



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 30, 2024 – 06:14 AM EDT

PDB ID : 4V8G
Title : Crystal structure of RMF bound to the 70S ribosome.
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.
Deposited on : 2011-12-11
Resolution : 3.00 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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

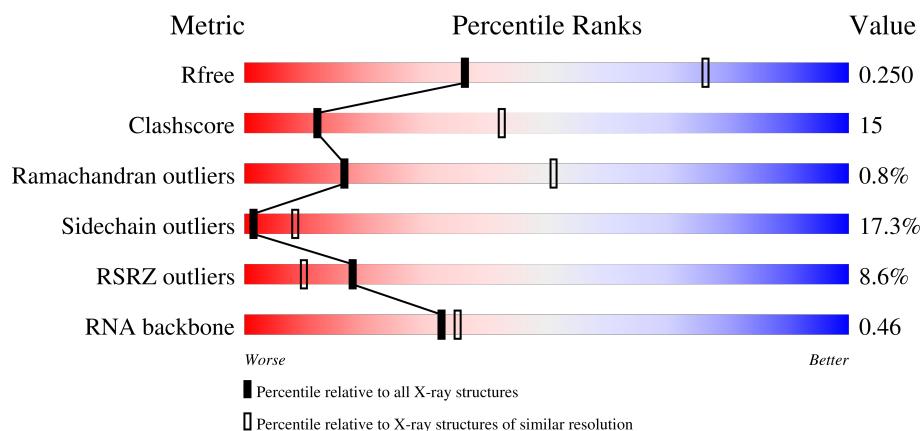
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)
RNA backbone	3690	1019 (3.20-2.80)

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	
1	CA	1522	
2	AB	256	
2	CB	256	

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

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	61	
22	CV	61	
23	BA	2915	
23	DA	2915	
24	BB	122	
24	DB	122	
25	BD	276	
25	DD	276	
26	BE	206	
26	DE	206	
27	BF	210	
27	DF	210	

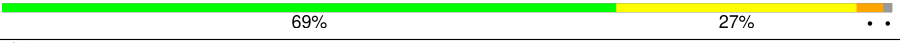










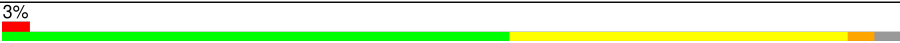




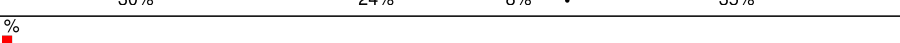
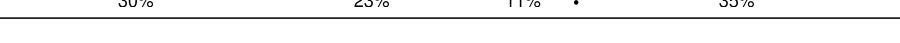







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Mol	Chain	Length	Quality of chain
28	BG	182	
28	DG	182	
29	BH	180	
29	DH	180	
30	BI	148	
30	DI	148	
31	BN	140	
31	DN	140	
32	BO	122	
32	DO	122	
33	BP	150	
33	DP	150	
34	BQ	141	
34	DQ	141	
35	BR	118	
35	DR	118	
36	BS	112	
36	DS	112	
37	BT	146	
37	DT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

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

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Mol	Chain	Length	Quality of chain
53	B9	37	
53	D9	37	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	AA	1620	-	-	-	X
54	MG	AA	1632	-	-	-	X
54	MG	AA	1641	-	-	-	X
54	MG	AA	1643	-	-	-	X
54	MG	AA	1661	-	-	-	X
54	MG	AA	1672	-	-	-	X
54	MG	AA	1676	-	-	-	X
54	MG	BA	3256	-	-	-	X
54	MG	CA	1610	-	-	-	X
54	MG	CA	1623	-	-	-	X
54	MG	CA	1624	-	-	-	X
54	MG	CA	1631	-	-	-	X
54	MG	DA	3206	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 283930 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	1505	Total	C	N	O	P	0	0	0
			32353	14399	5995	10454	1505			
1	CA	1501	Total	C	N	O	P	0	0	0
			32270	14362	5983	10424	1501			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	229	Total	C	N	O	S	0	0	0
			1775	1132	318	320	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			
			663	410	132	121	0	0	0

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

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

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

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

- 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		
			804	497	164	142	1	0	0
13	CM	114	Total	C	N	O	S		
			804	497	164	142	1	0	0

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

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

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

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

- Molecule 16 is a protein called 30S Ribosomal Protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			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	97	Total	C	N	O	S	0	0	0
			713	438	152	121	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 Ribosome modulation factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	53	Total	C	N	O	S	0	0	0
			333	204	66	61	2			
22	CV	53	Total	C	N	O	S	0	0	0
			353	218	67	66	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AV	56	HIS	-	expression tag	UNP P0AFW2
AV	57	HIS	-	expression tag	UNP P0AFW2
AV	58	HIS	-	expression tag	UNP P0AFW2
AV	59	HIS	-	expression tag	UNP P0AFW2
AV	60	HIS	-	expression tag	UNP P0AFW2
AV	61	HIS	-	expression tag	UNP P0AFW2
CV	56	HIS	-	expression tag	UNP P0AFW2
CV	57	HIS	-	expression tag	UNP P0AFW2
CV	58	HIS	-	expression tag	UNP P0AFW2
CV	59	HIS	-	expression tag	UNP P0AFW2
CV	60	HIS	-	expression tag	UNP P0AFW2
CV	61	HIS	-	expression tag	UNP P0AFW2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BA	2809	Total	C	N	O	P	0	0	0
			60512	26930	11328	19446	2808			
23	DA	2814	Total	C	N	O	P	0	0	0
			60620	26978	11348	19481	2813			

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	203	Total	C	N	O	S	0	0	1
			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
			1040	669	180	190	1			
30	DI	146	Total	C	N	O	S	0	0	0
			1038	668	180	189	1			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BS	110	Total	C	N	O	S	0	0	0
			865	544	172	149				
36	DS	110	Total	C	N	O	S	0	0	0
			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	100	Total	C	N	O	S	0	0	0
			760	490	136	133	1			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	AA	106	Total	Mg	0	0
			106	106		
54	AD	1	Total	Mg	0	0
			1	1		
54	BA	618	Total	Mg	0	0
			618	618		
54	BB	17	Total	Mg	0	0
			17	17		
54	BD	3	Total	Mg	0	0
			3	3		
54	BE	6	Total	Mg	0	0
			6	6		
54	BF	2	Total	Mg	0	0
			2	2		
54	BP	1	Total	Mg	0	0
			1	1		
54	BQ	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BR	2	Total 2	Mg 2	0	0
54	BU	2	Total 2	Mg 2	0	0
54	BV	1	Total 1	Mg 1	0	0
54	BW	1	Total 1	Mg 1	0	0
54	B0	2	Total 2	Mg 2	0	0
54	B1	1	Total 1	Mg 1	0	0
54	B2	2	Total 2	Mg 2	0	0
54	B3	2	Total 2	Mg 2	0	0
54	B5	2	Total 2	Mg 2	0	0
54	B8	3	Total 3	Mg 3	0	0
54	B9	1	Total 1	Mg 1	0	0
54	CA	69	Total 69	Mg 69	0	0
54	DA	430	Total 430	Mg 430	0	0
54	DB	5	Total 5	Mg 5	0	0
54	DD	1	Total 1	Mg 1	0	0
54	DE	1	Total 1	Mg 1	0	0
54	DF	2	Total 2	Mg 2	0	0
54	DP	1	Total 1	Mg 1	0	0
54	D6	1	Total 1	Mg 1	0	0
54	D7	1	Total 1	Mg 1	0	0
54	D8	1	Total 1	Mg 1	0	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	145	Total 145	O 145	0	0
56	AF	1	Total 1	O 1	0	0
56	AK	1	Total 1	O 1	0	0
56	AQ	1	Total 1	O 1	0	0
56	BA	1422	Total 1422	O 1422	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BB	31	Total 31	O 31	0	0
56	BD	10	Total 10	O 10	0	0
56	BE	8	Total 8	O 8	0	0
56	BF	11	Total 11	O 11	0	0
56	BH	2	Total 2	O 2	0	0
56	BN	2	Total 2	O 2	0	0
56	BO	3	Total 3	O 3	0	0
56	BP	6	Total 6	O 6	0	0
56	BQ	2	Total 2	O 2	0	0
56	BR	6	Total 6	O 6	0	0
56	BT	1	Total 1	O 1	0	0
56	BU	2	Total 2	O 2	0	0
56	BV	2	Total 2	O 2	0	0
56	BW	4	Total 4	O 4	0	0
56	BX	2	Total 2	O 2	0	0
56	BY	1	Total 1	O 1	0	0
56	B0	4	Total 4	O 4	0	0
56	B3	1	Total 1	O 1	0	0
56	B4	1	Total 1	O 1	0	0
56	B5	3	Total 3	O 3	0	0
56	B7	3	Total 3	O 3	0	0

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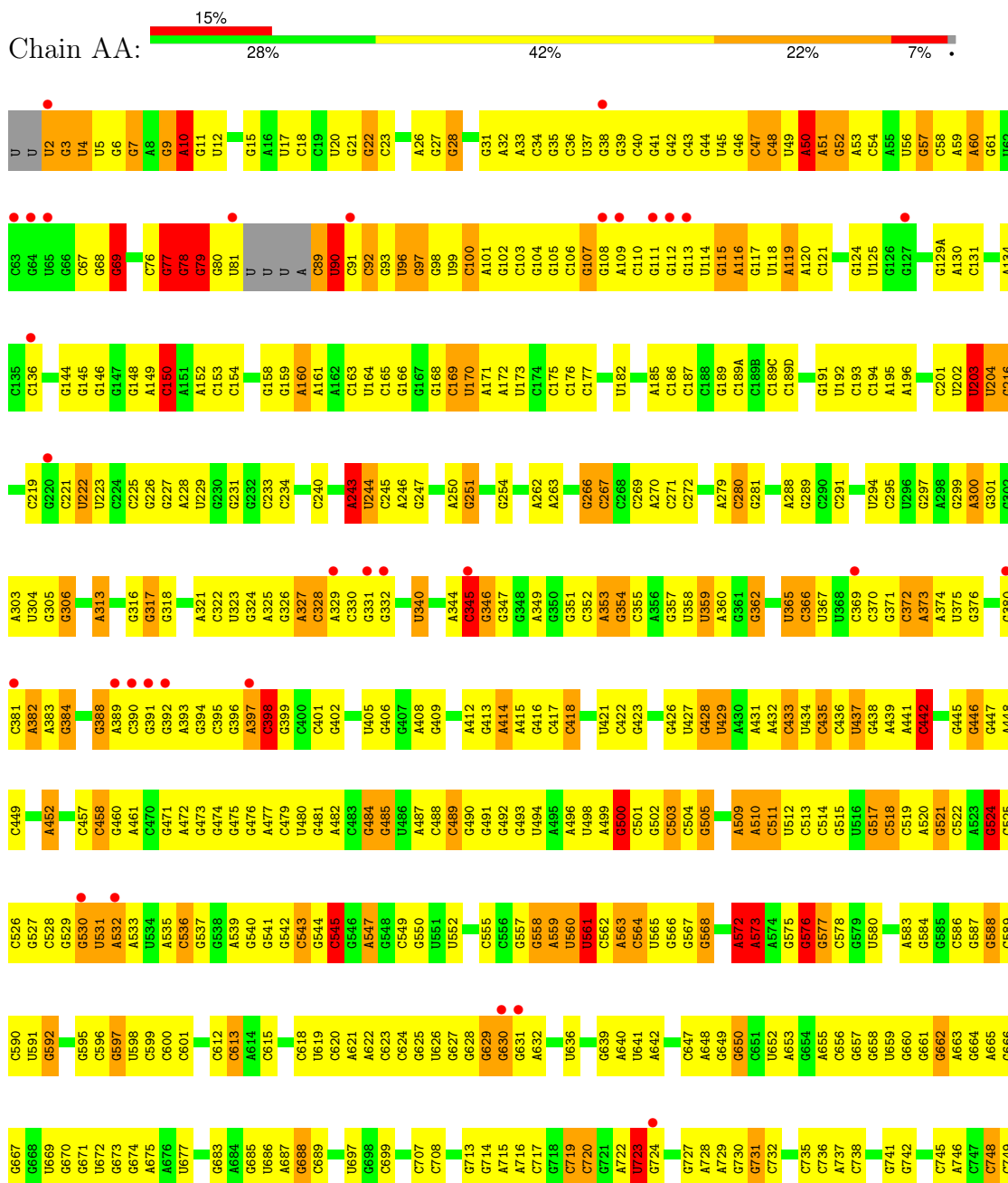
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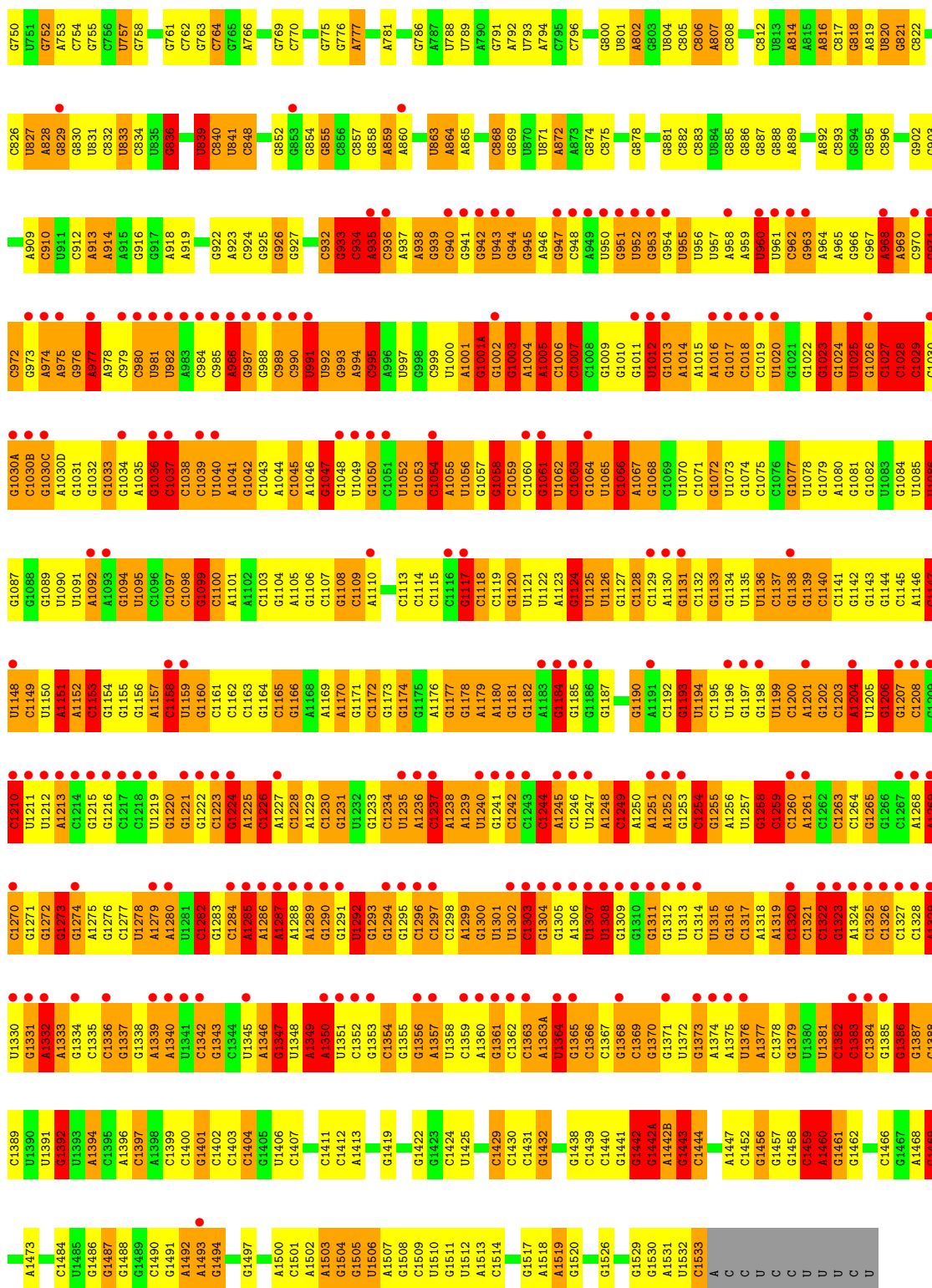
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56	B9	2	Total 2	O 2	0	0
56	CA	119	Total 119	O 119	0	0
56	CD	1	Total 1	O 1	0	0
56	CK	2	Total 2	O 2	0	0
56	CP	1	Total 1	O 1	0	0
56	CT	2	Total 2	O 2	0	0
56	DA	696	Total 696	O 696	0	0
56	DB	9	Total 9	O 9	0	0
56	DD	3	Total 3	O 3	0	0
56	DE	2	Total 2	O 2	0	0
56	DF	5	Total 5	O 5	0	0
56	DP	5	Total 5	O 5	0	0
56	DQ	2	Total 2	O 2	0	0
56	DR	1	Total 1	O 1	0	0
56	DV	1	Total 1	O 1	0	0
56	DX	1	Total 1	O 1	0	0
56	DY	1	Total 1	O 1	0	0
56	D0	1	Total 1	O 1	0	0
56	D1	2	Total 2	O 2	0	0

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.

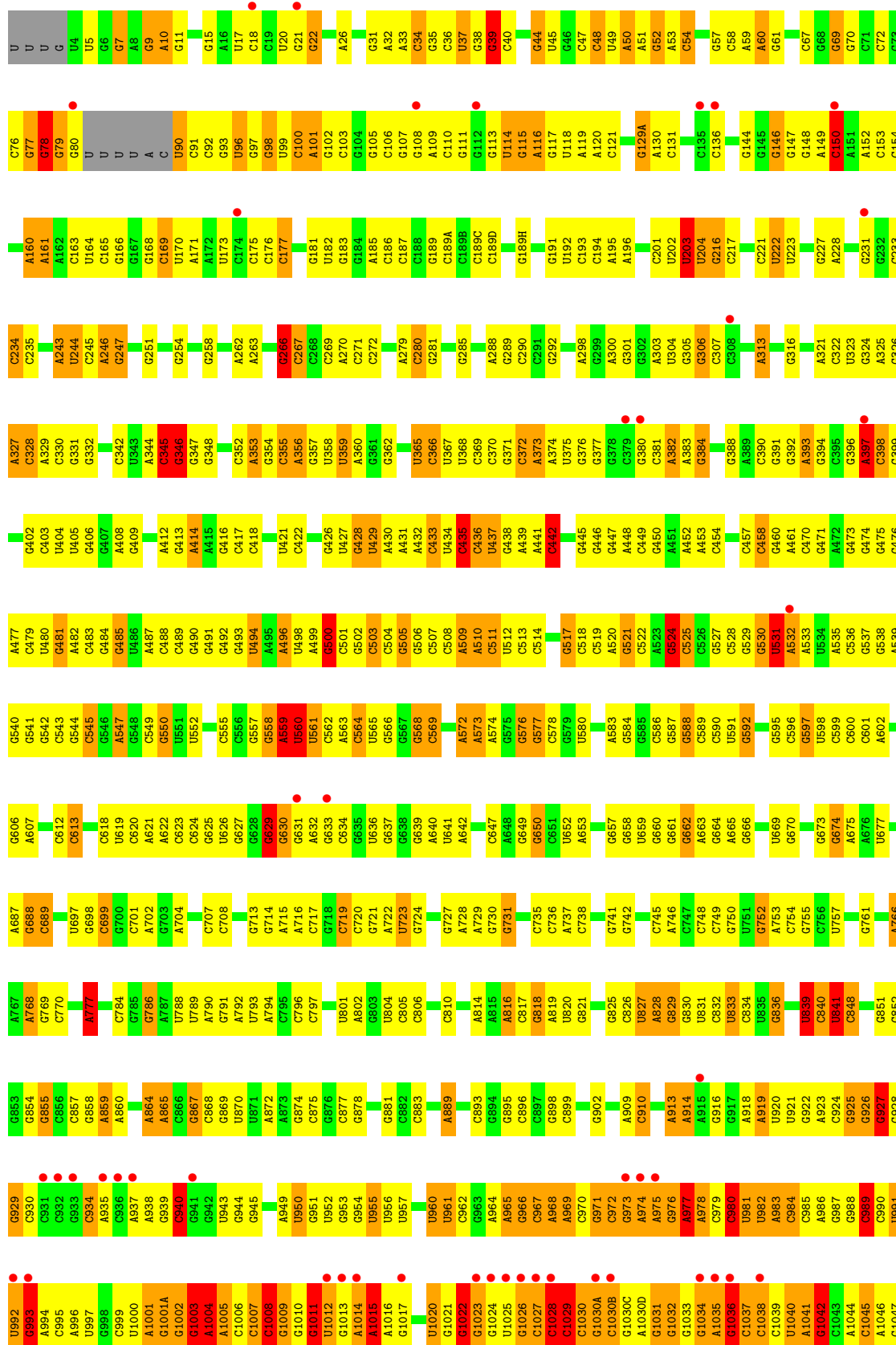
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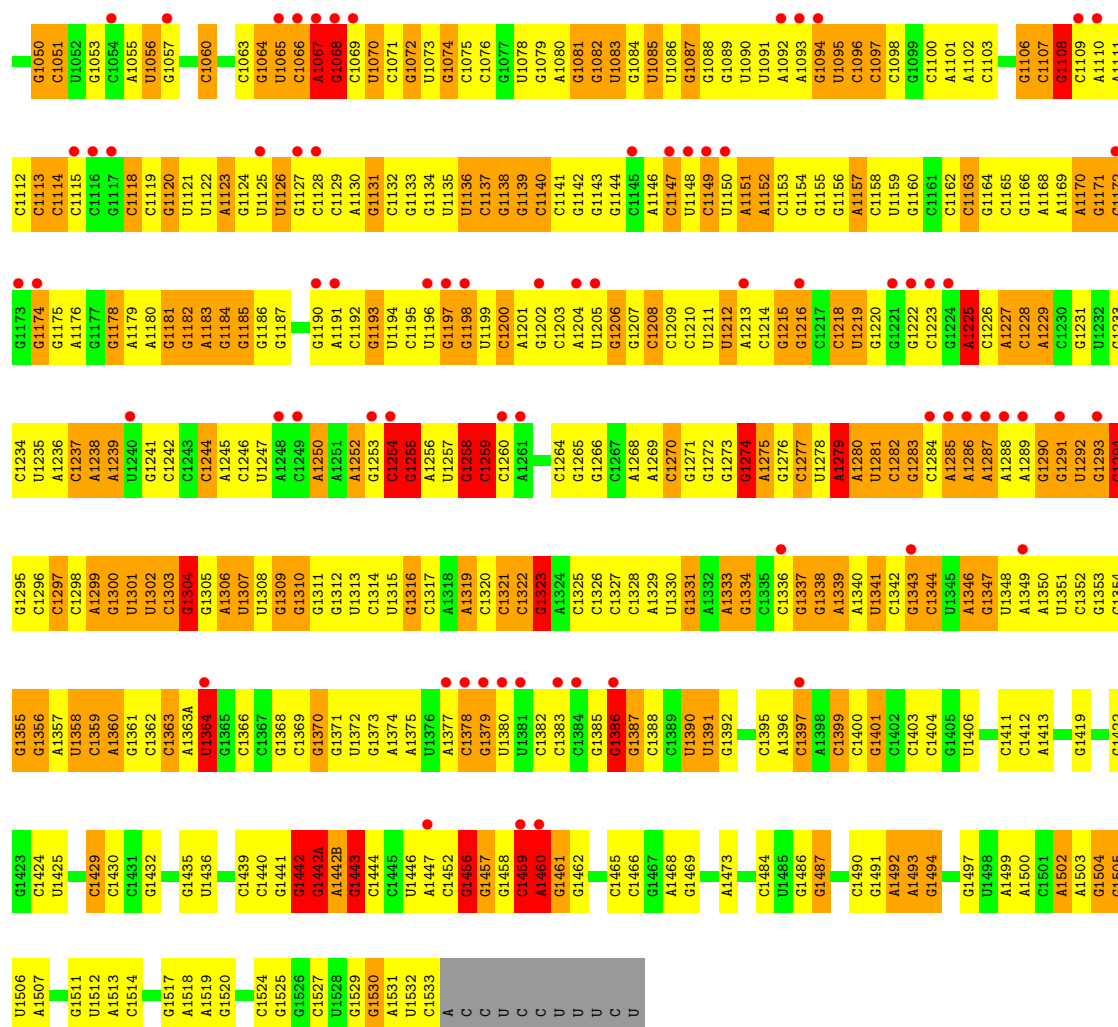




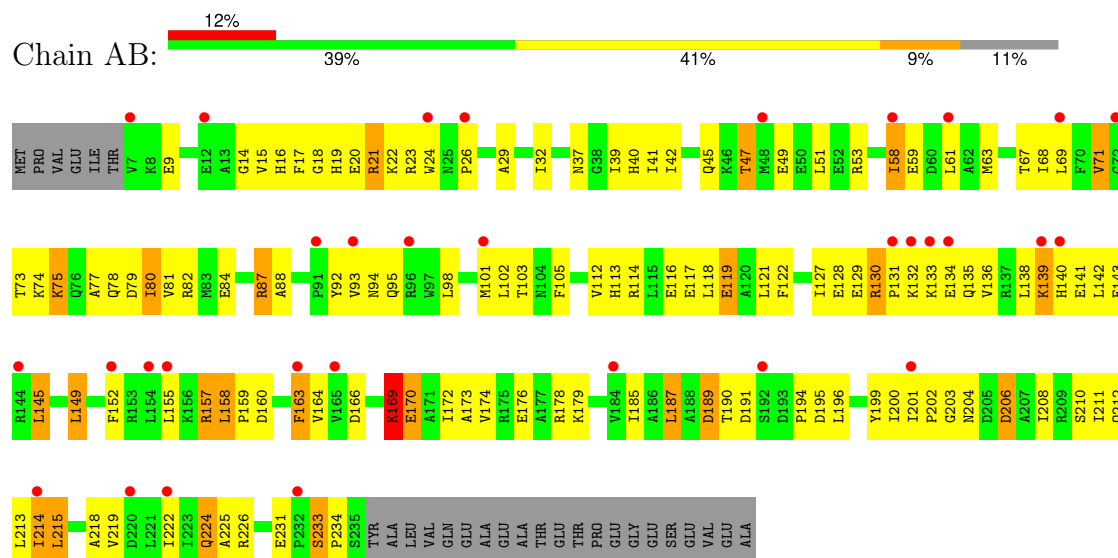
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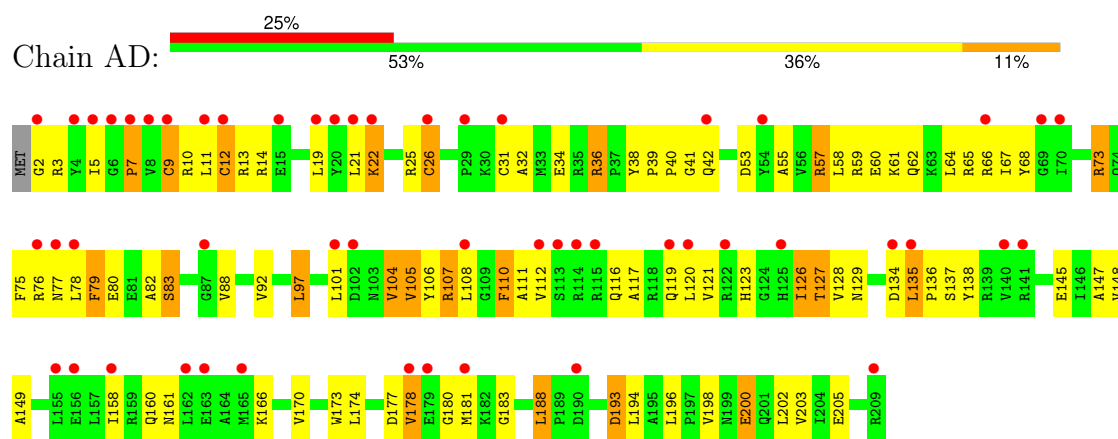




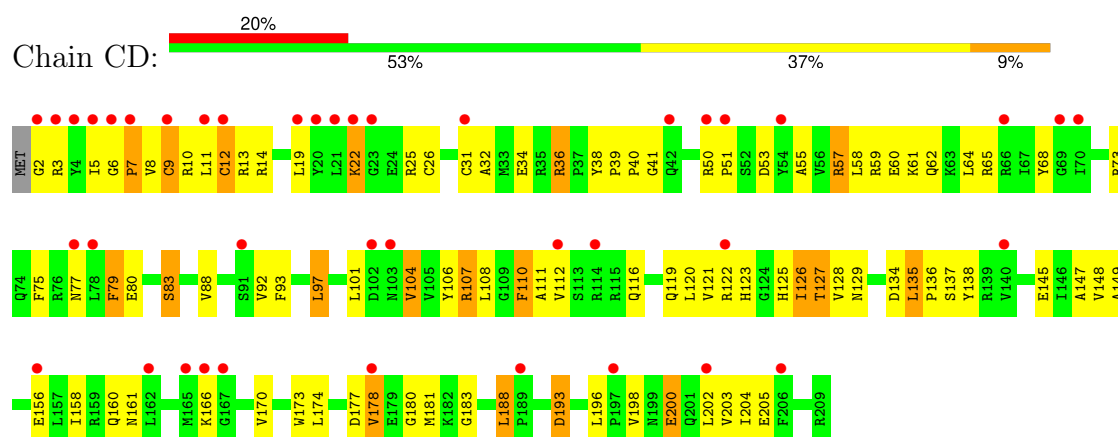
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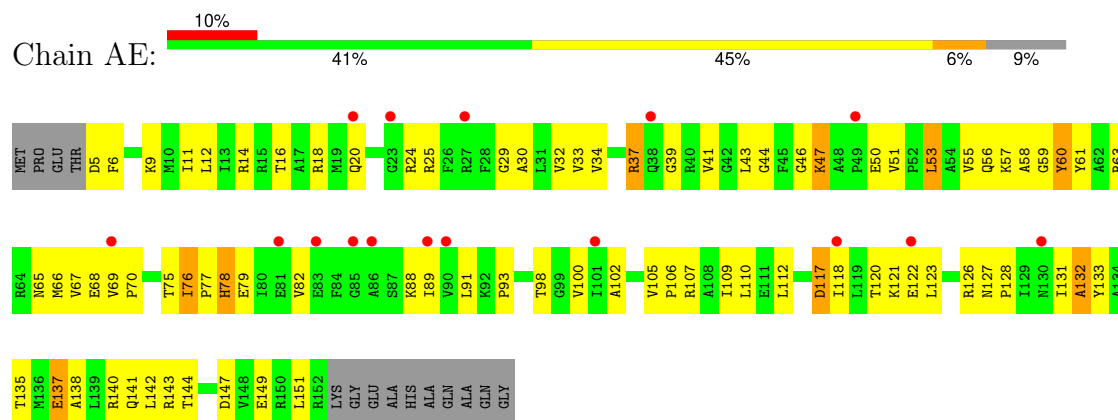
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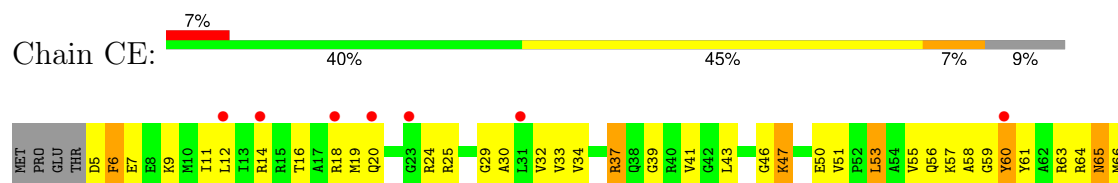
• Molecule 4: 30S Ribosomal Protein S4

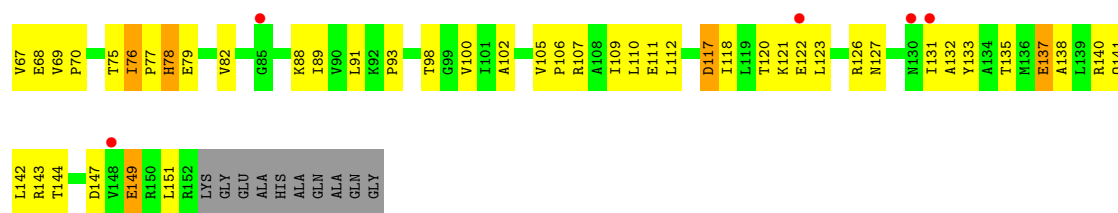


• Molecule 5: 30S Ribosomal Protein S5

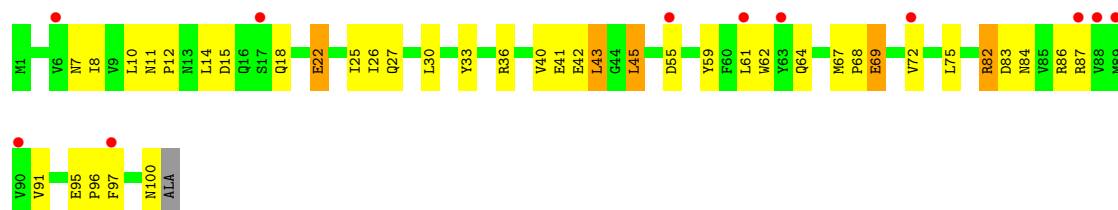


• Molecule 5: 30S Ribosomal Protein S5





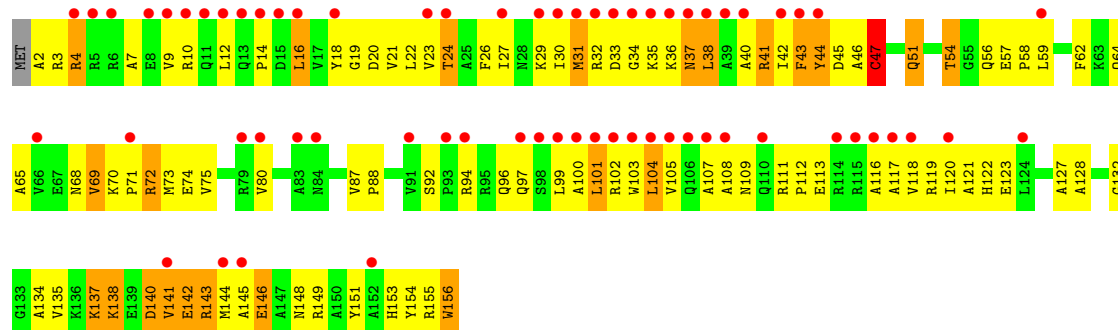
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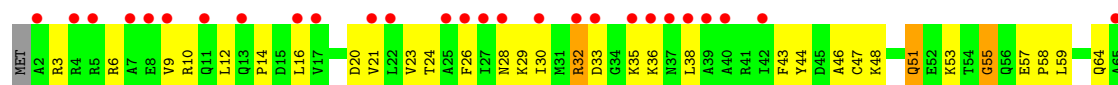
● Molecule 6: 30S Ribosomal Protein S6

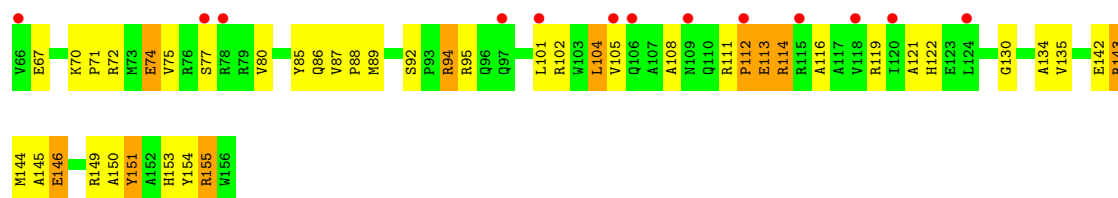


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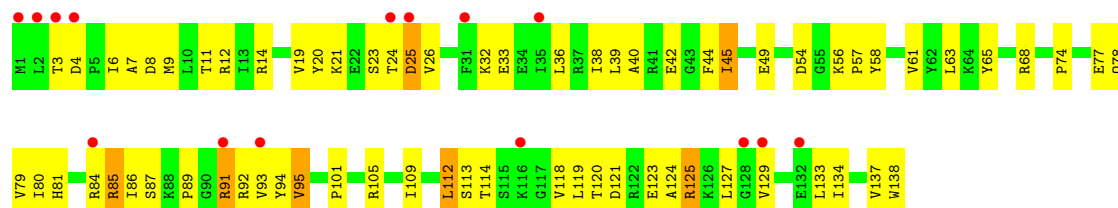


● Molecule 7: 30S Ribosomal Protein S7

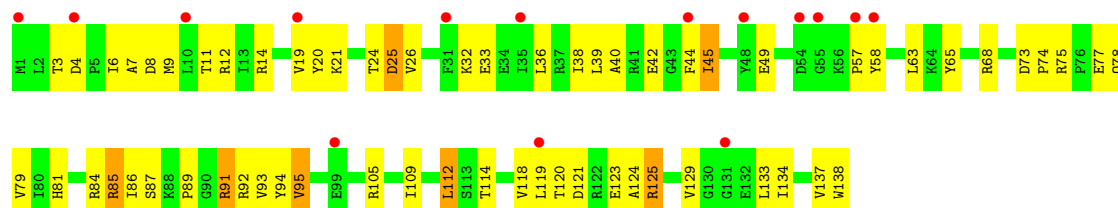




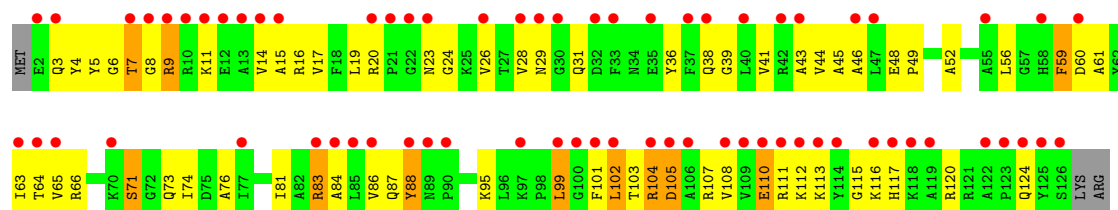
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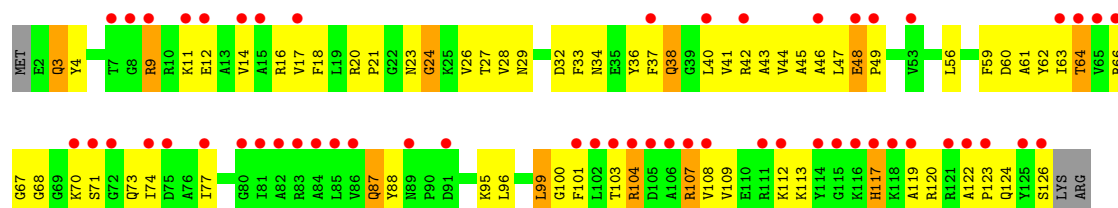
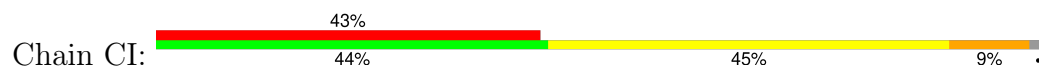
• Molecule 8: 30S Ribosomal Protein S8



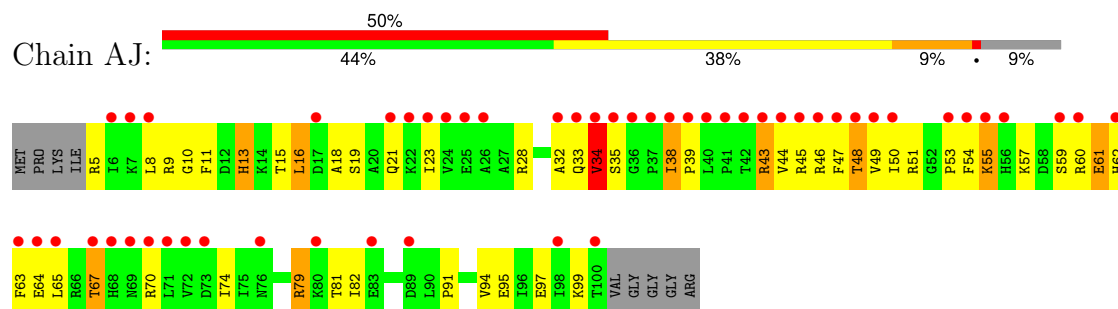
• Molecule 9: 30S Ribosomal Protein S9



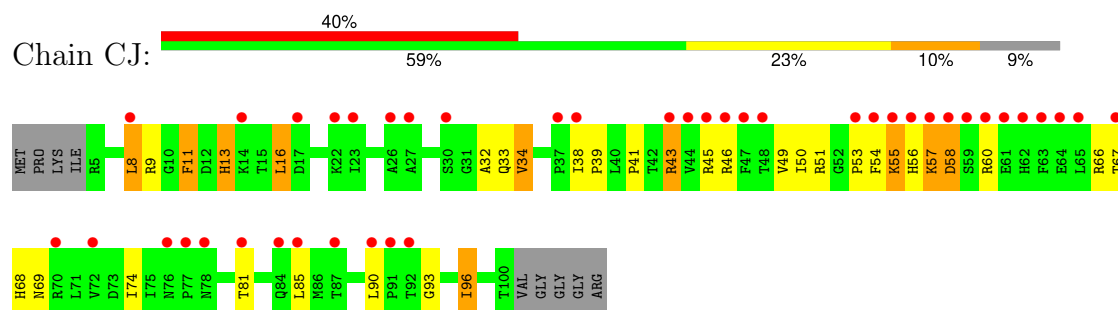
• Molecule 9: 30S Ribosomal Protein S9



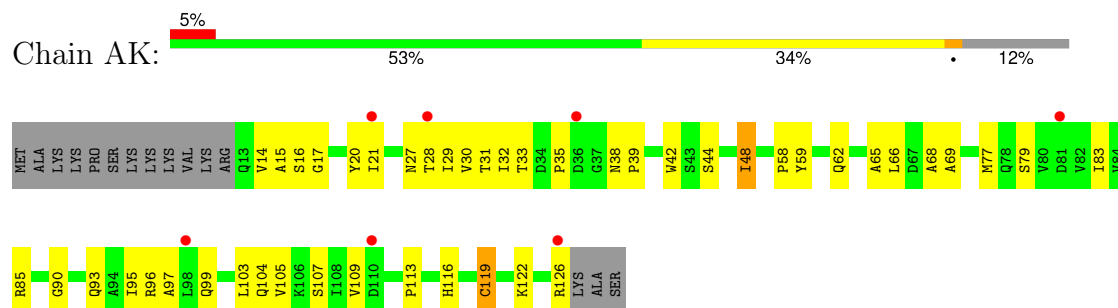
- Molecule 10: 30S Ribosomal Protein S10



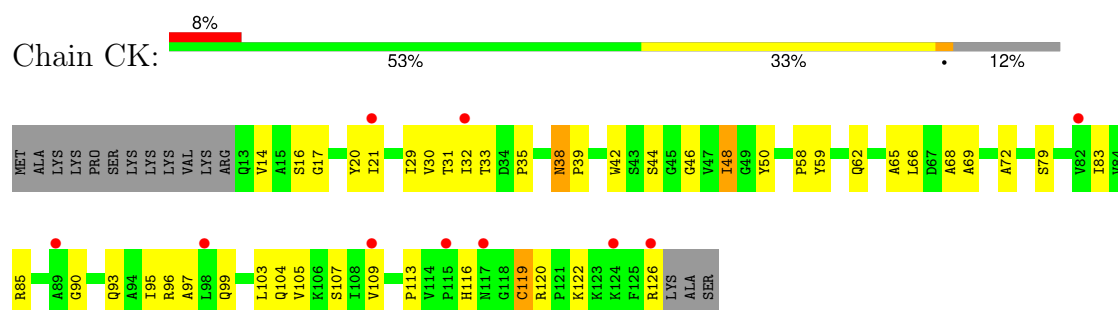
- Molecule 10: 30S Ribosomal Protein S10



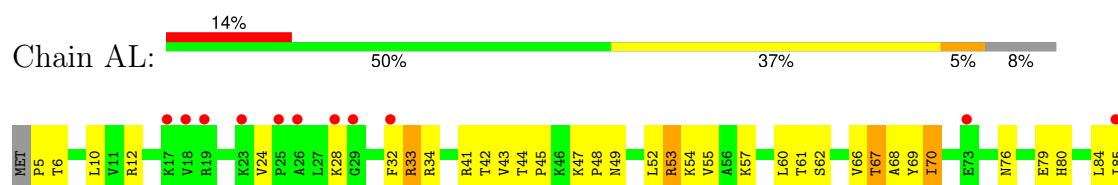
- Molecule 11: 30S Ribosomal Protein S11

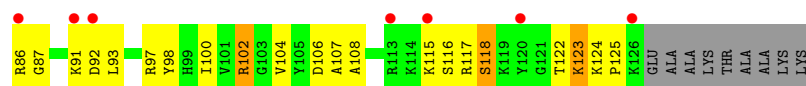


- Molecule 11: 30S Ribosomal Protein S11



- Molecule 12: 30S Ribosomal Protein S12

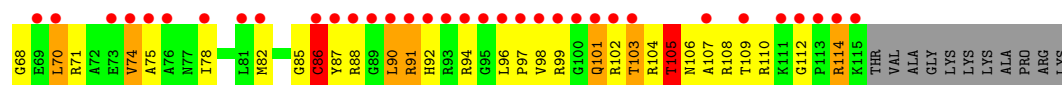
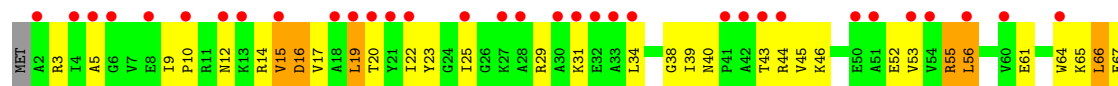




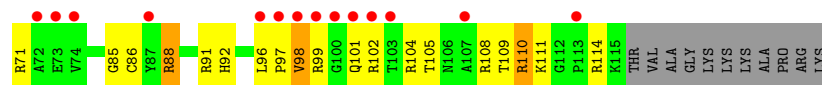
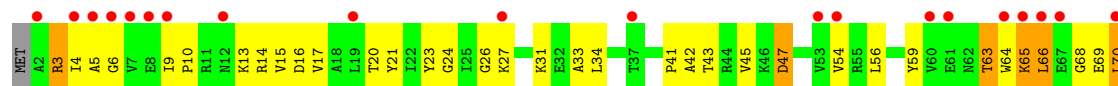
• Molecule 12: 30S Ribosomal Protein S12



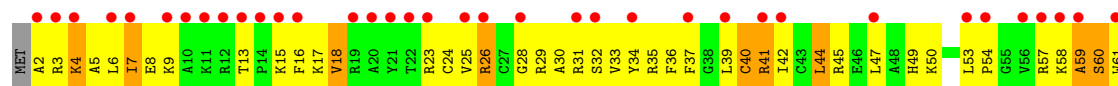
• Molecule 13: 30S Ribosomal Protein S13



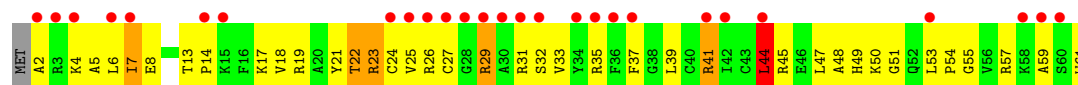
• Molecule 13: 30S Ribosomal Protein S13



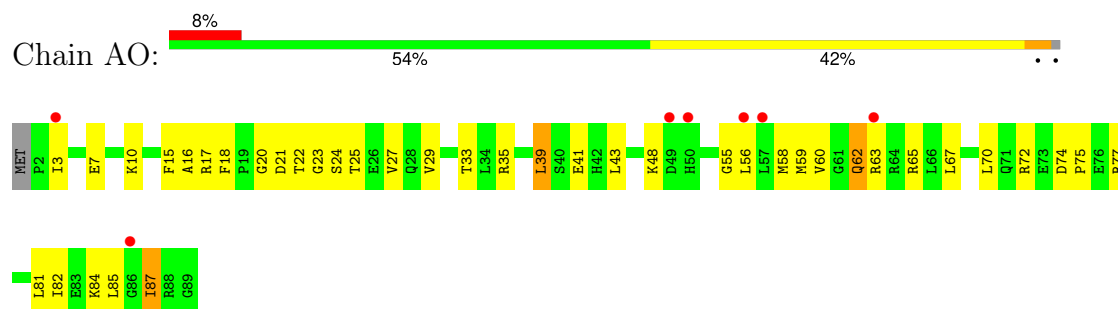
• Molecule 14: 30S Ribosomal Protein S14



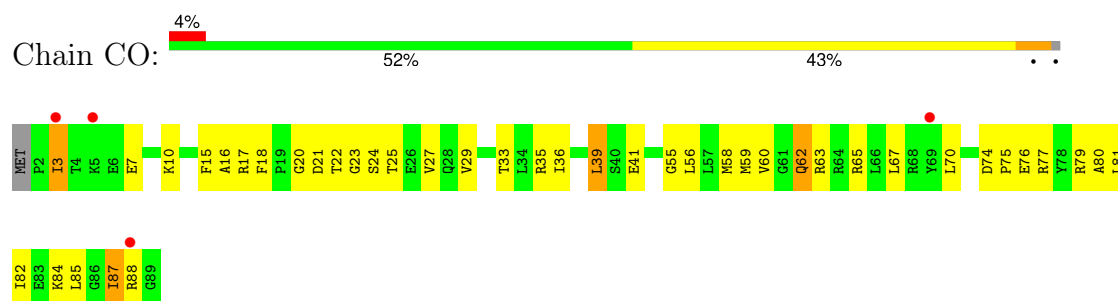
• Molecule 14: 30S Ribosomal Protein S14



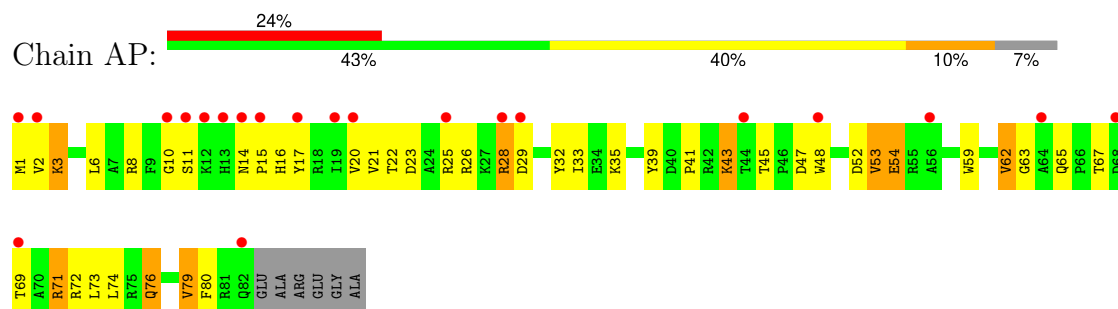
- Molecule 15: 30S Ribosomal Protein S15



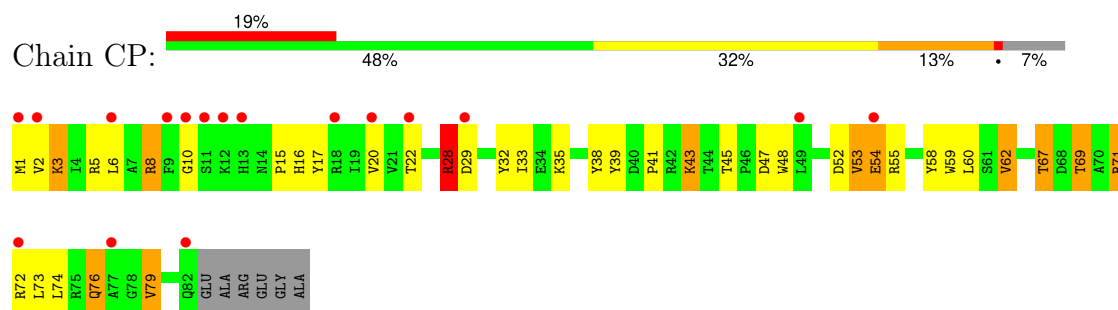
- Molecule 15: 30S Ribosomal Protein S15



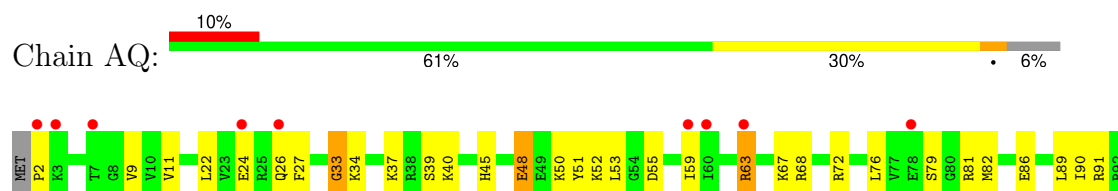
- Molecule 16: 30S Ribosomal Protein S16

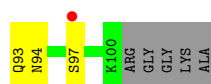


- Molecule 16: 30S Ribosomal Protein S16



- Molecule 17: 30S Ribosomal Protein S17

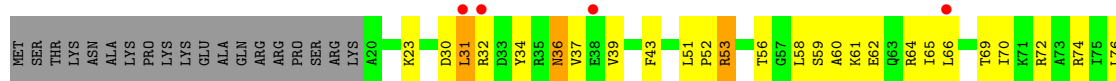
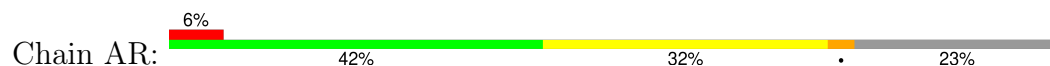




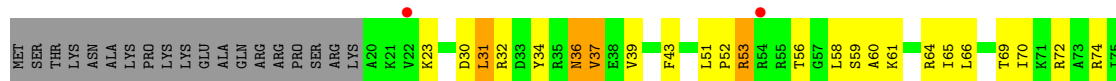
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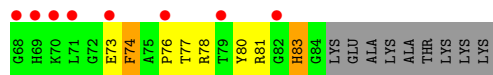
• Molecule 18: 30S Ribosomal Protein S18



• Molecule 18: 30S Ribosomal Protein S18



• Molecule 19: 30S Ribosomal Protein S19



• Molecule 19: 30S Ribosomal Protein S19

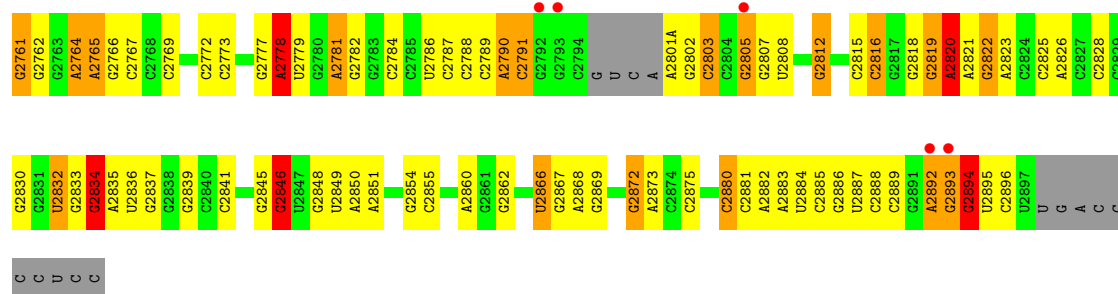


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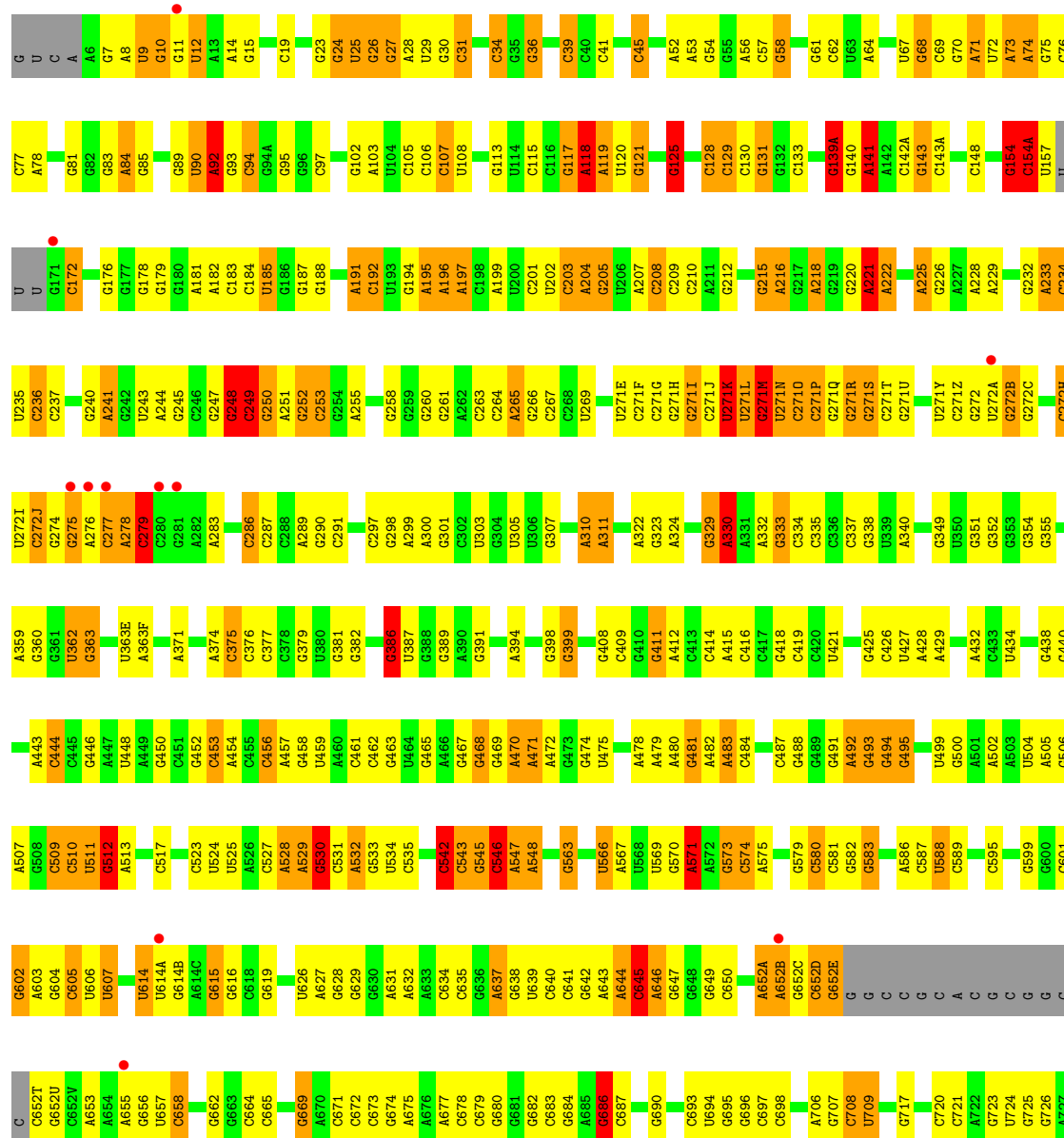
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|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|
| G684 | G685 | G686 | G687 | G688 | G689 | G690 | G691 | G692 | G693 | G694 | G695 | G696 | G697 | G698 | G699 | G700 | G701 | G702 | G703 | G704 | G705 | G706 | G707 | G708 | G709 | G710 | G711 | G712 | G713 | G714 | G715 | G716 | G717 | G718 | G719 | G720 | G721 | G722 | G723 | G724 | G725 | G726 | G727 | G728 | G729 | G730 | G731 | G732 | G733 | G734 | G735 | G736 | G737 | G738 | G739 | G740 | G741 | G742 | G743 | G744 | G745 | G746 | G747 | G748 | G749 | G750 | G751 | G752 | G753 | G754 | G755 | G756 | G757 | G758 | G759 | G760 | G761 | G762 | G763 | G764 | G765 | G766 | G767 | G768 | G769 | G770 | G771 | G772 | G773 | G774 | G775 | G776 | G777 | G778 | G779 | G780 | G781 | G782 | G783 | G784 | G785 | G786 | G787 | G788 | G789 | G790 | G791 | G792 | G793 | G794 | G795 | G796 | G797 | G798 | G799 | G800 | G801 | G802 | G803 | G804 | G805 | G806 | G807 | G808 | G809 | G810 | G811 | G812 | G813 | G814 | G815 | G816 | G817 | G818 | G819 | G820 | G821 | G822 | G823 | G824 | G825 | G826 | G827 | G828 | G829 | G830 | G831 | G832 | G833 | G834 | G835 | G836 | G837 | G838 | G839 | G840 | G841 | G842 | G843 | G844 | G845 | G846 | G847 | G848 | G849 | G850 | G851 | G852 | G853 | G854 | G855 | G856 | G857 | G858 | G859 | G860 | G861 | G862 | G863 | G864 | G865 | G866 | G867 | G868 | G869 | G870 | G871 | G872 | G873 | G874 | G875 | G876 | G877 | G878 | G879 | G880 | G881 | G882 | G883 | G884 | G885 | G886 | G887 | G888 | G889 | G890 | G891 | G892 | G893 | G894 | G895 | G896 | G897 | G898 | G899 | G900 | G901 | G902 | G903 | G904 | G905 | G906 | G907 | G908 | G909 | G910 | G911 | G912 | G913 | G914 | G915 | G916 | G917 | G918 | G919 | G920 | G921 | G922 | G923 | G924 | G925 | G926 | G927 | G928 | G929 | G930 | G931 | G932 | G933 | G934 | G935 | G936 | G937 | G938 | G939 | G940 | G941 | G942 | G943 | G944 | G945 | G946 | G947 | G948 | G949 | G950 | G951 | G952 | G953 | G954 | G955 | G956 | G957 | G958 | G959 | G960 | G961 | G962 | G963 | G964 | G965 | G966 | G967 | G968 | G969 | G970 | G971 | G972 | G973 | G974 | G975 | G976 | G977 | G978 | G979 | G980 | G981 | G982 | G983 | G984 | G985 | G986 | G987 | G988 | G989 | G990 | G991 | G992 | G993 | G994 | G995 | G996 | G997 | G998 | G999 | G1000 |
| A643 | A644 | A645 | A646 | A647 | A648 | A649 | A650 | A651 | A652 | A653 | A654 | A655 | A656 | A657 | A658 | A659 | A660 | A661 | A662 | A663 | A664 | A665 | A666 | A667 | A668 | A669 | A670 | A671 | A672 | A673 | A674 | A675 | A676 | A677 | A678 | A679 | A680 | A681 | A682 | A683 | A684 | A685 | A686 | A687 | A688 | A689 | A690 | A691 | A692 | A693 | A694 | A695 | A696 | A697 | A698 | A699 | A700 | A701 | A702 | A703 | A704 | A705 | A706 | A707 | A708 | A709 | A710 | A711 | A712 | A713 | A714 | A715 | A716 | A717 | A718 | A719 | A720 | A721 | A722 | A723 | A724 | A725 | A726 | A727 | A728 | A729 | A730 | A731 | A732 | A733 | A734 | A735 | A736 | A737 | A738 | A739 | A740 | A741 | A742 | A743 | A744 | A745 | A746 | A747 | A748 | A749 | A750 | A751 | A752 | A753 | A754 | A755 | A756 | A757 | A758 | A759 | A760 | A761 | A762 | A763 | A764 | A765 | A766 | A767 | A768 | A769 | A770 | A771 | 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 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G577 | A505 | C433 | C434 | C435 | C436 | C437 | C438 | C439 | C440 | C441 | C442 | C443 | C444 | C445 | C446 | C447 | C448 | C449 | C450 | C451 | C452 | C453 | C454 | C455 | C456 | C457 | C458 | C459 | C460 | C461 | C462 | C463 | C464 | C465 | C4 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

A1668	A1669	C1598	G1526	A1449	G1377	C1306	G1236	C1158	A	U1035	C970	A899	U827	U762
C1670	U1671	C1599	A1528	A1450	A1378	A1307	A1237	G1164	A	G1036	C971	A900	U828	G763
C1672	C1673	C1600	A1528A	C1450A	G1380	A1309	G1238	G1165	U	G1037	A973	C901	A829	A764
U1602	U1673	G1601	G1381	U1453	G1382	G1310	U1240	C1166	C	C1038	G974	C902	G830	G765
A1603	A1603	C1530	C1383	U1453	C1382	G1311	U1241	C	G	C1039	G975A	C904	G831	G766
C1604	C1674	C1531	C1383	U1453	C1382	G1312	A1242	G1171	U	C1041	G976	U905	U833	U767
C1605	A1676	G	A1384	G1469	G1469	U1313	G1243	G	C	G1042	C977	G906	C894	G768
G1606	A1677	U	C1385	G1461	G1385	C1314	G1244	A	C	A835	G978	U907	C894	G769
C1607	U	A	U1391	G1461	U1391	C1315	G1245	U	C	A836	G979	G907	C895	G770
A1608	G1681	C	A1392	G1467	A1392	G1319	A1247	A	U	A1045	G980	A911	C837	C772
A1609	A1609	A1393	A1393	A1471	A1393	G1320	G1248	G1107	G1047	A1046	A881	C914	U839	U774
A1610	U1611	U1394	U1394	A1472	U1394	A1321	U1249	U1108	A1048	C915	C882	C915	G844	G775
C1611	U1540	A1472	A1395	A1472	A1395	U1322	G1250	C1109	C1049	A1050	A883	G916	U847	G776
A1614	A1614	A1477	U1396	A1477	U1396	G1323	C1251	C1110	C1049	A1051	A884	A917	U847	A777
C1615	A1542	G1478	C1397	G1478	C1397	G1324	G1252	A1111	C1051	C986	C985	A917	U847	G778
A1616	A1543	G1479	C1398	G1479	C1398	G1325	G1253	G1112	C1052	C987	C986	A917	U847	U779
C1617	A1544	G1480	C1403	G1480	C1403	U1326	A1254	C1185	C	C987	C987	U922	A849	G780
A1618	A1545	U1481	C1404	U1481	C1404	G1327	U1255	G1186	A	A888	C988	C923	G852	A781
G1619	C1546	G1482	U1405	G1482	U1405	G1328	U1256	G1187	G	G889	C989	G928	G852	A782
G1620	C1547	G1482	U1406	G1482	U1406	U1329	C1257	A1188	G	A890	A990	G928	G855	A783
C1548	C1548	A1486	C1407	A1486	C1407	A1331	G1260	G1191	A	G993	C993	G931	C857	A784
G1622	G1487	C1408	C1408	G1487	C1408	G1332	C1261	G1192	G	C994	C994	G932	C857	G785
G1623	C1488	C1408	C1408	C1488	C1408	C1333	C1261	G1193	U	C995	A933	G933	U856	A788
A1554	G1555	U1489	C1411	U1489	C1411	G1334	U1266	A1194	U	A996	A996	G934	G859	C791
C1556	C1556	A1490	A1412	A1490	A1412	G1335	U1267	G1195	G	C997	A997	C935	U860	G792
C1557	C1557	U1490	G1413	U1490	G1413	G1336	A1268	C1196	G	C998	C998	C936	A861	A793
A1558	C1558	C1493	G1414	C1493	G1414	G1337	A1269	G1197	C	G1003	G1003	C937	C862	G794
G1559	G1559	A1494	U1415	A1494	U1415	G1338	G1270	C1200	U	C1004	C1004	G938	A863	G795
A1562	A1496	U1496	G1416	A1496	G1416	U1341	G1271	C1201	U	C1005	C1005	G939	C864	C796
G1563	C1497	U1497	C1417	C1497	C1417	G1344	A1272	C1202	A	C1006	C1006	G940	C865	C797
A1566	G1498	A1498	G1418	G1498	G1418	G1344	A1273	G1203	G	C1008	C1008	A941	A866	G798
A1567	G1500	G1500	U1420	G1500	U1420	G1344	A1274	G1204	A	C1009	C1009	G942	G869	G799
G1568	C1501	C1501	G1421	G1501	G1421	G1348	A1275	U1205	C	A1010	A1010	G944	U871	A800
A1569	C1502	C1502	G1424	A1569	G1424	A1349	A1278	G1206	C	G1011	G1011	A945	A872	G801
A1570	C1503	C1503	G1425	A1570	G1425	C1350	A1279	C1207	A	C1012	C1012	G946	G873	A802
A1571	C1504	C1504	G1426	A1571	G1426	C1351	A1284	C1208	G	C1013	C1013	C949	G879	G805
A1572	C1505	C1505	A1427	A1572	A1427	U1362	G1285	G1209	C	U1014	U1014	C950	C806	C806
C1506	C1506	C1506	G1428	C1506	G1428	G1368	G1285	A1210	C	G1015	G1015	C951	U807	U807
A1507	A1507	G1429	G1429	A1507	G1429	A1359	U1288	U1211	U	C1016	C1016	C952	C881	G808
A1508	C1509	A1508	C1430	A1508	C1430	A1360	G1289	A1212	C	U1019	U1019	A953	G882	G809
C1509B	A1509B	C1509B	C1431	C1509B	C1431	G1361	C1290	A1213	C	A1020	A1020	C954	G	U810
G1510	A1433	A1433	U1433	G1510	U1433	G1364	C1291	A1142A	U	A1021	A1021	C955	C	U811
C1511	G1435	G1435	G1435	C1511	G1435	A1365	U1292	G1144	U	U1023	U1023	C956	C	C812
U1514	C1437	C1437	C1437	U1514	C1437	A1367	C1293	C1217	A	G1024	G1024	A957	A	C815
G1515	U1438	U1438	U1438	G1515	U1438	A1368	G1296	G1145	A	U1025	U1025	A958	C	C816
C1583	A1583	A1583	A1439	C1583	A1439	G1369	C1297	G1149	A	A1027	A1027	A959	C	C817
C1584	A1584	A1584	U1439	C1584	U1439	G1370	C1298	C1150	G	A	A	C961	A	G818
A1586	A1586	A1586	G1440	A1586	G1440	G1371	C1299	G1151	A	A1028	A1028	C964	C893	A819
A1587	G1441	G1441	G1441	A1587	G1441	U1372	U1300	C1152	G	A1029	A1029	C965	C894	A820
C1520	G1442	G1442	G1442	C1520	G1442	A1373	A1301	C1153	U	G1030	G1030	C966	U895	A821
U1523	A1445	A1445	A1445	U1523	A1445	A1374	A1302	G1154	G	A1032	A1032	C967	A896	U822
G1524	C1445A	C1445A	C1445A	G1524	C1445A	C1375	G1303	A1155	C	A1033	A1033	C968	C897	A824
G1525	C1445A	C1445A	C1445A	G1525	C1445A	C1376	C1305	G1157	U	G1034	G1034	U969	C898	

G2694	U2611	G2548	G2476	G2410	G2337	A2274	U2197	C2129	U2068	C2008	G1930	G1828	G2694	G2702	G2701	G2700	G2699	G2698	G2697
G2612	G2548	G2477	G2476	G2411	G2358	G2275	A2196	U2130	G2069	G2009	U1931	A1829	G2697	G2703	G2617	G2616	G2615	G2614	G2613
G2613	G2549	G2478	G2477	G2412	G2359	G2280	A2197	U2131	G2070	G2010	G1934	G1830	G2698	G2704	G2621	G2620	G2619	G2618	G2617
G2614	G2550	G2479	G2478	G2413	G2360	G2281	A2198	U2132	G2071	G2011	G1935	G1831	G2699	G2705	G2622	G2621	G2620	G2619	G2618
G2615	G2551	G2480	G2479	G2414	G2361	G2282	U2203	G2133	G2072	G2012	A1936	G1832	G2700	G2706	G2623	G2622	G2621	G2620	G2619
G2616	G2552	G2481	G2480	G2415	G2362	G2283	C2205	A2134	G2073	G2013	A1937	G1833	G2701	G2707	G2624	G2623	G2622	G2621	G2620
G2617	G2553	G2482	G2481	G2416	U2344	G2284	G2206	A2135	U2074	A2014	A1938	G1834	G2702	G2708	G2625	G2624	G2623	G2622	G2621
G2618	G2554	G2483	G2482	G2417	G2345	G2285	G2207	G2136	U2075	A2015	A1939	G1835	G2703	G2709	G2626	G2625	G2624	G2623	G2622
G2619	G2555	G2484	G2483	G2418	G2346	G2286	G2208	G2137	U2076	A2016	U1940	G1836	G2704	G2710	G2627	G2626	G2625	G2624	G2623
G2620	G2556	G2485	G2484	G2419	A2346	G2287	G2209	C2140	U2077	U2017	G1945	G1837	G2705	G2711	G2628	G2627	G2626	G2625	G2624
G2621	G2557	G2486	G2485	G2420	A2347	G2288	G2210	G2141	U2078	G2018	G1946	G1838	G2706	G2712	G2629	G2628	G2627	G2626	G2625
G2622	G2558	G2487	G2486	G2421	U2348	G2289	G2211	G2142	U2079	A2019	U1947	G1839	G2707	G2713	G2630	G2629	G2628	G2627	G2626
G2623	G2559	G2488	G2487	G2422	G2349	G2290	G2212	G2143	G2080	A2020	C1947	G1840	G2708	G2714	G2631	G2630	G2629	G2628	G2627
G2624	G2560	G2489	G2488	G2423	G2350	G2291	G2213	C2144	G2081	U2021	U1951	G1841	G2709	G2715	G2632	G2631	G2630	G2629	G2628
G2625	G2561	G2490	G2489	G2424	A2352	G2292	G2214	C2145	A2082	G2022	U1952	G1842	G2710	G2716	G2633	G2632	G2631	G2630	G2629
G2626	G2562	G2491	G2490	G2425	G2353	G2293	G2215	C2146	U2083	G2023	A1953	A1843	G2711	G2717	G2634	G2633	G2632	G2631	G2630
G2627	G2563	G2492	G2491	A2426	G2354	G2294	A2226	G2147	G2084	G2024	A1954	A1780	G2712	G2718	G2635	G2634	G2633	G2632	G2631
G2628	G2564	G2493	G2492	G2427	G2355	G2295	A2227	G2148	G2085	C2026	U1955	G1844	G2713	G2719	G2636	G2635	G2634	G2633	G2632
G2629	G2565	G2494	G2493	G2428	G2356	G2296	G2228	G2149	G2086	G2027	U1956	G1845	G2714	G2720	G2637	G2636	G2635	G2634	G2633
G2630	G2566	G2495	G2494	G2429	U2357	G2297	G2229	G2150	U2089	G2028	U1957	G1846	G2715	G2721	G2638	G2637	G2636	G2635	G2634
G2631	G2567	G2496	G2495	G2430	G2358	G2298	G2230	G2151	G2090	G2029	C1958	G1847	G2716	G2722	G2639	G2638	G2637	G2636	G2635
G2632	G2568	G2497	G2496	A2431	A2360	G2299	U2232	G2152	U2091	A2030	G1959	G1848	G2717	G2723	G2640	G2639	G2638	G2637	G2636
G2633	G2569	G2498	G2497	G2432	A2361	G2300	G2233	G2153	G2092	G2031	G1960	G1849	G2718	G2724	G2641	G2640	G2639	G2638	G2637
G2634	G2570	G2499	G2498	A2433	G2362	G2301	G2234	G2154	G2093	G2032	G1961	G1850	G2719	G2725	G2642	G2641	G2640	G2639	G2638
G2635	G2571	G2500	G2499	G2434	G2363	G2302	G2235	G2155	G2094	G2033	G1962	G1851	G2720	G2726	G2643	G2642	G2641	G2640	G2639
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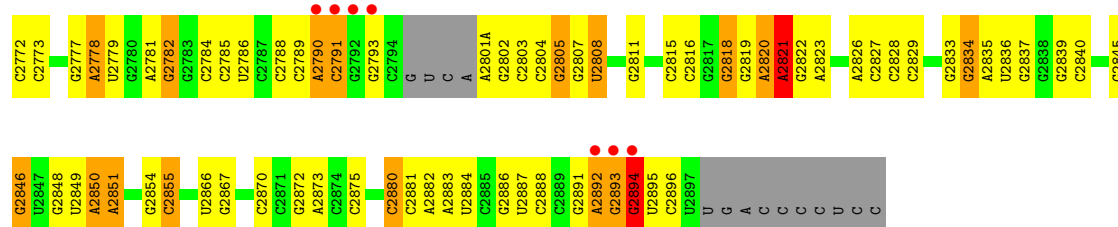


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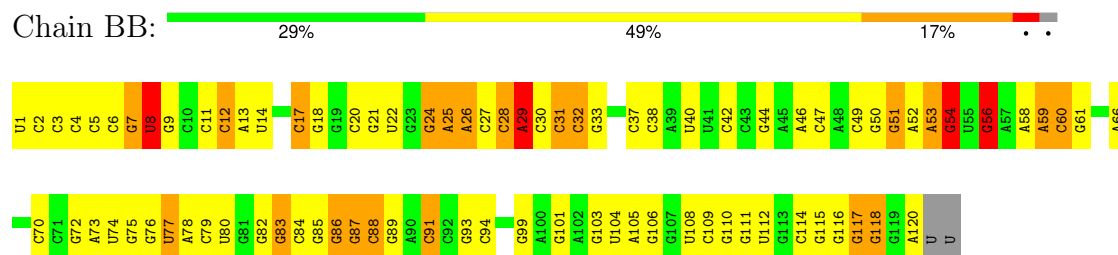


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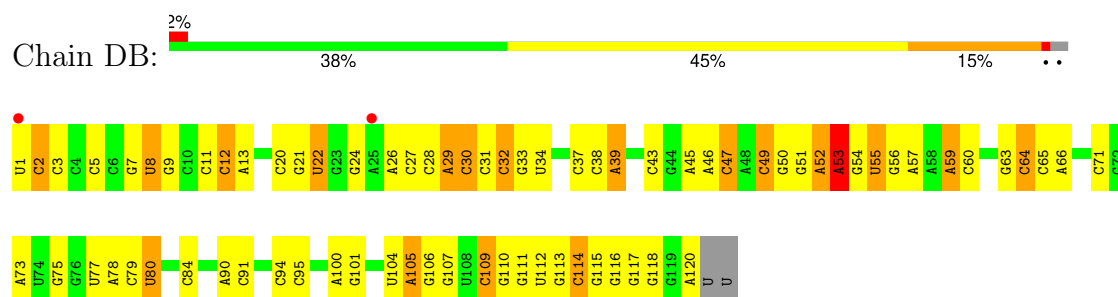




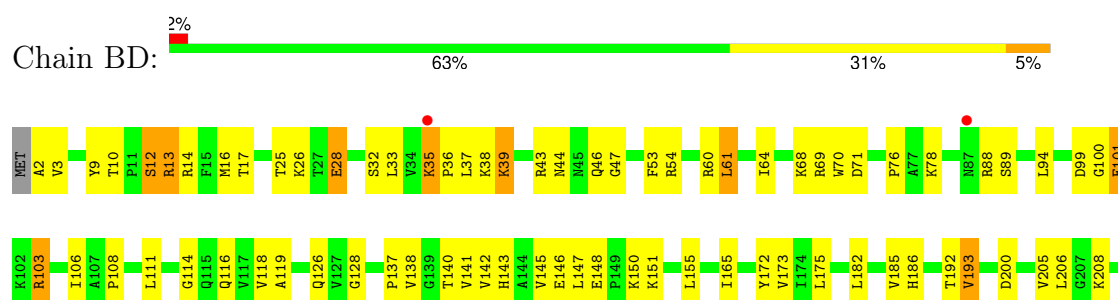
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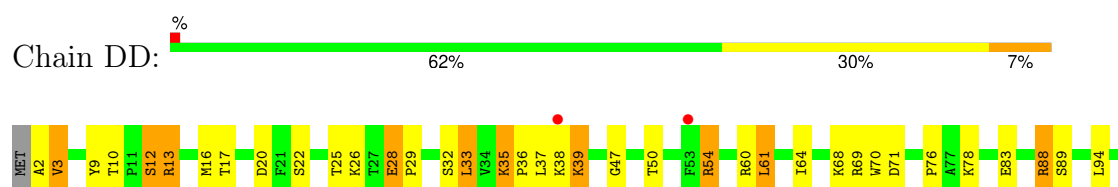
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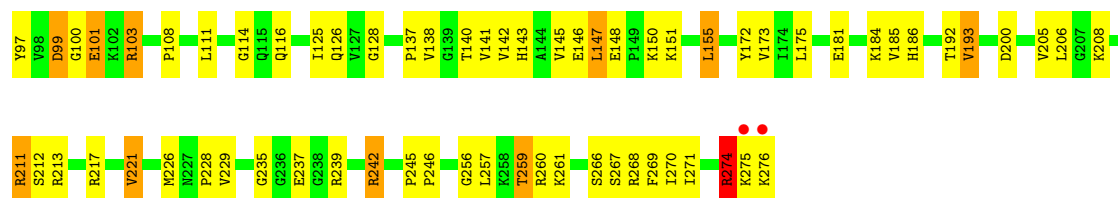


• Molecule 25: 50S Ribosomal Protein L2

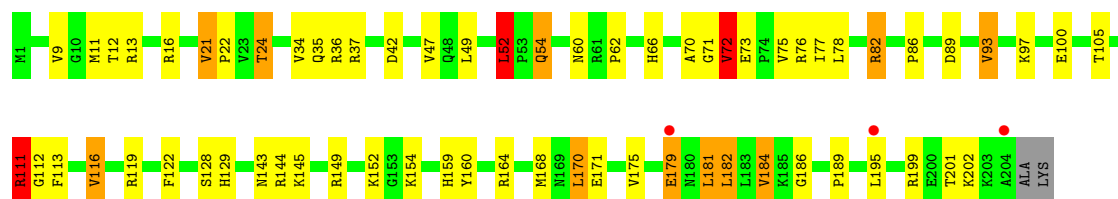


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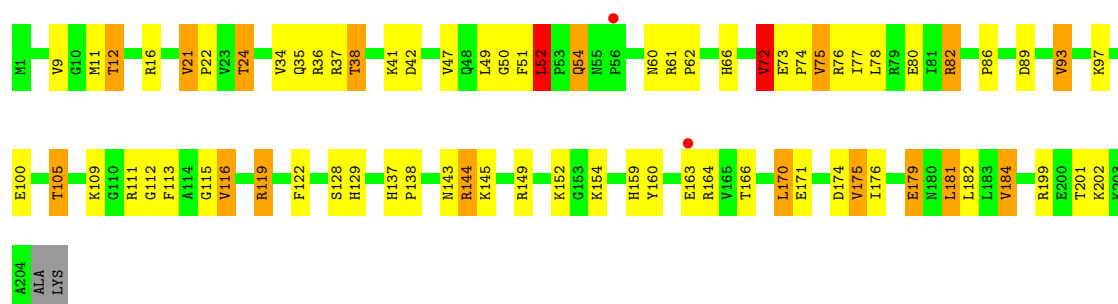




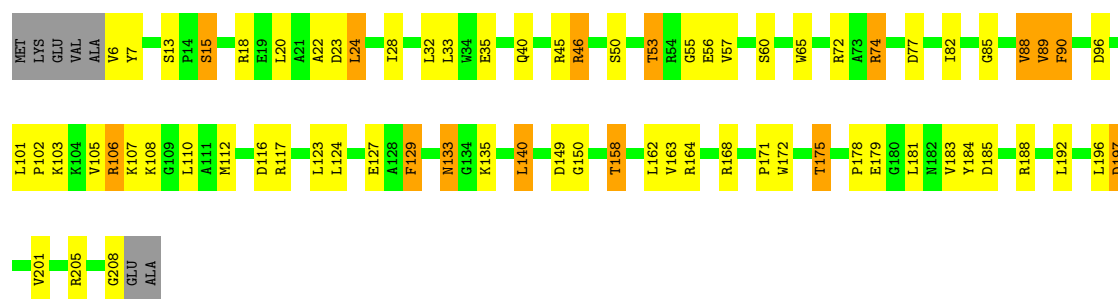
• Molecule 26: 50S Ribosomal Protein L3



• Molecule 26: 50S Ribosomal Protein L3

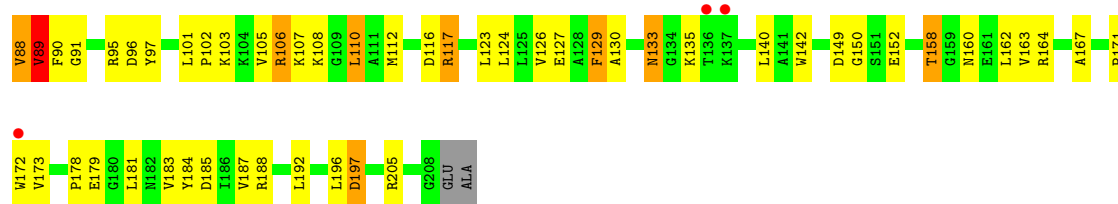


• Molecule 27: 50S Ribosomal Protein L4

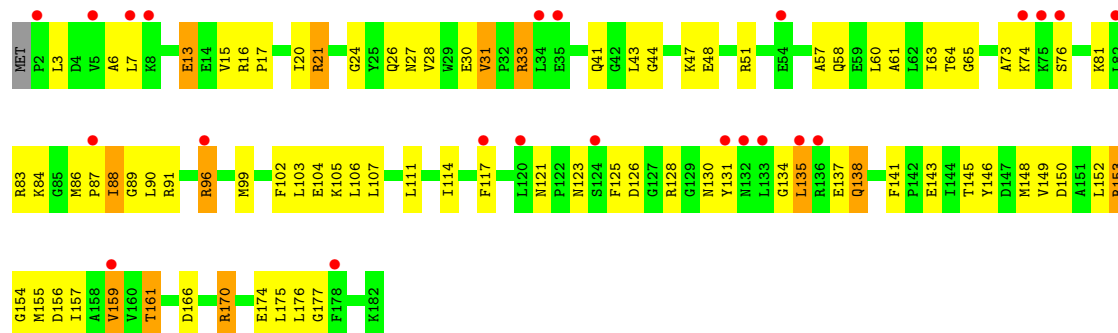


• Molecule 27: 50S Ribosomal Protein L4

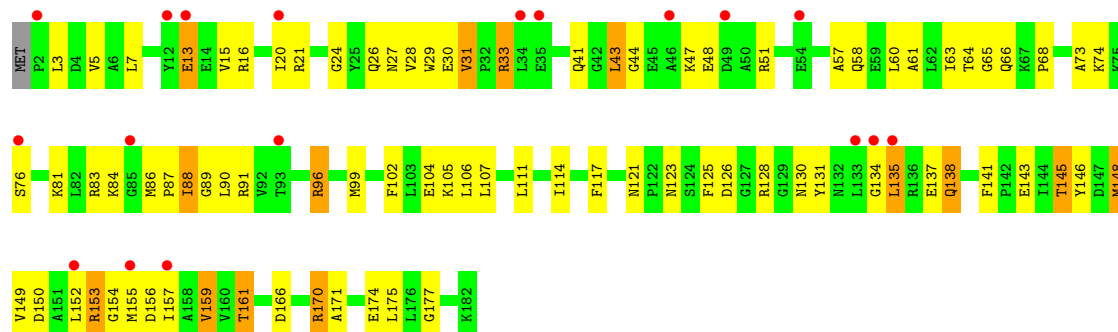




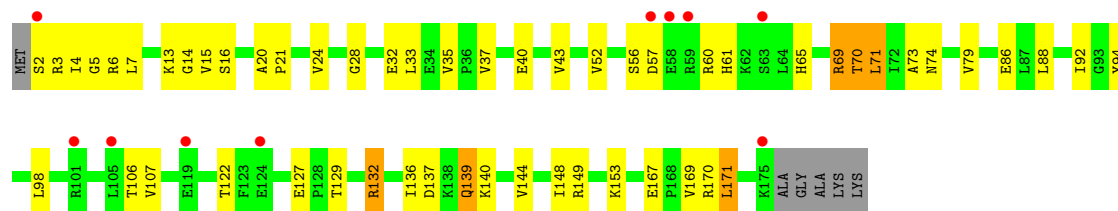
• Molecule 28: 50S Ribosomal Protein L5



• Molecule 28: 50S Ribosomal Protein L5

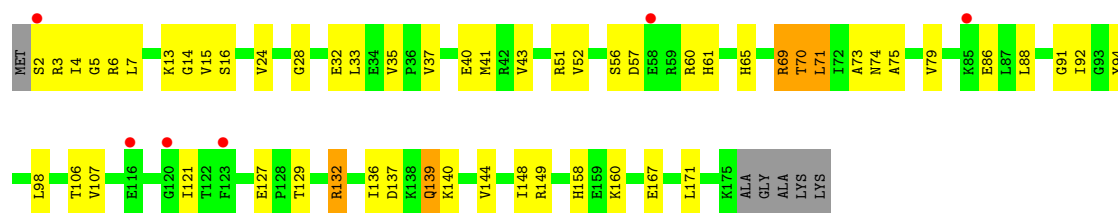


• Molecule 29: 50S Ribosomal Protein L6

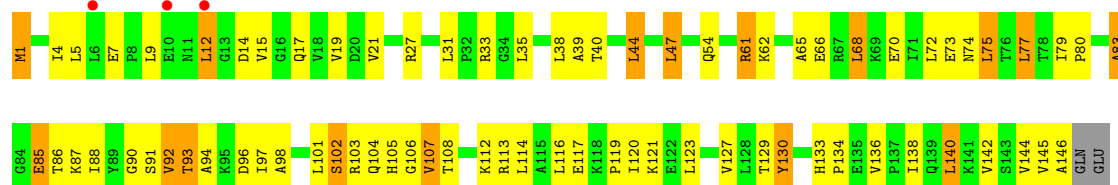


• Molecule 29: 50S Ribosomal Protein L6

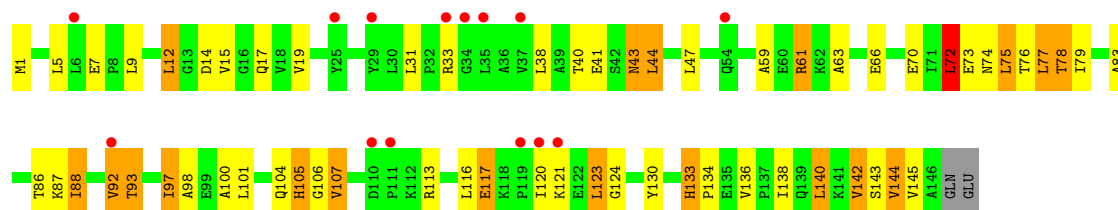




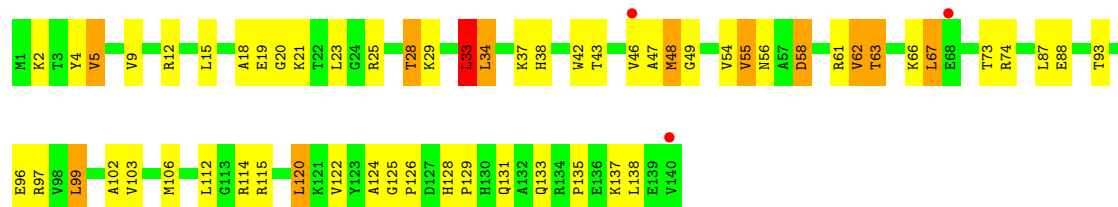
• Molecule 30: 50S Ribosomal Protein L9



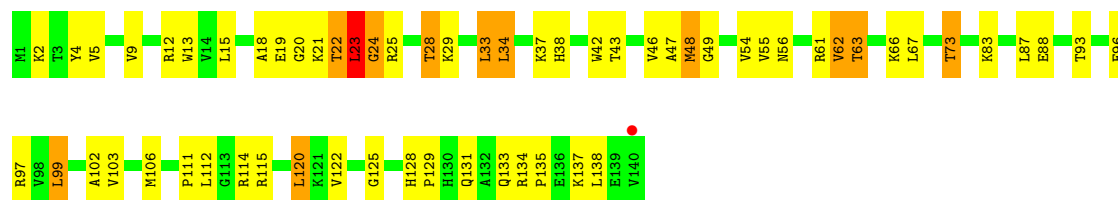
• Molecule 30: 50S Ribosomal Protein L9



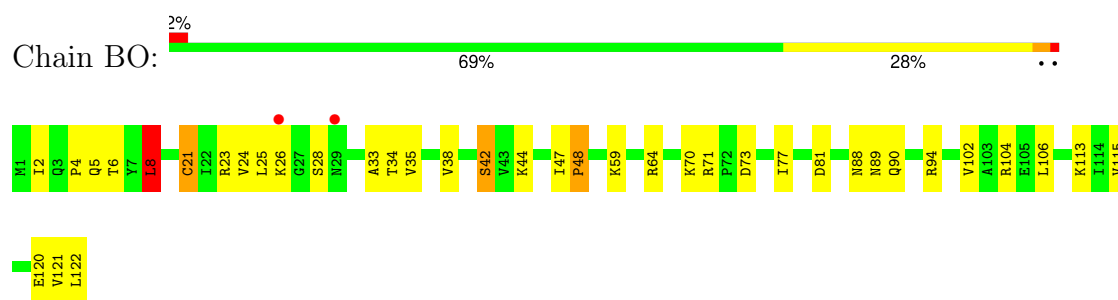
• Molecule 31: 50S Ribosomal Protein L13



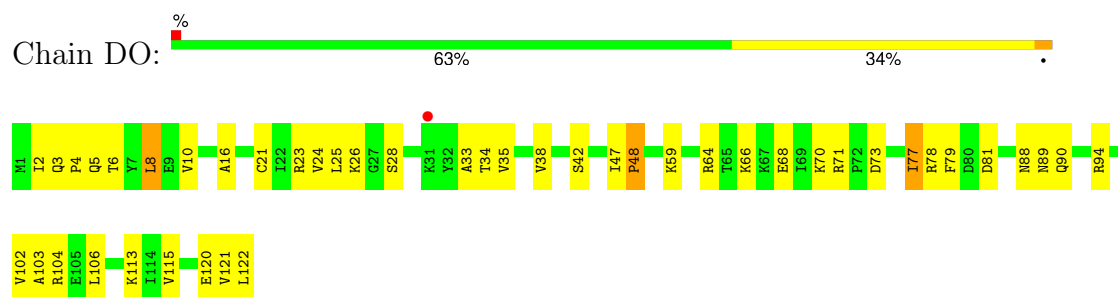
• Molecule 31: 50S Ribosomal Protein L13



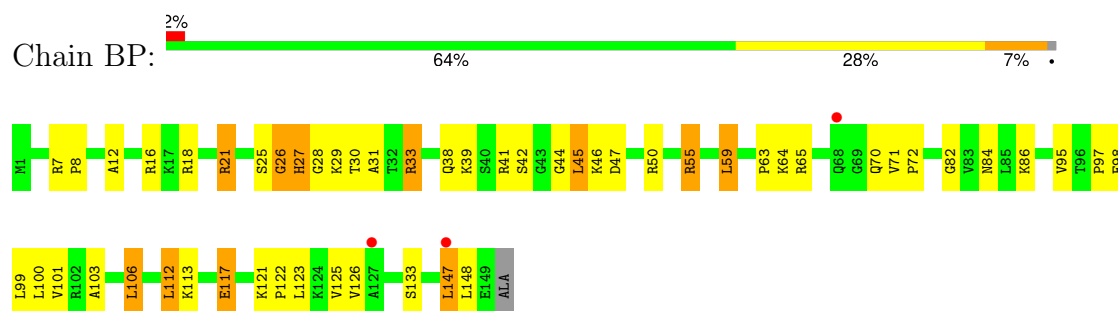
• Molecule 32: 50S Ribosomal Protein L14



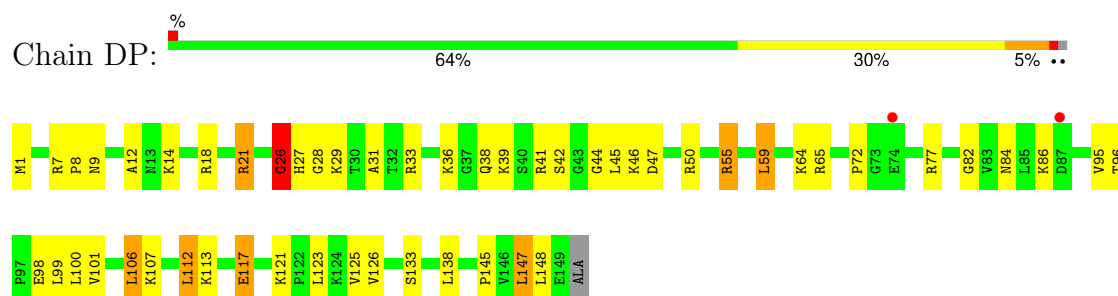
• Molecule 32: 50S Ribosomal Protein L14



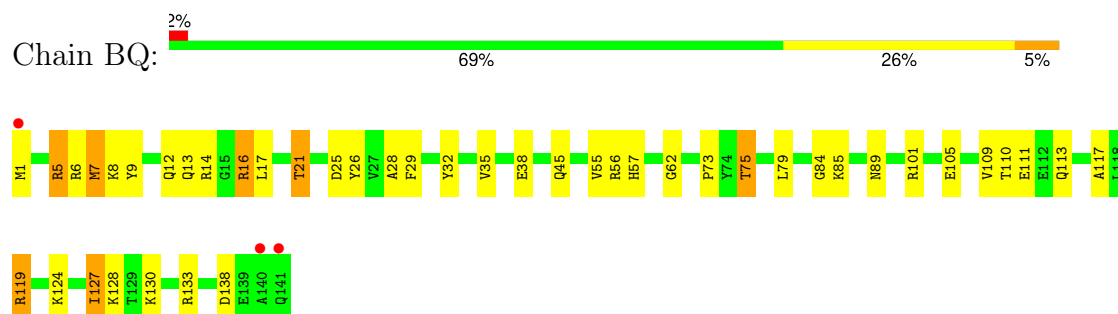
• Molecule 33: 50S Ribosomal Protein L15



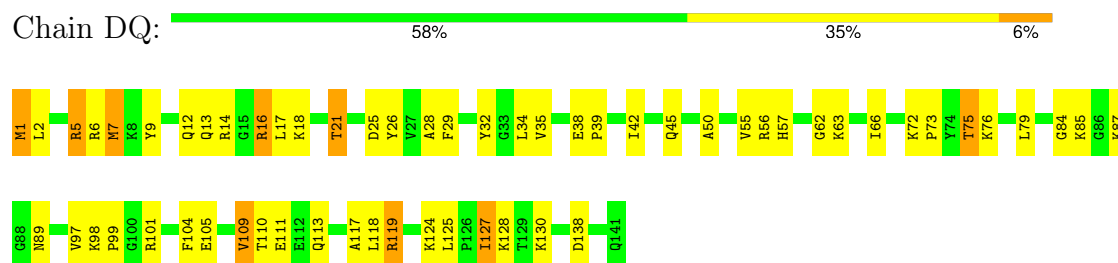
• Molecule 33: 50S Ribosomal Protein L15



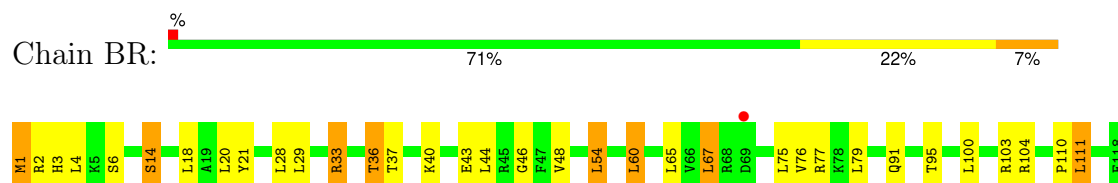
• Molecule 34: 50S Ribosomal Protein L16



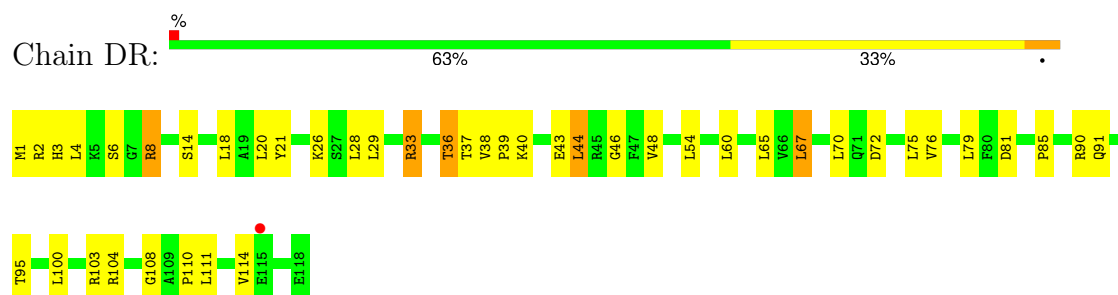
- Molecule 34: 50S Ribosomal Protein L16



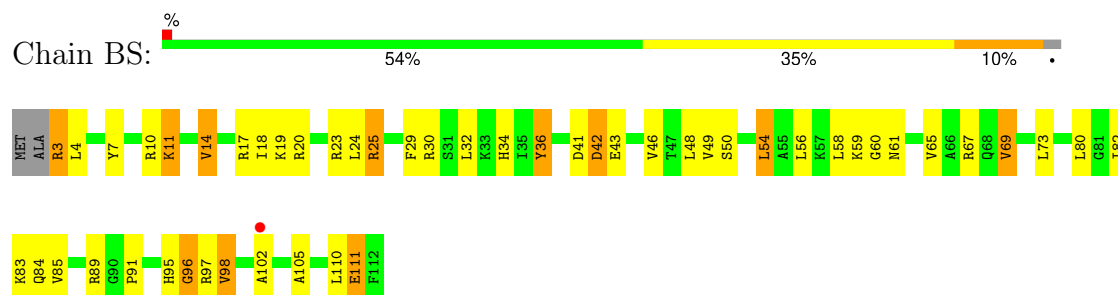
- Molecule 35: 50S Ribosomal Protein L17



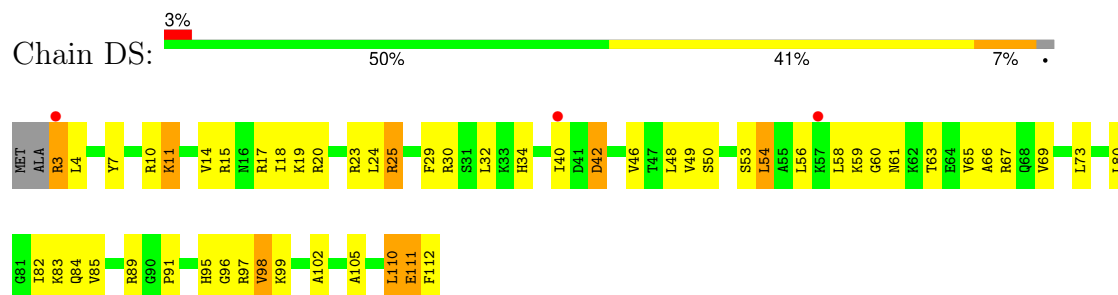
- Molecule 35: 50S Ribosomal Protein L17



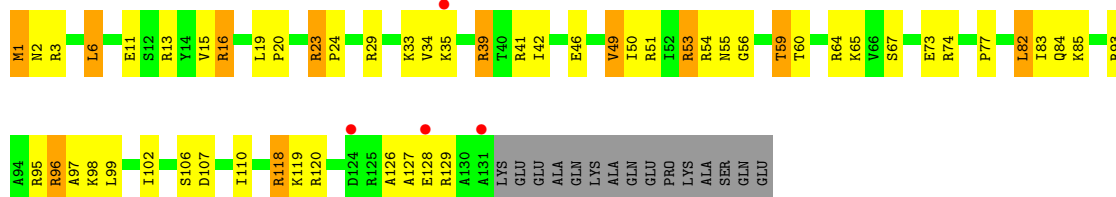
- Molecule 36: 50S Ribosomal Protein L18



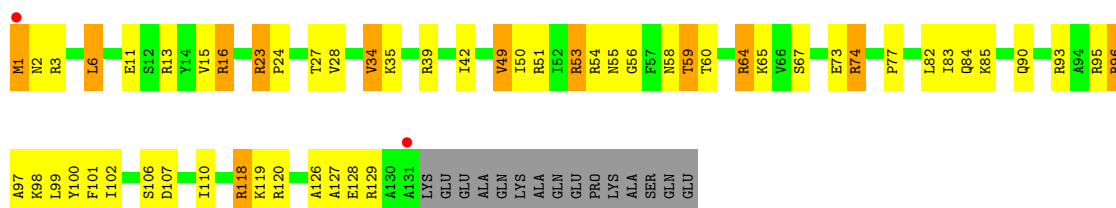
- Molecule 36: 50S Ribosomal Protein L18



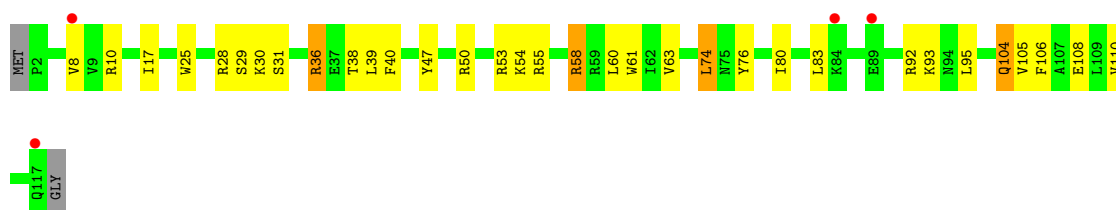
- Molecule 37: 50S Ribosomal Protein L19



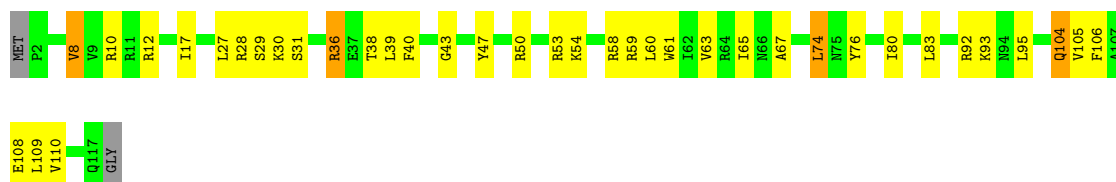
- Molecule 37: 50S Ribosomal Protein L19



- Molecule 38: 50S Ribosomal Protein L20

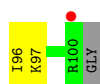


- Molecule 38: 50S Ribosomal Protein L20



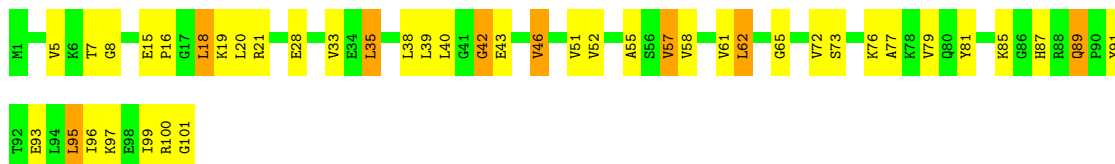
- Molecule 39: 50S Ribosomal Protein L21





• Molecule 39: 50S Ribosomal Protein L21

Chain DV: 57% 35% 8%



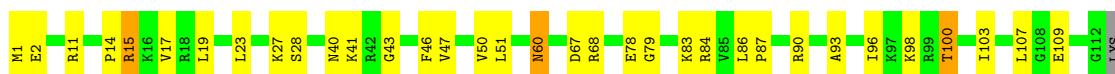
• Molecule 40: 50S Ribosomal Protein L22

Chain BW: 2% 73% 23% ..



• Molecule 40: 50S Ribosomal Protein L22

Chain DW: 69% 27% ..



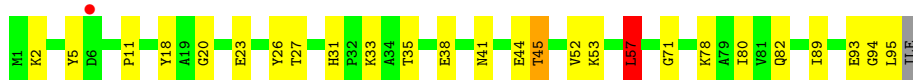
• Molecule 41: 50S Ribosomal Protein L23

Chain BX: 4% 73% 23% ..



• Molecule 41: 50S Ribosomal Protein L23

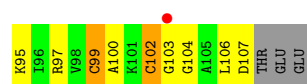
Chain DX: 72% 25% ..



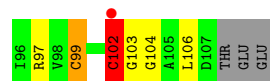
• Molecule 42: 50S Ribosomal Protein L24

Chain BY: 5% 54% 39% 2%

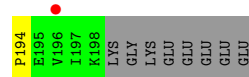
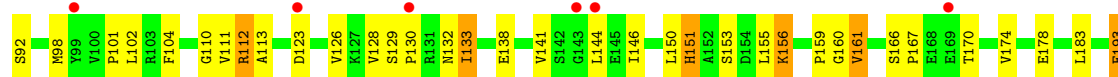
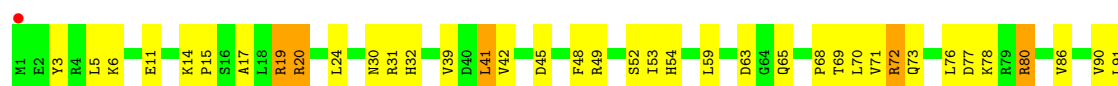




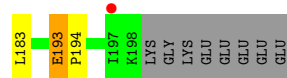
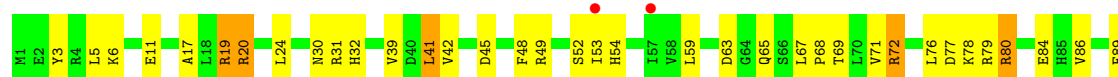
• Molecule 42: 50S Ribosomal Protein L24



• Molecule 43: 50S Ribosomal Protein L25



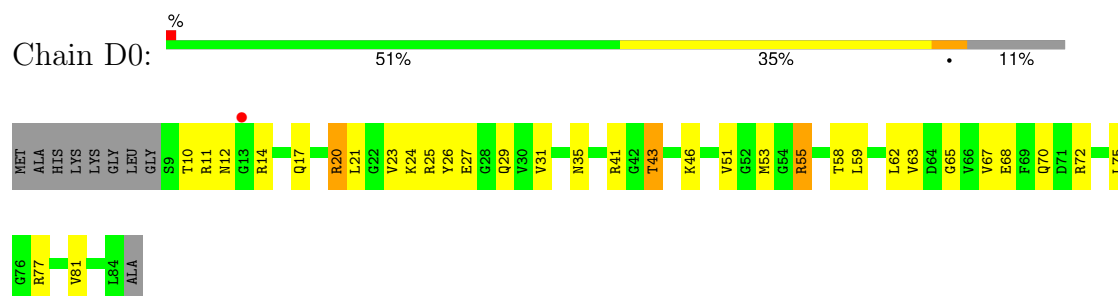
• Molecule 43: 50S Ribosomal Protein L25



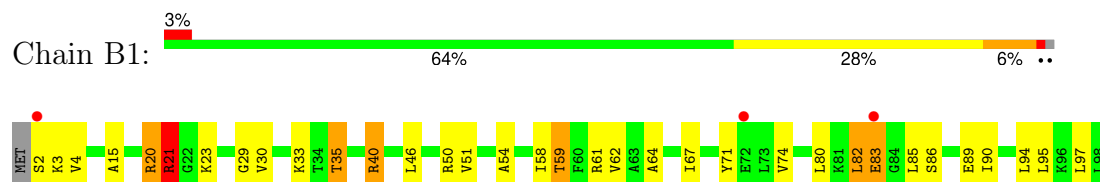
• Molecule 44: 50S Ribosomal Protein L27



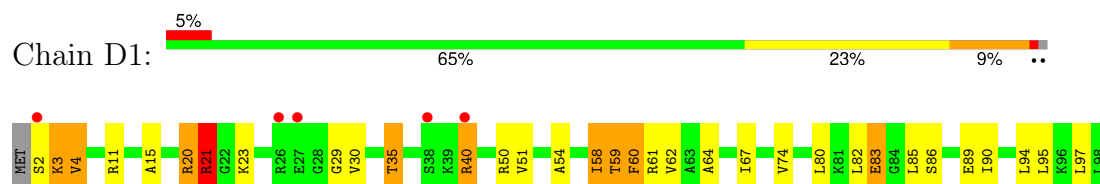
• Molecule 44: 50S Ribosomal Protein L27



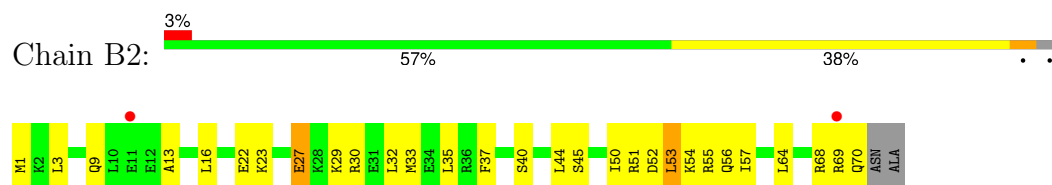
• Molecule 45: 50S Ribosomal Protein L28



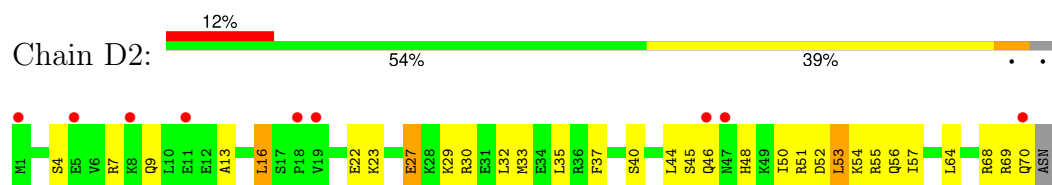
• Molecule 45: 50S Ribosomal Protein L28



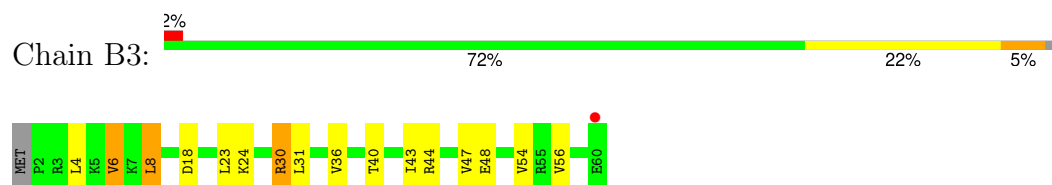
• Molecule 46: 50S Ribosomal Protein L29



• Molecule 46: 50S Ribosomal Protein L29

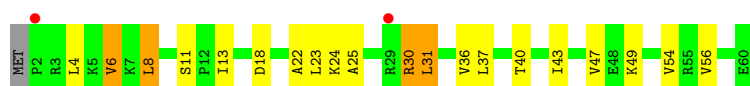


• Molecule 47: 50S Ribosomal Protein L30

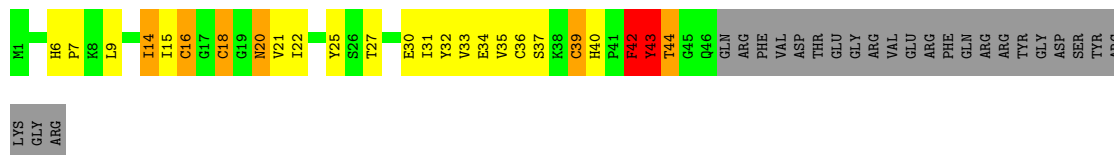
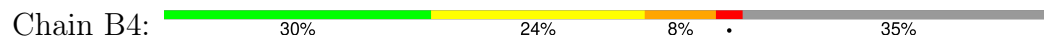


• Molecule 47: 50S Ribosomal Protein L30

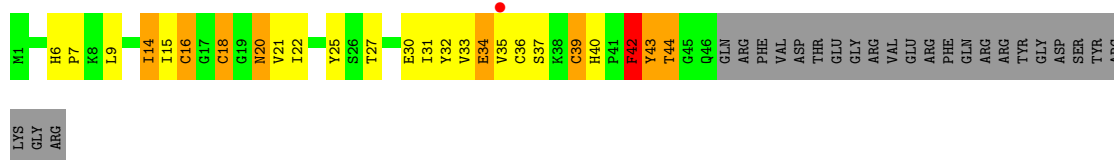
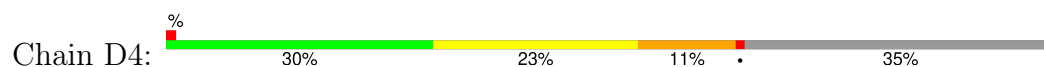




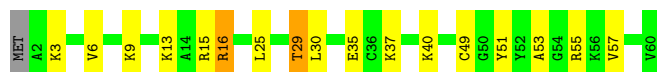
• Molecule 48: 50S Ribosomal Protein L31



• 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



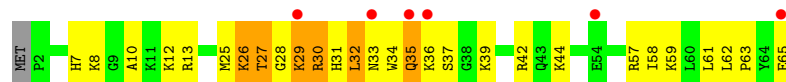
• Molecule 51: 50S Ribosomal Protein L34



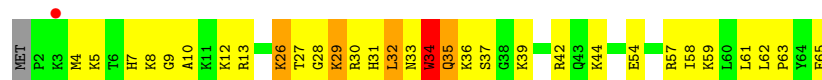
• Molecule 51: 50S Ribosomal Protein L34



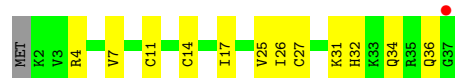
• Molecule 52: 50S Ribosomal Protein L35



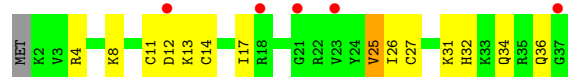
• Molecule 52: 50S Ribosomal Protein L35



• 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	210.24Å 451.44Å 621.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 3.00 49.75 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.75-3.00) 97.9 (49.75-3.00)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.218 , 0.254 0.215 , 0.250	Depositor DCC
R_{free} test set	57194 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	283930	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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: ZN, MG

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	0.99	24/36215 (0.1%)	1.43	546/56522 (1.0%)
1	CA	0.91	21/36123 (0.1%)	1.38	452/56379 (0.8%)
2	AB	0.59	0/1809	0.73	1/2450 (0.0%)
2	CB	0.61	0/1809	0.73	1/2450 (0.0%)
3	AC	0.72	0/1474	0.82	2/2003 (0.1%)
3	CC	0.68	0/1474	0.79	2/2003 (0.1%)
4	AD	0.69	3/1556 (0.2%)	0.76	2/2113 (0.1%)
4	CD	0.64	2/1556 (0.1%)	0.74	2/2113 (0.1%)
5	AE	0.58	0/1121	0.79	0/1517
5	CE	0.58	0/1121	0.78	1/1517 (0.1%)
6	AF	0.55	0/790	0.71	0/1077
6	CF	0.54	0/790	0.70	0/1077
7	AG	0.83	0/1183	0.89	1/1599 (0.1%)
7	CG	0.72	0/1183	0.77	0/1599
8	AH	0.51	0/1065	0.67	0/1445
8	CH	0.50	0/1065	0.67	0/1445
9	AI	0.84	0/867	0.84	0/1180
9	CI	0.74	0/867	0.84	1/1180 (0.1%)
10	AJ	0.78	0/676	0.86	0/924
10	CJ	0.75	0/676	0.88	2/924 (0.2%)
11	AK	0.51	0/843	0.71	0/1144
11	CK	0.53	0/843	0.69	0/1144
12	AL	0.56	0/921	0.74	0/1247
12	CL	0.54	0/921	0.73	0/1247
13	AM	0.92	0/814	0.92	2/1107 (0.2%)
13	CM	0.72	0/814	0.83	0/1107
14	AN	0.79	0/487	0.93	0/649
14	CN	0.66	0/487	0.71	1/649 (0.2%)
15	AO	0.52	0/735	0.72	0/981
15	CO	0.52	0/735	0.72	0/981
16	AP	0.56	0/667	0.82	0/905
16	CP	0.54	0/667	0.84	1/905 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.56	0/836	0.72	0/1117
17	CQ	0.57	0/836	0.72	0/1117
18	AR	0.54	0/519	0.79	0/699
18	CR	0.56	0/519	0.79	0/699
19	AS	0.92	0/574	0.92	0/781
19	CS	0.69	0/574	0.81	0/781
20	AT	0.54	0/715	0.78	0/947
20	CT	0.52	0/715	0.77	0/947
21	AU	0.78	0/203	0.77	0/266
21	CU	0.73	0/203	0.68	0/266
22	AV	0.63	0/339	0.75	0/464
22	CV	0.65	0/360	0.85	1/492 (0.2%)
23	BA	1.60	727/67771 (1.1%)	1.72	2179/105789 (2.1%)
23	DA	1.16	149/67893 (0.2%)	1.60	1664/105982 (1.6%)
24	BB	1.11	3/2878 (0.1%)	1.57	62/4490 (1.4%)
24	DB	0.97	4/2878 (0.1%)	1.46	37/4490 (0.8%)
25	BD	0.88	3/2186 (0.1%)	0.96	0/2944
25	DD	0.80	2/2186 (0.1%)	0.91	1/2944 (0.0%)
26	BE	0.89	0/1588	0.96	3/2145 (0.1%)
26	DE	0.75	0/1588	0.92	0/2145
27	BF	0.88	1/1615 (0.1%)	0.86	0/2188
27	DF	0.70	0/1615	0.90	2/2188 (0.1%)
28	BG	0.53	0/1393	0.71	0/1892
28	DG	0.59	0/1393	0.71	0/1892
29	BH	0.68	0/1343	0.80	3/1820 (0.2%)
29	DH	0.60	0/1343	0.77	2/1820 (0.1%)
30	BI	0.64	0/1055	0.83	0/1445
30	DI	0.65	0/1053	0.84	1/1442 (0.1%)
31	BN	0.86	0/1139	0.87	2/1538 (0.1%)
31	DN	0.65	0/1139	0.87	1/1538 (0.1%)
32	BO	0.79	1/933 (0.1%)	0.86	1/1257 (0.1%)
32	DO	0.70	0/933	0.86	1/1257 (0.1%)
33	BP	0.80	0/1148	0.93	1/1529 (0.1%)
33	DP	0.67	0/1148	0.93	2/1529 (0.1%)
34	BQ	0.79	0/1143	0.89	0/1527
34	DQ	0.70	0/1143	0.86	0/1527
35	BR	0.82	0/982	0.94	2/1312 (0.2%)
35	DR	0.74	0/982	0.93	2/1312 (0.2%)
36	BS	0.65	0/875	0.88	0/1168
36	DS	0.66	0/875	0.84	0/1168
37	BT	0.74	0/1077	0.87	0/1444
37	DT	0.66	0/1077	0.85	0/1444
38	BU	1.02	0/977	0.89	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DU	0.79	0/977	0.88	0/1301
39	BV	0.89	0/771	0.84	0/1037
39	DV	0.70	0/782	0.84	1/1049 (0.1%)
40	BW	1.04	0/891	0.99	2/1197 (0.2%)
40	DW	0.87	0/891	0.91	0/1197
41	BX	0.87	0/756	0.88	1/1016 (0.1%)
41	DX	0.78	0/756	0.84	1/1016 (0.1%)
42	BY	0.81	0/798	0.88	0/1073
42	DY	0.72	1/798 (0.1%)	0.87	1/1073 (0.1%)
43	BZ	0.62	0/1555	0.82	1/2118 (0.0%)
43	DZ	0.63	0/1555	0.80	1/2118 (0.0%)
44	B0	0.83	0/602	0.86	0/804
44	D0	0.73	0/602	0.81	0/804
45	B1	0.80	0/752	1.00	3/1003 (0.3%)
45	D1	0.77	0/752	0.99	2/1003 (0.2%)
46	B2	0.81	0/590	0.82	0/781
46	D2	0.71	0/590	0.83	0/781
47	B3	0.79	0/463	0.86	1/623 (0.2%)
47	D3	0.64	0/463	0.82	0/623
48	B4	0.64	0/358	0.82	1/487 (0.2%)
48	D4	0.70	0/358	0.82	1/487 (0.2%)
49	B5	1.01	0/469	0.99	1/634 (0.2%)
49	D5	0.75	0/469	0.95	1/634 (0.2%)
50	B6	0.84	1/456 (0.2%)	0.86	0/609
50	D6	0.92	2/456 (0.4%)	0.89	2/609 (0.3%)
51	B7	1.07	0/426	1.16	2/561 (0.4%)
51	D7	0.92	0/426	1.00	0/561
52	B8	0.88	0/516	1.00	2/679 (0.3%)
52	D8	0.73	1/516 (0.2%)	0.92	1/679 (0.1%)
53	B9	0.85	0/300	0.91	0/395
53	D9	0.68	0/300	0.83	0/395
All	All	1.12	945/304490 (0.3%)	1.42	5009/455973 (1.1%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	CC	0	2
5	CE	0	1
7	AG	0	4
7	CG	0	1
9	AI	0	2
9	CI	0	1
10	AJ	0	3
12	AL	0	1
12	CL	0	1
13	AM	0	3
13	CM	0	1
14	AN	0	3
17	AQ	0	1
17	CQ	0	1
19	AS	0	1
20	AT	0	2
20	CT	0	1
22	CV	0	3
25	BD	0	1
25	DD	0	1
26	BE	0	2
26	DE	0	1
27	BF	0	2
27	DF	0	3
28	BG	0	1
28	DG	0	1
30	BI	0	1
30	DI	0	1
31	BN	0	1
31	DN	0	2
32	BO	0	1
32	DO	0	1
33	BP	0	4
33	DP	0	2
36	BS	0	2
36	DS	0	1
37	BT	0	1
37	DT	0	1
41	BX	0	1
41	DX	0	1
42	BY	0	1
42	DY	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
43	BZ	0	1
45	B1	0	1
45	D1	0	1
48	B4	0	3
48	D4	0	2
52	D8	0	2
All	All	0	83

The worst 5 of 945 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1459	C	N1-C2	17.17	1.57	1.40
1	AA	1459	C	N1-C2	16.97	1.57	1.40
1	AA	1442(A)	G	N9-C4	16.14	1.50	1.38
1	CA	1442(A)	G	N9-C4	15.91	1.50	1.38
23	DA	528	A	N9-C4	-14.88	1.28	1.37

The worst 5 of 5009 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1442(A)	G	N3-C4-C5	-27.29	114.95	128.60
1	CA	1459	C	N3-C2-O2	-27.00	103.00	121.90
1	AA	1442(A)	G	N3-C4-C5	-26.82	115.19	128.60
1	CA	1459	C	C6-N1-C2	-26.34	109.77	120.30
1	AA	1459	C	N3-C2-O2	-25.91	103.77	121.90

There are no chirality outliers.

5 of 83 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	128	GLU	Peptide
2	AB	14	GLY	Peptide
2	AB	71	VAL	Peptide
3	AC	186	PHE	Peptide
7	AG	19	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	32353	0	16329	1267	0
1	CA	32270	0	16287	987	1
2	AB	1775	0	1743	99	0
2	CB	1775	0	1743	93	0
3	AC	1450	0	1314	80	0
3	CC	1450	0	1314	99	0
4	AD	1526	0	1417	79	0
4	CD	1526	0	1415	91	0
5	AE	1105	0	1130	55	0
5	CE	1105	0	1130	60	0
6	AF	777	0	737	26	0
6	CF	777	0	737	24	0
7	AG	1164	0	1106	100	0
7	CG	1164	0	1106	54	0
8	AH	1045	0	1033	52	0
8	CH	1045	0	1033	52	0
9	AI	852	0	742	69	0
9	CI	852	0	742	62	0
10	AJ	663	0	558	56	0
10	CJ	663	0	558	30	0
11	AK	828	0	822	28	0
11	CK	828	0	822	31	0
12	AL	905	0	916	44	0
12	CL	905	0	916	44	0
13	AM	804	0	752	62	0
13	CM	804	0	752	48	0
14	AN	478	0	497	50	0
14	CN	478	0	497	35	0
15	AO	724	0	749	25	0
15	CO	724	0	749	29	0
16	AP	651	0	638	33	0
16	CP	651	0	638	35	0
17	AQ	823	0	891	16	0
17	CQ	823	0	891	18	0
18	AR	514	0	530	24	0
18	CR	514	0	530	24	0
19	AS	560	0	466	41	0
19	CS	560	0	466	23	0
20	AT	713	0	766	36	0
20	CT	713	0	766	30	0
21	AU	199	0	208	26	0
21	CU	199	0	208	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	AV	333	0	235	14	0
22	CV	353	0	266	13	0
23	BA	60512	0	30492	877	0
23	DA	60620	0	30560	944	0
24	BB	2573	0	1304	45	0
24	DB	2573	0	1304	52	0
25	BD	2136	0	2218	67	0
25	DD	2136	0	2218	68	0
26	BE	1555	0	1607	39	0
26	DE	1555	0	1607	52	0
27	BF	1580	0	1621	51	0
27	DF	1580	0	1621	65	0
28	BG	1368	0	1324	51	0
28	DG	1368	0	1324	56	0
29	BH	1317	0	1376	30	0
29	DH	1317	0	1376	31	0
30	BI	1040	0	1045	55	1
30	DI	1038	0	1040	38	0
31	BN	1112	0	1180	37	0
31	DN	1112	0	1180	37	0
32	BO	923	0	981	24	0
32	DO	923	0	981	29	0
33	BP	1131	0	1201	38	0
33	DP	1131	0	1201	39	0
34	BQ	1122	0	1179	33	0
34	DQ	1122	0	1179	45	0
35	BR	968	0	1033	22	0
35	DR	968	0	1033	29	0
36	BS	865	0	905	46	0
36	DS	865	0	905	52	0
37	BT	1063	0	1103	41	0
37	DT	1063	0	1103	40	0
38	BU	959	0	1019	24	0
38	DU	959	0	1019	29	0
39	BV	760	0	816	20	0
39	DV	771	0	830	24	0
40	BW	881	0	935	17	0
40	DW	881	0	935	21	0
41	BX	742	0	799	17	0
41	DX	742	0	799	18	0
42	BY	785	0	828	31	0
42	DY	785	0	828	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	BZ	1522	0	1511	49	0
43	DZ	1522	0	1511	52	0
44	B0	594	0	604	23	0
44	D0	594	0	604	31	0
45	B1	745	0	804	31	0
45	D1	745	0	804	31	0
46	B2	588	0	643	19	0
46	D2	588	0	643	24	0
47	B3	458	0	503	9	0
47	D3	458	0	503	13	0
48	B4	349	0	336	20	0
48	D4	349	0	336	20	0
49	B5	455	0	472	14	0
49	D5	455	0	472	17	0
50	B6	449	0	462	19	0
50	D6	449	0	462	18	0
51	B7	418	0	467	11	0
51	D7	418	0	467	15	0
52	B8	509	0	565	23	0
52	D8	509	0	565	28	0
53	B9	297	0	316	8	0
53	D9	297	0	316	10	0
54	AA	106	0	0	0	0
54	AD	1	0	0	0	0
54	B0	2	0	0	0	0
54	B1	1	0	0	0	0
54	B2	2	0	0	0	0
54	B3	2	0	0	0	0
54	B5	2	0	0	0	0
54	B8	3	0	0	0	0
54	B9	1	0	0	0	0
54	BA	618	0	0	0	0
54	BB	17	0	0	0	0
54	BD	3	0	0	0	0
54	BE	6	0	0	0	0
54	BF	2	0	0	0	0
54	BP	1	0	0	0	0
54	BQ	3	0	0	0	0
54	BR	2	0	0	0	0
54	BU	2	0	0	0	0
54	BV	1	0	0	0	0
54	BW	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	CA	69	0	0	0	0
54	D6	1	0	0	0	0
54	D7	1	0	0	0	0
54	D8	1	0	0	0	0
54	DA	430	0	0	0	0
54	DB	5	0	0	0	0
54	DD	1	0	0	0	0
54	DE	1	0	0	0	0
54	DF	2	0	0	0	0
54	DP	1	0	0	0	0
55	AD	1	0	0	0	0
55	AN	1	0	0	0	0
55	B4	1	0	0	0	0
55	B5	1	0	0	0	0
55	B6	1	0	0	0	0
55	B9	1	0	0	0	0
55	BY	1	0	0	0	0
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	145	0	0	23	0
56	AF	1	0	0	0	0
56	AK	1	0	0	0	0
56	AQ	1	0	0	0	0
56	B0	4	0	0	0	0
56	B3	1	0	0	0	0
56	B4	1	0	0	0	0
56	B5	3	0	0	1	0
56	B7	3	0	0	0	0
56	B8	7	0	0	0	0
56	B9	2	0	0	1	0
56	BA	1422	0	0	86	0
56	BB	31	0	0	1	0
56	BD	10	0	0	4	0
56	BE	8	0	0	0	0
56	BF	11	0	0	0	0
56	BH	2	0	0	0	0
56	BN	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BO	3	0	0	0	0
56	BP	6	0	0	0	0
56	BQ	2	0	0	0	0
56	BR	6	0	0	0	0
56	BT	1	0	0	0	0
56	BU	2	0	0	0	0
56	BV	2	0	0	0	0
56	BW	4	0	0	0	0
56	BX	2	0	0	0	0
56	BY	1	0	0	0	0
56	CA	119	0	0	13	0
56	CD	1	0	0	0	0
56	CK	2	0	0	0	0
56	CP	1	0	0	0	0
56	CT	2	0	0	0	0
56	D0	1	0	0	0	0
56	D1	2	0	0	0	0
56	DA	696	0	0	56	0
56	DB	9	0	0	0	0
56	DD	3	0	0	0	0
56	DE	2	0	0	0	0
56	DF	5	0	0	0	0
56	DP	5	0	0	0	0
56	DQ	2	0	0	0	0
56	DR	1	0	0	0	0
56	DV	1	0	0	0	0
56	DX	1	0	0	0	0
56	DY	1	0	0	0	0
All	All	283930	0	186520	7011	1

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 15.

The worst 5 of 7011 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:1303:C:N4	1:AA:1334:G:H1	1.41	1.17
23:BA:2296:U:O4	23:BA:2335:A:N6	1.76	1.15
23:DA:2296:U:O4	23:DA:2335:A:N6	1.79	1.15
1:AA:1003:G:H1	1:AA:1037:C:N4	1.46	1.14
1:AA:559:A:H4'	1:AA:560:U:H3'	1.35	1.07

All (1) 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)
30:BI:91:SER:OG	1:CA:368:U:OP1[3_654]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	227/256 (89%)	188 (83%)	37 (16%)	2 (1%)	14	49
2	CB	227/256 (89%)	192 (85%)	33 (14%)	2 (1%)	14	49
3	AC	204/239 (85%)	179 (88%)	25 (12%)	0	100	100
3	CC	204/239 (85%)	177 (87%)	27 (13%)	0	100	100
4	AD	206/209 (99%)	179 (87%)	25 (12%)	2 (1%)	13	46
4	CD	206/209 (99%)	180 (87%)	24 (12%)	2 (1%)	13	46
5	AE	146/162 (90%)	125 (86%)	20 (14%)	1 (1%)	19	54
5	CE	146/162 (90%)	126 (86%)	20 (14%)	0	100	100
6	AF	98/101 (97%)	88 (90%)	10 (10%)	0	100	100
6	CF	98/101 (97%)	88 (90%)	10 (10%)	0	100	100
7	AG	153/156 (98%)	132 (86%)	19 (12%)	2 (1%)	10	39
7	CG	153/156 (98%)	128 (84%)	23 (15%)	2 (1%)	10	39
8	AH	136/138 (99%)	122 (90%)	14 (10%)	0	100	100
8	CH	136/138 (99%)	125 (92%)	11 (8%)	0	100	100
9	AI	123/128 (96%)	106 (86%)	15 (12%)	2 (2%)	8	34
9	CI	123/128 (96%)	109 (89%)	12 (10%)	2 (2%)	8	34
10	AJ	94/105 (90%)	78 (83%)	14 (15%)	2 (2%)	5	28
10	CJ	94/105 (90%)	74 (79%)	18 (19%)	2 (2%)	5	28
11	AK	112/129 (87%)	100 (89%)	12 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	CK	112/129 (87%)	100 (89%)	12 (11%)	0	100	100
12	AL	120/132 (91%)	109 (91%)	10 (8%)	1 (1%)	16	51
12	CL	120/132 (91%)	107 (89%)	11 (9%)	2 (2%)	7	33
13	AM	112/126 (89%)	82 (73%)	27 (24%)	3 (3%)	4	22
13	CM	112/126 (89%)	84 (75%)	27 (24%)	1 (1%)	14	49
14	AN	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	1	9
14	CN	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	7	33
15	AO	86/89 (97%)	71 (83%)	15 (17%)	0	100	100
15	CO	86/89 (97%)	72 (84%)	14 (16%)	0	100	100
16	AP	80/88 (91%)	69 (86%)	9 (11%)	2 (2%)	4	24
16	CP	80/88 (91%)	71 (89%)	7 (9%)	2 (2%)	4	24
17	AQ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
17	CQ	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
18	AR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
18	CR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
19	AS	79/93 (85%)	62 (78%)	16 (20%)	1 (1%)	10	39
19	CS	79/93 (85%)	60 (76%)	16 (20%)	3 (4%)	2	15
20	AT	95/106 (90%)	82 (86%)	10 (10%)	3 (3%)	3	19
20	CT	95/106 (90%)	81 (85%)	11 (12%)	3 (3%)	3	19
21	AU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
21	CU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
22	AV	51/61 (84%)	42 (82%)	9 (18%)	0	100	100
22	CV	51/61 (84%)	34 (67%)	14 (28%)	3 (6%)	1	7
25	BD	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	30	66
25	DD	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	30	66
26	BE	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	13	46
26	DE	202/206 (98%)	189 (94%)	11 (5%)	2 (1%)	13	46
27	BF	201/210 (96%)	187 (93%)	13 (6%)	1 (0%)	25	61
27	DF	201/210 (96%)	188 (94%)	12 (6%)	1 (0%)	25	61
28	BG	179/182 (98%)	151 (84%)	28 (16%)	0	100	100
28	DG	179/182 (98%)	151 (84%)	27 (15%)	1 (1%)	22	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	BH	172/180 (96%)	156 (91%)	14 (8%)	2 (1%)	11	41
29	DH	172/180 (96%)	158 (92%)	12 (7%)	2 (1%)	11	41
30	BI	144/148 (97%)	114 (79%)	27 (19%)	3 (2%)	5	28
30	DI	144/148 (97%)	113 (78%)	29 (20%)	2 (1%)	9	37
31	BN	138/140 (99%)	128 (93%)	6 (4%)	4 (3%)	3	20
31	DN	138/140 (99%)	126 (91%)	7 (5%)	5 (4%)	3	16
32	BO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
32	DO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
33	BP	147/150 (98%)	134 (91%)	12 (8%)	1 (1%)	19	54
33	DP	147/150 (98%)	134 (91%)	13 (9%)	0	100	100
34	BQ	139/141 (99%)	127 (91%)	12 (9%)	0	100	100
34	DQ	139/141 (99%)	125 (90%)	14 (10%)	0	100	100
35	BR	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
35	DR	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
36	BS	108/112 (96%)	96 (89%)	11 (10%)	1 (1%)	14	49
36	DS	108/112 (96%)	97 (90%)	10 (9%)	1 (1%)	14	49
37	BT	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
37	DT	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
38	BU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
38	DU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
39	BV	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
39	DV	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
40	BW	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
40	DW	110/113 (97%)	106 (96%)	4 (4%)	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%)	9 (9%)	2 (2%)	6	31
42	DY	105/110 (96%)	95 (90%)	8 (8%)	2 (2%)	6	31
43	BZ	196/206 (95%)	178 (91%)	15 (8%)	3 (2%)	8	36
43	DZ	196/206 (95%)	177 (90%)	16 (8%)	3 (2%)	8	36
44	B0	74/85 (87%)	71 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	D0	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
45	B1	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
45	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	12	44
46	B2	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
46	D2	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
47	B3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
47	D3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
48	B4	44/71 (62%)	37 (84%)	7 (16%)	0	100	100
48	D4	44/71 (62%)	38 (86%)	6 (14%)	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
50	B6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
50	D6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
51	B7	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	5	27
51	D7	46/49 (94%)	45 (98%)	0	1 (2%)	5	27
52	B8	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	8	34
52	D8	62/65 (95%)	59 (95%)	1 (2%)	2 (3%)	3	19
53	B9	34/37 (92%)	34 (100%)	0	0	100	100
53	D9	34/37 (92%)	34 (100%)	0	0	100	100
All	All	11473/12250 (94%)	10289 (90%)	1089 (10%)	95 (1%)	16	51

5 of 95 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	AM	91	ARG
33	BP	27	HIS
12	CL	92	ASP
31	DN	23	LEU
31	DN	24	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	177/220 (80%)	135 (76%)	42 (24%)	0	3
2	CB	177/220 (80%)	135 (76%)	42 (24%)	0	3
3	AC	114/188 (61%)	74 (65%)	40 (35%)	0	1
3	CC	114/188 (61%)	78 (68%)	36 (32%)	0	1
4	AD	141/181 (78%)	113 (80%)	28 (20%)	1	6
4	CD	141/181 (78%)	114 (81%)	27 (19%)	1	7
5	AE	108/123 (88%)	84 (78%)	24 (22%)	1	4
5	CE	108/123 (88%)	84 (78%)	24 (22%)	1	4
6	AF	76/90 (84%)	68 (90%)	8 (10%)	5	23
6	CF	76/90 (84%)	69 (91%)	7 (9%)	7	29
7	AG	103/127 (81%)	68 (66%)	35 (34%)	0	1
7	CG	103/127 (81%)	77 (75%)	26 (25%)	0	2
8	AH	103/119 (87%)	83 (81%)	20 (19%)	1	6
8	CH	103/119 (87%)	84 (82%)	19 (18%)	1	7
9	AI	62/99 (63%)	49 (79%)	13 (21%)	1	4
9	CI	62/99 (63%)	48 (77%)	14 (23%)	1	3
10	AJ	53/92 (58%)	41 (77%)	12 (23%)	1	3
10	CJ	53/92 (58%)	39 (74%)	14 (26%)	0	2
11	AK	81/99 (82%)	70 (86%)	11 (14%)	3	14
11	CK	81/99 (82%)	70 (86%)	11 (14%)	3	14
12	AL	91/109 (84%)	80 (88%)	11 (12%)	4	18
12	CL	91/109 (84%)	79 (87%)	12 (13%)	3	15
13	AM	64/101 (63%)	45 (70%)	19 (30%)	0	1
13	CM	64/101 (63%)	49 (77%)	15 (23%)	0	3
14	AN	46/50 (92%)	37 (80%)	9 (20%)	1	6
14	CN	46/50 (92%)	33 (72%)	13 (28%)	0	1
15	AO	77/80 (96%)	70 (91%)	7 (9%)	7	30
15	CO	77/80 (96%)	71 (92%)	6 (8%)	10	36
16	AP	63/74 (85%)	47 (75%)	16 (25%)	0	2
16	CP	63/74 (85%)	47 (75%)	16 (25%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AQ	94/97 (97%)	80 (85%)	14 (15%)	2	12
17	CQ	94/97 (97%)	80 (85%)	14 (15%)	2	12
18	AR	49/77 (64%)	43 (88%)	6 (12%)	4	18
18	CR	49/77 (64%)	42 (86%)	7 (14%)	2	13
19	AS	43/80 (54%)	24 (56%)	19 (44%)	0	0
19	CS	43/80 (54%)	32 (74%)	11 (26%)	0	2
20	AT	65/82 (79%)	56 (86%)	9 (14%)	3	14
20	CT	65/82 (79%)	55 (85%)	10 (15%)	2	11
21	AU	18/22 (82%)	11 (61%)	7 (39%)	0	0
21	CU	18/22 (82%)	13 (72%)	5 (28%)	0	1
22	AV	16/50 (32%)	13 (81%)	3 (19%)	1	7
22	CV	21/50 (42%)	14 (67%)	7 (33%)	0	1
25	BD	215/218 (99%)	181 (84%)	34 (16%)	2	10
25	DD	215/218 (99%)	180 (84%)	35 (16%)	2	9
26	BE	163/166 (98%)	138 (85%)	25 (15%)	2	11
26	DE	163/166 (98%)	135 (83%)	28 (17%)	1	8
27	BF	159/166 (96%)	133 (84%)	26 (16%)	2	9
27	DF	159/166 (96%)	133 (84%)	26 (16%)	2	9
28	BG	128/156 (82%)	106 (83%)	22 (17%)	1	8
28	DG	128/156 (82%)	106 (83%)	22 (17%)	1	8
29	BH	141/148 (95%)	127 (90%)	14 (10%)	6	26
29	DH	141/148 (95%)	127 (90%)	14 (10%)	6	26
30	BI	99/124 (80%)	75 (76%)	24 (24%)	0	3
30	DI	98/124 (79%)	67 (68%)	31 (32%)	0	1
31	BN	117/119 (98%)	92 (79%)	25 (21%)	1	4
31	DN	117/119 (98%)	93 (80%)	24 (20%)	1	5
32	BO	98/100 (98%)	90 (92%)	8 (8%)	9	34
32	DO	98/100 (98%)	90 (92%)	8 (8%)	9	34
33	BP	114/116 (98%)	98 (86%)	16 (14%)	3	13
33	DP	114/116 (98%)	100 (88%)	14 (12%)	4	18
34	BQ	111/111 (100%)	95 (86%)	16 (14%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	DQ	111/111 (100%)	96 (86%)	15 (14%)	3	14
35	BR	101/101 (100%)	82 (81%)	19 (19%)	1	7
35	DR	101/101 (100%)	83 (82%)	18 (18%)	1	8
36	BS	84/88 (96%)	69 (82%)	15 (18%)	1	8
36	DS	84/88 (96%)	72 (86%)	12 (14%)	2	13
37	BT	110/127 (87%)	95 (86%)	15 (14%)	3	14
37	DT	110/127 (87%)	92 (84%)	18 (16%)	2	9
38	BU	93/94 (99%)	84 (90%)	9 (10%)	6	27
38	DU	93/94 (99%)	84 (90%)	9 (10%)	6	27
39	BV	79/82 (96%)	62 (78%)	17 (22%)	1	4
39	DV	80/82 (98%)	64 (80%)	16 (20%)	1	5
40	BW	89/92 (97%)	78 (88%)	11 (12%)	4	17
40	DW	89/92 (97%)	76 (85%)	13 (15%)	2	12
41	BX	75/78 (96%)	70 (93%)	5 (7%)	13	43
41	DX	75/78 (96%)	70 (93%)	5 (7%)	13	43
42	BY	80/91 (88%)	66 (82%)	14 (18%)	1	8
42	DY	80/91 (88%)	63 (79%)	17 (21%)	1	4
43	BZ	159/179 (89%)	141 (89%)	18 (11%)	4	21
43	DZ	159/179 (89%)	141 (89%)	18 (11%)	4	21
44	B0	59/67 (88%)	54 (92%)	5 (8%)	8	33
44	D0	59/67 (88%)	54 (92%)	5 (8%)	8	33
45	B1	78/83 (94%)	67 (86%)	11 (14%)	3	13
45	D1	78/83 (94%)	67 (86%)	11 (14%)	3	13
46	B2	65/67 (97%)	59 (91%)	6 (9%)	7	29
46	D2	65/67 (97%)	58 (89%)	7 (11%)	5	22
47	B3	49/52 (94%)	43 (88%)	6 (12%)	4	18
47	D3	49/52 (94%)	42 (86%)	7 (14%)	2	13
48	B4	39/63 (62%)	29 (74%)	10 (26%)	0	2
48	D4	39/63 (62%)	29 (74%)	10 (26%)	0	2
49	B5	50/52 (96%)	45 (90%)	5 (10%)	6	25
49	D5	50/52 (96%)	45 (90%)	5 (10%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	B6	50/52 (96%)	39 (78%)	11 (22%)	1	4
50	D6	50/52 (96%)	37 (74%)	13 (26%)	0	2
51	B7	41/42 (98%)	32 (78%)	9 (22%)	1	4
51	D7	41/42 (98%)	34 (83%)	7 (17%)	1	8
52	B8	52/55 (94%)	43 (83%)	9 (17%)	1	8
52	D8	52/55 (94%)	43 (83%)	9 (17%)	1	8
53	B9	32/34 (94%)	29 (91%)	3 (9%)	7	28
53	D9	32/34 (94%)	29 (91%)	3 (9%)	7	28
All	All	8753/10166 (86%)	7236 (83%)	1517 (17%)	1	8

5 of 1517 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	CH	21	LYS
26	DE	105	THR
9	CI	104	ARG
8	CH	19	VAL
16	CP	69	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
28	DG	123	ASN
41	DX	55	ASN
28	DG	138	GLN
34	DQ	89	ASN
51	D7	6	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	425 (28%)	31 (2%)
1	CA	1499/1522 (98%)	383 (25%)	29 (1%)
23	BA	2802/2915 (96%)	556 (19%)	62 (2%)
23	DA	2808/2915 (96%)	552 (19%)	63 (2%)
24	BB	119/122 (97%)	21 (17%)	0
24	DB	119/122 (97%)	21 (17%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	8850/9118 (97%)	1958 (22%)	185 (2%)

5 of 1958 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	9	G
1	AA	10	A
1	AA	22	G

5 of 185 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	1201	A
23	DA	856	C
1	CA	1442	G
23	DA	277	C
23	DA	1047	G

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 1302 ligands modelled in this entry, 1302 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	1505/1522 (98%)	0.95	231 (15%) 6 4	52, 116, 177, 188	0
1	CA	1501/1522 (98%)	0.63	117 (7%) 20 11	53, 112, 168, 181	0
2	AB	229/256 (89%)	1.09	32 (13%) 7 4	114, 135, 150, 160	0
2	CB	229/256 (89%)	0.97	32 (13%) 7 4	113, 135, 150, 160	0
3	AC	206/239 (86%)	1.38	51 (24%) 2 2	122, 148, 164, 172	0
3	CC	206/239 (86%)	1.01	28 (13%) 8 5	119, 140, 153, 162	0
4	AD	208/209 (99%)	1.41	52 (25%) 2 2	100, 116, 133, 143	0
4	CD	208/209 (99%)	1.22	41 (19%) 3 3	95, 111, 129, 142	0
5	AE	148/162 (91%)	0.96	16 (10%) 12 7	85, 109, 124, 129	0
5	CE	148/162 (91%)	0.69	12 (8%) 19 11	87, 108, 124, 132	0
6	AF	100/101 (99%)	0.84	11 (11%) 12 7	88, 102, 122, 136	0
6	CF	100/101 (99%)	0.56	5 (5%) 35 20	93, 107, 123, 135	0
7	AG	155/156 (99%)	2.07	65 (41%) 1 1	134, 156, 166, 168	0
7	CG	155/156 (99%)	1.26	40 (25%) 2 2	118, 144, 151, 158	0
8	AH	138/138 (100%)	0.80	15 (10%) 12 7	93, 111, 121, 131	0
8	CH	138/138 (100%)	0.81	15 (10%) 12 7	89, 110, 120, 133	0
9	AI	125/128 (97%)	2.46	68 (54%) 0 0	131, 157, 170, 176	0
9	CI	125/128 (97%)	2.10	55 (44%) 1 1	129, 151, 161, 173	0
10	AJ	96/105 (91%)	2.39	52 (54%) 0 0	137, 155, 170, 176	0
10	CJ	96/105 (91%)	2.00	42 (43%) 1 1	130, 149, 161, 169	0
11	AK	114/129 (88%)	0.66	7 (6%) 28 16	74, 109, 123, 127	0
11	CK	114/129 (88%)	0.76	10 (8%) 17 9	79, 109, 122, 124	0
12	AL	122/132 (92%)	0.96	18 (14%) 7 4	72, 95, 111, 120	0
12	CL	122/132 (92%)	0.83	9 (7%) 22 12	72, 92, 106, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/126 (90%)	2.67	67 (58%) 0 0	147, 160, 171, 177	0
13	CM	114/126 (90%)	1.65	34 (29%) 1 1	124, 145, 155, 158	0
14	AN	60/61 (98%)	2.72	36 (60%) 0 0	134, 160, 169, 174	0
14	CN	60/61 (98%)	1.99	27 (45%) 1 1	136, 146, 152, 155	0
15	AO	88/89 (98%)	0.78	7 (7%) 20 11	78, 103, 120, 131	0
15	CO	88/89 (98%)	0.58	4 (4%) 39 22	79, 102, 122, 129	0
16	AP	82/88 (93%)	1.73	21 (25%) 2 2	98, 112, 132, 138	0
16	CP	82/88 (93%)	1.37	17 (20%) 3 2	89, 105, 122, 132	0
17	AQ	99/105 (94%)	0.96	10 (10%) 14 8	86, 99, 113, 118	0
17	CQ	99/105 (94%)	0.65	7 (7%) 23 13	84, 98, 113, 117	0
18	AR	68/88 (77%)	0.80	5 (7%) 22 12	93, 104, 138, 141	0
18	CR	68/88 (77%)	0.69	2 (2%) 54 32	95, 107, 138, 143	0
19	AS	81/93 (87%)	2.08	38 (46%) 0 1	131, 164, 174, 179	0
19	CS	81/93 (87%)	1.24	15 (18%) 4 3	125, 146, 153, 155	0
20	AT	97/106 (91%)	1.49	28 (28%) 1 1	90, 106, 127, 131	0
20	CT	97/106 (91%)	1.30	22 (22%) 3 2	84, 103, 125, 132	0
21	AU	23/27 (85%)	4.77	21 (91%) 0 0	147, 161, 169, 174	0
21	CU	23/27 (85%)	2.92	16 (69%) 0 0	130, 145, 153, 154	0
22	AV	53/61 (86%)	0.57	4 (7%) 22 12	93, 105, 121, 143	0
22	CV	53/61 (86%)	0.60	6 (11%) 11 6	90, 115, 141, 151	0
23	BA	2809/2915 (96%)	-0.26	70 (2%) 58 36	31, 50, 134, 186	0
23	DA	2814/2915 (96%)	-0.24	68 (2%) 59 37	34, 56, 138, 189	0
24	BB	120/122 (98%)	-0.17	0 100 100	46, 72, 94, 119	0
24	DB	120/122 (98%)	0.24	2 (1%) 69 47	63, 90, 111, 129	0
25	BD	275/276 (99%)	0.03	6 (2%) 62 40	34, 52, 69, 117	0
25	DD	275/276 (99%)	-0.21	4 (1%) 71 50	36, 55, 72, 119	0
26	BE	204/206 (99%)	-0.02	3 (1%) 71 50	32, 55, 78, 95	0
26	DE	204/206 (99%)	-0.09	2 (0%) 79 60	35, 61, 84, 101	0
27	BF	203/210 (96%)	-0.09	0 100 100	30, 60, 92, 136	0
27	DF	203/210 (96%)	0.08	4 (1%) 64 43	34, 67, 96, 136	0
28	BG	181/182 (99%)	0.97	23 (12%) 9 5	80, 120, 143, 152	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	181/182 (99%)	1.03	18 (9%) 14 8	92, 126, 146, 156	0
29	BH	174/180 (96%)	0.51	10 (5%) 30 17	58, 79, 97, 110	0
29	DH	174/180 (96%)	0.63	6 (3%) 48 28	70, 92, 107, 122	0
30	BI	146/148 (98%)	0.22	3 (2%) 63 41	57, 90, 108, 120	0
30	DI	146/148 (98%)	0.74	14 (9%) 15 8	60, 108, 127, 131	0
31	BN	140/140 (100%)	0.01	3 (2%) 63 41	39, 55, 83, 98	0
31	DN	140/140 (100%)	-0.07	1 (0%) 84 68	45, 63, 89, 101	0
32	BO	122/122 (100%)	-0.03	2 (1%) 70 49	43, 58, 79, 85	0
32	DO	122/122 (100%)	-0.21	1 (0%) 82 66	46, 62, 82, 86	0
33	BP	149/150 (99%)	0.15	3 (2%) 64 43	34, 63, 98, 109	0
33	DP	149/150 (99%)	0.10	2 (1%) 74 54	38, 70, 102, 111	0
34	BQ	141/141 (100%)	0.07	3 (2%) 63 41	43, 61, 77, 91	0
34	DQ	141/141 (100%)	0.11	0 100 100	47, 67, 85, 94	0
35	BR	118/118 (100%)	-0.12	1 (0%) 82 66	38, 50, 70, 78	0
35	DR	118/118 (100%)	-0.07	1 (0%) 82 66	42, 55, 73, 82	0
36	BS	110/112 (98%)	0.18	1 (0%) 81 63	58, 75, 93, 101	0
36	DS	110/112 (98%)	0.46	3 (2%) 56 34	64, 82, 99, 110	0
37	BT	131/146 (89%)	0.06	4 (3%) 51 30	51, 63, 98, 117	0
37	DT	131/146 (89%)	0.04	2 (1%) 71 50	55, 67, 101, 118	0
38	BU	116/118 (98%)	-0.11	4 (3%) 48 28	35, 48, 69, 81	0
38	DU	116/118 (98%)	-0.16	0 100 100	40, 56, 76, 86	0
39	BV	100/101 (99%)	0.00	2 (2%) 64 43	34, 62, 81, 91	0
39	DV	101/101 (100%)	0.03	0 100 100	40, 72, 90, 98	0
40	BW	112/113 (99%)	-0.26	2 (1%) 67 45	36, 43, 64, 102	0
40	DW	112/113 (99%)	-0.18	0 100 100	40, 48, 69, 95	0
41	BX	95/96 (98%)	0.04	4 (4%) 41 24	41, 51, 74, 98	0
41	DX	95/96 (98%)	0.11	1 (1%) 77 58	47, 56, 80, 102	0
42	BY	107/110 (97%)	0.54	5 (4%) 37 21	52, 64, 89, 107	0
42	DY	107/110 (97%)	0.73	8 (7%) 22 12	59, 72, 96, 116	0
43	BZ	198/206 (96%)	0.45	8 (4%) 43 25	65, 85, 111, 126	0
43	DZ	198/206 (96%)	0.43	7 (3%) 47 28	73, 92, 115, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	B0	76/85 (89%)	-0.07	0 100 100	48, 55, 71, 87	0
44	D0	76/85 (89%)	0.08	1 (1%) 74 54	53, 61, 76, 90	0
45	B1	97/98 (98%)	-0.02	3 (3%) 51 30	37, 57, 89, 103	0
45	D1	97/98 (98%)	0.19	5 (5%) 34 19	41, 61, 91, 108	0
46	B2	70/72 (97%)	0.25	2 (2%) 54 32	50, 66, 84, 103	0
46	D2	70/72 (97%)	0.70	9 (12%) 9 5	55, 71, 88, 112	0
47	B3	59/60 (98%)	0.26	1 (1%) 69 47	43, 57, 85, 101	0
47	D3	59/60 (98%)	0.28	2 (3%) 48 28	49, 64, 92, 112	0
48	B4	46/71 (64%)	0.36	0 100 100	106, 140, 151, 154	0
48	D4	46/71 (64%)	0.57	1 (2%) 62 40	113, 141, 152, 163	0
49	B5	59/60 (98%)	-0.25	0 100 100	33, 51, 68, 89	0
49	D5	59/60 (98%)	-0.22	0 100 100	37, 55, 73, 95	0
50	B6	53/54 (98%)	-0.13	1 (1%) 66 44	53, 61, 75, 78	0
50	D6	53/54 (98%)	-0.04	2 (3%) 44 26	56, 65, 79, 82	0
51	B7	48/49 (97%)	-0.12	4 (8%) 19 10	32, 37, 61, 78	0
51	D7	48/49 (97%)	-0.14	2 (4%) 41 24	36, 40, 64, 83	0
52	B8	64/65 (98%)	0.40	6 (9%) 15 9	42, 49, 58, 70	0
52	D8	64/65 (98%)	0.02	1 (1%) 70 49	46, 53, 62, 72	0
53	B9	36/37 (97%)	0.19	1 (2%) 55 33	49, 59, 72, 83	0
53	D9	36/37 (97%)	0.87	5 (13%) 7 4	58, 68, 81, 91	0
All	All	20542/21368 (96%)	0.40	1758 (8%) 18 10	30, 80, 160, 189	0

The worst 5 of 1758 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
21	AU	16	GLY	10.6
42	BY	1	MET	10.2
7	CG	2	ALA	10.1
21	AU	4	GLY	9.6
10	AJ	72	VAL	9.2

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1641	1/1	0.48	0.49	93,93,93,93	0
54	MG	BA	3280	1/1	0.53	0.27	89,89,89,89	0
54	MG	BA	3243	1/1	0.54	0.19	117,117,117,117	0
54	MG	BA	3363	1/1	0.55	0.21	74,74,74,74	0
54	MG	CA	1604	1/1	0.57	0.25	110,110,110,110	0
54	MG	AA	1643	1/1	0.60	0.62	96,96,96,96	0
54	MG	CA	1624	1/1	0.61	0.43	82,82,82,82	0
54	MG	DA	3297	1/1	0.61	0.19	66,66,66,66	0
54	MG	AA	1608	1/1	0.62	0.30	90,90,90,90	0
54	MG	AA	1625	1/1	0.62	0.33	102,102,102,102	0
54	MG	CA	1631	1/1	0.62	0.51	88,88,88,88	0
54	MG	AA	1665	1/1	0.62	0.18	86,86,86,86	0
54	MG	DA	3346	1/1	0.65	0.12	89,89,89,89	0
54	MG	DA	3030	1/1	0.66	0.21	52,52,52,52	0
54	MG	DA	3133	1/1	0.66	0.16	78,78,78,78	0
54	MG	AA	1606	1/1	0.66	0.38	74,74,74,74	0
54	MG	AA	1670	1/1	0.66	0.24	115,115,115,115	0
54	MG	BA	3569	1/1	0.67	0.28	68,68,68,68	0
54	MG	BB	208	1/1	0.68	0.23	70,70,70,70	0
54	MG	AA	1682	1/1	0.68	0.16	111,111,111,111	0
54	MG	AD	302	1/1	0.68	0.23	120,120,120,120	0
54	MG	AA	1632	1/1	0.68	0.50	93,93,93,93	0
54	MG	BA	3614	1/1	0.69	0.18	94,94,94,94	0
54	MG	DA	3180	1/1	0.69	0.34	78,78,78,78	0
54	MG	DA	3378	1/1	0.69	0.25	98,98,98,98	0
54	MG	DA	3379	1/1	0.69	0.17	94,94,94,94	0
54	MG	CA	1623	1/1	0.70	0.48	73,73,73,73	0
54	MG	BA	3340	1/1	0.70	0.18	65,65,65,65	0
54	MG	CA	1634	1/1	0.71	0.35	101,101,101,101	0
54	MG	CA	1610	1/1	0.71	0.41	80,80,80,80	0
54	MG	BA	3365	1/1	0.72	0.14	84,84,84,84	0
54	MG	DA	3200	1/1	0.72	0.22	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3308	1/1	0.72	0.25	51,51,51,51	0
54	MG	AA	1620	1/1	0.72	0.43	77,77,77,77	0
54	MG	DA	3050	1/1	0.72	0.28	90,90,90,90	0
54	MG	BA	3139	1/1	0.72	0.25	53,53,53,53	0
54	MG	BA	3157	1/1	0.73	0.15	46,46,46,46	0
54	MG	DA	3151	1/1	0.73	0.32	58,58,58,58	0
54	MG	BA	3093	1/1	0.73	0.31	81,81,81,81	0
54	MG	AA	1676	1/1	0.73	0.48	84,84,84,84	0
54	MG	DA	3194	1/1	0.74	0.37	77,77,77,77	0
54	MG	BA	3013	1/1	0.74	0.10	103,103,103,103	0
54	MG	DA	3219	1/1	0.74	0.27	38,38,38,38	0
54	MG	BA	3545	1/1	0.74	0.14	79,79,79,79	0
54	MG	AA	1655	1/1	0.74	0.34	90,90,90,90	0
54	MG	DA	3172	1/1	0.74	0.20	50,50,50,50	0
54	MG	AA	1630	1/1	0.74	0.29	76,76,76,76	0
54	MG	DA	3391	1/1	0.74	0.17	67,67,67,67	0
54	MG	DA	3091	1/1	0.75	0.27	70,70,70,70	0
54	MG	DA	3214	1/1	0.75	0.23	74,74,74,74	0
54	MG	DA	3128	1/1	0.75	0.33	72,72,72,72	0
54	MG	BB	207	1/1	0.75	0.23	69,69,69,69	0
54	MG	BA	3176	1/1	0.75	0.25	69,69,69,69	0
54	MG	BA	3055	1/1	0.75	0.21	58,58,58,58	0
54	MG	BA	3351	1/1	0.75	0.15	57,57,57,57	0
54	MG	BA	3160	1/1	0.75	0.24	46,46,46,46	0
55	ZN	CN	101	1/1	0.75	0.23	188,188,188,188	0
54	MG	BA	3034	1/1	0.76	0.12	46,46,46,46	0
54	MG	DA	3108	1/1	0.76	0.31	80,80,80,80	0
54	MG	BA	3549	1/1	0.76	0.16	68,68,68,68	0
54	MG	DA	3129	1/1	0.76	0.14	78,78,78,78	0
54	MG	BA	3195	1/1	0.76	0.25	84,84,84,84	0
54	MG	BA	3201	1/1	0.76	0.24	79,79,79,79	0
54	MG	BA	3203	1/1	0.76	0.25	69,69,69,69	0
54	MG	BA	3051	1/1	0.76	0.15	52,52,52,52	0
54	MG	DA	3189	1/1	0.76	0.34	66,66,66,66	0
54	MG	B0	101	1/1	0.76	0.22	75,75,75,75	0
54	MG	AA	1602	1/1	0.76	0.28	111,111,111,111	0
54	MG	AA	1654	1/1	0.76	0.16	87,87,87,87	0
54	MG	CA	1615	1/1	0.76	0.36	76,76,76,76	0
54	MG	AA	1639	1/1	0.76	0.22	74,74,74,74	0
54	MG	BA	3145	1/1	0.76	0.21	78,78,78,78	0
54	MG	DA	3360	1/1	0.76	0.14	63,63,63,63	0
54	MG	AA	1662	1/1	0.76	0.25	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1607	1/1	0.76	0.36	69,69,69,69	0
54	MG	BA	3487	1/1	0.76	0.16	94,94,94,94	0
54	MG	DB	201	1/1	0.76	0.37	75,75,75,75	0
54	MG	BA	3514	1/1	0.76	0.11	97,97,97,97	0
54	MG	AA	1619	1/1	0.77	0.32	68,68,68,68	0
54	MG	AA	1646	1/1	0.77	0.34	73,73,73,73	0
54	MG	BA	3553	1/1	0.77	0.19	70,70,70,70	0
54	MG	CA	1622	1/1	0.77	0.39	74,74,74,74	0
54	MG	BA	3076	1/1	0.77	0.21	70,70,70,70	0
54	MG	BA	3274	1/1	0.77	0.26	81,81,81,81	0
54	MG	AA	1671	1/1	0.77	0.23	89,89,89,89	0
54	MG	DA	3175	1/1	0.77	0.18	69,69,69,69	0
54	MG	AA	1653	1/1	0.77	0.40	80,80,80,80	0
54	MG	BA	3519	1/1	0.77	0.24	90,90,90,90	0
54	MG	B8	102	1/1	0.77	0.27	61,61,61,61	0
54	MG	AA	1700	1/1	0.78	0.13	114,114,114,114	0
54	MG	DA	3225	1/1	0.78	0.34	64,64,64,64	0
54	MG	BA	3375	1/1	0.78	0.22	46,46,46,46	0
54	MG	DA	3084	1/1	0.78	0.20	62,62,62,62	0
54	MG	AA	1628	1/1	0.78	0.22	84,84,84,84	0
54	MG	BA	3558	1/1	0.78	0.17	61,61,61,61	0
54	MG	BA	3197	1/1	0.78	0.25	62,62,62,62	0
54	MG	AA	1683	1/1	0.78	0.12	139,139,139,139	0
54	MG	DA	3410	1/1	0.78	0.14	72,72,72,72	0
54	MG	DA	3206	1/1	0.78	0.41	75,75,75,75	0
54	MG	CA	1657	1/1	0.78	0.29	86,86,86,86	0
54	MG	BA	3256	1/1	0.79	0.50	69,69,69,69	0
54	MG	DA	3037	1/1	0.79	0.26	49,49,49,49	0
54	MG	DA	3316	1/1	0.79	0.15	75,75,75,75	0
54	MG	AA	1698	1/1	0.79	0.35	68,68,68,68	0
54	MG	DA	3054	1/1	0.79	0.36	75,75,75,75	0
54	MG	BA	3061	1/1	0.79	0.32	64,64,64,64	0
54	MG	AA	1656	1/1	0.79	0.19	74,74,74,74	0
54	MG	AA	1609	1/1	0.79	0.25	91,91,91,91	0
54	MG	CA	1609	1/1	0.79	0.34	70,70,70,70	0
54	MG	CA	1638	1/1	0.79	0.28	71,71,71,71	0
55	ZN	AN	101	1/1	0.79	0.14	213,213,213,213	0
54	MG	BA	3124	1/1	0.79	0.29	68,68,68,68	0
54	MG	AA	1627	1/1	0.80	0.23	70,70,70,70	0
54	MG	BA	3148	1/1	0.80	0.27	54,54,54,54	0
54	MG	DA	3192	1/1	0.80	0.31	66,66,66,66	0
54	MG	AA	1694	1/1	0.80	0.22	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3320	1/1	0.80	0.16	57,57,57,57	0
54	MG	BB	204	1/1	0.80	0.26	67,67,67,67	0
54	MG	DA	3209	1/1	0.80	0.33	79,79,79,79	0
54	MG	DA	3033	1/1	0.80	0.27	68,68,68,68	0
54	MG	BA	3159	1/1	0.80	0.10	66,66,66,66	0
54	MG	DA	3223	1/1	0.80	0.21	104,104,104,104	0
54	MG	AA	1623	1/1	0.80	0.36	74,74,74,74	0
54	MG	DA	3278	1/1	0.80	0.13	46,46,46,46	0
54	MG	BA	3063	1/1	0.80	0.30	84,84,84,84	0
54	MG	AA	1658	1/1	0.80	0.18	60,60,60,60	0
54	MG	BA	3196	1/1	0.80	0.29	80,80,80,80	0
54	MG	BA	3439	1/1	0.80	0.15	53,53,53,53	0
54	MG	BA	3079	1/1	0.80	0.30	68,68,68,68	0
54	MG	CA	1612	1/1	0.80	0.30	84,84,84,84	0
54	MG	AA	1672	1/1	0.80	0.45	82,82,82,82	0
54	MG	DA	3134	1/1	0.80	0.22	64,64,64,64	0
54	MG	AA	1661	1/1	0.80	0.46	77,77,77,77	0
54	MG	BA	3136	1/1	0.80	0.31	73,73,73,73	0
54	MG	AA	1638	1/1	0.80	0.24	78,78,78,78	0
54	MG	DA	3069	1/1	0.81	0.32	61,61,61,61	0
54	MG	DA	3078	1/1	0.81	0.36	53,53,53,53	0
54	MG	DA	3025	1/1	0.81	0.34	57,57,57,57	0
54	MG	BA	3166	1/1	0.81	0.23	58,58,58,58	0
54	MG	DA	3298	1/1	0.81	0.13	71,71,71,71	0
54	MG	DA	3185	1/1	0.81	0.34	47,47,47,47	0
54	MG	DA	3345	1/1	0.81	0.10	100,100,100,100	0
54	MG	DA	3102	1/1	0.81	0.28	79,79,79,79	0
54	MG	DA	3190	1/1	0.81	0.19	57,57,57,57	0
54	MG	DA	3107	1/1	0.81	0.20	47,47,47,47	0
54	MG	BA	3068	1/1	0.81	0.26	70,70,70,70	0
54	MG	BA	3240	1/1	0.81	0.29	64,64,64,64	0
54	MG	DA	3399	1/1	0.81	0.29	60,60,60,60	0
54	MG	DA	3047	1/1	0.81	0.26	65,65,65,65	0
54	MG	BA	3184	1/1	0.81	0.25	66,66,66,66	0
54	MG	DB	202	1/1	0.81	0.51	86,86,86,86	0
54	MG	BA	3499	1/1	0.81	0.10	107,107,107,107	0
54	MG	DA	3147	1/1	0.81	0.43	78,78,78,78	0
54	MG	AA	1669	1/1	0.82	0.09	96,96,96,96	0
54	MG	BB	215	1/1	0.82	0.14	77,77,77,77	0
54	MG	BA	3086	1/1	0.82	0.22	57,57,57,57	0
54	MG	DA	3075	1/1	0.82	0.21	71,71,71,71	0
54	MG	DA	3310	1/1	0.82	0.15	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3152	1/1	0.82	0.24	73,73,73,73	0
54	MG	DA	3327	1/1	0.82	0.17	94,94,94,94	0
54	MG	DA	3341	1/1	0.82	0.22	39,39,39,39	0
54	MG	BA	3062	1/1	0.82	0.21	69,69,69,69	0
54	MG	CA	1648	1/1	0.82	0.13	100,100,100,100	0
54	MG	BA	3041	1/1	0.82	0.31	56,56,56,56	0
54	MG	CA	1659	1/1	0.82	0.22	60,60,60,60	0
54	MG	BA	3459	1/1	0.82	0.09	130,130,130,130	0
54	MG	DA	3390	1/1	0.82	0.12	69,69,69,69	0
54	MG	DA	3127	1/1	0.82	0.15	63,63,63,63	0
54	MG	AA	1697	1/1	0.82	0.14	75,75,75,75	0
54	MG	DA	3400	1/1	0.82	0.17	95,95,95,95	0
54	MG	AA	1677	1/1	0.82	0.46	81,81,81,81	0
54	MG	CA	1621	1/1	0.82	0.30	64,64,64,64	0
54	MG	DA	3217	1/1	0.82	0.41	69,69,69,69	0
54	MG	BA	3226	1/1	0.82	0.29	62,62,62,62	0
54	MG	DA	3141	1/1	0.82	0.29	74,74,74,74	0
54	MG	DA	3130	1/1	0.83	0.14	59,59,59,59	0
54	MG	DA	3232	1/1	0.83	0.25	46,46,46,46	0
54	MG	DA	3259	1/1	0.83	0.23	64,64,64,64	0
54	MG	DA	3034	1/1	0.83	0.24	74,74,74,74	0
54	MG	BA	3279	1/1	0.83	0.13	54,54,54,54	0
54	MG	DA	3043	1/1	0.83	0.18	63,63,63,63	0
54	MG	AA	1616	1/1	0.83	0.29	79,79,79,79	0
54	MG	DA	3313	1/1	0.83	0.15	64,64,64,64	0
54	MG	BA	3287	1/1	0.83	0.39	65,65,65,65	0
54	MG	BA	3497	1/1	0.83	0.19	55,55,55,55	0
54	MG	BA	3029	1/1	0.83	0.12	83,83,83,83	0
54	MG	CA	1626	1/1	0.83	0.25	86,86,86,86	0
54	MG	BB	209	1/1	0.83	0.20	79,79,79,79	0
54	MG	AA	1621	1/1	0.83	0.47	80,80,80,80	0
54	MG	DA	3089	1/1	0.83	0.41	82,82,82,82	0
54	MG	BR	201	1/1	0.83	0.30	58,58,58,58	0
54	MG	BA	3091	1/1	0.83	0.20	47,47,47,47	0
54	MG	DA	3103	1/1	0.83	0.24	71,71,71,71	0
54	MG	DA	3205	1/1	0.83	0.35	82,82,82,82	0
54	MG	BA	3520	1/1	0.83	0.30	67,67,67,67	0
54	MG	BA	3242	1/1	0.83	0.25	66,66,66,66	0
54	MG	DA	3126	1/1	0.83	0.21	80,80,80,80	0
54	MG	AA	1657	1/1	0.83	0.30	81,81,81,81	0
54	MG	BA	3102	1/1	0.83	0.15	59,59,59,59	0
54	MG	AA	1605	1/1	0.83	0.37	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1645	1/1	0.84	0.44	77,77,77,77	0
54	MG	BA	3205	1/1	0.84	0.21	61,61,61,61	0
54	MG	BA	3210	1/1	0.84	0.18	57,57,57,57	0
54	MG	BA	3535	1/1	0.84	0.12	70,70,70,70	0
54	MG	DA	3139	1/1	0.84	0.35	65,65,65,65	0
54	MG	BA	3218	1/1	0.84	0.27	54,54,54,54	0
54	MG	AA	1622	1/1	0.84	0.30	67,67,67,67	0
54	MG	DA	3299	1/1	0.84	0.10	54,54,54,54	0
54	MG	DA	3049	1/1	0.84	0.28	58,58,58,58	0
54	MG	DA	3155	1/1	0.84	0.20	57,57,57,57	0
54	MG	DA	3163	1/1	0.84	0.14	56,56,56,56	0
54	MG	BA	3080	1/1	0.84	0.34	42,42,42,42	0
54	MG	BA	3178	1/1	0.84	0.21	58,58,58,58	0
54	MG	BA	3565	1/1	0.84	0.13	90,90,90,90	0
54	MG	AA	1652	1/1	0.84	0.32	82,82,82,82	0
54	MG	BA	3428	1/1	0.84	0.18	35,35,35,35	0
54	MG	CA	1625	1/1	0.84	0.59	88,88,88,88	0
54	MG	BA	3618	1/1	0.84	0.09	85,85,85,85	0
54	MG	DA	3388	1/1	0.84	0.10	72,72,72,72	0
54	MG	AA	1634	1/1	0.84	0.34	95,95,95,95	0
54	MG	DA	3199	1/1	0.84	0.27	74,74,74,74	0
54	MG	BA	3267	1/1	0.84	0.32	53,53,53,53	0
54	MG	BA	3485	1/1	0.84	0.10	60,60,60,60	0
54	MG	AA	1675	1/1	0.84	0.40	73,73,73,73	0
54	MG	BA	3098	1/1	0.84	0.44	54,54,54,54	0
54	MG	BD	303	1/1	0.84	0.15	58,58,58,58	0
54	MG	DF	301	1/1	0.84	0.28	58,58,58,58	0
54	MG	DA	3008	1/1	0.84	0.17	48,48,48,48	0
54	MG	AA	1668	1/1	0.84	0.22	83,83,83,83	0
54	MG	AA	1637	1/1	0.85	0.33	82,82,82,82	0
54	MG	CA	1633	1/1	0.85	0.31	71,71,71,71	0
54	MG	AA	1696	1/1	0.85	0.08	74,74,74,74	0
54	MG	BA	3183	1/1	0.85	0.20	76,76,76,76	0
54	MG	DA	3123	1/1	0.85	0.14	56,56,56,56	0
54	MG	CA	1639	1/1	0.85	0.43	61,61,61,61	0
54	MG	BA	3213	1/1	0.85	0.30	64,64,64,64	0
54	MG	BP	201	1/1	0.85	0.27	43,43,43,43	0
54	MG	BA	3217	1/1	0.85	0.12	51,51,51,51	0
54	MG	BA	3073	1/1	0.85	0.15	67,67,67,67	0
54	MG	DA	3012	1/1	0.85	0.23	60,60,60,60	0
54	MG	B5	101	1/1	0.85	0.13	51,51,51,51	0
54	MG	BA	3188	1/1	0.85	0.12	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1602	1/1	0.85	0.37	82,82,82,82	0
54	MG	BA	3233	1/1	0.85	0.18	59,59,59,59	0
54	MG	BA	3360	1/1	0.85	0.12	53,53,53,53	0
54	MG	BA	3239	1/1	0.85	0.24	38,38,38,38	0
54	MG	BA	3194	1/1	0.85	0.26	79,79,79,79	0
54	MG	BA	3001	1/1	0.85	0.14	56,56,56,56	0
54	MG	CA	1619	1/1	0.85	0.25	69,69,69,69	0
54	MG	BA	3386	1/1	0.85	0.10	77,77,77,77	0
54	MG	DA	3183	1/1	0.85	0.19	50,50,50,50	0
54	MG	DA	3063	1/1	0.85	0.18	54,54,54,54	0
54	MG	BA	3425	1/1	0.85	0.15	37,37,37,37	0
54	MG	AA	1644	1/1	0.85	0.32	74,74,74,74	0
54	MG	AA	1692	1/1	0.85	0.17	113,113,113,113	0
54	MG	BA	3032	1/1	0.85	0.23	67,67,67,67	0
54	MG	DA	3195	1/1	0.85	0.30	75,75,75,75	0
54	MG	DA	3198	1/1	0.85	0.25	55,55,55,55	0
54	MG	BA	3481	1/1	0.85	0.13	76,76,76,76	0
54	MG	CA	1629	1/1	0.85	0.34	72,72,72,72	0
54	MG	DA	3097	1/1	0.85	0.30	64,64,64,64	0
54	MG	DA	3099	1/1	0.85	0.13	40,40,40,40	0
54	MG	BA	3023	1/1	0.86	0.21	52,52,52,52	0
54	MG	CA	1640	1/1	0.86	0.32	62,62,62,62	0
54	MG	BA	3167	1/1	0.86	0.31	68,68,68,68	0
54	MG	DA	3210	1/1	0.86	0.29	60,60,60,60	0
54	MG	DA	3109	1/1	0.86	0.28	70,70,70,70	0
54	MG	DA	3216	1/1	0.86	0.17	53,53,53,53	0
54	MG	BA	3498	1/1	0.86	0.10	69,69,69,69	0
54	MG	DA	3125	1/1	0.86	0.39	66,66,66,66	0
54	MG	B2	101	1/1	0.86	0.26	75,75,75,75	0
54	MG	BA	3170	1/1	0.86	0.33	52,52,52,52	0
54	MG	BA	3329	1/1	0.86	0.11	45,45,45,45	0
54	MG	DA	3250	1/1	0.86	0.26	41,41,41,41	0
54	MG	CA	1601	1/1	0.86	0.29	50,50,50,50	0
54	MG	BA	3517	1/1	0.86	0.15	51,51,51,51	0
54	MG	BA	3339	1/1	0.86	0.10	91,91,91,91	0
54	MG	AA	1618	1/1	0.86	0.22	69,69,69,69	0
54	MG	BA	3111	1/1	0.86	0.27	57,57,57,57	0
54	MG	AA	1673	1/1	0.86	0.26	67,67,67,67	0
54	MG	CA	1614	1/1	0.86	0.39	69,69,69,69	0
54	MG	AA	1601	1/1	0.86	0.37	68,68,68,68	0
54	MG	DA	3152	1/1	0.86	0.28	58,58,58,58	0
54	MG	DA	3336	1/1	0.86	0.12	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3077	1/1	0.86	0.26	43,43,43,43	0
54	MG	AA	1604	1/1	0.86	0.19	81,81,81,81	0
54	MG	DA	3059	1/1	0.86	0.22	55,55,55,55	0
54	MG	BA	3147	1/1	0.86	0.27	57,57,57,57	0
54	MG	DA	3367	1/1	0.86	0.26	68,68,68,68	0
54	MG	BA	3396	1/1	0.86	0.26	23,23,23,23	0
54	MG	DA	3070	1/1	0.86	0.12	53,53,53,53	0
54	MG	DA	3383	1/1	0.86	0.16	63,63,63,63	0
54	MG	DA	3071	1/1	0.86	0.23	60,60,60,60	0
54	MG	BA	3254	1/1	0.86	0.20	67,67,67,67	0
54	MG	AA	1640	1/1	0.86	0.53	80,80,80,80	0
54	MG	BA	3082	1/1	0.86	0.19	71,71,71,71	0
54	MG	AA	1649	1/1	0.86	0.20	66,66,66,66	0
54	MG	BA	3465	1/1	0.86	0.12	38,38,38,38	0
54	MG	DA	3196	1/1	0.86	0.34	63,63,63,63	0
54	MG	BA	3480	1/1	0.86	0.10	70,70,70,70	0
54	MG	AA	1617	1/1	0.86	0.23	82,82,82,82	0
54	MG	AA	1660	1/1	0.86	0.45	91,91,91,91	0
54	MG	DA	3203	1/1	0.86	0.24	48,48,48,48	0
54	MG	BA	3097	1/1	0.87	0.24	58,58,58,58	0
54	MG	BA	3015	1/1	0.87	0.22	42,42,42,42	0
54	MG	AA	1678	1/1	0.87	0.28	75,75,75,75	0
54	MG	DA	3224	1/1	0.87	0.35	80,80,80,80	0
54	MG	BA	3067	1/1	0.87	0.17	35,35,35,35	0
54	MG	BA	3249	1/1	0.87	0.26	70,70,70,70	0
54	MG	DA	3240	1/1	0.87	0.35	67,67,67,67	0
54	MG	DA	3249	1/1	0.87	0.23	67,67,67,67	0
54	MG	BA	3529	1/1	0.87	0.13	86,86,86,86	0
54	MG	BA	3374	1/1	0.87	0.09	75,75,75,75	0
54	MG	DA	3045	1/1	0.87	0.38	72,72,72,72	0
54	MG	BA	3542	1/1	0.87	0.17	60,60,60,60	0
54	MG	BA	3116	1/1	0.87	0.23	56,56,56,56	0
54	MG	BA	3546	1/1	0.87	0.09	57,57,57,57	0
54	MG	BA	3081	1/1	0.87	0.33	66,66,66,66	0
54	MG	DA	3058	1/1	0.87	0.12	51,51,51,51	0
54	MG	BA	3257	1/1	0.87	0.26	64,64,64,64	0
54	MG	DA	3062	1/1	0.87	0.14	65,65,65,65	0
54	MG	BA	3420	1/1	0.87	0.16	41,41,41,41	0
54	MG	BA	3563	1/1	0.87	0.10	67,67,67,67	0
54	MG	DA	3342	1/1	0.87	0.16	41,41,41,41	0
54	MG	BA	3135	1/1	0.87	0.23	54,54,54,54	0
54	MG	BA	3024	1/1	0.87	0.11	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3347	1/1	0.87	0.08	76,76,76,76	0
54	MG	BA	3207	1/1	0.87	0.13	59,59,59,59	0
54	MG	BA	3174	1/1	0.87	0.14	71,71,71,71	0
54	MG	BA	3464	1/1	0.87	0.12	41,41,41,41	0
54	MG	BA	3283	1/1	0.87	0.23	56,56,56,56	0
54	MG	BA	3070	1/1	0.87	0.20	61,61,61,61	0
54	MG	DA	3197	1/1	0.87	0.30	66,66,66,66	0
54	MG	BA	3140	1/1	0.87	0.16	59,59,59,59	0
54	MG	CA	1636	1/1	0.87	0.32	77,77,77,77	0
54	MG	BB	213	1/1	0.87	0.10	69,69,69,69	0
54	MG	BA	3314	1/1	0.87	0.11	71,71,71,71	0
54	MG	BA	3180	1/1	0.87	0.19	51,51,51,51	0
54	MG	BA	3491	1/1	0.87	0.17	65,65,65,65	0
54	MG	CA	1650	1/1	0.87	0.19	100,100,100,100	0
54	MG	AA	1674	1/1	0.87	0.16	73,73,73,73	0
54	MG	BU	202	1/1	0.87	0.28	62,62,62,62	0
54	MG	AA	1659	1/1	0.87	0.28	62,62,62,62	0
54	MG	DA	3221	1/1	0.88	0.15	69,69,69,69	0
54	MG	DA	3138	1/1	0.88	0.58	60,60,60,60	0
54	MG	BA	3269	1/1	0.88	0.22	54,54,54,54	0
54	MG	BA	3562	1/1	0.88	0.20	43,43,43,43	0
54	MG	DA	3143	1/1	0.88	0.31	62,62,62,62	0
54	MG	DA	3235	1/1	0.88	0.26	36,36,36,36	0
54	MG	DA	3238	1/1	0.88	0.42	52,52,52,52	0
54	MG	BA	3490	1/1	0.88	0.14	53,53,53,53	0
54	MG	DA	3064	1/1	0.88	0.20	53,53,53,53	0
54	MG	BA	3039	1/1	0.88	0.14	44,44,44,44	0
54	MG	DA	3252	1/1	0.88	0.21	41,41,41,41	0
54	MG	DA	3255	1/1	0.88	0.37	63,63,63,63	0
54	MG	BA	3220	1/1	0.88	0.13	79,79,79,79	0
54	MG	DA	3261	1/1	0.88	0.21	56,56,56,56	0
54	MG	DA	3159	1/1	0.88	0.36	59,59,59,59	0
54	MG	BA	3007	1/1	0.88	0.17	36,36,36,36	0
54	MG	BA	3100	1/1	0.88	0.31	72,72,72,72	0
54	MG	DA	3173	1/1	0.88	0.18	49,49,49,49	0
54	MG	CA	1613	1/1	0.88	0.33	71,71,71,71	0
54	MG	DA	3080	1/1	0.88	0.40	73,73,73,73	0
54	MG	DA	3181	1/1	0.88	0.29	51,51,51,51	0
54	MG	CA	1663	1/1	0.88	0.09	91,91,91,91	0
54	MG	CA	1669	1/1	0.88	0.13	117,117,117,117	0
54	MG	DA	3188	1/1	0.88	0.21	54,54,54,54	0
54	MG	BA	3505	1/1	0.88	0.10	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3093	1/1	0.88	0.46	66,66,66,66	0
54	MG	DA	3191	1/1	0.88	0.19	50,50,50,50	0
54	MG	AA	1706	1/1	0.88	0.08	100,100,100,100	0
54	MG	AA	1666	1/1	0.88	0.19	62,62,62,62	0
54	MG	BA	3112	1/1	0.88	0.35	47,47,47,47	0
54	MG	BA	3179	1/1	0.88	0.26	48,48,48,48	0
54	MG	BA	3092	1/1	0.88	0.34	55,55,55,55	0
54	MG	DA	3035	1/1	0.88	0.31	68,68,68,68	0
54	MG	DA	3036	1/1	0.88	0.15	65,65,65,65	0
54	MG	DA	3111	1/1	0.88	0.33	60,60,60,60	0
54	MG	BA	3534	1/1	0.88	0.18	76,76,76,76	0
54	MG	BA	3118	1/1	0.88	0.27	57,57,57,57	0
54	MG	AA	1702	1/1	0.88	0.11	97,97,97,97	0
54	MG	BA	3216	1/1	0.88	0.18	52,52,52,52	0
54	MG	DA	3411	1/1	0.88	0.11	90,90,90,90	0
54	MG	CA	1630	1/1	0.88	0.24	72,72,72,72	0
54	MG	BA	3356	1/1	0.88	0.26	59,59,59,59	0
54	MG	DA	3053	1/1	0.88	0.31	54,54,54,54	0
54	MG	BA	3358	1/1	0.88	0.09	64,64,64,64	0
54	MG	BA	3096	1/1	0.88	0.25	63,63,63,63	0
54	MG	AA	1667	1/1	0.89	0.25	63,63,63,63	0
54	MG	AA	1699	1/1	0.89	0.11	69,69,69,69	0
54	MG	AA	1648	1/1	0.89	0.18	62,62,62,62	0
54	MG	DA	3220	1/1	0.89	0.20	48,48,48,48	0
54	MG	BA	3286	1/1	0.89	0.15	52,52,52,52	0
54	MG	BA	3026	1/1	0.89	0.13	68,68,68,68	0
54	MG	BA	3555	1/1	0.89	0.12	49,49,49,49	0
54	MG	DA	3131	1/1	0.89	0.21	39,39,39,39	0
54	MG	BA	3225	1/1	0.89	0.14	61,61,61,61	0
54	MG	AA	1687	1/1	0.89	0.12	70,70,70,70	0
54	MG	DA	3135	1/1	0.89	0.17	44,44,44,44	0
54	MG	CA	1618	1/1	0.89	0.34	75,75,75,75	0
54	MG	DA	3241	1/1	0.89	0.21	63,63,63,63	0
54	MG	DA	3244	1/1	0.89	0.34	35,35,35,35	0
54	MG	DA	3246	1/1	0.89	0.29	41,41,41,41	0
54	MG	DA	3247	1/1	0.89	0.33	52,52,52,52	0
54	MG	AA	1688	1/1	0.89	0.11	111,111,111,111	0
54	MG	BA	3154	1/1	0.89	0.15	49,49,49,49	0
54	MG	BA	3335	1/1	0.89	0.10	55,55,55,55	0
54	MG	DA	3254	1/1	0.89	0.25	43,43,43,43	0
54	MG	AA	1636	1/1	0.89	0.19	86,86,86,86	0
54	MG	BA	3489	1/1	0.89	0.18	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3057	1/1	0.89	0.19	67,67,67,67	0
54	MG	DA	3262	1/1	0.89	0.09	46,46,46,46	0
54	MG	AA	1611	1/1	0.89	0.14	69,69,69,69	0
54	MG	BA	3003	1/1	0.89	0.23	29,29,29,29	0
54	MG	DA	3160	1/1	0.89	0.29	48,48,48,48	0
54	MG	AA	1612	1/1	0.89	0.28	76,76,76,76	0
54	MG	BA	3251	1/1	0.89	0.23	63,63,63,63	0
54	MG	BA	3052	1/1	0.89	0.33	61,61,61,61	0
54	MG	DA	3314	1/1	0.89	0.15	54,54,54,54	0
54	MG	BA	3169	1/1	0.89	0.20	60,60,60,60	0
54	MG	BA	3506	1/1	0.89	0.17	61,61,61,61	0
54	MG	BA	3507	1/1	0.89	0.12	53,53,53,53	0
54	MG	BQ	201	1/1	0.89	0.14	49,49,49,49	0
54	MG	DA	3076	1/1	0.89	0.28	70,70,70,70	0
54	MG	DA	3077	1/1	0.89	0.17	66,66,66,66	0
54	MG	AA	1642	1/1	0.89	0.12	64,64,64,64	0
54	MG	BR	202	1/1	0.89	0.17	49,49,49,49	0
54	MG	DA	3349	1/1	0.89	0.22	54,54,54,54	0
54	MG	BA	3209	1/1	0.89	0.33	67,67,67,67	0
54	MG	BV	201	1/1	0.89	0.22	74,74,74,74	0
54	MG	DA	3193	1/1	0.89	0.35	63,63,63,63	0
54	MG	CA	1654	1/1	0.89	0.16	95,95,95,95	0
54	MG	DA	3092	1/1	0.89	0.29	63,63,63,63	0
54	MG	BA	3057	1/1	0.89	0.15	46,46,46,46	0
54	MG	BA	3014	1/1	0.89	0.16	57,57,57,57	0
54	MG	CA	1661	1/1	0.89	0.15	100,100,100,100	0
54	MG	DA	3396	1/1	0.89	0.14	37,37,37,37	0
54	MG	B3	102	1/1	0.89	0.19	54,54,54,54	0
54	MG	BA	3388	1/1	0.89	0.12	54,54,54,54	0
54	MG	DA	3402	1/1	0.89	0.18	59,59,59,59	0
54	MG	DA	3106	1/1	0.89	0.20	56,56,56,56	0
54	MG	DA	3001	1/1	0.89	0.17	62,62,62,62	0
54	MG	DA	3004	1/1	0.89	0.23	59,59,59,59	0
54	MG	BA	3276	1/1	0.89	0.30	56,56,56,56	0
54	MG	BA	3415	1/1	0.89	0.08	49,49,49,49	0
54	MG	DA	3023	1/1	0.89	0.34	61,61,61,61	0
54	MG	DA	3215	1/1	0.89	0.16	58,58,58,58	0
54	MG	CA	1627	1/1	0.90	0.09	79,79,79,79	0
54	MG	BA	3031	1/1	0.90	0.15	41,41,41,41	0
54	MG	BA	3182	1/1	0.90	0.18	69,69,69,69	0
54	MG	BA	3219	1/1	0.90	0.28	62,62,62,62	0
54	MG	DA	3207	1/1	0.90	0.33	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1632	1/1	0.90	0.30	65,65,65,65	0
54	MG	BA	3581	1/1	0.90	0.10	47,47,47,47	0
54	MG	BA	3612	1/1	0.90	0.09	100,100,100,100	0
54	MG	DA	3095	1/1	0.90	0.40	71,71,71,71	0
54	MG	CA	1635	1/1	0.90	0.17	68,68,68,68	0
54	MG	DA	3098	1/1	0.90	0.24	62,62,62,62	0
54	MG	AA	1615	1/1	0.90	0.30	56,56,56,56	0
54	MG	CA	1637	1/1	0.90	0.33	67,67,67,67	0
54	MG	BA	3285	1/1	0.90	0.32	59,59,59,59	0
54	MG	BB	203	1/1	0.90	0.19	80,80,80,80	0
54	MG	BA	3150	1/1	0.90	0.14	61,61,61,61	0
54	MG	BA	3106	1/1	0.90	0.23	48,48,48,48	0
54	MG	DA	3228	1/1	0.90	0.37	51,51,51,51	0
54	MG	DA	3229	1/1	0.90	0.23	55,55,55,55	0
54	MG	DA	3231	1/1	0.90	0.33	54,54,54,54	0
54	MG	BA	3469	1/1	0.90	0.21	77,77,77,77	0
54	MG	CA	1653	1/1	0.90	0.15	83,83,83,83	0
54	MG	DA	3113	1/1	0.90	0.25	42,42,42,42	0
54	MG	DA	3118	1/1	0.90	0.28	44,44,44,44	0
54	MG	DA	3119	1/1	0.90	0.33	57,57,57,57	0
54	MG	DA	3242	1/1	0.90	0.30	38,38,38,38	0
54	MG	DA	3120	1/1	0.90	0.25	52,52,52,52	0
54	MG	DA	3121	1/1	0.90	0.38	53,53,53,53	0
54	MG	BA	3289	1/1	0.90	0.27	50,50,50,50	0
54	MG	BA	3292	1/1	0.90	0.14	44,44,44,44	0
54	MG	BB	214	1/1	0.90	0.12	67,67,67,67	0
54	MG	BA	3301	1/1	0.90	0.07	62,62,62,62	0
54	MG	DA	3253	1/1	0.90	0.23	42,42,42,42	0
54	MG	BB	216	1/1	0.90	0.26	46,46,46,46	0
54	MG	BA	3230	1/1	0.90	0.27	50,50,50,50	0
54	MG	DA	3256	1/1	0.90	0.35	59,59,59,59	0
54	MG	BA	3193	1/1	0.90	0.14	50,50,50,50	0
54	MG	BA	3315	1/1	0.90	0.11	84,84,84,84	0
54	MG	BA	3316	1/1	0.90	0.20	34,34,34,34	0
54	MG	BA	3495	1/1	0.90	0.10	70,70,70,70	0
54	MG	DA	3284	1/1	0.90	0.13	61,61,61,61	0
54	MG	DA	3018	1/1	0.90	0.15	42,42,42,42	0
54	MG	DA	3136	1/1	0.90	0.28	42,42,42,42	0
54	MG	BA	3108	1/1	0.90	0.25	56,56,56,56	0
54	MG	BA	3053	1/1	0.90	0.25	53,53,53,53	0
54	MG	BA	3332	1/1	0.90	0.18	60,60,60,60	0
54	MG	BA	3500	1/1	0.90	0.17	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3054	1/1	0.90	0.17	52,52,52,52	0
54	MG	DA	3320	1/1	0.90	0.12	57,57,57,57	0
54	MG	DA	3326	1/1	0.90	0.10	95,95,95,95	0
54	MG	BA	3088	1/1	0.90	0.25	46,46,46,46	0
54	MG	DA	3335	1/1	0.90	0.23	72,72,72,72	0
54	MG	BA	3089	1/1	0.90	0.26	46,46,46,46	0
54	MG	BA	3513	1/1	0.90	0.09	66,66,66,66	0
54	MG	DA	3158	1/1	0.90	0.25	72,72,72,72	0
54	MG	DA	3343	1/1	0.90	0.13	35,35,35,35	0
54	MG	BA	3072	1/1	0.90	0.20	59,59,59,59	0
54	MG	CA	1603	1/1	0.90	0.27	73,73,73,73	0
54	MG	AA	1681	1/1	0.90	0.12	65,65,65,65	0
54	MG	DA	3170	1/1	0.90	0.25	52,52,52,52	0
54	MG	DA	3359	1/1	0.90	0.17	49,49,49,49	0
54	MG	CA	1605	1/1	0.90	0.28	74,74,74,74	0
54	MG	DA	3363	1/1	0.90	0.12	72,72,72,72	0
54	MG	CA	1608	1/1	0.90	0.38	67,67,67,67	0
54	MG	DA	3052	1/1	0.90	0.34	71,71,71,71	0
54	MG	BA	3518	1/1	0.90	0.27	59,59,59,59	0
54	MG	AA	1603	1/1	0.90	0.21	68,68,68,68	0
54	MG	DA	3055	1/1	0.90	0.26	43,43,43,43	0
54	MG	BA	3004	1/1	0.90	0.17	41,41,41,41	0
54	MG	BA	3361	1/1	0.90	0.16	53,53,53,53	0
54	MG	BA	3261	1/1	0.90	0.20	59,59,59,59	0
54	MG	BA	3263	1/1	0.90	0.33	41,41,41,41	0
54	MG	BA	3264	1/1	0.90	0.34	38,38,38,38	0
54	MG	BA	3078	1/1	0.90	0.22	38,38,38,38	0
54	MG	DA	3407	1/1	0.90	0.19	59,59,59,59	0
54	MG	BA	3384	1/1	0.90	0.08	62,62,62,62	0
54	MG	BA	3141	1/1	0.90	0.31	65,65,65,65	0
54	MG	DA	3414	1/1	0.90	0.09	68,68,68,68	0
54	MG	BA	3270	1/1	0.90	0.35	74,74,74,74	0
54	MG	DA	3074	1/1	0.90	0.31	38,38,38,38	0
54	MG	BA	3272	1/1	0.90	0.23	65,65,65,65	0
54	MG	D6	102	1/1	0.90	0.33	64,64,64,64	0
54	MG	BA	3049	1/1	0.90	0.18	54,54,54,54	0
54	MG	BA	3417	1/1	0.90	0.13	37,37,37,37	0
54	MG	BA	3613	1/1	0.91	0.10	109,109,109,109	0
54	MG	BA	3331	1/1	0.91	0.11	51,51,51,51	0
54	MG	AA	1614	1/1	0.91	0.20	62,62,62,62	0
54	MG	BA	3043	1/1	0.91	0.17	54,54,54,54	0
54	MG	BA	3046	1/1	0.91	0.23	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1679	1/1	0.91	0.28	64,64,64,64	0
54	MG	BA	3492	1/1	0.91	0.10	78,78,78,78	0
54	MG	BA	3265	1/1	0.91	0.16	30,30,30,30	0
54	MG	AA	1663	1/1	0.91	0.34	70,70,70,70	0
54	MG	DA	3066	1/1	0.91	0.15	56,56,56,56	0
54	MG	DA	3068	1/1	0.91	0.20	48,48,48,48	0
54	MG	AA	1626	1/1	0.91	0.28	67,67,67,67	0
54	MG	BA	3087	1/1	0.91	0.24	56,56,56,56	0
54	MG	BA	3271	1/1	0.91	0.17	60,60,60,60	0
54	MG	DA	3072	1/1	0.91	0.27	50,50,50,50	0
54	MG	DA	3073	1/1	0.91	0.23	54,54,54,54	0
54	MG	BA	3016	1/1	0.91	0.15	57,57,57,57	0
54	MG	BA	3020	1/1	0.91	0.10	34,34,34,34	0
54	MG	DA	3292	1/1	0.91	0.11	39,39,39,39	0
54	MG	DA	3294	1/1	0.91	0.13	52,52,52,52	0
54	MG	BA	3369	1/1	0.91	0.11	74,74,74,74	0
54	MG	BA	3512	1/1	0.91	0.26	45,45,45,45	0
54	MG	CA	1646	1/1	0.91	0.17	92,92,92,92	0
54	MG	DA	3309	1/1	0.91	0.35	48,48,48,48	0
54	MG	DA	3184	1/1	0.91	0.29	39,39,39,39	0
54	MG	BA	3229	1/1	0.91	0.25	51,51,51,51	0
54	MG	DA	3081	1/1	0.91	0.25	52,52,52,52	0
54	MG	BA	3090	1/1	0.91	0.10	45,45,45,45	0
54	MG	CA	1651	1/1	0.91	0.19	61,61,61,61	0
54	MG	BA	3379	1/1	0.91	0.09	56,56,56,56	0
54	MG	BA	3232	1/1	0.91	0.13	54,54,54,54	0
54	MG	B1	101	1/1	0.91	0.12	50,50,50,50	0
54	MG	BA	3156	1/1	0.91	0.19	57,57,57,57	0
54	MG	BA	3235	1/1	0.91	0.21	45,45,45,45	0
54	MG	BA	3521	1/1	0.91	0.12	41,41,41,41	0
54	MG	BA	3237	1/1	0.91	0.27	56,56,56,56	0
54	MG	DA	3101	1/1	0.91	0.43	62,62,62,62	0
54	MG	B9	102	1/1	0.91	0.18	45,45,45,45	0
54	MG	BA	3075	1/1	0.91	0.28	53,53,53,53	0
54	MG	BA	3120	1/1	0.91	0.18	42,42,42,42	0
54	MG	DA	3355	1/1	0.91	0.06	37,37,37,37	0
54	MG	DA	3204	1/1	0.91	0.19	37,37,37,37	0
54	MG	DA	3011	1/1	0.91	0.32	46,46,46,46	0
54	MG	BA	3241	1/1	0.91	0.38	62,62,62,62	0
54	MG	BA	3543	1/1	0.91	0.14	59,59,59,59	0
54	MG	DA	3368	1/1	0.91	0.11	78,78,78,78	0
54	MG	DA	3370	1/1	0.91	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3294	1/1	0.91	0.09	37,37,37,37	0
54	MG	BA	3021	1/1	0.91	0.12	33,33,33,33	0
54	MG	DA	3116	1/1	0.91	0.32	46,46,46,46	0
54	MG	DA	3387	1/1	0.91	0.06	71,71,71,71	0
54	MG	DA	3117	1/1	0.91	0.27	34,34,34,34	0
54	MG	DA	3029	1/1	0.91	0.26	72,72,72,72	0
54	MG	BA	3125	1/1	0.91	0.18	50,50,50,50	0
54	MG	DA	3393	1/1	0.91	0.08	81,81,81,81	0
54	MG	BA	3456	1/1	0.91	0.09	89,89,89,89	0
54	MG	BA	3458	1/1	0.91	0.10	45,45,45,45	0
54	MG	BA	3311	1/1	0.91	0.24	60,60,60,60	0
54	MG	BA	3130	1/1	0.91	0.28	32,32,32,32	0
54	MG	BA	3250	1/1	0.91	0.14	47,47,47,47	0
54	MG	DA	3041	1/1	0.91	0.25	49,49,49,49	0
54	MG	CA	1617	1/1	0.91	0.41	70,70,70,70	0
54	MG	BA	3131	1/1	0.91	0.13	44,44,44,44	0
54	MG	DA	3420	1/1	0.91	0.11	97,97,97,97	0
54	MG	DA	3423	1/1	0.91	0.07	79,79,79,79	0
54	MG	BA	3473	1/1	0.91	0.20	59,59,59,59	0
54	MG	BA	3577	1/1	0.91	0.19	58,58,58,58	0
54	MG	DB	203	1/1	0.91	0.42	61,61,61,61	0
54	MG	BA	3022	1/1	0.91	0.11	57,57,57,57	0
54	MG	DA	3237	1/1	0.91	0.29	39,39,39,39	0
54	MG	BA	3173	1/1	0.91	0.38	65,65,65,65	0
55	ZN	B4	101	1/1	0.91	0.08	200,200,200,200	0
54	MG	DA	3239	1/1	0.91	0.21	39,39,39,39	0
55	ZN	DY	201	1/1	0.91	0.09	128,128,128,128	0
54	MG	DA	3137	1/1	0.92	0.30	64,64,64,64	0
54	MG	BA	3036	1/1	0.92	0.22	49,49,49,49	0
54	MG	DA	3243	1/1	0.92	0.33	53,53,53,53	0
54	MG	BA	3215	1/1	0.92	0.23	61,61,61,61	0
54	MG	DA	3245	1/1	0.92	0.14	47,47,47,47	0
54	MG	AA	1664	1/1	0.92	0.14	85,85,85,85	0
54	MG	DA	3142	1/1	0.92	0.12	46,46,46,46	0
54	MG	DA	3248	1/1	0.92	0.39	44,44,44,44	0
54	MG	BA	3113	1/1	0.92	0.18	35,35,35,35	0
54	MG	AA	1631	1/1	0.92	0.36	64,64,64,64	0
54	MG	DA	3251	1/1	0.92	0.34	39,39,39,39	0
54	MG	BA	3344	1/1	0.92	0.09	52,52,52,52	0
54	MG	BA	3345	1/1	0.92	0.17	45,45,45,45	0
54	MG	BA	3494	1/1	0.92	0.24	44,44,44,44	0
54	MG	DA	3157	1/1	0.92	0.21	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3042	1/1	0.92	0.26	47,47,47,47	0
54	MG	BA	3005	1/1	0.92	0.13	42,42,42,42	0
54	MG	BA	3222	1/1	0.92	0.07	51,51,51,51	0
54	MG	DA	3162	1/1	0.92	0.18	55,55,55,55	0
54	MG	BA	3224	1/1	0.92	0.19	61,61,61,61	0
54	MG	DA	3165	1/1	0.92	0.21	58,58,58,58	0
54	MG	DA	3166	1/1	0.92	0.20	55,55,55,55	0
54	MG	DA	3168	1/1	0.92	0.19	42,42,42,42	0
54	MG	BA	3155	1/1	0.92	0.34	64,64,64,64	0
54	MG	BA	3503	1/1	0.92	0.13	68,68,68,68	0
54	MG	BA	3121	1/1	0.92	0.07	38,38,38,38	0
54	MG	BA	3228	1/1	0.92	0.20	26,26,26,26	0
54	MG	DA	3178	1/1	0.92	0.31	58,58,58,58	0
54	MG	BA	3273	1/1	0.92	0.09	66,66,66,66	0
54	MG	BA	3189	1/1	0.92	0.22	46,46,46,46	0
54	MG	DA	3182	1/1	0.92	0.23	59,59,59,59	0
54	MG	DA	3317	1/1	0.92	0.07	94,94,94,94	0
54	MG	DA	3318	1/1	0.92	0.07	66,66,66,66	0
54	MG	BA	3275	1/1	0.92	0.08	41,41,41,41	0
54	MG	DA	3082	1/1	0.92	0.12	51,51,51,51	0
54	MG	DA	3083	1/1	0.92	0.24	55,55,55,55	0
54	MG	BA	3191	1/1	0.92	0.17	45,45,45,45	0
54	MG	DA	3086	1/1	0.92	0.32	54,54,54,54	0
54	MG	BW	201	1/1	0.92	0.14	51,51,51,51	0
54	MG	BA	3383	1/1	0.92	0.11	71,71,71,71	0
54	MG	BA	3231	1/1	0.92	0.21	45,45,45,45	0
54	MG	BA	3045	1/1	0.92	0.26	62,62,62,62	0
54	MG	B3	101	1/1	0.92	0.14	60,60,60,60	0
54	MG	BA	3019	1/1	0.92	0.09	39,39,39,39	0
54	MG	BA	3392	1/1	0.92	0.12	55,55,55,55	0
54	MG	DA	3351	1/1	0.92	0.12	78,78,78,78	0
54	MG	DA	3006	1/1	0.92	0.15	44,44,44,44	0
54	MG	BA	3522	1/1	0.92	0.15	68,68,68,68	0
54	MG	BA	3525	1/1	0.92	0.06	112,112,112,112	0
54	MG	BA	3234	1/1	0.92	0.23	34,34,34,34	0
54	MG	DA	3105	1/1	0.92	0.32	33,33,33,33	0
54	MG	DA	3017	1/1	0.92	0.22	61,61,61,61	0
54	MG	BA	3533	1/1	0.92	0.15	48,48,48,48	0
54	MG	DA	3375	1/1	0.92	0.09	50,50,50,50	0
54	MG	DA	3020	1/1	0.92	0.18	39,39,39,39	0
54	MG	BA	3047	1/1	0.92	0.20	50,50,50,50	0
54	MG	BA	3165	1/1	0.92	0.20	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3028	1/1	0.92	0.17	53,53,53,53	0
54	MG	BA	3541	1/1	0.92	0.20	54,54,54,54	0
54	MG	CA	1606	1/1	0.92	0.41	81,81,81,81	0
54	MG	AA	1635	1/1	0.92	0.20	71,71,71,71	0
54	MG	BA	3290	1/1	0.92	0.21	47,47,47,47	0
54	MG	DA	3394	1/1	0.92	0.17	56,56,56,56	0
54	MG	BA	3200	1/1	0.92	0.16	51,51,51,51	0
54	MG	BA	3069	1/1	0.92	0.31	53,53,53,53	0
54	MG	DA	3122	1/1	0.92	0.30	47,47,47,47	0
54	MG	BA	3547	1/1	0.92	0.15	31,31,31,31	0
54	MG	BA	3450	1/1	0.92	0.11	71,71,71,71	0
54	MG	DA	3408	1/1	0.92	0.09	65,65,65,65	0
54	MG	BA	3453	1/1	0.92	0.12	74,74,74,74	0
54	MG	DA	3227	1/1	0.92	0.20	65,65,65,65	0
54	MG	CA	1616	1/1	0.92	0.30	72,72,72,72	0
54	MG	BA	3103	1/1	0.92	0.37	67,67,67,67	0
54	MG	DA	3230	1/1	0.92	0.27	67,67,67,67	0
54	MG	BA	3011	1/1	0.92	0.20	50,50,50,50	0
54	MG	BA	3244	1/1	0.92	0.26	45,45,45,45	0
54	MG	DA	3233	1/1	0.92	0.22	43,43,43,43	0
54	MG	DA	3234	1/1	0.92	0.34	56,56,56,56	0
54	MG	BA	3247	1/1	0.92	0.23	53,53,53,53	0
54	MG	AA	1610	1/1	0.92	0.34	75,75,75,75	0
54	MG	BA	3109	1/1	0.92	0.13	57,57,57,57	0
54	MG	BA	3175	1/1	0.92	0.36	70,70,70,70	0
54	MG	BA	3252	1/1	0.92	0.17	44,44,44,44	0
54	MG	AA	1650	1/1	0.93	0.33	70,70,70,70	0
54	MG	BA	3185	1/1	0.93	0.13	44,44,44,44	0
54	MG	BA	3528	1/1	0.93	0.11	43,43,43,43	0
54	MG	BA	3355	1/1	0.93	0.14	54,54,54,54	0
54	MG	BA	3530	1/1	0.93	0.10	84,84,84,84	0
54	MG	DA	3169	1/1	0.93	0.17	39,39,39,39	0
54	MG	DA	3079	1/1	0.93	0.23	60,60,60,60	0
54	MG	DA	3171	1/1	0.93	0.38	53,53,53,53	0
54	MG	DA	3257	1/1	0.93	0.30	59,59,59,59	0
54	MG	BA	3532	1/1	0.93	0.07	35,35,35,35	0
54	MG	CA	1656	1/1	0.93	0.09	97,97,97,97	0
54	MG	DA	3174	1/1	0.93	0.36	60,60,60,60	0
54	MG	DA	3263	1/1	0.93	0.08	70,70,70,70	0
54	MG	BA	3282	1/1	0.93	0.17	43,43,43,43	0
54	MG	DA	3176	1/1	0.93	0.21	61,61,61,61	0
54	MG	BA	3357	1/1	0.93	0.08	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3293	1/1	0.93	0.13	50,50,50,50	0
54	MG	DA	3179	1/1	0.93	0.37	62,62,62,62	0
54	MG	BA	3467	1/1	0.93	0.10	73,73,73,73	0
54	MG	DA	3085	1/1	0.93	0.28	51,51,51,51	0
54	MG	BA	3030	1/1	0.93	0.14	37,37,37,37	0
54	MG	CA	1664	1/1	0.93	0.06	94,94,94,94	0
54	MG	BA	3009	1/1	0.93	0.17	59,59,59,59	0
54	MG	B8	101	1/1	0.93	0.17	64,64,64,64	0
54	MG	DA	3186	1/1	0.93	0.17	42,42,42,42	0
54	MG	DA	3003	1/1	0.93	0.20	35,35,35,35	0
54	MG	BA	3476	1/1	0.93	0.12	44,44,44,44	0
54	MG	DA	3096	1/1	0.93	0.23	46,46,46,46	0
54	MG	BA	3161	1/1	0.93	0.23	54,54,54,54	0
54	MG	BA	3162	1/1	0.93	0.33	62,62,62,62	0
54	MG	AA	1633	1/1	0.93	0.39	72,72,72,72	0
54	MG	AA	1695	1/1	0.93	0.08	93,93,93,93	0
54	MG	DA	3016	1/1	0.93	0.15	41,41,41,41	0
54	MG	DA	3338	1/1	0.93	0.12	50,50,50,50	0
54	MG	DA	3340	1/1	0.93	0.21	44,44,44,44	0
54	MG	BA	3551	1/1	0.93	0.21	40,40,40,40	0
54	MG	AA	1680	1/1	0.93	0.15	83,83,83,83	0
54	MG	BA	3554	1/1	0.93	0.15	58,58,58,58	0
54	MG	DA	3021	1/1	0.93	0.26	53,53,53,53	0
54	MG	BA	3168	1/1	0.93	0.20	52,52,52,52	0
54	MG	BA	3557	1/1	0.93	0.31	42,42,42,42	0
54	MG	DA	3026	1/1	0.93	0.07	49,49,49,49	0
54	MG	DA	3350	1/1	0.93	0.14	50,50,50,50	0
54	MG	DA	3112	1/1	0.93	0.30	60,60,60,60	0
54	MG	BA	3377	1/1	0.93	0.10	69,69,69,69	0
54	MG	DA	3357	1/1	0.93	0.08	53,53,53,53	0
54	MG	DA	3114	1/1	0.93	0.12	51,51,51,51	0
54	MG	CA	1611	1/1	0.93	0.14	64,64,64,64	0
54	MG	BA	3142	1/1	0.93	0.34	53,53,53,53	0
54	MG	DA	3364	1/1	0.93	0.10	67,67,67,67	0
54	MG	DA	3366	1/1	0.93	0.07	35,35,35,35	0
54	MG	BA	3115	1/1	0.93	0.30	43,43,43,43	0
54	MG	BA	3064	1/1	0.93	0.14	45,45,45,45	0
54	MG	BA	3566	1/1	0.93	0.16	40,40,40,40	0
54	MG	BA	3496	1/1	0.93	0.08	79,79,79,79	0
54	MG	DA	3218	1/1	0.93	0.41	53,53,53,53	0
54	MG	BA	3571	1/1	0.93	0.08	76,76,76,76	0
54	MG	DA	3380	1/1	0.93	0.07	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3266	1/1	0.93	0.50	48,48,48,48	0
54	MG	DA	3386	1/1	0.93	0.08	63,63,63,63	0
54	MG	BA	3065	1/1	0.93	0.14	47,47,47,47	0
54	MG	BA	3590	1/1	0.93	0.10	82,82,82,82	0
54	MG	DA	3046	1/1	0.93	0.43	43,43,43,43	0
54	MG	BA	3391	1/1	0.93	0.16	38,38,38,38	0
54	MG	DA	3226	1/1	0.93	0.23	53,53,53,53	0
54	MG	DA	3048	1/1	0.93	0.11	53,53,53,53	0
54	MG	BA	3066	1/1	0.93	0.13	43,43,43,43	0
54	MG	BA	3501	1/1	0.93	0.08	61,61,61,61	0
54	MG	BA	3502	1/1	0.93	0.10	41,41,41,41	0
54	MG	BA	3236	1/1	0.93	0.27	50,50,50,50	0
54	MG	BA	3151	1/1	0.93	0.25	62,62,62,62	0
54	MG	CA	1628	1/1	0.93	0.23	55,55,55,55	0
54	MG	BA	3038	1/1	0.93	0.06	36,36,36,36	0
54	MG	BA	3153	1/1	0.93	0.23	53,53,53,53	0
54	MG	AA	1624	1/1	0.93	0.44	66,66,66,66	0
54	MG	DA	3415	1/1	0.93	0.13	89,89,89,89	0
54	MG	BA	3084	1/1	0.93	0.28	56,56,56,56	0
54	MG	BA	3434	1/1	0.93	0.19	36,36,36,36	0
54	MG	BA	3436	1/1	0.93	0.15	38,38,38,38	0
54	MG	DA	3065	1/1	0.93	0.18	58,58,58,58	0
54	MG	BA	3006	1/1	0.93	0.11	44,44,44,44	0
54	MG	BA	3449	1/1	0.93	0.10	49,49,49,49	0
54	MG	DF	302	1/1	0.93	0.11	64,64,64,64	0
54	MG	DP	201	1/1	0.93	0.40	58,58,58,58	0
54	MG	BF	301	1/1	0.93	0.22	56,56,56,56	0
54	MG	D8	101	1/1	0.93	0.32	49,49,49,49	0
55	ZN	AD	301	1/1	0.93	0.17	107,107,107,107	0
54	MG	BA	3341	1/1	0.93	0.10	69,69,69,69	0
54	MG	BA	3277	1/1	0.93	0.20	66,66,66,66	0
54	MG	BQ	202	1/1	0.93	0.29	53,53,53,53	0
54	MG	CA	1642	1/1	0.93	0.11	87,87,87,87	0
54	MG	BA	3171	1/1	0.94	0.30	67,67,67,67	0
54	MG	BA	3584	1/1	0.94	0.09	68,68,68,68	0
54	MG	DA	3153	1/1	0.94	0.23	38,38,38,38	0
54	MG	BA	3587	1/1	0.94	0.12	66,66,66,66	0
54	MG	BA	3588	1/1	0.94	0.14	86,86,86,86	0
54	MG	BA	3028	1/1	0.94	0.19	46,46,46,46	0
54	MG	DA	3061	1/1	0.94	0.21	52,52,52,52	0
54	MG	BA	3594	1/1	0.94	0.08	70,70,70,70	0
54	MG	DA	3258	1/1	0.94	0.11	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3291	1/1	0.94	0.21	59,59,59,59	0
54	MG	DA	3260	1/1	0.94	0.21	44,44,44,44	0
54	MG	BA	3144	1/1	0.94	0.21	54,54,54,54	0
54	MG	DA	3164	1/1	0.94	0.14	46,46,46,46	0
54	MG	BA	3211	1/1	0.94	0.22	53,53,53,53	0
54	MG	BA	3110	1/1	0.94	0.27	23,23,23,23	0
54	MG	BB	202	1/1	0.94	0.13	46,46,46,46	0
54	MG	DA	3286	1/1	0.94	0.11	50,50,50,50	0
54	MG	BA	3302	1/1	0.94	0.16	45,45,45,45	0
54	MG	BA	3397	1/1	0.94	0.07	31,31,31,31	0
54	MG	BA	3214	1/1	0.94	0.30	34,34,34,34	0
54	MG	BA	3018	1/1	0.94	0.15	72,72,72,72	0
54	MG	BA	3313	1/1	0.94	0.13	42,42,42,42	0
54	MG	CA	1641	1/1	0.94	0.17	74,74,74,74	0
54	MG	DA	3301	1/1	0.94	0.07	55,55,55,55	0
54	MG	BA	3008	1/1	0.94	0.15	32,32,32,32	0
54	MG	CA	1643	1/1	0.94	0.08	109,109,109,109	0
54	MG	DA	3177	1/1	0.94	0.34	59,59,59,59	0
54	MG	CA	1644	1/1	0.94	0.12	74,74,74,74	0
54	MG	CA	1645	1/1	0.94	0.18	63,63,63,63	0
54	MG	AA	1690	1/1	0.94	0.07	59,59,59,59	0
54	MG	BA	3114	1/1	0.94	0.16	43,43,43,43	0
54	MG	BA	3435	1/1	0.94	0.14	36,36,36,36	0
54	MG	DA	3324	1/1	0.94	0.14	64,64,64,64	0
54	MG	BA	3318	1/1	0.94	0.10	73,73,73,73	0
54	MG	BA	3258	1/1	0.94	0.27	56,56,56,56	0
54	MG	DA	3331	1/1	0.94	0.17	69,69,69,69	0
54	MG	BA	3441	1/1	0.94	0.12	35,35,35,35	0
54	MG	BA	3448	1/1	0.94	0.18	33,33,33,33	0
54	MG	DA	3187	1/1	0.94	0.37	47,47,47,47	0
54	MG	BA	3526	1/1	0.94	0.14	28,28,28,28	0
54	MG	DA	3088	1/1	0.94	0.29	65,65,65,65	0
54	MG	BA	3327	1/1	0.94	0.08	34,34,34,34	0
54	MG	AA	1629	1/1	0.94	0.25	63,63,63,63	0
54	MG	BA	3048	1/1	0.94	0.22	42,42,42,42	0
54	MG	BA	3094	1/1	0.94	0.11	41,41,41,41	0
54	MG	CA	1666	1/1	0.94	0.08	131,131,131,131	0
54	MG	BA	3223	1/1	0.94	0.24	57,57,57,57	0
54	MG	AA	1685	1/1	0.94	0.08	77,77,77,77	0
54	MG	BA	3463	1/1	0.94	0.09	36,36,36,36	0
54	MG	DA	3352	1/1	0.94	0.10	61,61,61,61	0
54	MG	DA	3354	1/1	0.94	0.12	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3536	1/1	0.94	0.06	82,82,82,82	0
54	MG	BA	3540	1/1	0.94	0.11	61,61,61,61	0
54	MG	DA	3007	1/1	0.94	0.08	36,36,36,36	0
54	MG	DA	3201	1/1	0.94	0.34	69,69,69,69	0
54	MG	DA	3202	1/1	0.94	0.13	37,37,37,37	0
54	MG	BA	3187	1/1	0.94	0.23	30,30,30,30	0
54	MG	DA	3104	1/1	0.94	0.11	57,57,57,57	0
54	MG	DA	3009	1/1	0.94	0.18	54,54,54,54	0
54	MG	BA	3050	1/1	0.94	0.08	46,46,46,46	0
54	MG	BA	3227	1/1	0.94	0.10	42,42,42,42	0
54	MG	DA	3372	1/1	0.94	0.20	40,40,40,40	0
54	MG	DA	3208	1/1	0.94	0.44	52,52,52,52	0
54	MG	DA	3014	1/1	0.94	0.13	52,52,52,52	0
54	MG	BA	3544	1/1	0.94	0.07	91,91,91,91	0
54	MG	AA	1686	1/1	0.94	0.08	115,115,115,115	0
54	MG	BA	3099	1/1	0.94	0.25	52,52,52,52	0
54	MG	BA	3475	1/1	0.94	0.17	53,53,53,53	0
54	MG	BA	3192	1/1	0.94	0.15	43,43,43,43	0
54	MG	DA	3115	1/1	0.94	0.20	39,39,39,39	0
54	MG	BA	3127	1/1	0.94	0.32	51,51,51,51	0
54	MG	DA	3024	1/1	0.94	0.13	49,49,49,49	0
54	MG	BA	3128	1/1	0.94	0.18	53,53,53,53	0
54	MG	AA	1651	1/1	0.94	0.41	69,69,69,69	0
54	MG	DA	3027	1/1	0.94	0.33	51,51,51,51	0
54	MG	CA	1607	1/1	0.94	0.21	72,72,72,72	0
54	MG	BA	3101	1/1	0.94	0.31	51,51,51,51	0
54	MG	BA	3556	1/1	0.94	0.10	58,58,58,58	0
54	MG	DA	3403	1/1	0.94	0.10	49,49,49,49	0
54	MG	DA	3405	1/1	0.94	0.15	70,70,70,70	0
54	MG	DA	3406	1/1	0.94	0.07	35,35,35,35	0
54	MG	DA	3031	1/1	0.94	0.27	43,43,43,43	0
54	MG	DA	3032	1/1	0.94	0.26	43,43,43,43	0
54	MG	DA	3409	1/1	0.94	0.06	79,79,79,79	0
54	MG	BA	3025	1/1	0.94	0.09	52,52,52,52	0
54	MG	BA	3085	1/1	0.94	0.42	63,63,63,63	0
54	MG	BA	3559	1/1	0.94	0.14	39,39,39,39	0
54	MG	BA	3105	1/1	0.94	0.09	40,40,40,40	0
54	MG	AA	1613	1/1	0.94	0.23	74,74,74,74	0
54	MG	DA	3038	1/1	0.94	0.25	39,39,39,39	0
54	MG	BA	3493	1/1	0.94	0.12	52,52,52,52	0
54	MG	BA	3284	1/1	0.94	0.07	40,40,40,40	0
54	MG	BA	3567	1/1	0.94	0.08	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3204	1/1	0.94	0.07	47,47,47,47	0
54	MG	BA	3071	1/1	0.94	0.12	49,49,49,49	0
54	MG	CA	1620	1/1	0.94	0.26	57,57,57,57	0
54	MG	BA	3572	1/1	0.94	0.14	49,49,49,49	0
54	MG	D7	101	1/1	0.94	0.21	52,52,52,52	0
54	MG	BA	3206	1/1	0.94	0.17	68,68,68,68	0
54	MG	BA	3579	1/1	0.94	0.11	53,53,53,53	0
54	MG	DA	3144	1/1	0.94	0.26	42,42,42,42	0
54	MG	DA	3146	1/1	0.94	0.28	35,35,35,35	0
54	MG	BA	3580	1/1	0.94	0.08	61,61,61,61	0
54	MG	DA	3148	1/1	0.94	0.38	70,70,70,70	0
54	MG	CA	1649	1/1	0.95	0.08	92,92,92,92	0
54	MG	BA	3561	1/1	0.95	0.15	49,49,49,49	0
54	MG	DA	3315	1/1	0.95	0.07	59,59,59,59	0
54	MG	BA	3442	1/1	0.95	0.10	31,31,31,31	0
54	MG	BA	3445	1/1	0.95	0.06	56,56,56,56	0
54	MG	BA	3299	1/1	0.95	0.10	38,38,38,38	0
54	MG	BA	3012	1/1	0.95	0.09	34,34,34,34	0
54	MG	DA	3321	1/1	0.95	0.10	53,53,53,53	0
54	MG	BA	3510	1/1	0.95	0.08	33,33,33,33	0
54	MG	BA	3186	1/1	0.95	0.25	64,64,64,64	0
54	MG	BA	3306	1/1	0.95	0.08	51,51,51,51	0
54	MG	DA	3330	1/1	0.95	0.11	44,44,44,44	0
54	MG	DA	3211	1/1	0.95	0.24	53,53,53,53	0
54	MG	BA	3455	1/1	0.95	0.22	42,42,42,42	0
54	MG	BA	3573	1/1	0.95	0.07	55,55,55,55	0
54	MG	CA	1665	1/1	0.95	0.11	76,76,76,76	0
54	MG	BA	3362	1/1	0.95	0.05	73,73,73,73	0
54	MG	CA	1668	1/1	0.95	0.12	105,105,105,105	0
54	MG	BA	3056	1/1	0.95	0.12	48,48,48,48	0
54	MG	BA	3310	1/1	0.95	0.11	44,44,44,44	0
54	MG	DA	3002	1/1	0.95	0.31	67,67,67,67	0
54	MG	DA	3222	1/1	0.95	0.18	47,47,47,47	0
54	MG	BA	3460	1/1	0.95	0.08	58,58,58,58	0
54	MG	BA	3143	1/1	0.95	0.32	45,45,45,45	0
54	MG	DA	3149	1/1	0.95	0.25	36,36,36,36	0
54	MG	DA	3005	1/1	0.95	0.21	64,64,64,64	0
54	MG	BA	3172	1/1	0.95	0.11	71,71,71,71	0
54	MG	DA	3353	1/1	0.95	0.08	40,40,40,40	0
54	MG	BA	3074	1/1	0.95	0.21	55,55,55,55	0
54	MG	BA	3129	1/1	0.95	0.15	49,49,49,49	0
54	MG	BA	3593	1/1	0.95	0.10	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3358	1/1	0.95	0.07	68,68,68,68	0
54	MG	BA	3468	1/1	0.95	0.08	38,38,38,38	0
54	MG	BA	3608	1/1	0.95	0.07	87,87,87,87	0
54	MG	DA	3361	1/1	0.95	0.06	67,67,67,67	0
54	MG	DA	3362	1/1	0.95	0.06	63,63,63,63	0
54	MG	BA	3253	1/1	0.95	0.18	38,38,38,38	0
54	MG	DA	3161	1/1	0.95	0.35	55,55,55,55	0
54	MG	DA	3015	1/1	0.95	0.27	71,71,71,71	0
54	MG	BA	3472	1/1	0.95	0.12	29,29,29,29	0
54	MG	DA	3087	1/1	0.95	0.21	58,58,58,58	0
54	MG	BA	3278	1/1	0.95	0.10	43,43,43,43	0
54	MG	DA	3371	1/1	0.95	0.06	50,50,50,50	0
54	MG	BA	3146	1/1	0.95	0.38	52,52,52,52	0
54	MG	DA	3167	1/1	0.95	0.18	59,59,59,59	0
54	MG	BA	3117	1/1	0.95	0.10	31,31,31,31	0
54	MG	AA	1704	1/1	0.95	0.06	90,90,90,90	0
54	MG	BA	3164	1/1	0.95	0.11	39,39,39,39	0
54	MG	BB	205	1/1	0.95	0.33	57,57,57,57	0
54	MG	BA	3537	1/1	0.95	0.11	38,38,38,38	0
54	MG	BA	3483	1/1	0.95	0.13	57,57,57,57	0
54	MG	BA	3259	1/1	0.95	0.16	51,51,51,51	0
54	MG	DA	3389	1/1	0.95	0.07	58,58,58,58	0
54	MG	BB	210	1/1	0.95	0.09	67,67,67,67	0
54	MG	DA	3100	1/1	0.95	0.45	61,61,61,61	0
54	MG	BA	3095	1/1	0.95	0.24	45,45,45,45	0
54	MG	BA	3337	1/1	0.95	0.11	33,33,33,33	0
54	MG	BA	3399	1/1	0.95	0.10	41,41,41,41	0
54	MG	BA	3405	1/1	0.95	0.10	38,38,38,38	0
54	MG	BA	3408	1/1	0.95	0.16	34,34,34,34	0
54	MG	BE	301	1/1	0.95	0.20	43,43,43,43	0
54	MG	BE	302	1/1	0.95	0.11	52,52,52,52	0
54	MG	BE	303	1/1	0.95	0.08	54,54,54,54	0
54	MG	BE	306	1/1	0.95	0.10	56,56,56,56	0
54	MG	DA	3110	1/1	0.95	0.10	46,46,46,46	0
54	MG	BA	3338	1/1	0.95	0.10	30,30,30,30	0
54	MG	DA	3039	1/1	0.95	0.16	41,41,41,41	0
54	MG	DA	3040	1/1	0.95	0.23	50,50,50,50	0
54	MG	DA	3265	1/1	0.95	0.09	39,39,39,39	0
54	MG	DA	3267	1/1	0.95	0.13	59,59,59,59	0
54	MG	BA	3548	1/1	0.95	0.09	41,41,41,41	0
54	MG	DA	3417	1/1	0.95	0.13	81,81,81,81	0
54	MG	DA	3279	1/1	0.95	0.17	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3421	1/1	0.95	0.07	69,69,69,69	0
54	MG	BA	3262	1/1	0.95	0.32	32,32,32,32	0
54	MG	DA	3044	1/1	0.95	0.27	51,51,51,51	0
54	MG	DA	3289	1/1	0.95	0.06	52,52,52,52	0
54	MG	BA	3198	1/1	0.95	0.21	29,29,29,29	0
54	MG	DE	301	1/1	0.95	0.35	37,37,37,37	0
54	MG	BA	3199	1/1	0.95	0.08	31,31,31,31	0
54	MG	BA	3059	1/1	0.95	0.19	49,49,49,49	0
54	MG	DA	3296	1/1	0.95	0.07	50,50,50,50	0
54	MG	BU	201	1/1	0.95	0.21	51,51,51,51	0
54	MG	BA	3221	1/1	0.95	0.22	51,51,51,51	0
54	MG	BA	3347	1/1	0.95	0.17	55,55,55,55	0
54	MG	BA	3122	1/1	0.95	0.24	56,56,56,56	0
54	MG	DA	3308	1/1	0.95	0.14	49,49,49,49	0
54	MG	BA	3002	1/1	0.95	0.10	98,98,98,98	0
54	MG	BA	3297	1/1	0.95	0.11	35,35,35,35	0
54	MG	DA	3312	1/1	0.95	0.07	67,67,67,67	0
54	MG	CA	1655	1/1	0.96	0.18	74,74,74,74	0
54	MG	DA	3322	1/1	0.96	0.11	35,35,35,35	0
54	MG	DA	3212	1/1	0.96	0.13	38,38,38,38	0
54	MG	DA	3325	1/1	0.96	0.13	36,36,36,36	0
54	MG	DA	3060	1/1	0.96	0.13	60,60,60,60	0
54	MG	BA	3509	1/1	0.96	0.08	85,85,85,85	0
54	MG	BA	3568	1/1	0.96	0.08	60,60,60,60	0
54	MG	BA	3298	1/1	0.96	0.07	53,53,53,53	0
54	MG	DA	3332	1/1	0.96	0.06	62,62,62,62	0
54	MG	DA	3334	1/1	0.96	0.07	56,56,56,56	0
54	MG	BA	3570	1/1	0.96	0.11	36,36,36,36	0
54	MG	BA	3511	1/1	0.96	0.07	33,33,33,33	0
54	MG	DA	3140	1/1	0.96	0.23	70,70,70,70	0
54	MG	AA	1647	1/1	0.96	0.27	61,61,61,61	0
54	MG	DA	3067	1/1	0.96	0.22	32,32,32,32	0
54	MG	BA	3359	1/1	0.96	0.06	49,49,49,49	0
54	MG	BA	3033	1/1	0.96	0.18	40,40,40,40	0
54	MG	CA	1667	1/1	0.96	0.13	64,64,64,64	0
54	MG	BA	3578	1/1	0.96	0.12	60,60,60,60	0
54	MG	BA	3208	1/1	0.96	0.25	54,54,54,54	0
54	MG	BA	3104	1/1	0.96	0.10	48,48,48,48	0
54	MG	BA	3163	1/1	0.96	0.31	42,42,42,42	0
54	MG	BA	3364	1/1	0.96	0.04	46,46,46,46	0
54	MG	BA	3585	1/1	0.96	0.09	54,54,54,54	0
54	MG	DA	3154	1/1	0.96	0.44	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3044	1/1	0.96	0.20	49,49,49,49	0
54	MG	DA	3156	1/1	0.96	0.23	52,52,52,52	0
54	MG	BA	3027	1/1	0.96	0.12	56,56,56,56	0
54	MG	DA	3236	1/1	0.96	0.36	44,44,44,44	0
54	MG	BA	3524	1/1	0.96	0.09	77,77,77,77	0
54	MG	BA	3123	1/1	0.96	0.12	43,43,43,43	0
54	MG	BA	3017	1/1	0.96	0.15	47,47,47,47	0
54	MG	DA	3010	1/1	0.96	0.10	43,43,43,43	0
54	MG	BA	3595	1/1	0.96	0.06	82,82,82,82	0
54	MG	BA	3190	1/1	0.96	0.19	46,46,46,46	0
54	MG	DA	3013	1/1	0.96	0.09	41,41,41,41	0
54	MG	BA	3611	1/1	0.96	0.06	70,70,70,70	0
54	MG	BA	3037	1/1	0.96	0.14	52,52,52,52	0
54	MG	DA	3369	1/1	0.96	0.13	57,57,57,57	0
54	MG	BA	3058	1/1	0.96	0.13	56,56,56,56	0
54	MG	BA	3245	1/1	0.96	0.11	36,36,36,36	0
54	MG	BA	3326	1/1	0.96	0.07	30,30,30,30	0
54	MG	DA	3374	1/1	0.96	0.14	44,44,44,44	0
54	MG	DA	3019	1/1	0.96	0.10	41,41,41,41	0
54	MG	BA	3083	1/1	0.96	0.32	56,56,56,56	0
54	MG	DA	3094	1/1	0.96	0.16	39,39,39,39	0
54	MG	BA	3389	1/1	0.96	0.11	33,33,33,33	0
54	MG	DA	3382	1/1	0.96	0.10	53,53,53,53	0
54	MG	DA	3022	1/1	0.96	0.30	52,52,52,52	0
54	MG	BA	3248	1/1	0.96	0.29	50,50,50,50	0
54	MG	BA	3479	1/1	0.96	0.08	35,35,35,35	0
54	MG	BB	206	1/1	0.96	0.24	62,62,62,62	0
54	MG	BA	3538	1/1	0.96	0.07	70,70,70,70	0
54	MG	BA	3330	1/1	0.96	0.11	36,36,36,36	0
54	MG	AA	1691	1/1	0.96	0.07	58,58,58,58	0
54	MG	BA	3060	1/1	0.96	0.18	45,45,45,45	0
54	MG	BB	212	1/1	0.96	0.06	68,68,68,68	0
54	MG	DA	3395	1/1	0.96	0.10	37,37,37,37	0
54	MG	BA	3333	1/1	0.96	0.15	36,36,36,36	0
54	MG	DA	3397	1/1	0.96	0.06	65,65,65,65	0
54	MG	BA	3334	1/1	0.96	0.07	43,43,43,43	0
54	MG	BA	3406	1/1	0.96	0.11	40,40,40,40	0
54	MG	DA	3266	1/1	0.96	0.07	58,58,58,58	0
54	MG	AA	1703	1/1	0.96	0.09	89,89,89,89	0
54	MG	DA	3268	1/1	0.96	0.12	43,43,43,43	0
54	MG	DA	3277	1/1	0.96	0.08	42,42,42,42	0
54	MG	BD	301	1/1	0.96	0.08	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3412	1/1	0.96	0.09	41,41,41,41	0
54	MG	BA	3413	1/1	0.96	0.12	31,31,31,31	0
54	MG	BA	3414	1/1	0.96	0.14	26,26,26,26	0
54	MG	BA	3132	1/1	0.96	0.20	31,31,31,31	0
54	MG	DA	3412	1/1	0.96	0.06	45,45,45,45	0
54	MG	DA	3291	1/1	0.96	0.16	43,43,43,43	0
54	MG	BE	304	1/1	0.96	0.09	32,32,32,32	0
54	MG	BA	3133	1/1	0.96	0.17	31,31,31,31	0
54	MG	DA	3042	1/1	0.96	0.26	46,46,46,46	0
54	MG	BA	3419	1/1	0.96	0.09	35,35,35,35	0
54	MG	BF	302	1/1	0.96	0.16	62,62,62,62	0
54	MG	DA	3424	1/1	0.96	0.04	130,130,130,130	0
54	MG	DA	3427	1/1	0.96	0.09	40,40,40,40	0
54	MG	BA	3134	1/1	0.96	0.29	44,44,44,44	0
54	MG	BA	3255	1/1	0.96	0.30	65,65,65,65	0
54	MG	BA	3177	1/1	0.96	0.10	45,45,45,45	0
54	MG	DB	204	1/1	0.96	0.11	74,74,74,74	0
54	MG	DA	3306	1/1	0.96	0.07	88,88,88,88	0
54	MG	BA	3432	1/1	0.96	0.10	31,31,31,31	0
54	MG	BA	3040	1/1	0.96	0.09	33,33,33,33	0
54	MG	DA	3124	1/1	0.96	0.26	35,35,35,35	0
54	MG	CA	1647	1/1	0.96	0.12	78,78,78,78	0
54	MG	BA	3202	1/1	0.96	0.19	65,65,65,65	0
54	MG	AA	1684	1/1	0.96	0.06	76,76,76,76	0
54	MG	BA	3260	1/1	0.96	0.27	50,50,50,50	0
54	MG	BA	3138	1/1	0.96	0.11	54,54,54,54	0
54	MG	BA	3181	1/1	0.96	0.16	48,48,48,48	0
54	MG	B0	102	1/1	0.96	0.12	56,56,56,56	0
54	MG	DA	3132	1/1	0.96	0.22	49,49,49,49	0
55	ZN	D4	101	1/1	0.96	0.09	176,176,176,176	0
54	MG	BA	3349	1/1	0.97	0.05	39,39,39,39	0
54	MG	BA	3350	1/1	0.97	0.09	60,60,60,60	0
54	MG	BA	3504	1/1	0.97	0.23	28,28,28,28	0
54	MG	BA	3288	1/1	0.97	0.34	33,33,33,33	0
54	MG	DA	3348	1/1	0.97	0.04	85,85,85,85	0
54	MG	BA	3564	1/1	0.97	0.13	36,36,36,36	0
54	MG	BQ	203	1/1	0.97	0.09	44,44,44,44	0
54	MG	BA	3452	1/1	0.97	0.09	62,62,62,62	0
54	MG	BA	3352	1/1	0.97	0.11	53,53,53,53	0
54	MG	BA	3454	1/1	0.97	0.09	34,34,34,34	0
54	MG	BA	3394	1/1	0.97	0.05	29,29,29,29	0
54	MG	BA	3119	1/1	0.97	0.07	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3356	1/1	0.97	0.12	42,42,42,42	0
54	MG	BA	3457	1/1	0.97	0.07	91,91,91,91	0
54	MG	BA	3238	1/1	0.97	0.06	32,32,32,32	0
54	MG	CA	1652	1/1	0.97	0.11	65,65,65,65	0
54	MG	BA	3281	1/1	0.97	0.07	56,56,56,56	0
54	MG	BA	3516	1/1	0.97	0.06	39,39,39,39	0
54	MG	DA	3051	1/1	0.97	0.13	43,43,43,43	0
54	MG	BA	3400	1/1	0.97	0.08	34,34,34,34	0
54	MG	B2	102	1/1	0.97	0.09	60,60,60,60	0
54	MG	DA	3365	1/1	0.97	0.06	50,50,50,50	0
54	MG	BA	3461	1/1	0.97	0.07	38,38,38,38	0
54	MG	CA	1658	1/1	0.97	0.13	83,83,83,83	0
54	MG	DA	3056	1/1	0.97	0.28	61,61,61,61	0
54	MG	BA	3401	1/1	0.97	0.07	45,45,45,45	0
54	MG	CA	1660	1/1	0.97	0.10	106,106,106,106	0
54	MG	AA	1701	1/1	0.97	0.04	96,96,96,96	0
54	MG	BA	3312	1/1	0.97	0.06	50,50,50,50	0
54	MG	BA	3010	1/1	0.97	0.08	48,48,48,48	0
54	MG	DA	3272	1/1	0.97	0.09	47,47,47,47	0
54	MG	DA	3376	1/1	0.97	0.06	43,43,43,43	0
54	MG	DA	3377	1/1	0.97	0.07	61,61,61,61	0
54	MG	BA	3410	1/1	0.97	0.07	34,34,34,34	0
54	MG	BA	3411	1/1	0.97	0.15	43,43,43,43	0
54	MG	BA	3126	1/1	0.97	0.30	57,57,57,57	0
54	MG	DA	3381	1/1	0.97	0.09	79,79,79,79	0
54	MG	DA	3280	1/1	0.97	0.11	40,40,40,40	0
54	MG	DA	3282	1/1	0.97	0.06	42,42,42,42	0
54	MG	DA	3385	1/1	0.97	0.18	49,49,49,49	0
54	MG	DA	3283	1/1	0.97	0.07	48,48,48,48	0
54	MG	BA	3527	1/1	0.97	0.09	51,51,51,51	0
54	MG	DA	3285	1/1	0.97	0.08	52,52,52,52	0
54	MG	BA	3137	1/1	0.97	0.05	38,38,38,38	0
54	MG	BA	3474	1/1	0.97	0.13	66,66,66,66	0
54	MG	BA	3336	1/1	0.97	0.06	46,46,46,46	0
54	MG	BA	3606	1/1	0.97	0.06	29,29,29,29	0
54	MG	BA	3531	1/1	0.97	0.07	49,49,49,49	0
54	MG	AA	1693	1/1	0.97	0.05	78,78,78,78	0
54	MG	DA	3295	1/1	0.97	0.07	42,42,42,42	0
54	MG	BA	3478	1/1	0.97	0.08	92,92,92,92	0
54	MG	BA	3416	1/1	0.97	0.06	46,46,46,46	0
54	MG	BA	3317	1/1	0.97	0.07	51,51,51,51	0
54	MG	BA	3617	1/1	0.97	0.08	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3367	1/1	0.97	0.17	33,33,33,33	0
54	MG	DA	3303	1/1	0.97	0.10	37,37,37,37	0
54	MG	DA	3305	1/1	0.97	0.05	55,55,55,55	0
54	MG	DA	3213	1/1	0.97	0.40	64,64,64,64	0
54	MG	BB	201	1/1	0.97	0.09	61,61,61,61	0
54	MG	DA	3145	1/1	0.97	0.27	47,47,47,47	0
54	MG	BA	3482	1/1	0.97	0.12	58,58,58,58	0
54	MG	BA	3368	1/1	0.97	0.23	34,34,34,34	0
54	MG	BA	3539	1/1	0.97	0.06	61,61,61,61	0
54	MG	DA	3413	1/1	0.97	0.09	37,37,37,37	0
54	MG	BA	3484	1/1	0.97	0.14	40,40,40,40	0
54	MG	DA	3150	1/1	0.97	0.27	41,41,41,41	0
54	MG	DA	3416	1/1	0.97	0.06	32,32,32,32	0
54	MG	BA	3422	1/1	0.97	0.09	27,27,27,27	0
54	MG	BA	3486	1/1	0.97	0.06	48,48,48,48	0
54	MG	BA	3300	1/1	0.97	0.07	37,37,37,37	0
54	MG	BA	3370	1/1	0.97	0.09	66,66,66,66	0
54	MG	BA	3430	1/1	0.97	0.13	30,30,30,30	0
54	MG	DA	3425	1/1	0.97	0.07	60,60,60,60	0
54	MG	BB	211	1/1	0.97	0.05	51,51,51,51	0
54	MG	DA	3428	1/1	0.97	0.04	81,81,81,81	0
54	MG	BA	3319	1/1	0.97	0.06	68,68,68,68	0
54	MG	BA	3158	1/1	0.97	0.29	51,51,51,51	0
54	MG	DA	3090	1/1	0.97	0.17	53,53,53,53	0
54	MG	BA	3342	1/1	0.97	0.08	57,57,57,57	0
54	MG	DB	205	1/1	0.97	0.10	70,70,70,70	0
54	MG	DA	3328	1/1	0.97	0.05	34,34,34,34	0
54	MG	DA	3329	1/1	0.97	0.06	47,47,47,47	0
54	MG	BA	3322	1/1	0.97	0.06	45,45,45,45	0
54	MG	BA	3550	1/1	0.97	0.08	37,37,37,37	0
54	MG	BA	3324	1/1	0.97	0.10	82,82,82,82	0
54	MG	DA	3333	1/1	0.97	0.05	53,53,53,53	0
54	MG	BD	302	1/1	0.97	0.19	38,38,38,38	0
54	MG	BA	3440	1/1	0.97	0.05	63,63,63,63	0
54	MG	BA	3346	1/1	0.97	0.05	45,45,45,45	0
54	MG	BA	3325	1/1	0.97	0.06	47,47,47,47	0
54	MG	BA	3444	1/1	0.97	0.05	61,61,61,61	0
54	MG	BA	3387	1/1	0.97	0.10	33,33,33,33	0
54	MG	BA	3447	1/1	0.97	0.17	37,37,37,37	0
55	ZN	D6	101	1/1	0.97	0.05	86,86,86,86	0
54	MG	BA	3348	1/1	0.98	0.10	37,37,37,37	0
54	MG	DA	3384	1/1	0.98	0.10	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3446	1/1	0.98	0.05	40,40,40,40	0
54	MG	DA	3271	1/1	0.98	0.07	57,57,57,57	0
54	MG	BA	3321	1/1	0.98	0.07	65,65,65,65	0
54	MG	DA	3275	1/1	0.98	0.04	48,48,48,48	0
54	MG	DA	3276	1/1	0.98	0.12	51,51,51,51	0
54	MG	BA	3508	1/1	0.98	0.12	40,40,40,40	0
54	MG	BA	3390	1/1	0.98	0.12	29,29,29,29	0
54	MG	DA	3392	1/1	0.98	0.04	56,56,56,56	0
54	MG	BA	3576	1/1	0.98	0.05	41,41,41,41	0
54	MG	AA	1705	1/1	0.98	0.07	68,68,68,68	0
54	MG	DA	3337	1/1	0.98	0.07	42,42,42,42	0
54	MG	BA	3149	1/1	0.98	0.18	49,49,49,49	0
54	MG	DA	3339	1/1	0.98	0.05	48,48,48,48	0
54	MG	DA	3398	1/1	0.98	0.04	52,52,52,52	0
54	MG	BA	3451	1/1	0.98	0.14	34,34,34,34	0
54	MG	BB	217	1/1	0.98	0.17	42,42,42,42	0
54	MG	BA	3418	1/1	0.98	0.07	54,54,54,54	0
54	MG	BA	3393	1/1	0.98	0.13	38,38,38,38	0
54	MG	DA	3404	1/1	0.98	0.07	53,53,53,53	0
54	MG	DA	3344	1/1	0.98	0.04	51,51,51,51	0
54	MG	DA	3287	1/1	0.98	0.04	46,46,46,46	0
54	MG	BA	3515	1/1	0.98	0.12	46,46,46,46	0
54	MG	DA	3290	1/1	0.98	0.10	42,42,42,42	0
54	MG	BA	3107	1/1	0.98	0.15	49,49,49,49	0
54	MG	BA	3035	1/1	0.98	0.19	45,45,45,45	0
54	MG	BA	3373	1/1	0.98	0.06	55,55,55,55	0
54	MG	BA	3589	1/1	0.98	0.05	70,70,70,70	0
54	MG	BA	3427	1/1	0.98	0.12	32,32,32,32	0
54	MG	BA	3592	1/1	0.98	0.04	51,51,51,51	0
54	MG	BA	3268	1/1	0.98	0.09	44,44,44,44	0
54	MG	BA	3552	1/1	0.98	0.08	38,38,38,38	0
54	MG	CA	1662	1/1	0.98	0.07	95,95,95,95	0
54	MG	DA	3300	1/1	0.98	0.14	62,62,62,62	0
54	MG	BA	3293	1/1	0.98	0.09	29,29,29,29	0
54	MG	BA	3596	1/1	0.98	0.05	46,46,46,46	0
54	MG	BA	3303	1/1	0.98	0.12	36,36,36,36	0
54	MG	BA	3607	1/1	0.98	0.09	38,38,38,38	0
54	MG	DA	3307	1/1	0.98	0.10	39,39,39,39	0
54	MG	BA	3523	1/1	0.98	0.04	79,79,79,79	0
54	MG	DA	3429	1/1	0.98	0.05	44,44,44,44	0
54	MG	BA	3609	1/1	0.98	0.12	51,51,51,51	0
54	MG	BA	3433	1/1	0.98	0.06	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3311	1/1	0.98	0.06	65,65,65,65	0
54	MG	BA	3402	1/1	0.98	0.07	47,47,47,47	0
54	MG	BA	3343	1/1	0.98	0.04	91,91,91,91	0
54	MG	DD	301	1/1	0.98	0.09	40,40,40,40	0
54	MG	BA	3304	1/1	0.98	0.07	27,27,27,27	0
54	MG	BA	3560	1/1	0.98	0.06	29,29,29,29	0
54	MG	BA	3438	1/1	0.98	0.09	38,38,38,38	0
54	MG	BA	3407	1/1	0.98	0.08	35,35,35,35	0
54	MG	DA	3373	1/1	0.98	0.11	38,38,38,38	0
54	MG	BA	3212	1/1	0.98	0.21	47,47,47,47	0
54	MG	DA	3319	1/1	0.98	0.06	59,59,59,59	0
54	MG	BA	3470	1/1	0.98	0.09	35,35,35,35	0
54	MG	BA	3471	1/1	0.98	0.11	38,38,38,38	0
55	ZN	BY	201	1/1	0.98	0.03	74,74,74,74	0
54	MG	BA	3385	1/1	0.98	0.07	73,73,73,73	0
55	ZN	B9	101	1/1	0.98	0.05	69,69,69,69	0
55	ZN	CD	301	1/1	0.98	0.22	96,96,96,96	0
54	MG	DA	3323	1/1	0.98	0.16	36,36,36,36	0
54	MG	BA	3295	1/1	0.98	0.07	44,44,44,44	0
54	MG	BA	3309	1/1	0.98	0.14	38,38,38,38	0
54	MG	B8	103	1/1	0.98	0.11	51,51,51,51	0
54	MG	BA	3426	1/1	0.99	0.11	28,28,28,28	0
54	MG	BA	3488	1/1	0.99	0.06	34,34,34,34	0
54	MG	BA	3296	1/1	0.99	0.05	48,48,48,48	0
54	MG	BA	3403	1/1	0.99	0.06	44,44,44,44	0
54	MG	BA	3429	1/1	0.99	0.11	29,29,29,29	0
54	MG	BA	3599	1/1	0.99	0.04	50,50,50,50	0
54	MG	DA	3401	1/1	0.99	0.03	85,85,85,85	0
54	MG	BA	3600	1/1	0.99	0.09	31,31,31,31	0
54	MG	BA	3602	1/1	0.99	0.04	24,24,24,24	0
54	MG	BA	3603	1/1	0.99	0.04	30,30,30,30	0
54	MG	BA	3404	1/1	0.99	0.05	46,46,46,46	0
54	MG	BA	3431	1/1	0.99	0.20	34,34,34,34	0
54	MG	BA	3328	1/1	0.99	0.06	27,27,27,27	0
54	MG	BA	3462	1/1	0.99	0.05	25,25,25,25	0
54	MG	DA	3302	1/1	0.99	0.13	36,36,36,36	0
54	MG	BA	3610	1/1	0.99	0.04	56,56,56,56	0
54	MG	DA	3304	1/1	0.99	0.05	38,38,38,38	0
54	MG	BA	3307	1/1	0.99	0.06	29,29,29,29	0
54	MG	BA	3323	1/1	0.99	0.03	40,40,40,40	0
54	MG	BA	3371	1/1	0.99	0.06	67,67,67,67	0
54	MG	BA	3466	1/1	0.99	0.04	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3615	1/1	0.99	0.04	91,91,91,91	0
54	MG	BA	3616	1/1	0.99	0.06	82,82,82,82	0
54	MG	DA	3419	1/1	0.99	0.03	50,50,50,50	0
54	MG	BA	3409	1/1	0.99	0.07	26,26,26,26	0
54	MG	B5	102	1/1	0.99	0.04	42,42,42,42	0
54	MG	DA	3422	1/1	0.99	0.03	75,75,75,75	0
54	MG	BA	3437	1/1	0.99	0.07	28,28,28,28	0
54	MG	BA	3372	1/1	0.99	0.11	50,50,50,50	0
54	MG	BA	3246	1/1	0.99	0.19	49,49,49,49	0
54	MG	DA	3426	1/1	0.99	0.04	94,94,94,94	0
54	MG	BA	3353	1/1	0.99	0.03	28,28,28,28	0
54	MG	BA	3354	1/1	0.99	0.09	49,49,49,49	0
54	MG	BA	3376	1/1	0.99	0.04	55,55,55,55	0
54	MG	DA	3430	1/1	0.99	0.04	72,72,72,72	0
54	MG	BA	3443	1/1	0.99	0.07	41,41,41,41	0
54	MG	DA	3264	1/1	0.99	0.12	46,46,46,46	0
54	MG	BA	3574	1/1	0.99	0.04	41,41,41,41	0
54	MG	BA	3575	1/1	0.99	0.05	54,54,54,54	0
54	MG	AA	1689	1/1	0.99	0.05	55,55,55,55	0
54	MG	BA	3395	1/1	0.99	0.06	32,32,32,32	0
54	MG	DA	3269	1/1	0.99	0.04	54,54,54,54	0
54	MG	BA	3477	1/1	0.99	0.04	45,45,45,45	0
54	MG	BA	3378	1/1	0.99	0.13	38,38,38,38	0
54	MG	DA	3273	1/1	0.99	0.04	37,37,37,37	0
54	MG	DA	3274	1/1	0.99	0.03	35,35,35,35	0
54	MG	BA	3305	1/1	0.99	0.03	37,37,37,37	0
54	MG	BA	3398	1/1	0.99	0.04	36,36,36,36	0
54	MG	BA	3582	1/1	0.99	0.12	54,54,54,54	0
54	MG	BA	3583	1/1	0.99	0.03	50,50,50,50	0
54	MG	BA	3380	1/1	0.99	0.05	50,50,50,50	0
54	MG	BA	3421	1/1	0.99	0.04	36,36,36,36	0
55	ZN	B6	101	1/1	0.99	0.03	54,54,54,54	0
54	MG	BA	3586	1/1	0.99	0.05	58,58,58,58	0
54	MG	BA	3382	1/1	0.99	0.07	58,58,58,58	0
54	MG	BA	3423	1/1	0.99	0.09	30,30,30,30	0
54	MG	BA	3424	1/1	0.99	0.12	32,32,32,32	0
54	MG	BA	3366	1/1	0.99	0.04	50,50,50,50	0
54	MG	BA	3591	1/1	0.99	0.06	56,56,56,56	0
55	ZN	D9	101	1/1	0.99	0.05	87,87,87,87	0
54	MG	BA	3381	1/1	1.00	0.04	49,49,49,49	0
54	MG	BA	3604	1/1	1.00	0.02	36,36,36,36	0
54	MG	BA	3605	1/1	1.00	0.03	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	ZN	B5	103	1/1	1.00	0.02	58,58,58,58	0
54	MG	BA	3597	1/1	1.00	0.02	26,26,26,26	0
54	MG	BE	305	1/1	1.00	0.09	32,32,32,32	0
54	MG	DA	3270	1/1	1.00	0.04	34,34,34,34	0
54	MG	DA	3418	1/1	1.00	0.02	39,39,39,39	0
54	MG	DA	3288	1/1	1.00	0.05	37,37,37,37	0
54	MG	BA	3601	1/1	1.00	0.02	33,33,33,33	0
55	ZN	D5	101	1/1	1.00	0.02	65,65,65,65	0
54	MG	BA	3598	1/1	1.00	0.02	39,39,39,39	0
54	MG	DA	3281	1/1	1.00	0.03	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.