



# wwPDB X-ray Structure Validation Summary Report i

Jun 16, 2014 – 09:16 PM BST

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

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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

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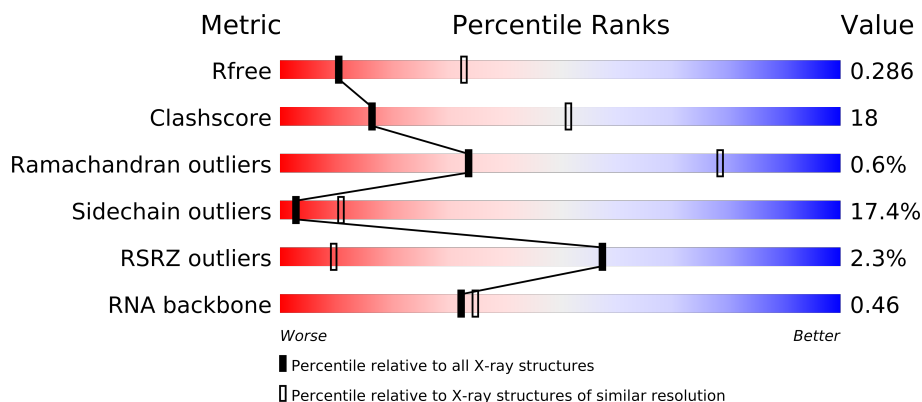
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

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  $\geq 3$ , 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	AX	101	
22	CX	101	
23	BA	2913	
23	DA	2913	
24	BB	122	
24	DB	122	
25	BD	276	
25	DD	276	
26	BE	206	
26	DE	206	
27	BF	210	
27	DF	210	



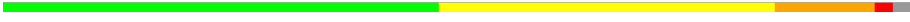



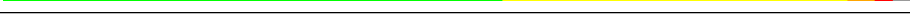

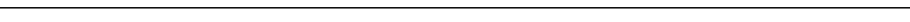

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Mol	Chain	Length	Quality of chain
28	BG	182	
28	DG	182	
29	BH	180	
29	DH	180	
30	BI	148	
30	DI	148	
31	BN	140	
31	DN	140	
32	BO	122	
32	DO	122	
33	BP	150	
33	DP	150	
34	BQ	141	
34	DQ	141	
35	BR	118	
35	DR	118	
36	BS	112	
36	DS	112	
37	BT	146	
37	DT	146	
38	BU	118	
38	DU	118	
39	BV	101	
39	DV	101	
40	BW	113	
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	
49	D5	60	
50	B6	54	
50	D6	54	
51	B7	49	
51	D7	49	
52	B8	65	
52	D8	65	
53	B9	37	
53	D9	37	

## 2 Entry composition

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	230	Total	C	N	O	S	0	0	0
			1787	1141	319	322	5			
2	CB	229	Total	C	N	O	S	0	0	0
			1775	1132	318	320	5			

- Molecule 3 is a protein called 30S Ribosomal Protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1450	906	279	264	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1450	906	279	264	1			

- Molecule 4 is a protein called 30S Ribosomal Protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1526	963	283	274	6			
4	CD	208	Total	C	N	O	S	0	0	0
			1526	963	283	274	6			

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	4			
5	CE	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	4			

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			777	493	137	144	3			
6	CF	100	Total	C	N	O	S	0	0	0
			777	493	137	144	3			

- Molecule 7 is a protein called 30S Ribosomal Protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1164	726	224	208	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1164	726	224	208	6			

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	AJ	96	Total	C	N	O	0	0	0
			663	410	132	121			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CJ	96	Total	C	N	O			
			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	0
11	CK	114	Total	C	N	O	S			
			828	516	155	154	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	122	Total	C	N	O	S			
			905	567	178	159	1	0	0	0
12	CL	122	Total	C	N	O	S			
			905	567	178	159	1	0	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	0
13	CM	114	Total	C	N	O	S			
			804	497	164	142	1	0	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	0
14	CN	60	Total	C	N	O	S			
			478	303	99	72	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S			
			724	453	143	126	2	0	0	0
15	CO	88	Total	C	N	O	S			
			724	453	143	126	2	0	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	87	Total	C	N	O	S	0	0	0
			665	410	142	111	2			
20	CT	97	Total	C	N	O	S	0	0	0
			713	438	152	121	2			

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

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

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

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

There are 12 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BD	275	Total	C	N	O	S	0	0	0
			2135	1349	422	361	3			
25	DD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	203	Total	C	N	O	S	0	0	1
			1580	1007	298	273	2			
27	DF	203	Total	C	N	O	S	0	0	1
			1580	1007	298	273	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BI	146	Total	C	N	O	S	0	0	0
			1037	666	180	190	1			
30	DI	146	Total	C	N	O	S	0	0	0
			953	608	168	176	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a protein called 50S Ribosomal Protein L36.

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

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BA	660	Total	Mg	0	0
			660	660		
54	CA	162	Total	Mg	0	0
			162	162		
54	DQ	2	Total	Mg	0	0
			2	2		
54	DF	1	Total	Mg	0	0
			1	1		
54	B8	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BE	5	Total 5	Mg 5	0	0
54	B1	1	Total 1	Mg 1	0	0
54	BP	1	Total 1	Mg 1	0	0
54	B5	2	Total 2	Mg 2	0	0
54	BB	23	Total 23	Mg 23	0	0
54	BT	2	Total 2	Mg 2	0	0
54	D8	2	Total 2	Mg 2	0	0
54	B9	1	Total 1	Mg 1	0	0
54	BF	2	Total 2	Mg 2	0	0
54	DR	3	Total 3	Mg 3	0	0
54	B2	1	Total 1	Mg 1	0	0
54	AA	135	Total 135	Mg 135	0	0
54	BQ	4	Total 4	Mg 4	0	0
54	CQ	1	Total 1	Mg 1	0	0
54	AD	1	Total 1	Mg 1	0	0
54	DD	2	Total 2	Mg 2	0	0
54	D0	2	Total 2	Mg 2	0	0
54	BG	1	Total 1	Mg 1	0	0
54	B3	1	Total 1	Mg 1	0	0
54	BR	1	Total 1	Mg 1	0	0
54	DA	598	Total 598	Mg 598	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	DP	1	Total 1	Mg 1	0	0
54	BV	1	Total 1	Mg 1	0	0
54	DO	2	Total 2	Mg 2	0	0
54	DE	4	Total 4	Mg 4	0	0
54	AQ	1	Total 1	Mg 1	0	0
54	D1	1	Total 1	Mg 1	0	0
54	BZ	1	Total 1	Mg 1	0	0
54	AC	1	Total 1	Mg 1	0	0
54	BS	1	Total 1	Mg 1	0	0
54	D5	1	Total 1	Mg 1	0	0
54	BD	3	Total 3	Mg 3	0	0
54	B0	3	Total 3	Mg 3	0	0
54	CE	1	Total 1	Mg 1	0	0
54	BW	2	Total 2	Mg 2	0	0
54	AF	1	Total 1	Mg 1	0	0
54	DB	8	Total 8	Mg 8	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

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

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

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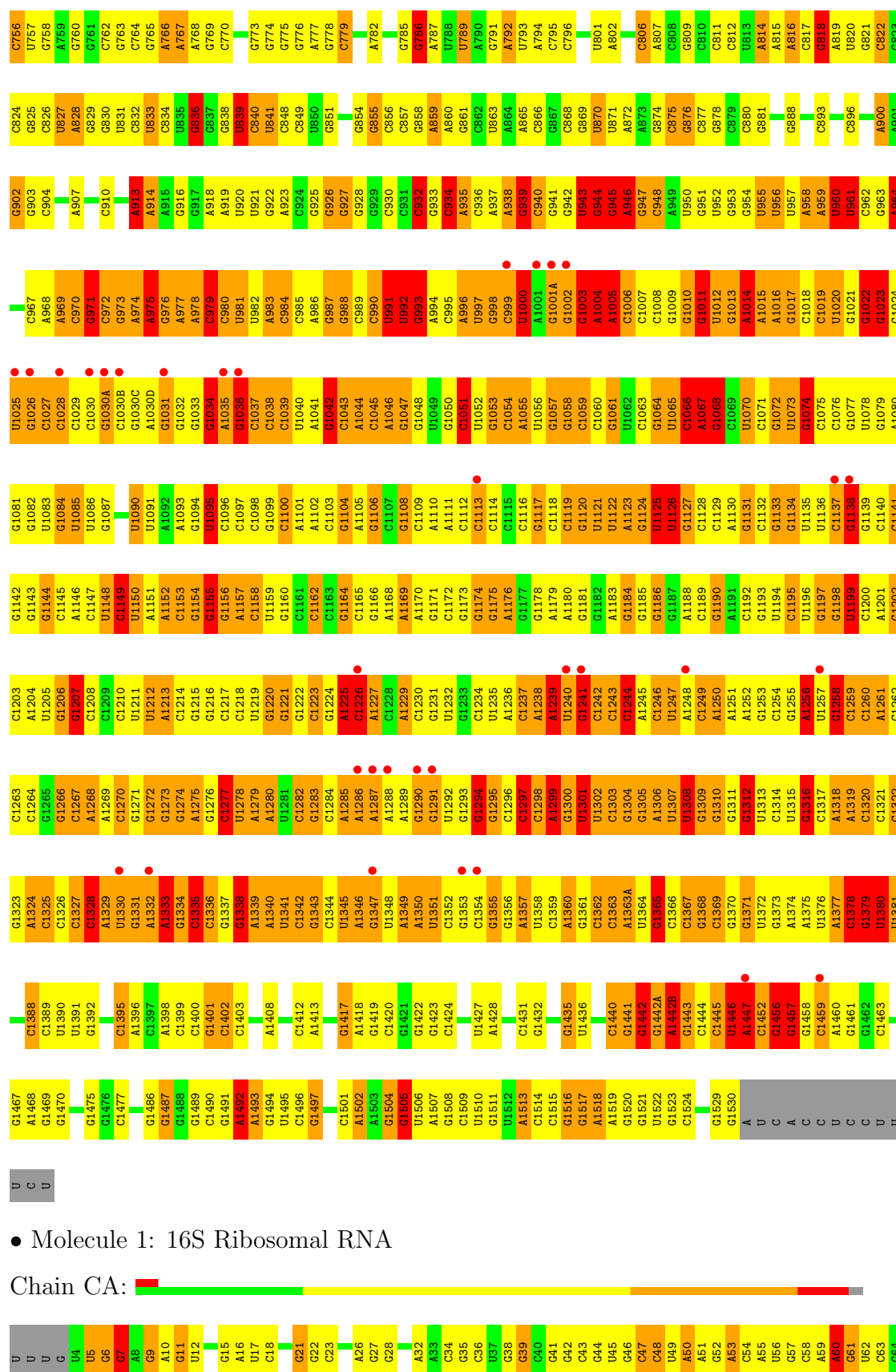
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56	B8	10	Total 10	O 10	0	0
56	B9	1	Total 1	O 1	0	0
56	CA	265	Total 265	O 265	0	0
56	CC	1	Total 1	O 1	0	0
56	CD	1	Total 1	O 1	0	0
56	CE	2	Total 2	O 2	0	0
56	CK	1	Total 1	O 1	0	0
56	CL	2	Total 2	O 2	0	0
56	CN	1	Total 1	O 1	0	0
56	CP	1	Total 1	O 1	0	0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

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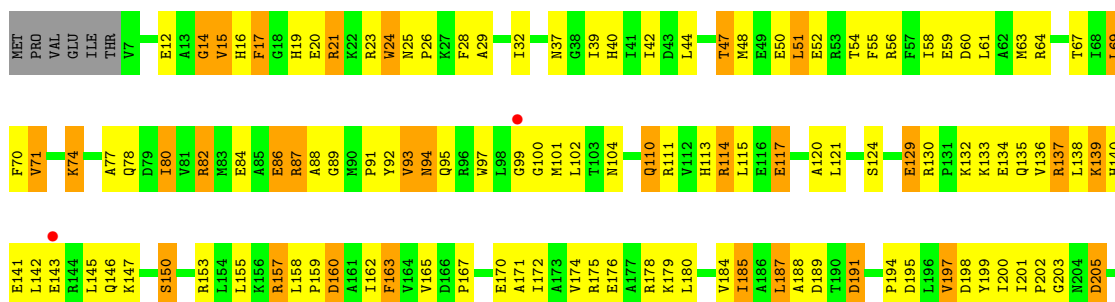
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			10	10		
56	DQ	3	Total	O	0	0
			3	3		
56	DR	2	Total	O	0	0
			2	2		
56	DT	2	Total	O	0	0
			2	2		
56	DU	5	Total	O	0	0
			5	5		
56	DV	2	Total	O	0	0
			2	2		
56	DW	2	Total	O	0	0
			2	2		
56	DX	1	Total	O	0	0
			1	1		
56	DY	2	Total	O	0	0
			2	2		
56	D0	1	Total	O	0	0
			1	1		
56	D1	5	Total	O	0	0
			5	5		
56	D3	1	Total	O	0	0
			1	1		
56	D4	1	Total	O	0	0
			1	1		
56	D7	3	Total	O	0	0
			3	3		
56	D8	1	Total	O	0	0
			1	1		

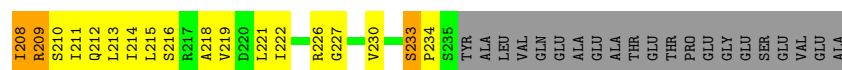






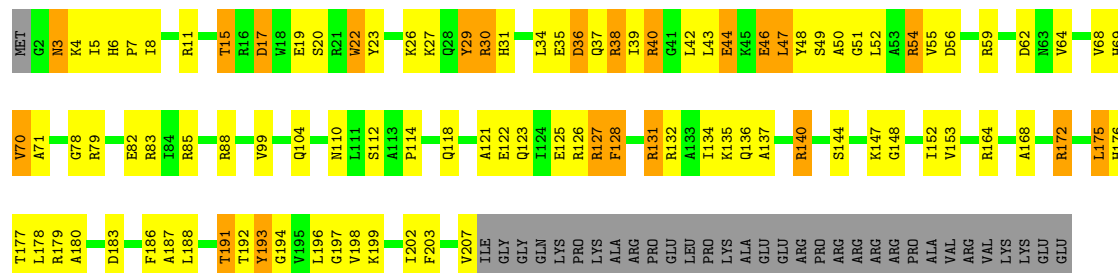
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A1111	C1051	G1060	C995	A935	C857	C783	G713	G637	C570	G505	G426	G361	C291	C201	G144	G66
C1112	U1052	A996	U997	C936	A858	C784	G714	G638	U571	A509	G428	U365	G292	U202	G145	C67
C1113	G1053	A938	C998	A937	A860	C785	G715	A642	A572	C511	A430	U367	U284	U203	G146	G68
C1114	C1054	G939	C999	A938	G861	C786	G717	A646	A573	C512	A431	U368	U285	U204	G147	G69
C1115	A1055	C940	U1000	C940	A865	A787	G718	U646	A574	C513	C433	U369	U286	G216	G148	G70
C1116	U1056	G941	A1001	C941	A866	G791	G721	C647	C575	C514	C434	C370	C287	G217	C150	C71
C1117	G1057	U942	G1001A	G942	C866	A792	A722	G650	G576	C515	A435	C371	A298	C221	A151	C72
C1118	C1058	U943	G1002	U943	C867	A793	U723	G651	G577	C516	C436	C372	A300	U222	G152	C76
C1119	G1059	G944	G1003	G944	C868	A794	G724	U652	U580	C517	A437	C373	G299	U223	G157	G77
G1120	C1060	G945	G1004	G945	C869	C795	G725	U653	U581	C518	G438	A374	A300	C224	G157	G78
U1121	A1005	U870	A1005	U870	A653	C796	C726	A653	U582	C519	A439	U375	G297	C225	G158	G79
U1122	C1066	U871	C1066	G947	U871	C796	C726	A653	U583	C520	A441	U376	A298	G226	G159	G
C1063	C1007	A872	C1007	C948	A872	A802	A729	G657	A583	A521	C442	G377	C307	G227	A160	U
G1064	C1008	A873	G1008	A949	A873	G803	A730	G658	A584	C522	C443	G378	C308	G232	A161	U
U1065	G1009	C874	U950	C874	A874	U804	G731	U659	G585	C523	C444	C379	G309	G233	A162	U
C1066	G1010	C875	C805	G951	C875	C805	G732	G660	C586	C524	C445	G380	G310	G234	G163	A
A1067	G1011	C876	C806	G952	C876	C806	G733	G661	C587	C525	C446	G381	G311	G235	G164	C
G1068	U1012	C877	A807	G953	C877	A807	G734	G662	C588	C526	C447	G382	G312	G236	U160	U90
C1069	G1013	C878	C808	G954	C878	C808	G735	G663	C589	C527	C448	G383	G313	G237	C165	C91
U1070	A1014	C879	G809	U955	C879	G809	A737	G664	C590	C528	C449	A384	G314	C240	C166	C92
C1071	A1015	C880	C810	U956	C880	C810	G738	G665	C591	C529	C450	G385	G315	C241	G167	G93
G1072	G1016	U957	C811	U957	C881	C811	G739	G666	C592	C530	C451	C386	G316	C242	G168	G94
U1073	A1017	C882	C812	U958	C882	C812	U740	G667	C593	C531	C452	C387	G317	C243	G169	U96
G1074	C1018	C883	U813	A959	C883	U813	G741	G668	C600	C532	C453	U387	G318	A244	G170	C97
C1075	C1019	U884	A814	U960	U884	A814	G742	G669	C601	C533	C454	G388	G319	G245	U171	C98
U1076	U1020	C885	A815	U961	C885	A815	G743	G670	C602	C534	C455	G389	G320	G246	A171	G99
G1077	G1021	G962	C817	C962	C886	A816	A746	U672	U603	C535	C456	C390	G321	C247	A172	U99
C1078	G1022	G963	C818	G963	C887	C818	G747	U673	C604	C536	C457	C391	G322	G248	U173	C100
G1079	G1023	C888	G818	A964	C888	G818	C747	U674	U605	C537	C458	G392	G323	U252	C174	A101
C1080	A965	C889	A819	G965	C889	A819	C748	U675	U606	C538	C459	G393	G324	U253	C175	G102
U1081	U1024	C890	C820	A966	C890	C820	G749	U676	A607	C539	C460	G394	G325	G254	C176	C103
G1082	G1026	C967	G821	C967	C891	G821	U750	U677	A608	C540	C461	G395	G326	G255	G104	G105
U1083	C1027	A968	C822	A968	C892	C822	U751	U678	A609	C541	C462	G396	G327	G256	C106	C106
G1084	A969	G901	G823	A969	C893	G823	G752	C679	G610	C542	C463	G397	G328	G257	U182	G183
U1085	C1028	G902	G824	C970	C894	G824	A753	C680	A611	C543	C464	C398	G329	G258	G184	A109
U1086	G1030	G903	C826	C971	C895	C826	G754	C681	A612	C544	C465	C401	G330	G259	A185	G113
U1087	U1030A	G904	U827	C972	C896	U827	G755	G682	A613	C545	C466	G402	G331	G260	G186	U114
G1088	C1030B	A909	A828	G973	C897	A828	G756	G683	C615	C546	C467	C403	G332	U261	C187	G115
U1089	G1030C	C910	G829	A974	C898	G829	U757	A684	G616	C547	C468	U404	G333	A262	G188	G116
U1090	A1030D	A975	G830	A975	C899	G830	G758	G685	G617	C548	C469	U405	G334	A263	G189	A116
U1091	G1031	C976	U831	G976	C900	U831	A759	U686	C618	C549	C470	U406	G335	C267	G189A	G117
A1092	G1032	A977	C832	A977	C901	C832	G760	U687	U619	C550	C471	G407	G336	C268	C189B	
G1093	G1033	A978	U833	A978	C902	U833	G761	G688	C620	C551	C472	A408	G337	C269	C189C	A120
U1094	A1034	C979	C834	A979	C903	C834	G762	C689	A621	C552	C473	A409	G338	A270	G189F	G122
G1095	G1035	C980	U835	A980	C904	U835	G763	G690	A622	C553	C474	A410	G339	A271	G189G	C123
C1096	G1036	U920	G836	A981	C905	G836	G764	G691	A623	C554	C475	A411	G340	C271	G189H	G124
U1097	C1037	U921	G837	A982	C906	G837	A766	U692	C624	C555	C476	A412	G341	G276	G189I	U125
C1098	C1038	G922	G838	A983	C907	G838	A767	G693	G625	C556	C477	A413	G342	C277	G189J	G126
U1099	U1039	C984	U839	C984	C908	U839	G768	A694	U626	C557	C478	A414	G343	G278	U189K	G127
G1100	C1039	C985	G925	C985	C909	G925	G769	G695	G627	C558	C479	A415	G344	G279	G189L	G129A
A1101	A1040	A986	G926	A986	C910	G926	C770	U697	G628	C559	C480	C417	G345	A279	U190	A130
C1102	G1042	G987	U841	C987	C911	U841	G771	U705	G629	C560	C481	C418	G346	C283	G191	C131
C1103	C1043	G988	C849	G988	C912	C849	G772	U706	G630	C561	C482	C419	G347	G284	U192	C132
G1104	A1044	C989	U850	G989	C913	U850	G773	A707	G631	C562	C483	C420	G348	G285	C193	G133
A1105	C1045	C990	G851	C990	C914	G851	G774	A708	A632	C563	C484	U421	G349	G286	C194	U133
G1106	A1046	C991	G852	C991	C915	G852	G775	C707	G633	C564	C485	C422	G350	G287	A195	G142
C1107	U992	C932	G854	C932	C916	G854	A777	C708	C634	C565	C486	G423	G351	G288	U196	
G1108	G1048	G993	G855	G993	C917	G855	G776	G709	G635	C566	C487	G424	G352	G289		





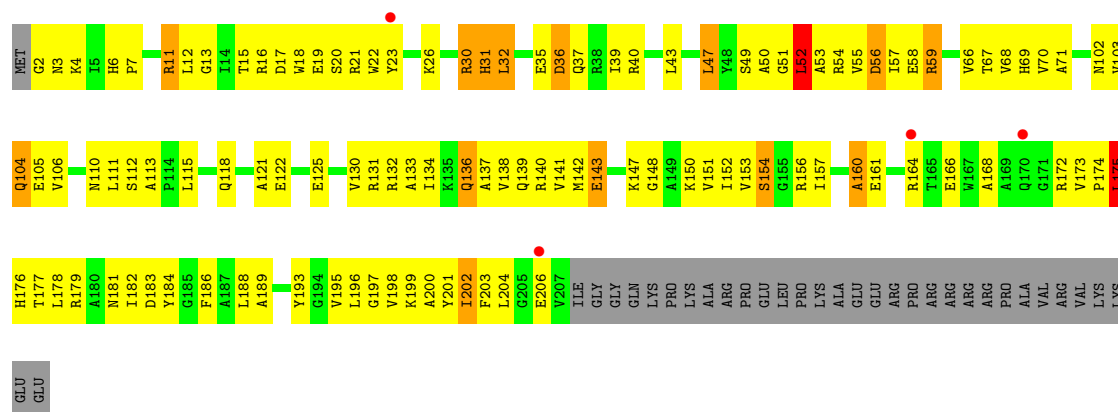
• Molecule 3: 30S Ribosomal Protein S3

Chain AC:



• Molecule 3: 30S Ribosomal Protein S3

Chain CC:



• Molecule 4: 30S Ribosomal Protein S4

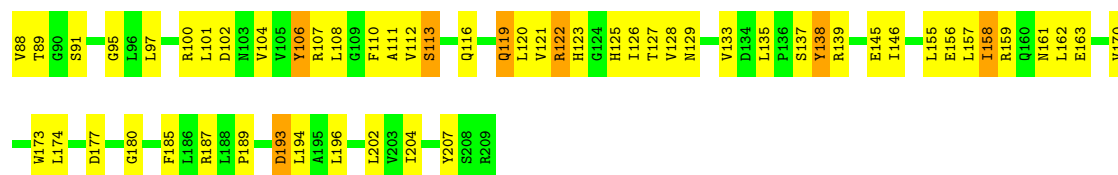
Chain AD:



• Molecule 4: 30S Ribosomal Protein S4

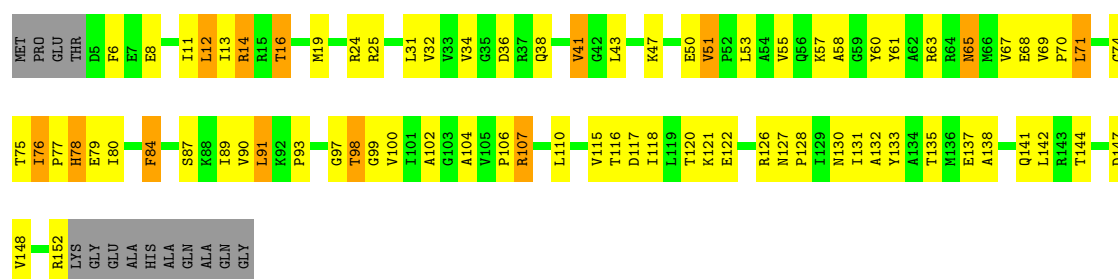
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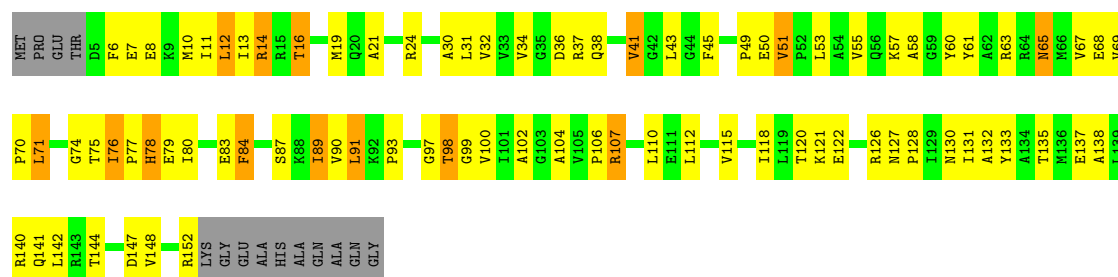
• Molecule 5: 30S Ribosomal Protein S5

Chain AE:



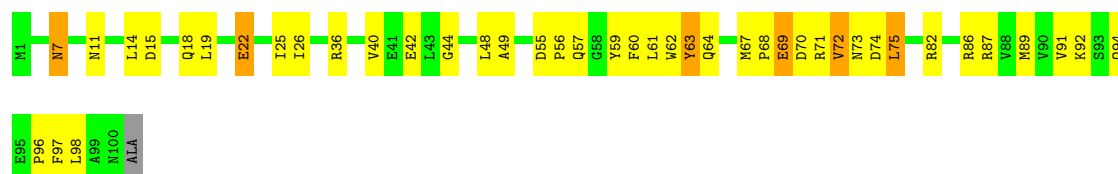
• Molecule 5: 30S Ribosomal Protein S5

Chain CE:



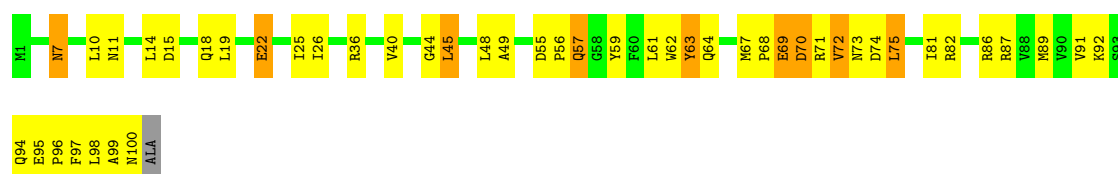
• Molecule 6: 30S Ribosomal Protein S6

Chain AF:



• Molecule 6: 30S Ribosomal Protein S6

Chain CF:



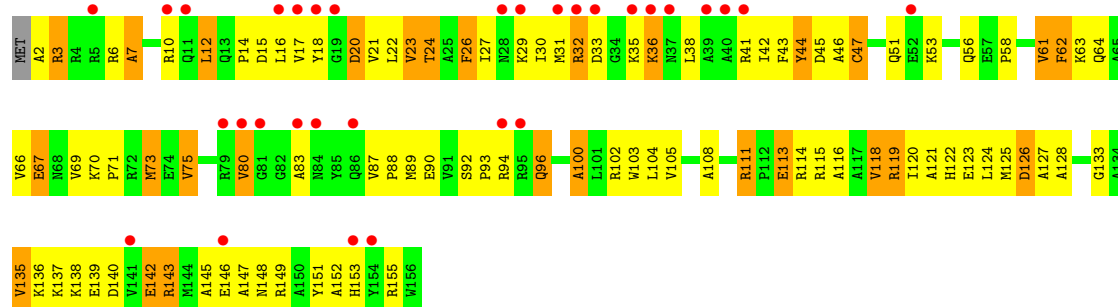
• Molecule 7: 30S Ribosomal Protein S7

Chain AG:



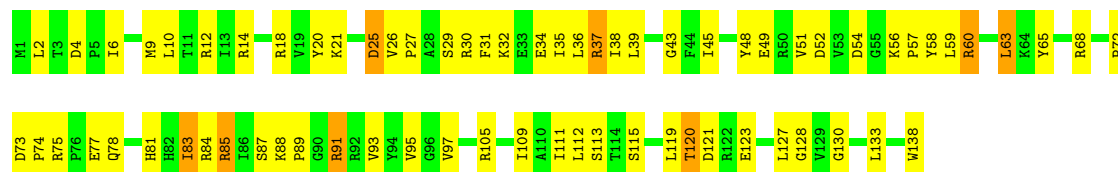
• Molecule 7: 30S Ribosomal Protein S7

Chain CG:



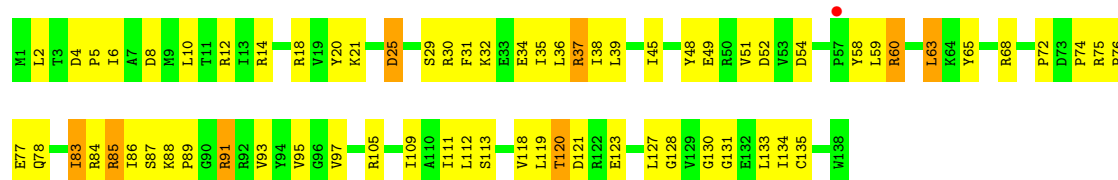
• Molecule 8: 30S Ribosomal Protein S8

Chain AH:



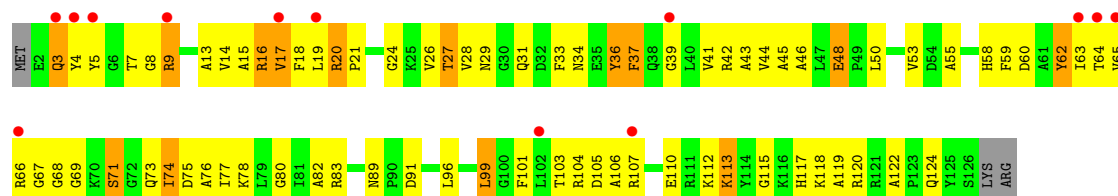
• Molecule 8: 30S Ribosomal Protein S8

Chain CH:

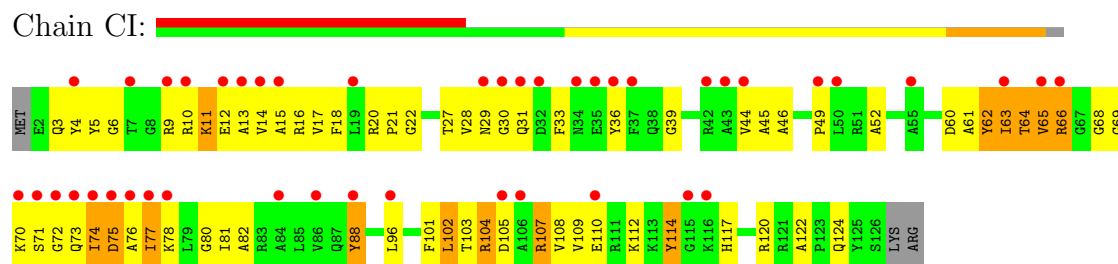


• Molecule 9: 30S Ribosomal Protein S9

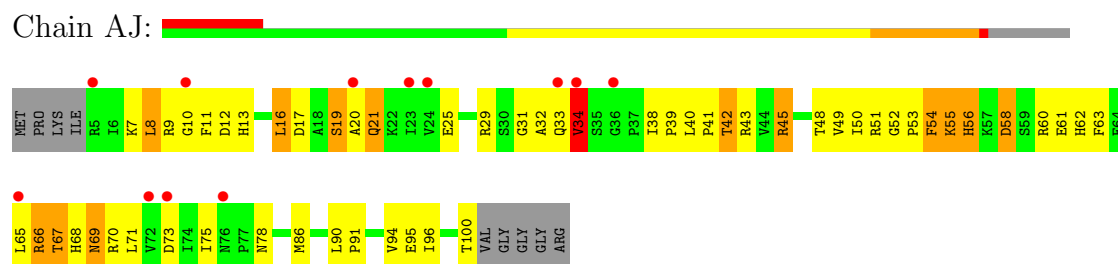
Chain AI:



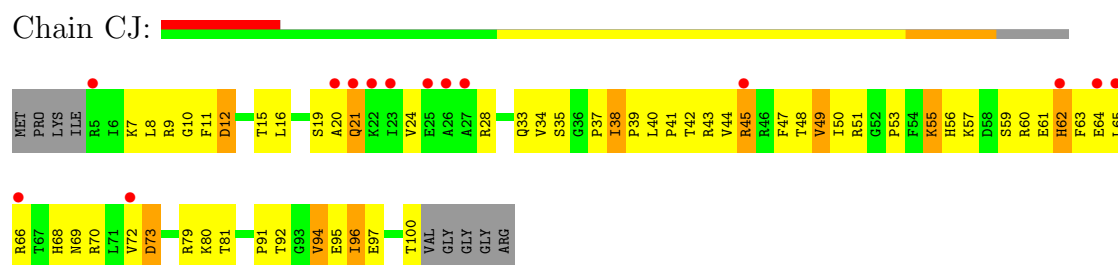
- Molecule 9: 30S Ribosomal Protein S9



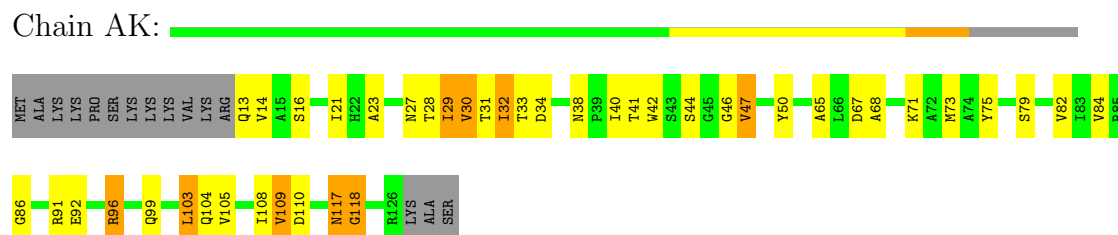
- Molecule 10: 30S Ribosomal Protein S10



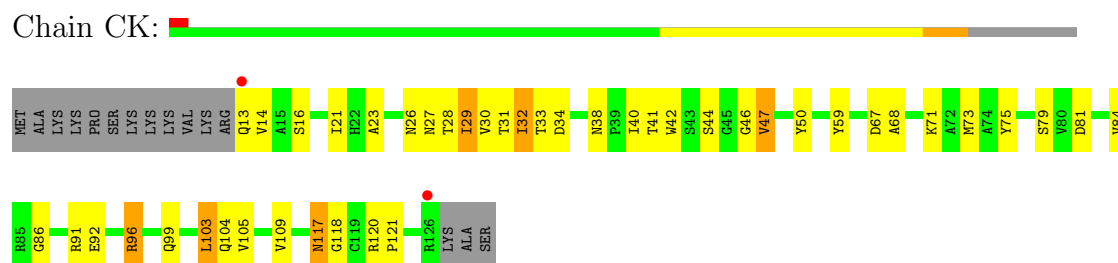
- Molecule 10: 30S Ribosomal Protein S10



- Molecule 11: 30S Ribosomal Protein S11

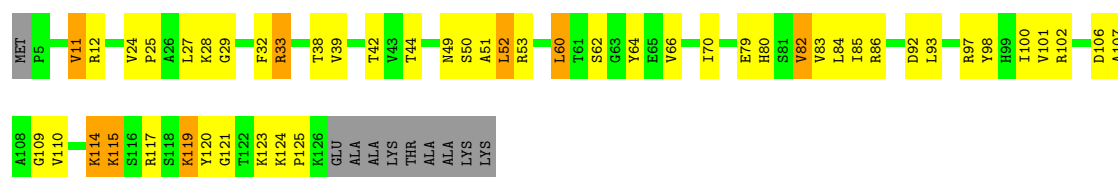


- Molecule 11: 30S Ribosomal Protein S11



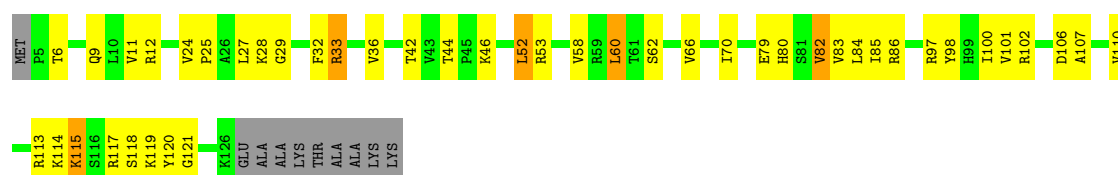
- Molecule 12: 30S Ribosomal Protein S12





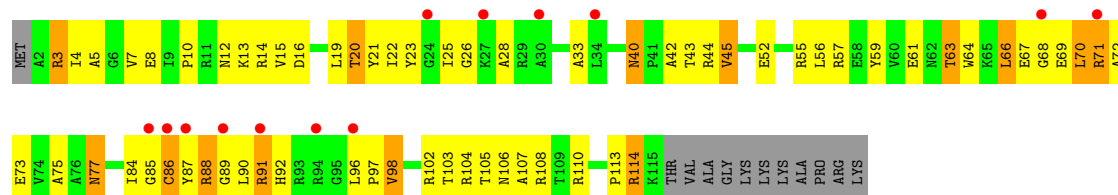
• Molecule 12: 30S Ribosomal Protein S12

Chain CL:



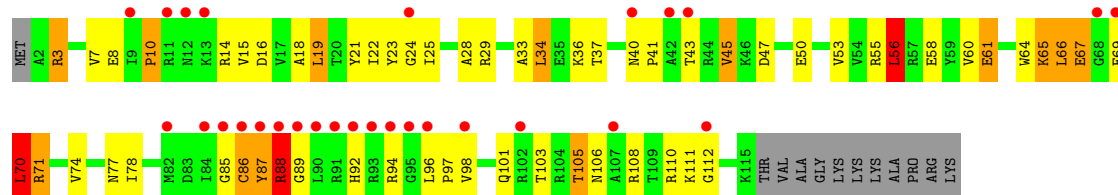
• Molecule 13: 30S Ribosomal Protein S13

Chain AM:



• Molecule 13: 30S Ribosomal Protein S13

Chain CM:



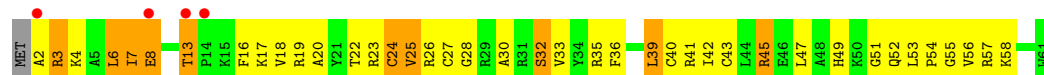
• Molecule 14: 30S Ribosomal Protein S14

Chain AN:



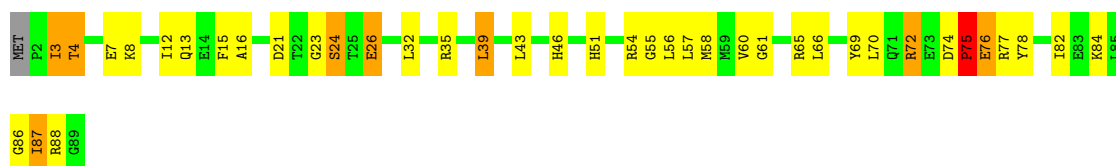
• Molecule 14: 30S Ribosomal Protein S14

Chain CN:



• Molecule 15: 30S Ribosomal Protein S15

Chain AO:



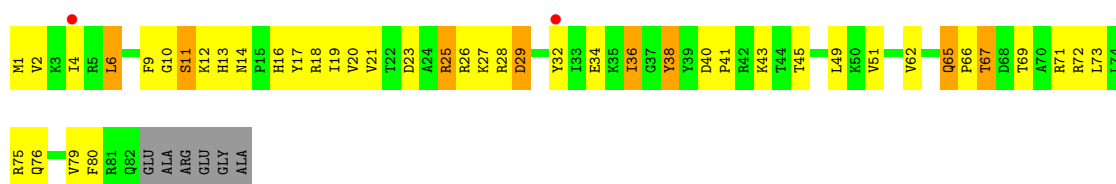
• Molecule 15: 30S Ribosomal Protein S15

Chain CO:



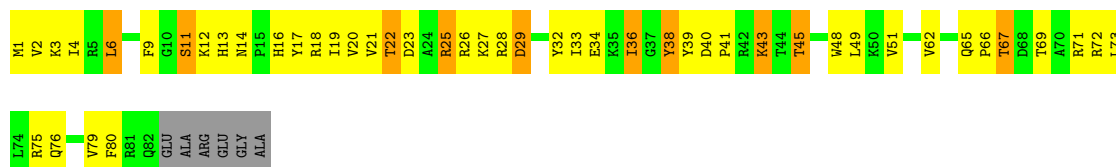
• Molecule 16: 30S Ribosomal Protein S16

Chain AP:



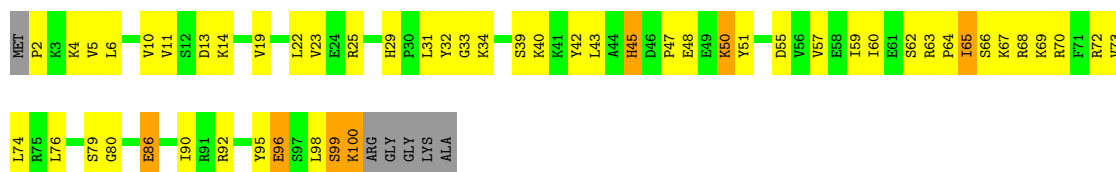
• Molecule 16: 30S Ribosomal Protein S16

Chain CP:



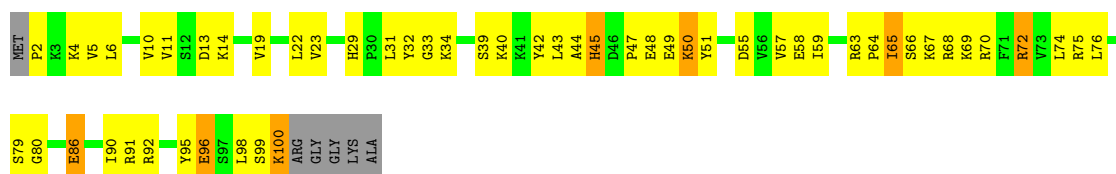
• Molecule 17: 30S Ribosomal Protein S17

Chain AQ:



• Molecule 17: 30S Ribosomal Protein S17

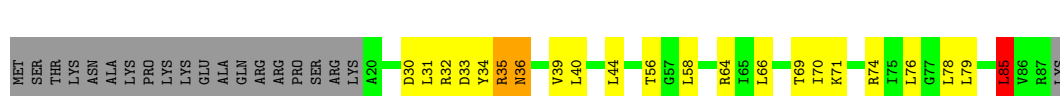
Chain CQ:





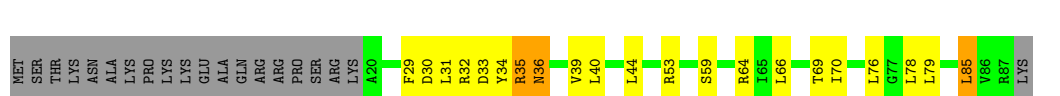
- Molecule 18: 30S Ribosomal Protein S18

Chain AR:



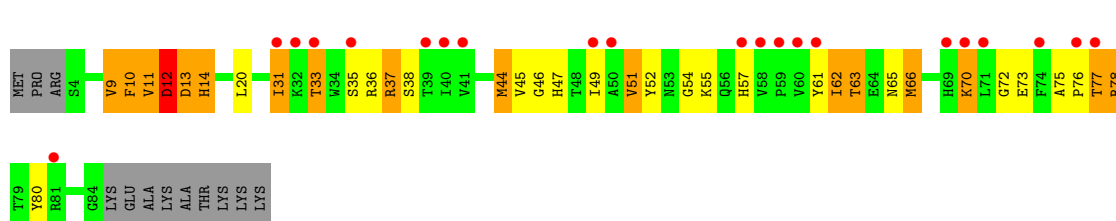
- Molecule 18: 30S Ribosomal Protein S18

Chain CR:



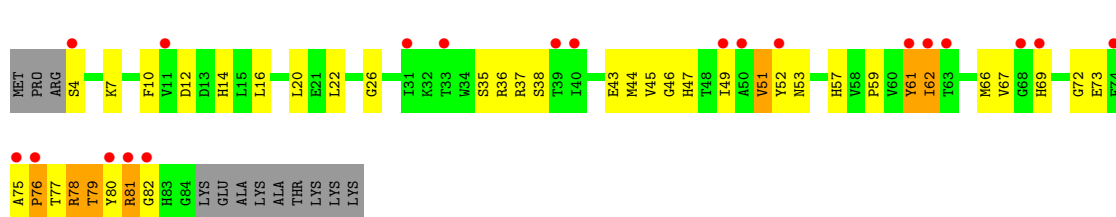
- Molecule 19: 30S Ribosomal Protein S19

Chain AS:



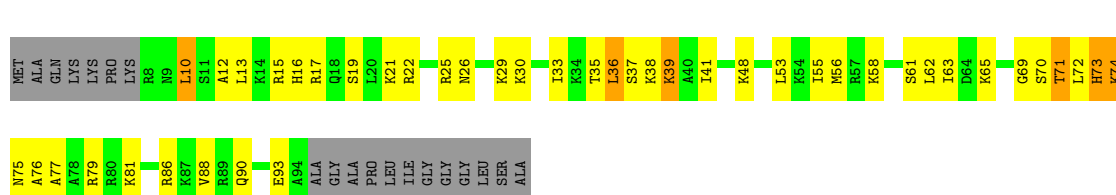
- Molecule 19: 30S Ribosomal Protein S19

Chain CS:



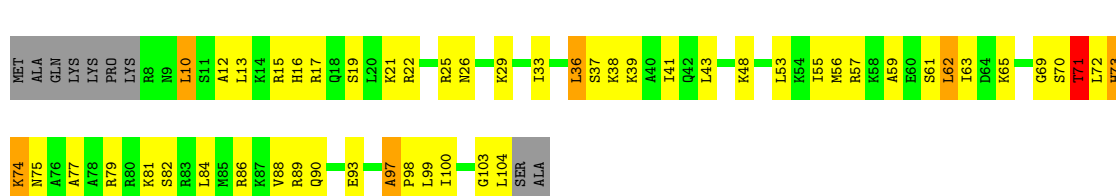
- Molecule 20: 30S Ribosomal Protein S20

Chain AT:



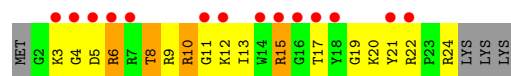
- Molecule 20: 30S Ribosomal Protein S20

Chain CT:



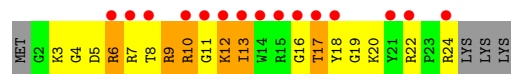
- Molecule 21: 30S Ribosomal Protein THX

Chain AU: 



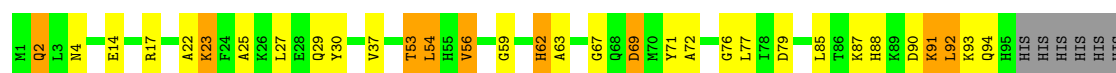
- Molecule 21: 30S Ribosomal Protein THX

Chain CU: 



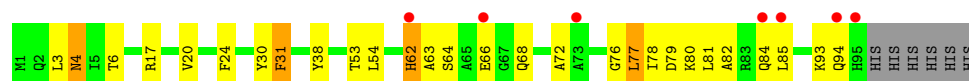
- Molecule 22: Probable sigma(54) modulation protein

Chain AX: 



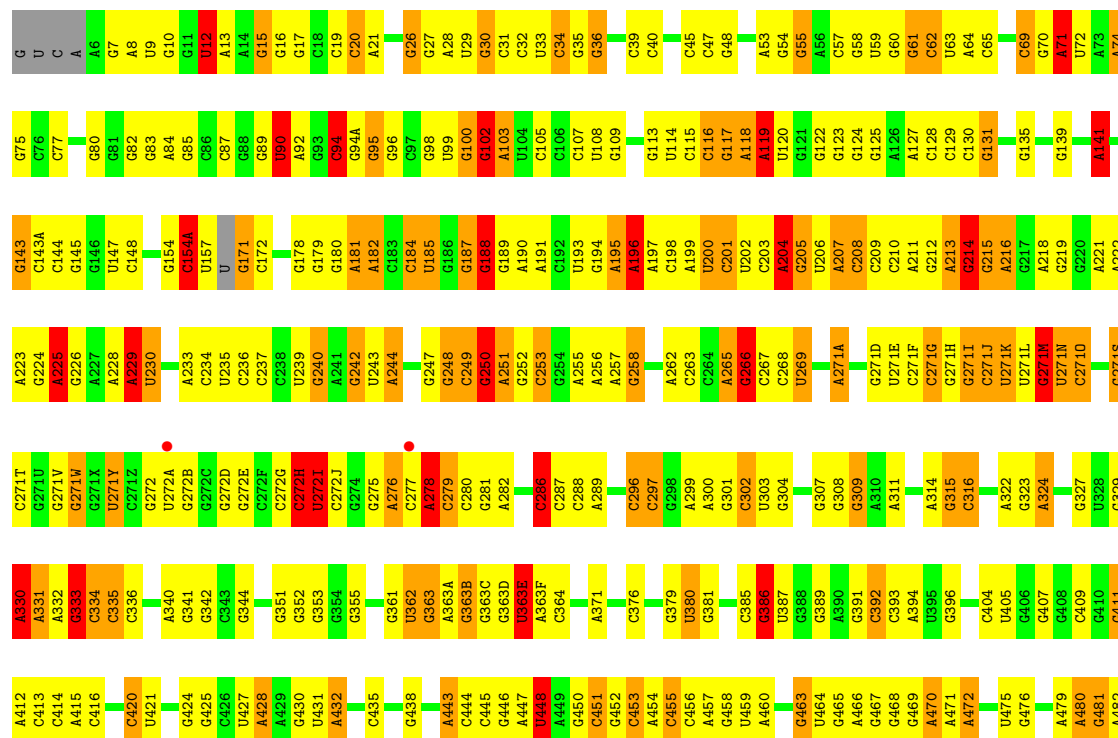
- Molecule 22: Probable sigma(54) modulation protein

Chain CX: 



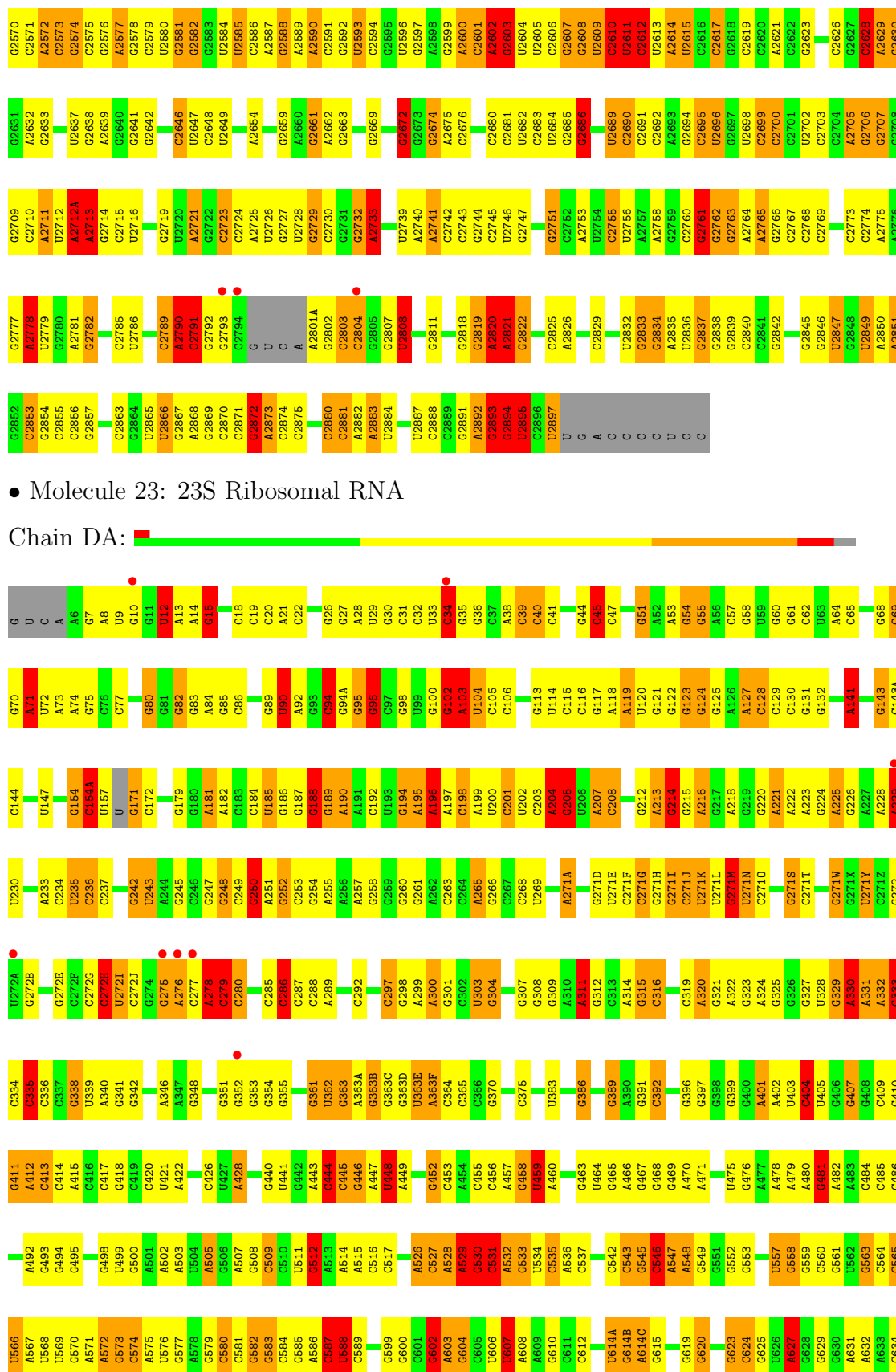
- Molecule 23: 23S Ribosomal RNA

Chain BA: 



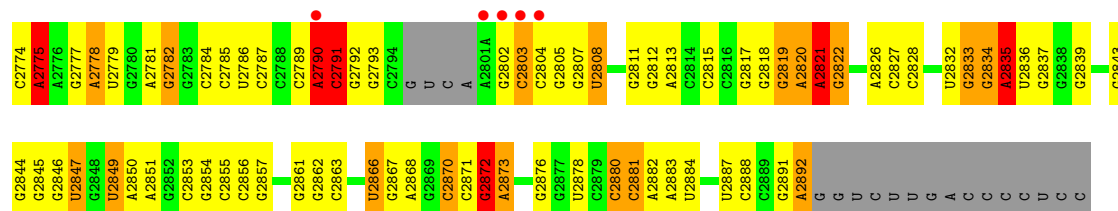
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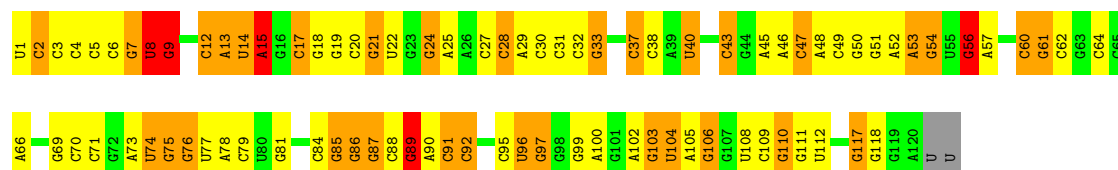
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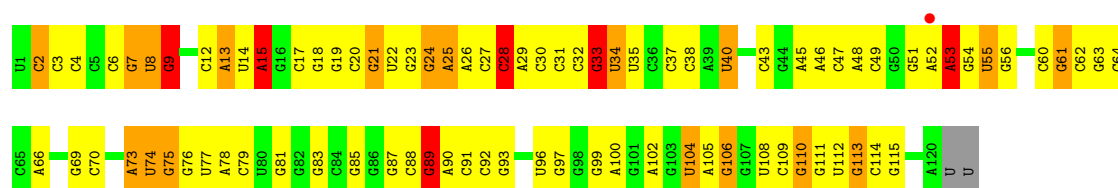
• Molecule 24: 5S Ribosomal RNA

Chain BB:



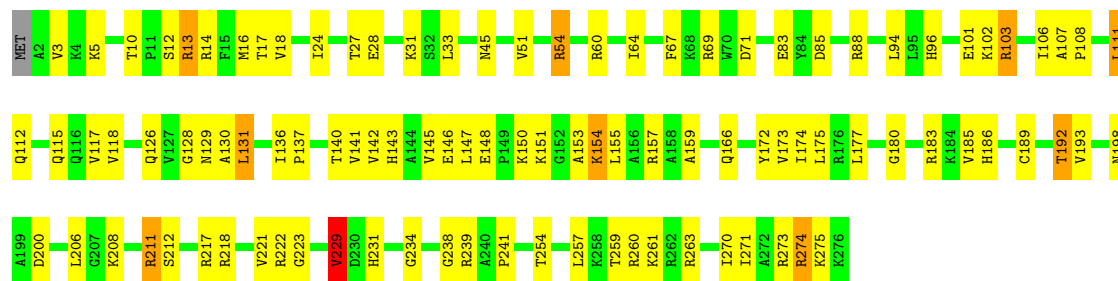
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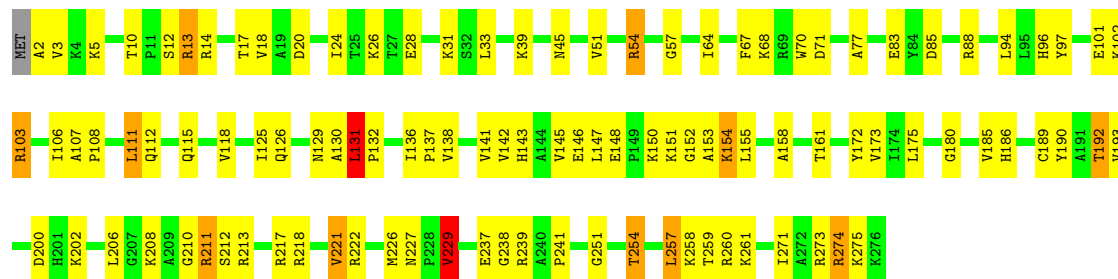
• Molecule 25: 50S Ribosomal Protein L2

Chain BD:



• Molecule 25: 50S Ribosomal Protein L2

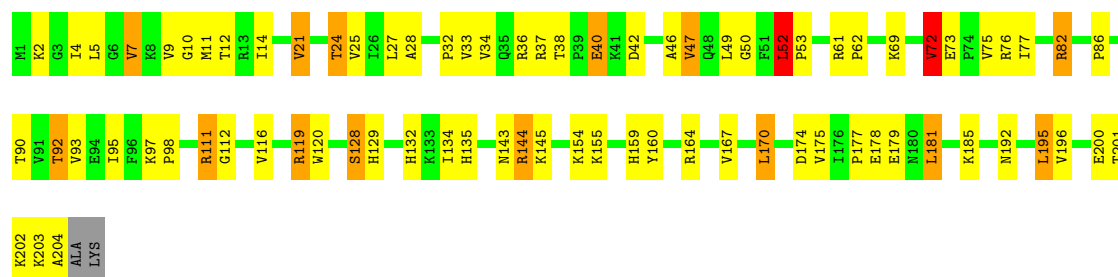
Chain DD:



• Molecule 26: 50S Ribosomal Protein L3

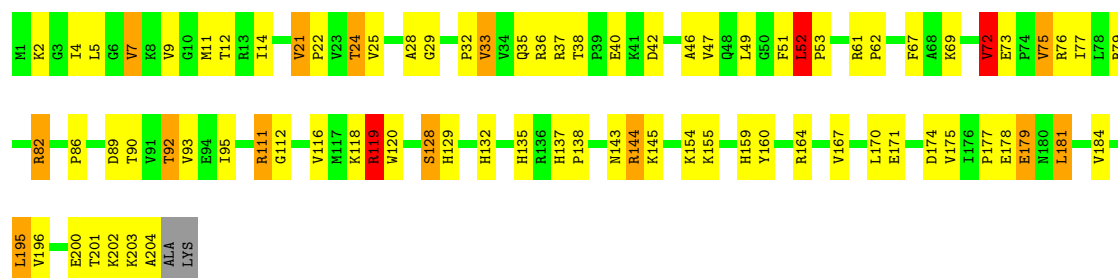


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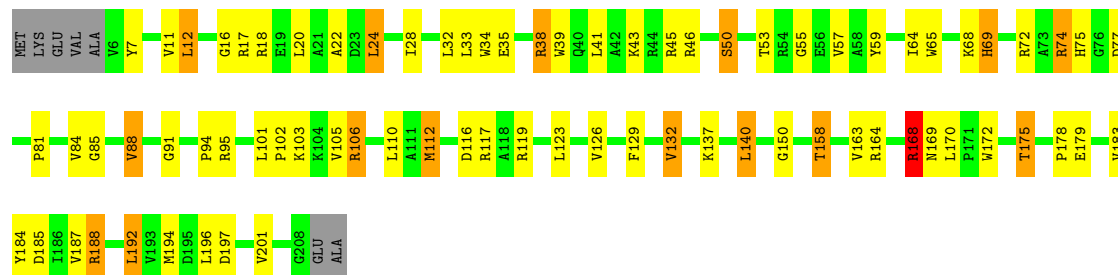
- Molecule 26: 50S Ribosomal Protein L3

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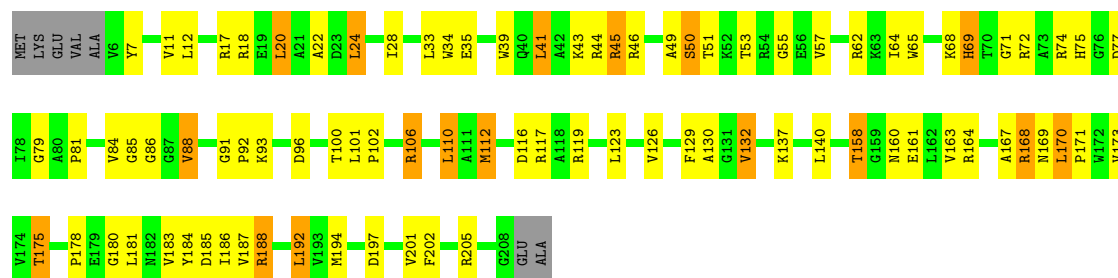
- Molecule 27: 50S Ribosomal Protein L4

Chain BF:



- Molecule 27: 50S Ribosomal Protein L4

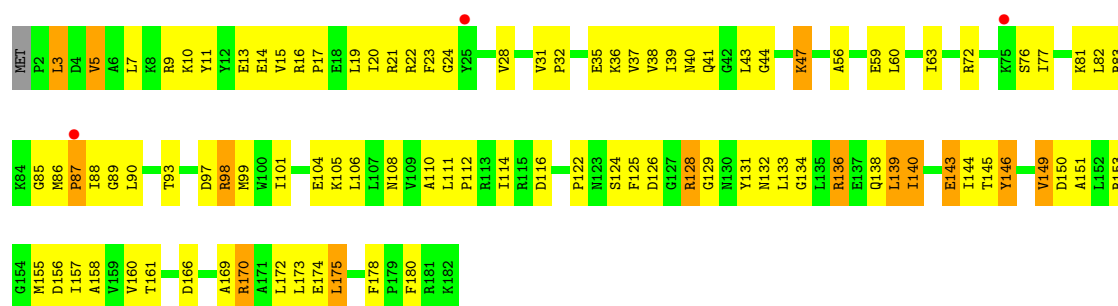
Chain DF:



- Molecule 28: 50S Ribosomal Protein L5

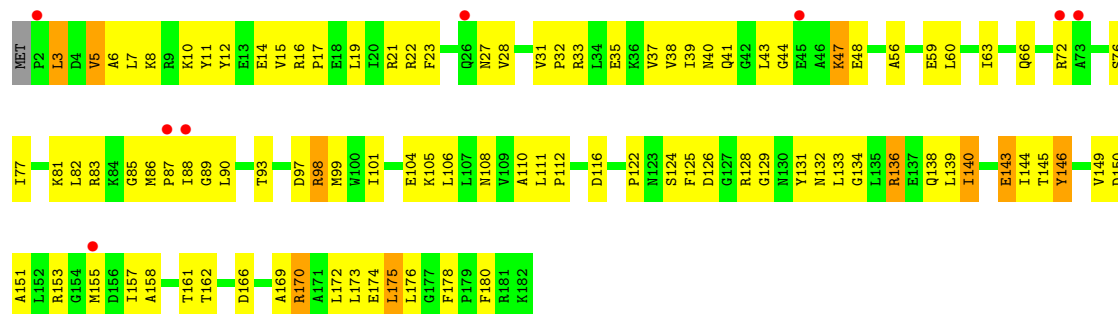
Chain BG:





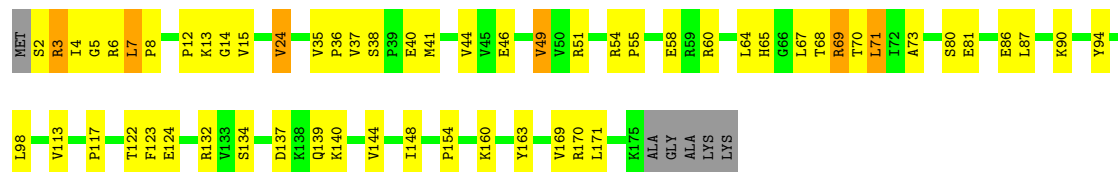
• Molecule 28: 50S Ribosomal Protein L5

Chain DG:



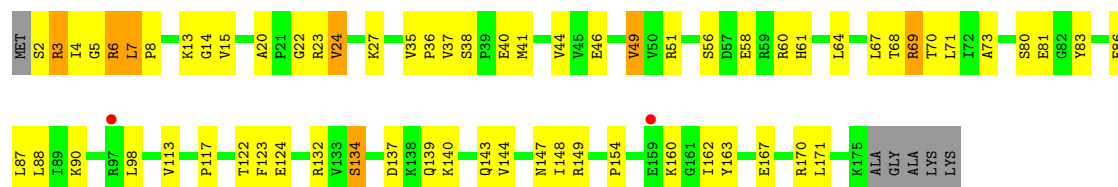
• Molecule 29: 50S Ribosomal Protein L6

Chain BH:



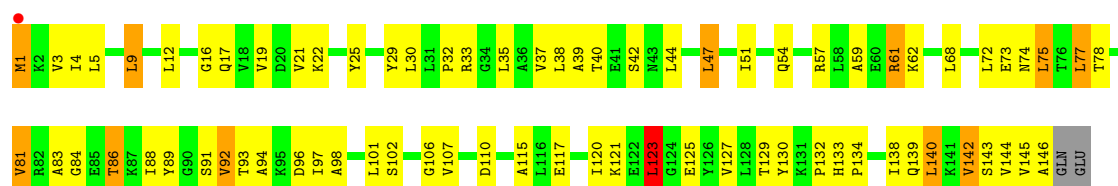
• Molecule 29: 50S Ribosomal Protein L6

Chain DH:

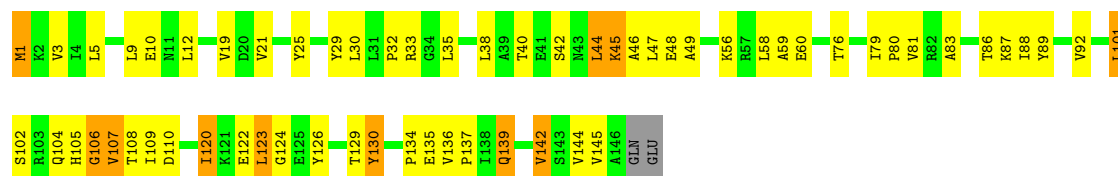


• Molecule 30: 50S Ribosomal Protein L9

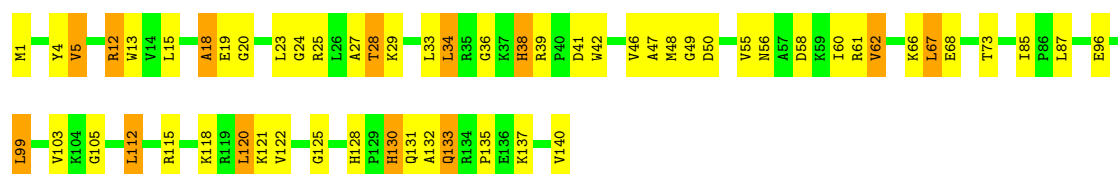
Chain BI:



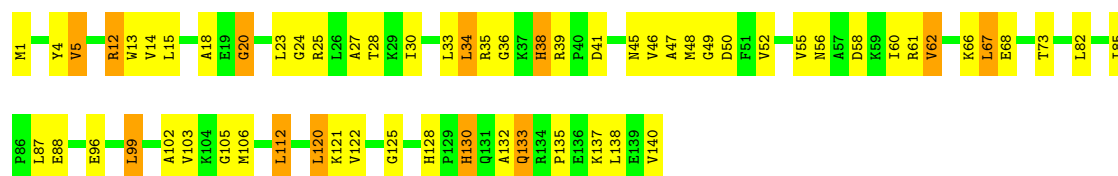
- Molecule 30: 50S Ribosomal Protein L9

Chain DI: 

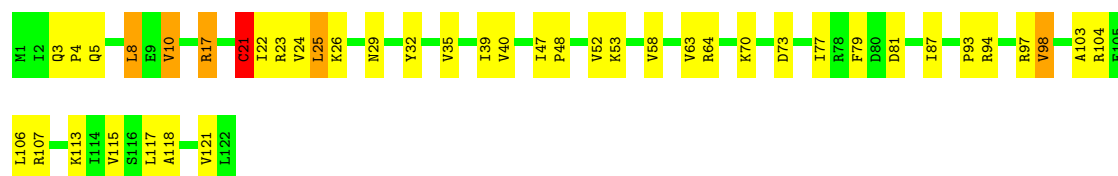
- Molecule 31: 50S Ribosomal Protein L13

Chain BN: 

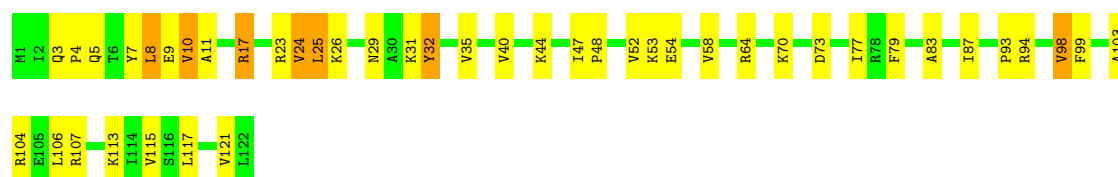
- Molecule 31: 50S Ribosomal Protein L13

Chain DN: 

- Molecule 32: 50S Ribosomal Protein L14

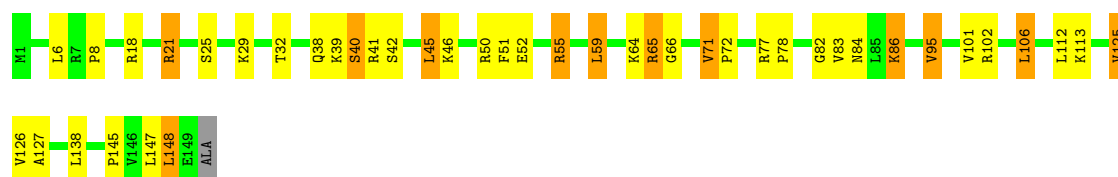
Chain BO: 

- Molecule 32: 50S Ribosomal Protein L14

Chain DO: 

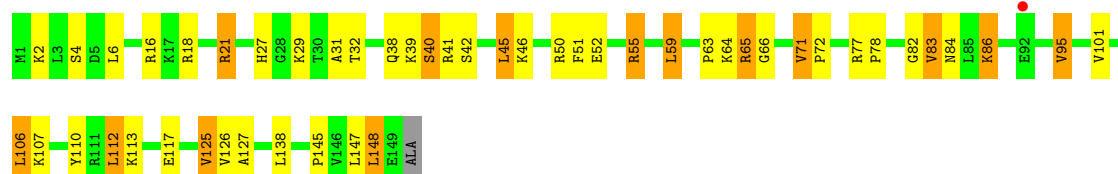
- Molecule 33: 50S Ribosomal Protein L15

Chain BP: 



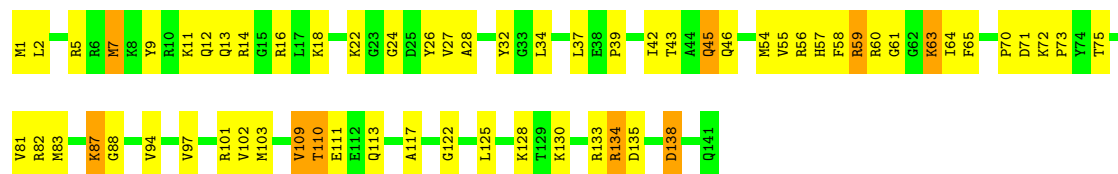
• Molecule 33: 50S Ribosomal Protein L15

Chain DP:



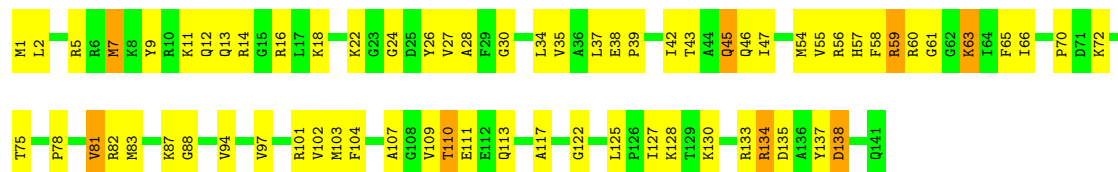
• Molecule 34: 50S Ribosomal Protein L16

Chain BQ:



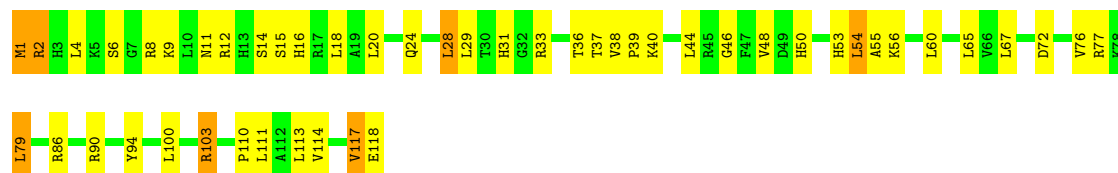
• Molecule 34: 50S Ribosomal Protein L16

Chain DQ:



• Molecule 35: 50S Ribosomal Protein L17

Chain BR:



• Molecule 35: 50S Ribosomal Protein L17

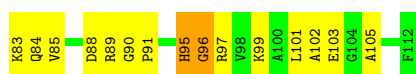
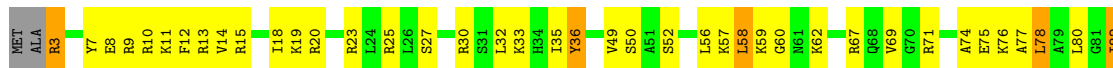
Chain DR:





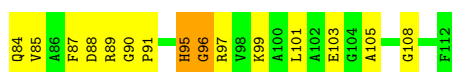
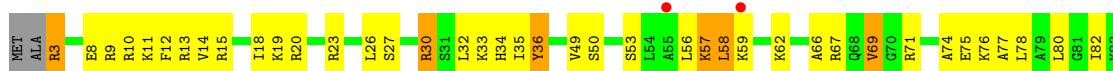
• Molecule 36: 50S Ribosomal Protein L18

Chain BS:



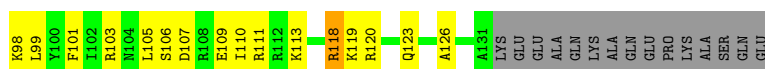
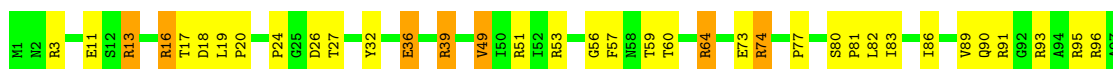
• Molecule 36: 50S Ribosomal Protein L18

Chain DS:



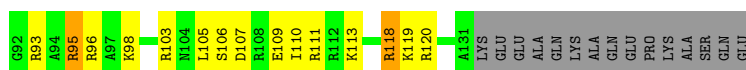
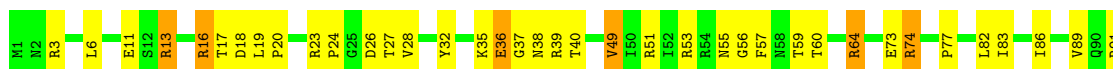
• Molecule 37: 50S Ribosomal Protein L19

Chain BT:



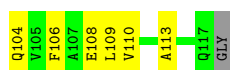
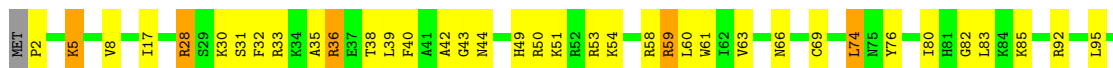
• Molecule 37: 50S Ribosomal Protein L19

Chain DT:



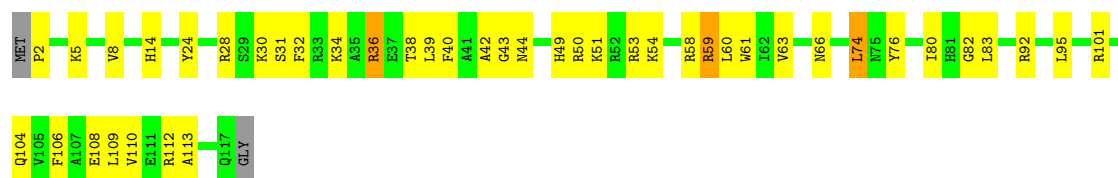
• Molecule 38: 50S Ribosomal Protein L20

Chain BU:



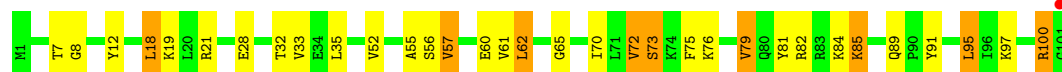
• Molecule 38: 50S Ribosomal Protein L20

Chain DU:



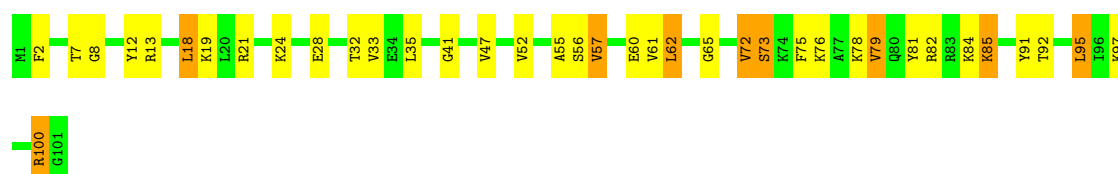
- Molecule 39: 50S Ribosomal Protein L21

Chain BV:



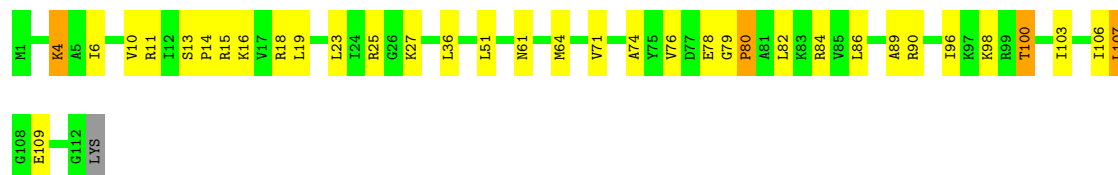
- Molecule 39: 50S Ribosomal Protein L21

Chain DV:



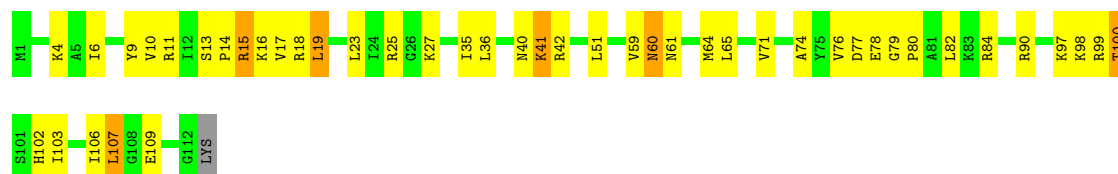
- Molecule 40: 50S Ribosomal Protein L22

Chain BW:



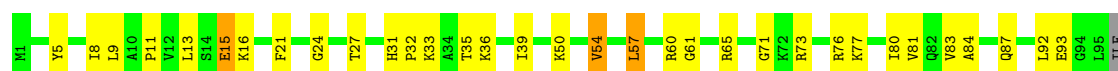
- Molecule 40: 50S Ribosomal Protein L22

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:



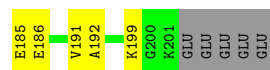
• Molecule 42: 50S Ribosomal Protein L24

Chain DY:



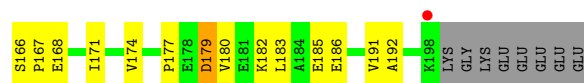
• Molecule 43: 50S Ribosomal Protein L25

Chain BZ:



• Molecule 43: 50S Ribosomal Protein L25

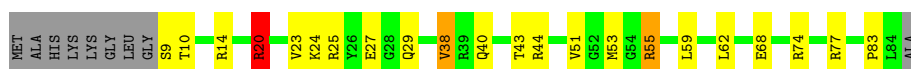
Chain DZ:



• 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:



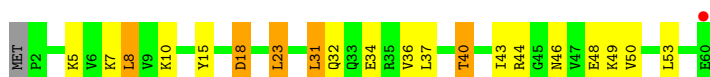
- Molecule 47: 50S Ribosomal Protein L30

Chain B3:



- Molecule 47: 50S Ribosomal Protein L30

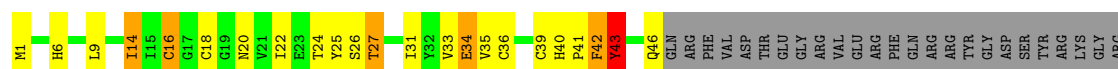
Chain D3:



- Molecule 48: 50S Ribosomal Protein L31

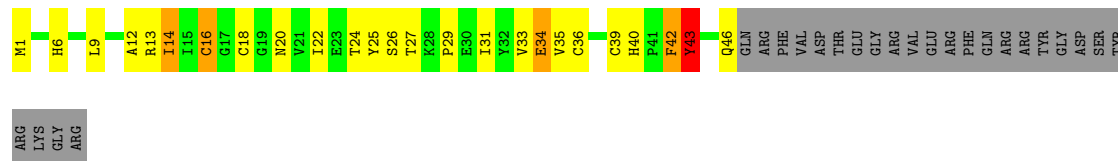
Chain B4:





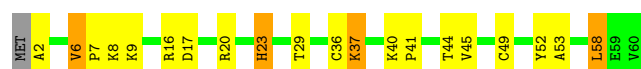
- Molecule 48: 50S Ribosomal Protein L31

Chain D4:



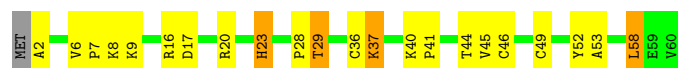
- Molecule 49: 50S Ribosomal Protein L32

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:



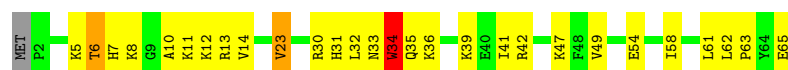
- Molecule 51: 50S Ribosomal Protein L34

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, $\alpha$ , $\beta$ , $\gamma$	208.97Å 447.24Å 617.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 3.10 49.98 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.98-3.10) 96.0 (49.98-3.10)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.216 , 0.258 0.243 , 0.286	Depositor DCC
$R_{free}$ test set	41403 reflections (4.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.0	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 29.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	1 of 993194 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	286308	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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	1.14	57/36123 (0.2%)	1.54	760/56379 (1.3%)
1	CA	1.11	53/36028 (0.1%)	1.55	750/56231 (1.3%)
2	AB	0.69	0/1822	0.79	1/2468 (0.0%)
2	CB	0.75	0/1809	0.79	1/2450 (0.0%)
3	AC	0.80	0/1474	0.88	0/2003
3	CC	0.78	0/1474	0.86	2/2003 (0.1%)
4	AD	0.68	2/1556 (0.1%)	0.87	3/2113 (0.1%)
4	CD	0.72	2/1556 (0.1%)	0.87	3/2113 (0.1%)
5	AE	0.61	0/1121	0.80	1/1517 (0.1%)
5	CE	0.63	0/1121	0.82	1/1517 (0.1%)
6	AF	0.59	0/790	0.73	0/1077
6	CF	0.62	0/790	0.73	0/1077
7	AG	1.04	0/1183	0.98	2/1599 (0.1%)
7	CG	0.96	0/1183	0.90	0/1599
8	AH	0.57	0/1065	0.73	0/1445
8	CH	0.58	0/1065	0.75	0/1445
9	AI	0.92	0/867	0.92	0/1180
9	CI	1.00	0/867	0.91	1/1180 (0.1%)
10	AJ	0.83	0/676	0.91	1/924 (0.1%)
10	CJ	0.90	0/676	0.97	0/924
11	AK	0.62	0/843	0.75	1/1144 (0.1%)
11	CK	0.61	0/843	0.75	1/1144 (0.1%)
12	AL	0.63	0/921	0.78	0/1247
12	CL	0.64	0/921	0.80	0/1247
13	AM	1.02	0/814	1.00	0/1107
13	CM	1.03	0/814	1.03	2/1107 (0.2%)
14	AN	0.76	0/487	0.90	0/649
14	CN	0.77	1/487 (0.2%)	0.87	1/649 (0.2%)
15	AO	0.62	0/735	0.84	0/981
15	CO	0.66	0/735	0.85	0/981
16	AP	0.63	0/667	0.82	0/905
16	CP	0.56	0/667	0.82	0/905

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.66	0/836	0.84	0/1117
17	CQ	0.69	1/836 (0.1%)	0.85	0/1117
18	AR	0.59	0/519	0.76	1/699 (0.1%)
18	CR	0.63	0/519	0.76	1/699 (0.1%)
19	AS	0.96	0/574	0.87	0/781
19	CS	0.98	0/574	0.93	0/781
20	AT	0.63	0/666	0.79	0/880
20	CT	0.62	0/715	0.84	1/947 (0.1%)
21	AU	0.82	0/203	0.92	0/266
21	CU	0.91	0/203	0.97	0/266
22	AX	0.69	0/637	0.84	1/864 (0.1%)
22	CX	0.77	0/606	0.82	0/828
23	BA	1.58	572/68445 (0.8%)	1.72	2187/106848 (2.0%)
23	DA	1.21	155/67893 (0.2%)	1.65	1848/105980 (1.7%)
24	BB	1.13	6/2878 (0.2%)	1.53	60/4490 (1.3%)
24	DB	1.13	2/2878 (0.1%)	1.52	49/4490 (1.1%)
25	BD	0.90	1/2185 (0.0%)	0.91	4/2942 (0.1%)
25	DD	0.82	0/2186	0.91	2/2944 (0.1%)
26	BE	0.90	0/1588	0.92	0/2145
26	DE	0.78	0/1588	0.92	3/2145 (0.1%)
27	BF	0.91	0/1615	0.95	3/2188 (0.1%)
27	DF	0.74	0/1615	0.92	2/2188 (0.1%)
28	BG	0.61	0/1393	0.79	0/1892
28	DG	0.72	0/1393	0.81	0/1892
29	BH	0.72	0/1343	0.82	1/1820 (0.1%)
29	DH	0.66	0/1343	0.81	0/1820
30	BI	0.64	0/1052	0.87	1/1441 (0.1%)
30	DI	0.63	0/967	0.84	1/1334 (0.1%)
31	BN	0.87	0/1139	0.87	0/1538
31	DN	0.71	0/1139	0.89	1/1538 (0.1%)
32	BO	0.87	1/933 (0.1%)	0.88	1/1257 (0.1%)
32	DO	0.73	0/933	0.83	1/1257 (0.1%)
33	BP	0.84	0/1148	0.91	1/1529 (0.1%)
33	DP	0.73	0/1148	0.89	1/1529 (0.1%)
34	BQ	0.84	0/1143	0.87	1/1527 (0.1%)
34	DQ	0.74	0/1143	0.86	0/1527
35	BR	0.80	0/982	0.92	0/1312
35	DR	0.75	0/982	0.92	1/1312 (0.1%)
36	BS	0.67	0/875	0.88	1/1168 (0.1%)
36	DS	0.69	0/875	0.87	1/1168 (0.1%)
37	BT	0.83	0/1077	0.92	0/1444
37	DT	0.73	0/1077	0.90	0/1444
38	BU	1.00	1/977 (0.1%)	0.87	1/1301 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DU	0.79	0/977	0.86	0/1301
39	BV	0.85	0/782	0.92	0/1049
39	DV	0.77	0/782	0.85	0/1049
40	BW	1.02	0/891	0.91	0/1197
40	DW	0.87	0/891	0.91	1/1197 (0.1%)
41	BX	0.91	0/756	0.88	2/1016 (0.2%)
41	DX	0.78	0/756	0.86	1/1016 (0.1%)
42	BY	0.80	1/798 (0.1%)	0.88	0/1073
42	DY	0.73	1/798 (0.1%)	0.89	0/1073
43	BZ	0.70	0/1569	0.82	1/2137 (0.0%)
43	DZ	0.72	0/1555	0.81	1/2118 (0.0%)
44	B0	0.85	0/602	0.92	1/804 (0.1%)
44	D0	0.78	0/602	0.92	0/804
45	B1	0.85	0/752	0.90	2/1003 (0.2%)
45	D1	0.80	0/752	0.89	1/1003 (0.1%)
46	B2	0.82	0/590	0.86	0/781
46	D2	0.79	0/590	0.86	0/781
47	B3	0.76	0/463	0.84	1/623 (0.2%)
47	D3	0.69	0/463	0.81	0/623
48	B4	0.68	0/358	0.84	1/487 (0.2%)
48	D4	0.85	0/358	0.83	1/487 (0.2%)
49	B5	0.93	1/469 (0.2%)	1.00	0/634
49	D5	0.86	1/469 (0.2%)	0.96	0/634
50	B6	0.93	2/456 (0.4%)	0.84	0/609
50	D6	0.75	0/456	0.87	2/609 (0.3%)
51	B7	1.03	1/426 (0.2%)	1.12	1/561 (0.2%)
51	D7	0.88	0/426	1.01	1/561 (0.2%)
52	B8	0.96	0/516	0.94	1/679 (0.1%)
52	D8	0.76	0/516	0.90	0/679
53	B9	0.79	0/300	0.95	0/395
53	D9	0.71	0/300	0.90	0/395
All	All	1.18	861/305420 (0.3%)	1.47	5724/457343 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	3
2	CB	0	4
3	AC	0	3

*Continued on next page...*

*Continued from previous page...*

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

The worst 5 of 861 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1442(A)	G	N9-C4	17.19	1.51	1.38
1	AA	1442(A)	G	N9-C4	15.23	1.50	1.38
1	AA	1442(A)	G	C2-N3	15.04	1.44	1.32
1	CA	1442(A)	G	C2-N3	14.30	1.44	1.32
1	AA	1442(A)	G	N3-C4	13.24	1.44	1.35

The worst 5 of 5724 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1442(A)	G	N3-C4-C5	-26.14	115.53	128.60
23	DA	2296	U	N3-C4-O4	-25.95	101.23	119.40
1	AA	1442(A)	G	N3-C4-C5	-25.64	115.78	128.60
1	CA	1442(A)	G	N3-C4-N9	25.18	141.10	126.00
1	AA	1442(A)	G	N3-C4-N9	25.11	141.07	126.00

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	129	GLU	Peptide
2	AB	14	GLY	Peptide
2	AB	71	VAL	Peptide
3	AC	19	GLU	Peptide
3	AC	51	GLY	Peptide

## 5.2 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	32270	0	16286	1214	0
1	CA	32185	0	16244	1267	1
2	AB	1787	0	1752	122	0
2	CB	1775	0	1743	121	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AC	1450	0	1314	92	0
3	CC	1450	0	1314	123	0
4	AD	1526	0	1415	71	0
4	CD	1526	0	1415	85	0
5	AE	1105	0	1130	56	0
5	CE	1105	0	1130	60	0
6	AF	777	0	737	31	0
6	CF	777	0	737	35	0
7	AG	1164	0	1106	87	0
7	CG	1164	0	1106	99	0
8	AH	1045	0	1033	48	0
8	CH	1045	0	1033	51	0
9	AI	852	0	742	83	0
9	CI	852	0	742	79	0
10	AJ	663	0	558	56	0
10	CJ	663	0	558	70	0
11	AK	828	0	822	29	0
11	CK	828	0	822	28	0
12	AL	905	0	916	41	0
12	CL	905	0	916	32	0
13	AM	804	0	752	58	0
13	CM	804	0	752	60	0
14	AN	478	0	497	33	0
14	CN	478	0	496	58	0
15	AO	724	0	749	34	0
15	CO	724	0	749	31	0
16	AP	651	0	638	31	0
16	CP	651	0	638	36	0
17	AQ	823	0	891	43	0
17	CQ	823	0	891	47	0
18	AR	514	0	530	25	0
18	CR	514	0	530	21	0
19	AS	560	0	466	46	0
19	CS	560	0	466	40	0
20	AT	665	0	731	34	0
20	CT	713	0	766	39	0
21	AU	199	0	208	31	0
21	CU	199	0	208	23	0
22	AX	631	0	540	20	0
22	CX	601	0	485	16	0
23	BA	61112	0	30809	1210	1
23	DA	60621	0	30566	1219	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	BB	2573	0	1306	56	0
24	DB	2573	0	1306	55	0
25	BD	2135	0	2214	73	0
25	DD	2136	0	2218	79	0
26	BE	1555	0	1607	52	0
26	DE	1555	0	1607	56	0
27	BF	1580	0	1621	63	0
27	DF	1580	0	1621	63	0
28	BG	1368	0	1324	74	0
28	DG	1368	0	1324	86	0
29	BH	1317	0	1376	35	0
29	DH	1317	0	1376	36	0
30	BI	1037	0	1036	54	1
30	DI	953	0	858	38	0
31	BN	1112	0	1180	33	0
31	DN	1112	0	1180	44	0
32	BO	923	0	981	26	0
32	DO	923	0	981	28	0
33	BP	1131	0	1201	45	0
33	DP	1131	0	1201	55	0
34	BQ	1122	0	1179	46	0
34	DQ	1122	0	1179	49	0
35	BR	968	0	1033	32	0
35	DR	968	0	1033	36	0
36	BS	865	0	905	50	0
36	DS	865	0	905	50	0
37	BT	1063	0	1103	42	0
37	DT	1063	0	1103	43	0
38	BU	959	0	1019	34	0
38	DU	959	0	1019	35	0
39	BV	771	0	830	23	0
39	DV	771	0	830	25	0
40	BW	881	0	935	21	0
40	DW	881	0	935	31	0
41	BX	742	0	799	23	0
41	DX	742	0	799	26	0
42	BY	785	0	828	23	0
42	DY	785	0	828	23	0
43	BZ	1536	0	1518	52	0
43	DZ	1522	0	1511	65	0
44	B0	594	0	604	16	0
44	D0	594	0	604	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	B1	745	0	804	21	0
45	D1	745	0	804	24	0
46	B2	588	0	643	16	0
46	D2	588	0	643	19	0
47	B3	458	0	503	8	0
47	D3	458	0	503	13	0
48	B4	349	0	336	23	0
48	D4	349	0	336	28	0
49	B5	455	0	472	13	0
49	D5	455	0	472	14	0
50	B6	449	0	462	18	0
50	D6	449	0	462	15	0
51	B7	418	0	467	14	0
51	D7	418	0	467	18	0
52	B8	509	0	565	18	0
52	D8	509	0	565	22	0
53	B9	297	0	316	9	0
53	D9	297	0	316	9	0
54	AA	135	0	0	0	0
54	AC	1	0	0	0	0
54	AD	1	0	0	0	0
54	AF	1	0	0	0	0
54	AQ	1	0	0	0	0
54	B0	3	0	0	0	0
54	B1	1	0	0	0	0
54	B2	1	0	0	0	0
54	B3	1	0	0	0	0
54	B5	2	0	0	0	0
54	B8	2	0	0	0	0
54	B9	1	0	0	0	0
54	BA	660	0	0	0	0
54	BB	23	0	0	0	0
54	BD	3	0	0	0	0
54	BE	5	0	0	0	0
54	BF	2	0	0	0	0
54	BG	1	0	0	0	0
54	BP	1	0	0	0	0
54	BQ	4	0	0	0	0
54	BR	1	0	0	0	0
54	BS	1	0	0	0	0
54	BT	2	0	0	0	0
54	BV	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	BW	2	0	0	0	0
54	BZ	1	0	0	0	0
54	CA	162	0	0	0	0
54	CE	1	0	0	0	0
54	CQ	1	0	0	0	0
54	D0	2	0	0	0	0
54	D1	1	0	0	0	0
54	D5	1	0	0	0	0
54	D8	2	0	0	0	0
54	DA	598	0	0	0	0
54	DB	8	0	0	0	0
54	DD	2	0	0	0	0
54	DE	4	0	0	0	0
54	DF	1	0	0	0	0
54	DO	2	0	0	0	0
54	DP	1	0	0	0	0
54	DQ	2	0	0	0	0
54	DR	3	0	0	0	0
55	AD	1	0	0	0	0
55	AN	1	0	0	0	0
55	B4	1	0	0	0	0
55	B5	1	0	0	0	0
55	B6	1	0	0	0	0
55	B9	1	0	0	0	0
55	BY	1	0	0	0	0
55	CD	1	0	0	0	0
55	CN	1	0	0	0	0
55	D4	1	0	0	0	0
55	D5	1	0	0	0	0
55	D6	1	0	0	0	0
55	D9	1	0	0	0	0
55	DY	1	0	0	0	0
56	AA	268	0	0	32	0
56	AE	1	0	0	0	0
56	AL	1	0	0	0	0
56	AO	1	0	0	0	0
56	AP	1	0	0	0	0
56	AT	1	0	0	0	0
56	AX	1	0	0	0	0
56	B0	8	0	0	0	0
56	B1	2	0	0	0	0
56	B3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	B5	3	0	0	0	0
56	B6	1	0	0	1	0
56	B7	5	0	0	0	0
56	B8	10	0	0	0	0
56	B9	1	0	0	1	0
56	BA	1694	0	0	169	0
56	BB	57	0	0	3	1
56	BD	20	0	0	3	0
56	BE	11	0	0	0	0
56	BF	6	0	0	1	0
56	BH	1	0	0	0	0
56	BN	2	0	0	0	0
56	BO	2	0	0	0	0
56	BP	11	0	0	2	0
56	BQ	5	0	0	0	0
56	BR	6	0	0	1	0
56	BT	1	0	0	0	0
56	BU	3	0	0	0	0
56	BV	3	0	0	0	0
56	BW	3	0	0	0	0
56	BX	2	0	0	0	0
56	BY	4	0	0	0	0
56	CA	265	0	0	25	0
56	CC	1	0	0	2	0
56	CD	1	0	0	0	0
56	CE	2	0	0	0	0
56	CK	1	0	0	1	0
56	CL	2	0	0	1	0
56	CN	1	0	0	0	0
56	CP	1	0	0	0	0
56	CQ	1	0	0	0	0
56	CT	1	0	0	0	0
56	CX	1	0	0	0	0
56	D0	1	0	0	0	0
56	D1	5	0	0	0	0
56	D3	1	0	0	0	0
56	D4	1	0	0	0	0
56	D7	3	0	0	0	0
56	D8	1	0	0	0	0
56	DA	1174	0	0	171	0
56	DB	17	0	0	0	0
56	DD	8	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DE	11	0	0	2	0
56	DF	7	0	0	1	0
56	DN	1	0	0	0	0
56	DO	5	0	0	1	0
56	DP	10	0	0	1	0
56	DQ	3	0	0	0	0
56	DR	2	0	0	1	0
56	DT	2	0	0	0	0
56	DU	5	0	0	0	0
56	DV	2	0	0	1	0
56	DW	2	0	0	0	0
56	DX	1	0	0	1	0
56	DY	2	0	0	0	0
All	All	286308	0	187082	8298	2

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 18.

The worst 5 of 8298 close contacts within the same asymmetric unit are listed below.

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

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:BA:1594:G:OP1	56:BB:323:HOH:O[1_455]	2.18	0.02
30:BI:91:SER:OG	1:CA:368:U:OP1[3_654]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	228/256 (89%)	199 (87%)	28 (12%)	1 (0%)	43	84
2	CB	227/256 (89%)	197 (87%)	29 (13%)	1 (0%)	43	84
3	AC	204/239 (85%)	175 (86%)	28 (14%)	1 (0%)	38	81
3	CC	204/239 (85%)	177 (87%)	27 (13%)	0	100	100
4	AD	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
4	CD	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
5	AE	146/162 (90%)	134 (92%)	12 (8%)	0	100	100
5	CE	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	30	76
6	AF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
6	CF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
7	AG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	18	60
7	CG	153/156 (98%)	132 (86%)	20 (13%)	1 (1%)	30	76
8	AH	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
8	CH	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
9	AI	123/128 (96%)	112 (91%)	10 (8%)	1 (1%)	27	74
9	CI	123/128 (96%)	111 (90%)	11 (9%)	1 (1%)	27	74
10	AJ	94/105 (90%)	78 (83%)	13 (14%)	3 (3%)	6	35
10	CJ	94/105 (90%)	76 (81%)	16 (17%)	2 (2%)	11	48
11	AK	112/129 (87%)	106 (95%)	6 (5%)	0	100	100
11	CK	112/129 (87%)	106 (95%)	6 (5%)	0	100	100
12	AL	120/132 (91%)	110 (92%)	9 (8%)	1 (1%)	27	74
12	CL	120/132 (91%)	109 (91%)	10 (8%)	1 (1%)	27	74
13	AM	112/126 (89%)	89 (80%)	21 (19%)	2 (2%)	13	52
13	CM	112/126 (89%)	87 (78%)	21 (19%)	4 (4%)	5	31
14	AN	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	6	32
14	CN	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
15	AO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	10	45
15	CO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	10	45
16	AP	80/88 (91%)	75 (94%)	4 (5%)	1 (1%)	18	60
16	CP	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	18	60
17	AQ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	CQ	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
18	AR	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
18	CR	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
19	AS	79/93 (85%)	67 (85%)	11 (14%)	1 (1%)	18	60
19	CS	79/93 (85%)	65 (82%)	13 (16%)	1 (1%)	18	60
20	AT	85/106 (80%)	78 (92%)	7 (8%)	0	100	100
20	CT	95/106 (90%)	84 (88%)	8 (8%)	3 (3%)	6	35
21	AU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
21	CU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
22	AX	93/101 (92%)	79 (85%)	13 (14%)	1 (1%)	21	65
22	CX	93/101 (92%)	84 (90%)	9 (10%)	0	100	100
25	BD	273/276 (99%)	260 (95%)	12 (4%)	1 (0%)	43	84
25	DD	273/276 (99%)	259 (95%)	13 (5%)	1 (0%)	43	84
26	BE	202/206 (98%)	190 (94%)	10 (5%)	2 (1%)	22	68
26	DE	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	22	68
27	BF	201/210 (96%)	195 (97%)	6 (3%)	0	100	100
27	DF	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	38	81
28	BG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	33	78
28	DG	179/182 (98%)	150 (84%)	29 (16%)	0	100	100
29	BH	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	33	78
29	DH	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	33	78
30	BI	144/148 (97%)	121 (84%)	21 (15%)	2 (1%)	16	58
30	DI	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	16	58
31	BN	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	10	46
31	DN	138/140 (99%)	128 (93%)	7 (5%)	3 (2%)	10	46
32	BO	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
32	DO	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
33	BP	147/150 (98%)	137 (93%)	10 (7%)	0	100	100
33	DP	147/150 (98%)	136 (92%)	11 (8%)	0	100	100
34	BQ	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	30	76
34	DQ	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	30	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	BR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
35	DR	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
36	BS	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
36	DS	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
37	BT	129/146 (88%)	127 (98%)	2 (2%)	0	100	100
37	DT	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
38	BU	114/118 (97%)	114 (100%)	0	0	100	100
38	DU	114/118 (97%)	114 (100%)	0	0	100	100
39	BV	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
39	DV	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
40	BW	110/113 (97%)	108 (98%)	1 (1%)	1 (1%)	25	71
40	DW	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
41	BX	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
41	DX	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
42	BY	105/110 (96%)	94 (90%)	10 (10%)	1 (1%)	22	68
42	DY	105/110 (96%)	94 (90%)	10 (10%)	1 (1%)	22	68
43	BZ	199/206 (97%)	183 (92%)	14 (7%)	2 (1%)	22	68
43	DZ	196/206 (95%)	180 (92%)	14 (7%)	2 (1%)	22	68
44	B0	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
44	D0	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
45	B1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	21	65
45	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	21	65
46	B2	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
46	D2	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
47	B3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
47	D3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
48	B4	44/71 (62%)	36 (82%)	8 (18%)	0	100	100
48	D4	44/71 (62%)	36 (82%)	8 (18%)	0	100	100
49	B5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
49	D5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
50	B6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	D6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
51	B7	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	10	46
51	D7	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	10	46
52	B8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
52	D8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
53	B9	34/37 (92%)	34 (100%)	0	0	100	100
53	D9	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
All	All	11552/12330 (94%)	10628 (92%)	855 (7%)	69 (1%)	33	78

5 of 69 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	178/220 (81%)	133 (75%)	45 (25%)	1	3
2	CB	177/220 (80%)	133 (75%)	44 (25%)	1	3
3	AC	114/188 (61%)	79 (69%)	35 (31%)	0	1
3	CC	114/188 (61%)	92 (81%)	22 (19%)	2	8
4	AD	141/181 (78%)	118 (84%)	23 (16%)	3	12
4	CD	141/181 (78%)	119 (84%)	22 (16%)	4	14
5	AE	108/123 (88%)	87 (81%)	21 (19%)	2	8
5	CE	108/123 (88%)	87 (81%)	21 (19%)	2	8
6	AF	76/90 (84%)	61 (80%)	15 (20%)	2	8
6	CF	76/90 (84%)	58 (76%)	18 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AG	103/127 (81%)	73 (71%)	30 (29%)	0	1
7	CG	103/127 (81%)	68 (66%)	35 (34%)	0	0
8	AH	103/119 (87%)	82 (80%)	21 (20%)	2	8
8	CH	103/119 (87%)	83 (81%)	20 (19%)	2	8
9	AI	62/99 (63%)	47 (76%)	15 (24%)	1	4
9	CI	62/99 (63%)	47 (76%)	15 (24%)	1	4
10	AJ	53/92 (58%)	38 (72%)	15 (28%)	0	1
10	CJ	53/92 (58%)	39 (74%)	14 (26%)	1	2
11	AK	81/99 (82%)	71 (88%)	10 (12%)	7	26
11	CK	81/99 (82%)	70 (86%)	11 (14%)	5	21
12	AL	91/109 (84%)	80 (88%)	11 (12%)	7	27
12	CL	91/109 (84%)	81 (89%)	10 (11%)	9	34
13	AM	64/101 (63%)	48 (75%)	16 (25%)	1	3
13	CM	64/101 (63%)	49 (77%)	15 (23%)	1	5
14	AN	46/50 (92%)	36 (78%)	10 (22%)	1	6
14	CN	46/50 (92%)	32 (70%)	14 (30%)	0	1
15	AO	77/80 (96%)	68 (88%)	9 (12%)	8	29
15	CO	77/80 (96%)	68 (88%)	9 (12%)	8	29
16	AP	63/74 (85%)	46 (73%)	17 (27%)	1	2
16	CP	63/74 (85%)	44 (70%)	19 (30%)	0	1
17	AQ	94/97 (97%)	80 (85%)	14 (15%)	4	17
17	CQ	94/97 (97%)	81 (86%)	13 (14%)	5	21
18	AR	49/77 (64%)	44 (90%)	5 (10%)	11	37
18	CR	49/77 (64%)	44 (90%)	5 (10%)	11	37
19	AS	43/80 (54%)	26 (60%)	17 (40%)	0	0
19	CS	43/80 (54%)	32 (74%)	11 (26%)	1	2
20	AT	64/82 (78%)	55 (86%)	9 (14%)	5	20
20	CT	65/82 (79%)	55 (85%)	10 (15%)	4	15
21	AU	18/22 (82%)	13 (72%)	5 (28%)	0	1
21	CU	18/22 (82%)	11 (61%)	7 (39%)	0	0
22	AX	45/87 (52%)	34 (76%)	11 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	CX	38/87 (44%)	29 (76%)	9 (24%)	1	4
25	BD	215/218 (99%)	182 (85%)	33 (15%)	4	15
25	DD	215/218 (99%)	183 (85%)	32 (15%)	4	17
26	BE	163/166 (98%)	135 (83%)	28 (17%)	3	11
26	DE	163/166 (98%)	137 (84%)	26 (16%)	3	13
27	BF	159/166 (96%)	135 (85%)	24 (15%)	4	16
27	DF	159/166 (96%)	134 (84%)	25 (16%)	4	14
28	BG	128/156 (82%)	109 (85%)	19 (15%)	4	17
28	DG	128/156 (82%)	109 (85%)	19 (15%)	4	17
29	BH	141/148 (95%)	123 (87%)	18 (13%)	6	24
29	DH	141/148 (95%)	123 (87%)	18 (13%)	6	24
30	BI	98/124 (79%)	81 (83%)	17 (17%)	3	11
30	DI	74/124 (60%)	60 (81%)	14 (19%)	2	9
31	BN	117/119 (98%)	98 (84%)	19 (16%)	3	13
31	DN	117/119 (98%)	98 (84%)	19 (16%)	3	13
32	BO	98/100 (98%)	82 (84%)	16 (16%)	3	12
32	DO	98/100 (98%)	83 (85%)	15 (15%)	4	15
33	BP	114/116 (98%)	99 (87%)	15 (13%)	6	23
33	DP	114/116 (98%)	99 (87%)	15 (13%)	6	23
34	BQ	111/111 (100%)	96 (86%)	15 (14%)	6	22
34	DQ	111/111 (100%)	96 (86%)	15 (14%)	6	22
35	BR	101/101 (100%)	79 (78%)	22 (22%)	1	6
35	DR	101/101 (100%)	77 (76%)	24 (24%)	1	4
36	BS	84/88 (96%)	67 (80%)	17 (20%)	2	8
36	DS	84/88 (96%)	68 (81%)	16 (19%)	2	9
37	BT	110/127 (87%)	98 (89%)	12 (11%)	9	34
37	DT	110/127 (87%)	95 (86%)	15 (14%)	5	21
38	BU	93/94 (99%)	82 (88%)	11 (12%)	8	29
38	DU	93/94 (99%)	83 (89%)	10 (11%)	9	34
39	BV	80/82 (98%)	63 (79%)	17 (21%)	1	7
39	DV	80/82 (98%)	63 (79%)	17 (21%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	BW	89/92 (97%)	81 (91%)	8 (9%)	14	47
40	DW	89/92 (97%)	78 (88%)	11 (12%)	7	25
41	BX	75/78 (96%)	71 (95%)	4 (5%)	32	72
41	DX	75/78 (96%)	70 (93%)	5 (7%)	23	63
42	BY	80/91 (88%)	64 (80%)	16 (20%)	2	8
42	DY	80/91 (88%)	63 (79%)	17 (21%)	1	7
43	BZ	159/179 (89%)	137 (86%)	22 (14%)	5	21
43	DZ	159/179 (89%)	139 (87%)	20 (13%)	7	24
44	B0	59/67 (88%)	51 (86%)	8 (14%)	5	21
44	D0	59/67 (88%)	50 (85%)	9 (15%)	4	15
45	B1	78/83 (94%)	63 (81%)	15 (19%)	2	9
45	D1	78/83 (94%)	66 (85%)	12 (15%)	4	15
46	B2	65/67 (97%)	54 (83%)	11 (17%)	3	11
46	D2	65/67 (97%)	55 (85%)	10 (15%)	4	15
47	B3	49/52 (94%)	44 (90%)	5 (10%)	11	37
47	D3	49/52 (94%)	44 (90%)	5 (10%)	11	37
48	B4	39/63 (62%)	33 (85%)	6 (15%)	4	15
48	D4	39/63 (62%)	33 (85%)	6 (15%)	4	15
49	B5	50/52 (96%)	42 (84%)	8 (16%)	3	13
49	D5	50/52 (96%)	41 (82%)	9 (18%)	2	10
50	B6	50/52 (96%)	39 (78%)	11 (22%)	1	6
50	D6	50/52 (96%)	40 (80%)	10 (20%)	2	8
51	B7	41/42 (98%)	34 (83%)	7 (17%)	3	11
51	D7	41/42 (98%)	34 (83%)	7 (17%)	3	11
52	B8	52/55 (94%)	42 (81%)	10 (19%)	2	9
52	D8	52/55 (94%)	42 (81%)	10 (19%)	2	9
53	B9	32/34 (94%)	28 (88%)	4 (12%)	7	25
53	D9	32/34 (94%)	28 (88%)	4 (12%)	7	25
All	All	8775/10240 (86%)	7244 (83%)	1531 (17%)	3	11

5 of 1531 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	B0	74	ARG
4	CD	158	ILE
42	DY	6	HIS
46	B2	32	LEU
2	CB	51	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
38	BU	49	HIS
2	CB	140	HIS
33	DP	84	ASN
39	BV	80	GLN
46	B2	9	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1499/1522 (98%)	385 (25%)	33 (2%)
1	CA	1495/1522 (98%)	396 (26%)	34 (2%)
23	BA	2833/2913 (97%)	609 (21%)	60 (2%)
23	DA	2807/2913 (96%)	600 (21%)	56 (1%)
24	BB	119/122 (97%)	25 (21%)	0
24	DB	119/122 (97%)	26 (21%)	0
All	All	8872/9114 (97%)	2041 (23%)	183 (2%)

5 of 2041 RNA backbone outliers are listed below:

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

5 of 183 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BA	2126	A
1	CA	495	A
23	DA	1819	A

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Mol	Chain	Res	Type
23	BA	2318	G
23	BA	2802	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 1662 ligands modelled in this entry, 1662 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1501/1522 (98%)	-0.13	38 (2%) 54 9	47, 95, 155, 169	0
1	CA	1497/1522 (98%)	-0.15	48 (3%) 45 7	50, 96, 158, 171	0
2	AB	230/256 (89%)	-0.10	2 (0%) 81 25	87, 114, 134, 148	0
2	CB	229/256 (89%)	0.13	2 (0%) 81 25	92, 116, 136, 149	0
3	AC	206/239 (86%)	-0.01	0 100 100	85, 109, 127, 136	0
3	CC	206/239 (86%)	0.16	4 (1%) 64 13	94, 120, 143, 158	0
4	AD	208/209 (99%)	-0.06	0 100 100	75, 94, 114, 125	0
4	CD	208/209 (99%)	-0.00	0 100 100	76, 93, 114, 124	0
5	AE	148/162 (91%)	-0.22	0 100 100	66, 86, 103, 125	0
5	CE	148/162 (91%)	-0.10	0 100 100	69, 88, 104, 127	0
6	AF	100/101 (99%)	-0.26	0 100 100	67, 82, 100, 116	0
6	CF	100/101 (99%)	-0.23	0 100 100	70, 86, 103, 117	0
7	AG	155/156 (99%)	1.22	37 (23%) 1 0	113, 139, 153, 159	0
7	CG	155/156 (99%)	1.13	31 (20%) 2 0	122, 137, 149, 159	0
8	AH	138/138 (100%)	0.08	0 100 100	71, 90, 100, 110	0
8	CH	138/138 (100%)	-0.07	1 (0%) 84 32	71, 92, 103, 113	0
9	AI	125/128 (97%)	0.79	13 (10%) 7 1	110, 137, 149, 154	0
9	CI	125/128 (97%)	1.69	44 (35%) 1 0	115, 139, 152, 163	0
10	AJ	96/105 (91%)	0.81	12 (12%) 5 1	92, 126, 141, 147	0
10	CJ	96/105 (91%)	1.10	14 (14%) 3 1	108, 134, 150, 160	0
11	AK	114/129 (88%)	-0.08	0 100 100	60, 86, 108, 120	0
11	CK	114/129 (88%)	-0.01	2 (1%) 65 14	63, 89, 107, 126	0
12	AL	122/132 (92%)	-0.07	0 100 100	62, 77, 95, 112	0
12	CL	122/132 (92%)	-0.02	0 100 100	63, 77, 96, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	114/126 (90%)	0.88	13 (11%) 6 1	112, 139, 150, 153	0
13	CM	114/126 (90%)	1.22	28 (24%) 1 0	116, 140, 151, 160	0
14	AN	60/61 (98%)	0.48	5 (8%) 11 2	93, 118, 131, 144	0
14	CN	60/61 (98%)	0.62	4 (6%) 17 3	103, 122, 134, 139	0
15	AO	88/89 (98%)	-0.07	0 100 100	63, 85, 103, 113	0
15	CO	88/89 (98%)	-0.03	0 100 100	63, 85, 105, 111	0
16	AP	82/88 (93%)	0.41	2 (2%) 56 9	76, 88, 110, 120	0
16	CP	82/88 (93%)	0.22	0 100 100	73, 85, 105, 117	0
17	AQ	99/105 (94%)	-0.01	0 100 100	68, 82, 102, 106	0
17	CQ	99/105 (94%)	-0.00	0 100 100	69, 83, 101, 108	0
18	AR	68/88 (77%)	-0.10	0 100 100	71, 82, 105, 112	0
18	CR	68/88 (77%)	0.11	0 100 100	75, 85, 105, 117	0
19	AS	81/93 (87%)	1.37	21 (25%) 1 0	113, 138, 147, 152	0
19	CS	81/93 (87%)	1.59	20 (24%) 1 0	114, 140, 150, 153	0
20	AT	87/106 (82%)	0.17	0 100 100	75, 88, 103, 111	0
20	CT	97/106 (91%)	0.01	0 100 100	72, 86, 105, 115	0
21	AU	23/27 (85%)	2.39	14 (60%) 0 0	128, 136, 145, 154	0
21	CU	23/27 (85%)	2.85	15 (65%) 0 0	129, 137, 148, 150	0
22	AX	95/101 (94%)	0.25	0 100 100	69, 94, 115, 123	0
22	CX	95/101 (94%)	0.79	7 (7%) 14 2	88, 106, 129, 145	0
23	BA	2837/2913 (97%)	-0.39	23 (0%) 83 28	26, 47, 132, 176	0
23	DA	2814/2913 (96%)	-0.52	55 (1%) 62 12	28, 50, 133, 176	0
24	BB	120/122 (98%)	-0.47	0 100 100	43, 72, 93, 110	0
24	DB	120/122 (98%)	-0.22	1 (0%) 83 28	48, 81, 106, 117	0
25	BD	275/276 (99%)	-0.30	0 100 100	29, 45, 63, 113	0
25	DD	275/276 (99%)	-0.28	0 100 100	30, 47, 66, 116	0
26	BE	204/206 (99%)	-0.30	0 100 100	28, 49, 72, 95	0
26	DE	204/206 (99%)	-0.32	0 100 100	29, 50, 76, 95	0
27	BF	203/210 (96%)	-0.29	0 100 100	29, 54, 88, 111	0
27	DF	203/210 (96%)	-0.25	0 100 100	31, 59, 90, 112	0
28	BG	181/182 (99%)	-0.05	3 (1%) 67 15	76, 110, 133, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DG	181/182 (99%)	0.45	8 (4%) 33 5	86, 117, 138, 148	0
29	BH	174/180 (96%)	-0.20	0 100 100	54, 73, 94, 110	0
29	DH	174/180 (96%)	0.18	2 (1%) 77 22	65, 82, 101, 119	0
30	BI	146/148 (98%)	-0.26	1 (0%) 84 32	54, 81, 99, 115	0
30	DI	146/148 (98%)	-0.03	0 100 100	56, 89, 108, 120	0
31	BN	140/140 (100%)	-0.29	0 100 100	38, 49, 78, 92	0
31	DN	140/140 (100%)	-0.19	0 100 100	40, 54, 82, 96	0
32	BO	122/122 (100%)	-0.30	0 100 100	35, 50, 69, 77	0
32	DO	122/122 (100%)	-0.39	0 100 100	36, 52, 69, 77	0
33	BP	149/150 (99%)	-0.22	0 100 100	30, 58, 89, 105	0
33	DP	149/150 (99%)	-0.11	1 (0%) 84 32	31, 62, 92, 112	0
34	BQ	141/141 (100%)	-0.26	0 100 100	39, 54, 71, 83	0
34	DQ	141/141 (100%)	-0.23	0 100 100	41, 58, 77, 88	0
35	BR	118/118 (100%)	-0.25	0 100 100	34, 44, 58, 77	0
35	DR	118/118 (100%)	-0.20	0 100 100	36, 47, 62, 78	0
36	BS	110/112 (98%)	-0.09	0 100 100	50, 69, 89, 96	0
36	DS	110/112 (98%)	0.25	2 (1%) 65 14	55, 74, 94, 102	0
37	BT	131/146 (89%)	-0.31	0 100 100	43, 55, 92, 119	0
37	DT	131/146 (89%)	-0.25	0 100 100	46, 57, 93, 128	0
38	BU	116/118 (98%)	-0.31	0 100 100	32, 44, 62, 71	0
38	DU	116/118 (98%)	-0.33	0 100 100	34, 48, 66, 73	0
39	BV	101/101 (100%)	-0.27	1 (0%) 79 23	29, 56, 79, 103	0
39	DV	101/101 (100%)	-0.16	0 100 100	32, 62, 85, 103	0
40	BW	112/113 (99%)	-0.29	0 100 100	33, 40, 62, 103	0
40	DW	112/113 (99%)	-0.32	0 100 100	35, 42, 67, 105	0
41	BX	95/96 (98%)	-0.19	0 100 100	38, 49, 72, 88	0
41	DX	95/96 (98%)	-0.20	1 (1%) 77 22	41, 52, 77, 90	0
42	BY	107/110 (97%)	-0.19	0 100 100	47, 61, 85, 108	0
42	DY	107/110 (97%)	0.11	2 (1%) 64 13	52, 65, 89, 113	0
43	BZ	201/206 (97%)	-0.28	0 100 100	53, 76, 99, 122	0
43	DZ	198/206 (96%)	-0.02	1 (0%) 88 39	62, 81, 102, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	B0	76/85 (89%)	-0.23	0 100 100	39, 48, 64, 91	0
44	D0	76/85 (89%)	0.02	0 100 100	43, 52, 66, 92	0
45	B1	97/98 (98%)	-0.15	0 100 100	36, 48, 82, 97	0
45	D1	97/98 (98%)	-0.11	0 100 100	36, 51, 83, 98	0
46	B2	70/72 (97%)	-0.17	1 (1%) 72 17	46, 60, 76, 107	0
46	D2	70/72 (97%)	-0.13	0 100 100	50, 64, 81, 103	0
47	B3	59/60 (98%)	-0.18	0 100 100	38, 49, 86, 97	0
47	D3	59/60 (98%)	0.13	1 (1%) 67 15	41, 53, 93, 102	0
48	B4	46/71 (64%)	-0.30	0 100 100	101, 129, 144, 148	0
48	D4	46/71 (64%)	0.09	0 100 100	113, 133, 144, 152	0
49	B5	59/60 (98%)	-0.41	0 100 100	30, 45, 66, 80	0
49	D5	59/60 (98%)	-0.38	0 100 100	32, 47, 68, 81	0
50	B6	53/54 (98%)	-0.43	0 100 100	42, 51, 70, 79	0
50	D6	53/54 (98%)	-0.20	0 100 100	43, 54, 72, 82	0
51	B7	48/49 (97%)	-0.21	0 100 100	30, 34, 55, 80	0
51	D7	48/49 (97%)	-0.08	0 100 100	32, 35, 58, 84	0
52	B8	64/65 (98%)	-0.21	0 100 100	38, 43, 52, 70	0
52	D8	64/65 (98%)	-0.11	0 100 100	40, 45, 55, 70	0
53	B9	36/37 (97%)	0.20	0 100 100	44, 55, 62, 73	0
53	D9	36/37 (97%)	0.40	0 100 100	47, 59, 68, 75	0
All	All	20641/21444 (96%)	-0.13	480 (2%) 57 9	26, 71, 144, 176	0

The worst 5 of 480 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
21	CU	12	LYS	8.0
1	CA	1030(B)	C	7.8
19	CS	69	HIS	7.7
21	CU	11	GLY	7.2
23	BA	888	C	6.7

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
54	MG	BA	3022	1/1	0.26	-	46,46,46,46	0
54	MG	AA	1735	1/1	0.14	-	110,110,110,110	0
54	MG	DQ	202	1/1	0.18	-	33,33,33,33	0
54	MG	BA	3563	1/1	0.08	-	70,70,70,70	0
54	MG	DA	3260	1/1	0.17	-	41,41,41,41	0
54	MG	DA	3572	1/1	0.10	-	71,71,71,71	0
54	MG	DA	3392	1/1	0.16	-	35,35,35,35	0
54	MG	DA	3159	1/1	0.20	-	45,45,45,45	0
54	MG	CA	1748	1/1	0.05	-	58,58,58,58	0
54	MG	BA	3328	1/1	0.20	-	30,30,30,30	0
54	MG	BA	3359	1/1	0.11	-	70,70,70,70	0
54	MG	BA	3228	1/1	0.41	-	37,37,37,37	0
54	MG	DA	3056	1/1	0.21	-	43,43,43,43	0
54	MG	CA	1610	1/1	0.27	-	60,60,60,60	0
54	MG	DA	3031	1/1	0.24	-	53,53,53,53	0
54	MG	BA	3050	1/1	0.20	-	35,35,35,35	0
54	MG	BA	3336	1/1	0.09	-	45,45,45,45	0
54	MG	BA	3375	1/1	0.15	-	34,34,34,34	0
54	MG	DB	207	1/1	0.24	-	57,57,57,57	0
54	MG	DA	3145	1/1	0.17	-	61,61,61,61	0
54	MG	BA	3579	1/1	0.09	-	100,100,100,100	0
54	MG	BA	3076	1/1	0.22	-	44,44,44,44	0
54	MG	CA	1658	1/1	0.33	-	58,58,58,58	0
54	MG	DA	3532	1/1	0.24	-	116,116,116,116	0
54	MG	DA	3504	1/1	0.10	-	63,63,63,63	0
54	MG	BA	3042	1/1	0.23	-	40,40,40,40	0
54	MG	BA	3617	1/1	0.08	-	94,94,94,94	0
54	MG	DA	3387	1/1	0.12	-	60,60,60,60	0
54	MG	BA	3089	1/1	0.34	-	41,41,41,41	0
54	MG	BA	3275	1/1	0.29	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3174	1/1	0.14	-	32,32,32,32	0
54	MG	BA	3596	1/1	0.08	-	48,48,48,48	0
54	MG	BA	3414	1/1	0.14	-	29,29,29,29	0
54	MG	BA	3027	1/1	0.16	-	38,38,38,38	0
54	MG	DA	3131	1/1	0.27	-	56,56,56,56	0
54	MG	BA	3144	1/1	0.25	-	46,46,46,46	0
54	MG	DA	3330	1/1	0.14	-	37,37,37,37	0
54	MG	DA	3503	1/1	0.24	-	34,34,34,34	0
54	MG	BA	3559	1/1	0.07	-	71,71,71,71	0
54	MG	BA	3448	1/1	0.14	-	38,38,38,38	0
54	MG	DA	3519	1/1	0.07	-	52,52,52,52	0
54	MG	AA	1605	1/1	0.17	-	66,66,66,66	0
54	MG	BA	3128	1/1	0.20	-	49,49,49,49	0
54	MG	DA	3050	1/1	0.27	-	34,34,34,34	0
54	MG	BA	3119	1/1	0.35	-	42,42,42,42	0
54	MG	AA	1644	1/1	0.34	-	39,39,39,39	0
54	MG	DA	3507	1/1	0.10	-	80,80,80,80	0
54	MG	DA	3413	1/1	0.12	-	56,56,56,56	0
54	MG	BA	3243	1/1	0.32	-	42,42,42,42	0
54	MG	BA	3624	1/1	0.11	-	36,36,36,36	0
54	MG	BA	3043	1/1	0.13	-	39,39,39,39	0
54	MG	DA	3341	1/1	0.12	-	43,43,43,43	0
54	MG	BA	3621	1/1	0.33	-	52,52,52,52	0
54	MG	DA	3333	1/1	0.15	-	37,37,37,37	0
54	MG	DA	3089	1/1	0.13	-	52,52,52,52	0
54	MG	BA	3049	1/1	0.36	-	53,53,53,53	0
54	MG	AA	1664	1/1	0.14	-	57,57,57,57	0
54	MG	AA	1603	1/1	0.40	-	79,79,79,79	0
54	MG	AA	1656	1/1	0.57	-	59,59,59,59	0
54	MG	DA	3229	1/1	0.33	-	44,44,44,44	0
54	MG	BA	3629	1/1	0.10	-	24,24,24,24	0
54	MG	DA	3103	1/1	0.18	-	54,54,54,54	0
54	MG	DA	3188	1/1	0.13	-	69,69,69,69	0
54	MG	DA	3376	1/1	0.13	-	30,30,30,30	0
54	MG	AA	1680	1/1	0.27	-	72,72,72,72	0
54	MG	DA	3316	1/1	0.77	-	69,69,69,69	0
54	MG	BA	3658	1/1	0.15	-	114,114,114,114	0
54	MG	BA	3411	1/1	0.08	-	63,63,63,63	0
54	MG	DA	3094	1/1	0.15	-	56,56,56,56	0
54	MG	DA	3569	1/1	0.12	-	104,104,104,104	0
54	MG	BA	3102	1/1	0.36	-	44,44,44,44	0
54	MG	DA	3269	1/1	0.29	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3209	1/1	0.25	-	51,51,51,51	0
54	MG	AA	1732	1/1	0.09	-	94,94,94,94	0
54	MG	CA	1717	1/1	0.12	-	110,110,110,110	0
54	MG	CA	1671	1/1	0.43	-	49,49,49,49	0
54	MG	BA	3230	1/1	0.22	-	30,30,30,30	0
54	MG	DA	3577	1/1	0.08	-	57,57,57,57	0
54	MG	DA	3033	1/1	0.15	-	66,66,66,66	0
54	MG	AA	1666	1/1	0.14	-	74,74,74,74	0
54	MG	BA	3335	1/1	0.08	-	66,66,66,66	0
54	MG	CA	1725	1/1	0.17	-	65,65,65,65	0
54	MG	BA	3576	1/1	0.18	-	21,21,21,21	0
54	MG	BA	3458	1/1	0.17	-	35,35,35,35	0
54	MG	DA	3342	1/1	0.18	-	38,38,38,38	0
54	MG	DA	3275	1/1	0.39	-	47,47,47,47	0
54	MG	DA	3288	1/1	0.22	-	39,39,39,39	0
54	MG	DA	3306	1/1	0.35	-	29,29,29,29	0
54	MG	BA	3653	1/1	0.14	-	104,104,104,104	0
55	ZN	AD	301	1/1	0.28	-	74,74,74,74	0
54	MG	CA	1704	1/1	0.13	-	92,92,92,92	0
54	MG	BA	3060	1/1	0.15	-	54,54,54,54	0
54	MG	BA	3487	1/1	0.15	-	20,20,20,20	0
54	MG	BA	3430	1/1	0.05	-	49,49,49,49	0
54	MG	CA	1666	1/1	0.32	-	64,64,64,64	0
54	MG	DA	3346	1/1	0.14	-	35,35,35,35	0
54	MG	DA	3268	1/1	0.58	-	54,54,54,54	0
54	MG	BA	3306	1/1	0.16	-	55,55,55,55	0
54	MG	BA	3634	1/1	0.12	-	53,53,53,53	0
54	MG	DA	3114	1/1	0.40	-	30,30,30,30	0
54	MG	BA	3515	1/1	0.17	-	72,72,72,72	0
54	MG	BA	3251	1/1	0.27	-	27,27,27,27	0
54	MG	BA	3129	1/1	0.35	-	37,37,37,37	0
54	MG	DA	3555	1/1	0.15	-	56,56,56,56	0
54	MG	BA	3450	1/1	0.10	-	38,38,38,38	0
54	MG	DA	3211	1/1	0.26	-	48,48,48,48	0
54	MG	DA	3168	1/1	0.20	-	42,42,42,42	0
54	MG	DA	3048	1/1	0.25	-	40,40,40,40	0
54	MG	BA	3610	1/1	0.08	-	63,63,63,63	0
54	MG	DA	3222	1/1	0.19	-	68,68,68,68	0
54	MG	DA	3217	1/1	0.48	-	32,32,32,32	0
54	MG	BA	3030	1/1	0.15	-	48,48,48,48	0
54	MG	DA	3298	1/1	0.29	-	49,49,49,49	0
54	MG	BA	3244	1/1	0.15	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1641	1/1	0.16	-	42,42,42,42	0
54	MG	CA	1760	1/1	0.10	-	87,87,87,87	0
54	MG	DA	3024	1/1	0.36	-	47,47,47,47	0
54	MG	DA	3041	1/1	0.53	-	36,36,36,36	0
54	MG	DA	3290	1/1	0.52	-	58,58,58,58	0
54	MG	DA	3526	1/1	0.10	-	98,98,98,98	0
54	MG	DA	3570	1/1	0.21	-	28,28,28,28	0
54	MG	DA	3055	1/1	0.29	-	56,56,56,56	0
54	MG	BA	3160	1/1	0.30	-	39,39,39,39	0
54	MG	DA	3453	1/1	0.07	-	79,79,79,79	0
54	MG	DA	3278	1/1	0.07	-	83,83,83,83	0
54	MG	BA	3006	1/1	0.19	-	25,25,25,25	0
54	MG	BA	3025	1/1	0.21	-	48,48,48,48	0
54	MG	BA	3274	1/1	0.27	-	26,26,26,26	0
54	MG	BA	3011	1/1	0.29	-	26,26,26,26	0
54	MG	BB	218	1/1	0.10	-	45,45,45,45	0
54	MG	AA	1661	1/1	0.28	-	55,55,55,55	0
54	MG	AA	1729	1/1	0.09	-	80,80,80,80	0
54	MG	DA	3489	1/1	0.12	-	79,79,79,79	0
54	MG	DA	3495	1/1	0.09	-	83,83,83,83	0
54	MG	DA	3108	1/1	0.13	-	42,42,42,42	0
54	MG	DA	3123	1/1	0.27	-	53,53,53,53	0
54	MG	BA	3304	1/1	0.31	-	54,54,54,54	0
54	MG	CA	1602	1/1	0.41	-	62,62,62,62	0
54	MG	BA	3341	1/1	0.05	-	44,44,44,44	0
54	MG	AA	1659	1/1	0.91	-	70,70,70,70	0
54	MG	DA	3302	1/1	0.51	-	21,21,21,21	0
54	MG	DA	3205	1/1	0.27	-	47,47,47,47	0
54	MG	AA	1681	1/1	0.24	-	50,50,50,50	0
54	MG	BA	3635	1/1	0.08	-	23,23,23,23	0
54	MG	AA	1727	1/1	0.12	-	61,61,61,61	0
54	MG	CA	1673	1/1	0.60	-	57,57,57,57	0
55	ZN	CD	301	1/1	0.26	-	71,71,71,71	0
54	MG	BA	3037	1/1	0.25	-	75,75,75,75	0
54	MG	DA	3571	1/1	0.14	-	55,55,55,55	0
54	MG	BA	3175	1/1	0.14	-	43,43,43,43	0
54	MG	BA	3202	1/1	0.17	-	48,48,48,48	0
54	MG	CA	1634	1/1	0.18	-	64,64,64,64	0
54	MG	BE	301	1/1	0.41	-	34,34,34,34	0
54	MG	CA	1723	1/1	0.15	-	55,55,55,55	0
54	MG	BA	3381	1/1	0.05	-	66,66,66,66	0
55	ZN	AN	101	1/1	0.12	-	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1604	1/1	0.14	-	73,73,73,73	0
54	MG	BA	3442	1/1	0.14	-	76,76,76,76	0
54	MG	BP	201	1/1	0.14	-	45,45,45,45	0
54	MG	BA	3068	1/1	0.38	-	50,50,50,50	0
54	MG	BA	3467	1/1	0.22	-	30,30,30,30	0
54	MG	D5	101	1/1	0.35	-	52,52,52,52	0
54	MG	DA	3388	1/1	0.17	-	43,43,43,43	0
54	MG	BA	3514	1/1	0.10	-	61,61,61,61	0
54	MG	CA	1641	1/1	0.09	-	52,52,52,52	0
54	MG	DA	3393	1/1	0.13	-	41,41,41,41	0
54	MG	DA	3417	1/1	0.15	-	31,31,31,31	0
54	MG	BA	3595	1/1	0.28	-	27,27,27,27	0
54	MG	DA	3010	1/1	0.20	-	42,42,42,42	0
54	MG	BA	3589	1/1	0.16	-	94,94,94,94	0
54	MG	DA	3381	1/1	0.04	-	42,42,42,42	0
54	MG	DA	3197	1/1	0.33	-	49,49,49,49	0
54	MG	CA	1617	1/1	0.10	-	87,87,87,87	0
54	MG	DB	202	1/1	0.23	-	50,50,50,50	0
54	MG	DA	3443	1/1	0.10	-	75,75,75,75	0
54	MG	BA	3094	1/1	0.22	-	54,54,54,54	0
54	MG	BA	3348	1/1	0.07	-	59,59,59,59	0
54	MG	DA	3109	1/1	0.18	-	59,59,59,59	0
54	MG	CA	1651	1/1	0.33	-	46,46,46,46	0
54	MG	BA	3331	1/1	0.16	-	48,48,48,48	0
54	MG	BA	3529	1/1	0.06	-	65,65,65,65	0
54	MG	BA	3550	1/1	0.06	-	87,87,87,87	0
55	ZN	D6	101	1/1	0.07	-	63,63,63,63	0
54	MG	CA	1694	1/1	0.18	-	62,62,62,62	0
54	MG	BA	3265	1/1	0.38	-	29,29,29,29	0
54	MG	CA	1665	1/1	0.28	-	84,84,84,84	0
54	MG	CA	1693	1/1	0.85	-	59,59,59,59	0
54	MG	BA	3419	1/1	0.40	-	21,21,21,21	0
54	MG	CA	1626	1/1	0.40	-	62,62,62,62	0
54	MG	DA	3292	1/1	0.26	-	33,33,33,33	0
54	MG	DA	3257	1/1	0.31	-	56,56,56,56	0
54	MG	CA	1747	1/1	0.11	-	95,95,95,95	0
54	MG	CA	1703	1/1	0.17	-	56,56,56,56	0
54	MG	DA	3074	1/1	0.18	-	54,54,54,54	0
54	MG	BA	3572	1/1	0.16	-	63,63,63,63	0
54	MG	BA	3148	1/1	0.22	-	47,47,47,47	0
54	MG	BA	3567	1/1	0.10	-	54,54,54,54	0
54	MG	BB	203	1/1	0.20	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3175	1/1	0.37	-	44,44,44,44	0
54	MG	BA	3426	1/1	0.10	-	37,37,37,37	0
54	MG	BA	3401	1/1	0.13	-	58,58,58,58	0
54	MG	AA	1614	1/1	0.51	-	56,56,56,56	0
54	MG	DA	3451	1/1	0.12	-	103,103,103,103	0
54	MG	DA	3043	1/1	0.14	-	54,54,54,54	0
54	MG	DA	3441	1/1	0.27	-	48,48,48,48	0
54	MG	BA	3223	1/1	0.54	-	60,60,60,60	0
54	MG	AA	1671	1/1	0.37	-	67,67,67,67	0
54	MG	AA	1678	1/1	0.51	-	74,74,74,74	0
54	MG	BA	3479	1/1	0.18	-	32,32,32,32	0
54	MG	BA	3180	1/1	0.25	-	41,41,41,41	0
54	MG	BA	3229	1/1	0.19	-	41,41,41,41	0
54	MG	DA	3464	1/1	0.10	-	89,89,89,89	0
54	MG	BA	3065	1/1	0.22	-	41,41,41,41	0
54	MG	DA	3235	1/1	0.37	-	54,54,54,54	0
54	MG	BA	3260	1/1	0.40	-	30,30,30,30	0
54	MG	AA	1638	1/1	0.14	-	53,53,53,53	0
54	MG	DA	3117	1/1	0.16	-	47,47,47,47	0
54	MG	DA	3557	1/1	0.15	-	103,103,103,103	0
54	MG	DA	3446	1/1	0.22	-	42,42,42,42	0
54	MG	BA	3343	1/1	0.08	-	73,73,73,73	0
54	MG	BA	3231	1/1	0.11	-	47,47,47,47	0
54	MG	DA	3597	1/1	0.16	-	93,93,93,93	0
54	MG	DA	3246	1/1	0.39	-	68,68,68,68	0
54	MG	BA	3564	1/1	0.12	-	59,59,59,59	0
54	MG	CA	1656	1/1	0.36	-	86,86,86,86	0
54	MG	DA	3273	1/1	0.34	-	50,50,50,50	0
54	MG	BA	3289	1/1	0.29	-	34,34,34,34	0
54	MG	DA	3334	1/1	0.12	-	52,52,52,52	0
54	MG	BA	3154	1/1	0.40	-	50,50,50,50	0
54	MG	AA	1667	1/1	0.20	-	38,38,38,38	0
54	MG	CA	1697	1/1	0.12	-	57,57,57,57	0
54	MG	BA	3204	1/1	0.13	-	38,38,38,38	0
54	MG	DA	3475	1/1	0.10	-	30,30,30,30	0
54	MG	CA	1664	1/1	0.11	-	80,80,80,80	0
54	MG	DA	3134	1/1	0.27	-	62,62,62,62	0
54	MG	AA	1653	1/1	0.06	-	49,49,49,49	0
54	MG	DA	3561	1/1	0.18	-	71,71,71,71	0
54	MG	BA	3575	1/1	0.09	-	41,41,41,41	0
54	MG	BS	201	1/1	0.53	-	49,49,49,49	0
54	MG	BA	3272	1/1	0.36	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3057	1/1	0.13	-	35,35,35,35	0
54	MG	DF	301	1/1	0.29	-	50,50,50,50	0
54	MG	BA	3312	1/1	0.09	-	51,51,51,51	0
54	MG	BA	3557	1/1	0.18	-	78,78,78,78	0
54	MG	AA	1652	1/1	0.28	-	49,49,49,49	0
54	MG	BA	3051	1/1	0.17	-	48,48,48,48	0
54	MG	DA	3063	1/1	0.31	-	60,60,60,60	0
54	MG	DA	3551	1/1	0.18	-	62,62,62,62	0
54	MG	BA	3555	1/1	0.12	-	47,47,47,47	0
54	MG	BA	3542	1/1	0.11	-	83,83,83,83	0
54	MG	BQ	202	1/1	0.24	-	34,34,34,34	0
54	MG	DB	208	1/1	0.10	-	104,104,104,104	0
54	MG	DA	3129	1/1	0.14	-	61,61,61,61	0
54	MG	DA	3343	1/1	0.06	-	37,37,37,37	0
54	MG	BA	3162	1/1	0.34	-	42,42,42,42	0
54	MG	BE	302	1/1	0.21	-	41,41,41,41	0
54	MG	DA	3181	1/1	0.24	-	49,49,49,49	0
54	MG	DA	3588	1/1	0.18	-	34,34,34,34	0
54	MG	BA	3626	1/1	0.10	-	64,64,64,64	0
54	MG	DA	3547	1/1	0.17	-	29,29,29,29	0
54	MG	DA	3444	1/1	0.15	-	41,41,41,41	0
54	MG	DB	205	1/1	0.16	-	55,55,55,55	0
54	MG	DA	3083	1/1	0.20	-	37,37,37,37	0
54	MG	DA	3271	1/1	0.39	-	57,57,57,57	0
54	MG	DA	3390	1/1	0.07	-	47,47,47,47	0
54	MG	AA	1651	1/1	0.34	-	60,60,60,60	0
54	MG	CA	1738	1/1	0.07	-	112,112,112,112	0
54	MG	BA	3095	1/1	0.19	-	48,48,48,48	0
54	MG	BA	3137	1/1	0.27	-	38,38,38,38	0
54	MG	BA	3181	1/1	0.20	-	38,38,38,38	0
54	MG	DA	3430	1/1	0.11	-	30,30,30,30	0
54	MG	BA	3015	1/1	0.20	-	48,48,48,48	0
54	MG	DA	3113	1/1	0.43	-	59,59,59,59	0
54	MG	DA	3508	1/1	0.10	-	60,60,60,60	0
54	MG	BA	3059	1/1	0.13	-	48,48,48,48	0
54	MG	BA	3032	1/1	0.12	-	40,40,40,40	0
54	MG	BA	3561	1/1	0.07	-	54,54,54,54	0
54	MG	B0	102	1/1	0.17	-	54,54,54,54	0
54	MG	BA	3212	1/1	0.23	-	68,68,68,68	0
54	MG	BA	3511	1/1	0.14	-	32,32,32,32	0
54	MG	BA	3183	1/1	0.35	-	29,29,29,29	0
54	MG	CA	1663	1/1	0.37	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3204	1/1	0.47	-	43,43,43,43	0
54	MG	BA	3071	1/1	0.16	-	34,34,34,34	0
54	MG	AA	1613	1/1	0.20	-	65,65,65,65	0
54	MG	BA	3643	1/1	0.11	-	59,59,59,59	0
54	MG	DA	3226	1/1	0.53	-	55,55,55,55	0
54	MG	DA	3192	1/1	0.17	-	50,50,50,50	0
54	MG	DA	3014	1/1	0.21	-	31,31,31,31	0
54	MG	BA	3554	1/1	0.09	-	88,88,88,88	0
54	MG	BA	3220	1/1	0.27	-	31,31,31,31	0
54	MG	BA	3641	1/1	0.25	-	72,72,72,72	0
54	MG	BA	3264	1/1	0.39	-	41,41,41,41	0
54	MG	BA	3057	1/1	0.23	-	51,51,51,51	0
54	MG	BA	3397	1/1	0.11	-	86,86,86,86	0
54	MG	DA	3553	1/1	0.07	-	54,54,54,54	0
54	MG	AA	1728	1/1	0.13	-	53,53,53,53	0
54	MG	BA	3357	1/1	0.15	-	25,25,25,25	0
54	MG	DA	3299	1/1	0.38	-	65,65,65,65	0
54	MG	BD	303	1/1	0.19	-	35,35,35,35	0
54	MG	DA	3574	1/1	0.07	-	41,41,41,41	0
54	MG	BA	3235	1/1	0.17	-	50,50,50,50	0
54	MG	BA	3121	1/1	0.35	-	36,36,36,36	0
54	MG	BA	3131	1/1	0.75	-	62,62,62,62	0
54	MG	DA	3154	1/1	0.32	-	26,26,26,26	0
54	MG	BA	3077	1/1	0.26	-	42,42,42,42	0
54	MG	DA	3576	1/1	0.08	-	48,48,48,48	0
54	MG	DA	3584	1/1	0.28	-	48,48,48,48	0
54	MG	BA	3116	1/1	0.17	-	53,53,53,53	0
54	MG	DD	301	1/1	0.22	-	47,47,47,47	0
54	MG	AA	1626	1/1	0.38	-	71,71,71,71	0
54	MG	BA	3577	1/1	0.14	-	77,77,77,77	0
54	MG	DA	3044	1/1	0.20	-	46,46,46,46	0
54	MG	DA	3421	1/1	0.09	-	93,93,93,93	0
54	MG	BB	219	1/1	0.07	-	105,105,105,105	0
54	MG	BA	3620	1/1	0.05	-	68,68,68,68	0
54	MG	BA	3364	1/1	0.07	-	81,81,81,81	0
54	MG	BA	3054	1/1	0.17	-	34,34,34,34	0
54	MG	BA	3503	1/1	0.11	-	64,64,64,64	0
54	MG	AA	1623	1/1	0.17	-	74,74,74,74	0
54	MG	BA	3488	1/1	0.17	-	24,24,24,24	0
54	MG	BA	3021	1/1	0.24	-	44,44,44,44	0
54	MG	BA	3386	1/1	0.10	-	40,40,40,40	0
54	MG	BA	3399	1/1	0.14	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	ZN	D9	101	1/1	0.05	-	65,65,65,65	0
54	MG	CA	1754	1/1	0.06	-	74,74,74,74	0
54	MG	DA	3236	1/1	0.24	-	47,47,47,47	0
54	MG	DA	3062	1/1	0.34	-	49,49,49,49	0
54	MG	DA	3106	1/1	0.41	-	37,37,37,37	0
54	MG	DA	3251	1/1	0.18	-	40,40,40,40	0
54	MG	BE	304	1/1	0.18	-	25,25,25,25	0
54	MG	DA	3493	1/1	0.05	-	63,63,63,63	0
54	MG	DA	3144	1/1	0.42	-	42,42,42,42	0
54	MG	DA	3544	1/1	0.06	-	72,72,72,72	0
54	MG	AA	1654	1/1	0.51	-	59,59,59,59	0
54	MG	AA	1612	1/1	0.34	-	86,86,86,86	0
54	MG	BA	3140	1/1	0.53	-	36,36,36,36	0
54	MG	BA	3167	1/1	0.41	-	31,31,31,31	0
54	MG	DA	3076	1/1	0.13	-	42,42,42,42	0
54	MG	BA	3615	1/1	0.12	-	52,52,52,52	0
54	MG	CA	1718	1/1	0.17	-	83,83,83,83	0
54	MG	BA	3569	1/1	0.09	-	69,69,69,69	0
54	MG	BA	3147	1/1	0.10	-	55,55,55,55	0
54	MG	BA	3283	1/1	0.45	-	21,21,21,21	0
54	MG	DA	3486	1/1	0.22	-	64,64,64,64	0
54	MG	DA	3253	1/1	0.09	-	50,50,50,50	0
54	MG	DA	3216	1/1	0.16	-	51,51,51,51	0
54	MG	BA	3505	1/1	0.19	-	41,41,41,41	0
54	MG	BA	3651	1/1	0.25	-	87,87,87,87	0
54	MG	BA	3081	1/1	0.35	-	42,42,42,42	0
54	MG	CA	1715	1/1	0.04	-	103,103,103,103	0
54	MG	DA	3366	1/1	0.18	-	31,31,31,31	0
54	MG	DA	3099	1/1	0.21	-	36,36,36,36	0
54	MG	BA	3473	1/1	0.22	-	30,30,30,30	0
54	MG	BA	3510	1/1	0.10	-	56,56,56,56	0
54	MG	AA	1601	1/1	0.29	-	55,55,55,55	0
54	MG	AA	1658	1/1	0.50	-	57,57,57,57	0
54	MG	CA	1729	1/1	0.15	-	81,81,81,81	0
54	MG	BA	3369	1/1	0.13	-	52,52,52,52	0
54	MG	DA	3294	1/1	0.16	-	42,42,42,42	0
54	MG	BA	3279	1/1	0.49	-	27,27,27,27	0
54	MG	CA	1720	1/1	0.15	-	89,89,89,89	0
54	MG	DA	3252	1/1	0.53	-	59,59,59,59	0
54	MG	BA	3323	1/1	0.17	-	23,23,23,23	0
54	MG	DA	3502	1/1	0.11	-	37,37,37,37	0
54	MG	BA	3363	1/1	0.14	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1700	1/1	0.08	-	42,42,42,42	0
54	MG	DA	3452	1/1	0.09	-	90,90,90,90	0
54	MG	DA	3191	1/1	0.20	-	51,51,51,51	0
54	MG	BA	3344	1/1	0.32	-	61,61,61,61	0
54	MG	BA	3438	1/1	0.18	-	65,65,65,65	0
54	MG	BA	3195	1/1	0.23	-	60,60,60,60	0
54	MG	BA	3176	1/1	0.15	-	60,60,60,60	0
54	MG	BA	3026	1/1	0.21	-	52,52,52,52	0
54	MG	BA	3636	1/1	0.05	-	28,28,28,28	0
54	MG	AA	1696	1/1	0.15	-	66,66,66,66	0
54	MG	BA	3261	1/1	0.38	-	34,34,34,34	0
54	MG	DA	3237	1/1	0.30	-	62,62,62,62	0
54	MG	BA	3556	1/1	0.26	-	57,57,57,57	0
54	MG	BA	3403	1/1	0.13	-	67,67,67,67	0
54	MG	DA	3231	1/1	0.27	-	36,36,36,36	0
54	MG	BA	3586	1/1	0.10	-	63,63,63,63	0
54	MG	DA	3195	1/1	0.27	-	48,48,48,48	0
54	MG	BA	3623	1/1	0.12	-	73,73,73,73	0
54	MG	BA	3471	1/1	0.20	-	27,27,27,27	0
54	MG	DA	3219	1/1	0.19	-	38,38,38,38	0
54	MG	DA	3071	1/1	0.20	-	44,44,44,44	0
54	MG	BA	3326	1/1	0.11	-	49,49,49,49	0
54	MG	DA	3398	1/1	0.27	-	88,88,88,88	0
54	MG	CA	1615	1/1	0.12	-	65,65,65,65	0
54	MG	CA	1661	1/1	0.64	-	67,67,67,67	0
54	MG	DA	3310	1/1	0.38	-	28,28,28,28	0
54	MG	DA	3420	1/1	0.20	-	37,37,37,37	0
54	MG	DA	3283	1/1	0.18	-	61,61,61,61	0
54	MG	CA	1603	1/1	0.31	-	56,56,56,56	0
54	MG	DA	3198	1/1	0.74	-	57,57,57,57	0
54	MG	DA	3317	1/1	0.21	-	47,47,47,47	0
54	MG	CA	1674	1/1	0.13	-	74,74,74,74	0
54	MG	CA	1633	1/1	0.55	-	77,77,77,77	0
54	MG	BA	3164	1/1	0.36	-	50,50,50,50	0
54	MG	AA	1648	1/1	0.41	-	44,44,44,44	0
54	MG	BA	3405	1/1	0.15	-	61,61,61,61	0
54	MG	BA	3187	1/1	0.59	-	42,42,42,42	0
54	MG	DA	3185	1/1	0.14	-	57,57,57,57	0
54	MG	D0	102	1/1	0.15	-	72,72,72,72	0
54	MG	DA	3541	1/1	0.09	-	130,130,130,130	0
54	MG	DA	3300	1/1	0.14	-	41,41,41,41	0
54	MG	BA	3029	1/1	0.18	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1762	1/1	0.07	-	156,156,156,156	0
54	MG	BA	3537	1/1	0.17	-	31,31,31,31	0
54	MG	DA	3225	1/1	0.49	-	51,51,51,51	0
54	MG	BA	3431	1/1	0.08	-	71,71,71,71	0
54	MG	BT	201	1/1	0.19	-	53,53,53,53	0
54	MG	DA	3029	1/1	0.37	-	40,40,40,40	0
54	MG	AA	1701	1/1	0.11	-	48,48,48,48	0
54	MG	CA	1636	1/1	0.35	-	59,59,59,59	0
54	MG	AA	1611	1/1	0.16	-	83,83,83,83	0
54	MG	CA	1710	1/1	0.09	-	48,48,48,48	0
54	MG	DA	3378	1/1	0.12	-	33,33,33,33	0
54	MG	BA	3548	1/1	0.12	-	29,29,29,29	0
54	MG	DA	3069	1/1	0.39	-	42,42,42,42	0
54	MG	BA	3110	1/1	0.23	-	66,66,66,66	0
54	MG	CA	1758	1/1	0.20	-	84,84,84,84	0
54	MG	DA	3040	1/1	0.29	-	48,48,48,48	0
54	MG	AA	1713	1/1	0.09	-	91,91,91,91	0
54	MG	BA	3300	1/1	0.45	-	48,48,48,48	0
54	MG	BA	3659	1/1	0.08	-	81,81,81,81	0
54	MG	BA	3252	1/1	0.32	-	36,36,36,36	0
54	MG	BA	3545	1/1	0.06	-	43,43,43,43	0
54	MG	DA	3038	1/1	0.07	-	37,37,37,37	0
54	MG	BA	3285	1/1	0.53	-	38,38,38,38	0
54	MG	BA	3543	1/1	0.16	-	119,119,119,119	0
54	MG	BA	3134	1/1	0.39	-	41,41,41,41	0
54	MG	DA	3280	1/1	0.42	-	58,58,58,58	0
54	MG	CA	1616	1/1	0.25	-	58,58,58,58	0
54	MG	BA	3638	1/1	0.14	-	67,67,67,67	0
54	MG	DA	3232	1/1	0.31	-	57,57,57,57	0
54	MG	DA	3078	1/1	0.16	-	48,48,48,48	0
54	MG	BA	3587	1/1	0.12	-	60,60,60,60	0
54	MG	BA	3402	1/1	0.06	-	54,54,54,54	0
54	MG	BA	3151	1/1	0.34	-	33,33,33,33	0
54	MG	DA	3431	1/1	0.10	-	59,59,59,59	0
54	MG	DA	3296	1/1	0.12	-	67,67,67,67	0
54	MG	BA	3591	1/1	0.10	-	34,34,34,34	0
54	MG	BA	3171	1/1	0.32	-	31,31,31,31	0
54	MG	DA	3059	1/1	0.22	-	45,45,45,45	0
54	MG	BA	3290	1/1	0.18	-	63,63,63,63	0
54	MG	BA	3469	1/1	0.14	-	40,40,40,40	0
54	MG	AA	1606	1/1	0.21	-	79,79,79,79	0
54	MG	CA	1614	1/1	0.55	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3250	1/1	0.41	-	26,26,26,26	0
54	MG	BB	206	1/1	0.22	-	57,57,57,57	0
54	MG	DA	3356	1/1	0.17	-	60,60,60,60	0
54	MG	DP	201	1/1	0.18	-	54,54,54,54	0
54	MG	AD	302	1/1	0.30	-	77,77,77,77	0
54	MG	CA	1684	1/1	0.35	-	91,91,91,91	0
54	MG	BA	3477	1/1	0.11	-	53,53,53,53	0
54	MG	DA	3234	1/1	0.20	-	41,41,41,41	0
54	MG	CA	1690	1/1	0.27	-	64,64,64,64	0
54	MG	DA	3466	1/1	0.11	-	68,68,68,68	0
54	MG	BA	3319	1/1	0.12	-	54,54,54,54	0
54	MG	BA	3016	1/1	0.20	-	47,47,47,47	0
54	MG	CA	1735	1/1	0.29	-	69,69,69,69	0
54	MG	DA	3301	1/1	0.46	-	50,50,50,50	0
54	MG	BA	3468	1/1	0.16	-	24,24,24,24	0
54	MG	CA	1698	1/1	0.11	-	47,47,47,47	0
54	MG	DA	3221	1/1	0.48	-	51,51,51,51	0
54	MG	DA	3167	1/1	0.20	-	51,51,51,51	0
54	MG	DA	3510	1/1	0.10	-	74,74,74,74	0
54	MG	BA	3245	1/1	0.34	-	23,23,23,23	0
54	MG	CA	1707	1/1	0.20	-	94,94,94,94	0
54	MG	BA	3035	1/1	0.18	-	45,45,45,45	0
54	MG	BA	3516	1/1	0.25	-	63,63,63,63	0
54	MG	DA	3516	1/1	0.19	-	32,32,32,32	0
54	MG	BA	3466	1/1	0.15	-	39,39,39,39	0
54	MG	BA	3480	1/1	0.15	-	31,31,31,31	0
54	MG	BA	3339	1/1	0.12	-	70,70,70,70	0
54	MG	BA	3527	1/1	0.18	-	29,29,29,29	0
54	MG	DA	3073	1/1	0.40	-	68,68,68,68	0
54	MG	CA	1685	1/1	0.35	-	71,71,71,71	0
54	MG	B0	101	1/1	0.17	-	39,39,39,39	0
54	MG	DA	3469	1/1	0.06	-	56,56,56,56	0
54	MG	AA	1615	1/1	0.46	-	54,54,54,54	0
54	MG	BA	3115	1/1	0.12	-	45,45,45,45	0
54	MG	BA	3210	1/1	0.16	-	40,40,40,40	0
54	MG	BA	3377	1/1	0.22	-	32,32,32,32	0
54	MG	DA	3266	1/1	0.37	-	47,47,47,47	0
54	MG	BA	3609	1/1	0.09	-	75,75,75,75	0
54	MG	BA	3288	1/1	0.23	-	66,66,66,66	0
54	MG	BA	3224	1/1	0.26	-	50,50,50,50	0
54	MG	DA	3429	1/1	0.04	-	56,56,56,56	0
54	MG	BA	3145	1/1	0.18	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1695	1/1	0.33	-	50,50,50,50	0
54	MG	BA	3538	1/1	0.10	-	66,66,66,66	0
54	MG	AA	1724	1/1	0.27	-	74,74,74,74	0
54	MG	BA	3580	1/1	0.16	-	49,49,49,49	0
54	MG	DA	3242	1/1	0.55	-	34,34,34,34	0
54	MG	BA	3513	1/1	0.09	-	86,86,86,86	0
54	MG	BA	3565	1/1	0.07	-	68,68,68,68	0
54	MG	DA	3157	1/1	0.34	-	44,44,44,44	0
54	MG	CA	1649	1/1	0.38	-	66,66,66,66	0
54	MG	BA	3197	1/1	0.29	-	41,41,41,41	0
54	MG	DA	3423	1/1	0.16	-	32,32,32,32	0
54	MG	BA	3257	1/1	0.39	-	23,23,23,23	0
54	MG	BA	3573	1/1	0.22	-	23,23,23,23	0
54	MG	BA	3640	1/1	0.10	-	116,116,116,116	0
54	MG	BA	3607	1/1	0.17	-	99,99,99,99	0
54	MG	CA	1639	1/1	0.30	-	76,76,76,76	0
54	MG	BA	3632	1/1	0.06	-	54,54,54,54	0
54	MG	BA	3130	1/1	0.24	-	43,43,43,43	0
54	MG	CA	1716	1/1	0.16	-	102,102,102,102	0
54	MG	DA	3383	1/1	0.10	-	54,54,54,54	0
54	MG	BA	3455	1/1	0.23	-	22,22,22,22	0
54	MG	BA	3150	1/1	0.12	-	42,42,42,42	0
54	MG	DA	3238	1/1	0.40	-	56,56,56,56	0
54	MG	DA	3477	1/1	0.13	-	53,53,53,53	0
54	MG	BA	3500	1/1	0.17	-	44,44,44,44	0
54	MG	DA	3200	1/1	0.19	-	34,34,34,34	0
54	MG	BB	211	1/1	0.21	-	47,47,47,47	0
54	MG	DA	3027	1/1	0.40	-	56,56,56,56	0
54	MG	BA	3424	1/1	0.20	-	72,72,72,72	0
54	MG	BA	3056	1/1	0.14	-	57,57,57,57	0
54	MG	BA	3657	1/1	0.46	-	65,65,65,65	0
54	MG	BB	207	1/1	0.18	-	52,52,52,52	0
54	MG	BA	3594	1/1	0.06	-	86,86,86,86	0
54	MG	BA	3276	1/1	0.25	-	23,23,23,23	0
54	MG	BA	3413	1/1	0.12	-	57,57,57,57	0
54	MG	BA	3295	1/1	0.62	-	54,54,54,54	0
54	MG	DA	3289	1/1	0.61	-	54,54,54,54	0
54	MG	AA	1715	1/1	0.11	-	61,61,61,61	0
54	MG	DA	3375	1/1	0.15	-	31,31,31,31	0
54	MG	DA	3336	1/1	0.17	-	41,41,41,41	0
54	MG	BA	3003	1/1	0.31	-	74,74,74,74	0
54	MG	D8	102	1/1	0.28	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	B5	103	1/1	0.09	-	57,57,57,57	0
54	MG	BA	3023	1/1	0.16	-	52,52,52,52	0
54	MG	DA	3337	1/1	0.27	-	30,30,30,30	0
54	MG	DA	3445	1/1	0.16	-	42,42,42,42	0
54	MG	DA	3438	1/1	0.15	-	90,90,90,90	0
54	MG	AA	1682	1/1	0.12	-	76,76,76,76	0
54	MG	CA	1635	1/1	0.14	-	60,60,60,60	0
54	MG	BA	3365	1/1	0.06	-	69,69,69,69	0
54	MG	AA	1718	1/1	0.05	-	96,96,96,96	0
54	MG	CE	201	1/1	0.54	-	77,77,77,77	0
54	MG	CA	1724	1/1	0.11	-	49,49,49,49	0
54	MG	DA	3549	1/1	0.20	-	45,45,45,45	0
54	MG	BA	3179	1/1	0.27	-	37,37,37,37	0
54	MG	BA	3310	1/1	0.33	-	23,23,23,23	0
54	MG	CA	1623	1/1	0.40	-	43,43,43,43	0
54	MG	BA	3010	1/1	0.24	-	39,39,39,39	0
54	MG	BA	3387	1/1	0.06	-	63,63,63,63	0
54	MG	BA	3490	1/1	0.09	-	28,28,28,28	0
54	MG	DA	3458	1/1	0.05	-	62,62,62,62	0
54	MG	BA	3083	1/1	0.20	-	43,43,43,43	0
54	MG	BA	3334	1/1	0.07	-	51,51,51,51	0
54	MG	DA	3239	1/1	0.54	-	58,58,58,58	0
54	MG	CA	1632	1/1	0.24	-	69,69,69,69	0
54	MG	BA	3392	1/1	0.11	-	110,110,110,110	0
54	MG	DA	3101	1/1	0.22	-	39,39,39,39	0
54	MG	BA	3047	1/1	0.30	-	35,35,35,35	0
54	MG	BA	3546	1/1	0.17	-	73,73,73,73	0
54	MG	CA	1659	1/1	0.22	-	48,48,48,48	0
54	MG	BA	3234	1/1	0.17	-	69,69,69,69	0
54	MG	DA	3163	1/1	0.33	-	30,30,30,30	0
54	MG	BA	3270	1/1	0.44	-	25,25,25,25	0
54	MG	CA	1605	1/1	0.29	-	67,67,67,67	0
54	MG	CA	1638	1/1	0.27	-	52,52,52,52	0
54	MG	BA	3412	1/1	0.14	-	78,78,78,78	0
54	MG	DA	3254	1/1	0.21	-	64,64,64,64	0
54	MG	DA	3170	1/1	0.12	-	56,56,56,56	0
54	MG	BA	3436	1/1	0.13	-	70,70,70,70	0
54	MG	BV	201	1/1	0.24	-	67,67,67,67	0
54	MG	DA	3005	1/1	0.20	-	77,77,77,77	0
54	MG	DA	3372	1/1	0.15	-	41,41,41,41	0
54	MG	BA	3075	1/1	0.18	-	46,46,46,46	0
54	MG	AA	1662	1/1	0.12	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3036	1/1	0.16	-	36,36,36,36	0
54	MG	BA	3630	1/1	0.08	-	34,34,34,34	0
54	MG	BA	3423	1/1	0.16	-	33,33,33,33	0
54	MG	BA	3277	1/1	0.39	-	22,22,22,22	0
54	MG	AA	1620	1/1	0.18	-	65,65,65,65	0
54	MG	AA	1704	1/1	0.16	-	86,86,86,86	0
54	MG	BA	3302	1/1	0.15	-	47,47,47,47	0
54	MG	DR	201	1/1	0.23	-	40,40,40,40	0
54	MG	AA	1698	1/1	0.18	-	69,69,69,69	0
54	MG	DA	3566	1/1	0.12	-	54,54,54,54	0
54	MG	AA	1655	1/1	0.46	-	43,43,43,43	0
54	MG	BA	3454	1/1	0.12	-	25,25,25,25	0
54	MG	DA	3322	1/1	0.33	-	49,49,49,49	0
54	MG	DA	3075	1/1	0.25	-	58,58,58,58	0
54	MG	BA	3410	1/1	0.08	-	77,77,77,77	0
54	MG	DA	3501	1/1	0.10	-	58,58,58,58	0
54	MG	DA	3285	1/1	0.04	-	64,64,64,64	0
54	MG	DB	203	1/1	0.37	-	58,58,58,58	0
54	MG	DA	3474	1/1	0.10	-	30,30,30,30	0
54	MG	BA	3581	1/1	0.11	-	86,86,86,86	0
54	MG	BA	3216	1/1	0.30	-	43,43,43,43	0
54	MG	DA	3457	1/1	0.08	-	64,64,64,64	0
54	MG	BA	3073	1/1	0.32	-	52,52,52,52	0
54	MG	BA	3086	1/1	0.68	-	57,57,57,57	0
54	MG	BA	3593	1/1	0.23	-	84,84,84,84	0
54	MG	DA	3424	1/1	0.12	-	52,52,52,52	0
54	MG	BA	3353	1/1	0.21	-	91,91,91,91	0
54	MG	DA	3118	1/1	0.23	-	43,43,43,43	0
54	MG	BA	3296	1/1	0.22	-	43,43,43,43	0
54	MG	AA	1665	1/1	0.09	-	51,51,51,51	0
54	MG	CA	1675	1/1	0.62	-	61,61,61,61	0
54	MG	AA	1687	1/1	0.15	-	62,62,62,62	0
54	MG	DA	3513	1/1	0.13	-	34,34,34,34	0
54	MG	BA	3647	1/1	0.14	-	70,70,70,70	0
54	MG	AA	1689	1/1	0.06	-	99,99,99,99	0
54	MG	DA	3598	1/1	0.10	-	76,76,76,76	0
54	MG	BB	214	1/1	0.12	-	40,40,40,40	0
54	MG	AA	1619	1/1	0.27	-	86,86,86,86	0
54	MG	BA	3005	1/1	0.30	-	60,60,60,60	0
54	MG	BA	3018	1/1	0.55	-	40,40,40,40	0
54	MG	DA	3533	1/1	0.12	-	89,89,89,89	0
54	MG	DA	3058	1/1	0.49	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3152	1/1	0.43	-	61,61,61,61	0
54	MG	DA	3389	1/1	0.06	-	51,51,51,51	0
54	MG	DA	3156	1/1	0.22	-	35,35,35,35	0
54	MG	AA	1609	1/1	0.28	-	51,51,51,51	0
54	MG	CA	1732	1/1	0.17	-	110,110,110,110	0
54	MG	CA	1686	1/1	0.26	-	61,61,61,61	0
54	MG	BA	3498	1/1	0.09	-	32,32,32,32	0
54	MG	BA	3002	1/1	0.29	-	51,51,51,51	0
54	MG	DA	3032	1/1	0.24	-	49,49,49,49	0
54	MG	DA	3472	1/1	0.32	-	50,50,50,50	0
54	MG	BA	3382	1/1	0.15	-	100,100,100,100	0
54	MG	CA	1739	1/1	0.15	-	87,87,87,87	0
54	MG	AA	1703	1/1	0.05	-	66,66,66,66	0
54	MG	BA	3222	1/1	0.49	-	60,60,60,60	0
54	MG	BA	3351	1/1	0.08	-	60,60,60,60	0
54	MG	AA	1720	1/1	0.06	-	68,68,68,68	0
54	MG	BA	3611	1/1	0.07	-	44,44,44,44	0
54	MG	DA	3284	1/1	0.22	-	55,55,55,55	0
54	MG	DA	3082	1/1	0.37	-	36,36,36,36	0
54	MG	BA	3486	1/1	0.16	-	75,75,75,75	0
54	MG	BA	3143	1/1	0.21	-	30,30,30,30	0
54	MG	AA	1607	1/1	0.19	-	78,78,78,78	0
54	MG	BA	3322	1/1	0.08	-	37,37,37,37	0
54	MG	CA	1744	1/1	0.06	-	83,83,83,83	0
54	MG	DA	3116	1/1	0.19	-	43,43,43,43	0
54	MG	B0	103	1/1	0.13	-	89,89,89,89	0
54	MG	BA	3345	1/1	0.10	-	71,71,71,71	0
54	MG	BA	3309	1/1	0.09	-	31,31,31,31	0
54	MG	DA	3011	1/1	0.20	-	42,42,42,42	0
54	MG	BA	3124	1/1	0.18	-	33,33,33,33	0
54	MG	DA	3196	1/1	0.43	-	58,58,58,58	0
54	MG	DA	3287	1/1	0.28	-	57,57,57,57	0
54	MG	BA	3217	1/1	0.21	-	41,41,41,41	0
54	MG	BA	3044	1/1	0.08	-	33,33,33,33	0
54	MG	DA	3326	1/1	0.18	-	46,46,46,46	0
54	MG	DA	3015	1/1	0.16	-	38,38,38,38	0
54	MG	BA	3263	1/1	0.41	-	36,36,36,36	0
54	MG	AA	1646	1/1	0.23	-	59,59,59,59	0
54	MG	CA	1727	1/1	0.16	-	46,46,46,46	0
54	MG	DE	302	1/1	0.33	-	21,21,21,21	0
54	MG	BA	3652	1/1	0.04	-	97,97,97,97	0
54	MG	DA	3355	1/1	0.12	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BB	220	1/1	0.15	-	60,60,60,60	0
54	MG	CA	1750	1/1	0.11	-	78,78,78,78	0
54	MG	BA	3106	1/1	0.20	-	52,52,52,52	0
54	MG	BA	3463	1/1	0.08	-	28,28,28,28	0
54	MG	BA	3159	1/1	0.25	-	46,46,46,46	0
54	MG	CA	1647	1/1	0.18	-	86,86,86,86	0
54	MG	DA	3384	1/1	0.08	-	45,45,45,45	0
54	MG	DA	3281	1/1	0.23	-	42,42,42,42	0
54	MG	BA	3646	1/1	0.16	-	142,142,142,142	0
54	MG	DA	3470	1/1	0.09	-	47,47,47,47	0
54	MG	DA	3025	1/1	0.29	-	49,49,49,49	0
54	MG	BA	3225	1/1	0.21	-	44,44,44,44	0
54	MG	BA	3069	1/1	0.34	-	42,42,42,42	0
54	MG	BA	3504	1/1	0.11	-	65,65,65,65	0
54	MG	BA	3024	1/1	0.32	-	41,41,41,41	0
54	MG	B9	102	1/1	0.14	-	28,28,28,28	0
54	MG	DA	3295	1/1	0.27	-	59,59,59,59	0
54	MG	BA	3269	1/1	0.50	-	35,35,35,35	0
54	MG	BA	3562	1/1	0.14	-	59,59,59,59	0
54	MG	BA	3186	1/1	0.35	-	26,26,26,26	0
54	MG	DA	3256	1/1	0.23	-	52,52,52,52	0
54	MG	BA	3242	1/1	0.18	-	38,38,38,38	0
54	MG	DA	3560	1/1	0.15	-	57,57,57,57	0
54	MG	DA	3416	1/1	0.12	-	66,66,66,66	0
54	MG	DA	3481	1/1	0.42	-	61,61,61,61	0
54	MG	DA	3492	1/1	0.07	-	56,56,56,56	0
55	ZN	B9	101	1/1	0.07	-	50,50,50,50	0
54	MG	AA	1712	1/1	0.33	-	86,86,86,86	0
54	MG	CA	1643	1/1	0.24	-	70,70,70,70	0
54	MG	DA	3203	1/1	0.41	-	33,33,33,33	0
54	MG	BA	3342	1/1	0.15	-	32,32,32,32	0
54	MG	CA	1668	1/1	0.56	-	87,87,87,87	0
54	MG	DA	3525	1/1	0.17	-	106,106,106,106	0
54	MG	AA	1645	1/1	0.27	-	60,60,60,60	0
54	MG	BA	3362	1/1	0.12	-	43,43,43,43	0
54	MG	CA	1637	1/1	0.42	-	73,73,73,73	0
54	MG	CA	1749	1/1	0.24	-	61,61,61,61	0
54	MG	BA	3123	1/1	0.27	-	43,43,43,43	0
54	MG	DA	3128	1/1	0.19	-	45,45,45,45	0
54	MG	CA	1752	1/1	0.15	-	71,71,71,71	0
54	MG	DA	3017	1/1	0.22	-	50,50,50,50	0
54	MG	BA	3492	1/1	0.21	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1722	1/1	0.22	-	66,66,66,66	0
54	MG	DA	3563	1/1	0.14	-	70,70,70,70	0
54	MG	BA	3227	1/1	0.17	-	32,32,32,32	0
54	MG	DA	3174	1/1	0.23	-	51,51,51,51	0
54	MG	BA	3445	1/1	0.17	-	31,31,31,31	0
54	MG	BA	3321	1/1	0.05	-	32,32,32,32	0
54	MG	DA	3001	1/1	0.27	-	48,48,48,48	0
54	MG	BA	3088	1/1	0.16	-	33,33,33,33	0
54	MG	DR	202	1/1	0.36	-	34,34,34,34	0
54	MG	CA	1708	1/1	0.09	-	80,80,80,80	0
54	MG	DA	3323	1/1	0.11	-	40,40,40,40	0
54	MG	BA	3409	1/1	0.05	-	68,68,68,68	0
54	MG	DA	3098	1/1	0.19	-	37,37,37,37	0
55	ZN	D4	101	1/1	0.07	-	214,214,214,214	0
54	MG	DA	3162	1/1	0.33	-	35,35,35,35	0
54	MG	BA	3547	1/1	0.27	-	105,105,105,105	0
54	MG	BA	3588	1/1	0.13	-	64,64,64,64	0
54	MG	DA	3179	1/1	0.25	-	68,68,68,68	0
54	MG	DA	3022	1/1	0.17	-	34,34,34,34	0
54	MG	CA	1655	1/1	0.25	-	98,98,98,98	0
54	MG	BA	3053	1/1	0.44	-	57,57,57,57	0
54	MG	BA	3142	1/1	0.24	-	42,42,42,42	0
54	MG	BA	3198	1/1	0.12	-	44,44,44,44	0
54	MG	BA	3218	1/1	0.12	-	55,55,55,55	0
54	MG	DA	3265	1/1	0.37	-	44,44,44,44	0
54	MG	DA	3051	1/1	0.17	-	38,38,38,38	0
54	MG	BA	3582	1/1	0.21	-	79,79,79,79	0
54	MG	DA	3517	1/1	0.23	-	66,66,66,66	0
54	MG	CA	1650	1/1	0.21	-	60,60,60,60	0
54	MG	BA	3172	1/1	0.39	-	47,47,47,47	0
54	MG	DA	3230	1/1	0.20	-	45,45,45,45	0
54	MG	CA	1629	1/1	0.22	-	87,87,87,87	0
54	MG	DA	3049	1/1	0.20	-	49,49,49,49	0
54	MG	DA	3578	1/1	0.23	-	29,29,29,29	0
54	MG	BA	3170	1/1	0.22	-	29,29,29,29	0
54	MG	BA	3262	1/1	0.37	-	27,27,27,27	0
54	MG	DA	3270	1/1	0.16	-	64,64,64,64	0
54	MG	DA	3208	1/1	0.34	-	53,53,53,53	0
54	MG	AA	1702	1/1	0.15	-	68,68,68,68	0
54	MG	CA	1721	1/1	0.23	-	64,64,64,64	0
54	MG	BA	3484	1/1	0.19	-	27,27,27,27	0
54	MG	BA	3427	1/1	0.18	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1612	1/1	0.16	-	65,65,65,65	0
54	MG	CA	1601	1/1	0.21	-	45,45,45,45	0
54	MG	BA	3443	1/1	0.24	-	47,47,47,47	0
54	MG	CA	1669	1/1	0.27	-	76,76,76,76	0
54	MG	BA	3249	1/1	0.35	-	25,25,25,25	0
54	MG	AA	1711	1/1	0.24	-	46,46,46,46	0
54	MG	BA	3478	1/1	0.16	-	41,41,41,41	0
54	MG	AA	1710	1/1	0.07	-	79,79,79,79	0
54	MG	B1	101	1/1	0.16	-	45,45,45,45	0
54	MG	DA	3339	1/1	0.06	-	44,44,44,44	0
54	MG	BA	3103	1/1	0.21	-	29,29,29,29	0
54	MG	DA	3002	1/1	0.15	-	69,69,69,69	0
54	MG	CA	1737	1/1	0.12	-	89,89,89,89	0
54	MG	DA	3297	1/1	0.18	-	78,78,78,78	0
54	MG	BA	3528	1/1	0.17	-	39,39,39,39	0
54	MG	BA	3526	1/1	0.12	-	22,22,22,22	0
54	MG	BA	3350	1/1	0.09	-	40,40,40,40	0
54	MG	BB	208	1/1	0.23	-	43,43,43,43	0
54	MG	AA	1730	1/1	0.10	-	51,51,51,51	0
54	MG	BA	3136	1/1	0.40	-	45,45,45,45	0
54	MG	BA	3502	1/1	0.24	-	34,34,34,34	0
54	MG	BA	3475	1/1	0.14	-	39,39,39,39	0
54	MG	DA	3460	1/1	0.20	-	65,65,65,65	0
54	MG	AA	1630	1/1	0.25	-	39,39,39,39	0
54	MG	BA	3406	1/1	0.06	-	66,66,66,66	0
54	MG	BA	3013	1/1	0.23	-	49,49,49,49	0
54	MG	BA	3101	1/1	0.12	-	37,37,37,37	0
54	MG	CA	1687	1/1	0.22	-	62,62,62,62	0
54	MG	BA	3418	1/1	0.12	-	49,49,49,49	0
54	MG	DA	3259	1/1	0.21	-	43,43,43,43	0
54	MG	DA	3087	1/1	0.11	-	54,54,54,54	0
54	MG	DA	3394	1/1	0.05	-	47,47,47,47	0
54	MG	DA	3187	1/1	0.12	-	71,71,71,71	0
54	MG	BA	3314	1/1	0.15	-	37,37,37,37	0
54	MG	DA	3291	1/1	0.42	-	53,53,53,53	0
54	MG	BA	3099	1/1	0.18	-	46,46,46,46	0
54	MG	DA	3437	1/1	0.17	-	85,85,85,85	0
54	MG	AA	1633	1/1	0.30	-	62,62,62,62	0
54	MG	BA	3092	1/1	0.40	-	26,26,26,26	0
54	MG	DA	3399	1/1	0.10	-	51,51,51,51	0
54	MG	BA	3189	1/1	0.33	-	41,41,41,41	0
54	MG	DA	3311	1/1	0.34	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3418	1/1	0.15	-	31,31,31,31	0
54	MG	DA	3305	1/1	0.24	-	35,35,35,35	0
54	MG	AA	1617	1/1	0.21	-	45,45,45,45	0
54	MG	DA	3137	1/1	0.10	-	38,38,38,38	0
54	MG	BA	3241	1/1	0.23	-	65,65,65,65	0
54	MG	DA	3534	1/1	0.13	-	28,28,28,28	0
54	MG	DR	203	1/1	0.48	-	51,51,51,51	0
54	MG	CA	1606	1/1	0.22	-	59,59,59,59	0
54	MG	BA	3157	1/1	0.31	-	48,48,48,48	0
54	MG	DA	3419	1/1	0.10	-	44,44,44,44	0
54	MG	BD	302	1/1	0.22	-	28,28,28,28	0
54	MG	BA	3165	1/1	0.28	-	51,51,51,51	0
54	MG	DA	3364	1/1	0.13	-	32,32,32,32	0
54	MG	DA	3338	1/1	0.20	-	42,42,42,42	0
54	MG	DA	3039	1/1	0.17	-	28,28,28,28	0
54	MG	BA	3329	1/1	0.21	-	74,74,74,74	0
54	MG	DA	3414	1/1	0.17	-	51,51,51,51	0
54	MG	BA	3138	1/1	0.35	-	42,42,42,42	0
54	MG	DA	3133	1/1	0.37	-	36,36,36,36	0
54	MG	DA	3449	1/1	0.20	-	42,42,42,42	0
54	MG	DA	3568	1/1	0.07	-	78,78,78,78	0
54	MG	DA	3523	1/1	0.06	-	74,74,74,74	0
54	MG	BA	3434	1/1	0.07	-	62,62,62,62	0
54	MG	BA	3446	1/1	0.14	-	30,30,30,30	0
54	MG	DA	3243	1/1	0.21	-	28,28,28,28	0
54	MG	BA	3389	1/1	0.20	-	46,46,46,46	0
54	MG	BA	3536	1/1	0.08	-	68,68,68,68	0
54	MG	BA	3055	1/1	0.17	-	53,53,53,53	0
54	MG	BA	3214	1/1	0.22	-	52,52,52,52	0
54	MG	CA	1702	1/1	0.12	-	64,64,64,64	0
54	MG	DA	3409	1/1	0.07	-	73,73,73,73	0
54	MG	BB	209	1/1	0.13	-	60,60,60,60	0
54	MG	BB	210	1/1	0.17	-	60,60,60,60	0
54	MG	BQ	201	1/1	0.20	-	51,51,51,51	0
54	MG	DA	3594	1/1	0.15	-	58,58,58,58	0
54	MG	CA	1609	1/1	0.26	-	70,70,70,70	0
54	MG	BA	3525	1/1	0.13	-	35,35,35,35	0
54	MG	BA	3379	1/1	0.09	-	22,22,22,22	0
54	MG	BA	3163	1/1	0.28	-	23,23,23,23	0
54	MG	CA	1604	1/1	0.51	-	81,81,81,81	0
54	MG	CA	1677	1/1	0.16	-	64,64,64,64	0
54	MG	BA	3111	1/1	0.23	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3102	1/1	0.48	-	40,40,40,40	0
54	MG	BA	3422	1/1	0.16	-	76,76,76,76	0
54	MG	DA	3589	1/1	0.11	-	75,75,75,75	0
54	MG	DA	3546	1/1	0.12	-	64,64,64,64	0
54	MG	BA	3639	1/1	0.21	-	65,65,65,65	0
54	MG	BA	3495	1/1	0.12	-	35,35,35,35	0
54	MG	BA	3465	1/1	0.15	-	44,44,44,44	0
54	MG	DA	3478	1/1	0.17	-	87,87,87,87	0
54	MG	DA	3463	1/1	0.06	-	69,69,69,69	0
54	MG	DA	3264	1/1	0.36	-	61,61,61,61	0
54	MG	DA	3019	1/1	0.18	-	40,40,40,40	0
54	MG	BA	3152	1/1	0.40	-	54,54,54,54	0
54	MG	BA	3041	1/1	0.22	-	40,40,40,40	0
54	MG	BA	3052	1/1	0.14	-	52,52,52,52	0
54	MG	DA	3374	1/1	0.22	-	37,37,37,37	0
54	MG	BA	3541	1/1	0.10	-	42,42,42,42	0
54	MG	BA	3090	1/1	0.14	-	62,62,62,62	0
54	MG	DA	3245	1/1	0.25	-	57,57,57,57	0
54	MG	CA	1680	1/1	0.28	-	78,78,78,78	0
54	MG	DA	3068	1/1	0.12	-	33,33,33,33	0
54	MG	DA	3096	1/1	0.52	-	59,59,59,59	0
54	MG	BQ	204	1/1	0.09	-	43,43,43,43	0
54	MG	CA	1701	1/1	0.09	-	72,72,72,72	0
54	MG	CA	1660	1/1	0.40	-	70,70,70,70	0
54	MG	BA	3303	1/1	0.12	-	64,64,64,64	0
54	MG	BA	3188	1/1	0.27	-	39,39,39,39	0
54	MG	DA	3340	1/1	0.12	-	45,45,45,45	0
54	MG	BA	3470	1/1	0.29	-	60,60,60,60	0
54	MG	BA	3637	1/1	0.15	-	108,108,108,108	0
54	MG	BA	3239	1/1	0.16	-	67,67,67,67	0
54	MG	BA	3518	1/1	0.12	-	50,50,50,50	0
54	MG	DA	3483	1/1	0.23	-	59,59,59,59	0
55	ZN	B6	101	1/1	0.11	-	48,48,48,48	0
54	MG	DA	3261	1/1	0.35	-	44,44,44,44	0
54	MG	AA	1629	1/1	0.29	-	44,44,44,44	0
54	MG	BA	3489	1/1	0.14	-	23,23,23,23	0
54	MG	DA	3558	1/1	0.14	-	36,36,36,36	0
54	MG	BA	3449	1/1	0.30	-	29,29,29,29	0
54	MG	DA	3224	1/1	0.36	-	32,32,32,32	0
54	MG	BA	3437	1/1	0.12	-	49,49,49,49	0
54	MG	BA	3256	1/1	0.33	-	23,23,23,23	0
54	MG	DA	3450	1/1	0.11	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3096	1/1	0.40	-	47,47,47,47	0
54	MG	DA	3410	1/1	0.12	-	86,86,86,86	0
54	MG	DA	3368	1/1	0.15	-	52,52,52,52	0
54	MG	DA	3468	1/1	0.06	-	53,53,53,53	0
54	MG	AA	1647	1/1	0.23	-	55,55,55,55	0
54	MG	AA	1688	1/1	0.15	-	96,96,96,96	0
54	MG	BA	3597	1/1	0.28	-	84,84,84,84	0
54	MG	DA	3161	1/1	0.36	-	39,39,39,39	0
54	MG	BA	3483	1/1	0.13	-	28,28,28,28	0
54	MG	BA	3435	1/1	0.14	-	48,48,48,48	0
54	MG	DA	3435	1/1	0.49	-	57,57,57,57	0
54	MG	DB	201	1/1	0.16	-	43,43,43,43	0
54	MG	BA	3320	1/1	0.17	-	42,42,42,42	0
54	MG	BA	3429	1/1	0.23	-	47,47,47,47	0
54	MG	DA	3142	1/1	0.22	-	37,37,37,37	0
54	MG	BA	3238	1/1	0.34	-	53,53,53,53	0
54	MG	DA	3540	1/1	0.11	-	53,53,53,53	0
54	MG	CA	1646	1/1	0.41	-	59,59,59,59	0
54	MG	BA	3354	1/1	0.09	-	37,37,37,37	0
54	MG	DA	3147	1/1	0.41	-	54,54,54,54	0
54	MG	DA	3240	1/1	0.16	-	53,53,53,53	0
54	MG	BA	3644	1/1	0.09	-	88,88,88,88	0
54	MG	BA	3232	1/1	0.21	-	64,64,64,64	0
54	MG	DA	3476	1/1	0.11	-	66,66,66,66	0
54	MG	BA	3246	1/1	0.47	-	20,20,20,20	0
54	MG	DA	3331	1/1	0.14	-	71,71,71,71	0
54	MG	BA	3373	1/1	0.07	-	44,44,44,44	0
54	MG	AA	1621	1/1	0.33	-	62,62,62,62	0
54	MG	DA	3365	1/1	0.07	-	40,40,40,40	0
54	MG	CA	1691	1/1	0.45	-	51,51,51,51	0
54	MG	DA	3521	1/1	0.11	-	86,86,86,86	0
54	MG	DA	3391	1/1	0.10	-	37,37,37,37	0
54	MG	DA	3407	1/1	0.06	-	70,70,70,70	0
54	MG	DA	3233	1/1	0.14	-	38,38,38,38	0
54	MG	BA	3299	1/1	0.23	-	66,66,66,66	0
54	MG	BA	3655	1/1	0.22	-	104,104,104,104	0
54	MG	BA	3366	1/1	0.19	-	83,83,83,83	0
54	MG	BA	3603	1/1	0.08	-	40,40,40,40	0
54	MG	BA	3460	1/1	0.27	-	61,61,61,61	0
54	MG	BA	3601	1/1	0.15	-	76,76,76,76	0
54	MG	CA	1730	1/1	0.10	-	62,62,62,62	0
54	MG	BA	3112	1/1	0.17	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3140	1/1	0.39	-	64,64,64,64	0
54	MG	DA	3505	1/1	0.13	-	91,91,91,91	0
54	MG	BA	3156	1/1	0.29	-	39,39,39,39	0
54	MG	BA	3519	1/1	0.05	-	64,64,64,64	0
54	MG	DA	3282	1/1	0.13	-	64,64,64,64	0
54	MG	DA	3003	1/1	0.20	-	46,46,46,46	0
54	MG	DA	3321	1/1	0.42	-	51,51,51,51	0
54	MG	DA	3490	1/1	0.12	-	33,33,33,33	0
54	MG	DA	3026	1/1	0.08	-	39,39,39,39	0
54	MG	BA	3417	1/1	0.07	-	48,48,48,48	0
54	MG	DA	3415	1/1	0.10	-	43,43,43,43	0
54	MG	DA	3149	1/1	0.37	-	53,53,53,53	0
54	MG	BA	3425	1/1	0.12	-	53,53,53,53	0
54	MG	DA	3328	1/1	0.36	-	57,57,57,57	0
54	MG	DA	3344	1/1	0.08	-	30,30,30,30	0
54	MG	DA	3479	1/1	0.18	-	62,62,62,62	0
54	MG	DA	3461	1/1	0.15	-	41,41,41,41	0
54	MG	BA	3093	1/1	0.17	-	42,42,42,42	0
54	MG	DQ	201	1/1	0.20	-	40,40,40,40	0
54	MG	AA	1631	1/1	0.16	-	41,41,41,41	0
54	MG	DA	3313	1/1	0.35	-	29,29,29,29	0
54	MG	BA	3654	1/1	0.14	-	126,126,126,126	0
54	MG	BA	3284	1/1	0.36	-	24,24,24,24	0
54	MG	CA	1714	1/1	0.15	-	87,87,87,87	0
54	MG	DB	206	1/1	0.27	-	58,58,58,58	0
54	MG	BA	3440	1/1	0.08	-	46,46,46,46	0
54	MG	AA	1642	1/1	0.88	-	54,54,54,54	0
54	MG	BA	3476	1/1	0.21	-	49,49,49,49	0
54	MG	BA	3286	1/1	0.46	-	52,52,52,52	0
54	MG	DA	3072	1/1	0.43	-	50,50,50,50	0
54	MG	BR	201	1/1	0.14	-	29,29,29,29	0
54	MG	DA	3586	1/1	0.14	-	49,49,49,49	0
54	MG	CA	1756	1/1	0.21	-	80,80,80,80	0
54	MG	AA	1627	1/1	0.34	-	59,59,59,59	0
54	MG	DA	3132	1/1	0.42	-	49,49,49,49	0
54	MG	DA	3121	1/1	0.11	-	34,34,34,34	0
54	MG	BA	3376	1/1	0.09	-	26,26,26,26	0
54	MG	BB	223	1/1	0.15	-	133,133,133,133	0
54	MG	DA	3085	1/1	0.20	-	43,43,43,43	0
54	MG	BA	3203	1/1	0.50	-	55,55,55,55	0
54	MG	DA	3406	1/1	0.10	-	58,58,58,58	0
54	MG	AA	1676	1/1	0.29	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1669	1/1	0.14	-	103,103,103,103	0
54	MG	BB	204	1/1	0.23	-	52,52,52,52	0
54	MG	DA	3111	1/1	0.18	-	50,50,50,50	0
54	MG	BA	3451	1/1	0.20	-	28,28,28,28	0
54	MG	BA	3017	1/1	0.13	-	31,31,31,31	0
54	MG	AA	1624	1/1	0.39	-	70,70,70,70	0
54	MG	BA	3482	1/1	0.20	-	27,27,27,27	0
54	MG	DA	3194	1/1	0.27	-	37,37,37,37	0
54	MG	CA	1648	1/1	0.31	-	60,60,60,60	0
54	MG	DA	3210	1/1	0.26	-	53,53,53,53	0
54	MG	BA	3656	1/1	0.13	-	68,68,68,68	0
54	MG	BA	3028	1/1	0.15	-	22,22,22,22	0
54	MG	CA	1628	1/1	0.12	-	75,75,75,75	0
54	MG	BA	3367	1/1	0.20	-	71,71,71,71	0
54	MG	BA	3522	1/1	0.11	-	74,74,74,74	0
54	MG	BA	3508	1/1	0.13	-	29,29,29,29	0
54	MG	DA	3166	1/1	0.33	-	45,45,45,45	0
54	MG	DA	3021	1/1	0.12	-	51,51,51,51	0
54	MG	BA	3501	1/1	0.08	-	29,29,29,29	0
54	MG	DA	3018	1/1	0.21	-	54,54,54,54	0
54	MG	CA	1741	1/1	0.30	-	79,79,79,79	0
54	MG	DA	3542	1/1	0.06	-	83,83,83,83	0
54	MG	DA	3158	1/1	0.28	-	46,46,46,46	0
54	MG	BA	3066	1/1	0.35	-	39,39,39,39	0
54	MG	DA	3462	1/1	0.12	-	51,51,51,51	0
54	MG	BA	3307	1/1	0.11	-	44,44,44,44	0
54	MG	DA	3482	1/1	0.18	-	56,56,56,56	0
54	MG	BA	3533	1/1	0.16	-	61,61,61,61	0
54	MG	AA	1684	1/1	0.81	-	60,60,60,60	0
54	MG	DA	3028	1/1	0.30	-	67,67,67,67	0
54	MG	BB	216	1/1	0.09	-	82,82,82,82	0
54	MG	DA	3500	1/1	0.10	-	74,74,74,74	0
54	MG	DA	3309	1/1	0.39	-	28,28,28,28	0
54	MG	BA	3602	1/1	0.05	-	56,56,56,56	0
54	MG	DA	3052	1/1	0.39	-	52,52,52,52	0
54	MG	BA	3153	1/1	0.41	-	51,51,51,51	0
54	MG	BA	3201	1/1	0.31	-	31,31,31,31	0
54	MG	CA	1743	1/1	0.08	-	61,61,61,61	0
54	MG	AA	1733	1/1	0.07	-	78,78,78,78	0
54	MG	CA	1753	1/1	0.13	-	86,86,86,86	0
54	MG	BQ	203	1/1	0.13	-	73,73,73,73	0
54	MG	BA	3133	1/1	0.26	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1653	1/1	0.78	-	57,57,57,57	0
54	MG	BA	3184	1/1	0.22	-	40,40,40,40	0
55	ZN	B5	101	1/1	0.09	-	45,45,45,45	0
54	MG	DA	3427	1/1	0.06	-	59,59,59,59	0
54	MG	DA	3359	1/1	0.11	-	33,33,33,33	0
54	MG	BA	3297	1/1	0.24	-	46,46,46,46	0
54	MG	BA	3383	1/1	0.10	-	70,70,70,70	0
54	MG	BA	3219	1/1	0.14	-	46,46,46,46	0
54	MG	DA	3201	1/1	0.31	-	49,49,49,49	0
54	MG	DA	3439	1/1	0.06	-	57,57,57,57	0
54	MG	DA	3567	1/1	0.24	-	46,46,46,46	0
54	MG	BA	3038	1/1	0.31	-	76,76,76,76	0
54	MG	BA	3080	1/1	0.21	-	39,39,39,39	0
54	MG	BW	202	1/1	0.19	-	33,33,33,33	0
54	MG	DA	3496	1/1	0.23	-	66,66,66,66	0
54	MG	BA	3291	1/1	0.12	-	39,39,39,39	0
54	MG	DA	3373	1/1	0.28	-	32,32,32,32	0
54	MG	BA	3368	1/1	0.22	-	53,53,53,53	0
54	MG	DA	3518	1/1	0.08	-	69,69,69,69	0
54	MG	BB	201	1/1	0.17	-	57,57,57,57	0
54	MG	DA	3046	1/1	0.16	-	42,42,42,42	0
54	MG	BA	3337	1/1	0.17	-	49,49,49,49	0
54	MG	DA	3583	1/1	0.11	-	65,65,65,65	0
54	MG	BA	3570	1/1	0.14	-	78,78,78,78	0
54	MG	CA	1662	1/1	0.37	-	75,75,75,75	0
54	MG	BA	3625	1/1	0.05	-	53,53,53,53	0
54	MG	CA	1640	1/1	0.28	-	82,82,82,82	0
54	MG	CA	1712	1/1	0.27	-	87,87,87,87	0
54	MG	BA	3540	1/1	0.11	-	35,35,35,35	0
54	MG	BA	3199	1/1	0.17	-	41,41,41,41	0
54	MG	AA	1731	1/1	0.18	-	119,119,119,119	0
54	MG	AA	1683	1/1	0.65	-	58,58,58,58	0
54	MG	DA	3218	1/1	0.63	-	62,62,62,62	0
54	MG	DA	3258	1/1	0.42	-	52,52,52,52	0
54	MG	DA	3348	1/1	0.15	-	41,41,41,41	0
54	MG	BA	3355	1/1	0.13	-	29,29,29,29	0
54	MG	BA	3404	1/1	0.09	-	45,45,45,45	0
54	MG	BW	201	1/1	0.10	-	32,32,32,32	0
54	MG	BA	3447	1/1	0.14	-	29,29,29,29	0
54	MG	BA	3190	1/1	0.19	-	27,27,27,27	0
54	MG	DA	3308	1/1	0.32	-	33,33,33,33	0
54	MG	DA	3432	1/1	0.10	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3370	1/1	0.09	-	32,32,32,32	0
54	MG	BA	3520	1/1	0.14	-	95,95,95,95	0
54	MG	BA	3613	1/1	0.07	-	65,65,65,65	0
54	MG	DA	3095	1/1	0.23	-	53,53,53,53	0
54	MG	BA	3113	1/1	0.10	-	60,60,60,60	0
54	MG	B8	102	1/1	0.10	-	61,61,61,61	0
54	MG	D1	101	1/1	0.17	-	38,38,38,38	0
54	MG	BT	202	1/1	0.39	-	52,52,52,52	0
54	MG	DA	3362	1/1	0.09	-	26,26,26,26	0
54	MG	BA	3127	1/1	0.25	-	38,38,38,38	0
54	MG	DA	3180	1/1	0.25	-	49,49,49,49	0
54	MG	DA	3007	1/1	0.17	-	48,48,48,48	0
54	MG	BA	3282	1/1	0.33	-	27,27,27,27	0
54	MG	BA	3120	1/1	0.13	-	51,51,51,51	0
54	MG	DA	3248	1/1	0.14	-	42,42,42,42	0
54	MG	BA	3493	1/1	0.21	-	40,40,40,40	0
54	MG	BA	3173	1/1	0.40	-	32,32,32,32	0
54	MG	BA	3118	1/1	0.17	-	44,44,44,44	0
54	MG	CA	1745	1/1	0.32	-	116,116,116,116	0
54	MG	AA	1690	1/1	0.10	-	72,72,72,72	0
54	MG	DA	3176	1/1	0.37	-	70,70,70,70	0
54	MG	AA	1717	1/1	0.14	-	93,93,93,93	0
54	MG	BA	3091	1/1	0.34	-	40,40,40,40	0
54	MG	BA	3539	1/1	0.11	-	47,47,47,47	0
54	MG	BA	3258	1/1	0.36	-	55,55,55,55	0
54	MG	DA	3097	1/1	0.26	-	23,23,23,23	0
54	MG	DA	3497	1/1	0.24	-	83,83,83,83	0
54	MG	DA	3426	1/1	0.09	-	81,81,81,81	0
54	MG	BA	3330	1/1	0.15	-	34,34,34,34	0
54	MG	AA	1719	1/1	0.14	-	144,144,144,144	0
54	MG	DA	3456	1/1	0.09	-	42,42,42,42	0
54	MG	CA	1670	1/1	0.66	-	73,73,73,73	0
54	MG	DA	3164	1/1	0.36	-	56,56,56,56	0
54	MG	DA	3293	1/1	0.28	-	33,33,33,33	0
54	MG	DA	3122	1/1	0.24	-	49,49,49,49	0
54	MG	CA	1672	1/1	0.21	-	66,66,66,66	0
54	MG	DA	3538	1/1	0.16	-	87,87,87,87	0
54	MG	BA	3132	1/1	0.13	-	33,33,33,33	0
54	MG	BA	3009	1/1	0.27	-	45,45,45,45	0
54	MG	DA	3433	1/1	0.11	-	47,47,47,47	0
54	MG	BA	3014	1/1	0.57	-	65,65,65,65	0
54	MG	BA	3211	1/1	0.09	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3045	1/1	0.12	-	38,38,38,38	0
54	MG	AA	1714	1/1	0.23	-	57,57,57,57	0
54	MG	BA	3196	1/1	0.13	-	46,46,46,46	0
54	MG	BA	3416	1/1	0.08	-	25,25,25,25	0
54	MG	AA	1673	1/1	0.59	-	60,60,60,60	0
54	MG	BA	3149	1/1	0.28	-	57,57,57,57	0
54	MG	DA	3084	1/1	0.23	-	37,37,37,37	0
54	MG	DA	3274	1/1	0.46	-	61,61,61,61	0
54	MG	CA	1761	1/1	0.19	-	65,65,65,65	0
54	MG	AA	1632	1/1	0.27	-	71,71,71,71	0
54	MG	BA	3308	1/1	0.17	-	52,52,52,52	0
54	MG	BA	3122	1/1	0.31	-	49,49,49,49	0
54	MG	BA	3200	1/1	0.20	-	31,31,31,31	0
54	MG	BA	3114	1/1	0.29	-	63,63,63,63	0
54	MG	AA	1734	1/1	0.12	-	96,96,96,96	0
54	MG	BA	3494	1/1	0.12	-	34,34,34,34	0
54	MG	BA	3394	1/1	0.14	-	50,50,50,50	0
54	MG	BA	3385	1/1	0.13	-	63,63,63,63	0
54	MG	BA	3317	1/1	0.17	-	34,34,34,34	0
54	MG	AA	1716	1/1	0.08	-	116,116,116,116	0
54	MG	AA	1691	1/1	0.12	-	43,43,43,43	0
54	MG	DA	3053	1/1	0.14	-	40,40,40,40	0
54	MG	DA	3065	1/1	0.13	-	53,53,53,53	0
54	MG	DA	3244	1/1	0.50	-	33,33,33,33	0
54	MG	DA	3349	1/1	0.14	-	35,35,35,35	0
54	MG	BA	3407	1/1	0.18	-	47,47,47,47	0
54	MG	DA	3512	1/1	0.13	-	42,42,42,42	0
54	MG	DA	3067	1/1	0.22	-	49,49,49,49	0
54	MG	BE	303	1/1	0.12	-	26,26,26,26	0
54	MG	DA	3199	1/1	0.16	-	44,44,44,44	0
54	MG	DA	3467	1/1	0.11	-	43,43,43,43	0
54	MG	BA	3352	1/1	0.11	-	81,81,81,81	0
54	MG	DA	3367	1/1	0.24	-	30,30,30,30	0
54	MG	CA	1709	1/1	0.12	-	63,63,63,63	0
54	MG	DA	3250	1/1	0.16	-	49,49,49,49	0
54	MG	DA	3088	1/1	0.36	-	55,55,55,55	0
54	MG	AA	1628	1/1	0.27	-	68,68,68,68	0
54	MG	BA	3248	1/1	0.39	-	27,27,27,27	0
54	MG	BA	3361	1/1	0.06	-	59,59,59,59	0
54	MG	AA	1637	1/1	0.22	-	84,84,84,84	0
54	MG	DA	3361	1/1	0.10	-	30,30,30,30	0
54	MG	BA	3532	1/1	0.25	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1734	1/1	0.21	-	66,66,66,66	0
54	MG	BA	3390	1/1	0.07	-	62,62,62,62	0
54	MG	DA	3081	1/1	0.64	-	58,58,58,58	0
54	MG	CA	1645	1/1	0.93	-	60,60,60,60	0
54	MG	BA	3178	1/1	0.31	-	43,43,43,43	0
54	MG	DA	3488	1/1	0.17	-	58,58,58,58	0
54	MG	BA	3067	1/1	0.16	-	43,43,43,43	0
54	MG	DA	3434	1/1	0.15	-	60,60,60,60	0
54	MG	BA	3549	1/1	0.04	-	55,55,55,55	0
54	MG	DA	3276	1/1	0.99	-	60,60,60,60	0
54	MG	DA	3212	1/1	0.30	-	75,75,75,75	0
54	MG	DA	3091	1/1	0.19	-	55,55,55,55	0
54	MG	AA	1643	1/1	0.57	-	47,47,47,47	0
54	MG	CA	1679	1/1	0.46	-	59,59,59,59	0
54	MG	BA	3660	1/1	0.12	-	104,104,104,104	0
54	MG	BA	3247	1/1	0.44	-	26,26,26,26	0
54	MG	AA	1721	1/1	0.06	-	62,62,62,62	0
54	MG	DA	3436	1/1	0.15	-	81,81,81,81	0
54	MG	BA	3292	1/1	0.24	-	70,70,70,70	0
54	MG	DA	3318	1/1	0.17	-	58,58,58,58	0
54	MG	D8	101	1/1	0.18	-	48,48,48,48	0
54	MG	DE	303	1/1	0.13	-	45,45,45,45	0
54	MG	DA	3035	1/1	0.20	-	60,60,60,60	0
54	MG	DA	3092	1/1	0.32	-	41,41,41,41	0
54	MG	CA	1700	1/1	0.09	-	70,70,70,70	0
54	MG	DA	3498	1/1	0.10	-	28,28,28,28	0
54	MG	BA	3318	1/1	0.22	-	35,35,35,35	0
54	MG	CA	1688	1/1	0.34	-	54,54,54,54	0
54	MG	BA	3125	1/1	0.36	-	45,45,45,45	0
54	MG	BA	3001	1/1	0.18	-	43,43,43,43	0
54	MG	BA	3388	1/1	0.10	-	47,47,47,47	0
54	MG	BA	3105	1/1	0.34	-	28,28,28,28	0
54	MG	BA	3191	1/1	0.28	-	40,40,40,40	0
54	MG	BA	3604	1/1	0.06	-	50,50,50,50	0
54	MG	DA	3524	1/1	0.15	-	79,79,79,79	0
54	MG	BA	3072	1/1	0.09	-	59,59,59,59	0
54	MG	DA	3385	1/1	0.07	-	49,49,49,49	0
54	MG	BA	3012	1/1	0.36	-	27,27,27,27	0
54	MG	BA	3433	1/1	0.11	-	55,55,55,55	0
54	MG	BB	212	1/1	0.28	-	60,60,60,60	0
54	MG	CA	1746	1/1	0.11	-	97,97,97,97	0
54	MG	BA	3592	1/1	0.12	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1624	1/1	0.55	-	63,63,63,63	0
54	MG	BA	3444	1/1	0.10	-	53,53,53,53	0
54	MG	BA	3481	1/1	0.15	-	25,25,25,25	0
54	MG	DA	3127	1/1	0.28	-	56,56,56,56	0
54	MG	BA	3325	1/1	0.11	-	40,40,40,40	0
54	MG	DA	3332	1/1	0.28	-	53,53,53,53	0
54	MG	DA	3487	1/1	0.15	-	48,48,48,48	0
54	MG	DA	3455	1/1	0.05	-	68,68,68,68	0
54	MG	BA	3332	1/1	0.10	-	50,50,50,50	0
54	MG	BA	3240	1/1	0.28	-	71,71,71,71	0
54	MG	DA	3377	1/1	0.06	-	33,33,33,33	0
54	MG	DA	3136	1/1	0.29	-	62,62,62,62	0
54	MG	DA	3223	1/1	0.21	-	54,54,54,54	0
54	MG	D0	101	1/1	0.08	-	41,41,41,41	0
54	MG	DA	3112	1/1	0.20	-	51,51,51,51	0
54	MG	DA	3151	1/1	0.08	-	43,43,43,43	0
54	MG	DA	3402	1/1	0.12	-	44,44,44,44	0
54	MG	DA	3004	1/1	0.07	-	88,88,88,88	0
54	MG	BF	302	1/1	0.26	-	42,42,42,42	0
54	MG	BA	3619	1/1	0.11	-	64,64,64,64	0
54	MG	AA	1693	1/1	0.10	-	51,51,51,51	0
54	MG	BA	3441	1/1	0.09	-	56,56,56,56	0
54	MG	BA	3459	1/1	0.16	-	38,38,38,38	0
54	MG	BA	3605	1/1	0.08	-	55,55,55,55	0
54	MG	DA	3107	1/1	0.09	-	54,54,54,54	0
54	MG	CA	1642	1/1	0.20	-	87,87,87,87	0
54	MG	DA	3573	1/1	0.25	-	31,31,31,31	0
54	MG	DA	3465	1/1	0.08	-	75,75,75,75	0
54	MG	BA	3534	1/1	0.19	-	25,25,25,25	0
54	MG	AA	1705	1/1	0.40	-	97,97,97,97	0
54	MG	DA	3190	1/1	0.09	-	59,59,59,59	0
54	MG	CA	1613	1/1	0.36	-	66,66,66,66	0
54	MG	BA	3146	1/1	0.60	-	65,65,65,65	0
54	MG	DA	3473	1/1	0.19	-	38,38,38,38	0
54	MG	BA	3378	1/1	0.18	-	25,25,25,25	0
54	MG	BA	3420	1/1	0.17	-	61,61,61,61	0
54	MG	BA	3324	1/1	0.10	-	42,42,42,42	0
54	MG	AA	1634	1/1	0.11	-	56,56,56,56	0
54	MG	DA	3126	1/1	0.51	-	63,63,63,63	0
54	MG	AA	1660	1/1	0.42	-	80,80,80,80	0
54	MG	BA	3408	1/1	0.25	-	50,50,50,50	0
54	MG	DA	3485	1/1	0.25	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3259	1/1	0.35	-	27,27,27,27	0
54	MG	DA	3141	1/1	0.54	-	60,60,60,60	0
54	MG	BA	3108	1/1	0.23	-	51,51,51,51	0
54	MG	BB	215	1/1	0.17	-	65,65,65,65	0
54	MG	BA	3141	1/1	0.31	-	36,36,36,36	0
54	MG	DA	3304	1/1	0.43	-	29,29,29,29	0
54	MG	DA	3104	1/1	0.23	-	34,34,34,34	0
55	ZN	D5	102	1/1	0.09	-	69,69,69,69	0
54	MG	CA	1678	1/1	0.23	-	55,55,55,55	0
54	MG	DA	3182	1/1	0.31	-	46,46,46,46	0
54	MG	BA	3578	1/1	0.11	-	44,44,44,44	0
54	MG	DA	3148	1/1	0.17	-	48,48,48,48	0
54	MG	BB	222	1/1	0.16	-	80,80,80,80	0
54	MG	BA	3098	1/1	0.23	-	40,40,40,40	0
54	MG	BA	3485	1/1	0.10	-	32,32,32,32	0
54	MG	BA	3642	1/1	0.14	-	139,139,139,139	0
54	MG	DA	3178	1/1	0.35	-	32,32,32,32	0
54	MG	BA	3007	1/1	0.29	-	28,28,28,28	0
54	MG	BA	3566	1/1	0.12	-	44,44,44,44	0
54	MG	DA	3404	1/1	0.14	-	36,36,36,36	0
54	MG	DA	3013	1/1	0.17	-	37,37,37,37	0
54	MG	DA	3550	1/1	0.17	-	58,58,58,58	0
54	MG	DA	3522	1/1	0.28	-	61,61,61,61	0
54	MG	DA	3173	1/1	0.11	-	52,52,52,52	0
54	MG	DA	3386	1/1	0.07	-	39,39,39,39	0
54	MG	DA	3494	1/1	0.13	-	37,37,37,37	0
54	MG	DA	3587	1/1	0.22	-	95,95,95,95	0
54	MG	AA	1707	1/1	0.14	-	102,102,102,102	0
54	MG	DA	3454	1/1	0.08	-	64,64,64,64	0
54	MG	BA	3608	1/1	0.24	-	71,71,71,71	0
54	MG	DA	3369	1/1	0.08	-	50,50,50,50	0
54	MG	AA	1635	1/1	0.13	-	61,61,61,61	0
54	MG	BB	217	1/1	0.09	-	67,67,67,67	0
54	MG	CA	1618	1/1	0.42	-	64,64,64,64	0
54	MG	DA	3120	1/1	0.24	-	43,43,43,43	0
54	MG	BA	3456	1/1	0.21	-	32,32,32,32	0
54	MG	DA	3405	1/1	0.16	-	32,32,32,32	0
54	MG	AA	1723	1/1	0.11	-	112,112,112,112	0
54	MG	AA	1726	1/1	0.17	-	86,86,86,86	0
54	MG	CA	1607	1/1	0.18	-	50,50,50,50	0
54	MG	DA	3562	1/1	0.12	-	58,58,58,58	0
54	MG	DE	301	1/1	0.19	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3215	1/1	0.07	-	49,49,49,49	0
54	MG	DA	3228	1/1	0.47	-	40,40,40,40	0
54	MG	BA	3380	1/1	0.12	-	26,26,26,26	0
54	MG	DA	3061	1/1	0.18	-	32,32,32,32	0
54	MG	DA	3115	1/1	0.43	-	59,59,59,59	0
54	MG	CA	1689	1/1	0.38	-	61,61,61,61	0
54	MG	BA	3360	1/1	0.25	-	35,35,35,35	0
54	MG	DA	3064	1/1	0.37	-	48,48,48,48	0
55	ZN	BY	201	1/1	0.11	-	69,69,69,69	0
54	MG	BA	3087	1/1	0.24	-	46,46,46,46	0
54	MG	DA	3380	1/1	0.10	-	42,42,42,42	0
54	MG	BA	3372	1/1	0.08	-	49,49,49,49	0
54	MG	BA	3453	1/1	0.07	-	46,46,46,46	0
54	MG	DA	3442	1/1	0.12	-	82,82,82,82	0
54	MG	DA	3535	1/1	0.17	-	64,64,64,64	0
54	MG	BA	3221	1/1	0.31	-	57,57,57,57	0
54	MG	BA	3062	1/1	0.30	-	45,45,45,45	0
54	MG	DA	3329	1/1	0.13	-	41,41,41,41	0
54	MG	BA	3266	1/1	0.45	-	22,22,22,22	0
54	MG	BA	3209	1/1	0.19	-	56,56,56,56	0
54	MG	DA	3515	1/1	0.27	-	37,37,37,37	0
54	MG	DA	3480	1/1	0.17	-	52,52,52,52	0
54	MG	BA	3255	1/1	0.29	-	25,25,25,25	0
54	MG	DA	3172	1/1	0.28	-	64,64,64,64	0
54	MG	DA	3202	1/1	0.35	-	66,66,66,66	0
54	MG	CA	1740	1/1	0.42	-	68,68,68,68	0
54	MG	DA	3130	1/1	0.33	-	47,47,47,47	0
54	MG	DA	3529	1/1	0.07	-	56,56,56,56	0
54	MG	DA	3189	1/1	0.23	-	84,84,84,84	0
54	MG	DA	3171	1/1	0.15	-	61,61,61,61	0
54	MG	DA	3425	1/1	0.08	-	47,47,47,47	0
54	MG	DA	3531	1/1	0.17	-	91,91,91,91	0
54	MG	DA	3552	1/1	0.39	-	35,35,35,35	0
54	MG	BA	3268	1/1	0.35	-	27,27,27,27	0
54	MG	AA	1677	1/1	0.28	-	62,62,62,62	0
54	MG	DA	3554	1/1	0.10	-	47,47,47,47	0
54	MG	BA	3004	1/1	0.07	-	76,76,76,76	0
54	MG	DA	3324	1/1	0.16	-	51,51,51,51	0
54	MG	DA	3030	1/1	0.30	-	55,55,55,55	0
54	MG	BA	3078	1/1	0.25	-	30,30,30,30	0
54	MG	DA	3352	1/1	0.11	-	33,33,33,33	0
54	MG	CQ	201	1/1	0.40	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3506	1/1	0.10	-	30,30,30,30	0
54	MG	BA	3301	1/1	0.65	-	75,75,75,75	0
54	MG	AA	1725	1/1	0.21	-	56,56,56,56	0
54	MG	DA	3155	1/1	0.25	-	64,64,64,64	0
54	MG	CA	1625	1/1	0.37	-	63,63,63,63	0
54	MG	BA	3395	1/1	0.10	-	60,60,60,60	0
54	MG	DA	3484	1/1	0.06	-	64,64,64,64	0
54	MG	DA	3351	1/1	0.11	-	40,40,40,40	0
54	MG	BA	3226	1/1	0.29	-	50,50,50,50	0
54	MG	BA	3599	1/1	0.16	-	30,30,30,30	0
54	MG	BA	3192	1/1	0.12	-	51,51,51,51	0
54	MG	BA	3616	1/1	0.31	-	131,131,131,131	0
54	MG	AA	1610	1/1	0.34	-	56,56,56,56	0
54	MG	BA	3315	1/1	0.16	-	31,31,31,31	0
54	MG	BA	3462	1/1	0.09	-	43,43,43,43	0
54	MG	CA	1759	1/1	0.25	-	69,69,69,69	0
54	MG	DA	3509	1/1	0.18	-	37,37,37,37	0
55	ZN	DY	201	1/1	0.05	-	94,94,94,94	0
54	MG	DA	3177	1/1	0.17	-	88,88,88,88	0
54	MG	DA	3537	1/1	0.10	-	63,63,63,63	0
54	MG	DA	3382	1/1	0.21	-	53,53,53,53	0
54	MG	CA	1652	1/1	0.45	-	76,76,76,76	0
54	MG	BA	3117	1/1	0.29	-	39,39,39,39	0
54	MG	DA	3565	1/1	0.19	-	34,34,34,34	0
54	MG	BA	3507	1/1	0.29	-	41,41,41,41	0
54	MG	CA	1751	1/1	0.28	-	61,61,61,61	0
54	MG	DA	3548	1/1	0.13	-	89,89,89,89	0
54	MG	DA	3459	1/1	0.07	-	53,53,53,53	0
54	MG	DA	3124	1/1	0.39	-	37,37,37,37	0
54	MG	CA	1733	1/1	0.16	-	82,82,82,82	0
54	MG	DA	3379	1/1	0.10	-	59,59,59,59	0
54	MG	BA	3205	1/1	0.12	-	54,54,54,54	0
54	MG	DA	3303	1/1	0.49	-	34,34,34,34	0
54	MG	DA	3335	1/1	0.10	-	36,36,36,36	0
54	MG	BA	3509	1/1	0.14	-	50,50,50,50	0
54	MG	B2	101	1/1	0.16	-	45,45,45,45	0
54	MG	CA	1667	1/1	0.34	-	77,77,77,77	0
54	MG	CA	1611	1/1	0.25	-	43,43,43,43	0
54	MG	BA	3535	1/1	0.14	-	55,55,55,55	0
54	MG	B3	101	1/1	0.26	-	51,51,51,51	0
54	MG	DA	3327	1/1	0.37	-	52,52,52,52	0
54	MG	DA	3506	1/1	0.14	-	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3042	1/1	0.24	-	33,33,33,33	0
54	MG	BA	3135	1/1	0.44	-	45,45,45,45	0
54	MG	BA	3491	1/1	0.08	-	28,28,28,28	0
54	MG	CA	1682	1/1	0.09	-	58,58,58,58	0
54	MG	BA	3461	1/1	0.17	-	79,79,79,79	0
54	MG	DA	3357	1/1	0.16	-	36,36,36,36	0
54	MG	BA	3233	1/1	0.42	-	41,41,41,41	0
54	MG	BA	3497	1/1	0.25	-	61,61,61,61	0
54	MG	BG	201	1/1	0.19	-	60,60,60,60	0
54	MG	BA	3253	1/1	0.45	-	19,19,19,19	0
54	MG	BE	305	1/1	0.16	-	60,60,60,60	0
54	MG	BA	3521	1/1	0.09	-	40,40,40,40	0
54	MG	BA	3045	1/1	0.25	-	45,45,45,45	0
54	MG	BA	3544	1/1	0.14	-	46,46,46,46	0
54	MG	BA	3552	1/1	0.26	-	82,82,82,82	0
54	MG	AQ	201	1/1	0.23	-	58,58,58,58	0
54	MG	BA	3627	1/1	0.10	-	50,50,50,50	0
54	MG	CA	1736	1/1	0.18	-	70,70,70,70	0
54	MG	BA	3598	1/1	0.10	-	65,65,65,65	0
54	MG	CA	1722	1/1	0.11	-	71,71,71,71	0
54	MG	BA	3558	1/1	0.23	-	28,28,28,28	0
54	MG	BA	3298	1/1	0.43	-	54,54,54,54	0
54	MG	DA	3150	1/1	0.37	-	42,42,42,42	0
54	MG	DA	3360	1/1	0.20	-	37,37,37,37	0
54	MG	DA	3408	1/1	0.15	-	51,51,51,51	0
54	MG	BA	3474	1/1	0.08	-	37,37,37,37	0
54	MG	AA	1674	1/1	0.34	-	63,63,63,63	0
54	MG	DA	3146	1/1	0.23	-	44,44,44,44	0
54	MG	BA	3215	1/1	0.21	-	50,50,50,50	0
54	MG	DA	3530	1/1	0.23	-	132,132,132,132	0
54	MG	BA	3524	1/1	0.12	-	38,38,38,38	0
54	MG	DA	3272	1/1	0.38	-	30,30,30,30	0
54	MG	AA	1668	1/1	0.57	-	62,62,62,62	0
54	MG	BB	221	1/1	0.07	-	50,50,50,50	0
54	MG	CA	1654	1/1	0.14	-	65,65,65,65	0
54	MG	DA	3090	1/1	0.10	-	53,53,53,53	0
54	MG	BA	3371	1/1	0.12	-	33,33,33,33	0
54	MG	BA	3109	1/1	0.42	-	62,62,62,62	0
54	MG	DA	3539	1/1	0.08	-	67,67,67,67	0
54	MG	BA	3161	1/1	0.20	-	40,40,40,40	0
54	MG	BZ	301	1/1	0.17	-	55,55,55,55	0
54	MG	DA	3354	1/1	0.07	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1705	1/1	0.15	-	96,96,96,96	0
54	MG	DA	3448	1/1	0.08	-	42,42,42,42	0
54	MG	BA	3551	1/1	0.10	-	82,82,82,82	0
54	MG	AA	1686	1/1	0.11	-	68,68,68,68	0
54	MG	DA	3520	1/1	0.13	-	56,56,56,56	0
54	MG	AA	1670	1/1	0.33	-	53,53,53,53	0
54	MG	BA	3168	1/1	0.27	-	28,28,28,28	0
54	MG	DA	3422	1/1	0.18	-	43,43,43,43	0
54	MG	BA	3400	1/1	0.22	-	47,47,47,47	0
54	MG	AA	1616	1/1	0.13	-	92,92,92,92	0
54	MG	CA	1742	1/1	0.06	-	113,113,113,113	0
54	MG	BA	3271	1/1	0.14	-	30,30,30,30	0
54	MG	BA	3628	1/1	0.16	-	35,35,35,35	0
54	MG	CA	1657	1/1	0.40	-	61,61,61,61	0
54	MG	DA	3220	1/1	0.23	-	51,51,51,51	0
54	MG	DA	3165	1/1	0.41	-	60,60,60,60	0
54	MG	BA	3177	1/1	0.12	-	57,57,57,57	0
54	MG	BA	3070	1/1	0.19	-	37,37,37,37	0
54	MG	DO	202	1/1	0.17	-	39,39,39,39	0
54	MG	DA	3263	1/1	0.19	-	40,40,40,40	0
54	MG	DA	3595	1/1	0.13	-	58,58,58,58	0
54	MG	DA	3511	1/1	0.07	-	49,49,49,49	0
54	MG	BA	3155	1/1	0.17	-	41,41,41,41	0
54	MG	DA	3105	1/1	0.12	-	46,46,46,46	0
54	MG	DA	3396	1/1	0.17	-	52,52,52,52	0
54	MG	BA	3457	1/1	0.17	-	27,27,27,27	0
54	MG	BA	3019	1/1	0.15	-	34,34,34,34	0
54	MG	BA	3415	1/1	0.07	-	33,33,33,33	0
54	MG	BA	3340	1/1	0.10	-	79,79,79,79	0
54	MG	DA	3008	1/1	0.48	-	58,58,58,58	0
54	MG	DA	3345	1/1	0.33	-	54,54,54,54	0
54	MG	BB	202	1/1	0.15	-	43,43,43,43	0
54	MG	BA	3313	1/1	0.09	-	37,37,37,37	0
54	MG	BA	3126	1/1	0.22	-	41,41,41,41	0
54	MG	DA	3581	1/1	0.07	-	52,52,52,52	0
54	MG	CA	1683	1/1	0.20	-	100,100,100,100	0
54	MG	CA	1731	1/1	0.11	-	74,74,74,74	0
54	MG	DA	3079	1/1	0.17	-	47,47,47,47	0
54	MG	BA	3166	1/1	0.28	-	36,36,36,36	0
54	MG	DA	3080	1/1	0.17	-	44,44,44,44	0
54	MG	BA	3280	1/1	0.29	-	46,46,46,46	0
54	MG	BA	3574	1/1	0.31	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3185	1/1	0.53	-	51,51,51,51	0
54	MG	BA	3622	1/1	0.12	-	45,45,45,45	0
54	MG	BA	3356	1/1	0.17	-	29,29,29,29	0
54	MG	AA	1622	1/1	0.19	-	81,81,81,81	0
54	MG	DA	3277	1/1	0.18	-	77,77,77,77	0
54	MG	DA	3066	1/1	0.20	-	62,62,62,62	0
54	MG	BA	3236	1/1	0.26	-	66,66,66,66	0
54	MG	BA	3649	1/1	0.21	-	125,125,125,125	0
54	MG	DA	3592	1/1	0.06	-	83,83,83,83	0
54	MG	DA	3279	1/1	0.13	-	44,44,44,44	0
54	MG	BA	3614	1/1	0.04	-	66,66,66,66	0
54	MG	AA	1692	1/1	0.65	-	144,144,144,144	0
54	MG	DA	3499	1/1	0.14	-	67,67,67,67	0
54	MG	BA	3063	1/1	0.13	-	54,54,54,54	0
54	MG	CA	1631	1/1	0.37	-	48,48,48,48	0
54	MG	CA	1696	1/1	0.44	-	61,61,61,61	0
54	MG	DA	3527	1/1	0.14	-	91,91,91,91	0
54	MG	DA	3036	1/1	0.29	-	44,44,44,44	0
54	MG	DA	3363	1/1	0.20	-	26,26,26,26	0
54	MG	BA	3645	1/1	0.07	-	102,102,102,102	0
54	MG	BA	3346	1/1	0.11	-	52,52,52,52	0
54	MG	BA	3374	1/1	0.08	-	34,34,34,34	0
54	MG	DA	3034	1/1	0.08	-	32,32,32,32	0
54	MG	BA	3064	1/1	0.24	-	34,34,34,34	0
54	MG	AF	201	1/1	0.17	-	62,62,62,62	0
54	MG	AA	1685	1/1	0.12	-	71,71,71,71	0
54	MG	B5	102	1/1	0.09	-	52,52,52,52	0
54	MG	DB	204	1/1	0.70	-	74,74,74,74	0
54	MG	BA	3421	1/1	0.07	-	68,68,68,68	0
54	MG	BA	3058	1/1	0.14	-	32,32,32,32	0
54	MG	AA	1697	1/1	0.21	-	106,106,106,106	0
54	MG	DA	3086	1/1	0.23	-	48,48,48,48	0
54	MG	DA	3307	1/1	0.20	-	35,35,35,35	0
54	MG	DA	3591	1/1	0.10	-	66,66,66,66	0
54	MG	BA	3650	1/1	0.16	-	88,88,88,88	0
54	MG	BA	3305	1/1	0.25	-	69,69,69,69	0
54	MG	AA	1602	1/1	0.33	-	89,89,89,89	0
54	MG	BA	3428	1/1	0.09	-	56,56,56,56	0
54	MG	CA	1719	1/1	0.06	-	54,54,54,54	0
54	MG	BA	3393	1/1	0.18	-	37,37,37,37	0
54	MG	AA	1709	1/1	0.14	-	101,101,101,101	0
54	MG	BA	3472	1/1	0.26	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3353	1/1	0.21	-	61,61,61,61	0
54	MG	CA	1706	1/1	0.11	-	103,103,103,103	0
54	MG	DA	3395	1/1	0.10	-	39,39,39,39	0
54	MG	DA	3227	1/1	0.32	-	52,52,52,52	0
54	MG	DA	3020	1/1	0.21	-	56,56,56,56	0
54	MG	DA	3590	1/1	0.23	-	82,82,82,82	0
54	MG	BA	3600	1/1	0.07	-	81,81,81,81	0
54	MG	BA	3517	1/1	0.11	-	26,26,26,26	0
54	MG	BB	205	1/1	0.33	-	45,45,45,45	0
54	MG	DA	3536	1/1	0.17	-	51,51,51,51	0
54	MG	BA	3169	1/1	0.20	-	31,31,31,31	0
54	MG	AA	1679	1/1	0.23	-	44,44,44,44	0
54	MG	DA	3593	1/1	0.14	-	83,83,83,83	0
54	MG	BA	3631	1/1	0.15	-	26,26,26,26	0
54	MG	DA	3183	1/1	0.45	-	26,26,26,26	0
54	MG	DA	3314	1/1	0.38	-	43,43,43,43	0
54	MG	DO	201	1/1	0.10	-	120,120,120,120	0
54	MG	AA	1625	1/1	0.43	-	79,79,79,79	0
54	MG	CA	1757	1/1	0.25	-	80,80,80,80	0
54	MG	CA	1630	1/1	0.58	-	72,72,72,72	0
54	MG	BA	3530	1/1	0.13	-	56,56,56,56	0
54	MG	BA	3107	1/1	0.23	-	60,60,60,60	0
54	MG	DE	304	1/1	0.18	-	42,42,42,42	0
54	MG	DA	3060	1/1	0.30	-	41,41,41,41	0
54	MG	DA	3016	1/1	0.20	-	62,62,62,62	0
54	MG	BA	3207	1/1	0.12	-	33,33,33,33	0
54	MG	DA	3153	1/1	0.39	-	58,58,58,58	0
54	MG	AA	1699	1/1	0.19	-	99,99,99,99	0
54	MG	DA	3125	1/1	0.31	-	50,50,50,50	0
54	MG	CA	1620	1/1	0.14	-	58,58,58,58	0
54	MG	DA	3213	1/1	0.28	-	48,48,48,48	0
54	MG	CA	1676	1/1	0.23	-	73,73,73,73	0
54	MG	CA	1621	1/1	0.58	-	64,64,64,64	0
54	MG	BA	3584	1/1	0.10	-	42,42,42,42	0
54	MG	DA	3139	1/1	0.45	-	59,59,59,59	0
54	MG	B8	101	1/1	0.23	-	51,51,51,51	0
54	MG	DA	3325	1/1	0.18	-	38,38,38,38	0
54	MG	BA	3034	1/1	0.11	-	41,41,41,41	0
54	MG	DA	3412	1/1	0.09	-	58,58,58,58	0
54	MG	DD	302	1/1	0.40	-	38,38,38,38	0
54	MG	BA	3208	1/1	0.28	-	38,38,38,38	0
54	MG	DA	3247	1/1	0.33	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3287	1/1	0.39	-	44,44,44,44	0
54	MG	DA	3207	1/1	0.28	-	54,54,54,54	0
54	MG	BA	3648	1/1	0.11	-	91,91,91,91	0
54	MG	DA	3491	1/1	0.17	-	44,44,44,44	0
54	MG	DA	3596	1/1	0.18	-	125,125,125,125	0
54	MG	BA	3347	1/1	0.18	-	94,94,94,94	0
54	MG	DA	3347	1/1	0.17	-	35,35,35,35	0
54	MG	DA	3312	1/1	0.51	-	29,29,29,29	0
54	MG	CA	1699	1/1	0.15	-	83,83,83,83	0
54	MG	DA	3267	1/1	0.29	-	54,54,54,54	0
54	MG	AA	1636	1/1	0.27	-	79,79,79,79	0
54	MG	BA	3633	1/1	0.11	-	43,43,43,43	0
54	MG	AC	301	1/1	0.17	-	57,57,57,57	0
54	MG	CA	1755	1/1	0.10	-	129,129,129,129	0
54	MG	DA	3214	1/1	0.21	-	37,37,37,37	0
54	MG	BA	3327	1/1	0.17	-	23,23,23,23	0
54	MG	DA	3037	1/1	0.13	-	43,43,43,43	0
54	MG	BA	3031	1/1	0.18	-	44,44,44,44	0
54	MG	DA	3193	1/1	0.60	-	40,40,40,40	0
54	MG	DA	3528	1/1	0.14	-	124,124,124,124	0
54	MG	CA	1622	1/1	0.29	-	47,47,47,47	0
54	MG	DA	3579	1/1	0.08	-	57,57,57,57	0
54	MG	AA	1706	1/1	0.10	-	91,91,91,91	0
54	MG	AA	1708	1/1	0.35	-	91,91,91,91	0
54	MG	CA	1726	1/1	0.20	-	52,52,52,52	0
54	MG	DA	3143	1/1	0.22	-	60,60,60,60	0
54	MG	DA	3077	1/1	0.18	-	49,49,49,49	0
54	MG	DA	3559	1/1	0.05	-	79,79,79,79	0
54	MG	DA	3249	1/1	0.27	-	49,49,49,49	0
54	MG	BA	3085	1/1	0.37	-	52,52,52,52	0
54	MG	CA	1728	1/1	0.17	-	60,60,60,60	0
54	MG	AA	1618	1/1	1.08	-	94,94,94,94	0
54	MG	BA	3396	1/1	0.16	-	29,29,29,29	0
54	MG	BA	3100	1/1	0.20	-	42,42,42,42	0
54	MG	DA	3186	1/1	0.14	-	54,54,54,54	0
54	MG	DA	3411	1/1	0.11	-	49,49,49,49	0
54	MG	BA	3139	1/1	0.27	-	46,46,46,46	0
54	MG	BA	3452	1/1	0.13	-	64,64,64,64	0
54	MG	BA	3316	1/1	0.12	-	45,45,45,45	0
54	MG	AA	1649	1/1	0.33	-	43,43,43,43	0
54	MG	CA	1644	1/1	0.25	-	53,53,53,53	0
54	MG	DA	3110	1/1	0.31	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3048	1/1	0.20	-	68,68,68,68	0
54	MG	BA	3033	1/1	0.10	-	36,36,36,36	0
54	MG	CA	1692	1/1	0.56	-	86,86,86,86	0
54	MG	BB	213	1/1	0.14	-	38,38,38,38	0
54	MG	DA	3009	1/1	0.28	-	46,46,46,46	0
54	MG	DA	3070	1/1	0.32	-	57,57,57,57	0
54	MG	DA	3397	1/1	0.18	-	34,34,34,34	0
54	MG	DA	3401	1/1	0.30	-	108,108,108,108	0
54	MG	BA	3273	1/1	0.38	-	37,37,37,37	0
54	MG	BA	3358	1/1	0.12	-	55,55,55,55	0
54	MG	AA	1675	1/1	0.21	-	76,76,76,76	0
54	MG	BA	3097	1/1	0.52	-	47,47,47,47	0
54	MG	DA	3262	1/1	0.32	-	53,53,53,53	0
54	MG	BA	3590	1/1	0.30	-	31,31,31,31	0
54	MG	DA	3315	1/1	0.12	-	31,31,31,31	0
54	MG	BA	3349	1/1	0.12	-	36,36,36,36	0
54	MG	DA	3320	1/1	0.17	-	38,38,38,38	0
54	MG	DA	3545	1/1	0.09	-	82,82,82,82	0
54	MG	BA	3384	1/1	0.11	-	88,88,88,88	0
54	MG	DA	3471	1/1	0.20	-	31,31,31,31	0
54	MG	BA	3079	1/1	0.21	-	50,50,50,50	0
54	MG	CA	1681	1/1	0.44	-	82,82,82,82	0
54	MG	DA	3184	1/1	0.17	-	46,46,46,46	0
54	MG	BA	3213	1/1	0.09	-	43,43,43,43	0
54	MG	DA	3575	1/1	0.21	-	35,35,35,35	0
54	MG	DA	3585	1/1	0.13	-	33,33,33,33	0
54	MG	BD	301	1/1	0.45	-	49,49,49,49	0
54	MG	BF	301	1/1	0.19	-	33,33,33,33	0
54	MG	AA	1657	1/1	0.37	-	58,58,58,58	0
54	MG	BA	3237	1/1	0.33	-	71,71,71,71	0
54	MG	BA	3293	1/1	0.27	-	48,48,48,48	0
54	MG	BA	3182	1/1	0.40	-	37,37,37,37	0
54	MG	CA	1627	1/1	0.38	-	55,55,55,55	0
54	MG	DA	3319	1/1	0.33	-	57,57,57,57	0
54	MG	DA	3564	1/1	0.13	-	61,61,61,61	0
54	MG	BA	3278	1/1	0.39	-	30,30,30,30	0
54	MG	BA	3560	1/1	0.08	-	74,74,74,74	0
54	MG	DA	3047	1/1	0.16	-	38,38,38,38	0
54	MG	DA	3447	1/1	0.31	-	74,74,74,74	0
54	MG	BA	3583	1/1	0.14	-	34,34,34,34	0
54	MG	BA	3571	1/1	0.17	-	44,44,44,44	0
54	MG	DA	3023	1/1	0.07	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3169	1/1	0.15	-	45,45,45,45	0
54	MG	BA	3158	1/1	0.11	-	40,40,40,40	0
54	MG	BA	3512	1/1	0.29	-	109,109,109,109	0
55	ZN	B4	101	1/1	0.06	-	199,199,199,199	0
54	MG	BA	3496	1/1	0.15	-	39,39,39,39	0
54	MG	BA	3281	1/1	0.25	-	24,24,24,24	0
54	MG	DA	3206	1/1	0.61	-	52,52,52,52	0
54	MG	AA	1639	1/1	0.49	-	67,67,67,67	0
54	MG	CA	1608	1/1	0.54	-	93,93,93,93	0
54	MG	DA	3138	1/1	0.32	-	41,41,41,41	0
54	MG	BA	3082	1/1	0.11	-	36,36,36,36	0
54	MG	BA	3553	1/1	0.10	-	89,89,89,89	0
54	MG	BA	3267	1/1	0.34	-	36,36,36,36	0
54	MG	CA	1713	1/1	0.16	-	73,73,73,73	0
54	MG	BA	3612	1/1	0.08	-	59,59,59,59	0
54	MG	BA	3370	1/1	0.21	-	41,41,41,41	0
54	MG	BA	3074	1/1	0.40	-	53,53,53,53	0
54	MG	DA	3006	1/1	0.29	-	38,38,38,38	0
54	MG	AA	1608	1/1	0.27	-	67,67,67,67	0
54	MG	BA	3391	1/1	0.09	-	39,39,39,39	0
54	MG	AA	1663	1/1	0.53	-	64,64,64,64	0
54	MG	BA	3398	1/1	0.14	-	52,52,52,52	0
54	MG	BA	3464	1/1	0.13	-	39,39,39,39	0
54	MG	DA	3135	1/1	0.35	-	47,47,47,47	0
54	MG	DA	3119	1/1	0.33	-	48,48,48,48	0
54	MG	DA	3556	1/1	0.06	-	56,56,56,56	0
54	MG	DA	3255	1/1	0.16	-	58,58,58,58	0
54	MG	BA	3432	1/1	0.04	-	67,67,67,67	0
54	MG	BA	3206	1/1	0.27	-	49,49,49,49	0
54	MG	BA	3061	1/1	0.49	-	54,54,54,54	0
54	MG	DA	3350	1/1	0.09	-	47,47,47,47	0
54	MG	DA	3428	1/1	0.05	-	68,68,68,68	0
54	MG	AA	1650	1/1	0.53	-	53,53,53,53	0
54	MG	BA	3254	1/1	0.35	-	25,25,25,25	0
54	MG	DA	3054	1/1	0.11	-	46,46,46,46	0
54	MG	DA	3012	1/1	0.18	-	30,30,30,30	0
54	MG	DA	3286	1/1	0.22	-	33,33,33,33	0
54	MG	BA	3294	1/1	0.18	-	39,39,39,39	0
54	MG	BA	3338	1/1	0.12	-	62,62,62,62	0
54	MG	CA	1619	1/1	0.11	-	50,50,50,50	0
54	MG	DA	3371	1/1	0.24	-	43,43,43,43	0
54	MG	DA	3440	1/1	0.29	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3523	1/1	0.12	-	110,110,110,110	0
54	MG	BA	3568	1/1	0.10	-	39,39,39,39	0
55	ZN	CN	101	1/1	0.07	-	107,107,107,107	0
54	MG	BA	3606	1/1	0.09	-	34,34,34,34	0
54	MG	DA	3582	1/1	0.21	-	63,63,63,63	0
54	MG	BA	3311	1/1	0.17	-	24,24,24,24	0
54	MG	AA	1695	1/1	0.12	-	74,74,74,74	0
54	MG	CA	1711	1/1	0.11	-	103,103,103,103	0
54	MG	BA	3046	1/1	0.18	-	36,36,36,36	0
54	MG	BA	3499	1/1	0.12	-	60,60,60,60	0
54	MG	DA	3400	1/1	0.16	-	66,66,66,66	0
54	MG	BA	3531	1/1	0.07	-	89,89,89,89	0
54	MG	DA	3160	1/1	0.09	-	42,42,42,42	0
54	MG	BA	3040	1/1	0.35	-	30,30,30,30	0
54	MG	AA	1640	1/1	0.24	-	58,58,58,58	0
54	MG	DA	3241	1/1	0.31	-	35,35,35,35	0
54	MG	DA	3514	1/1	0.19	-	42,42,42,42	0
54	MG	BA	3104	1/1	0.29	-	63,63,63,63	0
54	MG	BA	3020	1/1	0.10	-	82,82,82,82	0
54	MG	DA	3100	1/1	0.24	-	38,38,38,38	0
54	MG	BA	3194	1/1	0.22	-	63,63,63,63	0
54	MG	DA	3093	1/1	0.26	-	56,56,56,56	0
54	MG	BA	3039	1/1	0.21	-	32,32,32,32	0
54	MG	BA	3618	1/1	0.09	-	52,52,52,52	0
54	MG	BA	3333	1/1	0.18	-	40,40,40,40	0
54	MG	BA	3193	1/1	0.63	-	35,35,35,35	0
54	MG	BA	3008	1/1	0.21	-	28,28,28,28	0
54	MG	DA	3580	1/1	0.16	-	52,52,52,52	0
54	MG	BA	3439	1/1	0.18	-	59,59,59,59	0
54	MG	BA	3585	1/1	0.12	-	52,52,52,52	0
54	MG	DA	3403	1/1	0.08	-	34,34,34,34	0
54	MG	DA	3543	1/1	0.13	-	53,53,53,53	0
54	MG	AA	1694	1/1	0.08	-	80,80,80,80	0
54	MG	BA	3084	1/1	0.13	-	59,59,59,59	0
54	MG	DA	3358	1/1	0.12	-	39,39,39,39	0
54	MG	AA	1672	1/1	0.41	-	46,46,46,46	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.