



wwPDB X-ray Structure Validation Summary Report i

Jun 16, 2014 – 07:04 PM BST

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 validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

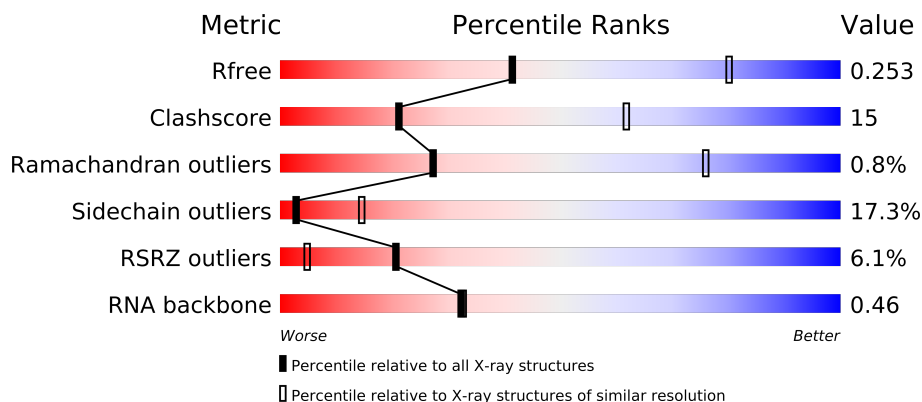
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance

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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1522	
1	CA	1522	
2	AB	256	
2	CB	256	
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	

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Mol	Chain	Length	Quality of chain
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	
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	
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	

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Mol	Chain	Length	Quality of chain
49	B5	60	<div><div></div></div>
49	D5	60	<div><div></div></div>
50	B6	54	<div><div></div></div>
50	D6	54	<div><div></div></div>
51	B7	49	<div><div></div></div>
51	D7	49	<div><div></div></div>
52	B8	65	<div><div></div></div>
52	D8	65	<div><div></div></div>
53	B9	37	<div><div></div></div>
53	D9	37	<div><div></div></div>

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 283930 atoms, of which 0 are hydrogen and 0 are deuterium.

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		0	0	0
			865	544	172	149				
36	DS	110	Total	C	N	O		0	0	0
			865	544	172	149				

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BV	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	BA	618	Total	Mg	0	0
			618	618		
54	CA	69	Total	Mg	0	0
			69	69		
54	DF	2	Total	Mg	0	0
			2	2		
54	B8	3	Total	Mg	0	0
			3	3		
54	BE	6	Total	Mg	0	0
			6	6		
54	B1	1	Total	Mg	0	0
			1	1		
54	BP	1	Total	Mg	0	0
			1	1		
54	D6	1	Total	Mg	0	0
			1	1		
54	B5	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BB	17	Total 17	Mg 17	0	0
54	D8	1	Total 1	Mg 1	0	0
54	B9	1	Total 1	Mg 1	0	0
54	BF	2	Total 2	Mg 2	0	0
54	B2	2	Total 2	Mg 2	0	0
54	AA	106	Total 106	Mg 106	0	0
54	BQ	3	Total 3	Mg 3	0	0
54	D7	1	Total 1	Mg 1	0	0
54	BU	2	Total 2	Mg 2	0	0
54	AD	1	Total 1	Mg 1	0	0
54	DD	1	Total 1	Mg 1	0	0
54	B3	2	Total 2	Mg 2	0	0
54	BR	2	Total 2	Mg 2	0	0
54	DA	430	Total 430	Mg 430	0	0
54	BV	1	Total 1	Mg 1	0	0
54	DE	1	Total 1	Mg 1	0	0
54	DP	1	Total 1	Mg 1	0	0
54	BD	3	Total 3	Mg 3	0	0
54	B0	2	Total 2	Mg 2	0	0
54	BW	1	Total 1	Mg 1	0	0
54	DB	5	Total 5	Mg 5	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	B5	1	Total 1	Zn 1	0	0
55	B4	1	Total 1	Zn 1	0	0
55	AD	1	Total 1	Zn 1	0	0
55	CD	1	Total 1	Zn 1	0	0
55	B9	1	Total 1	Zn 1	0	0
55	BY	1	Total 1	Zn 1	0	0
55	DY	1	Total 1	Zn 1	0	0
55	D5	1	Total 1	Zn 1	0	0
55	D4	1	Total 1	Zn 1	0	0
55	AN	1	Total 1	Zn 1	0	0
55	CN	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
55	B6	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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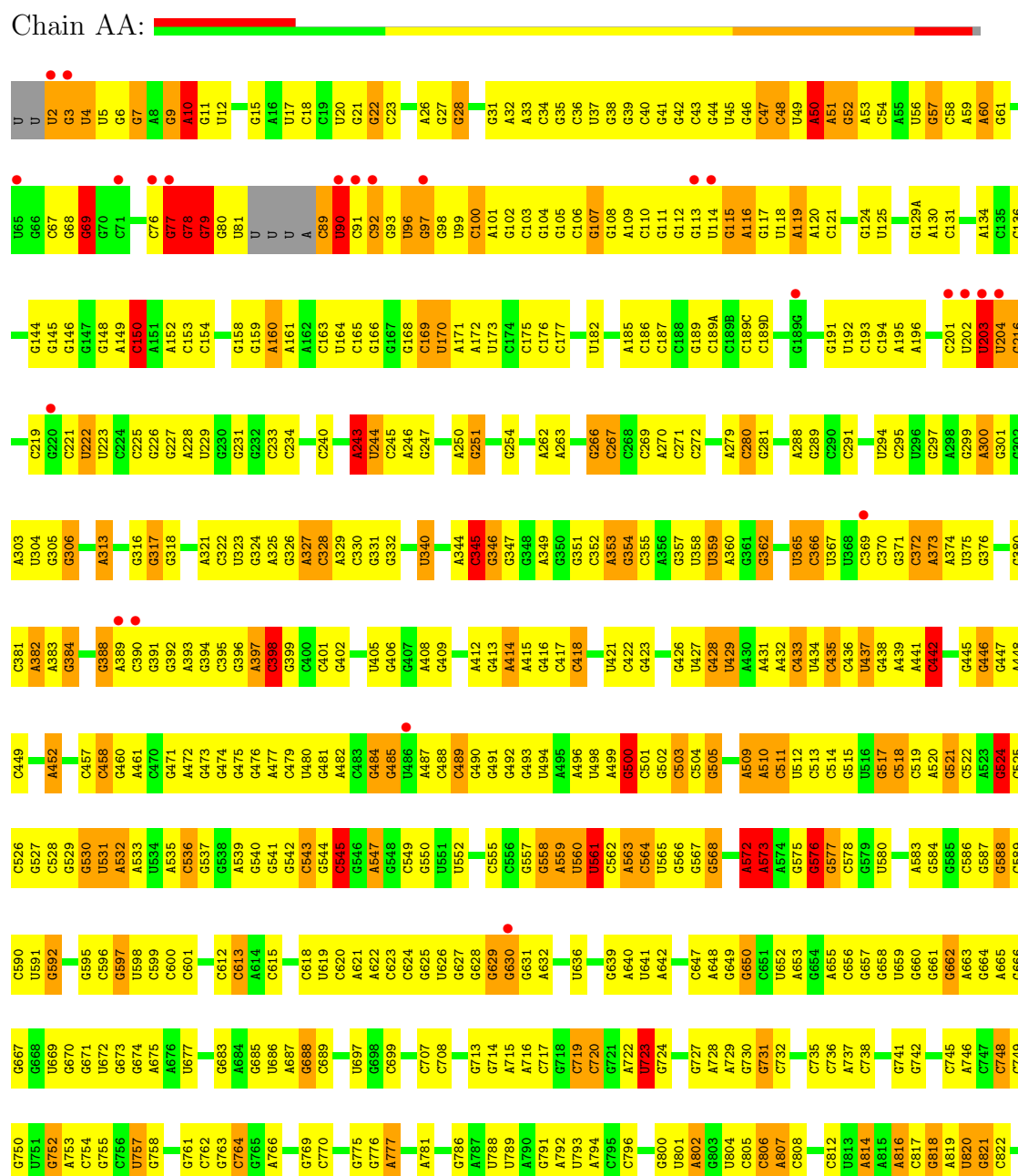
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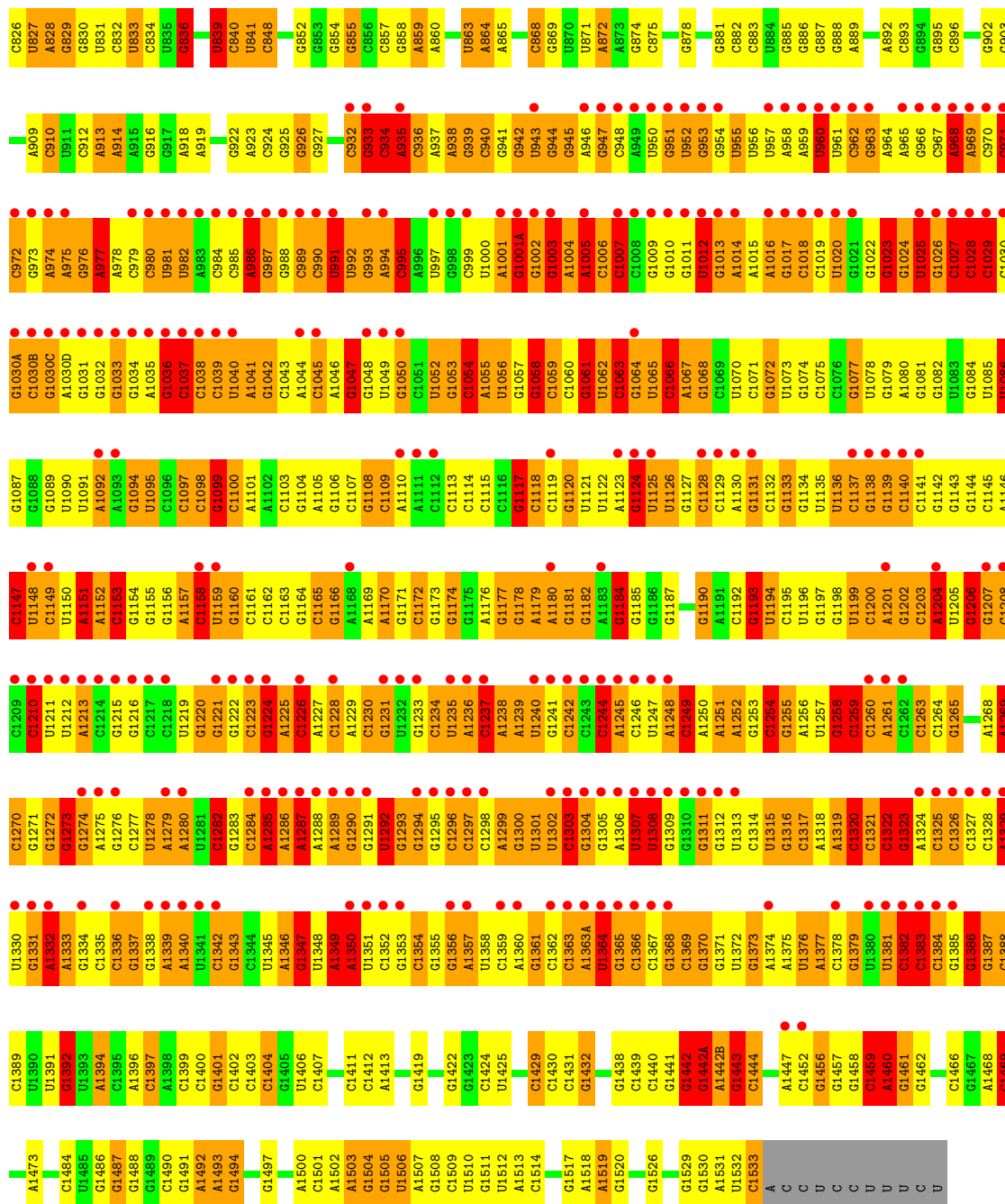
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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56	B9	2	Total 2	O 2	0	0
56	CA	119	Total 119	O 119	0	0
56	CD	1	Total 1	O 1	0	0
56	CK	2	Total 2	O 2	0	0
56	CP	1	Total 1	O 1	0	0
56	CT	2	Total 2	O 2	0	0
56	DA	696	Total 696	O 696	0	0
56	DB	9	Total 9	O 9	0	0
56	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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

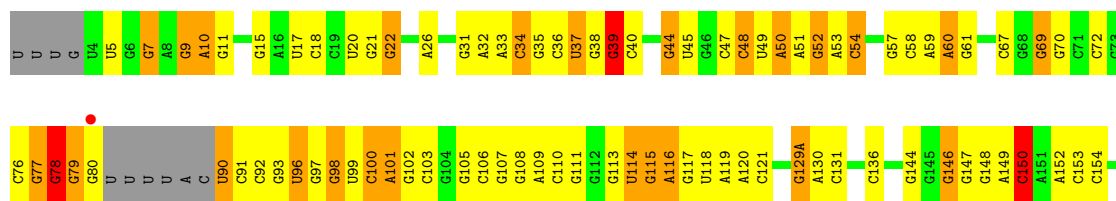
• Molecule 1: 16S Ribosomal RNA



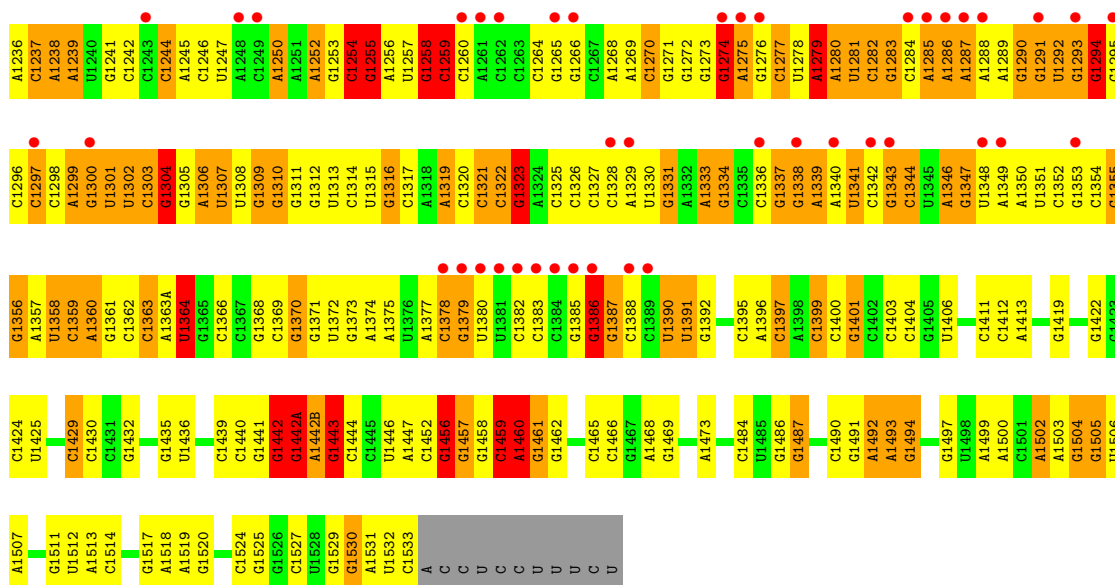


● Molecule 1: 16S Ribosomal RNA

Chain CA:

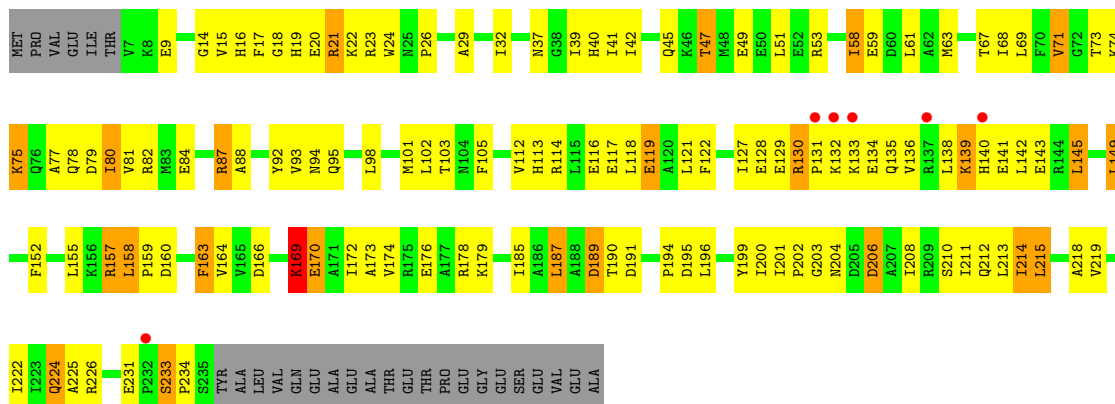


G1175	G1176	G1177	G1178	G1179	G1180	G1181	G1182	G1183	G1184	G1185	G1186	G1187	G1188	G1189	G1190	G1191	G1192	G1193	G1194	G1195	G1196	G1197	G1198	G1199	G1200	G1201	G1202	G1203	G1204	G1205	G1206	G1207	G1208	G1209	G1210	G1211	G1212	G1213	G1214	G1215	G1216	G1217	G1218	G1219	G1220	G1221	G1222	G1223	G1224	G1225	G1226	G1227	G1228	G1229	G1230	G1231	G1232	G1233	G1234	G1235																																																																																																																																																																																																																																																																																																																																																																																										
C1114	C1115	C1116	C1117	C1118	C1119	C1120	C1121	C1122	C1123	C1124	C1125	C1126	C1127	C1128	C1129	C1130	C1131	C1132	C1133	C1134	C1135	C1136	C1137	C1138	C1139	C1140	C1141	C1142	C1143	C1144	C1145	C1146	C1147	C1148	C1149	C1150	C1151	C1152	C1153	C1154	C1155	C1156	C1157	C1158	C1159	C1160	C1161	C1162	C1163	C1164	C1165	C1166	C1167	C1168	C1169	C1170	C1171	C1172	C1173	C1174																																																																																																																																																																																																																																																																																																																																																																																										
G1051	G1052	G1053	G1054	G1055	G1056	G1057	G1058	G1059	G1060	G1061	G1062	G1063	G1064	G1065	G1066	G1067	G1068	G1069	G1070	G1071	G1072	G1073	G1074	G1075	G1076	G1077	G1078	G1079	G1080	G1081	G1082	G1083	G1084	G1085	G1086	G1087	G1088	G1089	G1090	G1091	G1092	G1093	G1094	G1095	G1096	G1097	G1098	G1099	G1100	G1101	G1102	G1103	G1104	G1105	G1106	G1107	G1108	G1109	G1110	G1111	G1112	G1113																																																																																																																																																																																																																																																																																																																																																																																								
C995	C996	C997	C998	C999	C1000	C1001	C1002	C1003	C1004	C1005	C1006	C1007	C1008	C1009	C1010	C1011	C1012	C1013	C1014	C1015	C1016	C1017	C1018	C1019	C1020	C1021	C1022	C1023	C1024	C1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033	C1034	C1035	C1036	C1037	C1038	C1039	C1040	C1041	C1042	C1043	C1044	C1045	C1046	C1047	C1048	C1049	C1050																																																																																																																																																																																																																																																																																																																																																																																															
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																																																																																																																																																																																																																																																																																																																																																																																								
C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931																																																																																																																																																																																																																																																																																																																																																																											
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	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																																																																																																																																																																																																																																																																																																																																																																			
U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732	U733	U734	U735	U736	U737	U738	U739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769																																																																																																																																																																																																																																																																																																																																																																														
C612	C613	C614	C615	C616	C617	C618	C619	C620	C621	C622	C623	C624	C625	C626	C627	C628	C629	C630	C631	C632	C633	C634	C635	C636	C637	C638	C639	C640	C641	C642	C643	C644	C645	C646	C647	C648	C649	C650	C651	C652	C653	C654	C655	C656	C657	C658	C659	C660	C661	C662	C663	C664	C665	C666	C667	C668	C669	C670	C671	C672	C673	C674	C675	C676	C677	C678	C679	C680	C681	C682	C683	C684	C685	C686	C687	C688	C689	C690	C691	C692	C693	C694	C695	C696	C697	C698	C699	C700	C701	C702	C703	C704	C705	C706	C707	C708	C709	C710	C711	C712	C713	C714	C715	C716	C717	C718	C719	C720	C721	C722	C723	C724	C725	C726	C727	C728	C729	C730	C731	C732	C733	C734	C735	C736	C737	C738	C739	C740	C741	C742	C743	C744	C745	C746	C747	C748	C749	C750	C751	C752	C753	C754	C755	C756	C757	C758	C759	C760	C761	C762	C763	C764	C765	C766	C767	C768	C769	C770	C771	C772	C773	C774	C775	C776	C777	C778	C779	C780	C781	C782	C783	C784	C785	C786	C787	C788	C789	C790	C791	C792	C793	C794	C795	C796	C797	C798	C799	C800	C801	C802	C803	C804	C805	C806	C807	C808	C809	C810	C811	C812	C813	C814	C815	C816	C817	C818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	C1000	C1001	C1002	C1003	C1004	C1005	C1006	C1007	C1008	C1009	C1010	C1011	C1012	C1013	C1014	C1015	C1016	C1017	C1018	C1019	C1020	C1021	C1022	C1023	C1024	C1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033	C1034	C1035	C1036	C1037	C1038	C1039	C1040	C1041	C1042	C1043	C1044	C1045	C1046	C1047	C1048	C1049	C1050
G481	G482	G483	G484	G485	G486	G487	G488	G489	G490	G491	G492	G493	G494	G495	G496	G497	G498	G499	G500	G501	G502	G503	G504	G505	G506	G507	G508	G509	G510	G511	G512	G513	G514	G515	G516	G517	G518	G519	G520	G521	G522	G523	G524	G525	G526	G527	G528	G529	G530	G531	G532	G533	G534	G535	G536	G537	G538	G539	G540	G541	G542																																																																																																																																																																																																																																																																																																																																																																																									
U404	U405	U406	U407	U408	U409	U410	U411	U412	U413	U414	U415	U416	U417	U418	U419	U420	U421	U422	U423	U424	U425	U426	U427	U428	U429	U430	U431	U432	U433	U434	U435	U436	U437	U438	U439	U440	U441	U442	U443	U444	U445	U446	U447	U448	U449	U450	U451	U452	U453	U454	U455	U456	U457	U458	U459	U460	U461	U462	U463	U464	U465	U466	U467	U468	U469	U470	U471	U472	U473	U474	U475	U476	U477	U478	U479	U480																																																																																																																																																																																																																																																																																																																																																																										
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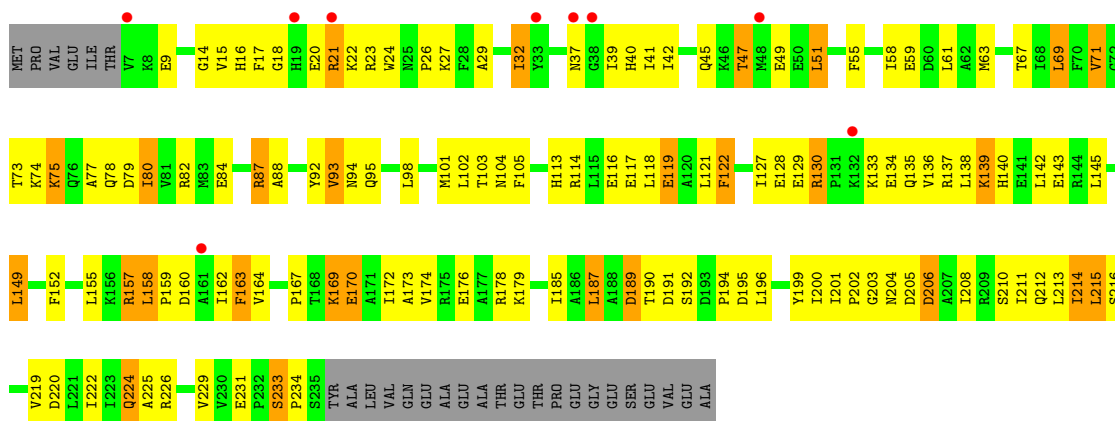
• Molecule 2: 30S Ribosomal Protein S2

Chain AB:



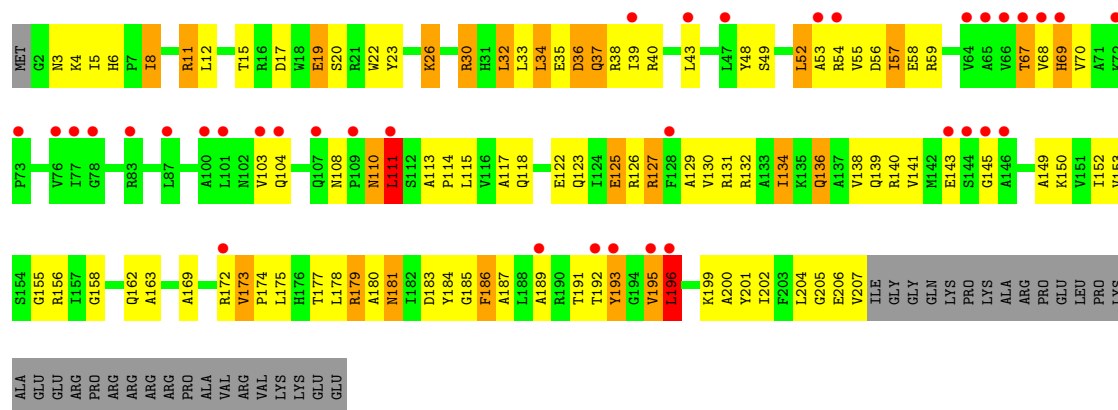
• Molecule 2: 30S Ribosomal Protein S2

Chain CB:



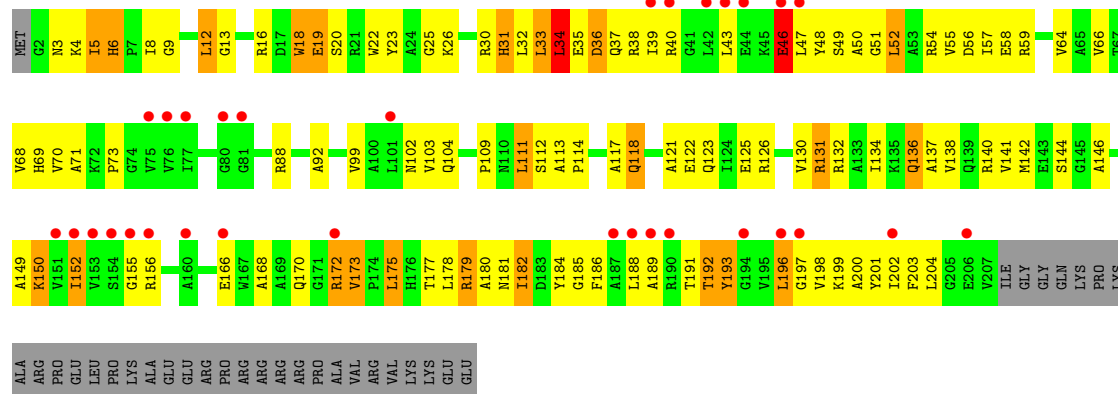
• Molecule 3: 30S Ribosomal Protein S3

Chain AC:



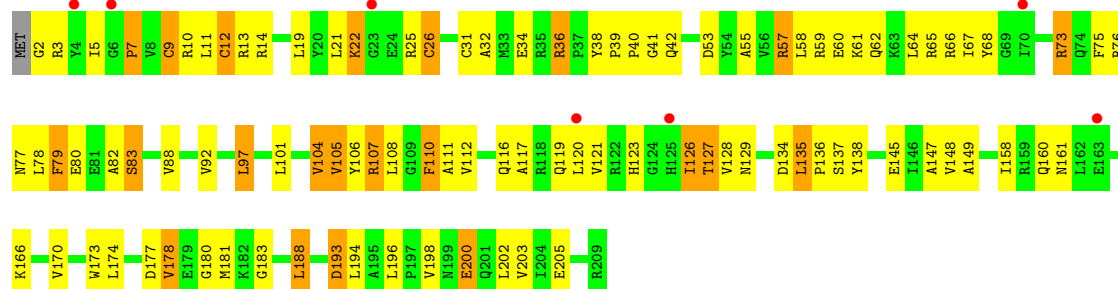
- Molecule 3: 30S Ribosomal Protein S3

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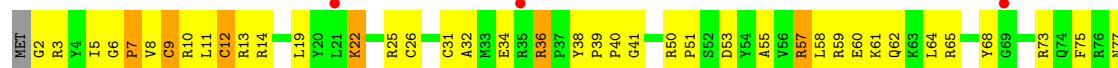
- Molecule 4: 30S Ribosomal Protein S4

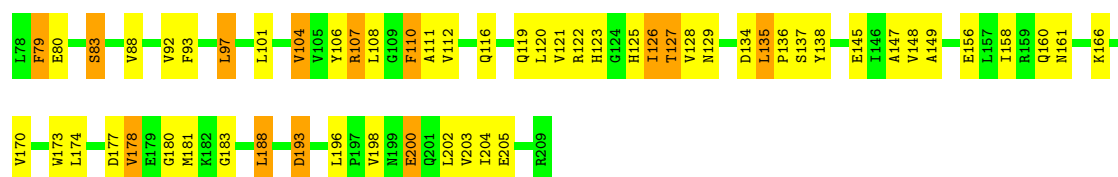
Chain AD:



- Molecule 4: 30S Ribosomal Protein S4

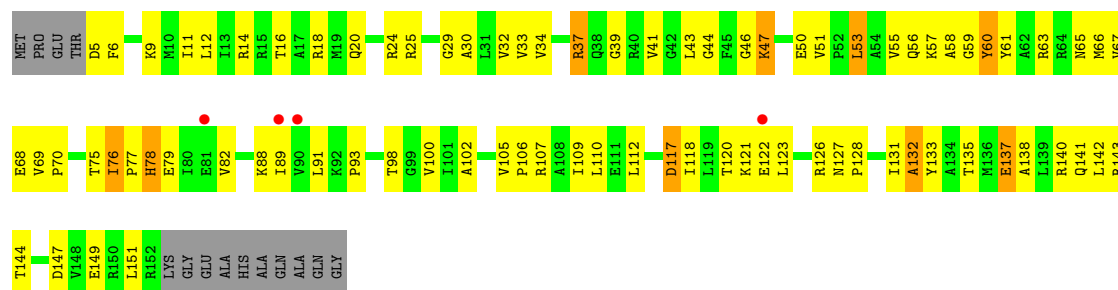
Chain CD:





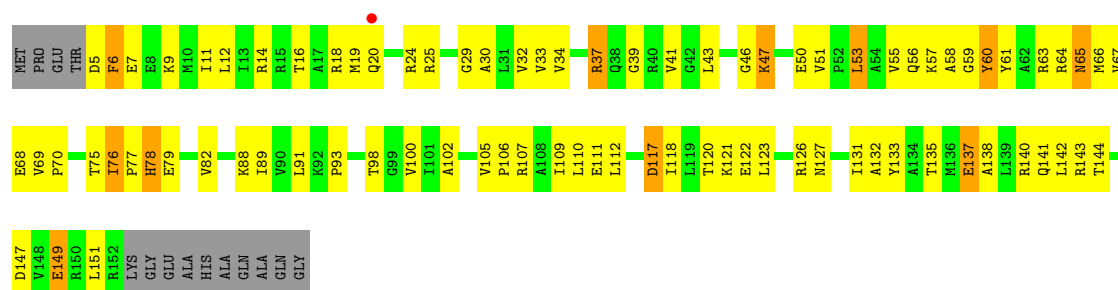
• Molecule 5: 30S Ribosomal Protein S5

Chain AE:



• Molecule 5: 30S Ribosomal Protein S5

Chain CE:



• Molecule 6: 30S Ribosomal Protein S6

Chain AF:



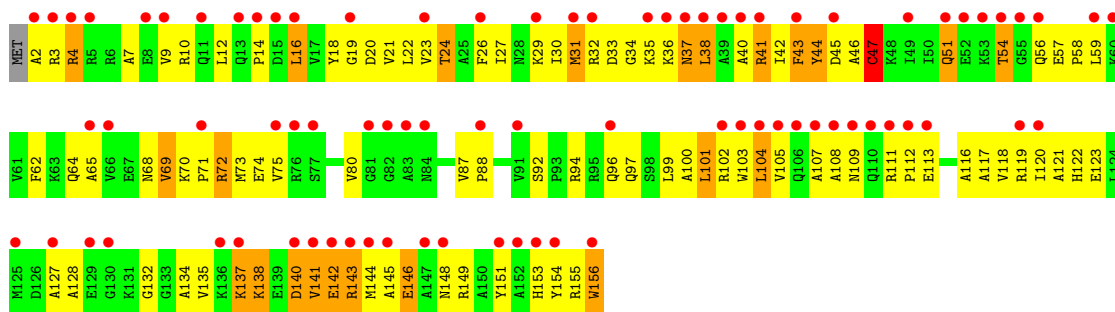
• Molecule 6: 30S Ribosomal Protein S6

Chain CF:



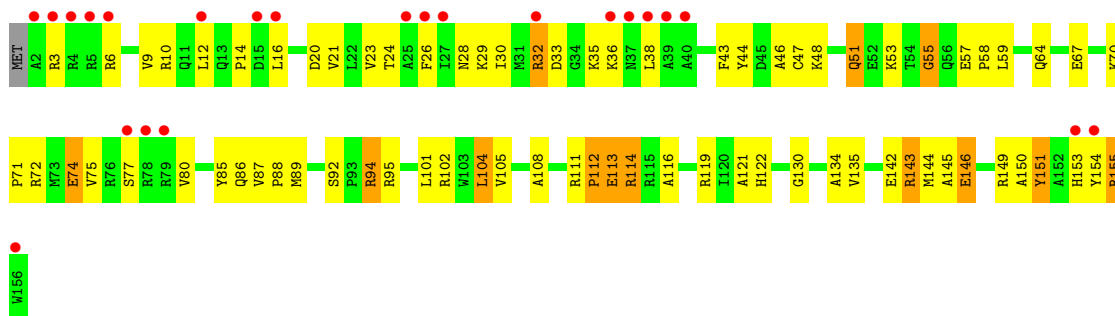
• Molecule 7: 30S Ribosomal Protein S7

Chain AG:



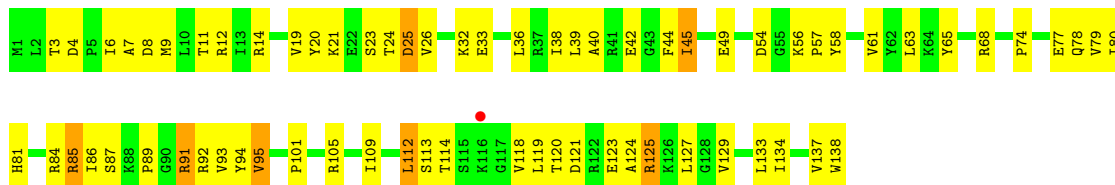
• Molecule 7: 30S Ribosomal Protein S7

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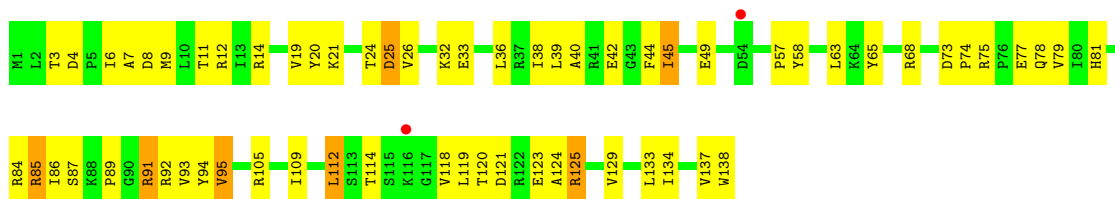
• Molecule 8: 30S Ribosomal Protein S8

Chain AH:



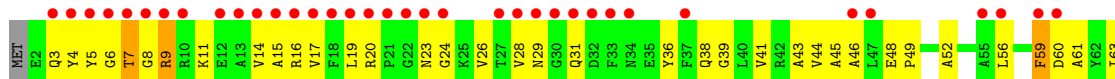
• Molecule 8: 30S Ribosomal Protein S8

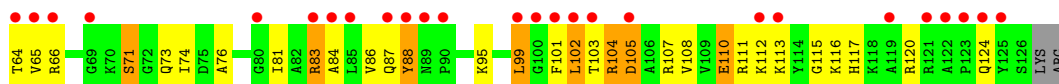
Chain CH:



• Molecule 9: 30S Ribosomal Protein S9

Chain AI:





• Molecule 9: 30S Ribosomal Protein S9

Chain CI:



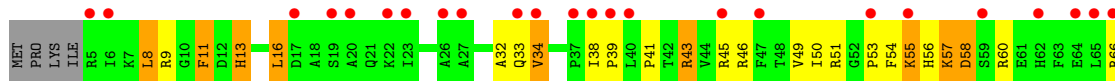
• Molecule 10: 30S Ribosomal Protein S10

Chain AJ:



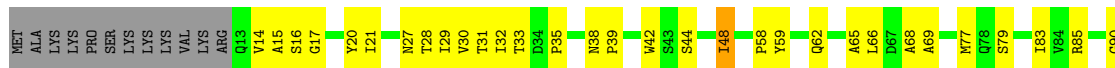
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Chain CJ:



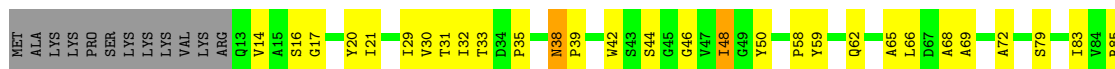
• Molecule 11: 30S Ribosomal Protein S11

Chain AK:



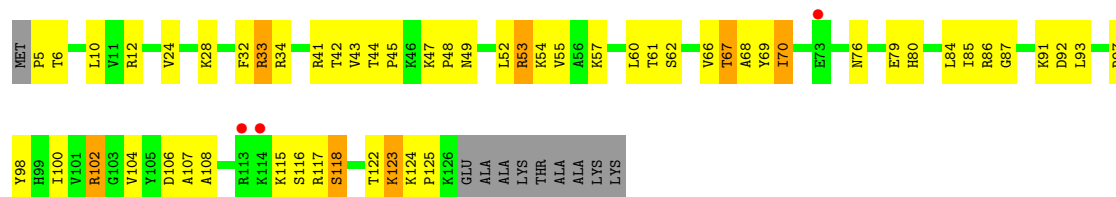
• Molecule 11: 30S Ribosomal Protein S11

Chain CK:



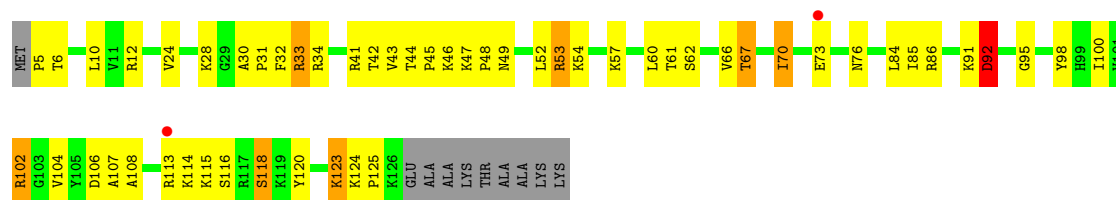
- Molecule 12: 30S Ribosomal Protein S12

Chain AL:



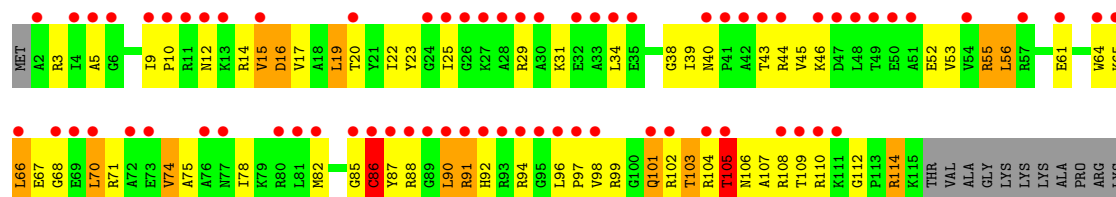
- Molecule 12: 30S Ribosomal Protein S12

Chain CL:



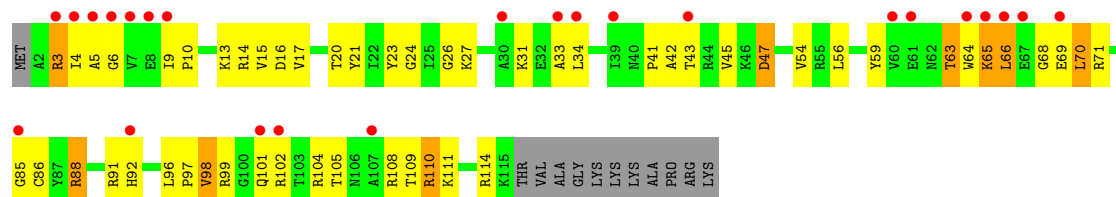
- Molecule 13: 30S Ribosomal Protein S13

Chain AM:



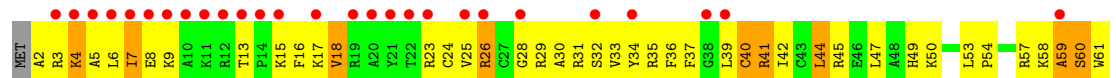
- Molecule 13: 30S Ribosomal Protein S13

Chain CM:



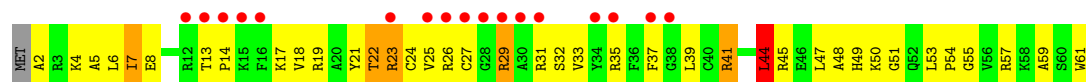
- Molecule 14: 30S Ribosomal Protein S14

Chain AN:



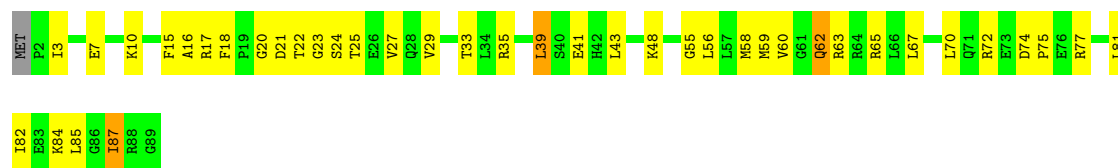
- Molecule 14: 30S Ribosomal Protein S14

Chain CN:



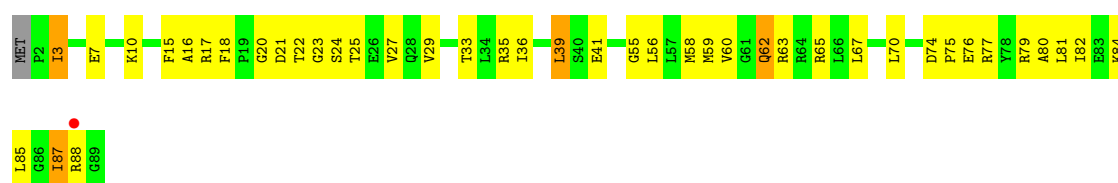
• Molecule 15: 30S Ribosomal Protein S15

Chain AO:



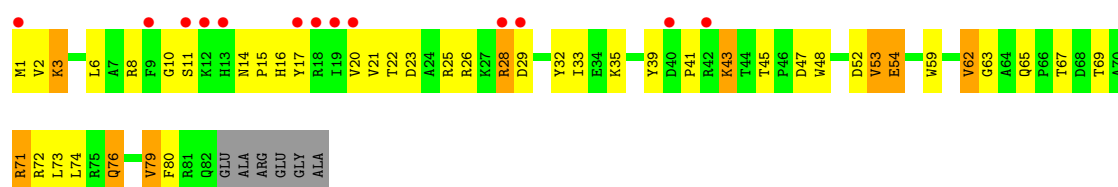
• Molecule 15: 30S Ribosomal Protein S15

Chain CO:



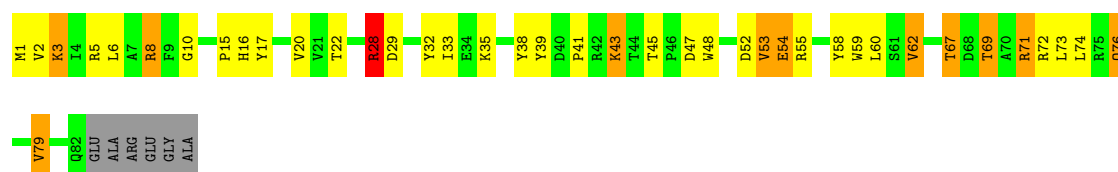
• Molecule 16: 30S Ribosomal Protein S16

Chain AP:



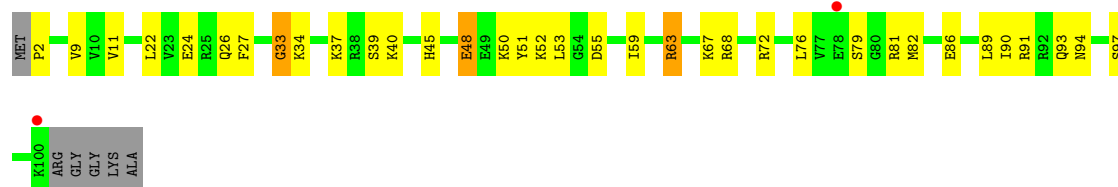
• Molecule 16: 30S Ribosomal Protein S16

Chain CP:



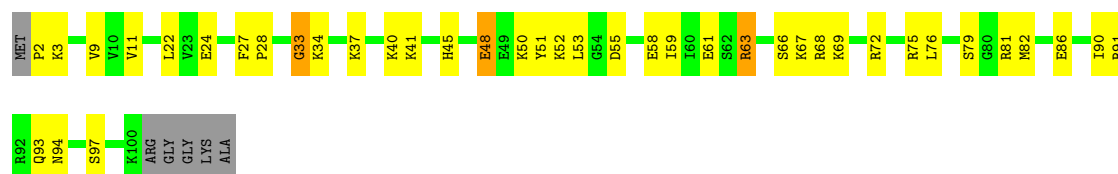
• Molecule 17: 30S Ribosomal Protein S17

Chain AQ:



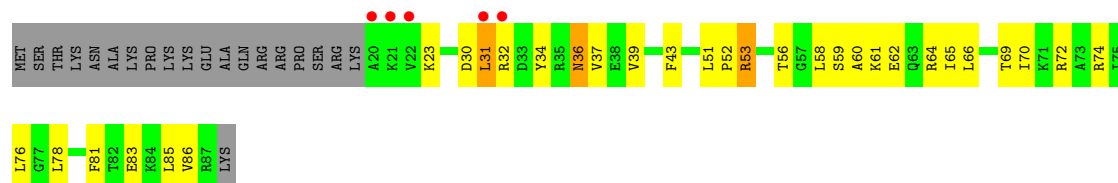
• Molecule 17: 30S Ribosomal Protein S17

Chain CQ:



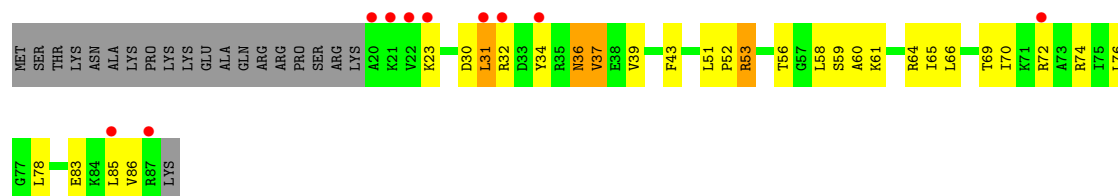
• Molecule 18: 30S Ribosomal Protein S18

Chain AR:



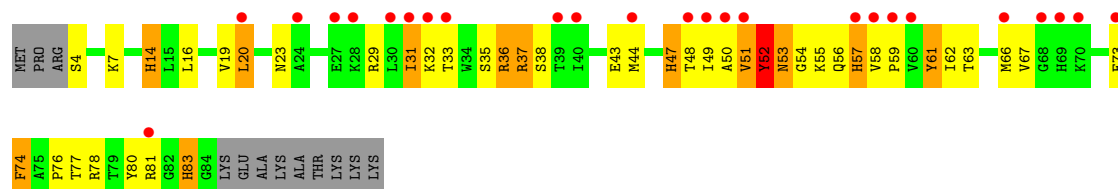
• Molecule 18: 30S Ribosomal Protein S18

Chain CR:



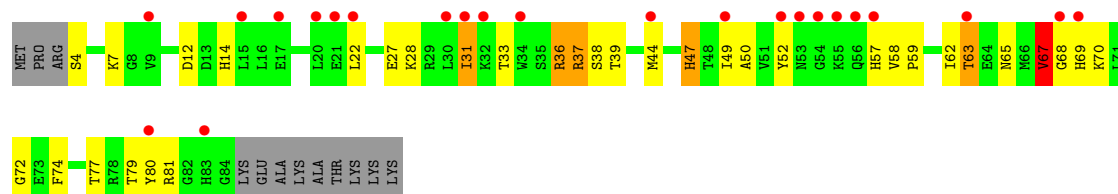
• Molecule 19: 30S Ribosomal Protein S19

Chain AS:



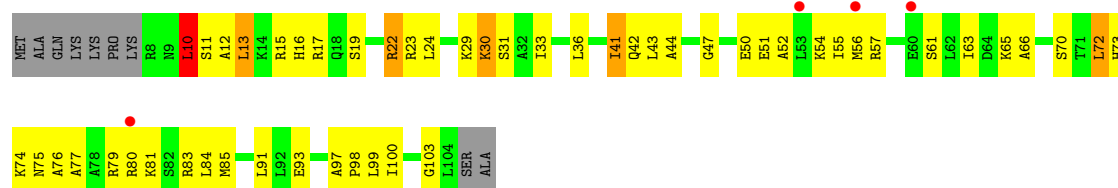
• Molecule 19: 30S Ribosomal Protein S19

Chain CS:



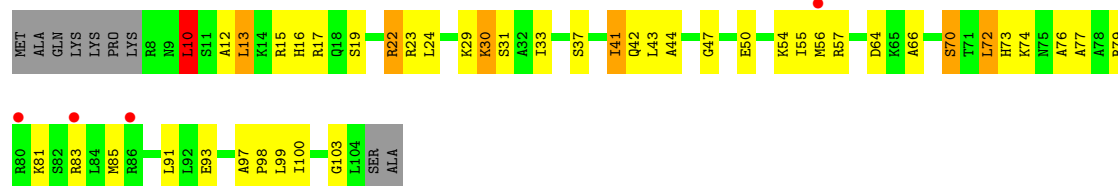
• Molecule 20: 30S Ribosomal Protein S20

Chain AT:



• Molecule 20: 30S Ribosomal Protein S20

Chain CT:



• Molecule 21: 30S Ribosomal Protein THX

Chain AU:



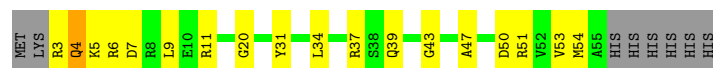
• Molecule 21: 30S Ribosomal Protein THX

Chain CU:



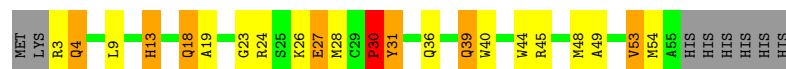
• Molecule 22: Ribosome modulation factor

Chain AV:



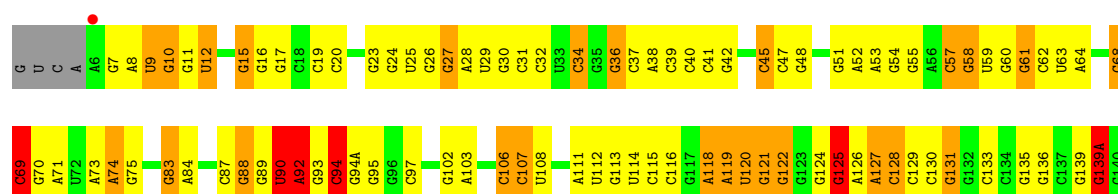
• Molecule 22: Ribosome modulation factor

Chain CV:

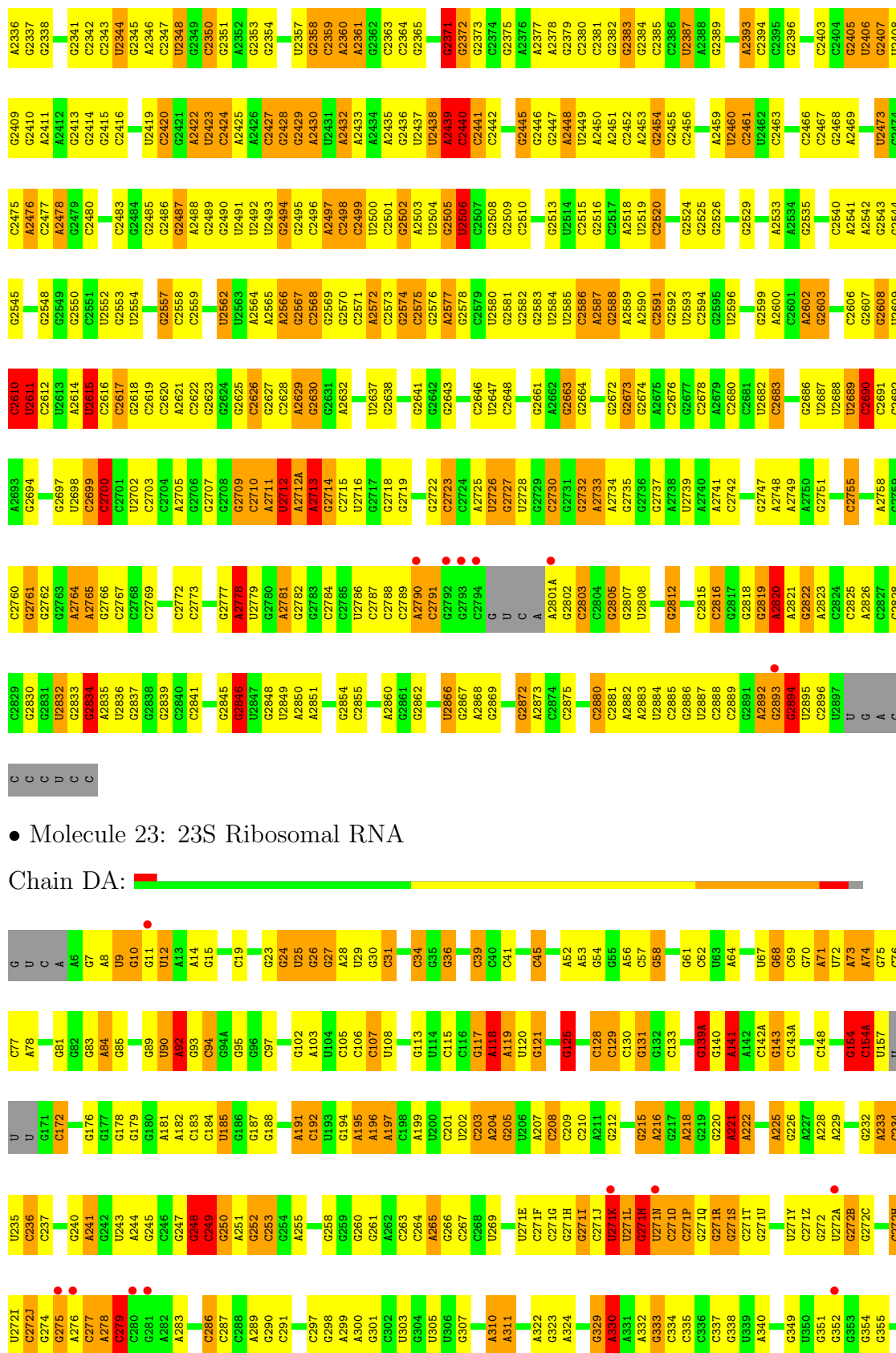


• Molecule 23: 23S Ribosomal RNA

Chain BA:

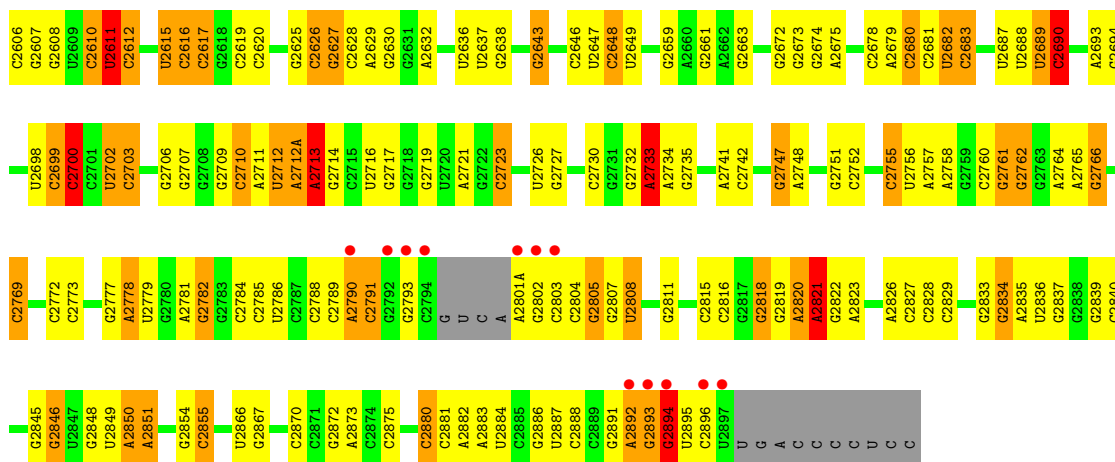






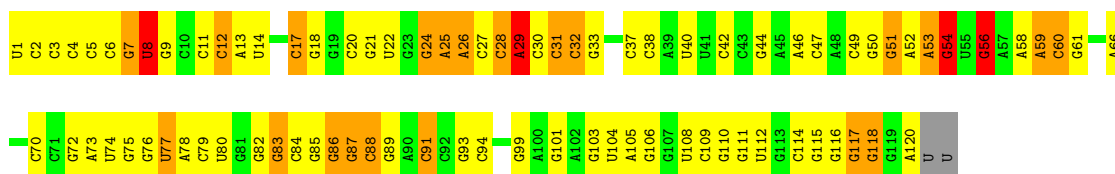
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G2548	A2476	G2409	G2339	C2275	G2194	G2131	U2068	A2006	A1928	G1828	G1763		C1588	
G2549	G2477	A2410	G2340		G2195	U2132	U2069	C2007	G1929	G1829	G1764	A1668	U1518	U1518
G2550	G2478	A2411	G2341	G2280	C2196	A2133	G2069	C2008	G1930	C1830	U1765	A1669	C1592	G1519
G2551	G2479	A2412	G2342	G2281	C2197	A2134	G2070	C2009	G1931	C1831	U1766	G1670	C1593	G1520
G2552	G2480	G2413	G2343	G2282	U2197	A2135	A2071	G2010	U1931	G1832	C1767	U1671	U1593	U1593
G2553	G2481	G2414	U2344	G2283	A2198	C2136	G2072	G2011	C1934	U1833	U1768		G1594	G1524
U2554	G2482	G2415	G2345	G2284	A2199	G2139	C2073	U2012	G1935	U1834	G1769	G1674	G1525	G1525
U2555	G2483	C2416	A2346	C2285	G2200	G2140	U2074	A2013	A1936	G1835		C1675	G1526	G1527
G2556	G2484	C2417	G2347	A2286		G2141	U2075	A2014	A1937	G1836	U1775	A1676	C1599	G1527
G2557	G2485	A2418	U2348	A2287	U2203	G2142		A2015	A1938	G1837	U1776	A1677	G1600	
G2558	G2486	U2419	G2349	A2288	G2206	G2143	U2079	U2016	U1939	G1838	G1777		G1601	G1529
G2559	G2487	C2420	G2350	G2289	G2207	U2144	G2080	U2017	U1940	G1839	U1778	G1678	U1602	C1530
G2560	A2488	G2421	G2351	G2290	G2207	C2145		G2018		U1840	U1779	G1681	A1603	C1531
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U2563	G2491	C2424	G2354	G2292	G2219	G2148	G2087	C2021	C1947	U1843	U1782	G1687	G1606	U1534
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A2565	G2494	A2426	C2356	G2295	G2221	U2150	U2089	G2023	U1955	G1846	U1784	U1689	A1608	C1536
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C2501	G2501	A2434	C2363	G2303		G2157	U2096	A2031	U1969	U1862	C1791	G1698	A1616	A1545
G2502	G2502	A2435	G2364	G2304	G2235	A2158	U2097	G2032	U1969	C1866	U1792	G1699	C1617	C1546
U2503	U2503	A2436	G2365	A2305	G2236	G2159	U2098	A2033	G1964	A1876	C1793	A1700	A1618	C1547
G2504	G2504	U2437	G2366	G2306	G2237	G2160	U2099	U2034	C1965	A1877	U1794	A1701		C1548
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		A2448	C2317	G2317	U2248	A2171	G2110	C2045	U1981	G1899	U1805	G1722	C1638	C1564
C2517	C2517	U2449	G2318	G2318	U2249	G2172	C2111	G2046	C1982	A1900	C1806	U1739	U1639	C1565
A2518	A2518	A2450	G2319	G2319	G2250	U2173	G2112	U2047	C1983	G1906	G1807	G1740	C1640	A1566
U2519	U2519	A2451	G2320	G2320	G2251	C2174	U2113	G2048	G1984	G1907			A1641	A1567
G2520	G2520	C2452	G2321	G2321	G2252	C2175	A2114	G2049	U1985	C1908	A1810	C1745A	G1642	G1568
C2521	C2521	U2387	A2322	A2322	G2253	G2176	G2115		A1986	G1909	A1812	G1746	G1648	A1571
U2522	U2522	A2388	G2323	G2323	G2254	C2177	G2116	G2052	G1987	U1911	G1813	G1747	C1648	
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G2525	G2525	G2391	G2326	G2326	G2257	U2180	A2119	C2055	G1991	A1914	G1816	C1754	G1653	C1577
		U2460	G2327	G2327	G2258	G2181	G2120	G2056	G1992	U1915	U1818	U1755	A1654	U1578
G2529	G2529	C2461	A2328	A2328	U2262	G2182	G2121	A2057	U1993					
A2602	A2602	U2462	G2329	G2329	C2263	G2183	U2122	A2058	G1997					
G2603	G2603	C2463	G2330	G2330	A2267	C2185	G2123	A2059						



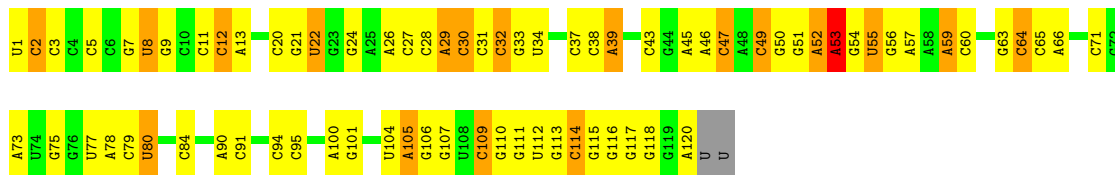
• Molecule 24: 5S Ribosomal RNA

Chain BB:



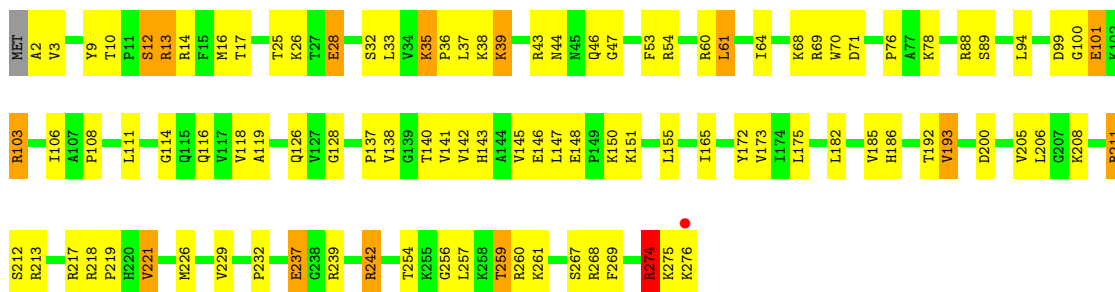
• Molecule 24: 5S Ribosomal RNA

Chain DB:



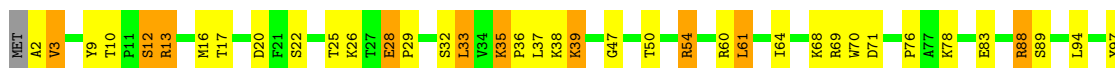
• Molecule 25: 50S Ribosomal Protein L2

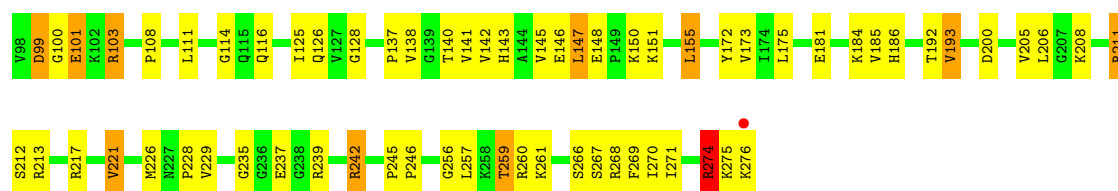
Chain BD:



• Molecule 25: 50S Ribosomal Protein L2

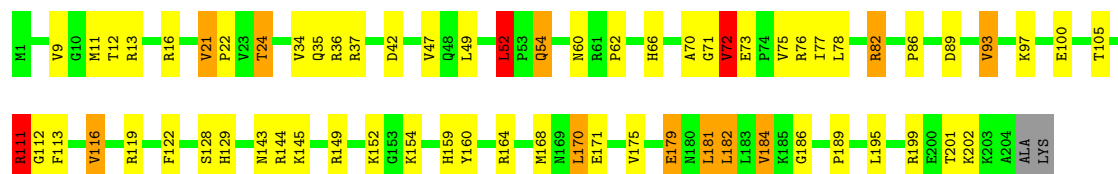
Chain DD:





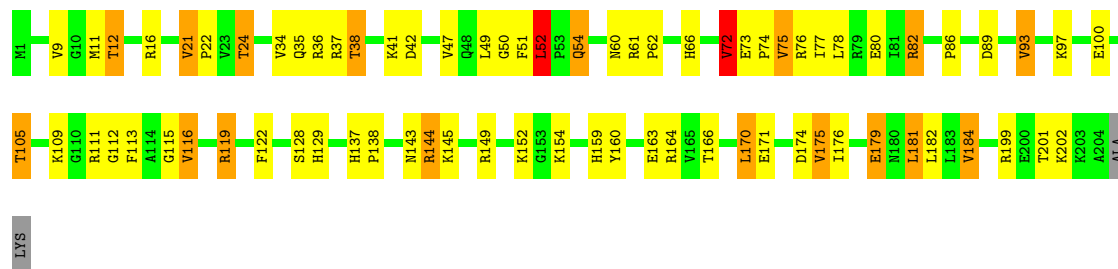
• Molecule 26: 50S Ribosomal Protein L3

Chain BE:



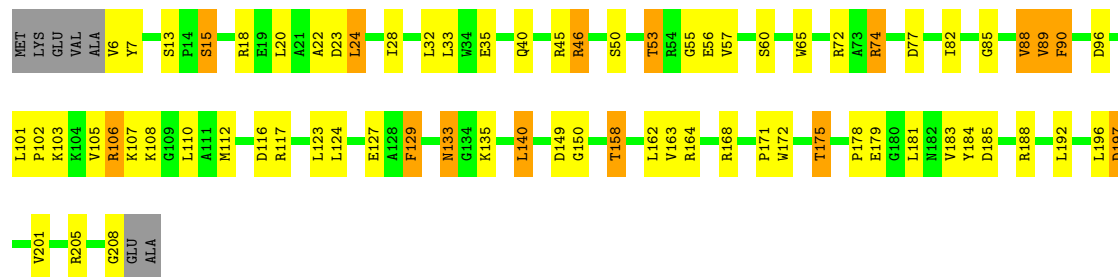
• Molecule 26: 50S Ribosomal Protein L3

Chain DE:



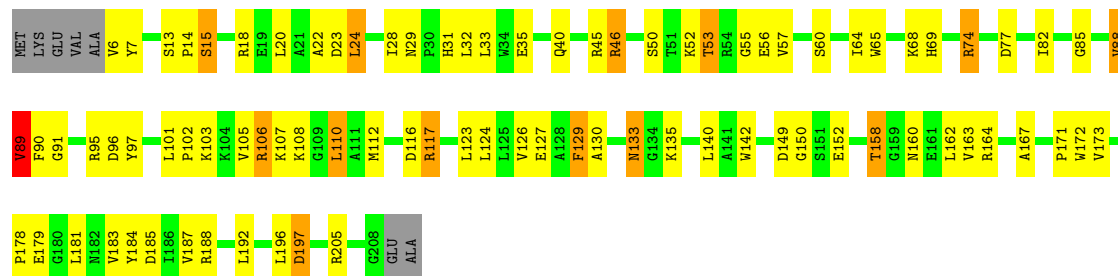
• Molecule 27: 50S Ribosomal Protein L4

Chain BF:

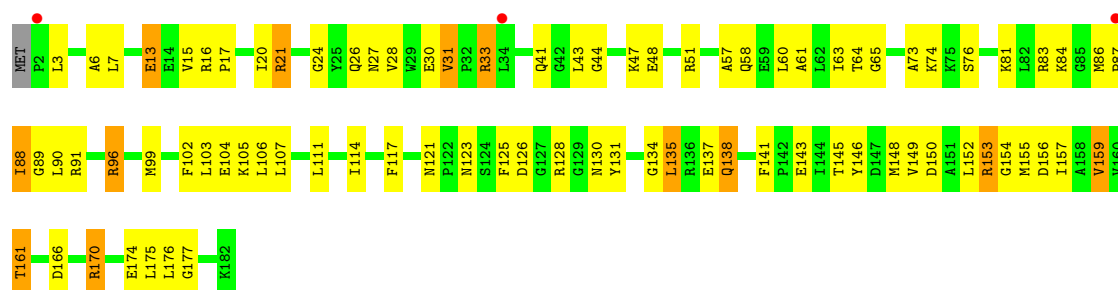


• Molecule 27: 50S Ribosomal Protein L4

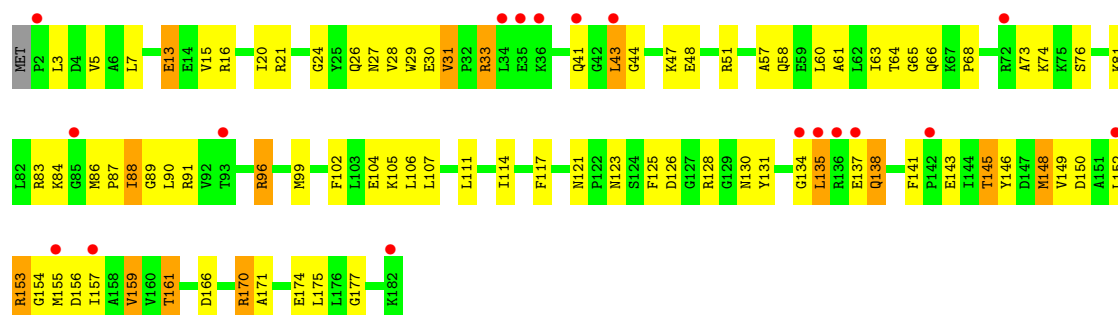
Chain DF:



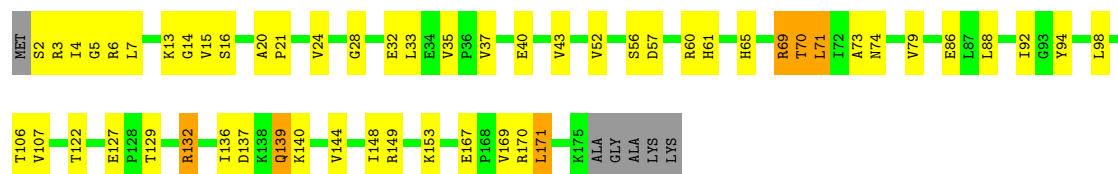
- Molecule 28: 50S Ribosomal Protein L5

Chain BG: 

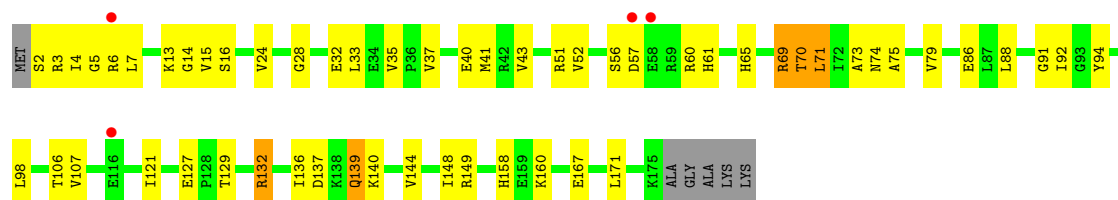
- Molecule 28: 50S Ribosomal Protein L5

Chain DG: 

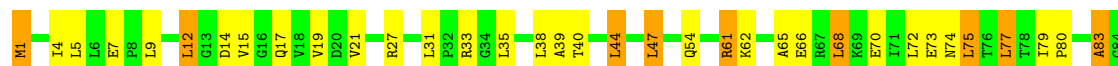
- Molecule 29: 50S Ribosomal Protein L6

Chain BH: 

- Molecule 29: 50S Ribosomal Protein L6

Chain DH: 

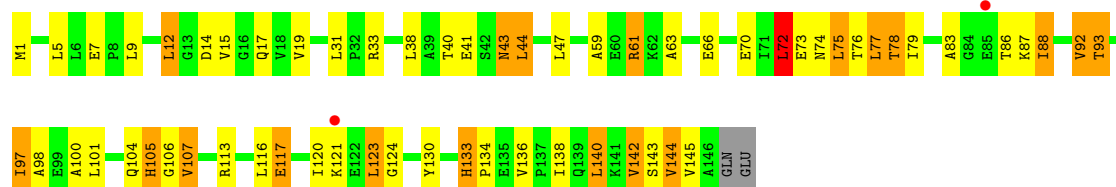
- Molecule 30: 50S Ribosomal Protein L9

Chain BI: 



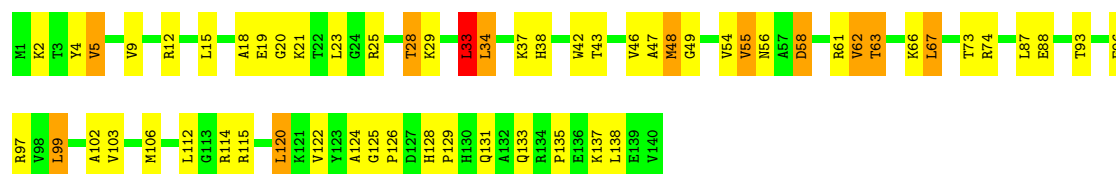
• Molecule 30: 50S Ribosomal Protein L9

Chain DI:



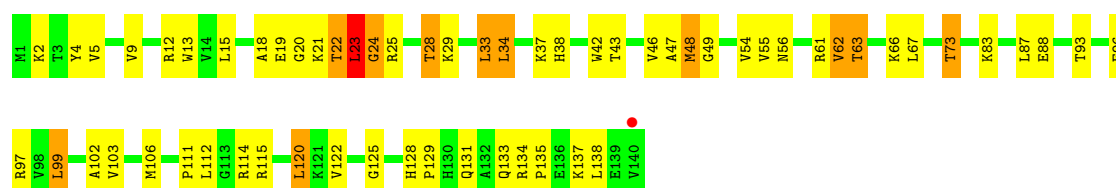
• Molecule 31: 50S Ribosomal Protein L13

Chain BN:



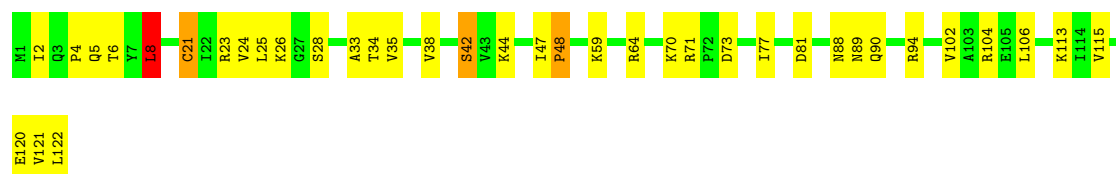
• Molecule 31: 50S Ribosomal Protein L13

Chain DN:



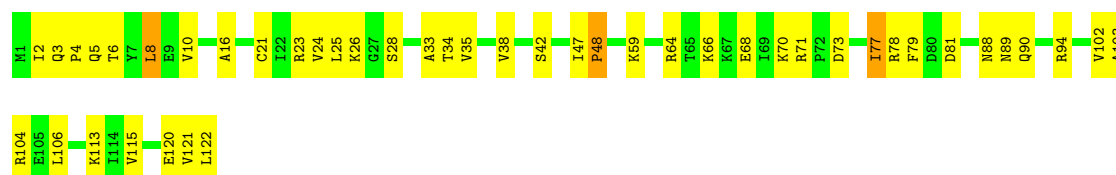
• Molecule 32: 50S Ribosomal Protein L14

Chain BO:



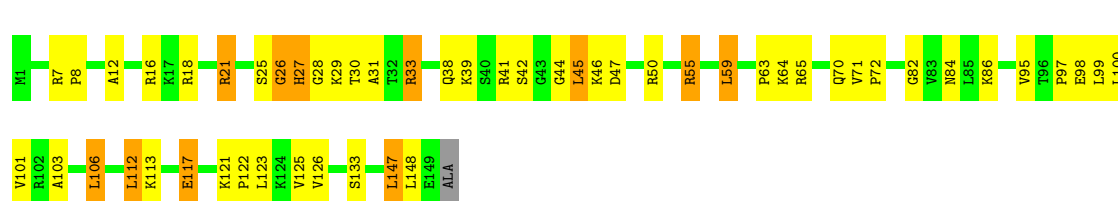
• Molecule 32: 50S Ribosomal Protein L14

Chain DO:



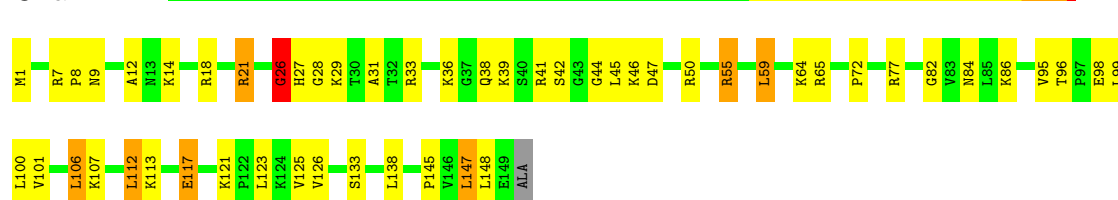
• Molecule 33: 50S Ribosomal Protein L15

Chain BP:



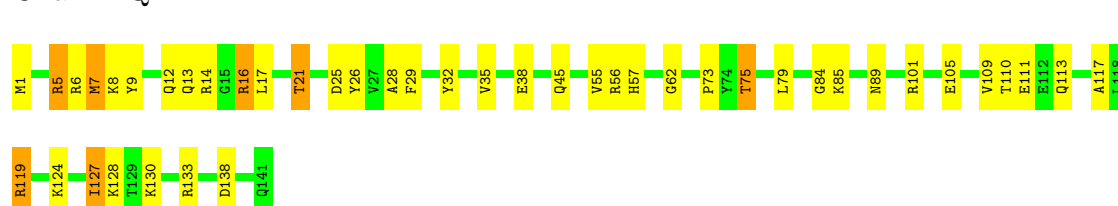
- Molecule 33: 50S Ribosomal Protein L15

Chain DP:



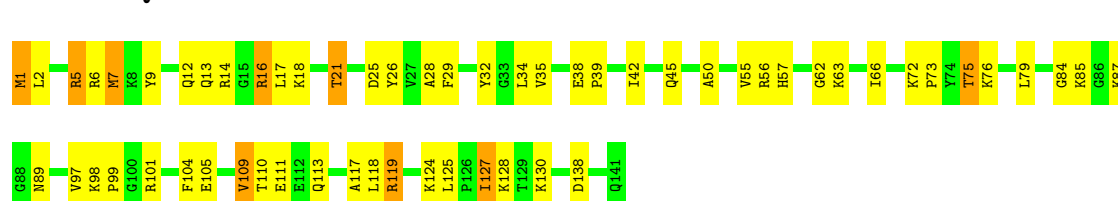
- Molecule 34: 50S Ribosomal Protein L16

Chain BQ:



- Molecule 34: 50S Ribosomal Protein L16

Chain DQ:



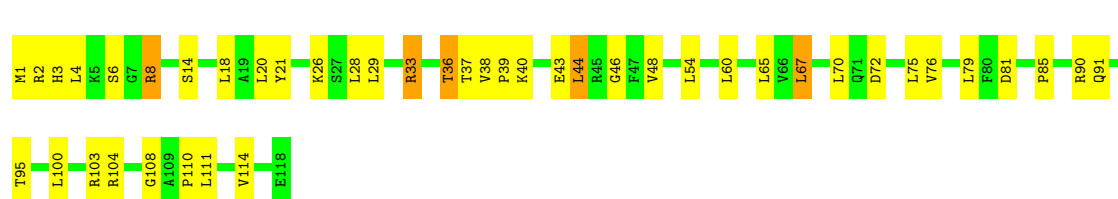
- Molecule 35: 50S Ribosomal Protein L17

Chain BR:



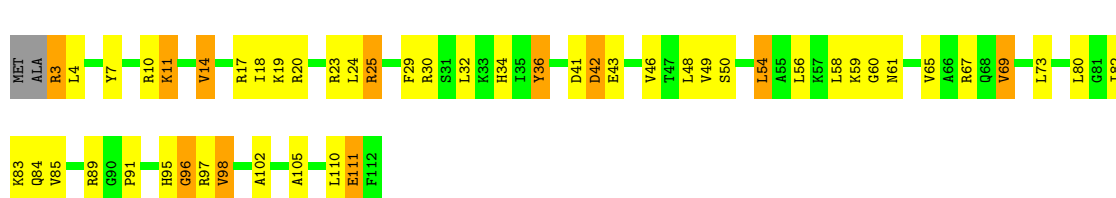
- Molecule 35: 50S Ribosomal Protein L17

Chain DR:



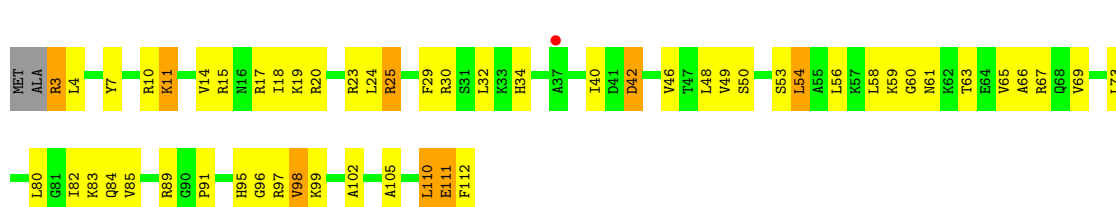
- Molecule 36: 50S Ribosomal Protein L18

Chain BS:



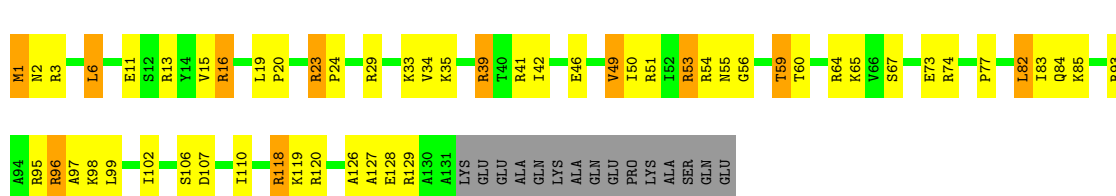
- Molecule 36: 50S Ribosomal Protein L18

Chain DS:



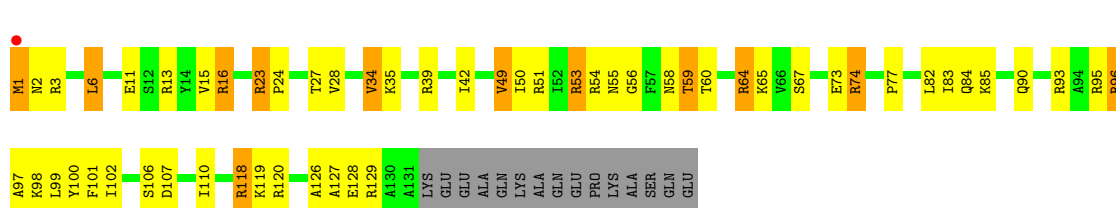
- Molecule 37: 50S Ribosomal Protein L19

Chain BT:



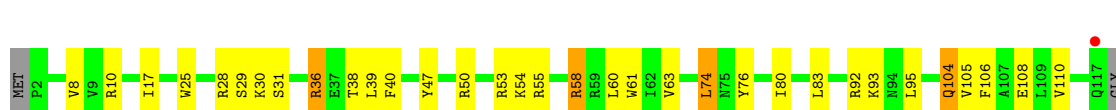
- Molecule 37: 50S Ribosomal Protein L19

Chain DT:



- Molecule 38: 50S Ribosomal Protein L20

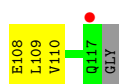
Chain BU:



- Molecule 38: 50S Ribosomal Protein L20

Chain DU:





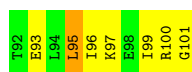
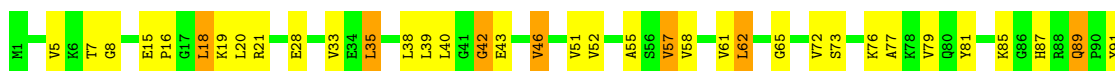
• Molecule 39: 50S Ribosomal Protein L21

Chain BV:



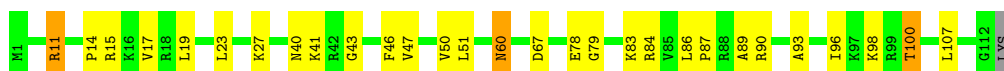
• Molecule 39: 50S Ribosomal Protein L21

Chain DV:



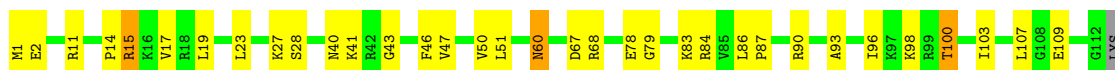
• Molecule 40: 50S Ribosomal Protein L22

Chain BW:



• Molecule 40: 50S Ribosomal Protein L22

Chain DW:



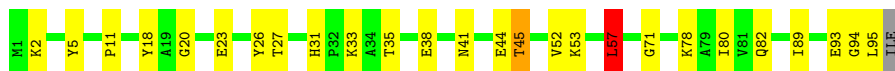
• Molecule 41: 50S Ribosomal Protein L23

Chain BX:



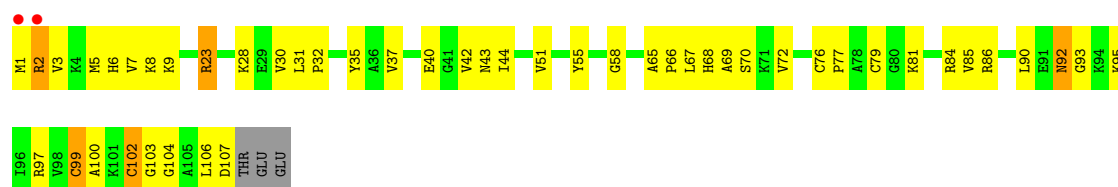
• Molecule 41: 50S Ribosomal Protein L23

Chain DX:



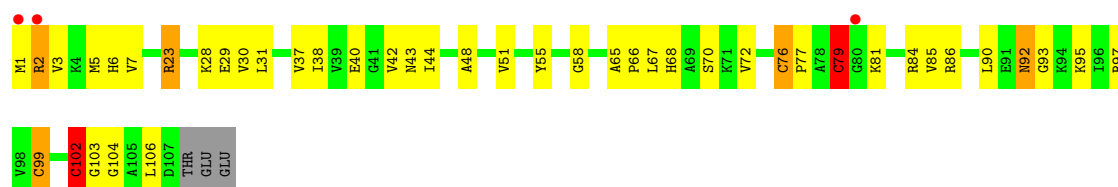
• Molecule 42: 50S Ribosomal Protein L24

Chain BY:



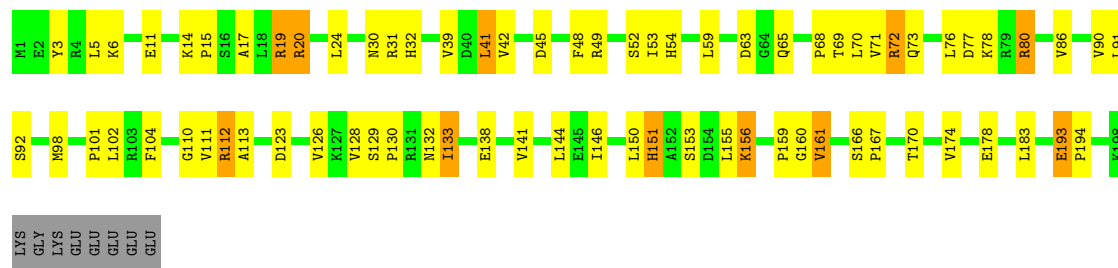
• Molecule 42: 50S Ribosomal Protein L24

Chain DY:



• Molecule 43: 50S Ribosomal Protein L25

Chain BZ:



• Molecule 43: 50S Ribosomal Protein L25

Chain DZ:



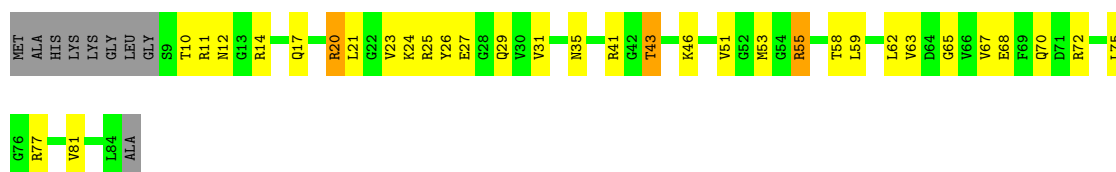
• Molecule 44: 50S Ribosomal Protein L27

Chain B0:



• Molecule 44: 50S Ribosomal Protein L27

Chain D0:



- Molecule 45: 50S Ribosomal Protein L28

Chain B1:



- Molecule 45: 50S Ribosomal Protein L28

Chain D1:



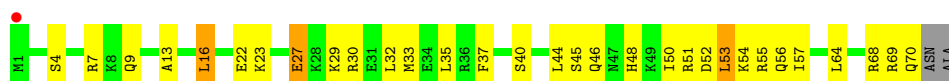
- Molecule 46: 50S Ribosomal Protein L29

Chain B2:



- Molecule 46: 50S Ribosomal Protein L29

Chain D2:



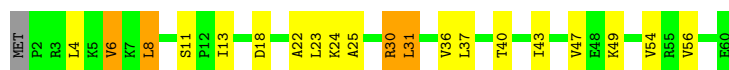
- Molecule 47: 50S Ribosomal Protein L30

Chain B3:



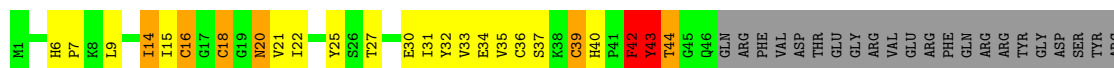
- Molecule 47: 50S Ribosomal Protein L30

Chain D3:



- Molecule 48: 50S Ribosomal Protein L31

Chain B4:



LYS
GLY
ARG

- Molecule 48: 50S Ribosomal Protein L31

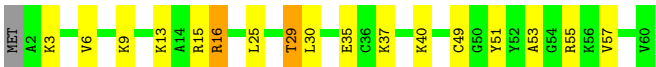
Chain D4: 



LYS
GLY
ARG

- Molecule 49: 50S Ribosomal Protein L32

Chain B5: 



- Molecule 49: 50S Ribosomal Protein L32

Chain D5: 



- Molecule 50: 50S Ribosomal Protein L33

Chain B6: 



- Molecule 50: 50S Ribosomal Protein L33

Chain D6: 



- Molecule 51: 50S Ribosomal Protein L34

Chain B7: 



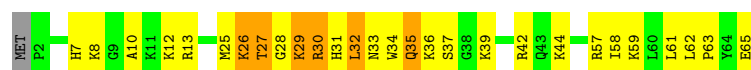
- Molecule 51: 50S Ribosomal Protein L34

Chain D7: 



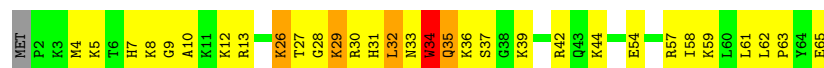
- Molecule 52: 50S Ribosomal Protein L35

Chain B8:



- Molecule 52: 50S Ribosomal Protein L35

Chain D8:



- Molecule 53: 50S Ribosomal Protein L36

Chain B9:



- Molecule 53: 50S Ribosomal Protein L36

Chain D9:



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) 98.0 (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 (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.218 , 0.254 0.218 , 0.253	Depositor DCC
R_{free} test set	57194 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 42.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 1142037 reflections	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	AU	199	0	208	26	0
21	CU	199	0	208	9	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	BY	785	0	828	31	0
42	DY	785	0	828	27	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	BV	1	0	0	0	0
54	BW	1	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BH	2	0	0	0	0
56	BN	2	0	0	0	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

The worst 5 of 7011 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(Å)
30:BI:91:SER:OG	1:CA:368:U:OP1[3.654]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	227/256 (89%)	188 (83%)	37 (16%)	2 (1%)	25	73
2	CB	227/256 (89%)	192 (85%)	33 (14%)	2 (1%)	25	73
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%)	22	70
4	CD	206/209 (99%)	180 (87%)	24 (12%)	2 (1%)	22	70
5	AE	146/162 (90%)	125 (86%)	20 (14%)	1 (1%)	30	78
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%)	18	62
7	CG	153/156 (98%)	128 (84%)	23 (15%)	2 (1%)	18	62
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%)	14	56
9	CI	123/128 (96%)	109 (89%)	12 (10%)	2 (2%)	14	56
10	AJ	94/105 (90%)	78 (83%)	14 (15%)	2 (2%)	11	47
10	CJ	94/105 (90%)	74 (79%)	18 (19%)	2 (2%)	11	47
11	AK	112/129 (87%)	100 (89%)	12 (11%)	0	100	100
11	CK	112/129 (87%)	100 (89%)	12 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AL	120/132 (91%)	109 (91%)	10 (8%)	1 (1%)	27	76
12	CL	120/132 (91%)	107 (89%)	11 (9%)	2 (2%)	14	54
13	AM	112/126 (89%)	82 (73%)	27 (24%)	3 (3%)	8	38
13	CM	112/126 (89%)	84 (75%)	27 (24%)	1 (1%)	25	73
14	AN	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	3	18
14	CN	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	14	54
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%)	9	40
16	CP	80/88 (91%)	71 (89%)	7 (9%)	2 (2%)	9	40
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%)	18	62
19	CS	79/93 (85%)	60 (76%)	16 (20%)	3 (4%)	5	27
20	AT	95/106 (90%)	82 (86%)	10 (10%)	3 (3%)	6	33
20	CT	95/106 (90%)	81 (85%)	11 (12%)	3 (3%)	6	33
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%)	2	14
25	BD	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	43	87
25	DD	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	43	87
26	BE	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	22	70
26	DE	202/206 (98%)	189 (94%)	11 (5%)	2 (1%)	22	70
27	BF	201/210 (96%)	187 (93%)	13 (6%)	1 (0%)	38	84
27	DF	201/210 (96%)	188 (94%)	12 (6%)	1 (0%)	38	84
28	BG	179/182 (98%)	151 (84%)	28 (16%)	0	100	100
28	DG	179/182 (98%)	151 (84%)	27 (15%)	1 (1%)	33	81
29	BH	172/180 (96%)	156 (91%)	14 (8%)	2 (1%)	19	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	DH	172/180 (96%)	158 (92%)	12 (7%)	2 (1%)	19	64
30	BI	144/148 (97%)	114 (79%)	27 (19%)	3 (2%)	11	47
30	DI	144/148 (97%)	113 (78%)	29 (20%)	2 (1%)	16	60
31	BN	138/140 (99%)	128 (93%)	6 (4%)	4 (3%)	7	35
31	DN	138/140 (99%)	126 (91%)	7 (5%)	5 (4%)	5	29
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%)	30	78
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%)	25	73
36	DS	108/112 (96%)	97 (90%)	10 (9%)	1 (1%)	25	73
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%)	12	51
42	DY	105/110 (96%)	95 (90%)	8 (8%)	2 (2%)	12	51
43	BZ	196/206 (95%)	178 (91%)	15 (8%)	3 (2%)	15	58
43	DZ	196/206 (95%)	177 (90%)	16 (8%)	3 (2%)	15	58
44	B0	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
44	D0	74/85 (87%)	71 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	B1	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
45	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	21	67
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%)	10	45
51	D7	46/49 (94%)	45 (98%)	0	1 (2%)	10	45
52	B8	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	14	56
52	D8	62/65 (95%)	59 (95%)	1 (2%)	2 (3%)	6	33
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%)	27	76

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%)	1	5
2	CB	177/220 (80%)	135 (76%)	42 (24%)	1	5
3	AC	114/188 (61%)	74 (65%)	40 (35%)	0	1
3	CC	114/188 (61%)	78 (68%)	36 (32%)	0	2
4	AD	141/181 (78%)	113 (80%)	28 (20%)	2	10
4	CD	141/181 (78%)	114 (81%)	27 (19%)	2	12
5	AE	108/123 (88%)	84 (78%)	24 (22%)	1	7
5	CE	108/123 (88%)	84 (78%)	24 (22%)	1	7
6	AF	76/90 (84%)	68 (90%)	8 (10%)	10	37
6	CF	76/90 (84%)	69 (91%)	7 (9%)	13	46
7	AG	103/127 (81%)	68 (66%)	35 (34%)	0	1
7	CG	103/127 (81%)	77 (75%)	26 (25%)	1	4
8	AH	103/119 (87%)	83 (81%)	20 (19%)	2	11
8	CH	103/119 (87%)	84 (82%)	19 (18%)	2	13
9	AI	62/99 (63%)	49 (79%)	13 (21%)	1	8
9	CI	62/99 (63%)	48 (77%)	14 (23%)	1	6
10	AJ	53/92 (58%)	41 (77%)	12 (23%)	1	6
10	CJ	53/92 (58%)	39 (74%)	14 (26%)	1	4
11	AK	81/99 (82%)	70 (86%)	11 (14%)	5	24
11	CK	81/99 (82%)	70 (86%)	11 (14%)	5	24
12	AL	91/109 (84%)	80 (88%)	11 (12%)	7	29
12	CL	91/109 (84%)	79 (87%)	12 (13%)	6	25
13	AM	64/101 (63%)	45 (70%)	19 (30%)	0	2
13	CM	64/101 (63%)	49 (77%)	15 (23%)	1	5
14	AN	46/50 (92%)	37 (80%)	9 (20%)	2	11
14	CN	46/50 (92%)	33 (72%)	13 (28%)	0	3
15	AO	77/80 (96%)	70 (91%)	7 (9%)	14	46
15	CO	77/80 (96%)	71 (92%)	6 (8%)	18	55
16	AP	63/74 (85%)	47 (75%)	16 (25%)	1	4
16	CP	63/74 (85%)	47 (75%)	16 (25%)	1	4
17	AQ	94/97 (97%)	80 (85%)	14 (15%)	4	20
17	CQ	94/97 (97%)	80 (85%)	14 (15%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AR	49/77 (64%)	43 (88%)	6 (12%)	7	29
18	CR	49/77 (64%)	42 (86%)	7 (14%)	5	22
19	AS	43/80 (54%)	24 (56%)	19 (44%)	0	0
19	CS	43/80 (54%)	32 (74%)	11 (26%)	1	4
20	AT	65/82 (79%)	56 (86%)	9 (14%)	5	24
20	CT	65/82 (79%)	55 (85%)	10 (15%)	4	19
21	AU	18/22 (82%)	11 (61%)	7 (39%)	0	1
21	CU	18/22 (82%)	13 (72%)	5 (28%)	0	3
22	AV	16/50 (32%)	13 (81%)	3 (19%)	2	12
22	CV	21/50 (42%)	14 (67%)	7 (33%)	0	2
25	BD	215/218 (99%)	181 (84%)	34 (16%)	4	18
25	DD	215/218 (99%)	180 (84%)	35 (16%)	3	17
26	BE	163/166 (98%)	138 (85%)	25 (15%)	4	19
26	DE	163/166 (98%)	135 (83%)	28 (17%)	3	14
27	BF	159/166 (96%)	133 (84%)	26 (16%)	3	16
27	DF	159/166 (96%)	133 (84%)	26 (16%)	3	16
28	BG	128/156 (82%)	106 (83%)	22 (17%)	3	14
28	DG	128/156 (82%)	106 (83%)	22 (17%)	3	14
29	BH	141/148 (95%)	127 (90%)	14 (10%)	11	40
29	DH	141/148 (95%)	127 (90%)	14 (10%)	11	40
30	BI	99/124 (80%)	75 (76%)	24 (24%)	1	5
30	DI	98/124 (79%)	67 (68%)	31 (32%)	0	2
31	BN	117/119 (98%)	92 (79%)	25 (21%)	1	8
31	DN	117/119 (98%)	93 (80%)	24 (20%)	2	9
32	BO	98/100 (98%)	90 (92%)	8 (8%)	17	52
32	DO	98/100 (98%)	90 (92%)	8 (8%)	17	52
33	BP	114/116 (98%)	98 (86%)	16 (14%)	5	23
33	DP	114/116 (98%)	100 (88%)	14 (12%)	7	28
34	BQ	111/111 (100%)	95 (86%)	16 (14%)	5	22
34	DQ	111/111 (100%)	96 (86%)	15 (14%)	6	24
35	BR	101/101 (100%)	82 (81%)	19 (19%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	DR	101/101 (100%)	83 (82%)	18 (18%)	2	14
36	BS	84/88 (96%)	69 (82%)	15 (18%)	2	13
36	DS	84/88 (96%)	72 (86%)	12 (14%)	5	22
37	BT	110/127 (87%)	95 (86%)	15 (14%)	5	24
37	DT	110/127 (87%)	92 (84%)	18 (16%)	3	16
38	BU	93/94 (99%)	84 (90%)	9 (10%)	12	42
38	DU	93/94 (99%)	84 (90%)	9 (10%)	12	42
39	BV	79/82 (96%)	62 (78%)	17 (22%)	1	8
39	DV	80/82 (98%)	64 (80%)	16 (20%)	2	10
40	BW	89/92 (97%)	78 (88%)	11 (12%)	7	28
40	DW	89/92 (97%)	76 (85%)	13 (15%)	5	21
41	BX	75/78 (96%)	70 (93%)	5 (7%)	23	64
41	DX	75/78 (96%)	70 (93%)	5 (7%)	23	64
42	BY	80/91 (88%)	66 (82%)	14 (18%)	3	14
42	DY	80/91 (88%)	63 (79%)	17 (21%)	1	8
43	BZ	159/179 (89%)	141 (89%)	18 (11%)	9	33
43	DZ	159/179 (89%)	141 (89%)	18 (11%)	9	33
44	B0	59/67 (88%)	54 (92%)	5 (8%)	15	51
44	D0	59/67 (88%)	54 (92%)	5 (8%)	15	51
45	B1	78/83 (94%)	67 (86%)	11 (14%)	5	23
45	D1	78/83 (94%)	67 (86%)	11 (14%)	5	23
46	B2	65/67 (97%)	59 (91%)	6 (9%)	13	46
46	D2	65/67 (97%)	58 (89%)	7 (11%)	9	35
47	B3	49/52 (94%)	43 (88%)	6 (12%)	7	29
47	D3	49/52 (94%)	42 (86%)	7 (14%)	5	22
48	B4	39/63 (62%)	29 (74%)	10 (26%)	1	4
48	D4	39/63 (62%)	29 (74%)	10 (26%)	1	4
49	B5	50/52 (96%)	45 (90%)	5 (10%)	11	39
49	D5	50/52 (96%)	45 (90%)	5 (10%)	11	39
50	B6	50/52 (96%)	39 (78%)	11 (22%)	1	7
50	D6	50/52 (96%)	37 (74%)	13 (26%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	B7	41/42 (98%)	32 (78%)	9 (22%)	1	7
51	D7	41/42 (98%)	34 (83%)	7 (17%)	3	15
52	B8	52/55 (94%)	43 (83%)	9 (17%)	3	14
52	D8	52/55 (94%)	43 (83%)	9 (17%)	3	14
53	B9	32/34 (94%)	29 (91%)	3 (9%)	13	44
53	D9	32/34 (94%)	29 (91%)	3 (9%)	13	44
All	All	8753/10166 (86%)	7236 (83%)	1517 (17%)	3	14

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

Mol	Chain	Res	Type
44	B0	20	ARG
4	CD	97	LEU
41	DX	45	THR
46	B2	53	LEU
2	CB	58	ILE

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

Mol	Chain	Res	Type
9	CI	38	GLN
15	CO	37	ASN
42	DY	6	HIS
9	CI	73	GLN
10	CJ	33	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
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
23	BA	2308	G
1	CA	484	G
23	DA	2126	A
23	BA	2439	A
1	CA	7	G

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	0.78	252 (16%) 2 1	52, 116, 177, 188	0
1	CA	1501/1522 (98%)	0.36	150 (9%) 8 2	53, 112, 168, 181	0
2	AB	229/256 (89%)	0.15	6 (2%) 53 10	114, 135, 150, 160	0
2	CB	229/256 (89%)	0.30	9 (3%) 37 7	113, 135, 150, 160	0
3	AC	206/239 (86%)	0.98	36 (17%) 2 1	122, 148, 164, 172	0
3	CC	206/239 (86%)	0.84	31 (15%) 3 1	119, 140, 153, 162	0
4	AD	208/209 (99%)	0.24	7 (3%) 43 8	100, 116, 133, 143	0
4	CD	208/209 (99%)	0.10	3 (1%) 72 18	95, 111, 129, 142	0
5	AE	148/162 (91%)	0.15	4 (2%) 52 10	85, 109, 124, 129	0
5	CE	148/162 (91%)	0.21	1 (0%) 84 28	87, 108, 124, 132	0
6	AF	100/101 (99%)	-0.13	1 (1%) 79 22	88, 102, 122, 136	0
6	CF	100/101 (99%)	0.03	1 (1%) 79 22	93, 107, 123, 135	0
7	AG	155/156 (99%)	2.24	81 (52%) 0 0	134, 156, 166, 168	0
7	CG	155/156 (99%)	1.12	23 (14%) 3 1	118, 144, 151, 158	0
8	AH	138/138 (100%)	-0.01	1 (0%) 84 28	93, 111, 121, 131	0
8	CH	138/138 (100%)	0.02	2 (1%) 72 18	89, 110, 120, 133	0
9	AI	125/128 (97%)	2.36	62 (49%) 1 0	131, 157, 170, 176	0
9	CI	125/128 (97%)	1.88	46 (36%) 1 0	129, 151, 161, 173	0
10	AJ	96/105 (91%)	1.85	37 (38%) 1 0	137, 155, 171, 176	0
10	CJ	96/105 (91%)	1.77	38 (39%) 1 0	130, 149, 161, 169	0
11	AK	114/129 (88%)	-0.01	0 100 100	74, 109, 123, 127	0
11	CK	114/129 (88%)	0.15	0 100 100	79, 109, 122, 124	0
12	AL	122/132 (92%)	0.05	3 (2%) 54 11	72, 95, 111, 120	0
12	CL	122/132 (92%)	0.16	2 (1%) 68 16	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%)	2.86	71 (62%) 0 0	147, 160, 171, 177	0
13	CM	114/126 (90%)	1.48	24 (21%) 1 1	124, 145, 155, 158	0
14	AN	60/61 (98%)	2.49	27 (45%) 1 0	134, 160, 169, 174	0
14	CN	60/61 (98%)	1.26	17 (28%) 1 0	136, 146, 152, 155	0
15	AO	88/89 (98%)	-0.02	0 100 100	78, 103, 120, 131	0
15	CO	88/89 (98%)	-0.01	1 (1%) 77 21	79, 102, 122, 129	0
16	AP	82/88 (93%)	0.91	13 (15%) 3 1	98, 112, 132, 138	0
16	CP	82/88 (93%)	0.32	0 100 100	89, 105, 123, 132	0
17	AQ	99/105 (94%)	0.28	2 (2%) 62 12	86, 99, 113, 118	0
17	CQ	99/105 (94%)	-0.10	0 100 100	84, 98, 113, 117	0
18	AR	68/88 (77%)	0.39	5 (7%) 14 3	93, 104, 138, 141	0
18	CR	68/88 (77%)	0.74	10 (14%) 3 1	95, 107, 138, 143	0
19	AS	81/93 (87%)	1.69	25 (30%) 1 0	131, 164, 174, 179	0
19	CS	81/93 (87%)	1.54	23 (28%) 1 0	125, 146, 153, 155	0
20	AT	97/106 (91%)	0.26	4 (4%) 35 7	90, 106, 127, 131	0
20	CT	97/106 (91%)	0.43	4 (4%) 35 7	84, 103, 125, 132	0
21	AU	23/27 (85%)	4.65	19 (82%) 0 0	147, 161, 169, 174	0
21	CU	23/27 (85%)	1.52	6 (26%) 1 1	130, 145, 153, 154	0
22	AV	53/61 (86%)	-0.11	0 100 100	93, 105, 121, 143	0
22	CV	53/61 (86%)	-0.37	0 100 100	90, 115, 141, 151	0
23	BA	2809/2915 (96%)	-0.14	66 (2%) 57 12	31, 50, 134, 186	0
23	DA	2814/2915 (96%)	-0.29	94 (3%) 44 8	34, 56, 138, 189	0
24	BB	120/122 (98%)	-0.48	0 100 100	46, 72, 94, 119	0
24	DB	120/122 (98%)	-0.33	0 100 100	63, 90, 111, 129	0
25	BD	275/276 (99%)	-0.23	1 (0%) 90 41	34, 52, 69, 117	0
25	DD	275/276 (99%)	-0.28	1 (0%) 90 41	36, 55, 72, 119	0
26	BE	204/206 (99%)	-0.20	0 100 100	32, 55, 78, 95	0
26	DE	204/206 (99%)	-0.23	0 100 100	35, 61, 84, 101	0
27	BF	203/210 (96%)	-0.26	0 100 100	30, 60, 92, 136	0
27	DF	203/210 (96%)	-0.21	0 100 100	34, 67, 96, 136	0
28	BG	181/182 (99%)	0.15	3 (1%) 67 15	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%)	0.65	18 (9%) 8 2	92, 126, 146, 156	0
29	BH	174/180 (96%)	-0.18	0 100 100	58, 79, 97, 110	0
29	DH	174/180 (96%)	0.24	4 (2%) 57 12	70, 92, 107, 122	0
30	BI	146/148 (98%)	-0.13	0 100 100	57, 90, 108, 120	0
30	DI	146/148 (98%)	0.31	2 (1%) 72 18	60, 108, 127, 131	0
31	BN	140/140 (100%)	-0.27	0 100 100	39, 55, 83, 98	0
31	DN	140/140 (100%)	-0.36	1 (0%) 84 28	45, 63, 89, 101	0
32	BO	122/122 (100%)	-0.22	0 100 100	43, 58, 79, 85	0
32	DO	122/122 (100%)	-0.32	0 100 100	46, 62, 82, 86	0
33	BP	149/150 (99%)	-0.02	0 100 100	34, 63, 98, 109	0
33	DP	149/150 (99%)	-0.16	0 100 100	38, 70, 102, 111	0
34	BQ	141/141 (100%)	-0.15	0 100 100	43, 61, 77, 91	0
34	DQ	141/141 (100%)	-0.12	0 100 100	47, 67, 85, 94	0
35	BR	118/118 (100%)	-0.23	0 100 100	38, 50, 70, 78	0
35	DR	118/118 (100%)	-0.23	0 100 100	42, 55, 73, 82	0
36	BS	110/112 (98%)	0.03	0 100 100	58, 75, 93, 101	0
36	DS	110/112 (98%)	0.05	1 (0%) 81 24	64, 82, 99, 110	0
37	BT	131/146 (89%)	-0.19	0 100 100	51, 63, 98, 117	0
37	DT	131/146 (89%)	-0.26	1 (0%) 83 26	55, 67, 101, 118	0
38	BU	116/118 (98%)	-0.17	1 (0%) 81 24	35, 48, 69, 81	0
38	DU	116/118 (98%)	-0.15	1 (0%) 81 24	40, 56, 76, 86	0
39	BV	100/101 (99%)	-0.24	0 100 100	34, 62, 81, 91	0
39	DV	101/101 (100%)	-0.06	0 100 100	40, 72, 90, 98	0
40	BW	112/113 (99%)	-0.32	0 100 100	36, 43, 64, 102	0
40	DW	112/113 (99%)	-0.42	0 100 100	40, 48, 69, 95	0
41	BX	95/96 (98%)	-0.15	0 100 100	41, 51, 74, 98	0
41	DX	95/96 (98%)	-0.30	0 100 100	47, 56, 80, 102	0
42	BY	107/110 (97%)	-0.17	2 (1%) 64 13	52, 64, 89, 107	0
42	DY	107/110 (97%)	0.11	3 (2%) 50 10	59, 72, 96, 116	0
43	BZ	198/206 (96%)	-0.13	0 100 100	65, 85, 111, 126	0
43	DZ	198/206 (96%)	0.13	1 (0%) 88 36	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%)	-0.28	0 100 100	48, 55, 71, 87	0
44	D0	76/85 (89%)	0.07	0 100 100	53, 61, 76, 90	0
45	B1	97/98 (98%)	-0.16	0 100 100	37, 57, 89, 103	0
45	D1	97/98 (98%)	-0.16	0 100 100	41, 61, 91, 108	0
46	B2	70/72 (97%)	-0.13	0 100 100	50, 66, 84, 103	0
46	D2	70/72 (97%)	0.07	1 (1%) 72 18	55, 71, 88, 112	0
47	B3	59/60 (98%)	-0.21	0 100 100	43, 57, 85, 101	0
47	D3	59/60 (98%)	0.07	0 100 100	49, 64, 92, 112	0
48	B4	46/71 (64%)	-0.42	0 100 100	106, 141, 151, 154	0
48	D4	46/71 (64%)	-0.25	0 100 100	113, 141, 152, 163	0
49	B5	59/60 (98%)	-0.32	0 100 100	33, 51, 68, 89	0
49	D5	59/60 (98%)	-0.29	0 100 100	37, 55, 73, 95	0
50	B6	53/54 (98%)	0.11	0 100 100	53, 61, 75, 78	0
50	D6	53/54 (98%)	0.39	3 (5%) 23 5	56, 65, 79, 82	0
51	B7	48/49 (97%)	0.02	0 100 100	32, 37, 61, 78	0
51	D7	48/49 (97%)	-0.10	0 100 100	36, 40, 64, 83	0
52	B8	64/65 (98%)	-0.10	0 100 100	42, 49, 58, 70	0
52	D8	64/65 (98%)	-0.31	0 100 100	46, 53, 62, 72	0
53	B9	36/37 (97%)	0.04	0 100 100	49, 59, 72, 83	0
53	D9	36/37 (97%)	0.48	3 (8%) 11 3	58, 68, 81, 91	0
All	All	20542/21368 (96%)	0.15	1254 (6%) 21 5	30, 80, 160, 189	0

The worst 5 of 1254 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AA	974	A	12.9
14	AN	13	THR	12.9
14	AN	12	ARG	12.2
1	AA	1290	G	11.3
1	AA	1351	U	11.3

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 carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
54	MG	BA	3098	1/1	0.40	-	54,54,54,54	0
54	MG	CA	1612	1/1	0.44	-	84,84,84,84	0
54	MG	AA	1646	1/1	0.42	-	73,73,73,73	0
54	MG	BA	3533	1/1	0.21	-	48,48,48,48	0
55	ZN	B5	103	1/1	0.14	-	58,58,58,58	0
54	MG	AA	1626	1/1	0.48	-	67,67,67,67	0
54	MG	BA	3058	1/1	0.09	-	56,56,56,56	0
54	MG	BA	3387	1/1	0.24	-	33,33,33,33	0
54	MG	DA	3192	1/1	0.18	-	66,66,66,66	0
54	MG	DA	3279	1/1	0.32	-	40,40,40,40	0
54	MG	BA	3197	1/1	0.28	-	62,62,62,62	0
54	MG	CA	1663	1/1	0.10	-	91,91,91,91	0
54	MG	DA	3265	1/1	0.21	-	39,39,39,39	0
54	MG	DA	3232	1/1	0.35	-	46,46,46,46	0
54	MG	BA	3193	1/1	0.20	-	50,50,50,50	0
54	MG	AA	1607	1/1	0.44	-	69,69,69,69	0
54	MG	DA	3148	1/1	0.39	-	70,70,70,70	0
54	MG	DA	3414	1/1	0.12	-	68,68,68,68	0
54	MG	BA	3451	1/1	0.23	-	34,34,34,34	0
54	MG	DP	201	1/1	0.69	-	58,58,58,58	0
54	MG	BA	3354	1/1	0.06	-	49,49,49,49	0
54	MG	BA	3030	1/1	0.25	-	37,37,37,37	0
54	MG	BA	3213	1/1	0.35	-	64,64,64,64	0
54	MG	BA	3467	1/1	0.15	-	73,73,73,73	0
54	MG	DA	3387	1/1	0.08	-	71,71,71,71	0
54	MG	DA	3108	1/1	0.18	-	80,80,80,80	0
54	MG	BA	3553	1/1	0.18	-	70,70,70,70	0
54	MG	BA	3293	1/1	0.19	-	29,29,29,29	0
54	MG	CA	1650	1/1	0.24	-	100,100,100,100	0
54	MG	BA	3611	1/1	0.07	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1615	1/1	0.63	-	76,76,76,76	0
54	MG	CA	1609	1/1	0.80	-	70,70,70,70	0
54	MG	BA	3483	1/1	0.16	-	57,57,57,57	0
54	MG	BA	3471	1/1	0.20	-	38,38,38,38	0
54	MG	BA	3070	1/1	0.18	-	61,61,61,61	0
54	MG	BA	3576	1/1	0.10	-	41,41,41,41	0
54	MG	BA	3425	1/1	0.14	-	37,37,37,37	0
54	MG	AA	1648	1/1	0.16	-	62,62,62,62	0
54	MG	BA	3430	1/1	0.21	-	30,30,30,30	0
54	MG	BA	3379	1/1	0.07	-	56,56,56,56	0
54	MG	DA	3240	1/1	0.20	-	67,67,67,67	0
54	MG	CA	1621	1/1	0.26	-	64,64,64,64	0
54	MG	AA	1657	1/1	0.54	-	81,81,81,81	0
54	MG	BA	3061	1/1	0.54	-	64,64,64,64	0
54	MG	AA	1688	1/1	0.23	-	111,111,111,111	0
54	MG	BA	3072	1/1	0.26	-	59,59,59,59	0
54	MG	DA	3079	1/1	0.22	-	60,60,60,60	0
54	MG	BA	3269	1/1	0.26	-	54,54,54,54	0
54	MG	BA	3146	1/1	0.48	-	52,52,52,52	0
54	MG	BA	3166	1/1	0.46	-	58,58,58,58	0
54	MG	DA	3115	1/1	0.43	-	39,39,39,39	0
54	MG	DA	3354	1/1	0.24	-	41,41,41,41	0
54	MG	DA	3298	1/1	0.13	-	71,71,71,71	0
54	MG	BA	3079	1/1	0.27	-	68,68,68,68	0
54	MG	DA	3014	1/1	0.12	-	52,52,52,52	0
54	MG	DA	3341	1/1	0.23	-	39,39,39,39	0
54	MG	CA	1603	1/1	0.29	-	73,73,73,73	0
54	MG	DA	3331	1/1	0.17	-	69,69,69,69	0
54	MG	BA	3019	1/1	0.10	-	39,39,39,39	0
54	MG	DA	3009	1/1	0.31	-	54,54,54,54	0
54	MG	BA	3353	1/1	0.12	-	28,28,28,28	0
54	MG	BA	3218	1/1	0.37	-	54,54,54,54	0
54	MG	DA	3229	1/1	0.31	-	55,55,55,55	0
54	MG	AA	1685	1/1	0.12	-	77,77,77,77	0
54	MG	DA	3183	1/1	0.14	-	50,50,50,50	0
54	MG	DA	3423	1/1	0.14	-	79,79,79,79	0
54	MG	DA	3271	1/1	0.11	-	57,57,57,57	0
54	MG	AA	1610	1/1	0.27	-	75,75,75,75	0
54	MG	AA	1656	1/1	0.79	-	74,74,74,74	0
54	MG	BA	3315	1/1	0.16	-	84,84,84,84	0
54	MG	BA	3536	1/1	0.08	-	82,82,82,82	0
54	MG	BA	3599	1/1	0.09	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3448	1/1	0.26	-	33,33,33,33	0
54	MG	BA	3374	1/1	0.12	-	75,75,75,75	0
54	MG	DA	3096	1/1	0.39	-	46,46,46,46	0
54	MG	BA	3001	1/1	0.39	-	56,56,56,56	0
54	MG	DA	3396	1/1	0.21	-	37,37,37,37	0
54	MG	BA	3377	1/1	0.10	-	69,69,69,69	0
54	MG	DA	3167	1/1	0.10	-	59,59,59,59	0
54	MG	BA	3196	1/1	0.82	-	80,80,80,80	0
54	MG	DA	3407	1/1	0.22	-	59,59,59,59	0
54	MG	DA	3044	1/1	0.22	-	51,51,51,51	0
54	MG	BA	3511	1/1	0.17	-	33,33,33,33	0
54	MG	BA	3145	1/1	0.34	-	78,78,78,78	0
54	MG	DA	3159	1/1	0.59	-	59,59,59,59	0
54	MG	BA	3047	1/1	0.25	-	50,50,50,50	0
54	MG	BA	3242	1/1	0.43	-	66,66,66,66	0
54	MG	DA	3110	1/1	0.05	-	46,46,46,46	0
54	MG	BA	3255	1/1	0.55	-	65,65,65,65	0
54	MG	CA	1608	1/1	0.43	-	67,67,67,67	0
54	MG	DE	301	1/1	0.47	-	37,37,37,37	0
54	MG	BU	202	1/1	0.39	-	62,62,62,62	0
54	MG	BA	3421	1/1	0.13	-	36,36,36,36	0
54	MG	BA	3606	1/1	0.11	-	29,29,29,29	0
54	MG	DA	3252	1/1	0.35	-	41,41,41,41	0
54	MG	BA	3149	1/1	0.19	-	49,49,49,49	0
54	MG	B8	101	1/1	0.35	-	64,64,64,64	0
54	MG	BA	3208	1/1	0.31	-	54,54,54,54	0
54	MG	BA	3601	1/1	0.06	-	33,33,33,33	0
54	MG	AA	1623	1/1	0.40	-	74,74,74,74	0
54	MG	DA	3185	1/1	0.40	-	47,47,47,47	0
54	MG	B0	102	1/1	0.16	-	56,56,56,56	0
54	MG	BA	3427	1/1	0.22	-	32,32,32,32	0
54	MG	BA	3028	1/1	0.24	-	46,46,46,46	0
54	MG	CA	1648	1/1	0.12	-	100,100,100,100	0
54	MG	DA	3125	1/1	0.41	-	66,66,66,66	0
54	MG	BA	3562	1/1	0.32	-	43,43,43,43	0
54	MG	DA	3259	1/1	0.39	-	64,64,64,64	0
54	MG	BA	3108	1/1	0.25	-	56,56,56,56	0
54	MG	BA	3301	1/1	0.06	-	62,62,62,62	0
54	MG	DA	3163	1/1	0.31	-	56,56,56,56	0
54	MG	BA	3288	1/1	0.49	-	33,33,33,33	0
54	MG	DA	3276	1/1	0.13	-	51,51,51,51	0
54	MG	BB	211	1/1	0.09	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3153	1/1	0.30	-	53,53,53,53	0
54	MG	BA	3209	1/1	0.37	-	67,67,67,67	0
54	MG	BA	3494	1/1	0.45	-	44,44,44,44	0
54	MG	AA	1658	1/1	0.18	-	60,60,60,60	0
54	MG	BA	3513	1/1	0.17	-	66,66,66,66	0
54	MG	DA	3286	1/1	0.18	-	50,50,50,50	0
54	MG	BA	3461	1/1	0.21	-	38,38,38,38	0
54	MG	DA	3415	1/1	0.09	-	89,89,89,89	0
54	MG	DA	3065	1/1	0.19	-	58,58,58,58	0
54	MG	BA	3617	1/1	0.15	-	93,93,93,93	0
54	MG	BA	3398	1/1	0.14	-	36,36,36,36	0
54	MG	AA	1638	1/1	0.22	-	78,78,78,78	0
54	MG	AA	1671	1/1	0.24	-	89,89,89,89	0
54	MG	AA	1636	1/1	0.15	-	86,86,86,86	0
54	MG	BA	3050	1/1	0.24	-	46,46,46,46	0
54	MG	BA	3549	1/1	0.13	-	68,68,68,68	0
54	MG	BA	3388	1/1	0.17	-	54,54,54,54	0
54	MG	BA	3025	1/1	0.13	-	52,52,52,52	0
54	MG	AA	1667	1/1	0.31	-	63,63,63,63	0
54	MG	DA	3272	1/1	0.16	-	47,47,47,47	0
54	MG	BA	3089	1/1	0.41	-	46,46,46,46	0
54	MG	BA	3125	1/1	0.24	-	50,50,50,50	0
54	MG	DA	3026	1/1	0.18	-	49,49,49,49	0
54	MG	DA	3084	1/1	0.34	-	62,62,62,62	0
54	MG	DA	3302	1/1	0.24	-	36,36,36,36	0
54	MG	BA	3287	1/1	0.46	-	65,65,65,65	0
54	MG	BA	3023	1/1	0.11	-	52,52,52,52	0
54	MG	DA	3130	1/1	0.23	-	59,59,59,59	0
54	MG	DA	3219	1/1	0.31	-	38,38,38,38	0
54	MG	BA	3508	1/1	0.12	-	40,40,40,40	0
54	MG	DA	3176	1/1	0.35	-	61,61,61,61	0
54	MG	BA	3176	1/1	0.44	-	69,69,69,69	0
54	MG	DA	3346	1/1	0.11	-	89,89,89,89	0
54	MG	DA	3339	1/1	0.11	-	48,48,48,48	0
54	MG	DA	3361	1/1	0.04	-	67,67,67,67	0
54	MG	DA	3355	1/1	0.11	-	37,37,37,37	0
54	MG	DA	3338	1/1	0.18	-	50,50,50,50	0
54	MG	AA	1604	1/1	0.32	-	81,81,81,81	0
54	MG	BA	3011	1/1	0.56	-	50,50,50,50	0
54	MG	BA	3515	1/1	0.12	-	46,46,46,46	0
54	MG	DA	3204	1/1	0.31	-	37,37,37,37	0
54	MG	BA	3144	1/1	0.25	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1683	1/1	0.25	-	139,139,139,139	0
54	MG	BA	3018	1/1	0.11	-	72,72,72,72	0
54	MG	BA	3080	1/1	0.52	-	42,42,42,42	0
54	MG	BA	3500	1/1	0.21	-	33,33,33,33	0
54	MG	DA	3307	1/1	0.18	-	39,39,39,39	0
54	MG	BA	3161	1/1	0.36	-	54,54,54,54	0
54	MG	BA	3413	1/1	0.26	-	31,31,31,31	0
54	MG	BA	3593	1/1	0.11	-	70,70,70,70	0
54	MG	AA	1706	1/1	0.09	-	100,100,100,100	0
54	MG	BA	3224	1/1	0.32	-	61,61,61,61	0
54	MG	BA	3495	1/1	0.18	-	70,70,70,70	0
54	MG	BA	3101	1/1	0.28	-	51,51,51,51	0
54	MG	BA	3041	1/1	0.13	-	56,56,56,56	0
54	MG	DA	3013	1/1	0.14	-	41,41,41,41	0
54	MG	DA	3239	1/1	0.28	-	39,39,39,39	0
54	MG	DA	3201	1/1	0.41	-	69,69,69,69	0
54	MG	BD	302	1/1	0.30	-	38,38,38,38	0
54	MG	DA	3106	1/1	0.36	-	56,56,56,56	0
54	MG	BA	3538	1/1	0.12	-	70,70,70,70	0
54	MG	DA	3102	1/1	0.38	-	79,79,79,79	0
54	MG	BB	205	1/1	0.31	-	57,57,57,57	0
54	MG	BA	3582	1/1	0.12	-	54,54,54,54	0
54	MG	DA	3077	1/1	0.20	-	66,66,66,66	0
54	MG	BA	3481	1/1	0.13	-	76,76,76,76	0
54	MG	AA	1601	1/1	0.27	-	68,68,68,68	0
54	MG	DA	3315	1/1	0.13	-	59,59,59,59	0
54	MG	BA	3318	1/1	0.22	-	73,73,73,73	0
54	MG	BA	3373	1/1	0.09	-	55,55,55,55	0
54	MG	DA	3345	1/1	0.27	-	100,100,100,100	0
54	MG	DA	3175	1/1	0.25	-	69,69,69,69	0
54	MG	DA	3072	1/1	0.31	-	50,50,50,50	0
54	MG	AA	1692	1/1	0.66	-	113,113,113,113	0
54	MG	BA	3456	1/1	0.11	-	89,89,89,89	0
54	MG	BA	3046	1/1	0.33	-	49,49,49,49	0
54	MG	DA	3342	1/1	0.25	-	41,41,41,41	0
54	MG	DA	3184	1/1	0.42	-	39,39,39,39	0
54	MG	DA	3216	1/1	0.17	-	53,53,53,53	0
54	MG	BA	3006	1/1	0.17	-	44,44,44,44	0
54	MG	DA	3016	1/1	0.11	-	41,41,41,41	0
54	MG	BA	3266	1/1	0.78	-	48,48,48,48	0
54	MG	BA	3401	1/1	0.16	-	45,45,45,45	0
54	MG	BA	3341	1/1	0.07	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	ZN	D6	101	1/1	0.09	-	86,86,86,86	0
54	MG	DA	3005	1/1	0.19	-	64,64,64,64	0
54	MG	BA	3074	1/1	0.42	-	55,55,55,55	0
54	MG	BA	3561	1/1	0.26	-	49,49,49,49	0
54	MG	BA	3476	1/1	0.23	-	44,44,44,44	0
54	MG	DA	3235	1/1	0.34	-	36,36,36,36	0
54	MG	BA	3578	1/1	0.22	-	60,60,60,60	0
54	MG	DA	3081	1/1	0.23	-	52,52,52,52	0
54	MG	B5	102	1/1	0.09	-	42,42,42,42	0
54	MG	BA	3179	1/1	0.44	-	48,48,48,48	0
54	MG	BA	3048	1/1	0.20	-	42,42,42,42	0
54	MG	AA	1633	1/1	0.54	-	72,72,72,72	0
54	MG	BA	3343	1/1	0.06	-	91,91,91,91	0
54	MG	DA	3169	1/1	0.24	-	39,39,39,39	0
54	MG	BA	3331	1/1	0.18	-	51,51,51,51	0
54	MG	BB	210	1/1	0.15	-	67,67,67,67	0
54	MG	BA	3537	1/1	0.16	-	38,38,38,38	0
54	MG	BA	3563	1/1	0.10	-	67,67,67,67	0
54	MG	DA	3426	1/1	0.06	-	94,94,94,94	0
54	MG	BA	3120	1/1	0.30	-	42,42,42,42	0
54	MG	BF	302	1/1	0.20	-	62,62,62,62	0
54	MG	DA	3260	1/1	0.46	-	44,44,44,44	0
54	MG	BA	3164	1/1	0.14	-	39,39,39,39	0
54	MG	DA	3223	1/1	0.07	-	104,104,104,104	0
54	MG	BA	3103	1/1	0.44	-	67,67,67,67	0
54	MG	DA	3172	1/1	0.26	-	50,50,50,50	0
54	MG	BA	3496	1/1	0.10	-	79,79,79,79	0
54	MG	CA	1636	1/1	0.47	-	77,77,77,77	0
54	MG	BA	3254	1/1	0.20	-	67,67,67,67	0
54	MG	DA	3424	1/1	0.15	-	130,130,130,130	0
54	MG	DA	3356	1/1	0.17	-	42,42,42,42	0
54	MG	BA	3186	1/1	0.38	-	64,64,64,64	0
54	MG	DA	3381	1/1	0.10	-	79,79,79,79	0
54	MG	DA	3336	1/1	0.15	-	87,87,87,87	0
54	MG	DA	3082	1/1	0.33	-	51,51,51,51	0
54	MG	BA	3021	1/1	0.32	-	33,33,33,33	0
54	MG	BA	3324	1/1	0.09	-	82,82,82,82	0
54	MG	DA	3021	1/1	0.24	-	53,53,53,53	0
54	MG	DA	3118	1/1	0.42	-	44,44,44,44	0
54	MG	BA	3600	1/1	0.19	-	31,31,31,31	0
54	MG	DA	3107	1/1	0.21	-	47,47,47,47	0
54	MG	DA	3289	1/1	0.19	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3008	1/1	0.23	-	48,48,48,48	0
54	MG	DA	3258	1/1	0.09	-	56,56,56,56	0
54	MG	BA	3534	1/1	0.27	-	76,76,76,76	0
54	MG	DA	3037	1/1	0.38	-	49,49,49,49	0
54	MG	BA	3068	1/1	0.23	-	70,70,70,70	0
54	MG	CA	1617	1/1	0.87	-	70,70,70,70	0
54	MG	BA	3444	1/1	0.06	-	61,61,61,61	0
54	MG	DA	3418	1/1	0.07	-	39,39,39,39	0
54	MG	DA	3048	1/1	0.56	-	53,53,53,53	0
54	MG	BA	3322	1/1	0.12	-	45,45,45,45	0
54	MG	BA	3516	1/1	0.13	-	39,39,39,39	0
54	MG	DA	3035	1/1	0.48	-	68,68,68,68	0
54	MG	BA	3133	1/1	0.30	-	31,31,31,31	0
54	MG	BA	3215	1/1	0.13	-	61,61,61,61	0
54	MG	DA	3290	1/1	0.23	-	42,42,42,42	0
54	MG	DA	3194	1/1	0.54	-	77,77,77,77	0
54	MG	AA	1627	1/1	0.47	-	70,70,70,70	0
54	MG	CA	1653	1/1	0.27	-	83,83,83,83	0
54	MG	BA	3295	1/1	0.11	-	44,44,44,44	0
54	MG	BA	3244	1/1	0.52	-	45,45,45,45	0
54	MG	BA	3044	1/1	0.14	-	49,49,49,49	0
54	MG	AA	1693	1/1	0.12	-	78,78,78,78	0
54	MG	BA	3595	1/1	0.09	-	82,82,82,82	0
54	MG	CA	1642	1/1	0.09	-	87,87,87,87	0
54	MG	DA	3165	1/1	0.16	-	58,58,58,58	0
54	MG	DA	3323	1/1	0.19	-	36,36,36,36	0
54	MG	BA	3470	1/1	0.24	-	35,35,35,35	0
54	MG	CA	1638	1/1	0.36	-	71,71,71,71	0
54	MG	DA	3364	1/1	0.11	-	67,67,67,67	0
54	MG	DA	3059	1/1	0.23	-	55,55,55,55	0
54	MG	BA	3143	1/1	0.33	-	45,45,45,45	0
54	MG	BA	3163	1/1	0.42	-	42,42,42,42	0
54	MG	AA	1608	1/1	0.15	-	90,90,90,90	0
54	MG	BA	3002	1/1	0.16	-	98,98,98,98	0
54	MG	CA	1662	1/1	0.15	-	95,95,95,95	0
54	MG	BA	3355	1/1	0.15	-	54,54,54,54	0
54	MG	BA	3280	1/1	0.39	-	89,89,89,89	0
54	MG	BA	3032	1/1	0.23	-	67,67,67,67	0
54	MG	DA	3129	1/1	0.40	-	78,78,78,78	0
54	MG	BA	3157	1/1	0.16	-	46,46,46,46	0
54	MG	DA	3273	1/1	0.10	-	37,37,37,37	0
54	MG	DA	3213	1/1	0.12	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3011	1/1	0.24	-	46,46,46,46	0
54	MG	DA	3006	1/1	0.23	-	44,44,44,44	0
54	MG	BA	3336	1/1	0.12	-	46,46,46,46	0
54	MG	BA	3603	1/1	0.18	-	30,30,30,30	0
54	MG	CA	1649	1/1	0.12	-	92,92,92,92	0
54	MG	BA	3198	1/1	0.24	-	29,29,29,29	0
54	MG	DA	3170	1/1	0.20	-	52,52,52,52	0
54	MG	AA	1635	1/1	0.23	-	71,71,71,71	0
54	MG	DA	3343	1/1	0.17	-	35,35,35,35	0
54	MG	DA	3372	1/1	0.35	-	40,40,40,40	0
54	MG	BA	3340	1/1	0.20	-	65,65,65,65	0
54	MG	BA	3615	1/1	0.04	-	91,91,91,91	0
54	MG	DA	3400	1/1	0.31	-	95,95,95,95	0
54	MG	DA	3371	1/1	0.15	-	50,50,50,50	0
54	MG	BA	3363	1/1	0.26	-	74,74,74,74	0
54	MG	DA	3151	1/1	0.34	-	58,58,58,58	0
54	MG	DF	301	1/1	0.38	-	58,58,58,58	0
54	MG	AA	1651	1/1	0.80	-	69,69,69,69	0
54	MG	BA	3434	1/1	0.37	-	36,36,36,36	0
54	MG	DA	3038	1/1	0.30	-	39,39,39,39	0
54	MG	DA	3083	1/1	0.32	-	55,55,55,55	0
54	MG	DA	3369	1/1	0.19	-	57,57,57,57	0
54	MG	DA	3018	1/1	0.18	-	42,42,42,42	0
54	MG	BA	3191	1/1	0.15	-	45,45,45,45	0
54	MG	B8	103	1/1	0.16	-	51,51,51,51	0
54	MG	DA	3388	1/1	0.12	-	72,72,72,72	0
54	MG	AD	302	1/1	0.21	-	120,120,120,120	0
54	MG	BA	3228	1/1	0.37	-	26,26,26,26	0
54	MG	DA	3296	1/1	0.12	-	50,50,50,50	0
54	MG	BA	3420	1/1	0.28	-	41,41,41,41	0
54	MG	DA	3393	1/1	0.10	-	81,81,81,81	0
54	MG	BA	3067	1/1	0.32	-	35,35,35,35	0
54	MG	DA	3350	1/1	0.14	-	50,50,50,50	0
54	MG	BA	3429	1/1	0.16	-	29,29,29,29	0
54	MG	BA	3579	1/1	0.11	-	53,53,53,53	0
54	MG	DA	3174	1/1	0.45	-	60,60,60,60	0
54	MG	AA	1654	1/1	0.06	-	87,87,87,87	0
54	MG	BA	3472	1/1	0.21	-	29,29,29,29	0
54	MG	DA	3267	1/1	0.21	-	59,59,59,59	0
55	ZN	B4	101	1/1	0.05	-	200,200,200,200	0
54	MG	DA	3285	1/1	0.14	-	52,52,52,52	0
54	MG	AA	1625	1/1	0.26	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3300	1/1	0.15	-	37,37,37,37	0
54	MG	BA	3501	1/1	0.11	-	61,61,61,61	0
54	MG	AA	1653	1/1	0.61	-	80,80,80,80	0
54	MG	CA	1635	1/1	0.20	-	68,68,68,68	0
54	MG	BA	3479	1/1	0.16	-	35,35,35,35	0
54	MG	DA	3116	1/1	0.35	-	46,46,46,46	0
54	MG	DA	3001	1/1	0.20	-	62,62,62,62	0
54	MG	BA	3081	1/1	0.22	-	66,66,66,66	0
54	MG	BA	3095	1/1	0.36	-	45,45,45,45	0
54	MG	BA	3241	1/1	0.72	-	62,62,62,62	0
54	MG	DA	3301	1/1	0.16	-	55,55,55,55	0
54	MG	BA	3170	1/1	0.50	-	52,52,52,52	0
54	MG	AA	1682	1/1	0.18	-	111,111,111,111	0
54	MG	BA	3222	1/1	0.13	-	51,51,51,51	0
54	MG	AA	1699	1/1	0.17	-	69,69,69,69	0
54	MG	AA	1609	1/1	0.33	-	91,91,91,91	0
54	MG	DA	3052	1/1	0.42	-	71,71,71,71	0
54	MG	BA	3455	1/1	0.33	-	42,42,42,42	0
54	MG	BA	3159	1/1	0.23	-	66,66,66,66	0
54	MG	DA	3020	1/1	0.12	-	39,39,39,39	0
54	MG	DA	3312	1/1	0.08	-	67,67,67,67	0
55	ZN	DY	201	1/1	0.09	-	128,128,128,128	0
54	MG	CA	1616	1/1	0.47	-	72,72,72,72	0
54	MG	DA	3027	1/1	0.39	-	51,51,51,51	0
54	MG	BA	3493	1/1	0.23	-	52,52,52,52	0
54	MG	BA	3323	1/1	0.08	-	40,40,40,40	0
54	MG	DA	3113	1/1	0.36	-	42,42,42,42	0
54	MG	CA	1654	1/1	0.12	-	95,95,95,95	0
54	MG	AA	1622	1/1	0.73	-	67,67,67,67	0
54	MG	BA	3059	1/1	0.32	-	49,49,49,49	0
54	MG	BA	3111	1/1	0.29	-	57,57,57,57	0
54	MG	BA	3405	1/1	0.21	-	38,38,38,38	0
54	MG	BA	3392	1/1	0.11	-	55,55,55,55	0
54	MG	BA	3348	1/1	0.23	-	37,37,37,37	0
54	MG	BA	3104	1/1	0.20	-	48,48,48,48	0
54	MG	BA	3201	1/1	0.57	-	79,79,79,79	0
54	MG	DA	3162	1/1	0.40	-	55,55,55,55	0
54	MG	DA	3410	1/1	0.20	-	72,72,72,72	0
54	MG	DA	3168	1/1	0.28	-	42,42,42,42	0
54	MG	BA	3350	1/1	0.16	-	60,60,60,60	0
54	MG	BA	3580	1/1	0.09	-	61,61,61,61	0
54	MG	AA	1618	1/1	0.11	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	204	1/1	0.10	-	74,74,74,74	0
54	MG	B0	101	1/1	0.17	-	75,75,75,75	0
54	MG	BA	3031	1/1	0.36	-	41,41,41,41	0
54	MG	DA	3365	1/1	0.09	-	50,50,50,50	0
54	MG	BA	3308	1/1	0.49	-	51,51,51,51	0
54	MG	DA	3029	1/1	0.14	-	72,72,72,72	0
54	MG	DA	3017	1/1	0.28	-	61,61,61,61	0
54	MG	BA	3366	1/1	0.08	-	50,50,50,50	0
54	MG	DA	3421	1/1	0.10	-	69,69,69,69	0
54	MG	BA	3020	1/1	0.10	-	34,34,34,34	0
54	MG	DA	3269	1/1	0.11	-	54,54,54,54	0
54	MG	BA	3174	1/1	0.42	-	71,71,71,71	0
54	MG	BA	3618	1/1	0.16	-	85,85,85,85	0
54	MG	AA	1649	1/1	0.15	-	66,66,66,66	0
54	MG	BA	3517	1/1	0.28	-	51,51,51,51	0
54	MG	BA	3118	1/1	0.82	-	57,57,57,57	0
54	MG	BA	3181	1/1	0.18	-	48,48,48,48	0
54	MG	BA	3232	1/1	0.14	-	54,54,54,54	0
54	MG	DA	3099	1/1	0.23	-	40,40,40,40	0
54	MG	DA	3150	1/1	0.38	-	41,41,41,41	0
54	MG	BA	3229	1/1	0.37	-	51,51,51,51	0
54	MG	DA	3225	1/1	0.27	-	64,64,64,64	0
54	MG	DA	3309	1/1	0.47	-	48,48,48,48	0
54	MG	DA	3249	1/1	0.38	-	67,67,67,67	0
54	MG	CA	1627	1/1	0.15	-	79,79,79,79	0
54	MG	DA	3126	1/1	0.12	-	80,80,80,80	0
54	MG	BA	3581	1/1	0.13	-	47,47,47,47	0
54	MG	CA	1630	1/1	0.42	-	72,72,72,72	0
54	MG	DA	3135	1/1	0.22	-	44,44,44,44	0
54	MG	BA	3049	1/1	0.16	-	54,54,54,54	0
54	MG	BA	3530	1/1	0.12	-	84,84,84,84	0
54	MG	BA	3436	1/1	0.33	-	38,38,38,38	0
54	MG	DA	3428	1/1	0.07	-	81,81,81,81	0
54	MG	CA	1652	1/1	0.09	-	65,65,65,65	0
54	MG	DA	3198	1/1	0.17	-	55,55,55,55	0
54	MG	BA	3477	1/1	0.08	-	45,45,45,45	0
54	MG	BA	3604	1/1	0.06	-	36,36,36,36	0
54	MG	DA	3187	1/1	0.57	-	47,47,47,47	0
54	MG	AA	1675	1/1	0.38	-	73,73,73,73	0
54	MG	BA	3082	1/1	0.30	-	71,71,71,71	0
54	MG	DA	3270	1/1	0.11	-	34,34,34,34	0
54	MG	AA	1640	1/1	0.49	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BE	302	1/1	0.22	-	52,52,52,52	0
54	MG	BA	3076	1/1	0.09	-	70,70,70,70	0
54	MG	BA	3115	1/1	0.37	-	43,43,43,43	0
54	MG	DA	3419	1/1	0.06	-	50,50,50,50	0
54	MG	BA	3286	1/1	0.23	-	52,52,52,52	0
54	MG	BA	3482	1/1	0.17	-	58,58,58,58	0
54	MG	DA	3337	1/1	0.10	-	42,42,42,42	0
54	MG	BA	3442	1/1	0.16	-	31,31,31,31	0
54	MG	BA	3404	1/1	0.12	-	46,46,46,46	0
54	MG	AA	1664	1/1	0.14	-	85,85,85,85	0
54	MG	BA	3527	1/1	0.14	-	51,51,51,51	0
54	MG	BA	3113	1/1	0.38	-	35,35,35,35	0
54	MG	BA	3507	1/1	0.15	-	53,53,53,53	0
54	MG	DA	3068	1/1	0.24	-	48,48,48,48	0
54	MG	DA	3210	1/1	0.28	-	60,60,60,60	0
54	MG	AA	1678	1/1	0.50	-	75,75,75,75	0
54	MG	DA	3353	1/1	0.18	-	40,40,40,40	0
54	MG	BA	3279	1/1	0.16	-	54,54,54,54	0
54	MG	DA	3250	1/1	0.40	-	41,41,41,41	0
54	MG	DA	3266	1/1	0.09	-	58,58,58,58	0
54	MG	DA	3230	1/1	0.16	-	67,67,67,67	0
54	MG	BA	3532	1/1	0.09	-	35,35,35,35	0
55	ZN	D4	101	1/1	0.04	-	176,176,176,176	0
54	MG	BA	3064	1/1	0.23	-	45,45,45,45	0
54	MG	BA	3319	1/1	0.05	-	68,68,68,68	0
54	MG	BA	3253	1/1	0.23	-	38,38,38,38	0
54	MG	BA	3443	1/1	0.26	-	41,41,41,41	0
54	MG	DA	3333	1/1	0.08	-	53,53,53,53	0
54	MG	AA	1617	1/1	0.10	-	82,82,82,82	0
54	MG	CA	1667	1/1	0.16	-	64,64,64,64	0
54	MG	BA	3216	1/1	0.21	-	52,52,52,52	0
54	MG	DA	3226	1/1	0.17	-	53,53,53,53	0
54	MG	DA	3195	1/1	0.80	-	75,75,75,75	0
54	MG	CA	1605	1/1	0.32	-	74,74,74,74	0
54	MG	BE	303	1/1	0.14	-	54,54,54,54	0
54	MG	BA	3251	1/1	0.38	-	63,63,63,63	0
54	MG	BA	3597	1/1	0.09	-	26,26,26,26	0
54	MG	DA	3109	1/1	0.28	-	70,70,70,70	0
54	MG	BA	3263	1/1	0.57	-	41,41,41,41	0
54	MG	BA	3220	1/1	0.20	-	79,79,79,79	0
54	MG	BA	3194	1/1	0.24	-	79,79,79,79	0
54	MG	BA	3410	1/1	0.17	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3408	1/1	0.18	-	65,65,65,65	0
54	MG	DA	3031	1/1	0.43	-	43,43,43,43	0
54	MG	BA	3171	1/1	0.23	-	67,67,67,67	0
54	MG	BA	3574	1/1	0.05	-	41,41,41,41	0
54	MG	DA	3254	1/1	0.38	-	43,43,43,43	0
54	MG	DA	3032	1/1	0.28	-	43,43,43,43	0
54	MG	BA	3591	1/1	0.15	-	56,56,56,56	0
54	MG	DA	3139	1/1	0.46	-	65,65,65,65	0
54	MG	BA	3248	1/1	0.15	-	50,50,50,50	0
54	MG	BA	3168	1/1	0.33	-	52,52,52,52	0
54	MG	AA	1628	1/1	0.34	-	84,84,84,84	0
54	MG	DA	3075	1/1	0.39	-	71,71,71,71	0
54	MG	BA	3296	1/1	0.06	-	48,48,48,48	0
54	MG	DA	3244	1/1	0.45	-	35,35,35,35	0
54	MG	BA	3214	1/1	0.55	-	34,34,34,34	0
54	MG	DA	3206	1/1	0.20	-	75,75,75,75	0
54	MG	DA	3330	1/1	0.23	-	44,44,44,44	0
54	MG	BA	3203	1/1	0.32	-	69,69,69,69	0
54	MG	DA	3211	1/1	0.24	-	53,53,53,53	0
54	MG	DA	3411	1/1	0.14	-	90,90,90,90	0
54	MG	BA	3073	1/1	0.12	-	67,67,67,67	0
54	MG	DA	3100	1/1	0.33	-	61,61,61,61	0
54	MG	BA	3488	1/1	0.13	-	34,34,34,34	0
54	MG	AA	1629	1/1	0.20	-	63,63,63,63	0
54	MG	BA	3462	1/1	0.12	-	25,25,25,25	0
54	MG	DA	3143	1/1	0.52	-	62,62,62,62	0
54	MG	DA	3156	1/1	0.22	-	52,52,52,52	0
54	MG	BB	202	1/1	0.12	-	46,46,46,46	0
54	MG	DA	3149	1/1	0.36	-	36,36,36,36	0
54	MG	DA	3253	1/1	0.29	-	42,42,42,42	0
54	MG	DA	3386	1/1	0.10	-	63,63,63,63	0
54	MG	BA	3610	1/1	0.05	-	56,56,56,56	0
54	MG	BA	3042	1/1	0.50	-	47,47,47,47	0
54	MG	DA	3316	1/1	0.12	-	75,75,75,75	0
54	MG	BA	3422	1/1	0.23	-	27,27,27,27	0
54	MG	DA	3278	1/1	0.15	-	46,46,46,46	0
54	MG	DA	3228	1/1	0.55	-	51,51,51,51	0
54	MG	BA	3142	1/1	0.45	-	53,53,53,53	0
54	MG	BA	3347	1/1	0.20	-	55,55,55,55	0
54	MG	DA	3193	1/1	0.32	-	63,63,63,63	0
54	MG	BA	3155	1/1	0.38	-	64,64,64,64	0
54	MG	BA	3233	1/1	0.14	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3379	1/1	0.09	-	94,94,94,94	0
54	MG	BA	3375	1/1	0.34	-	46,46,46,46	0
54	MG	AA	1652	1/1	0.68	-	82,82,82,82	0
54	MG	BA	3558	1/1	0.13	-	61,61,61,61	0
54	MG	DA	3141	1/1	0.49	-	74,74,74,74	0
54	MG	DA	3351	1/1	0.17	-	78,78,78,78	0
54	MG	DA	3399	1/1	0.45	-	60,60,60,60	0
54	MG	BA	3015	1/1	0.40	-	42,42,42,42	0
54	MG	BA	3129	1/1	0.35	-	49,49,49,49	0
54	MG	BF	301	1/1	0.36	-	56,56,56,56	0
54	MG	BA	3260	1/1	0.49	-	50,50,50,50	0
54	MG	BB	212	1/1	0.05	-	68,68,68,68	0
54	MG	BA	3054	1/1	0.15	-	52,52,52,52	0
54	MG	DA	3103	1/1	0.29	-	71,71,71,71	0
54	MG	B9	102	1/1	0.32	-	45,45,45,45	0
54	MG	BB	214	1/1	0.15	-	67,67,67,67	0
54	MG	BA	3199	1/1	0.22	-	31,31,31,31	0
54	MG	DA	3275	1/1	0.10	-	48,48,48,48	0
54	MG	DA	3104	1/1	0.12	-	57,57,57,57	0
54	MG	BA	3358	1/1	0.07	-	64,64,64,64	0
54	MG	AA	1663	1/1	0.44	-	70,70,70,70	0
54	MG	DA	3049	1/1	0.32	-	58,58,58,58	0
54	MG	BA	3109	1/1	0.42	-	57,57,57,57	0
54	MG	BA	3135	1/1	0.40	-	54,54,54,54	0
54	MG	BA	3239	1/1	0.28	-	38,38,38,38	0
54	MG	BA	3469	1/1	0.37	-	77,77,77,77	0
54	MG	DA	3320	1/1	0.10	-	57,57,57,57	0
54	MG	DA	3299	1/1	0.13	-	54,54,54,54	0
54	MG	BA	3027	1/1	0.15	-	56,56,56,56	0
54	MG	DA	3310	1/1	0.27	-	56,56,56,56	0
54	MG	BA	3564	1/1	0.25	-	36,36,36,36	0
54	MG	DA	3374	1/1	0.24	-	44,44,44,44	0
54	MG	BA	3485	1/1	0.17	-	60,60,60,60	0
54	MG	DA	3304	1/1	0.17	-	38,38,38,38	0
54	MG	DA	3091	1/1	0.15	-	70,70,70,70	0
54	MG	DB	201	1/1	0.37	-	75,75,75,75	0
54	MG	DA	3093	1/1	0.70	-	66,66,66,66	0
54	MG	DA	3171	1/1	0.28	-	53,53,53,53	0
54	MG	BA	3440	1/1	0.09	-	63,63,63,63	0
54	MG	DA	3251	1/1	0.47	-	39,39,39,39	0
54	MG	CA	1631	1/1	0.99	-	88,88,88,88	0
54	MG	BA	3506	1/1	0.16	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3234	1/1	0.50	-	56,56,56,56	0
54	MG	DA	3220	1/1	0.22	-	48,48,48,48	0
54	MG	DA	3023	1/1	0.59	-	61,61,61,61	0
54	MG	BA	3184	1/1	0.23	-	66,66,66,66	0
54	MG	AA	1687	1/1	0.14	-	70,70,70,70	0
54	MG	DA	3412	1/1	0.16	-	45,45,45,45	0
54	MG	B3	101	1/1	0.39	-	60,60,60,60	0
55	ZN	AN	101	1/1	0.13	-	213,213,213,213	0
54	MG	BA	3345	1/1	0.20	-	45,45,45,45	0
54	MG	BA	3359	1/1	0.12	-	49,49,49,49	0
54	MG	BA	3352	1/1	0.10	-	53,53,53,53	0
54	MG	BA	3547	1/1	0.23	-	31,31,31,31	0
54	MG	BP	201	1/1	0.27	-	43,43,43,43	0
54	MG	BA	3062	1/1	0.07	-	69,69,69,69	0
54	MG	BA	3396	1/1	0.42	-	23,23,23,23	0
54	MG	DA	3222	1/1	0.25	-	47,47,47,47	0
54	MG	BA	3386	1/1	0.12	-	77,77,77,77	0
54	MG	DA	3182	1/1	0.23	-	59,59,59,59	0
54	MG	BA	3463	1/1	0.19	-	36,36,36,36	0
54	MG	BA	3316	1/1	0.31	-	34,34,34,34	0
54	MG	BA	3150	1/1	0.22	-	61,61,61,61	0
54	MG	DA	3218	1/1	0.73	-	53,53,53,53	0
54	MG	BA	3147	1/1	0.29	-	57,57,57,57	0
54	MG	CA	1657	1/1	0.23	-	86,86,86,86	0
54	MG	BA	3567	1/1	0.09	-	62,62,62,62	0
54	MG	CA	1619	1/1	0.42	-	69,69,69,69	0
54	MG	BA	3037	1/1	0.20	-	52,52,52,52	0
54	MG	DA	3293	1/1	0.26	-	50,50,50,50	0
55	ZN	D9	101	1/1	0.04	-	87,87,87,87	0
54	MG	DA	3404	1/1	0.08	-	53,53,53,53	0
54	MG	BA	3034	1/1	0.28	-	46,46,46,46	0
54	MG	CA	1651	1/1	0.18	-	61,61,61,61	0
54	MG	DA	3321	1/1	0.20	-	53,53,53,53	0
54	MG	CA	1632	1/1	0.27	-	65,65,65,65	0
54	MG	AA	1620	1/1	0.98	-	77,77,77,77	0
54	MG	DA	3332	1/1	0.05	-	62,62,62,62	0
54	MG	DA	3359	1/1	0.37	-	49,49,49,49	0
54	MG	DA	3003	1/1	0.35	-	35,35,35,35	0
54	MG	BA	3539	1/1	0.05	-	61,61,61,61	0
54	MG	BA	3335	1/1	0.14	-	55,55,55,55	0
54	MG	BA	3453	1/1	0.19	-	74,74,74,74	0
54	MG	BA	3188	1/1	0.26	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3255	1/1	0.36	-	63,63,63,63	0
54	MG	BA	3502	1/1	0.14	-	41,41,41,41	0
54	MG	DA	3161	1/1	0.43	-	55,55,55,55	0
54	MG	BA	3608	1/1	0.13	-	87,87,87,87	0
54	MG	BA	3490	1/1	0.23	-	53,53,53,53	0
54	MG	CA	1610	1/1	0.50	-	80,80,80,80	0
54	MG	DA	3362	1/1	0.12	-	63,63,63,63	0
54	MG	DA	3166	1/1	0.20	-	55,55,55,55	0
54	MG	DA	3124	1/1	0.49	-	35,35,35,35	0
54	MG	DA	3274	1/1	0.09	-	35,35,35,35	0
54	MG	BA	3349	1/1	0.13	-	39,39,39,39	0
54	MG	BA	3616	1/1	0.11	-	82,82,82,82	0
54	MG	BA	3400	1/1	0.20	-	34,34,34,34	0
54	MG	BA	3504	1/1	0.37	-	28,28,28,28	0
54	MG	BA	3235	1/1	0.13	-	45,45,45,45	0
54	MG	AA	1637	1/1	0.29	-	82,82,82,82	0
54	MG	DA	3363	1/1	0.10	-	72,72,72,72	0
54	MG	DA	3042	1/1	0.48	-	46,46,46,46	0
54	MG	DA	3191	1/1	0.24	-	50,50,50,50	0
54	MG	BA	3008	1/1	0.27	-	32,32,32,32	0
54	MG	DA	3247	1/1	0.35	-	52,52,52,52	0
54	MG	DA	3063	1/1	0.22	-	54,54,54,54	0
54	MG	BA	3369	1/1	0.27	-	74,74,74,74	0
54	MG	BA	3459	1/1	0.14	-	130,130,130,130	0
54	MG	DA	3089	1/1	0.43	-	82,82,82,82	0
54	MG	DA	3153	1/1	0.44	-	38,38,38,38	0
54	MG	BA	3321	1/1	0.10	-	65,65,65,65	0
54	MG	BA	3128	1/1	0.18	-	53,53,53,53	0
54	MG	D7	101	1/1	0.27	-	52,52,52,52	0
54	MG	BA	3250	1/1	0.23	-	47,47,47,47	0
54	MG	BA	3541	1/1	0.29	-	54,54,54,54	0
54	MG	BA	3542	1/1	0.22	-	60,60,60,60	0
54	MG	DA	3308	1/1	0.42	-	49,49,49,49	0
54	MG	AA	1665	1/1	0.54	-	86,86,86,86	0
54	MG	BE	305	1/1	0.20	-	32,32,32,32	0
54	MG	DA	3062	1/1	0.24	-	65,65,65,65	0
54	MG	BA	3365	1/1	0.11	-	84,84,84,84	0
54	MG	DA	3281	1/1	0.08	-	36,36,36,36	0
54	MG	AA	1611	1/1	0.30	-	69,69,69,69	0
54	MG	BA	3505	1/1	0.09	-	76,76,76,76	0
54	MG	CA	1606	1/1	0.64	-	81,81,81,81	0
54	MG	DA	3105	1/1	0.56	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3545	1/1	0.19	-	79,79,79,79	0
54	MG	DA	3212	1/1	0.21	-	38,38,38,38	0
54	MG	BA	3381	1/1	0.07	-	49,49,49,49	0
54	MG	BA	3238	1/1	0.15	-	32,32,32,32	0
54	MG	DA	3241	1/1	0.21	-	63,63,63,63	0
54	MG	DA	3384	1/1	0.18	-	57,57,57,57	0
54	MG	AA	1659	1/1	0.42	-	62,62,62,62	0
54	MG	DA	3287	1/1	0.06	-	46,46,46,46	0
54	MG	CA	1629	1/1	0.23	-	72,72,72,72	0
54	MG	DA	3257	1/1	0.54	-	59,59,59,59	0
54	MG	BA	3586	1/1	0.08	-	58,58,58,58	0
54	MG	CA	1618	1/1	0.38	-	75,75,75,75	0
54	MG	BA	3100	1/1	0.30	-	72,72,72,72	0
54	MG	DA	3208	1/1	0.46	-	52,52,52,52	0
54	MG	BA	3518	1/1	0.34	-	59,59,59,59	0
54	MG	BA	3566	1/1	0.22	-	40,40,40,40	0
54	MG	DA	3034	1/1	0.27	-	74,74,74,74	0
54	MG	BA	3402	1/1	0.08	-	47,47,47,47	0
54	MG	BA	3602	1/1	0.08	-	24,24,24,24	0
54	MG	AA	1631	1/1	0.40	-	64,64,64,64	0
54	MG	BA	3327	1/1	0.15	-	34,34,34,34	0
54	MG	BA	3140	1/1	0.41	-	59,59,59,59	0
54	MG	BA	3114	1/1	0.25	-	43,43,43,43	0
54	MG	BA	3124	1/1	0.22	-	68,68,68,68	0
54	MG	DA	3248	1/1	0.59	-	44,44,44,44	0
54	MG	DA	3200	1/1	0.20	-	67,67,67,67	0
54	MG	BA	3225	1/1	0.32	-	61,61,61,61	0
54	MG	AA	1689	1/1	0.09	-	55,55,55,55	0
54	MG	BA	3380	1/1	0.05	-	50,50,50,50	0
54	MG	AA	1680	1/1	0.17	-	83,83,83,83	0
54	MG	DA	3303	1/1	0.20	-	37,37,37,37	0
54	MG	BA	3299	1/1	0.20	-	38,38,38,38	0
54	MG	DA	3367	1/1	0.15	-	68,68,68,68	0
54	MG	BA	3278	1/1	0.30	-	43,43,43,43	0
54	MG	BB	203	1/1	0.21	-	80,80,80,80	0
54	MG	BA	3584	1/1	0.16	-	68,68,68,68	0
54	MG	DA	3318	1/1	0.08	-	66,66,66,66	0
54	MG	AA	1606	1/1	0.84	-	74,74,74,74	0
54	MG	BA	3294	1/1	0.19	-	37,37,37,37	0
54	MG	DA	3422	1/1	0.10	-	75,75,75,75	0
54	MG	AA	1615	1/1	0.35	-	56,56,56,56	0
54	MG	BA	3475	1/1	0.23	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3347	1/1	0.08	-	76,76,76,76	0
54	MG	DA	3406	1/1	0.25	-	35,35,35,35	0
54	MG	DA	3025	1/1	0.25	-	57,57,57,57	0
54	MG	DA	3157	1/1	0.31	-	69,69,69,69	0
54	MG	AA	1641	1/1	0.61	-	93,93,93,93	0
54	MG	BD	301	1/1	0.27	-	41,41,41,41	0
54	MG	BA	3424	1/1	0.23	-	32,32,32,32	0
54	MG	DA	3322	1/1	0.14	-	35,35,35,35	0
54	MG	AA	1612	1/1	0.36	-	76,76,76,76	0
54	MG	BA	3247	1/1	0.26	-	53,53,53,53	0
54	MG	BA	3313	1/1	0.14	-	42,42,42,42	0
54	MG	DA	3173	1/1	0.35	-	49,49,49,49	0
54	MG	BA	3391	1/1	0.27	-	38,38,38,38	0
54	MG	DA	3236	1/1	0.53	-	44,44,44,44	0
54	MG	BA	3589	1/1	0.06	-	70,70,70,70	0
54	MG	AA	1621	1/1	0.99	-	80,80,80,80	0
54	MG	D6	102	1/1	0.44	-	64,64,64,64	0
54	MG	DA	3128	1/1	0.30	-	72,72,72,72	0
54	MG	DA	3427	1/1	0.13	-	40,40,40,40	0
54	MG	BE	304	1/1	0.16	-	32,32,32,32	0
54	MG	BA	3521	1/1	0.20	-	41,41,41,41	0
54	MG	BA	3383	1/1	0.22	-	71,71,71,71	0
54	MG	BA	3526	1/1	0.30	-	28,28,28,28	0
54	MG	BA	3024	1/1	0.38	-	48,48,48,48	0
54	MG	BA	3131	1/1	0.17	-	44,44,44,44	0
54	MG	BA	3230	1/1	0.32	-	50,50,50,50	0
54	MG	DA	3028	1/1	0.17	-	53,53,53,53	0
54	MG	BA	3342	1/1	0.08	-	57,57,57,57	0
54	MG	DA	3057	1/1	0.17	-	67,67,67,67	0
54	MG	CA	1661	1/1	0.25	-	100,100,100,100	0
54	MG	DA	3069	1/1	0.45	-	61,61,61,61	0
54	MG	AA	1605	1/1	0.30	-	74,74,74,74	0
54	MG	BA	3026	1/1	0.17	-	68,68,68,68	0
54	MG	DA	3295	1/1	0.16	-	42,42,42,42	0
54	MG	BA	3524	1/1	0.17	-	77,77,77,77	0
54	MG	BA	3570	1/1	0.18	-	36,36,36,36	0
54	MG	BA	3270	1/1	0.31	-	74,74,74,74	0
54	MG	BA	3206	1/1	0.13	-	68,68,68,68	0
54	MG	CA	1669	1/1	0.10	-	117,117,117,117	0
54	MG	DA	3189	1/1	0.72	-	66,66,66,66	0
54	MG	DA	3051	1/1	0.13	-	43,43,43,43	0
54	MG	DA	3227	1/1	0.32	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3487	1/1	0.22	-	94,94,94,94	0
54	MG	AA	1634	1/1	0.77	-	95,95,95,95	0
54	MG	BA	3180	1/1	0.24	-	51,51,51,51	0
54	MG	DA	3311	1/1	0.06	-	65,65,65,65	0
54	MG	DA	3403	1/1	0.16	-	49,49,49,49	0
54	MG	BA	3464	1/1	0.29	-	41,41,41,41	0
54	MG	AA	1677	1/1	0.90	-	81,81,81,81	0
54	MG	DA	3158	1/1	0.42	-	72,72,72,72	0
54	MG	BA	3438	1/1	0.18	-	38,38,38,38	0
54	MG	BA	3165	1/1	0.14	-	56,56,56,56	0
54	MG	BA	3519	1/1	0.35	-	90,90,90,90	0
54	MG	DA	3147	1/1	0.70	-	78,78,78,78	0
54	MG	BA	3085	1/1	0.33	-	63,63,63,63	0
54	MG	BA	3356	1/1	0.30	-	59,59,59,59	0
54	MG	BV	201	1/1	0.45	-	74,74,74,74	0
54	MG	AA	1603	1/1	0.12	-	68,68,68,68	0
54	MG	DA	3401	1/1	0.08	-	85,85,85,85	0
54	MG	BB	215	1/1	0.18	-	77,77,77,77	0
54	MG	BA	3446	1/1	0.09	-	40,40,40,40	0
54	MG	BA	3102	1/1	0.34	-	59,59,59,59	0
54	MG	BA	3568	1/1	0.16	-	60,60,60,60	0
54	MG	BA	3298	1/1	0.10	-	53,53,53,53	0
54	MG	BA	3491	1/1	0.13	-	65,65,65,65	0
54	MG	BA	3189	1/1	0.31	-	46,46,46,46	0
54	MG	BA	3445	1/1	0.08	-	56,56,56,56	0
54	MG	AA	1672	1/1	0.67	-	82,82,82,82	0
54	MG	DA	3024	1/1	0.51	-	49,49,49,49	0
54	MG	DA	3335	1/1	0.26	-	72,72,72,72	0
54	MG	BA	3273	1/1	0.22	-	66,66,66,66	0
54	MG	AA	1643	1/1	0.79	-	96,96,96,96	0
54	MG	BA	3418	1/1	0.08	-	54,54,54,54	0
54	MG	BA	3035	1/1	0.26	-	45,45,45,45	0
54	MG	DA	3039	1/1	0.26	-	41,41,41,41	0
54	MG	BA	3007	1/1	0.22	-	36,36,36,36	0
54	MG	BA	3127	1/1	0.23	-	51,51,51,51	0
54	MG	BA	3306	1/1	0.15	-	51,51,51,51	0
54	MG	DA	3376	1/1	0.13	-	43,43,43,43	0
54	MG	DA	3119	1/1	0.58	-	57,57,57,57	0
54	MG	DA	3138	1/1	0.74	-	60,60,60,60	0
54	MG	DA	3120	1/1	0.71	-	52,52,52,52	0
54	MG	DA	3131	1/1	0.28	-	39,39,39,39	0
54	MG	AA	1704	1/1	0.11	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3256	1/1	0.51	-	59,59,59,59	0
54	MG	DA	3352	1/1	0.10	-	61,61,61,61	0
54	MG	DA	3137	1/1	0.55	-	64,64,64,64	0
54	MG	BA	3291	1/1	0.11	-	59,59,59,59	0
54	MG	BA	3588	1/1	0.27	-	86,86,86,86	0
54	MG	BA	3523	1/1	0.05	-	79,79,79,79	0
54	MG	BW	201	1/1	0.15	-	51,51,51,51	0
54	MG	BA	3473	1/1	0.47	-	59,59,59,59	0
54	MG	BA	3339	1/1	0.07	-	91,91,91,91	0
54	MG	DA	3164	1/1	0.27	-	46,46,46,46	0
54	MG	DA	3368	1/1	0.14	-	78,78,78,78	0
54	MG	BA	3236	1/1	0.22	-	50,50,50,50	0
54	MG	BA	3284	1/1	0.12	-	40,40,40,40	0
54	MG	AA	1681	1/1	0.12	-	65,65,65,65	0
54	MG	DA	3348	1/1	0.11	-	85,85,85,85	0
54	MG	CA	1634	1/1	0.38	-	101,101,101,101	0
54	MG	BA	3529	1/1	0.26	-	86,86,86,86	0
54	MG	AA	1644	1/1	0.28	-	74,74,74,74	0
54	MG	BA	3077	1/1	0.47	-	43,43,43,43	0
54	MG	DA	3140	1/1	0.55	-	70,70,70,70	0
54	MG	DA	3349	1/1	0.28	-	54,54,54,54	0
54	MG	BA	3261	1/1	0.23	-	59,59,59,59	0
54	MG	CA	1620	1/1	0.34	-	57,57,57,57	0
54	MG	DA	3066	1/1	0.16	-	56,56,56,56	0
54	MG	BA	3450	1/1	0.15	-	71,71,71,71	0
54	MG	BA	3364	1/1	0.11	-	46,46,46,46	0
54	MG	AA	1661	1/1	0.76	-	77,77,77,77	0
54	MG	BA	3397	1/1	0.16	-	31,31,31,31	0
54	MG	CA	1623	1/1	0.86	-	73,73,73,73	0
54	MG	BA	3075	1/1	0.27	-	53,53,53,53	0
54	MG	BA	3489	1/1	0.20	-	38,38,38,38	0
54	MG	BA	3172	1/1	0.24	-	71,71,71,71	0
54	MG	DA	3179	1/1	0.32	-	62,62,62,62	0
54	MG	BA	3614	1/1	0.32	-	94,94,94,94	0
54	MG	BA	3569	1/1	0.30	-	68,68,68,68	0
54	MG	DA	3291	1/1	0.34	-	43,43,43,43	0
54	MG	BA	3426	1/1	0.23	-	28,28,28,28	0
54	MG	BA	3390	1/1	0.22	-	29,29,29,29	0
54	MG	BA	3577	1/1	0.23	-	58,58,58,58	0
54	MG	DA	3280	1/1	0.28	-	40,40,40,40	0
54	MG	CA	1656	1/1	0.12	-	97,97,97,97	0
54	MG	DA	3144	1/1	0.30	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3310	1/1	0.24	-	44,44,44,44	0
54	MG	BA	3257	1/1	0.45	-	64,64,64,64	0
54	MG	BA	3612	1/1	0.12	-	100,100,100,100	0
54	MG	DA	3357	1/1	0.12	-	53,53,53,53	0
54	MG	DA	3389	1/1	0.13	-	58,58,58,58	0
54	MG	BA	3478	1/1	0.23	-	92,92,92,92	0
54	MG	BA	3378	1/1	0.15	-	38,38,38,38	0
54	MG	CA	1613	1/1	1.02	-	71,71,71,71	0
54	MG	BA	3088	1/1	0.35	-	46,46,46,46	0
54	MG	BA	3452	1/1	0.12	-	62,62,62,62	0
54	MG	BA	3466	1/1	0.07	-	67,67,67,67	0
54	MG	BA	3560	1/1	0.11	-	29,29,29,29	0
54	MG	BA	3449	1/1	0.17	-	49,49,49,49	0
54	MG	AA	1632	1/1	0.54	-	93,93,93,93	0
54	MG	DA	3076	1/1	0.19	-	70,70,70,70	0
54	MG	DA	3180	1/1	0.21	-	78,78,78,78	0
54	MG	BB	217	1/1	0.24	-	42,42,42,42	0
54	MG	BA	3531	1/1	0.14	-	49,49,49,49	0
54	MG	BA	3503	1/1	0.21	-	68,68,68,68	0
54	MG	BA	3362	1/1	0.10	-	73,73,73,73	0
54	MG	DA	3197	1/1	0.61	-	66,66,66,66	0
54	MG	BA	3272	1/1	0.07	-	65,65,65,65	0
54	MG	DA	3329	1/1	0.11	-	47,47,47,47	0
54	MG	BA	3465	1/1	0.19	-	38,38,38,38	0
54	MG	BA	3012	1/1	0.20	-	34,34,34,34	0
54	MG	AA	1698	1/1	0.43	-	68,68,68,68	0
54	MG	BA	3234	1/1	0.31	-	34,34,34,34	0
54	MG	DA	3058	1/1	0.09	-	51,51,51,51	0
54	MG	AA	1650	1/1	0.28	-	70,70,70,70	0
54	MG	BA	3325	1/1	0.10	-	47,47,47,47	0
54	MG	DA	3022	1/1	0.38	-	52,52,52,52	0
54	MG	BA	3116	1/1	0.34	-	56,56,56,56	0
54	MG	DA	3300	1/1	0.20	-	62,62,62,62	0
54	MG	DA	3095	1/1	0.24	-	71,71,71,71	0
54	MG	BA	3187	1/1	0.29	-	30,30,30,30	0
54	MG	BA	3439	1/1	0.17	-	53,53,53,53	0
54	MG	BA	3190	1/1	0.29	-	46,46,46,46	0
54	MG	BA	3585	1/1	0.22	-	54,54,54,54	0
54	MG	BA	3092	1/1	0.39	-	55,55,55,55	0
54	MG	AA	1690	1/1	0.12	-	59,59,59,59	0
54	MG	BA	3096	1/1	0.51	-	63,63,63,63	0
54	MG	BA	3415	1/1	0.12	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1645	1/1	0.86	-	77,77,77,77	0
54	MG	AA	1679	1/1	0.35	-	64,64,64,64	0
54	MG	BA	3441	1/1	0.25	-	35,35,35,35	0
54	MG	BA	3550	1/1	0.27	-	37,37,37,37	0
54	MG	BA	3099	1/1	0.26	-	52,52,52,52	0
54	MG	BA	3368	1/1	0.30	-	34,34,34,34	0
54	MG	BA	3419	1/1	0.24	-	35,35,35,35	0
54	MG	DA	3430	1/1	0.04	-	72,72,72,72	0
54	MG	BA	3162	1/1	0.45	-	62,62,62,62	0
54	MG	BA	3182	1/1	0.06	-	69,69,69,69	0
54	MG	BA	3160	1/1	0.40	-	46,46,46,46	0
54	MG	AA	1701	1/1	0.16	-	96,96,96,96	0
54	MG	BA	3154	1/1	0.15	-	49,49,49,49	0
54	MG	BA	3609	1/1	0.20	-	51,51,51,51	0
54	MG	BA	3333	1/1	0.30	-	36,36,36,36	0
54	MG	BA	3433	1/1	0.13	-	35,35,35,35	0
54	MG	BB	204	1/1	0.18	-	67,67,67,67	0
54	MG	DA	3385	1/1	0.35	-	49,49,49,49	0
54	MG	AA	1639	1/1	0.19	-	74,74,74,74	0
54	MG	B5	101	1/1	0.24	-	51,51,51,51	0
54	MG	BA	3384	1/1	0.10	-	62,62,62,62	0
54	MG	DB	203	1/1	0.46	-	61,61,61,61	0
54	MG	DA	3045	1/1	0.39	-	72,72,72,72	0
54	MG	DA	3391	1/1	0.17	-	67,67,67,67	0
54	MG	BA	3264	1/1	0.59	-	38,38,38,38	0
54	MG	BA	3158	1/1	0.39	-	51,51,51,51	0
54	MG	BA	3177	1/1	0.06	-	45,45,45,45	0
54	MG	BA	3431	1/1	0.24	-	34,34,34,34	0
54	MG	DA	3050	1/1	0.18	-	90,90,90,90	0
54	MG	BA	3403	1/1	0.14	-	44,44,44,44	0
54	MG	BA	3571	1/1	0.14	-	76,76,76,76	0
54	MG	BA	3056	1/1	0.36	-	48,48,48,48	0
54	MG	BA	3065	1/1	0.10	-	47,47,47,47	0
54	MG	BA	3252	1/1	0.22	-	44,44,44,44	0
54	MG	DA	3152	1/1	0.47	-	58,58,58,58	0
54	MG	BA	3408	1/1	0.30	-	34,34,34,34	0
54	MG	DA	3111	1/1	0.37	-	60,60,60,60	0
54	MG	DA	3097	1/1	0.64	-	64,64,64,64	0
54	MG	DA	3056	1/1	0.45	-	61,61,61,61	0
54	MG	BA	3138	1/1	0.27	-	54,54,54,54	0
54	MG	BA	3428	1/1	0.23	-	35,35,35,35	0
54	MG	BA	3605	1/1	0.11	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1644	1/1	0.14	-	74,74,74,74	0
54	MG	BA	3126	1/1	0.39	-	57,57,57,57	0
54	MG	DA	3325	1/1	0.22	-	36,36,36,36	0
54	MG	AA	1642	1/1	0.13	-	64,64,64,64	0
54	MG	DA	3098	1/1	0.31	-	62,62,62,62	0
54	MG	DA	3390	1/1	0.16	-	69,69,69,69	0
54	MG	DA	3012	1/1	0.21	-	60,60,60,60	0
54	MG	CA	1665	1/1	0.14	-	76,76,76,76	0
54	MG	DA	3360	1/1	0.14	-	63,63,63,63	0
54	MG	CA	1628	1/1	0.26	-	55,55,55,55	0
54	MG	BA	3309	1/1	0.14	-	38,38,38,38	0
54	MG	AA	1668	1/1	0.12	-	83,83,83,83	0
54	MG	BA	3005	1/1	0.12	-	42,42,42,42	0
54	MG	DA	3136	1/1	0.53	-	42,42,42,42	0
54	MG	BA	3573	1/1	0.10	-	55,55,55,55	0
54	MG	BE	306	1/1	0.10	-	56,56,56,56	0
54	MG	BA	3412	1/1	0.20	-	41,41,41,41	0
54	MG	DA	3085	1/1	0.47	-	51,51,51,51	0
54	MG	B2	102	1/1	0.28	-	60,60,60,60	0
54	MG	BA	3212	1/1	0.17	-	47,47,47,47	0
54	MG	BA	3093	1/1	0.17	-	81,81,81,81	0
54	MG	BA	3492	1/1	0.13	-	78,78,78,78	0
54	MG	AA	1676	1/1	0.55	-	84,84,84,84	0
54	MG	B8	102	1/1	0.29	-	61,61,61,61	0
54	MG	BA	3066	1/1	0.11	-	43,43,43,43	0
54	MG	DA	3188	1/1	0.28	-	54,54,54,54	0
54	MG	BA	3376	1/1	0.09	-	55,55,55,55	0
54	MG	DA	3047	1/1	0.44	-	65,65,65,65	0
54	MG	DA	3202	1/1	0.19	-	37,37,37,37	0
54	MG	BA	3414	1/1	0.27	-	26,26,26,26	0
54	MG	BA	3361	1/1	0.19	-	53,53,53,53	0
54	MG	DA	3242	1/1	0.56	-	38,38,38,38	0
54	MG	DA	3074	1/1	0.48	-	38,38,38,38	0
54	MG	DA	3429	1/1	0.13	-	44,44,44,44	0
54	MG	DA	3417	1/1	0.24	-	81,81,81,81	0
54	MG	BA	3167	1/1	0.36	-	68,68,68,68	0
54	MG	BU	201	1/1	0.38	-	51,51,51,51	0
54	MG	BA	3033	1/1	0.36	-	40,40,40,40	0
54	MG	BA	3231	1/1	0.39	-	45,45,45,45	0
54	MG	BA	3134	1/1	0.40	-	44,44,44,44	0
54	MG	BB	206	1/1	0.14	-	62,62,62,62	0
54	MG	DA	3088	1/1	0.28	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1604	1/1	0.19	-	110,110,110,110	0
54	MG	CA	1668	1/1	0.21	-	105,105,105,105	0
54	MG	DA	3215	1/1	0.24	-	58,58,58,58	0
54	MG	DA	3294	1/1	0.14	-	52,52,52,52	0
54	MG	BA	3382	1/1	0.11	-	58,58,58,58	0
54	MG	BA	3055	1/1	0.29	-	58,58,58,58	0
54	MG	CA	1660	1/1	0.17	-	106,106,106,106	0
54	MG	BA	3275	1/1	0.23	-	41,41,41,41	0
54	MG	DA	3297	1/1	0.25	-	66,66,66,66	0
54	MG	BA	3406	1/1	0.18	-	40,40,40,40	0
54	MG	BA	3211	1/1	0.16	-	53,53,53,53	0
54	MG	AA	1613	1/1	0.26	-	74,74,74,74	0
54	MG	BA	3245	1/1	0.11	-	36,36,36,36	0
54	MG	BA	3265	1/1	0.37	-	30,30,30,30	0
54	MG	DA	3145	1/1	0.46	-	47,47,47,47	0
54	MG	BA	3613	1/1	0.13	-	109,109,109,109	0
54	MG	BA	3528	1/1	0.12	-	43,43,43,43	0
54	MG	BA	3185	1/1	0.27	-	44,44,44,44	0
54	MG	DA	3146	1/1	0.42	-	35,35,35,35	0
54	MG	BA	3087	1/1	0.25	-	56,56,56,56	0
54	MG	BA	3063	1/1	0.23	-	84,84,84,84	0
54	MG	B2	101	1/1	0.29	-	75,75,75,75	0
54	MG	BA	3338	1/1	0.15	-	30,30,30,30	0
54	MG	BA	3317	1/1	0.09	-	51,51,51,51	0
54	MG	CA	1659	1/1	0.20	-	60,60,60,60	0
54	MG	DA	3070	1/1	0.26	-	53,53,53,53	0
54	MG	CA	1626	1/1	0.30	-	86,86,86,86	0
54	MG	BB	207	1/1	0.56	-	69,69,69,69	0
54	MG	BA	3078	1/1	0.35	-	38,38,38,38	0
54	MG	BA	3003	1/1	0.36	-	29,29,29,29	0
54	MG	BB	213	1/1	0.18	-	69,69,69,69	0
54	MG	BA	3432	1/1	0.17	-	31,31,31,31	0
54	MG	BA	3598	1/1	0.11	-	39,39,39,39	0
54	MG	CA	1666	1/1	0.12	-	131,131,131,131	0
54	MG	BA	3285	1/1	0.56	-	59,59,59,59	0
54	MG	BA	3514	1/1	0.20	-	97,97,97,97	0
54	MG	DA	3190	1/1	0.29	-	57,57,57,57	0
54	MG	BA	3053	1/1	0.30	-	53,53,53,53	0
54	MG	DA	3263	1/1	0.07	-	70,70,70,70	0
54	MG	BA	3204	1/1	0.15	-	47,47,47,47	0
54	MG	BA	3004	1/1	0.27	-	41,41,41,41	0
54	MG	BA	3346	1/1	0.07	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3080	1/1	1.03	-	73,73,73,73	0
54	MG	DA	3370	1/1	0.19	-	51,51,51,51	0
54	MG	BA	3393	1/1	0.20	-	38,38,38,38	0
55	ZN	CN	101	1/1	0.17	-	188,188,188,188	0
54	MG	CA	1645	1/1	0.27	-	63,63,63,63	0
55	ZN	BY	201	1/1	0.13	-	74,74,74,74	0
54	MG	BA	3136	1/1	0.25	-	73,73,73,73	0
54	MG	BD	303	1/1	0.18	-	58,58,58,58	0
54	MG	CA	1602	1/1	0.57	-	82,82,82,82	0
54	MG	DA	3392	1/1	0.08	-	56,56,56,56	0
54	MG	DA	3261	1/1	0.37	-	56,56,56,56	0
54	MG	BA	3399	1/1	0.21	-	41,41,41,41	0
54	MG	BA	3084	1/1	0.16	-	56,56,56,56	0
54	MG	BA	3535	1/1	0.24	-	70,70,70,70	0
54	MG	DA	3378	1/1	0.14	-	98,98,98,98	0
54	MG	BA	3423	1/1	0.21	-	30,30,30,30	0
54	MG	BA	3029	1/1	0.07	-	83,83,83,83	0
54	MG	DA	3233	1/1	0.32	-	43,43,43,43	0
54	MG	DA	3155	1/1	0.26	-	57,57,57,57	0
54	MG	DA	3207	1/1	0.39	-	53,53,53,53	0
54	MG	AA	1662	1/1	0.25	-	83,83,83,83	0
54	MG	BA	3297	1/1	0.18	-	35,35,35,35	0
54	MG	BA	3013	1/1	0.51	-	103,103,103,103	0
54	MG	DA	3394	1/1	0.35	-	56,56,56,56	0
54	MG	BA	3022	1/1	0.08	-	57,57,57,57	0
54	MG	CA	1611	1/1	0.18	-	64,64,64,64	0
54	MG	DA	3224	1/1	0.34	-	80,80,80,80	0
54	MG	CA	1622	1/1	0.34	-	74,74,74,74	0
54	MG	DA	3073	1/1	0.16	-	54,54,54,54	0
54	MG	BA	3036	1/1	0.45	-	49,49,49,49	0
54	MG	DA	3375	1/1	0.13	-	50,50,50,50	0
54	MG	DA	3358	1/1	0.14	-	68,68,68,68	0
54	MG	BA	3307	1/1	0.19	-	29,29,29,29	0
54	MG	BA	3110	1/1	0.37	-	23,23,23,23	0
54	MG	DA	3306	1/1	0.11	-	88,88,88,88	0
54	MG	BA	3217	1/1	0.36	-	51,51,51,51	0
54	MG	CA	1625	1/1	0.29	-	88,88,88,88	0
54	MG	BA	3389	1/1	0.20	-	33,33,33,33	0
54	MG	BA	3192	1/1	0.26	-	43,43,43,43	0
54	MG	CA	1641	1/1	0.20	-	74,74,74,74	0
54	MG	DA	3060	1/1	0.19	-	60,60,60,60	0
54	MG	BA	3195	1/1	0.32	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3288	1/1	0.10	-	37,37,37,37	0
54	MG	BR	202	1/1	0.29	-	49,49,49,49	0
54	MG	BA	3282	1/1	0.28	-	43,43,43,43	0
54	MG	DA	3221	1/1	0.42	-	69,69,69,69	0
54	MG	BA	3592	1/1	0.08	-	51,51,51,51	0
54	MG	BA	3290	1/1	0.33	-	47,47,47,47	0
54	MG	AA	1614	1/1	0.23	-	62,62,62,62	0
54	MG	DA	3380	1/1	0.10	-	91,91,91,91	0
54	MG	BB	216	1/1	0.33	-	46,46,46,46	0
54	MG	BA	3223	1/1	0.17	-	57,57,57,57	0
54	MG	DA	3231	1/1	0.42	-	54,54,54,54	0
54	MG	BA	3337	1/1	0.22	-	33,33,33,33	0
54	MG	DA	3413	1/1	0.18	-	37,37,37,37	0
54	MG	DA	3090	1/1	0.20	-	53,53,53,53	0
54	MG	DA	3326	1/1	0.11	-	95,95,95,95	0
54	MG	DA	3314	1/1	0.22	-	54,54,54,54	0
54	MG	AA	1616	1/1	0.38	-	79,79,79,79	0
54	MG	D8	101	1/1	0.57	-	49,49,49,49	0
54	MG	BA	3141	1/1	0.27	-	65,65,65,65	0
54	MG	DD	301	1/1	0.17	-	40,40,40,40	0
54	MG	BA	3510	1/1	0.17	-	33,33,33,33	0
54	MG	BA	3246	1/1	0.19	-	49,49,49,49	0
54	MG	BA	3311	1/1	0.28	-	60,60,60,60	0
55	ZN	CD	301	1/1	0.31	-	96,96,96,96	0
54	MG	BA	3183	1/1	0.29	-	76,76,76,76	0
54	MG	BA	3458	1/1	0.18	-	45,45,45,45	0
54	MG	BA	3328	1/1	0.18	-	27,27,27,27	0
54	MG	BQ	203	1/1	0.20	-	44,44,44,44	0
54	MG	CA	1607	1/1	0.23	-	72,72,72,72	0
54	MG	BA	3572	1/1	0.15	-	49,49,49,49	0
54	MG	DB	202	1/1	1.12	-	86,86,86,86	0
54	MG	AA	1630	1/1	0.51	-	76,76,76,76	0
54	MG	BB	209	1/1	0.17	-	79,79,79,79	0
54	MG	BA	3277	1/1	0.24	-	66,66,66,66	0
54	MG	BA	3360	1/1	0.16	-	53,53,53,53	0
54	MG	BA	3543	1/1	0.20	-	59,59,59,59	0
54	MG	BA	3069	1/1	0.47	-	53,53,53,53	0
54	MG	DA	3015	1/1	0.38	-	71,71,71,71	0
55	ZN	B9	101	1/1	0.13	-	69,69,69,69	0
54	MG	DA	3262	1/1	0.18	-	46,46,46,46	0
54	MG	BA	3051	1/1	0.14	-	52,52,52,52	0
54	MG	DA	3117	1/1	0.32	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1696	1/1	0.18	-	74,74,74,74	0
54	MG	DA	3071	1/1	0.30	-	60,60,60,60	0
54	MG	DA	3101	1/1	0.21	-	62,62,62,62	0
54	MG	BA	3009	1/1	0.20	-	59,59,59,59	0
54	MG	DA	3317	1/1	0.13	-	94,94,94,94	0
54	MG	BA	3202	1/1	0.38	-	65,65,65,65	0
54	MG	BA	3416	1/1	0.14	-	46,46,46,46	0
54	MG	BA	3344	1/1	0.11	-	52,52,52,52	0
54	MG	BA	3590	1/1	0.18	-	82,82,82,82	0
54	MG	BA	3205	1/1	0.39	-	61,61,61,61	0
54	MG	BA	3540	1/1	0.06	-	61,61,61,61	0
54	MG	BA	3551	1/1	0.25	-	40,40,40,40	0
54	MG	DA	3133	1/1	0.35	-	78,78,78,78	0
54	MG	DA	3214	1/1	0.65	-	74,74,74,74	0
54	MG	DA	3238	1/1	0.59	-	52,52,52,52	0
54	MG	DA	3313	1/1	0.20	-	64,64,64,64	0
54	MG	BA	3305	1/1	0.09	-	37,37,37,37	0
54	MG	AA	1703	1/1	0.18	-	89,89,89,89	0
55	ZN	AD	301	1/1	0.23	-	107,107,107,107	0
54	MG	DA	3160	1/1	0.48	-	48,48,48,48	0
54	MG	BA	3334	1/1	0.17	-	43,43,43,43	0
54	MG	BA	3289	1/1	0.65	-	50,50,50,50	0
54	MG	BA	3259	1/1	0.30	-	51,51,51,51	0
54	MG	BA	3499	1/1	0.20	-	107,107,107,107	0
54	MG	BA	3227	1/1	0.17	-	42,42,42,42	0
54	MG	DA	3046	1/1	0.69	-	43,43,43,43	0
54	MG	DA	3405	1/1	0.17	-	70,70,70,70	0
54	MG	BA	3040	1/1	0.21	-	33,33,33,33	0
54	MG	BA	3370	1/1	0.08	-	66,66,66,66	0
54	MG	DA	3041	1/1	0.21	-	49,49,49,49	0
54	MG	CA	1614	1/1	0.25	-	69,69,69,69	0
54	MG	DA	3061	1/1	0.31	-	52,52,52,52	0
54	MG	BA	3385	1/1	0.11	-	73,73,73,73	0
54	MG	DA	3283	1/1	0.13	-	48,48,48,48	0
54	MG	BA	3071	1/1	0.19	-	49,49,49,49	0
54	MG	BA	3221	1/1	0.17	-	51,51,51,51	0
54	MG	B3	102	1/1	0.23	-	54,54,54,54	0
54	MG	DA	3087	1/1	0.29	-	58,58,58,58	0
54	MG	BR	201	1/1	0.55	-	58,58,58,58	0
54	MG	DA	3186	1/1	0.21	-	42,42,42,42	0
54	MG	BA	3480	1/1	0.15	-	70,70,70,70	0
54	MG	AA	1647	1/1	0.37	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3122	1/1	0.49	-	47,47,47,47	0
54	MG	DA	3154	1/1	0.79	-	62,62,62,62	0
54	MG	BA	3060	1/1	0.21	-	45,45,45,45	0
54	MG	DA	3373	1/1	0.28	-	38,38,38,38	0
54	MG	DA	3055	1/1	0.46	-	43,43,43,43	0
54	MG	BA	3302	1/1	0.28	-	45,45,45,45	0
54	MG	AA	1691	1/1	0.10	-	58,58,58,58	0
54	MG	BA	3552	1/1	0.17	-	38,38,38,38	0
54	MG	BA	3121	1/1	0.14	-	38,38,38,38	0
54	MG	BA	3371	1/1	0.08	-	67,67,67,67	0
54	MG	DA	3217	1/1	0.27	-	69,69,69,69	0
54	MG	BA	3351	1/1	0.22	-	57,57,57,57	0
54	MG	DA	3177	1/1	0.83	-	59,59,59,59	0
54	MG	DA	3383	1/1	0.25	-	63,63,63,63	0
54	MG	DA	3114	1/1	0.16	-	51,51,51,51	0
54	MG	CA	1664	1/1	0.11	-	94,94,94,94	0
54	MG	BA	3594	1/1	0.15	-	70,70,70,70	0
54	MG	BA	3320	1/1	0.18	-	57,57,57,57	0
54	MG	BA	3123	1/1	0.18	-	43,43,43,43	0
54	MG	DA	3237	1/1	0.53	-	39,39,39,39	0
54	MG	BA	3151	1/1	0.26	-	62,62,62,62	0
54	MG	BA	3112	1/1	0.39	-	47,47,47,47	0
54	MG	BA	3409	1/1	0.17	-	26,26,26,26	0
54	MG	BE	301	1/1	0.54	-	43,43,43,43	0
54	MG	BA	3326	1/1	0.13	-	30,30,30,30	0
54	MG	DA	3246	1/1	0.44	-	41,41,41,41	0
54	MG	CA	1658	1/1	0.16	-	83,83,83,83	0
54	MG	DA	3196	1/1	0.48	-	63,63,63,63	0
54	MG	AA	1669	1/1	0.37	-	96,96,96,96	0
54	MG	AA	1695	1/1	0.10	-	93,93,93,93	0
54	MG	BA	3268	1/1	0.23	-	44,44,44,44	0
54	MG	DA	3245	1/1	0.33	-	47,47,47,47	0
54	MG	DA	3409	1/1	0.06	-	79,79,79,79	0
54	MG	BA	3314	1/1	0.15	-	71,71,71,71	0
54	MG	BA	3417	1/1	0.20	-	37,37,37,37	0
54	MG	BA	3200	1/1	0.25	-	51,51,51,51	0
54	MG	AA	1624	1/1	0.86	-	66,66,66,66	0
54	MG	DA	3033	1/1	0.24	-	68,68,68,68	0
54	MG	DA	3203	1/1	0.72	-	48,48,48,48	0
54	MG	DA	3402	1/1	0.21	-	59,59,59,59	0
54	MG	CA	1601	1/1	0.39	-	50,50,50,50	0
54	MG	DA	3377	1/1	0.10	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3327	1/1	0.41	-	94,94,94,94	0
54	MG	BA	3525	1/1	0.08	-	112,112,112,112	0
54	MG	BA	3094	1/1	0.15	-	41,41,41,41	0
54	MG	AA	1670	1/1	0.17	-	115,115,115,115	0
54	MG	BA	3139	1/1	0.24	-	53,53,53,53	0
54	MG	BA	3394	1/1	0.10	-	29,29,29,29	0
54	MG	CA	1637	1/1	0.62	-	67,67,67,67	0
54	MG	BA	3548	1/1	0.19	-	41,41,41,41	0
54	MG	DA	3092	1/1	0.27	-	63,63,63,63	0
54	MG	DA	3264	1/1	0.18	-	46,46,46,46	0
54	MG	BB	208	1/1	0.26	-	70,70,70,70	0
54	MG	DA	3121	1/1	0.64	-	53,53,53,53	0
54	MG	DF	302	1/1	0.20	-	64,64,64,64	0
54	MG	BA	3587	1/1	0.08	-	66,66,66,66	0
54	MG	CA	1639	1/1	0.65	-	61,61,61,61	0
54	MG	CA	1647	1/1	0.10	-	78,78,78,78	0
54	MG	DA	3134	1/1	0.24	-	64,64,64,64	0
54	MG	BA	3274	1/1	0.15	-	81,81,81,81	0
54	MG	BA	3435	1/1	0.27	-	36,36,36,36	0
54	MG	AA	1705	1/1	0.13	-	68,68,68,68	0
54	MG	DA	3334	1/1	0.15	-	56,56,56,56	0
54	MG	BA	3267	1/1	0.54	-	53,53,53,53	0
54	MG	DA	3067	1/1	0.32	-	32,32,32,32	0
54	MG	BA	3447	1/1	0.27	-	37,37,37,37	0
54	MG	DA	3340	1/1	0.38	-	44,44,44,44	0
54	MG	DA	3277	1/1	0.10	-	42,42,42,42	0
54	MG	CA	1640	1/1	0.34	-	62,62,62,62	0
54	MG	DA	3420	1/1	0.09	-	97,97,97,97	0
54	MG	DA	3344	1/1	0.07	-	51,51,51,51	0
54	MG	BA	3468	1/1	0.15	-	38,38,38,38	0
54	MG	AA	1655	1/1	0.19	-	90,90,90,90	0
54	MG	BA	3303	1/1	0.20	-	36,36,36,36	0
54	MG	BA	3554	1/1	0.22	-	58,58,58,58	0
54	MG	BA	3152	1/1	0.22	-	73,73,73,73	0
54	MG	AA	1619	1/1	0.32	-	68,68,68,68	0
54	MG	BA	3097	1/1	0.43	-	58,58,58,58	0
54	MG	BA	3544	1/1	0.16	-	91,91,91,91	0
54	MG	DA	3382	1/1	0.09	-	53,53,53,53	0
54	MG	DA	3078	1/1	0.37	-	53,53,53,53	0
54	MG	BA	3210	1/1	0.20	-	57,57,57,57	0
54	MG	AA	1702	1/1	0.20	-	97,97,97,97	0
54	MG	BA	3090	1/1	0.15	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3132	1/1	0.38	-	49,49,49,49	0
54	MG	BB	201	1/1	0.15	-	61,61,61,61	0
54	MG	DA	3284	1/1	0.15	-	61,61,61,61	0
54	MG	BA	3045	1/1	0.17	-	62,62,62,62	0
54	MG	DA	3416	1/1	0.12	-	32,32,32,32	0
54	MG	BA	3237	1/1	0.32	-	56,56,56,56	0
54	MG	BA	3107	1/1	0.14	-	49,49,49,49	0
54	MG	BA	3014	1/1	0.17	-	57,57,57,57	0
54	MG	BA	3486	1/1	0.11	-	48,48,48,48	0
54	MG	DA	3292	1/1	0.18	-	39,39,39,39	0
54	MG	BA	3575	1/1	0.04	-	54,54,54,54	0
54	MG	DA	3053	1/1	0.33	-	54,54,54,54	0
54	MG	BQ	201	1/1	0.15	-	49,49,49,49	0
54	MG	BA	3312	1/1	0.08	-	50,50,50,50	0
54	MG	BA	3105	1/1	0.12	-	40,40,40,40	0
54	MG	BA	3509	1/1	0.22	-	85,85,85,85	0
54	MG	B1	101	1/1	0.28	-	50,50,50,50	0
54	MG	BA	3137	1/1	0.17	-	38,38,38,38	0
54	MG	BA	3372	1/1	0.14	-	50,50,50,50	0
54	MG	DA	3123	1/1	0.19	-	56,56,56,56	0
54	MG	DA	3086	1/1	0.63	-	54,54,54,54	0
54	MG	DA	3112	1/1	0.32	-	60,60,60,60	0
54	MG	BA	3148	1/1	0.32	-	54,54,54,54	0
54	MG	DA	3010	1/1	0.17	-	43,43,43,43	0
54	MG	DA	3324	1/1	0.21	-	64,64,64,64	0
54	MG	DA	3425	1/1	0.07	-	60,60,60,60	0
54	MG	BA	3437	1/1	0.20	-	28,28,28,28	0
54	MG	BA	3522	1/1	0.47	-	68,68,68,68	0
54	MG	CA	1655	1/1	0.28	-	74,74,74,74	0
54	MG	BA	3520	1/1	0.22	-	67,67,67,67	0
54	MG	BA	3460	1/1	0.09	-	58,58,58,58	0
54	MG	BA	3304	1/1	0.16	-	27,27,27,27	0
54	MG	BA	3557	1/1	0.51	-	42,42,42,42	0
54	MG	BA	3474	1/1	0.18	-	66,66,66,66	0
54	MG	BA	3556	1/1	0.18	-	58,58,58,58	0
54	MG	DA	3395	1/1	0.26	-	37,37,37,37	0
54	MG	BA	3395	1/1	0.12	-	32,32,32,32	0
54	MG	DA	3007	1/1	0.20	-	36,36,36,36	0
54	MG	DA	3064	1/1	0.20	-	53,53,53,53	0
54	MG	DA	3205	1/1	0.07	-	82,82,82,82	0
54	MG	BA	3262	1/1	0.41	-	32,32,32,32	0
54	MG	DA	3305	1/1	0.09	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3052	1/1	0.25	-	61,61,61,61	0
54	MG	BA	3271	1/1	0.15	-	60,60,60,60	0
54	MG	BA	3039	1/1	0.27	-	44,44,44,44	0
54	MG	BA	3240	1/1	0.38	-	64,64,64,64	0
54	MG	DA	3019	1/1	0.17	-	41,41,41,41	0
54	MG	DA	3268	1/1	0.15	-	43,43,43,43	0
54	MG	BA	3249	1/1	0.24	-	70,70,70,70	0
54	MG	BA	3243	1/1	0.12	-	117,117,117,117	0
54	MG	DA	3040	1/1	0.31	-	50,50,50,50	0
54	MG	BA	3454	1/1	0.15	-	34,34,34,34	0
54	MG	CA	1643	1/1	0.05	-	109,109,109,109	0
54	MG	DA	3054	1/1	0.64	-	75,75,75,75	0
54	MG	BA	3292	1/1	0.19	-	44,44,44,44	0
54	MG	BA	3607	1/1	0.12	-	38,38,38,38	0
54	MG	DA	3004	1/1	0.19	-	59,59,59,59	0
54	MG	BA	3219	1/1	0.33	-	62,62,62,62	0
54	MG	DA	3002	1/1	0.62	-	67,67,67,67	0
54	MG	BA	3407	1/1	0.21	-	35,35,35,35	0
54	MG	DA	3397	1/1	0.04	-	65,65,65,65	0
54	MG	DA	3127	1/1	0.25	-	63,63,63,63	0
54	MG	BA	3010	1/1	0.19	-	48,48,48,48	0
54	MG	AA	1674	1/1	0.22	-	73,73,73,73	0
54	MG	DA	3366	1/1	0.13	-	35,35,35,35	0
54	MG	BA	3329	1/1	0.13	-	45,45,45,45	0
55	ZN	D5	101	1/1	0.07	-	65,65,65,65	0
54	MG	BQ	202	1/1	0.37	-	53,53,53,53	0
54	MG	AA	1673	1/1	0.27	-	67,67,67,67	0
54	MG	AA	1700	1/1	0.37	-	114,114,114,114	0
54	MG	DA	3142	1/1	0.25	-	46,46,46,46	0
54	MG	BA	3156	1/1	0.15	-	57,57,57,57	0
54	MG	BA	3332	1/1	0.29	-	60,60,60,60	0
54	MG	BA	3016	1/1	0.37	-	57,57,57,57	0
54	MG	BA	3173	1/1	0.28	-	65,65,65,65	0
54	MG	BA	3207	1/1	0.14	-	59,59,59,59	0
54	MG	DA	3181	1/1	0.67	-	51,51,51,51	0
54	MG	DA	3328	1/1	0.08	-	34,34,34,34	0
54	MG	BA	3283	1/1	0.53	-	56,56,56,56	0
54	MG	DA	3030	1/1	0.17	-	52,52,52,52	0
54	MG	BA	3281	1/1	0.26	-	56,56,56,56	0
54	MG	BA	3132	1/1	0.32	-	31,31,31,31	0
54	MG	BA	3457	1/1	0.13	-	91,91,91,91	0
54	MG	CA	1624	1/1	0.41	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3367	1/1	0.22	-	33,33,33,33	0
54	MG	DA	3319	1/1	0.10	-	59,59,59,59	0
54	MG	AA	1694	1/1	0.17	-	110,110,110,110	0
54	MG	BA	3555	1/1	0.27	-	49,49,49,49	0
55	ZN	B6	101	1/1	0.12	-	54,54,54,54	0
54	MG	BA	3122	1/1	0.33	-	56,56,56,56	0
54	MG	DA	3199	1/1	0.06	-	74,74,74,74	0
54	MG	BA	3119	1/1	0.16	-	39,39,39,39	0
54	MG	BA	3498	1/1	0.15	-	69,69,69,69	0
54	MG	AA	1697	1/1	0.17	-	75,75,75,75	0
54	MG	DA	3282	1/1	0.07	-	42,42,42,42	0
54	MG	BA	3130	1/1	0.39	-	32,32,32,32	0
54	MG	DA	3043	1/1	0.22	-	63,63,63,63	0
54	MG	BA	3178	1/1	0.17	-	58,58,58,58	0
54	MG	BA	3512	1/1	0.32	-	45,45,45,45	0
54	MG	AA	1666	1/1	0.53	-	62,62,62,62	0
54	MG	BA	3357	1/1	0.16	-	47,47,47,47	0
54	MG	BA	3017	1/1	0.13	-	47,47,47,47	0
54	MG	BA	3091	1/1	0.35	-	47,47,47,47	0
54	MG	DA	3398	1/1	0.10	-	52,52,52,52	0
54	MG	BA	3559	1/1	0.28	-	39,39,39,39	0
54	MG	BA	3106	1/1	0.38	-	48,48,48,48	0
54	MG	BA	3596	1/1	0.13	-	46,46,46,46	0
54	MG	DA	3036	1/1	0.19	-	65,65,65,65	0
54	MG	BA	3169	1/1	0.51	-	60,60,60,60	0
54	MG	CA	1646	1/1	0.46	-	92,92,92,92	0
54	MG	BA	3057	1/1	0.21	-	46,46,46,46	0
54	MG	DA	3209	1/1	0.26	-	79,79,79,79	0
54	MG	AA	1660	1/1	0.98	-	91,91,91,91	0
54	MG	AA	1684	1/1	0.05	-	76,76,76,76	0
54	MG	AA	1602	1/1	0.27	-	111,111,111,111	0
54	MG	DA	3094	1/1	0.16	-	39,39,39,39	0
54	MG	BA	3565	1/1	0.26	-	90,90,90,90	0
54	MG	BA	3043	1/1	0.31	-	54,54,54,54	0
54	MG	BA	3258	1/1	0.41	-	56,56,56,56	0
54	MG	BA	3086	1/1	0.26	-	57,57,57,57	0
54	MG	BA	3083	1/1	0.43	-	56,56,56,56	0
54	MG	BA	3497	1/1	0.17	-	55,55,55,55	0
54	MG	BA	3038	1/1	0.09	-	36,36,36,36	0
54	MG	DA	3243	1/1	0.35	-	53,53,53,53	0
54	MG	BA	3484	1/1	0.12	-	40,40,40,40	0
54	MG	DA	3178	1/1	0.48	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3330	1/1	0.26	-	36,36,36,36	0
54	MG	BA	3175	1/1	0.34	-	70,70,70,70	0
54	MG	BA	3411	1/1	0.28	-	43,43,43,43	0
54	MG	AA	1686	1/1	0.17	-	115,115,115,115	0
54	MG	BA	3276	1/1	0.63	-	56,56,56,56	0
54	MG	BA	3226	1/1	0.32	-	62,62,62,62	0
54	MG	BA	3256	1/1	0.65	-	69,69,69,69	0
54	MG	CA	1633	1/1	0.29	-	71,71,71,71	0
54	MG	BA	3583	1/1	0.05	-	50,50,50,50	0
54	MG	BA	3546	1/1	0.08	-	57,57,57,57	0
54	MG	BA	3117	1/1	0.25	-	31,31,31,31	0
54	MG	DB	205	1/1	0.14	-	70,70,70,70	0

6.5 Other polymers ⓘ

There are no such residues in this entry.