



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 07:29 PM BST

PDB ID : 4V84
Title : Crystal structure of a complex containing domain 3 of CrPV IGR IRES RNA bound to the 70S ribosome.
Authors : Zhu, J.; Korostelev, A.; Costantino, D.; Noller, H.F.; Kieft, J.S.
Deposited on : 2010-12-13
Resolution : 3.40 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

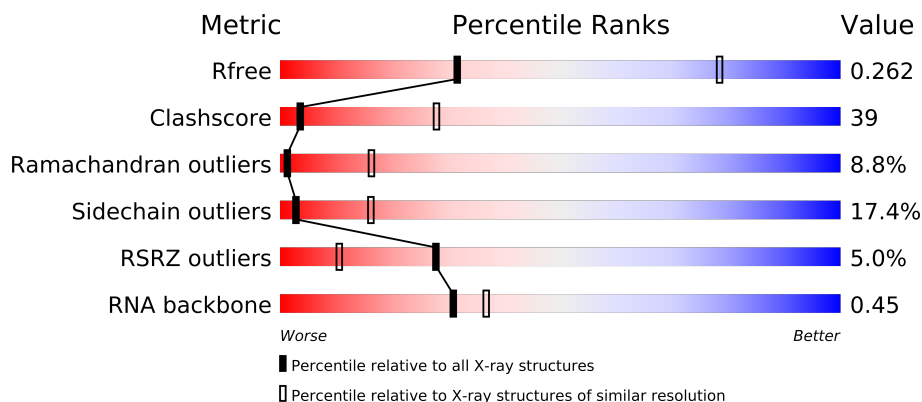
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.40 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	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)
RNA backbone	1838	1002 (4.02-2.76)

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

Mol	Chain	Length	Quality of chain
1	AA	1506	
1	CA	1506	
2	AB	234	
2	CB	234	
3	AC	206	
3	CC	206	
4	AD	208	
4	CD	208	
5	AE	151	
5	CE	151	
6	AF	101	
6	CF	101	

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Mol	Chain	Length	Quality of chain
7	AG	155	
7	CG	155	
8	AH	138	
8	CH	138	
9	AI	127	
9	CI	127	
10	AJ	98	
10	CJ	98	
11	AK	119	
11	CK	119	
12	AL	124	
12	CL	124	
13	AM	116	
13	CM	116	
14	AN	60	
14	CN	60	
15	AO	88	
15	CO	88	
16	AP	83	
16	CP	83	
17	AQ	99	
17	CQ	99	
18	AR	70	
18	CR	70	
19	AS	78	
19	CS	78	
20	AT	99	
20	CT	99	
21	AU	24	
21	CU	24	
22	AV	43	
22	CV	43	
23	BA	2879	
23	DA	2879	
24	BB	119	
24	DB	119	
25	BC	271	
25	DC	271	
26	BD	204	
26	DD	204	
27	BE	202	
27	DE	202	

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Mol	Chain	Length	Quality of chain
28	BF	181	
28	DF	181	
29	BG	159	
29	DG	159	
30	BH	145	
30	DH	145	
31	BI	65	
31	DI	65	
32	BJ	137	
32	DJ	137	
33	BK	122	
33	DK	122	
34	BL	146	
34	DL	146	
35	BM	136	
35	DM	136	
36	BN	117	
36	DN	117	
37	BO	98	
37	DO	98	
38	BP	137	
38	DP	137	
39	BQ	116	
39	DQ	116	
40	BR	101	
40	DR	101	
41	BS	112	
41	DS	112	
42	BT	92	
42	DT	92	
43	BU	100	
43	DU	100	
44	BV	188	
44	DV	188	
45	BW	76	
45	DW	76	
46	BX	88	
46	DX	88	
47	BY	62	
47	DY	62	
48	BZ	59	
48	DZ	59	

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Mol	Chain	Length	Quality of chain
49	B1	30	<div><div></div></div>
49	D1	30	<div><div></div></div>
50	B2	52	<div><div></div></div>
50	D2	52	<div><div></div></div>
51	B3	44	<div><div></div></div>
51	D3	44	<div><div></div></div>
52	B4	48	<div><div></div></div>
52	D4	48	<div><div></div></div>
53	B5	63	<div><div></div></div>
53	D5	63	<div><div></div></div>

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 282142 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 ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1506	Total	C	N	O	P	0	0	0
			32372	14409	5999	10459	1505			
1	CA	1506	Total	C	N	O	P	0	0	0
			32372	14409	5999	10459	1505			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			
2	CB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	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
			1613	1016	314	282	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	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
			1703	1066	339	291	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			
5	CE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	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
			1257	781	252	218	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	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
			1116	705	215	193	3			
8	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O		0	0	0
			1011	639	198	174				
9	CI	127	Total	C	N	O		0	0	0
			1011	639	198	174				

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			
12	CL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	116	Total	C	N	O	S	0	0	0
			929	574	191	162	2			
13	CM	116	Total	C	N	O	S	0	0	0
			929	574	191	162	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			
16	CP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	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
			824	528	152	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			824	528	152	142	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			
19	CS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			

- Molecule 20 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
20	CT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 21 is a protein called domain 3 of CrPV IGR IRES RNA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	24	Total	C	N	O	0	0	0
			209	128	50	31			
21	CU	24	Total	C	N	O	0	0	0
			209	128	50	31			

- Molecule 22 is a RNA chain called RNA (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	34	Total	C	N	O	P	0	0	0
			719	323	125	238	33			
22	CV	34	Total	C	N	O	P	0	0	0
			719	323	125	238	33			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BA	2760	Total	C	N	O	P	0	0	0
			59440	26455	11114	19112	2759			
23	DA	2760	Total	C	N	O	P	0	0	0
			59442	26456	11114	19113	2759			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	1142	U	C	SEE REMARK 999	GB AE017221.1
BA	2825	U	G	SEE REMARK 999	GB AE017221.1
DA	1142	U	C	SEE REMARK 999	GB AE017221.1
DA	2825	U	G	SEE REMARK 999	GB AE017221.1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
24	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	DC	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BD	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			
26	DD	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BE	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			
27	DE	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BF	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			
28	DF	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BG	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			
29	DG	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BH	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			
30	DH	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			

- Molecule 31 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
31	BI	32	Total	C	N	O	0	0	0
			254	157	49	48			
31	DI	32	Total	C	N	O	0	0	0
			254	157	49	48			

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BJ	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			
32	DJ	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BK	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			
33	DK	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BL	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
34	DL	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BM	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	5			
35	DM	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	5			

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BN	117	Total	C	N	O	0	0	0
			960	599	202	159			
36	DN	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BO	98	Total	C	N	O	0	0	0
			771	486	154	131			
37	DO	98	Total	C	N	O	0	0	0
			771	486	154	131			

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BP	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			
38	DP	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BQ	116	Total	C	N	O	S	0	0	0
			953	601	201	150	1			
39	DQ	116	Total	C	N	O	S	0	0	0
			953	601	201	150	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	?	-	PHE	DELETION	UNP Q72L76
DQ	?	-	PHE	DELETION	UNP Q72L76

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BR	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
40	DR	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BS	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			
41	DS	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BT	92	Total	C	N	O		0	0	0
			726	471	131	124				
42	DT	92	Total	C	N	O		0	0	0
			726	471	131	124				

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BU	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			
43	DU	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BV	188	Total	C	N	O	S	0	0	0
			1492	950	265	275	2			
44	DV	188	Total	C	N	O	S	0	0	0
			1492	950	265	275	2			

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BW	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			
45	DW	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	BX	88	Total	C	N	O	0	0	0
			695	435	141	119			
46	DX	88	Total	C	N	O	0	0	0
			695	435	141	119			

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BY	62	Total	C	N	O	S	0	0	0
			521	325	102	92	2			
47	DY	62	Total	C	N	O	S	0	0	0
			521	325	102	92	2			

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BZ	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			
48	DZ	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B1	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			
49	D1	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			

- Molecule 50 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B2	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			
50	D2	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B3	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	D3	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B4	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			
52	D4	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B5	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			
53	D5	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BB	17	Total	Mg	0	0
			17	17		
54	DE	1	Total	Mg	0	0
			1	1		
54	BA	408	Total	Mg	0	0
			408	408		
54	CA	140	Total	Mg	0	0
			140	140		
54	DG	1	Total	Mg	0	0
			1	1		
54	CV	1	Total	Mg	0	0
			1	1		
54	AV	4	Total	Mg	0	0
			4	4		
54	D2	1	Total	Mg	0	0
			1	1		
54	DA	436	Total	Mg	0	0
			436	436		
54	B2	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	CP	1	Total 1	Mg 1	0	0
54	AA	163	Total 163	Mg 163	0	0
54	D4	1	Total 1	Mg 1	0	0
54	BK	1	Total 1	Mg 1	0	0
54	AD	1	Total 1	Mg 1	0	0
54	DB	17	Total 17	Mg 17	0	0

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

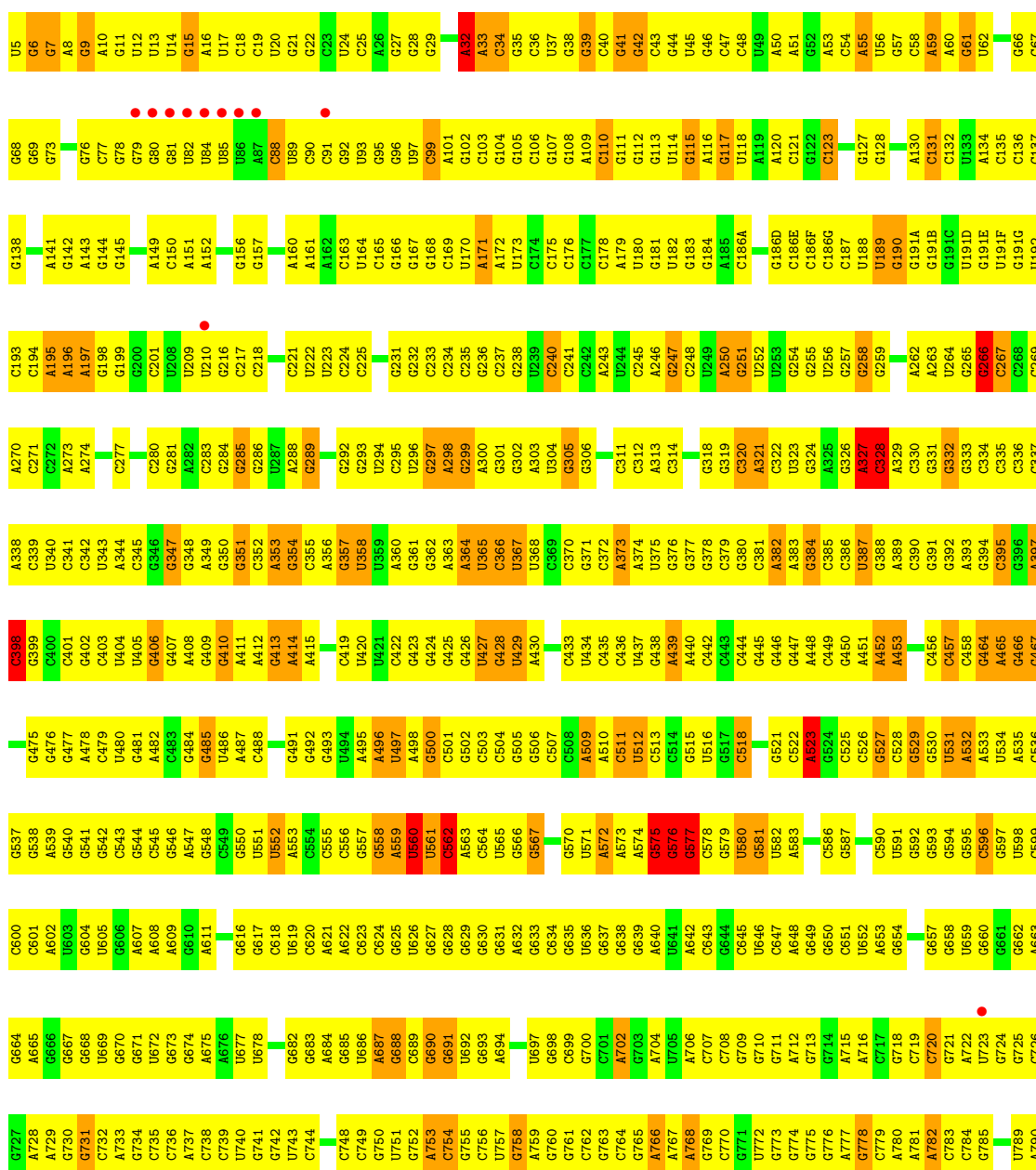
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	CN	1	Total 1	Zn 1	0	0
55	AD	1	Total 1	Zn 1	0	0
55	CD	1	Total 1	Zn 1	0	0
55	AN	1	Total 1	Zn 1	0	0

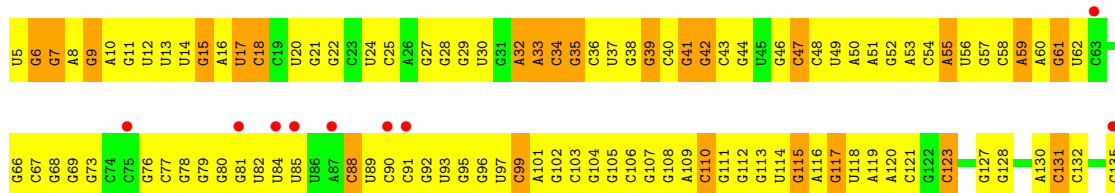
3 Residue-property plots

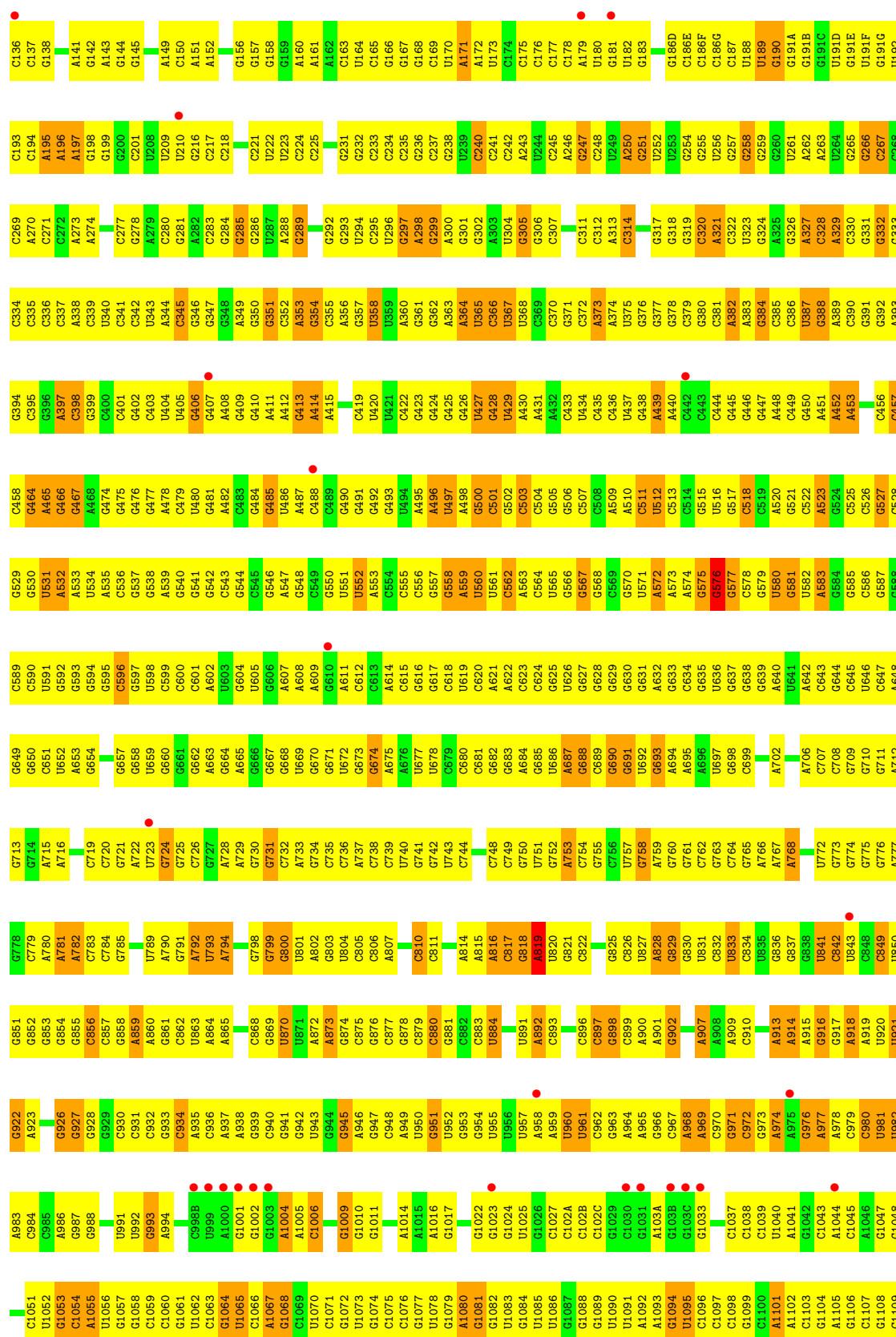
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

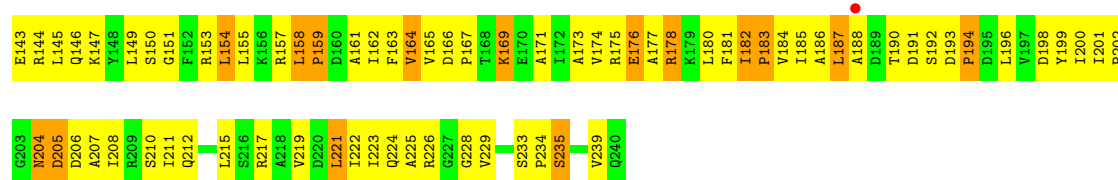
• Molecule 1: ribosomal RNA 16S

Chain AA: 



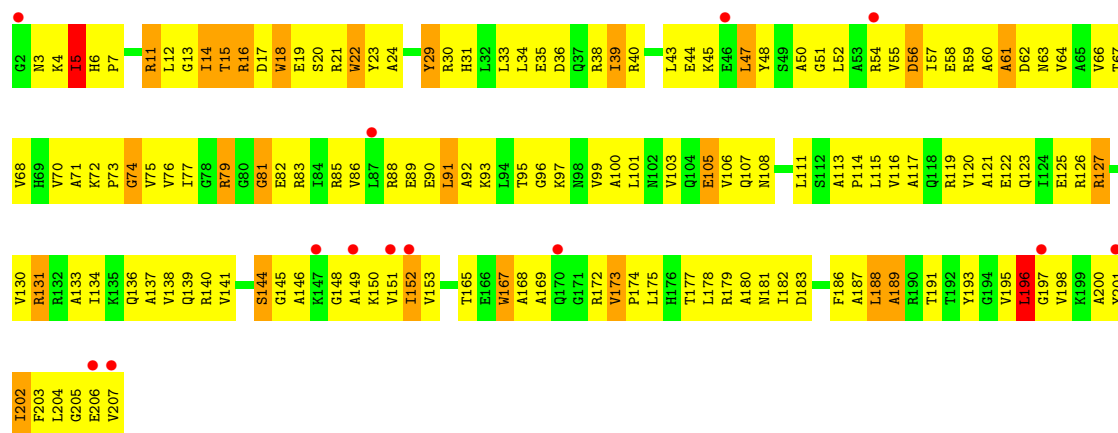






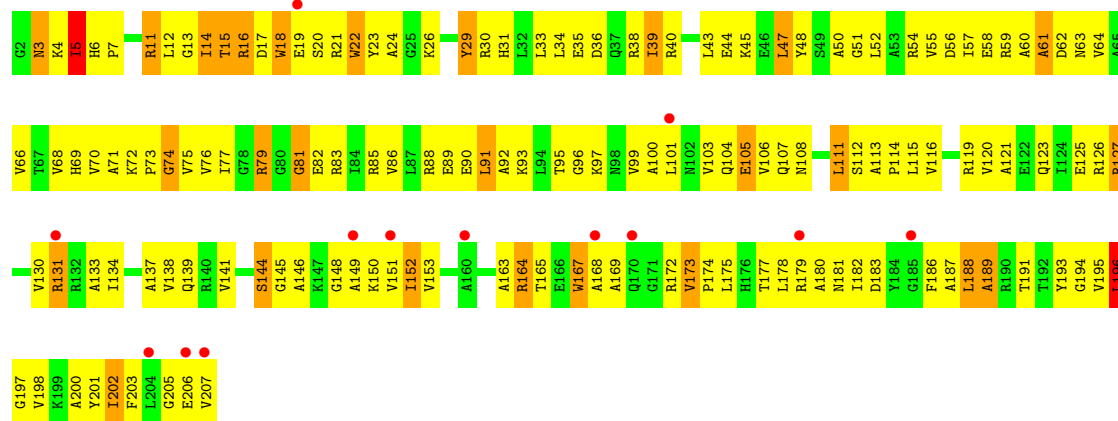
• Molecule 3: 30S ribosomal protein S3

Chain AC:



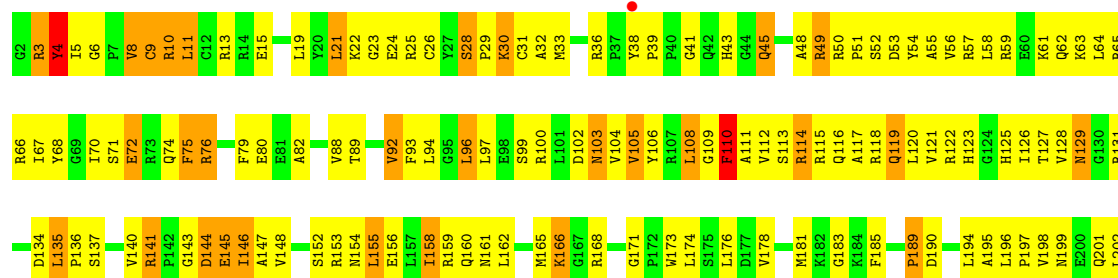
• Molecule 3: 30S ribosomal protein S3

Chain CC:



• Molecule 4: 30S ribosomal protein S4

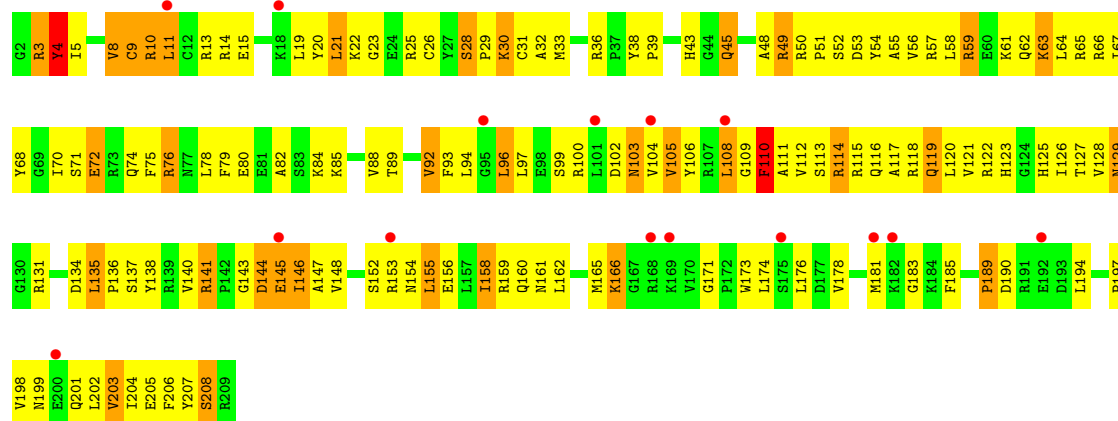
Chain AD:

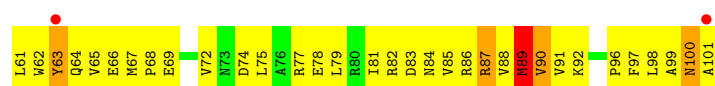


V203
I204
E205
F206
Y207
S208
R209

• Molecule 4: 30S ribosomal protein S4

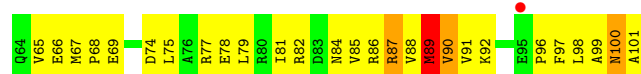
Chain CD:





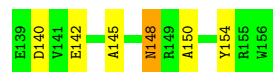
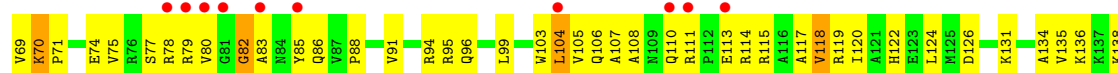
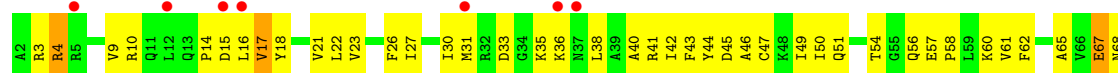
• Molecule 6: 30S ribosomal protein S6

Chain CF:



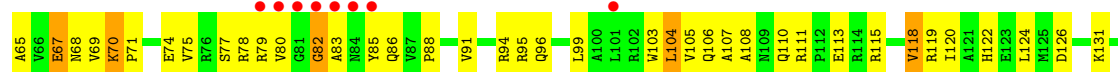
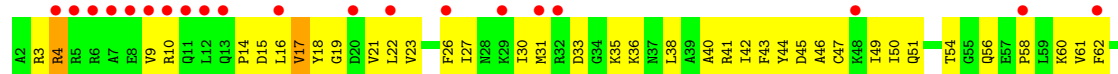
• Molecule 7: 30S ribosomal protein S7

Chain AG:



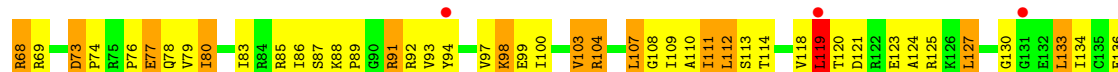
• Molecule 7: 30S ribosomal protein S7

Chain CG:



• Molecule 8: 30S ribosomal protein S8

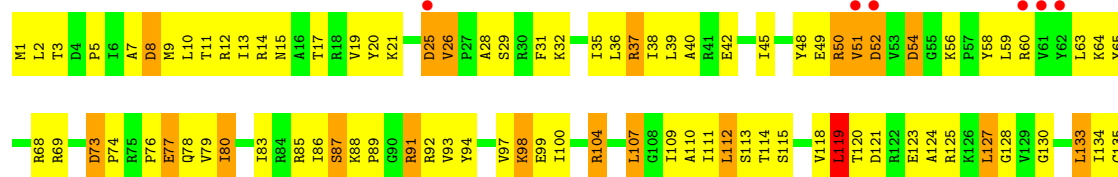
Chain AH:



V137
W138

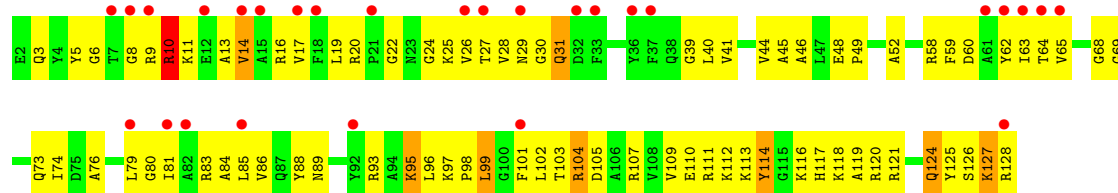
- Molecule 8: 30S ribosomal protein S8

Chain CH:

E136
V137
W138

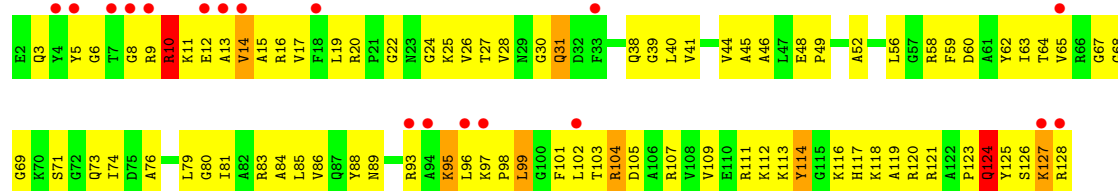
- Molecule 9: 30S ribosomal protein S9

Chain AI:



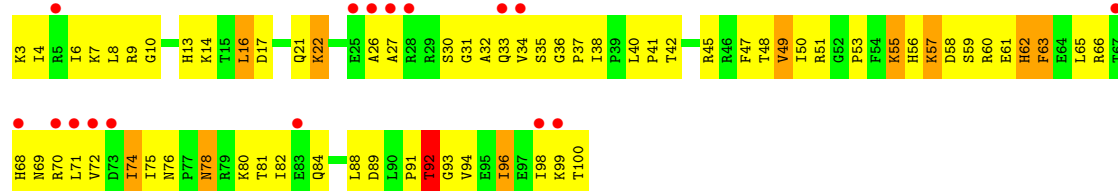
- Molecule 9: 30S ribosomal protein S9

Chain CI:



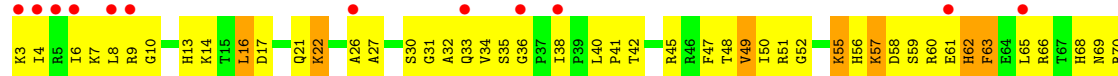
- Molecule 10: 30S ribosomal protein S10

Chain AJ:



- Molecule 10: 30S ribosomal protein S10

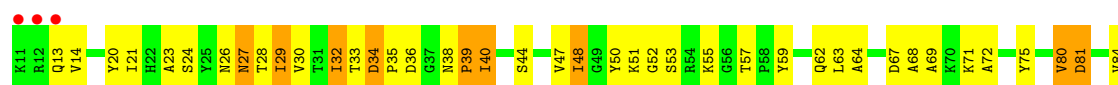
Chain CJ:





- Molecule 11: 30S ribosomal protein S11

Chain AK:



- Molecule 11: 30S ribosomal protein S11

Chain CK:



- Molecule 12: 30S ribosomal protein S12

Chain AL:



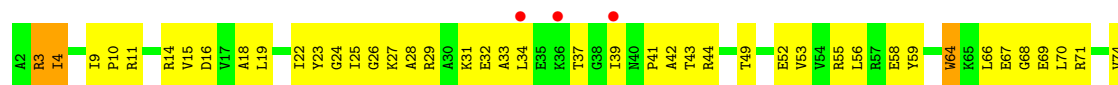
- Molecule 12: 30S ribosomal protein S12

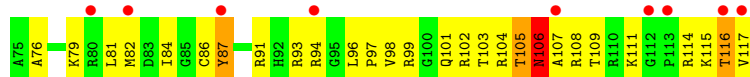
Chain CL:



- Molecule 13: 30S ribosomal protein S13

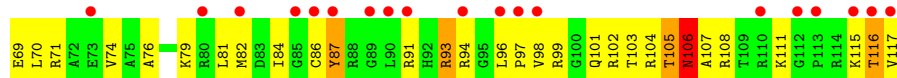
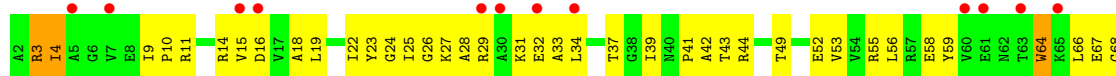
Chain AM:





- Molecule 13: 30S ribosomal protein S13

Chain CM:



- Molecule 14: 30S ribosomal protein S14 type Z

Chain AN:



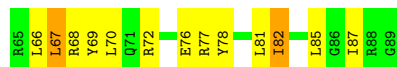
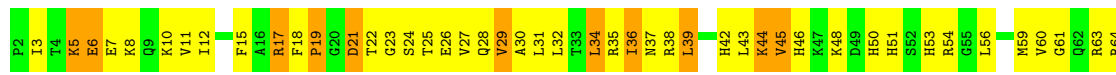
- Molecule 14: 30S ribosomal protein S14 type Z

Chain CN:



- Molecule 15: 30S ribosomal protein S15

Chain AO:



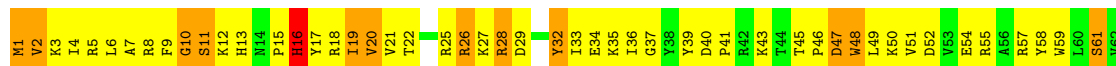
- Molecule 15: 30S ribosomal protein S15

Chain CO:



- Molecule 16: 30S ribosomal protein S16

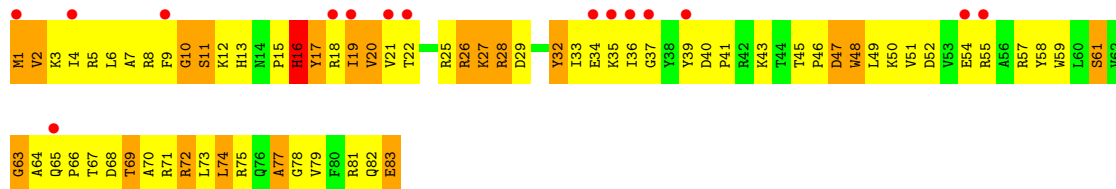
Chain AP:





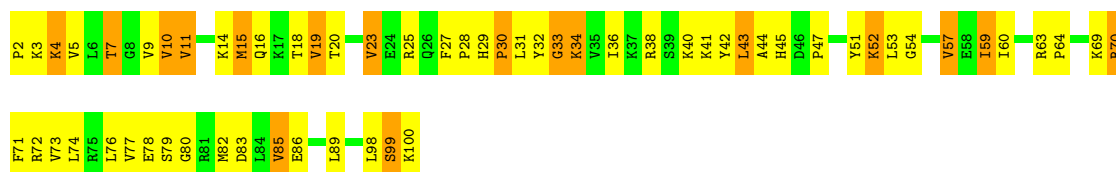
- Molecule 16: 30S ribosomal protein S16

Chain CP:



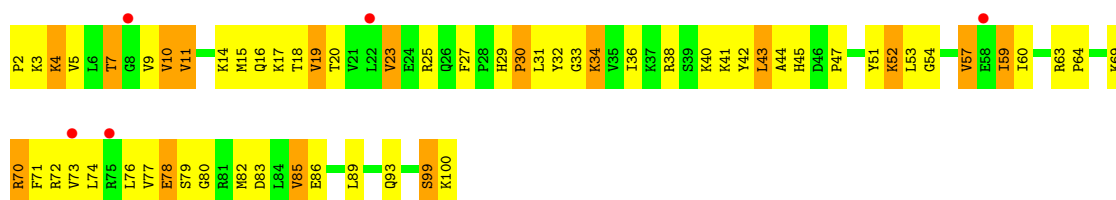
- Molecule 17: 30S ribosomal protein S17

Chain AQ:



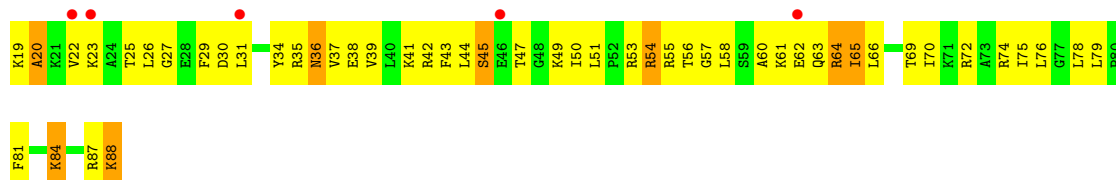
- Molecule 17: 30S ribosomal protein S17

Chain CQ:



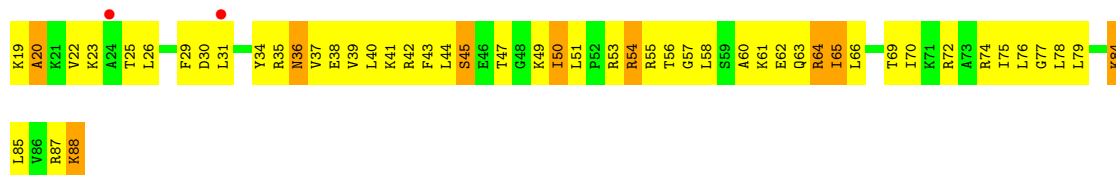
- Molecule 18: 30S ribosomal protein S18

Chain AR:

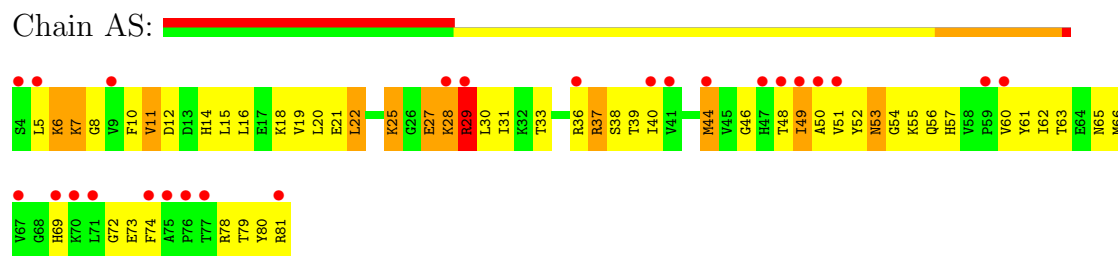


- Molecule 18: 30S ribosomal protein S18

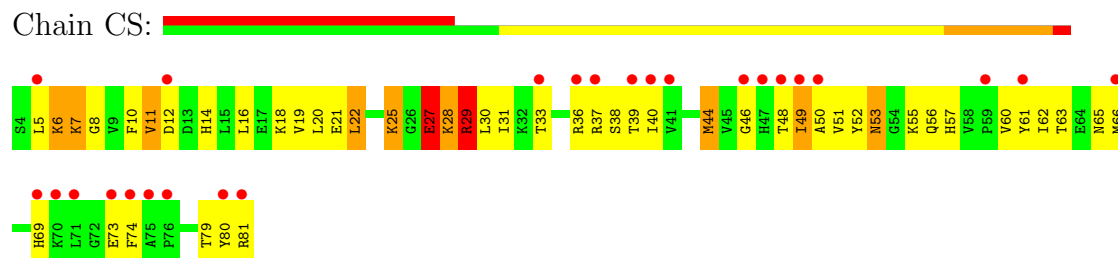
Chain CR:



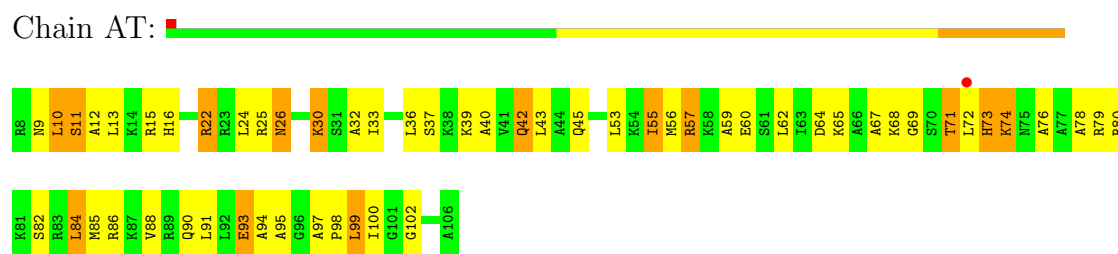
- Molecule 19: 30S ribosomal protein S19



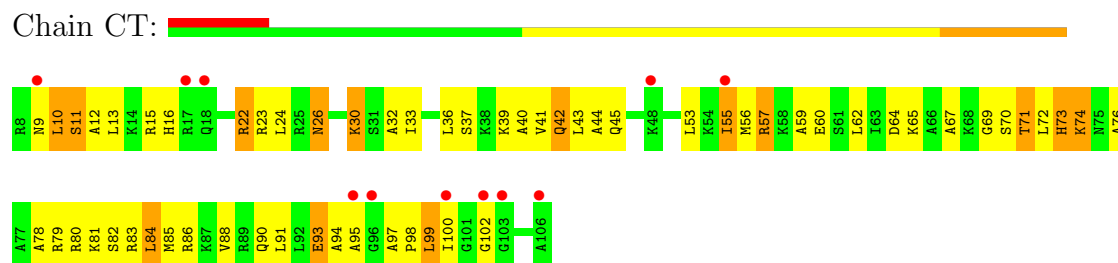
- Molecule 19: 30S ribosomal protein S19



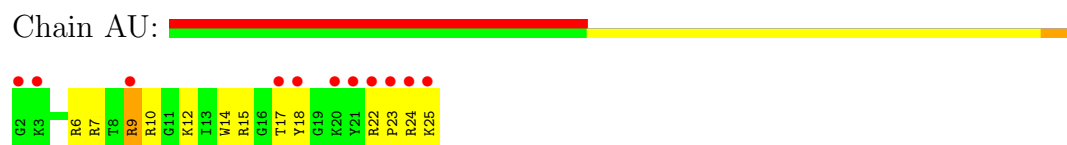
- Molecule 20: 30S ribosomal protein Thx



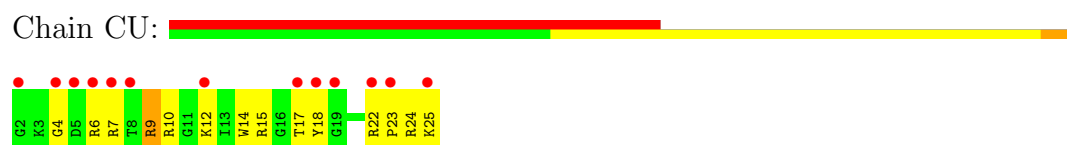
- Molecule 20: 30S ribosomal protein Thx



- Molecule 21: domain 3 of CrPV IGR IRES RNA



- Molecule 21: domain 3 of CrPV IGR IRES RNA



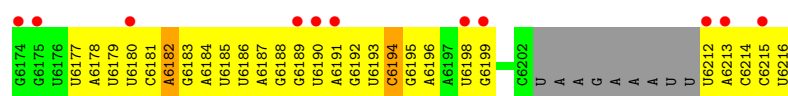
- Molecule 22: RNA (34-MER)

Chain AV:



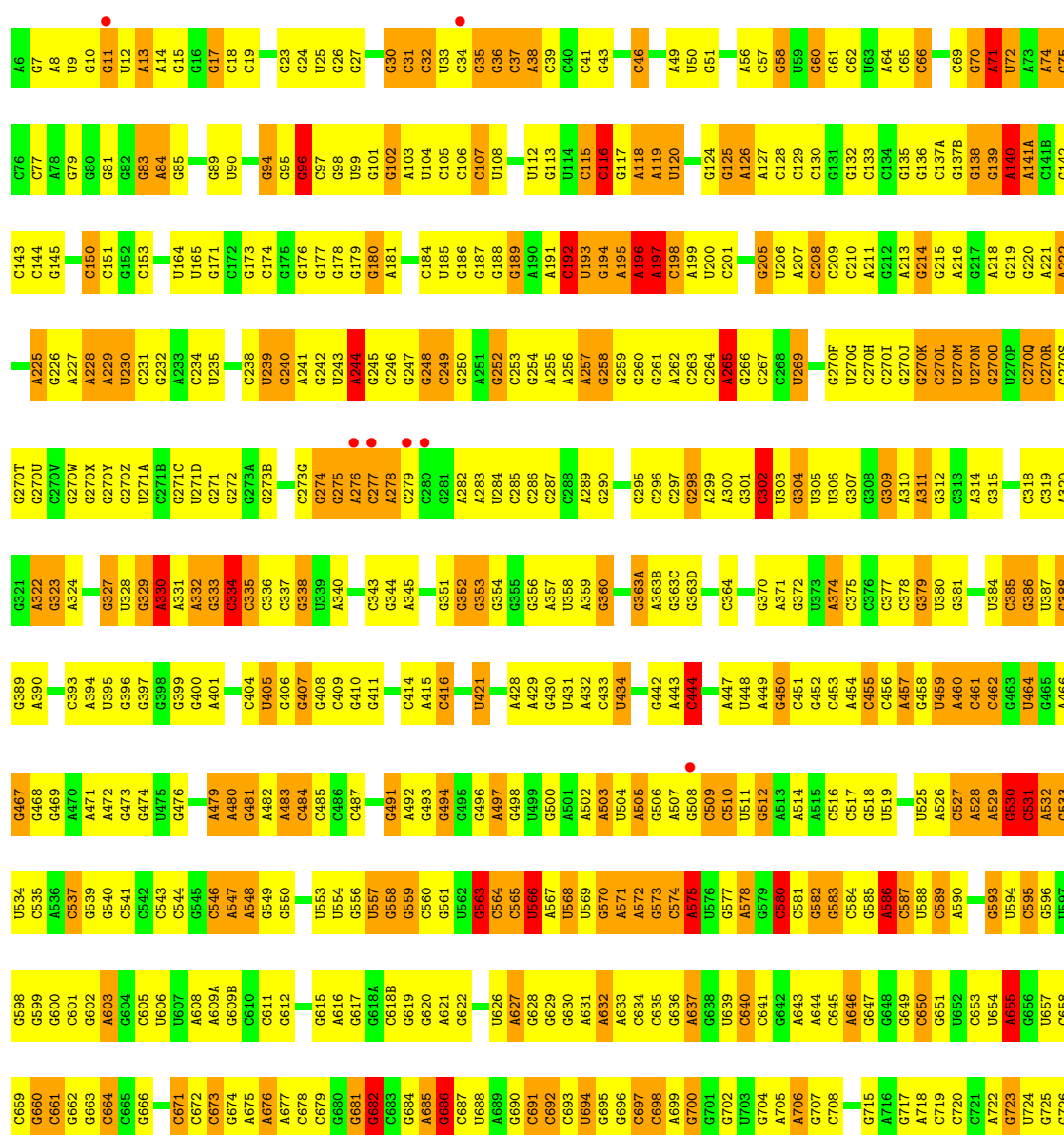
- Molecule 22: RNA (34-MER)

Chain CV:



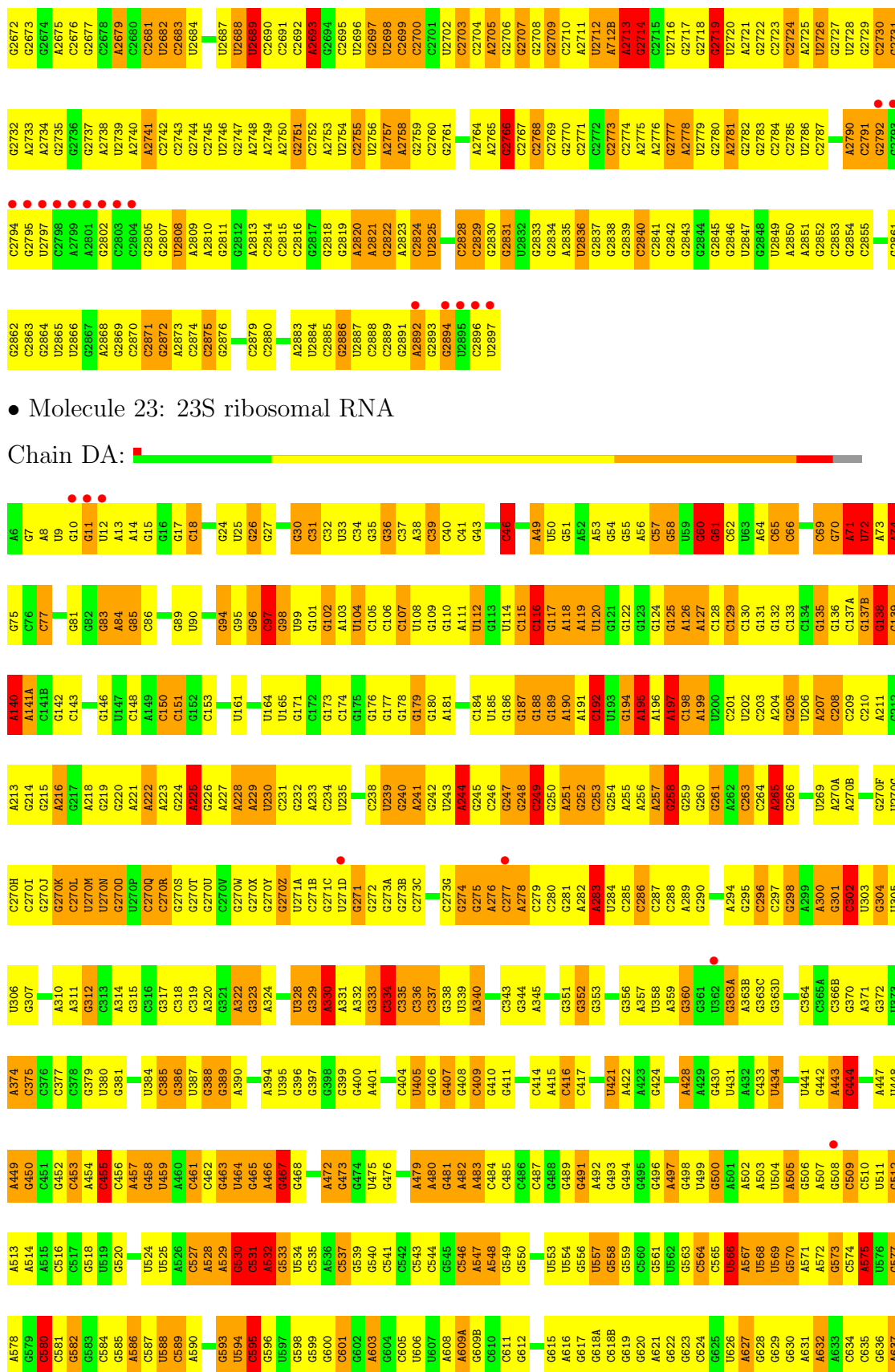
- Molecule 23: 23S ribosomal RNA

Chain BA:



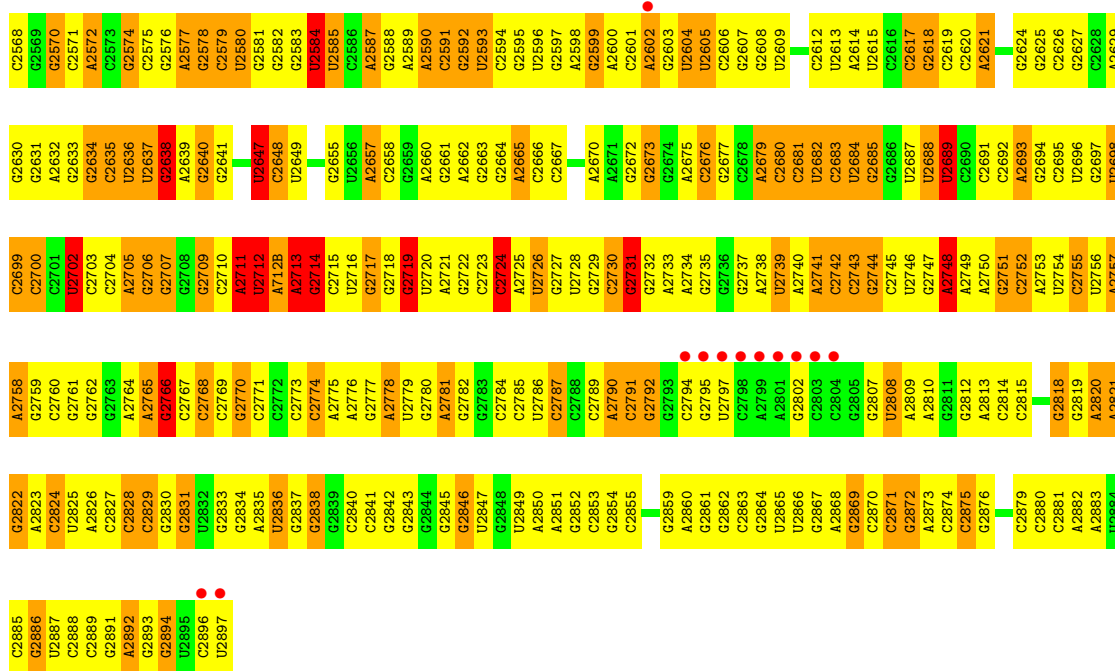


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A2604	C2539	A2478	A2418	G2352	G2290	A2225	G	C2095	C1973	C1909	U1834	G1771	C1687
U2605	C2540	G2479	G2419	U2291	U2290	G2226	G	U2096	C1974	C1909	U1835	G1772	U1688
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G2607	A2542	G2481	G2421	C2293	C2293	G2228	A	U2098	U1976	C1913	C1837	C1774	A1690
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G2648	U2583	C2517	U2457	G2396	G2329	A2270	A	A	A2013	A1952	A1886	A1812	G1750
U2649	U2584	A2518	G2458	C2397	G2330	G2271	C	C	A2014	G1953	C1887	G1813	C1751
U2650	C2585	U2519	A2459	G2398	G2331	U2272	C	C	A2015	U1955	G1888	A1814	G1752
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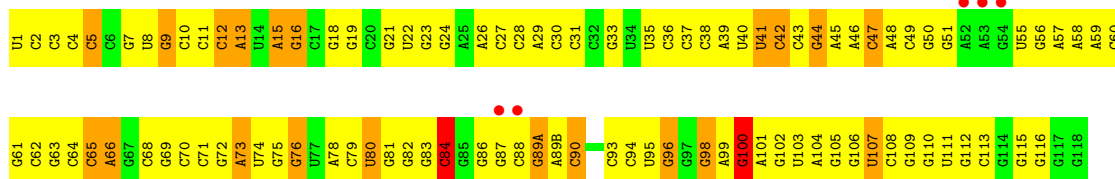


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C2507	G2445	G2385	G2321	G2260	G2187	C	C2064	A2005	G1945	C1871	G1800	A1729	C1656	A1597
	G2446	C2386	G2322	C2261	C2188	G	C2065	C2006	U1946	A1872	A1801	G1733	C1657	C1598
G2510	G2448	U2387	G2324	U2262	U2189	C	G2066	C2007	C1947	C1881	A1803	G1734	U1659	C1599
U2511	U2449	G2389	G2325	C2264	G2190	U	U2068	C2008	G1948	C1882	C1804	U1735	C1660	C1600
G2512	A2450	U2390	G2326		G2192	U	G2069	G2009	G1949	G1883	U1805	G1741	G1661	G1601
G2513	A2451	A2392	A2327	A2267	G2193	G	G2070	G2010	U1951	G1884	G1811	G1742	G1662	U1602
U2514	C2452	A2392	A2328	A2268	C2194	A	A2071	U2011	U1952	A1885	G1812	G1743	C1663	A1603
G2515	A2453	A2393	A2329	A2269	C2195	A	G2072	G2012	U1953	A1886	G1813	G1746	C1664	C1604
G2516	G2454	C2394	G2330	G2270	C2196	C		A2013	U1954	C1887	G1814	G1747	A1665	G1606
G2517	G2455	G2395	G2331	G2271	U2197	C	U2075	A2014	G1955	G1888	G1815	G1748	G1666	C1607
A2518	C2456	G2396	U2332	U2272	A2198	C		A2015	U1956	G1889	G1816	A1749	G1667	A1608
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A2566	C2501	G2502	C2441	G2256	C2256	U								
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				C2183	G2184	G								
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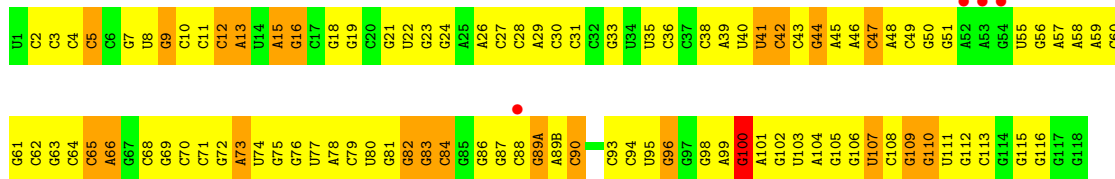
• Molecule 24: 5S ribosomal RNA

Chain BB:



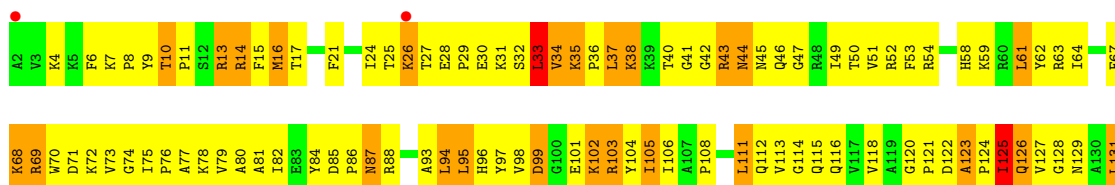
• Molecule 24: 5S ribosomal RNA

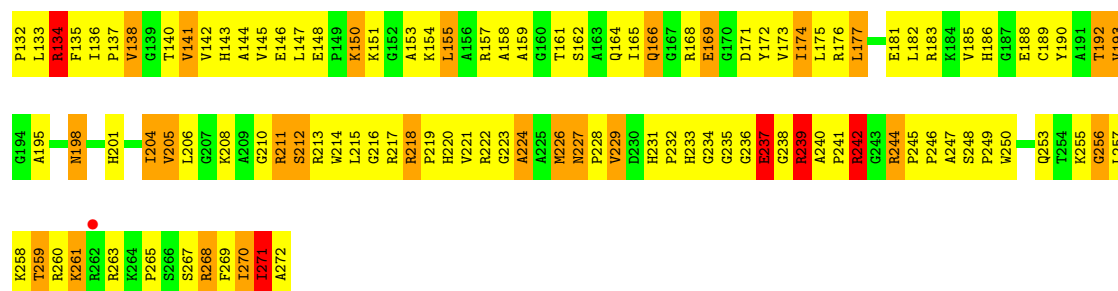
Chain DB:



• Molecule 25: 50S ribosomal protein L2

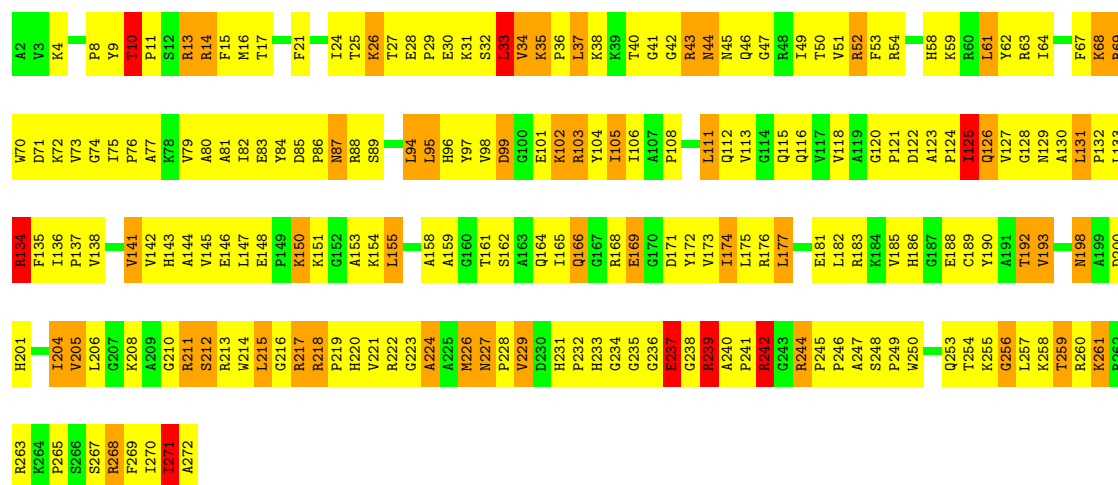
Chain BC:





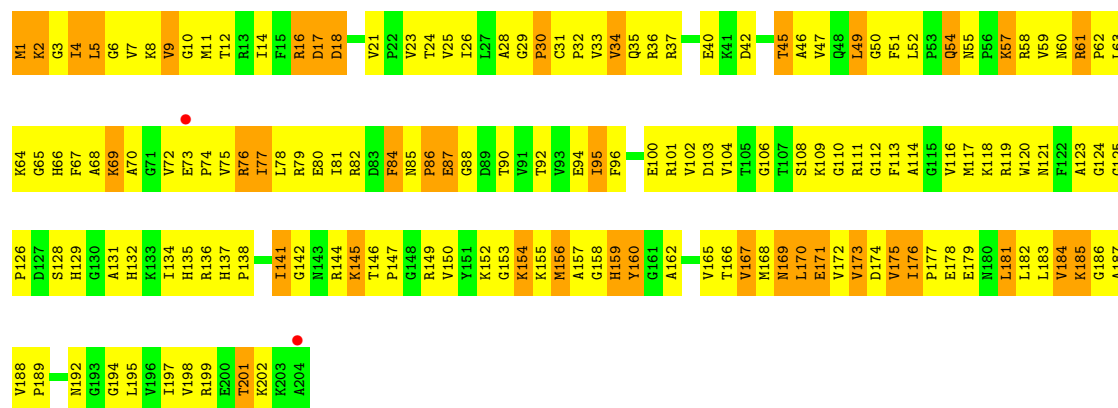
• Molecule 25: 50S ribosomal protein L2

Chain DC:



• Molecule 26: 50S ribosomal protein L3

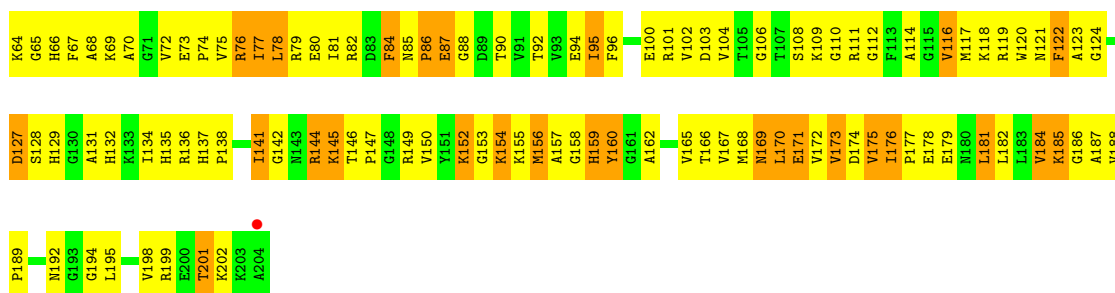
Chain BD:



• Molecule 26: 50S ribosomal protein L3

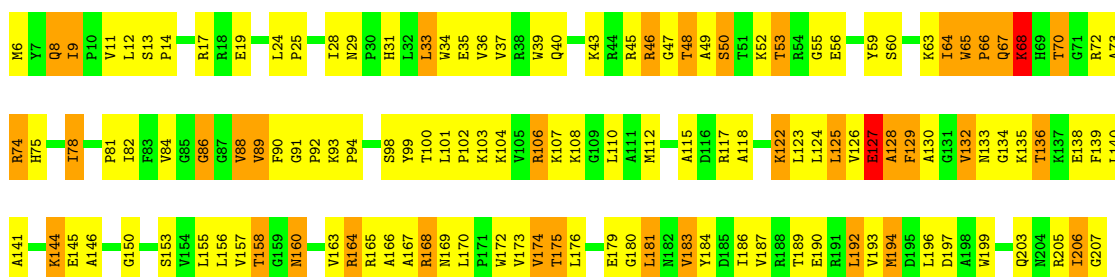
Chain DD:





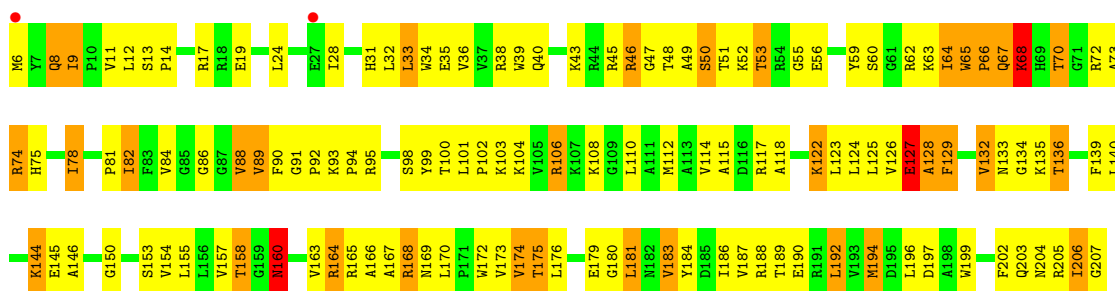
• Molecule 27: 50S ribosomal protein L4

Chain BE:



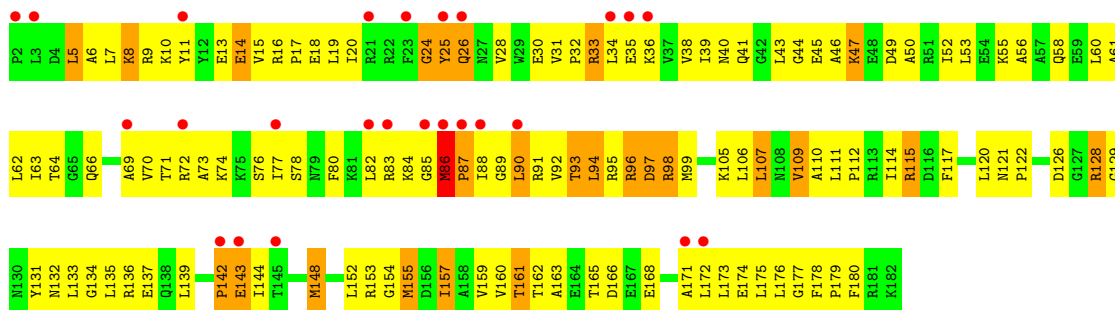
• Molecule 27: 50S ribosomal protein L4

Chain DE:



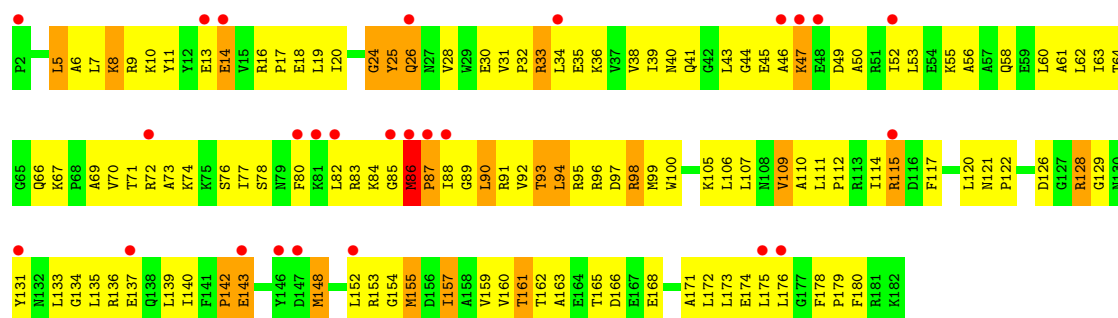
• Molecule 28: 50S ribosomal protein L5

Chain BF:



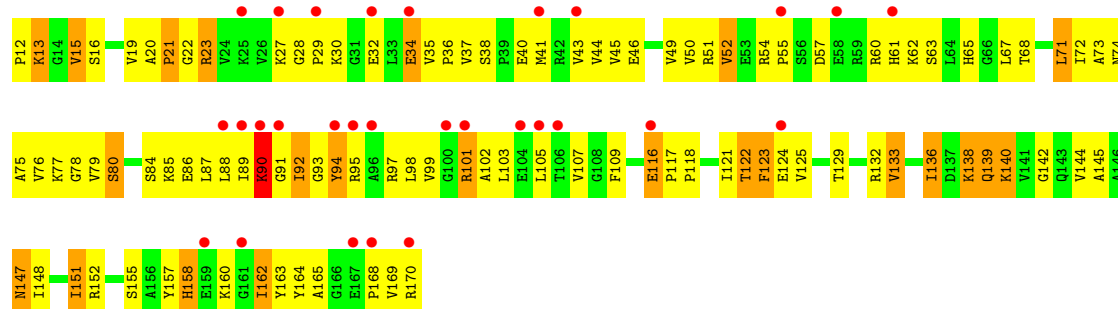
• Molecule 28: 50S ribosomal protein L5

Chain DF:



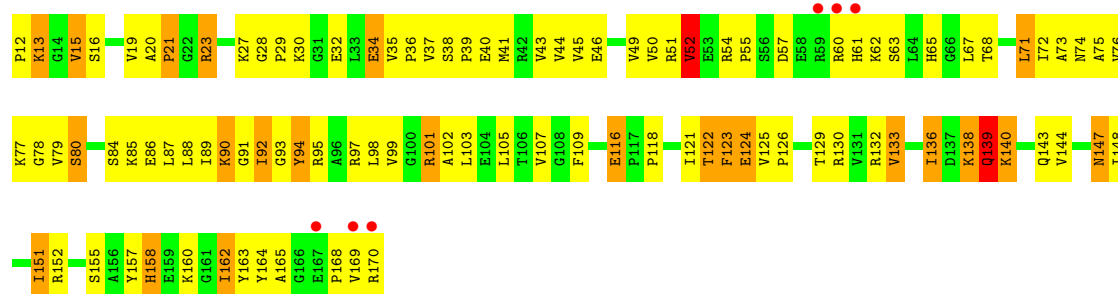
- Molecule 29: 50S ribosomal protein L6

Chain BG:



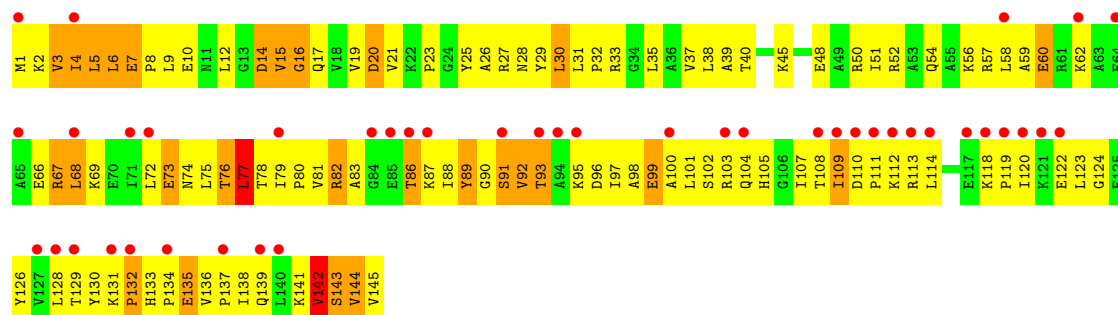
- Molecule 29: 50S ribosomal protein L6

Chain DG:

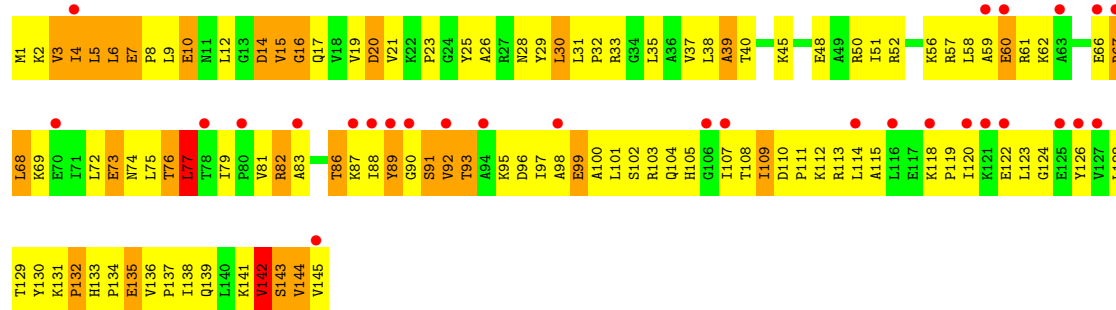


- Molecule 30: 50S ribosomal protein L9

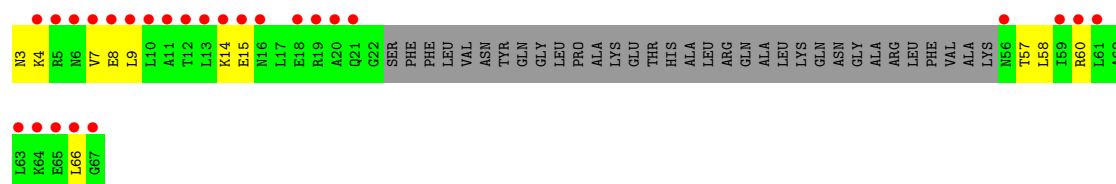
Chain BH:



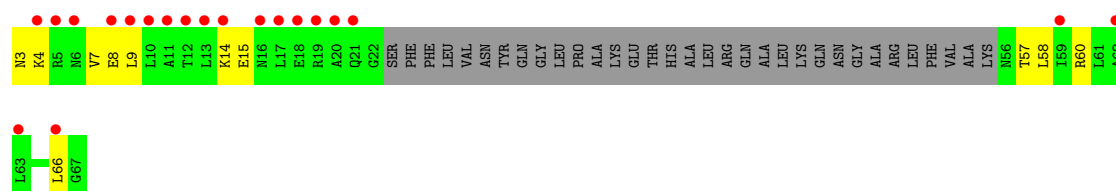
- Molecule 30: 50S ribosomal protein L9

Chain DH: 

- Molecule 31: 50S ribosomal protein L10

Chain BI: 

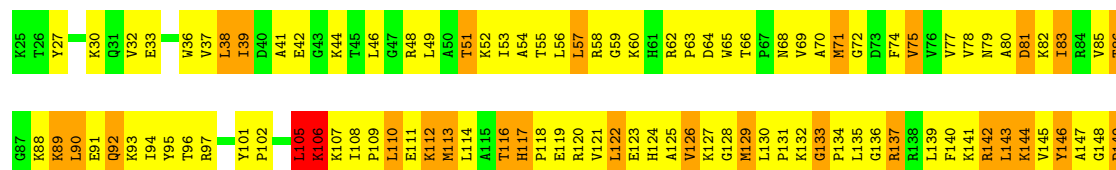
- Molecule 31: 50S ribosomal protein L10

Chain DI: 

- Molecule 32: 50S ribosomal protein L13

Chain BJ: 

- Molecule 32: 50S ribosomal protein L13

Chain DJ: 



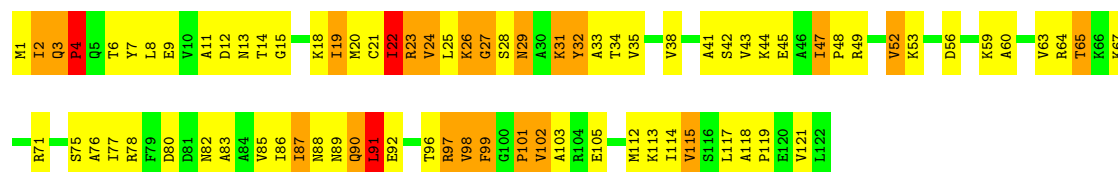
• Molecule 33: 50S ribosomal protein L14

Chain BK:



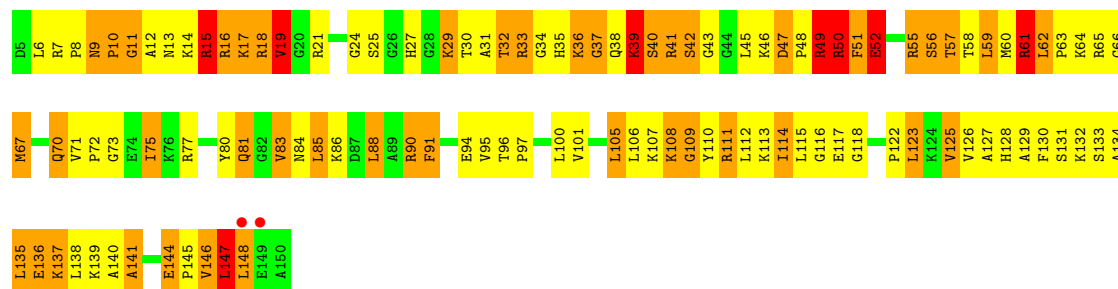
• Molecule 33: 50S ribosomal protein L14

Chain DK:



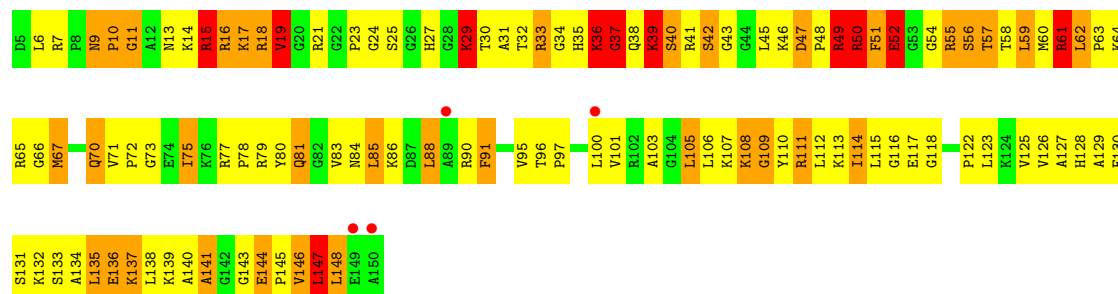
• Molecule 34: 50S ribosomal protein L15

Chain BL:



• Molecule 34: 50S ribosomal protein L15

Chain DL:

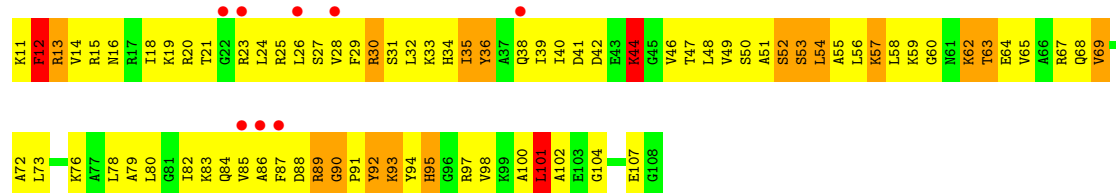


• Molecule 35: 50S ribosomal protein L16

Chain BM:

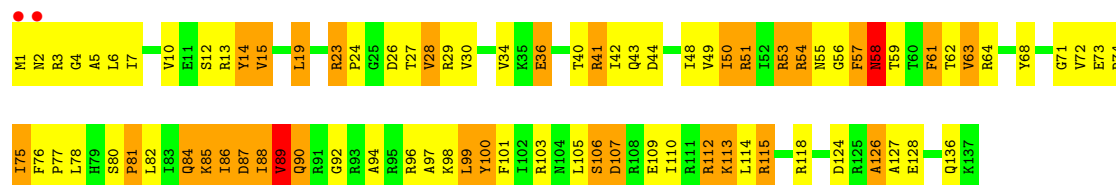


Chain DO:



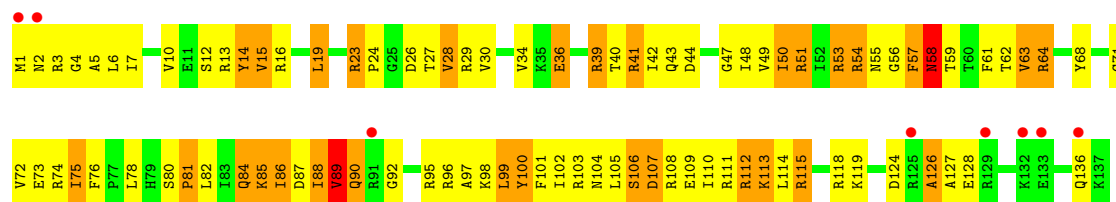
- Molecule 38: 50S ribosomal protein L19

Chain BP:



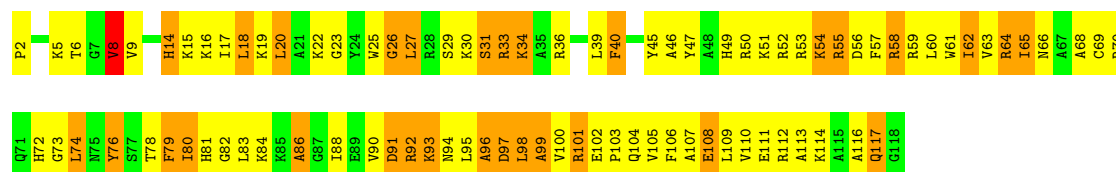
- Molecule 38: 50S ribosomal protein L19

Chain DP:



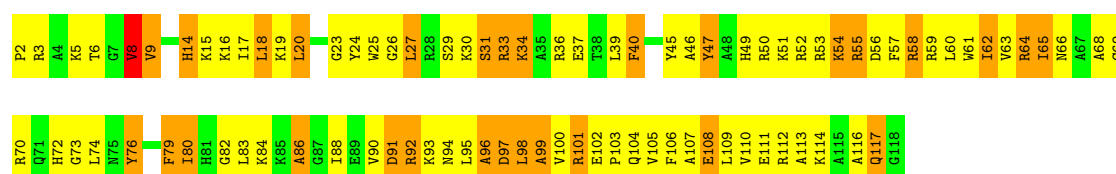
- Molecule 39: 50S ribosomal protein L20

Chain BQ:



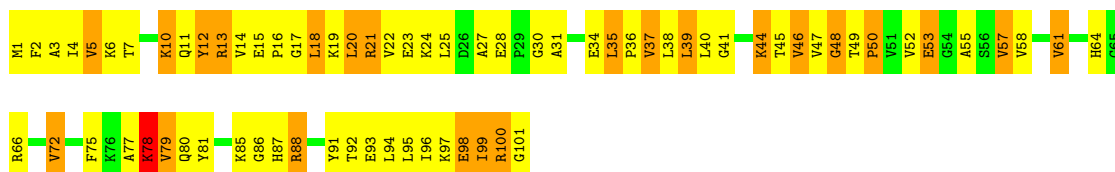
- Molecule 39: 50S ribosomal protein L20

Chain DQ:



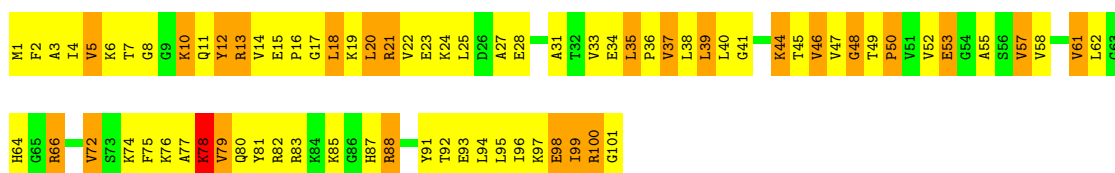
- Molecule 40: 50S ribosomal protein L21

Chain BR:



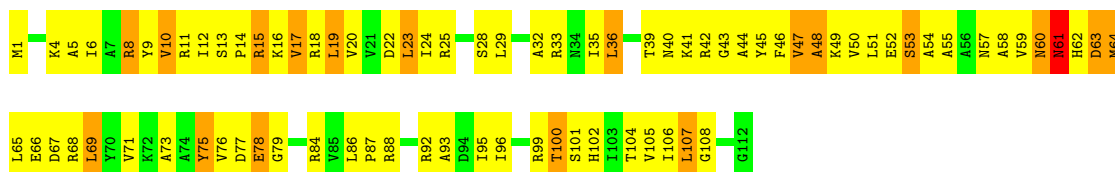
• Molecule 40: 50S ribosomal protein L21

Chain DR:



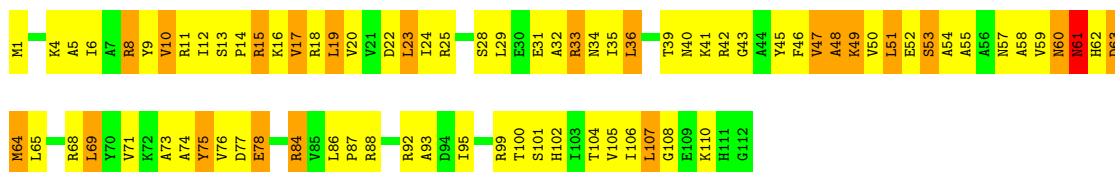
• Molecule 41: 50S ribosomal protein L22

Chain BS:



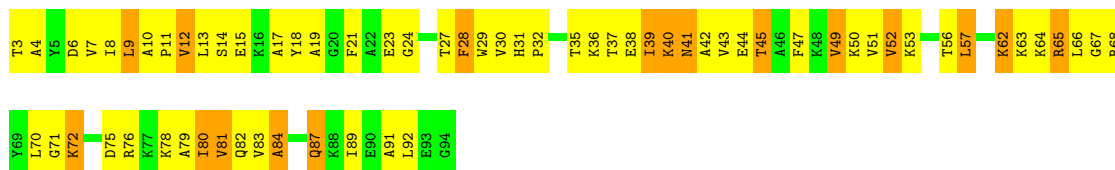
• Molecule 41: 50S ribosomal protein L22

Chain DS:



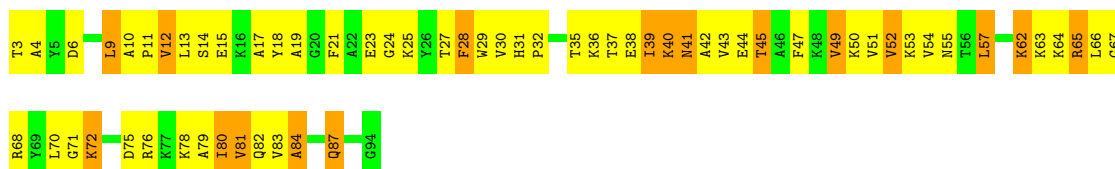
• Molecule 42: 50S ribosomal protein L23

Chain BT:

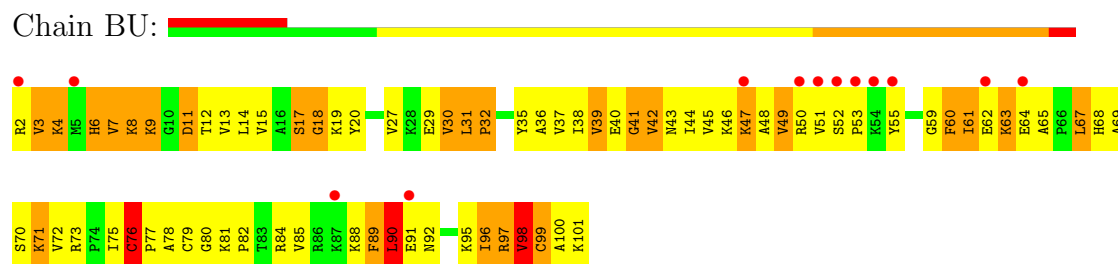


• Molecule 42: 50S ribosomal protein L23

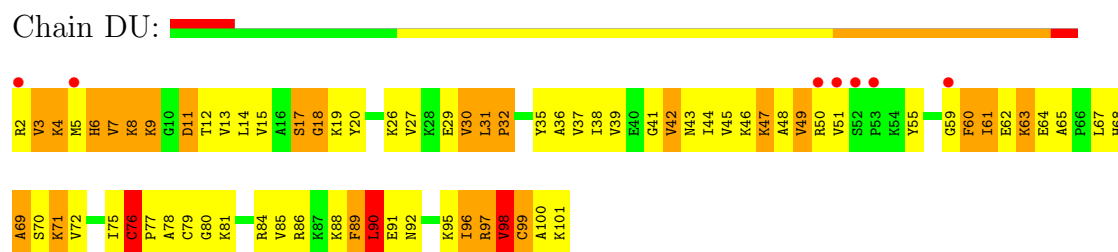
Chain DT:



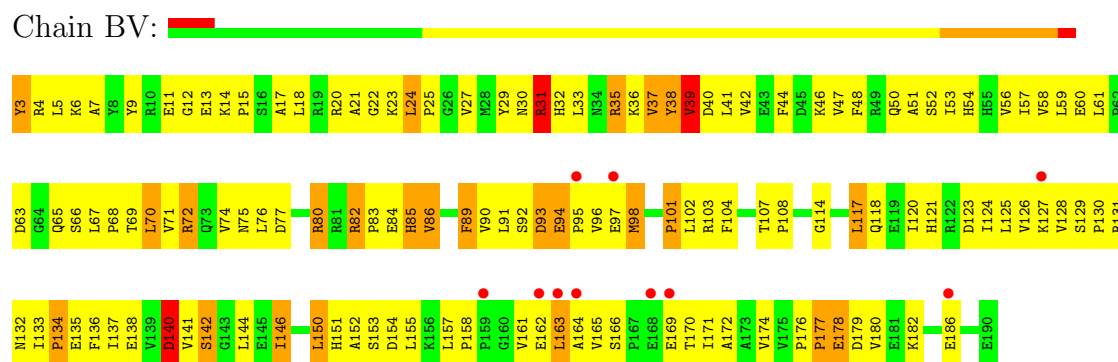
- Molecule 43: 50S ribosomal protein L24



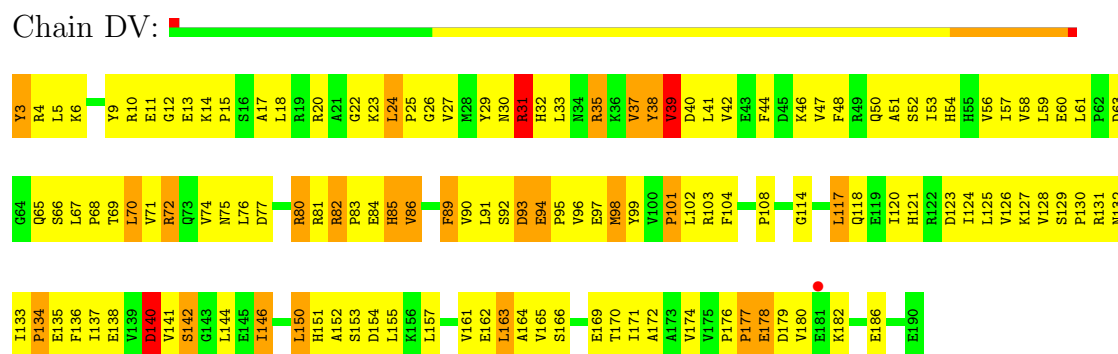
- Molecule 43: 50S ribosomal protein L24



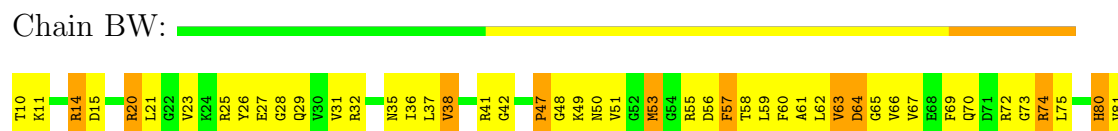
- Molecule 44: 50S ribosomal protein L25



- Molecule 44: 50S ribosomal protein L25



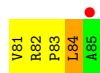
- Molecule 45: 50S ribosomal protein L27





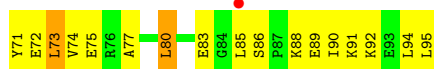
- Molecule 45: 50S ribosomal protein L27

Chain DW:



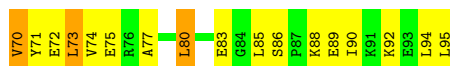
- Molecule 46: 50S ribosomal protein L28

Chain BX:



- Molecule 46: 50S ribosomal protein L28

Chain DX:



- Molecule 47: 50S ribosomal protein L29

Chain BY:



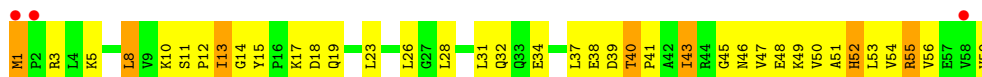
- Molecule 47: 50S ribosomal protein L29

Chain DY:



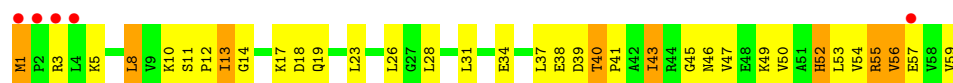
- Molecule 48: 50S ribosomal protein L30

Chain BZ:



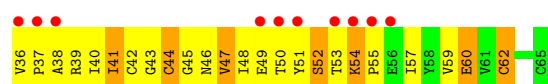
- Molecule 48: 50S ribosomal protein L30

Chain DZ: 



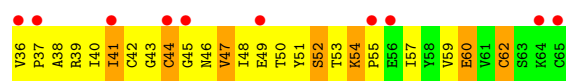
- Molecule 49: 50S ribosomal protein L31

Chain B1: 



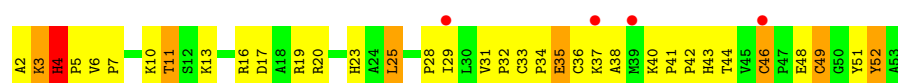
- Molecule 49: 50S ribosomal protein L31

Chain D1: 



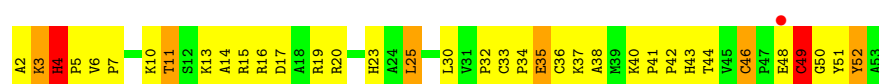
- Molecule 50: 50S ribosomal protein L32

Chain B2: 



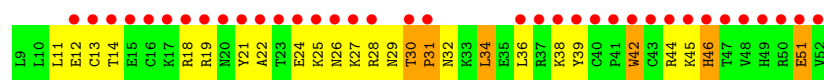
- Molecule 50: 50S ribosomal protein L32

Chain D2: 



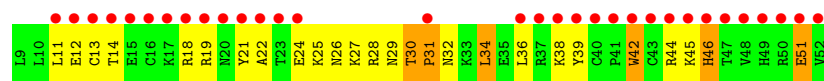
- Molecule 51: 50S ribosomal protein L33

Chain B3: 



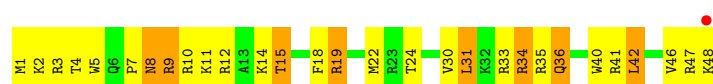
- Molecule 51: 50S ribosomal protein L33

Chain D3: 



- Molecule 52: 50S ribosomal protein L34

Chain B4: 



- Molecule 52: 50S ribosomal protein L34

Chain D4:



- Molecule 53: 50S ribosomal protein L35

Chain B5:



- Molecule 53: 50S ribosomal protein L35

Chain D5:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.69Å 451.66Å 614.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.52 – 3.40 49.52 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.52-3.40) 97.6 (49.52-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.228 , 0.266 0.227 , 0.262	Depositor DCC
R_{free} test set	7701 reflections (1.00%)	DCC
Wilson B-factor (Å ²)	86.0	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 68.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 775950 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	282142	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.63	4/36238 (0.0%)	1.02	99/56561 (0.2%)
1	CA	0.57	0/36238	0.96	75/56561 (0.1%)
2	AB	0.31	0/1936	0.51	0/2609
2	CB	0.28	0/1936	0.50	0/2609
3	AC	0.31	0/1637	0.47	0/2205
3	CC	0.29	0/1637	0.47	0/2205
4	AD	0.41	0/1733	0.59	0/2318
4	CD	0.34	0/1733	0.56	0/2318
5	AE	0.41	0/1172	0.61	0/1576
5	CE	0.36	0/1172	0.57	0/1576
6	AF	0.33	0/856	0.57	0/1154
6	CF	0.37	0/856	0.59	0/1154
7	AG	0.27	0/1276	0.46	0/1709
7	CG	0.27	0/1276	0.46	0/1709
8	AH	0.39	0/1136	0.61	0/1527
8	CH	0.33	0/1136	0.58	0/1527
9	AI	0.29	0/1029	0.45	0/1378
9	CI	0.27	0/1029	0.45	0/1378
10	AJ	0.28	0/808	0.48	0/1085
10	CJ	0.27	0/808	0.46	0/1085
11	AK	0.39	0/900	0.59	0/1213
11	CK	0.41	0/900	0.61	0/1213
12	AL	0.47	0/987	0.70	1/1320 (0.1%)
12	CL	0.44	0/987	0.68	0/1320
13	AM	0.25	0/939	0.44	0/1258
13	CM	0.24	0/939	0.44	0/1258
14	AN	0.31	0/501	0.50	0/664
14	CN	0.31	0/501	0.52	0/664
15	AO	0.39	0/745	0.57	0/992
15	CO	0.37	0/745	0.56	0/992
16	AP	0.42	0/717	0.62	0/963
16	CP	0.34	0/717	0.59	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.43	0/837	0.60	0/1117
17	CQ	0.37	0/837	0.56	0/1117
18	AR	0.38	0/579	0.61	0/768
18	CR	0.37	0/579	0.60	0/768
19	AS	0.25	0/643	0.43	0/865
19	CS	0.25	0/643	0.42	0/865
20	AT	0.38	0/764	0.57	0/1006
20	CT	0.33	0/764	0.54	0/1006
21	AU	0.23	0/213	0.43	0/277
21	CU	0.24	0/213	0.42	0/277
22	AV	0.43	0/802	0.68	0/1245
22	CV	0.43	0/802	0.69	0/1245
23	BA	1.07	153/66570 (0.2%)	1.48	1344/103918 (1.3%)
23	DA	1.19	253/66575 (0.4%)	1.59	1756/103930 (1.7%)
24	BB	0.58	0/2853	1.00	9/4451 (0.2%)
24	DB	0.59	0/2853	1.04	3/4451 (0.1%)
25	BC	0.71	1/2155 (0.0%)	0.90	3/2905 (0.1%)
25	DC	0.74	1/2155 (0.0%)	0.91	5/2905 (0.2%)
26	BD	0.58	0/1597	0.77	0/2153
26	DD	0.62	1/1597 (0.1%)	0.81	0/2153
27	BE	0.63	0/1622	0.77	0/2194
27	DE	0.67	0/1622	0.78	0/2194
28	BF	0.28	0/1500	0.49	0/2017
28	DF	0.28	0/1500	0.49	0/2017
29	BG	0.32	0/1246	0.58	0/1682
29	DG	0.44	0/1246	0.64	0/1682
30	BH	0.33	0/1148	0.56	0/1552
30	DH	0.38	0/1148	0.56	0/1552
31	BI	0.25	0/252	0.44	0/333
31	DI	0.27	0/252	0.46	0/333
32	BJ	0.56	0/1124	0.75	0/1515
32	DJ	0.59	0/1124	0.76	0/1515
33	BK	0.57	0/942	0.76	0/1268
33	DK	0.61	0/942	0.77	0/1268
34	BL	0.74	1/1131 (0.1%)	1.01	1/1504 (0.1%)
34	DL	0.75	2/1131 (0.2%)	1.03	5/1504 (0.3%)
35	BM	0.61	0/1099	0.83	2/1468 (0.1%)
35	DM	0.60	0/1099	0.83	1/1468 (0.1%)
36	BN	0.59	0/974	0.85	0/1302
36	DN	0.59	0/974	0.83	1/1302 (0.1%)
37	BO	0.36	0/779	0.58	0/1036
37	DO	0.39	0/779	0.61	0/1036
38	BP	0.50	0/1158	0.68	0/1544

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DP	0.51	0/1158	0.69	0/1544
39	BQ	0.63	0/970	0.81	0/1290
39	DQ	0.67	0/970	0.81	0/1290
40	BR	0.58	0/790	0.73	1/1057 (0.1%)
40	DR	0.61	0/790	0.74	1/1057 (0.1%)
41	BS	0.63	0/902	0.78	0/1209
41	DS	0.66	0/902	0.76	0/1209
42	BT	0.64	0/740	0.79	0/993
42	DT	0.74	0/740	0.84	0/993
43	BU	0.53	0/789	0.76	0/1051
43	DU	0.56	0/789	0.76	0/1051
44	BV	0.36	0/1524	0.57	0/2068
44	DV	0.38	0/1524	0.57	0/2068
45	BW	0.50	0/613	0.71	0/816
45	DW	0.52	0/613	0.72	0/816
46	BX	0.73	0/702	0.98	2/932 (0.2%)
46	DX	0.82	0/702	1.04	2/932 (0.2%)
47	BY	0.55	0/523	0.87	1/690 (0.1%)
47	DY	0.72	0/523	0.98	3/690 (0.4%)
48	BZ	0.52	0/473	0.68	0/634
48	DZ	0.50	0/473	0.65	0/634
49	B1	0.23	0/229	0.40	0/309
49	D1	0.22	0/229	0.41	0/309
50	B2	0.61	0/419	0.80	0/567
50	D2	0.58	0/419	0.79	0/567
51	B3	0.28	0/388	0.46	0/518
51	D3	0.27	0/388	0.46	0/518
52	B4	0.72	0/427	0.89	0/561
52	D4	0.84	0/427	1.05	1/561 (0.2%)
53	B5	0.68	0/516	0.88	0/679
53	D5	0.69	0/516	0.88	1/679 (0.1%)
All	All	0.85	416/305211 (0.1%)	1.21	3317/456064 (0.7%)

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
25	DC	0	1
27	BE	0	1
27	DE	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
34	BL	0	5
34	DL	0	5
35	BM	0	1
35	DM	0	1
36	BN	0	1
36	DN	0	1
39	BQ	0	2
39	DQ	0	2
All	All	0	21

The worst 5 of 416 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	DA	774	A	N9-C4	-13.87	1.29	1.37
23	DA	1332	G	N9-C4	-11.99	1.28	1.38
23	DA	1602	U	C4-O4	11.31	1.32	1.23
23	BA	1332	G	N9-C4	-11.02	1.29	1.38
23	DA	2249	U	C4-O4	10.67	1.32	1.23

The worst 5 of 3317 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DA	761	A	N1-C6-N6	30.82	137.09	118.60
23	BA	761	A	N1-C6-N6	25.08	133.65	118.60
23	DA	1332	G	N3-C4-N9	-24.42	111.35	126.00
23	DA	1332	G	N3-C4-C5	23.85	140.52	128.60
23	BA	1332	G	N3-C4-N9	-22.46	112.52	126.00

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	BE	47	GLY	Peptide
34	BL	29	LYS	Peptide
34	BL	37	GLY	Peptide
34	BL	39	LYS	Peptide
34	BL	9	ASN	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	32372	0	16339	1680	0
1	CA	32372	0	16339	1784	0
2	AB	1901	0	1951	173	0
2	CB	1901	0	1951	180	0
3	AC	1613	0	1677	180	0
3	CC	1613	0	1677	186	0
4	AD	1703	0	1764	192	0
4	CD	1703	0	1764	182	1
5	AE	1156	0	1213	141	0
5	CE	1156	0	1213	141	0
6	AF	843	0	857	96	1
6	CF	843	0	857	93	0
7	AG	1257	0	1296	95	0
7	CG	1257	0	1296	92	0
8	AH	1116	0	1177	133	0
8	CH	1116	0	1177	140	0
9	AI	1011	0	1043	100	0
9	CI	1011	0	1043	112	0
10	AJ	795	0	840	93	0
10	CJ	795	0	840	92	0
11	AK	885	0	904	76	0
11	CK	885	0	904	72	0
12	AL	971	0	1057	126	0
12	CL	971	0	1057	139	0
13	AM	929	0	987	83	0
13	CM	929	0	987	83	0
14	AN	492	0	530	49	0
14	CN	492	0	532	61	0
15	AO	734	0	771	66	0
15	CO	734	0	771	60	0
16	AP	701	0	720	96	0
16	CP	701	0	720	90	0
17	AQ	824	0	893	66	0
17	CQ	824	0	893	77	0
18	AR	574	0	644	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	CR	574	0	644	70	0
19	AS	630	0	652	70	0
19	CS	630	0	652	60	0
20	AT	762	0	859	64	0
20	CT	762	0	859	70	0
21	AU	209	0	221	16	0
21	CU	209	0	221	17	0
22	AV	719	0	366	58	0
22	CV	719	0	366	57	0
23	BA	59440	0	29964	2618	0
23	DA	59442	0	29965	2593	0
24	BB	2551	0	1295	147	0
24	DB	2551	0	1295	148	0
25	BC	2105	0	2182	353	0
25	DC	2105	0	2182	347	0
26	BD	1564	0	1629	224	0
26	DD	1564	0	1629	224	0
27	BE	1587	0	1632	147	0
27	DE	1587	0	1632	155	0
28	BF	1475	0	1537	155	0
28	DF	1475	0	1537	150	0
29	BG	1223	0	1282	114	0
29	DG	1223	0	1282	121	0
30	BH	1133	0	1220	131	0
30	DH	1133	0	1220	133	0
31	BI	254	0	275	8	0
31	DI	254	0	275	8	0
32	BJ	1097	0	1168	170	0
32	DJ	1097	0	1168	158	0
33	BK	932	0	994	97	0
33	DK	932	0	994	100	0
34	BL	1114	0	1187	270	0
34	DL	1114	0	1187	279	0
35	BM	1079	0	1127	170	0
35	DM	1079	0	1127	172	0
36	BN	960	0	1021	153	0
36	DN	960	0	1021	142	0
37	BO	771	0	832	95	0
37	DO	771	0	832	100	0
38	BP	1144	0	1211	129	0
38	DP	1144	0	1211	132	0
39	BQ	953	0	1013	150	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	DQ	953	0	1013	155	0
40	BR	779	0	852	131	0
40	DR	779	0	852	128	0
41	BS	891	0	951	106	0
41	DS	891	0	951	110	0
42	BT	726	0	778	88	0
42	DT	726	0	778	92	0
43	BU	776	0	870	138	0
43	DU	776	0	870	139	0
44	BV	1492	0	1513	174	0
44	DV	1492	0	1513	171	0
45	BW	605	0	628	71	0
45	DW	605	0	628	63	0
46	BX	695	0	764	112	0
46	DX	695	0	764	106	0
47	BY	521	0	575	81	0
47	DY	521	0	575	81	0
48	BZ	468	0	523	46	0
48	DZ	468	0	523	46	0
49	B1	226	0	225	23	0
49	D1	226	0	225	24	0
50	B2	405	0	420	61	0
50	D2	405	0	420	64	0
51	B3	381	0	391	25	0
51	D3	381	0	391	26	0
52	B4	419	0	467	50	0
52	D4	419	0	467	48	0
53	B5	508	0	576	111	0
53	D5	508	0	576	110	0
54	AA	163	0	0	0	0
54	AD	1	0	0	0	0
54	AV	4	0	0	0	0
54	B2	1	0	0	0	0
54	BA	408	0	0	0	0
54	BB	17	0	0	0	0
54	BK	1	0	0	0	0
54	CA	140	0	0	0	0
54	CP	1	0	0	0	0
54	CV	1	0	0	0	0
54	D2	1	0	0	0	0
54	D4	1	0	0	0	0
54	DA	436	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	DB	17	0	0	0	0
54	DE	1	0	0	0	0
54	DG	1	0	0	0	0
55	AD	1	0	0	0	0
55	AN	1	0	0	0	0
55	CD	1	0	0	0	0
55	CN	1	0	0	0	0
All	All	282142	0	191729	18333	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 39.

The worst 5 of 18333 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
34:DL:59:LEU:HA	34:DL:61:ARG:NE	1.55	1.20
34:DL:57:THR:HG23	34:DL:59:LEU:HD22	1.22	1.20
35:BM:81:VAL:O	35:BM:82:ARG:HG2	1.39	1.19
34:BL:57:THR:HG23	34:BL:59:LEU:HD22	1.21	1.19
52:D4:8:ASN:C	52:D4:8:ASN:HD22	1.42	1.18

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:AF:15:ASP:OD1	4:CD:20:TYR:OH[4_555]	2.18	0.02

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	232/234 (99%)	172 (74%)	40 (17%)	20 (9%)	1	17
2	CB	232/234 (99%)	173 (75%)	38 (16%)	21 (9%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	204/206 (99%)	136 (67%)	43 (21%)	25 (12%)	1	8
3	CC	204/206 (99%)	134 (66%)	45 (22%)	25 (12%)	1	8
4	AD	206/208 (99%)	152 (74%)	38 (18%)	16 (8%)	1	20
4	CD	206/208 (99%)	151 (73%)	40 (19%)	15 (7%)	2	22
5	AE	149/151 (99%)	103 (69%)	34 (23%)	12 (8%)	1	19
5	CE	149/151 (99%)	104 (70%)	34 (23%)	11 (7%)	2	22
6	AF	99/101 (98%)	71 (72%)	17 (17%)	11 (11%)	1	10
6	CF	99/101 (98%)	71 (72%)	18 (18%)	10 (10%)	1	12
7	AG	153/155 (99%)	121 (79%)	27 (18%)	5 (3%)	6	50
7	CG	153/155 (99%)	121 (79%)	27 (18%)	5 (3%)	6	50
8	AH	136/138 (99%)	97 (71%)	29 (21%)	10 (7%)	2	22
8	CH	136/138 (99%)	98 (72%)	28 (21%)	10 (7%)	2	22
9	AI	125/127 (98%)	91 (73%)	31 (25%)	3 (2%)	9	58
9	CI	125/127 (98%)	89 (71%)	32 (26%)	4 (3%)	6	51
10	AJ	96/98 (98%)	72 (75%)	20 (21%)	4 (4%)	4	41
10	CJ	96/98 (98%)	74 (77%)	18 (19%)	4 (4%)	4	41
11	AK	117/119 (98%)	83 (71%)	29 (25%)	5 (4%)	4	40
11	CK	117/119 (98%)	82 (70%)	30 (26%)	5 (4%)	4	40
12	AL	122/124 (98%)	78 (64%)	28 (23%)	16 (13%)	0	7
12	CL	122/124 (98%)	80 (66%)	27 (22%)	15 (12%)	1	8
13	AM	114/116 (98%)	93 (82%)	17 (15%)	4 (4%)	6	48
13	CM	114/116 (98%)	93 (82%)	17 (15%)	4 (4%)	6	48
14	AN	58/60 (97%)	46 (79%)	9 (16%)	3 (5%)	3	32
14	CN	58/60 (97%)	46 (79%)	9 (16%)	3 (5%)	3	32
15	AO	86/88 (98%)	62 (72%)	17 (20%)	7 (8%)	1	19
15	CO	86/88 (98%)	61 (71%)	19 (22%)	6 (7%)	2	23
16	AP	81/83 (98%)	46 (57%)	24 (30%)	11 (14%)	0	6
16	CP	81/83 (98%)	46 (57%)	25 (31%)	10 (12%)	1	8
17	AQ	97/99 (98%)	74 (76%)	16 (16%)	7 (7%)	2	23
17	CQ	97/99 (98%)	75 (77%)	16 (16%)	6 (6%)	2	27
18	AR	68/70 (97%)	40 (59%)	19 (28%)	9 (13%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CR	68/70 (97%)	41 (60%)	18 (26%)	9 (13%)	0	7
19	AS	76/78 (97%)	51 (67%)	21 (28%)	4 (5%)	3	32
19	CS	76/78 (97%)	50 (66%)	21 (28%)	5 (7%)	2	25
20	AT	97/99 (98%)	67 (69%)	23 (24%)	7 (7%)	2	23
20	CT	97/99 (98%)	67 (69%)	23 (24%)	7 (7%)	2	23
21	AU	22/24 (92%)	13 (59%)	8 (36%)	1 (4%)	4	38
21	CU	22/24 (92%)	13 (59%)	8 (36%)	1 (4%)	4	38
25	BC	269/271 (99%)	213 (79%)	36 (13%)	20 (7%)	2	22
25	DC	269/271 (99%)	210 (78%)	39 (14%)	20 (7%)	2	22
26	BD	202/204 (99%)	154 (76%)	34 (17%)	14 (7%)	2	24
26	DD	202/204 (99%)	155 (77%)	32 (16%)	15 (7%)	2	22
27	BE	200/202 (99%)	152 (76%)	32 (16%)	16 (8%)	1	19
27	DE	200/202 (99%)	155 (78%)	30 (15%)	15 (8%)	2	22
28	BF	179/181 (99%)	136 (76%)	31 (17%)	12 (7%)	2	25
28	DF	179/181 (99%)	136 (76%)	31 (17%)	12 (7%)	2	25
29	BG	157/159 (99%)	112 (71%)	35 (22%)	10 (6%)	2	26
29	DG	157/159 (99%)	111 (71%)	36 (23%)	10 (6%)	2	26
30	BH	143/145 (99%)	95 (66%)	29 (20%)	19 (13%)	0	7
30	DH	143/145 (99%)	91 (64%)	31 (22%)	21 (15%)	0	5
31	BI	28/65 (43%)	25 (89%)	3 (11%)	0	100	100
31	DI	28/65 (43%)	25 (89%)	3 (11%)	0	100	100
32	BJ	135/137 (98%)	97 (72%)	26 (19%)	12 (9%)	1	16
32	DJ	135/137 (98%)	97 (72%)	24 (18%)	14 (10%)	1	11
33	BK	120/122 (98%)	100 (83%)	11 (9%)	9 (8%)	2	22
33	DK	120/122 (98%)	98 (82%)	14 (12%)	8 (7%)	2	25
34	BL	144/146 (99%)	87 (60%)	31 (22%)	26 (18%)	0	3
34	DL	144/146 (99%)	86 (60%)	35 (24%)	23 (16%)	0	4
35	BM	134/136 (98%)	86 (64%)	28 (21%)	20 (15%)	0	4
35	DM	134/136 (98%)	86 (64%)	30 (22%)	18 (13%)	0	6
36	BN	115/117 (98%)	91 (79%)	13 (11%)	11 (10%)	1	14
36	DN	115/117 (98%)	90 (78%)	15 (13%)	10 (9%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	96/98 (98%)	57 (59%)	23 (24%)	16 (17%)	0	4
37	DO	96/98 (98%)	54 (56%)	25 (26%)	17 (18%)	0	3
38	BP	135/137 (98%)	101 (75%)	18 (13%)	16 (12%)	1	9
38	DP	135/137 (98%)	100 (74%)	19 (14%)	16 (12%)	1	9
39	BQ	114/116 (98%)	78 (68%)	22 (19%)	14 (12%)	1	8
39	DQ	114/116 (98%)	82 (72%)	20 (18%)	12 (10%)	1	11
40	BR	99/101 (98%)	70 (71%)	20 (20%)	9 (9%)	1	15
40	DR	99/101 (98%)	70 (71%)	20 (20%)	9 (9%)	1	15
41	BS	110/112 (98%)	88 (80%)	17 (16%)	5 (4%)	4	38
41	DS	110/112 (98%)	87 (79%)	17 (16%)	6 (6%)	3	31
42	BT	90/92 (98%)	69 (77%)	16 (18%)	5 (6%)	3	30
42	DT	90/92 (98%)	67 (74%)	18 (20%)	5 (6%)	3	30
43	BU	98/100 (98%)	55 (56%)	24 (24%)	19 (19%)	0	2
43	DU	98/100 (98%)	58 (59%)	21 (21%)	19 (19%)	0	2
44	BV	186/188 (99%)	135 (73%)	34 (18%)	17 (9%)	1	15
44	DV	186/188 (99%)	135 (73%)	34 (18%)	17 (9%)	1	15
45	BW	74/76 (97%)	61 (82%)	10 (14%)	3 (4%)	4	42
45	DW	74/76 (97%)	60 (81%)	10 (14%)	4 (5%)	3	31
46	BX	86/88 (98%)	57 (66%)	16 (19%)	13 (15%)	0	4
46	DX	86/88 (98%)	54 (63%)	19 (22%)	13 (15%)	0	4
47	BY	60/62 (97%)	45 (75%)	8 (13%)	7 (12%)	1	9
47	DY	60/62 (97%)	41 (68%)	12 (20%)	7 (12%)	1	9
48	BZ	57/59 (97%)	49 (86%)	7 (12%)	1 (2%)	13	65
48	DZ	57/59 (97%)	50 (88%)	6 (10%)	1 (2%)	13	65
49	B1	28/30 (93%)	15 (54%)	7 (25%)	6 (21%)	0	2
49	D1	28/30 (93%)	15 (54%)	7 (25%)	6 (21%)	0	2
50	B2	50/52 (96%)	40 (80%)	6 (12%)	4 (8%)	1	19
50	D2	50/52 (96%)	39 (78%)	7 (14%)	4 (8%)	1	19
51	B3	42/44 (96%)	26 (62%)	11 (26%)	5 (12%)	1	9
51	D3	42/44 (96%)	26 (62%)	11 (26%)	5 (12%)	1	9
52	B4	46/48 (96%)	42 (91%)	3 (6%)	1 (2%)	10	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	D4	46/48 (96%)	42 (91%)	3 (6%)	1 (2%)	10	60
53	B5	61/63 (97%)	43 (70%)	12 (20%)	6 (10%)	1	13
53	D5	61/63 (97%)	44 (72%)	10 (16%)	7 (12%)	1	9
All	All	11192/11458 (98%)	8080 (72%)	2125 (19%)	987 (9%)	1	16

5 of 987 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	204	ASN
3	AC	189	ALA
3	AC	196	LEU
4	AD	28	SER
4	AD	30	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	202/202 (100%)	178 (88%)	24 (12%)	8	36
2	CB	202/202 (100%)	179 (89%)	23 (11%)	8	38
3	AC	160/160 (100%)	146 (91%)	14 (9%)	14	55
3	CC	160/160 (100%)	145 (91%)	15 (9%)	13	50
4	AD	180/180 (100%)	150 (83%)	30 (17%)	3	19
4	CD	180/180 (100%)	150 (83%)	30 (17%)	3	19
5	AE	116/116 (100%)	92 (79%)	24 (21%)	2	8
5	CE	116/116 (100%)	94 (81%)	22 (19%)	2	11
6	AF	90/90 (100%)	82 (91%)	8 (9%)	14	55
6	CF	90/90 (100%)	83 (92%)	7 (8%)	18	62
7	AG	126/126 (100%)	121 (96%)	5 (4%)	42	84
7	CG	126/126 (100%)	121 (96%)	5 (4%)	42	84
8	AH	119/119 (100%)	102 (86%)	17 (14%)	5	27
8	CH	119/119 (100%)	104 (87%)	15 (13%)	7	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	AI	98/98 (100%)	88 (90%)	10 (10%)	11	46
9	CI	98/98 (100%)	88 (90%)	10 (10%)	11	46
10	AJ	88/88 (100%)	78 (89%)	10 (11%)	8	38
10	CJ	88/88 (100%)	78 (89%)	10 (11%)	8	38
11	AK	90/90 (100%)	75 (83%)	15 (17%)	3	19
11	CK	90/90 (100%)	76 (84%)	14 (16%)	4	23
12	AL	104/104 (100%)	83 (80%)	21 (20%)	2	9
12	CL	104/104 (100%)	83 (80%)	21 (20%)	2	9
13	AM	94/94 (100%)	87 (93%)	7 (7%)	20	65
13	CM	94/94 (100%)	87 (93%)	7 (7%)	20	65
14	AN	49/49 (100%)	45 (92%)	4 (8%)	17	60
14	CN	49/49 (100%)	45 (92%)	4 (8%)	17	60
15	AO	79/79 (100%)	69 (87%)	10 (13%)	6	33
15	CO	79/79 (100%)	69 (87%)	10 (13%)	6	33
16	AP	72/72 (100%)	57 (79%)	15 (21%)	2	8
16	CP	72/72 (100%)	56 (78%)	16 (22%)	1	7
17	AQ	94/94 (100%)	78 (83%)	16 (17%)	3	18
17	CQ	94/94 (100%)	79 (84%)	15 (16%)	3	21
18	AR	61/61 (100%)	58 (95%)	3 (5%)	35	79
18	CR	61/61 (100%)	58 (95%)	3 (5%)	35	79
19	AS	69/69 (100%)	60 (87%)	9 (13%)	6	31
19	CS	69/69 (100%)	60 (87%)	9 (13%)	6	31
20	AT	76/76 (100%)	65 (86%)	11 (14%)	5	26
20	CT	76/76 (100%)	65 (86%)	11 (14%)	5	26
21	AU	19/19 (100%)	19 (100%)	0	100	100
21	CU	19/19 (100%)	19 (100%)	0	100	100
25	BC	213/213 (100%)	164 (77%)	49 (23%)	1	6
25	DC	213/213 (100%)	162 (76%)	51 (24%)	1	5
26	BD	165/165 (100%)	129 (78%)	36 (22%)	1	7
26	DD	165/165 (100%)	129 (78%)	36 (22%)	1	7
27	BE	161/161 (100%)	124 (77%)	37 (23%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	DE	161/161 (100%)	124 (77%)	37 (23%)	1	6
28	BF	155/155 (100%)	132 (85%)	23 (15%)	4	25
28	DF	155/155 (100%)	134 (86%)	21 (14%)	6	29
29	BG	132/132 (100%)	108 (82%)	24 (18%)	2	13
29	DG	132/132 (100%)	107 (81%)	25 (19%)	2	12
30	BH	122/122 (100%)	103 (84%)	19 (16%)	4	23
30	DH	122/122 (100%)	103 (84%)	19 (16%)	4	23
31	BI	27/53 (51%)	25 (93%)	2 (7%)	20	65
31	DI	27/53 (51%)	25 (93%)	2 (7%)	20	65
32	BJ	116/116 (100%)	84 (72%)	32 (28%)	0	3
32	DJ	116/116 (100%)	85 (73%)	31 (27%)	1	4
33	BK	100/100 (100%)	78 (78%)	22 (22%)	1	7
33	DK	100/100 (100%)	78 (78%)	22 (22%)	1	7
34	BL	112/112 (100%)	75 (67%)	37 (33%)	0	2
34	DL	112/112 (100%)	76 (68%)	36 (32%)	0	2
35	BM	106/106 (100%)	82 (77%)	24 (23%)	1	6
35	DM	106/106 (100%)	81 (76%)	25 (24%)	1	6
36	BN	100/100 (100%)	75 (75%)	25 (25%)	1	5
36	DN	100/100 (100%)	76 (76%)	24 (24%)	1	5
37	BO	77/77 (100%)	63 (82%)	14 (18%)	2	13
37	DO	77/77 (100%)	63 (82%)	14 (18%)	2	13
38	BP	121/121 (100%)	96 (79%)	25 (21%)	2	8
38	DP	121/121 (100%)	94 (78%)	27 (22%)	1	7
39	BQ	92/92 (100%)	71 (77%)	21 (23%)	1	6
39	DQ	92/92 (100%)	71 (77%)	21 (23%)	1	6
40	BR	82/82 (100%)	63 (77%)	19 (23%)	1	6
40	DR	82/82 (100%)	61 (74%)	21 (26%)	1	4
41	BS	91/91 (100%)	65 (71%)	26 (29%)	0	3
41	DS	91/91 (100%)	65 (71%)	26 (29%)	0	3
42	BT	74/74 (100%)	60 (81%)	14 (19%)	2	12
42	DT	74/74 (100%)	60 (81%)	14 (19%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	BU	84/84 (100%)	66 (79%)	18 (21%)	1	8
43	DU	84/84 (100%)	67 (80%)	17 (20%)	2	9
44	BV	163/163 (100%)	142 (87%)	21 (13%)	6	32
44	DV	163/163 (100%)	141 (86%)	22 (14%)	6	29
45	BW	61/61 (100%)	52 (85%)	9 (15%)	4	25
45	DW	61/61 (100%)	53 (87%)	8 (13%)	6	31
46	BX	73/73 (100%)	50 (68%)	23 (32%)	0	3
46	DX	73/73 (100%)	50 (68%)	23 (32%)	0	3
47	BY	58/58 (100%)	46 (79%)	12 (21%)	2	8
47	DY	58/58 (100%)	46 (79%)	12 (21%)	2	8
48	BZ	51/51 (100%)	43 (84%)	8 (16%)	4	23
48	DZ	51/51 (100%)	43 (84%)	8 (16%)	4	23
49	B1	27/27 (100%)	26 (96%)	1 (4%)	45	85
49	D1	27/27 (100%)	26 (96%)	1 (4%)	45	85
50	B2	45/45 (100%)	40 (89%)	5 (11%)	9	40
50	D2	45/45 (100%)	39 (87%)	6 (13%)	6	30
51	B3	43/43 (100%)	38 (88%)	5 (12%)	8	37
51	D3	43/43 (100%)	38 (88%)	5 (12%)	8	37
52	B4	41/41 (100%)	29 (71%)	12 (29%)	0	3
52	D4	41/41 (100%)	28 (68%)	13 (32%)	0	3
53	B5	53/53 (100%)	42 (79%)	11 (21%)	2	8
53	D5	53/53 (100%)	43 (81%)	10 (19%)	2	12
All	All	9462/9514 (100%)	7811 (83%)	1651 (17%)	3	16

5 of 1651 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	BW	63	VAL
7	CG	67	GLU
42	DT	81	VAL
46	BX	73	LEU
2	CB	117	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 245 such sidechains are listed below:

Mol	Chain	Res	Type
46	BX	45	ASN
7	CG	13	GLN
44	DV	121	HIS
47	BY	56	GLN
2	CB	37	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1505/1506 (99%)	293 (19%)	14 (0%)
1	CA	1505/1506 (99%)	294 (19%)	14 (0%)
22	AV	32/43 (74%)	3 (9%)	0
22	CV	32/43 (74%)	3 (9%)	0
23	BA	2755/2879 (95%)	584 (21%)	27 (0%)
23	DA	2757/2879 (95%)	589 (21%)	29 (1%)
24	BB	118/119 (99%)	26 (22%)	0
24	DB	118/119 (99%)	27 (22%)	0
All	All	8822/9094 (97%)	1819 (20%)	84 (0%)

5 of 1819 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	13	U
1	AA	14	U

5 of 84 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BA	2433	A
1	CA	793	U
23	DA	2272	U
23	BA	2542	A
1	CA	327	A

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 1198 ligands modelled in this entry, 1198 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	AA	1506/1506 (100%)	0.17	39 (2%)	53	21	51, 122, 245, 498	0
1	CA	1506/1506 (100%)	0.24	58 (3%)	37	14	51, 126, 251, 414	0
2	AB	234/234 (100%)	0.61	24 (10%)	7	4	113, 174, 244, 298	0
2	CB	234/234 (100%)	0.56	14 (5%)	21	8	111, 177, 259, 325	0
3	AC	206/206 (100%)	0.44	13 (6%)	19	8	106, 160, 225, 263	0
3	CC	206/206 (100%)	0.52	13 (6%)	19	8	105, 161, 226, 271	0
4	AD	208/208 (100%)	0.31	1 (0%)	88	61	90, 142, 199, 247	0
4	CD	208/208 (100%)	0.77	15 (7%)	15	6	94, 146, 220, 300	0
5	AE	151/151 (100%)	0.20	2 (1%)	74	37	73, 114, 172, 272	0
5	CE	151/151 (100%)	0.34	2 (1%)	74	37	73, 117, 188, 252	0
6	AF	101/101 (100%)	0.44	3 (2%)	48	20	83, 135, 192, 270	0
6	CF	101/101 (100%)	0.13	2 (1%)	62	28	79, 131, 184, 246	0
7	AG	155/155 (100%)	0.85	17 (10%)	6	4	118, 187, 237, 333	0
7	CG	155/155 (100%)	1.13	30 (19%)	2	2	119, 187, 237, 286	0
8	AH	138/138 (100%)	0.31	4 (2%)	49	21	77, 121, 166, 199	0
8	CH	138/138 (100%)	0.46	6 (4%)	34	13	81, 123, 167, 219	0
9	AI	127/127 (100%)	1.24	28 (22%)	1	2	119, 225, 289, 345	0
9	CI	127/127 (100%)	1.06	18 (14%)	3	2	121, 225, 286, 354	0
10	AJ	98/98 (100%)	1.18	16 (16%)	2	2	118, 198, 278, 356	0
10	CJ	98/98 (100%)	1.11	16 (16%)	2	2	122, 197, 264, 351	0
11	AK	119/119 (100%)	0.27	5 (4%)	35	13	71, 111, 171, 263	0
11	CK	119/119 (100%)	0.17	5 (4%)	35	13	74, 111, 178, 264	0
12	AL	124/124 (100%)	0.30	2 (1%)	68	32	67, 107, 165, 268	0
12	CL	124/124 (100%)	0.53	6 (4%)	29	12	70, 109, 178, 252	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	116/116 (100%)	0.81	12 (10%) 7 4	134, 213, 299, 335	0
13	CM	116/116 (100%)	1.42	31 (26%) 1 1	135, 214, 309, 362	0
14	AN	60/60 (100%)	0.85	7 (11%) 5 3	114, 166, 217, 235	0
14	CN	60/60 (100%)	0.85	4 (6%) 17 7	116, 167, 227, 281	0
15	AO	88/88 (100%)	0.15	0 100 100	66, 108, 159, 227	0
15	CO	88/88 (100%)	0.20	0 100 100	67, 110, 166, 241	0
16	AP	83/83 (100%)	0.30	0 100 100	84, 118, 174, 214	0
16	CP	83/83 (100%)	1.27	15 (18%) 2 2	87, 123, 177, 210	0
17	AQ	99/99 (100%)	0.14	0 100 100	78, 112, 169, 216	0
17	CQ	99/99 (100%)	0.67	5 (5%) 27 10	79, 116, 166, 215	0
18	AR	70/70 (100%)	0.69	5 (7%) 16 6	84, 128, 183, 284	0
18	CR	70/70 (100%)	0.32	2 (2%) 49 21	82, 128, 192, 232	0
19	AS	78/78 (100%)	1.59	25 (32%) 1 1	152, 210, 275, 321	0
19	CS	78/78 (100%)	1.88	25 (32%) 1 1	151, 216, 291, 350	0
20	AT	99/99 (100%)	0.47	1 (1%) 79 44	86, 134, 203, 241	0
20	CT	99/99 (100%)	0.87	11 (11%) 6 3	92, 136, 212, 269	0
21	AU	24/24 (100%)	2.04	11 (45%) 1 1	160, 225, 264, 322	0
21	CU	24/24 (100%)	2.32	13 (54%) 0 1	163, 218, 265, 364	0
22	AV	34/43 (79%)	1.21	8 (23%) 1 2	89, 196, 324, 362	0
22	CV	34/43 (79%)	1.87	11 (32%) 1 1	92, 198, 333, 339	0
23	BA	2760/2879 (95%)	-0.15	43 (1%) 68 32	27, 65, 180, 398	0
23	DA	2760/2879 (95%)	-0.11	35 (1%) 74 37	25, 63, 178, 410	0
24	BB	119/119 (100%)	0.09	5 (4%) 35 13	77, 129, 182, 232	0
24	DB	119/119 (100%)	0.06	4 (3%) 43 17	78, 129, 184, 236	0
25	BC	271/271 (100%)	-0.04	3 (1%) 77 40	25, 58, 109, 175	0
25	DC	271/271 (100%)	-0.07	0 100 100	18, 57, 109, 177	0
26	BD	204/204 (100%)	0.20	2 (0%) 79 44	36, 73, 146, 341	0
26	DD	204/204 (100%)	0.17	1 (0%) 88 61	33, 71, 145, 347	0
27	BE	202/202 (100%)	-0.11	0 100 100	31, 73, 155, 246	0
27	DE	202/202 (100%)	0.08	2 (0%) 79 44	25, 73, 155, 192	0
28	BF	181/181 (100%)	0.87	25 (13%) 4 2	102, 182, 254, 314	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DF	181/181 (100%)	0.83	26 (14%) 3 2	104, 185, 268, 331	0
29	BG	159/159 (100%)	0.99	29 (18%) 2 2	85, 143, 221, 343	0
29	DG	159/159 (100%)	0.41	6 (3%) 38 15	79, 136, 186, 235	0
30	BH	145/145 (100%)	1.92	43 (29%) 1 1	67, 243, 391, 482	0
30	DH	145/145 (100%)	1.10	29 (20%) 2 2	64, 236, 379, 480	0
31	BI	32/65 (49%)	3.68	26 (81%) 0 0	171, 246, 347, 355	0
31	DI	32/65 (49%)	2.07	20 (62%) 0 0	168, 253, 310, 334	0
32	BJ	137/137 (100%)	0.06	0 100 100	51, 81, 142, 201	0
32	DJ	137/137 (100%)	-0.06	0 100 100	52, 81, 146, 194	0
33	BK	122/122 (100%)	0.04	0 100 100	42, 70, 111, 150	0
33	DK	122/122 (100%)	0.08	0 100 100	41, 69, 111, 162	0
34	BL	146/146 (100%)	0.29	2 (1%) 72 35	34, 97, 166, 309	0
34	DL	146/146 (100%)	0.34	4 (2%) 52 21	32, 97, 163, 293	0
35	BM	136/136 (100%)	0.16	4 (2%) 49 21	49, 89, 199, 370	0
35	DM	136/136 (100%)	0.36	4 (2%) 49 21	48, 88, 205, 406	0
36	BN	117/117 (100%)	0.22	0 100 100	45, 73, 137, 249	0
36	DN	117/117 (100%)	0.14	0 100 100	43, 73, 134, 235	0
37	BO	98/98 (100%)	0.77	3 (3%) 47 19	82, 137, 197, 223	0
37	DO	98/98 (100%)	0.63	8 (8%) 12 6	80, 136, 190, 215	0
38	BP	137/137 (100%)	0.10	2 (1%) 70 33	58, 93, 185, 250	0
38	DP	137/137 (100%)	0.29	8 (5%) 22 8	55, 92, 190, 273	0
39	BQ	116/116 (100%)	-0.03	0 100 100	35, 75, 124, 239	0
39	DQ	116/116 (100%)	-0.14	0 100 100	26, 74, 126, 248	0
40	BR	101/101 (100%)	0.08	0 100 100	41, 105, 164, 264	0
40	DR	101/101 (100%)	0.29	0 100 100	41, 110, 156, 259	0
41	BS	112/112 (100%)	0.12	0 100 100	44, 59, 137, 254	0
41	DS	112/112 (100%)	0.01	0 100 100	43, 59, 134, 255	0
42	BT	92/92 (100%)	0.13	0 100 100	45, 77, 129, 170	0
42	DT	92/92 (100%)	0.13	0 100 100	36, 73, 127, 169	0
43	BU	100/100 (100%)	0.97	13 (13%) 4 2	62, 104, 257, 396	0
43	DU	100/100 (100%)	0.84	7 (7%) 16 6	61, 102, 251, 408	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BV	188/188 (100%)	0.46	10 (5%) 25 9	83, 138, 195, 245	0
44	DV	188/188 (100%)	0.19	1 (0%) 88 61	83, 139, 194, 230	0
45	BW	76/76 (100%)	0.31	0 100 100	58, 84, 139, 261	0
45	DW	76/76 (100%)	0.42	3 (3%) 37 14	59, 84, 135, 256	0
46	BX	88/88 (100%)	0.26	1 (1%) 77 40	37, 74, 153, 322	0
46	DX	88/88 (100%)	0.28	0 100 100	39, 70, 153, 326	0
47	BY	62/62 (100%)	0.34	5 (8%) 12 6	57, 98, 209, 292	0
47	DY	62/62 (100%)	0.49	4 (6%) 18 7	51, 96, 212, 328	0
48	BZ	59/59 (100%)	0.57	3 (5%) 27 10	43, 81, 156, 299	0
48	DZ	59/59 (100%)	0.93	5 (8%) 11 5	45, 85, 157, 305	0
49	B1	30/30 (100%)	1.46	10 (33%) 1 1	184, 253, 295, 311	0
49	D1	30/30 (100%)	1.57	10 (33%) 1 1	183, 261, 306, 358	0
50	B2	52/52 (100%)	0.31	4 (7%) 13 6	26, 71, 187, 233	0
50	D2	52/52 (100%)	-0.05	1 (1%) 64 29	21, 72, 197, 229	0
51	B3	44/44 (100%)	5.10	36 (81%) 0 0	139, 249, 299, 320	0
51	D3	44/44 (100%)	5.02	32 (72%) 0 0	141, 245, 312, 333	0
52	B4	48/48 (100%)	-0.02	1 (2%) 60 27	33, 43, 93, 194	0
52	D4	48/48 (100%)	-0.04	0 100 100	21, 41, 91, 200	0
53	B5	63/63 (100%)	0.16	0 100 100	45, 68, 131, 215	0
53	D5	63/63 (100%)	0.27	0 100 100	45, 70, 132, 216	0
All	All	20230/20552 (98%)	0.29	1005 (4%) 28 10	18, 104, 241, 498	0

The worst 5 of 1005 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AA	82	U	21.1
1	AA	85	U	17.8
51	D3	47	THR	15.8
51	B3	41	PRO	15.6
51	B3	13	CYS	14.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
54	MG	BA	3191	1/1	0.36	-	76,76,76,76	0
54	MG	DA	3144	1/1	0.24	-	72,72,72,72	0
54	MG	AA	1655	1/1	0.63	-	72,72,72,72	0
54	MG	DA	3076	1/1	0.16	-	63,63,63,63	0
54	MG	CA	1632	1/1	0.28	-	79,79,79,79	0
54	MG	DA	3195	1/1	0.25	-	51,51,51,51	0
54	MG	AA	1658	1/1	0.11	-	94,94,94,94	0
54	MG	AA	1641	1/1	0.39	-	85,85,85,85	0
54	MG	BA	3283	1/1	0.20	-	76,76,76,76	0
54	MG	BA	2912	1/1	0.66	-	36,36,36,36	0
54	MG	BA	3050	1/1	0.19	-	41,41,41,41	0
54	MG	DA	3095	1/1	0.17	-	67,67,67,67	0
54	MG	BA	3114	1/1	0.73	-	78,78,78,78	0
54	MG	DA	3099	1/1	0.15	-	81,81,81,81	0
54	MG	BA	2951	1/1	0.39	-	28,28,28,28	0
54	MG	BA	3200	1/1	0.32	-	64,64,64,64	0
54	MG	CA	1615	1/1	0.25	-	51,51,51,51	0
54	MG	AA	1731	1/1	0.32	-	76,76,76,76	0
54	MG	DA	3142	1/1	0.20	-	109,109,109,109	0
54	MG	DA	3128	1/1	0.24	-	114,114,114,114	0
54	MG	AD	302	1/1	0.17	-	87,87,87,87	0
54	MG	BB	212	1/1	0.14	-	89,89,89,89	0
54	MG	DA	3320	1/1	0.42	-	58,58,58,58	0
54	MG	AA	1718	1/1	0.62	-	98,98,98,98	0
54	MG	DA	3071	1/1	0.39	-	64,64,64,64	0
54	MG	BA	3135	1/1	0.14	-	77,77,77,77	0
54	MG	BA	3057	1/1	0.44	-	63,63,63,63	0
54	MG	DA	3209	1/1	0.61	-	80,80,80,80	0
54	MG	DA	3084	1/1	0.14	-	146,146,146,146	0
54	MG	DA	3040	1/1	0.34	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1640	1/1	0.48	-	106,106,106,106	0
54	MG	AA	1649	1/1	0.35	-	89,89,89,89	0
54	MG	BA	2965	1/1	0.26	-	47,47,47,47	0
54	MG	BA	3077	1/1	0.12	-	75,75,75,75	0
54	MG	AA	1629	1/1	0.35	-	72,72,72,72	0
54	MG	DA	2949	1/1	0.54	-	41,41,41,41	0
54	MG	DA	3323	1/1	0.30	-	69,69,69,69	0
54	MG	BA	3100	1/1	0.07	-	77,77,77,77	0
54	MG	CA	1663	1/1	0.31	-	86,86,86,86	0
54	MG	DA	3230	1/1	0.21	-	63,63,63,63	0
54	MG	DA	3306	1/1	0.35	-	51,51,51,51	0
54	MG	DA	3185	1/1	0.31	-	108,108,108,108	0
54	MG	DA	3025	1/1	0.19	-	69,69,69,69	0
54	MG	BA	3153	1/1	0.29	-	67,67,67,67	0
54	MG	AA	1738	1/1	0.33	-	70,70,70,70	0
54	MG	DA	2966	1/1	0.36	-	70,70,70,70	0
54	MG	CA	1646	1/1	0.14	-	78,78,78,78	0
54	MG	AA	1698	1/1	0.40	-	88,88,88,88	0
54	MG	CA	1659	1/1	0.30	-	71,71,71,71	0
54	MG	DA	3089	1/1	0.24	-	76,76,76,76	0
54	MG	BA	3024	1/1	0.50	-	67,67,67,67	0
54	MG	BA	3059	1/1	0.18	-	60,60,60,60	0
54	MG	DA	3220	1/1	0.29	-	70,70,70,70	0
54	MG	BA	3212	1/1	0.23	-	69,69,69,69	0
54	MG	BB	203	1/1	0.17	-	83,83,83,83	0
54	MG	DA	3105	1/1	0.52	-	75,75,75,75	0
54	MG	DA	3061	1/1	0.28	-	75,75,75,75	0
54	MG	BA	3088	1/1	0.56	-	73,73,73,73	0
54	MG	AA	1707	1/1	0.20	-	100,100,100,100	0
54	MG	AA	1666	1/1	0.07	-	100,100,100,100	0
54	MG	AA	1628	1/1	0.38	-	62,62,62,62	0
54	MG	BA	3284	1/1	0.59	-	85,85,85,85	0
54	MG	CA	1714	1/1	0.19	-	74,74,74,74	0
54	MG	BA	3020	1/1	0.28	-	62,62,62,62	0
54	MG	AA	1633	1/1	0.17	-	73,73,73,73	0
54	MG	BA	3123	1/1	0.37	-	52,52,52,52	0
54	MG	AA	1654	1/1	0.34	-	76,76,76,76	0
54	MG	DA	3094	1/1	0.28	-	76,76,76,76	0
54	MG	DA	3026	1/1	0.10	-	48,48,48,48	0
54	MG	DA	2993	1/1	0.06	-	69,69,69,69	0
54	MG	DA	3024	1/1	0.39	-	36,36,36,36	0
54	MG	DA	2955	1/1	0.42	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
54	MG	BA	2962	1/1	0.17	-	17,17,17,17	0
54	MG	CA	1648	1/1	0.34	-	64,64,64,64	0
54	MG	AA	1692	1/1	0.31	-	84,84,84,84	0
54	MG	BA	3223	1/1	0.28	-	54,54,54,54	0
54	MG	DA	3274	1/1	0.36	-	62,62,62,62	0
54	MG	BA	3106	1/1	0.20	-	70,70,70,70	0
54	MG	BA	3293	1/1	0.18	-	86,86,86,86	0
54	MG	CA	1703	1/1	0.42	-	108,108,108,108	0
54	MG	BA	3152	1/1	0.14	-	75,75,75,75	0
54	MG	DA	2994	1/1	0.15	-	67,67,67,67	0
54	MG	BB	201	1/1	0.35	-	56,56,56,56	0
54	MG	BA	3197	1/1	0.38	-	57,57,57,57	0
54	MG	DA	3235	1/1	0.73	-	90,90,90,90	0
54	MG	DA	3263	1/1	0.34	-	63,63,63,63	0
54	MG	CA	1620	1/1	0.14	-	79,79,79,79	0
54	MG	DA	3273	1/1	0.26	-	85,85,85,85	0
54	MG	BA	3091	1/1	0.42	-	56,56,56,56	0
54	MG	BA	2958	1/1	0.34	-	42,42,42,42	0
54	MG	DB	210	1/1	0.07	-	74,74,74,74	0
54	MG	BA	3304	1/1	0.06	-	124,124,124,124	0
54	MG	DA	3078	1/1	0.52	-	79,79,79,79	0
54	MG	BA	3263	1/1	0.27	-	80,80,80,80	0
54	MG	DA	3293	1/1	0.11	-	67,67,67,67	0
54	MG	BA	3267	1/1	0.47	-	86,86,86,86	0
54	MG	DA	3233	1/1	0.32	-	57,57,57,57	0
54	MG	BA	3214	1/1	0.38	-	53,53,53,53	0
54	MG	AA	1681	1/1	0.22	-	99,99,99,99	0
54	MG	BA	3090	1/1	0.43	-	69,69,69,69	0
54	MG	BB	211	1/1	0.48	-	112,112,112,112	0
54	MG	BA	2915	1/1	0.17	-	4,4,4,4	0
54	MG	BA	3301	1/1	0.71	-	66,66,66,66	0
54	MG	BA	3166	1/1	0.35	-	74,74,74,74	0
54	MG	AA	1700	1/1	0.62	-	98,98,98,98	0
54	MG	DA	2990	1/1	0.16	-	35,35,35,35	0
54	MG	CA	1666	1/1	0.06	-	116,116,116,116	0
54	MG	DA	2946	1/1	0.53	-	24,24,24,24	0
54	MG	AA	1626	1/1	0.17	-	62,62,62,62	0
54	MG	DA	3208	1/1	0.41	-	49,49,49,49	0
54	MG	BB	217	1/1	0.13	-	78,78,78,78	0
54	MG	DA	3250	1/1	0.33	-	74,74,74,74	0
54	MG	BA	3206	1/1	0.10	-	60,60,60,60	0
54	MG	CA	1644	1/1	0.45	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1633	1/1	0.55	-	102,102,102,102	0
54	MG	BA	2903	1/1	0.39	-	14,14,14,14	0
54	MG	BA	3189	1/1	0.45	-	88,88,88,88	0
54	MG	AA	1603	1/1	0.33	-	35,35,35,35	0
54	MG	CA	1670	1/1	0.48	-	128,128,128,128	0
54	MG	BA	3036	1/1	0.13	-	92,92,92,92	0
54	MG	BA	3201	1/1	0.16	-	80,80,80,80	0
54	MG	DA	3037	1/1	0.17	-	77,77,77,77	0
54	MG	BA	3219	1/1	0.80	-	66,66,66,66	0
54	MG	AA	1611	1/1	0.26	-	49,49,49,49	0
54	MG	AA	1704	1/1	0.15	-	81,81,81,81	0
54	MG	BA	2952	1/1	0.29	-	38,38,38,38	0
54	MG	CP	101	1/1	0.18	-	96,96,96,96	0
54	MG	AA	1751	1/1	0.17	-	72,72,72,72	0
54	MG	DA	3124	1/1	0.08	-	90,90,90,90	0
54	MG	CA	1699	1/1	0.74	-	71,71,71,71	0
54	MG	AA	1753	1/1	0.33	-	102,102,102,102	0
54	MG	AA	1716	1/1	0.18	-	120,120,120,120	0
54	MG	AA	1728	1/1	0.93	-	105,105,105,105	0
54	MG	DE	301	1/1	0.21	-	44,44,44,44	0
54	MG	DA	3023	1/1	0.30	-	49,49,49,49	0
54	MG	DA	3052	1/1	0.19	-	107,107,107,107	0
54	MG	CA	1735	1/1	0.25	-	61,61,61,61	0
54	MG	BA	3157	1/1	0.33	-	68,68,68,68	0
54	MG	CA	1715	1/1	0.31	-	74,74,74,74	0
54	MG	BA	3276	1/1	0.23	-	65,65,65,65	0
54	MG	AA	1630	1/1	0.36	-	70,70,70,70	0
54	MG	DA	2983	1/1	0.34	-	70,70,70,70	0
54	MG	AA	1676	1/1	0.10	-	63,63,63,63	0
54	MG	CA	1651	1/1	0.09	-	99,99,99,99	0
54	MG	DA	3289	1/1	0.40	-	92,92,92,92	0
54	MG	DA	3310	1/1	0.30	-	52,52,52,52	0
54	MG	DA	2927	1/1	0.24	-	22,22,22,22	0
54	MG	CA	1658	1/1	0.42	-	110,110,110,110	0
55	ZN	CD	301	1/1	0.24	-	131,131,131,131	0
54	MG	BA	3208	1/1	0.23	-	48,48,48,48	0
54	MG	BA	3174	1/1	0.23	-	84,84,84,84	0
54	MG	BA	3259	1/1	0.39	-	75,75,75,75	0
54	MG	DA	3034	1/1	0.27	-	65,65,65,65	0
54	MG	DA	3183	1/1	0.10	-	83,83,83,83	0
54	MG	DA	3001	1/1	0.16	-	56,56,56,56	0
54	MG	CA	1723	1/1	0.30	-	141,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3040	1/1	0.27	-	58,58,58,58	0
54	MG	BA	3245	1/1	0.28	-	54,54,54,54	0
54	MG	BA	3085	1/1	0.40	-	68,68,68,68	0
54	MG	BA	3299	1/1	0.27	-	80,80,80,80	0
54	MG	BA	3252	1/1	0.10	-	92,92,92,92	0
54	MG	BA	2940	1/1	0.30	-	29,29,29,29	0
54	MG	CV	6301	1/1	0.19	-	98,98,98,98	0
54	MG	AA	1740	1/1	0.30	-	80,80,80,80	0
54	MG	DA	3221	1/1	0.19	-	68,68,68,68	0
54	MG	CA	1619	1/1	0.43	-	61,61,61,61	0
54	MG	BA	3017	1/1	0.23	-	69,69,69,69	0
54	MG	CA	1731	1/1	0.13	-	90,90,90,90	0
54	MG	DA	3079	1/1	0.28	-	38,38,38,38	0
54	MG	AV	6301	1/1	0.11	-	72,72,72,72	0
54	MG	DA	3154	1/1	0.33	-	94,94,94,94	0
54	MG	DA	2996	1/1	0.35	-	43,43,43,43	0
54	MG	BA	3289	1/1	0.23	-	65,65,65,65	0
54	MG	BA	3232	1/1	0.45	-	24,24,24,24	0
54	MG	BA	3138	1/1	0.14	-	100,100,100,100	0
54	MG	CA	1716	1/1	0.23	-	77,77,77,77	0
54	MG	BA	2905	1/1	0.55	-	12,12,12,12	0
54	MG	BA	2947	1/1	0.30	-	14,14,14,14	0
54	MG	CA	1711	1/1	0.42	-	87,87,87,87	0
54	MG	DA	3178	1/1	0.24	-	83,83,83,83	0
54	MG	AA	1653	1/1	0.35	-	89,89,89,89	0
54	MG	DB	215	1/1	0.43	-	103,103,103,103	0
54	MG	DA	3069	1/1	0.18	-	81,81,81,81	0
54	MG	AA	1645	1/1	0.58	-	79,79,79,79	0
54	MG	DA	3087	1/1	0.30	-	67,67,67,67	0
54	MG	AA	1760	1/1	0.13	-	84,84,84,84	0
54	MG	DA	3210	1/1	0.11	-	59,59,59,59	0
54	MG	DA	2988	1/1	0.58	-	41,41,41,41	0
54	MG	DA	2962	1/1	0.35	-	37,37,37,37	0
54	MG	DA	3121	1/1	0.19	-	69,69,69,69	0
54	MG	BA	3182	1/1	0.47	-	20,20,20,20	0
54	MG	BA	2977	1/1	0.33	-	52,52,52,52	0
54	MG	CA	1603	1/1	0.27	-	48,48,48,48	0
54	MG	BA	2917	1/1	0.39	-	8,8,8,8	0
54	MG	AA	1754	1/1	0.23	-	110,110,110,110	0
54	MG	AA	1757	1/1	0.47	-	89,89,89,89	0
54	MG	DA	3010	1/1	0.67	-	51,51,51,51	0
54	MG	DB	214	1/1	0.25	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	2922	1/1	0.32	-	7,7,7,7	0
54	MG	CA	1642	1/1	0.18	-	71,71,71,71	0
54	MG	BA	3075	1/1	0.17	-	67,67,67,67	0
54	MG	BA	2967	1/1	0.39	-	24,24,24,24	0
54	MG	DA	3093	1/1	0.35	-	69,69,69,69	0
54	MG	BB	209	1/1	0.34	-	83,83,83,83	0
54	MG	BA	3250	1/1	0.11	-	95,95,95,95	0
54	MG	DA	3049	1/1	0.22	-	56,56,56,56	0
54	MG	DA	2915	1/1	0.47	-	14,14,14,14	0
54	MG	DA	3102	1/1	0.21	-	68,68,68,68	0
54	MG	AA	1722	1/1	0.25	-	83,83,83,83	0
54	MG	DA	2976	1/1	0.30	-	37,37,37,37	0
54	MG	BA	3107	1/1	0.30	-	87,87,87,87	0
54	MG	BA	2936	1/1	0.19	-	43,43,43,43	0
54	MG	CA	1640	1/1	0.36	-	69,69,69,69	0
54	MG	DA	3017	1/1	0.25	-	93,93,93,93	0
54	MG	CA	1602	1/1	0.08	-	64,64,64,64	0
54	MG	DA	3194	1/1	0.34	-	10,10,10,10	0
54	MG	BA	2927	1/1	0.30	-	37,37,37,37	0
54	MG	DA	2982	1/1	0.20	-	33,33,33,33	0
54	MG	BA	3074	1/1	0.20	-	61,61,61,61	0
54	MG	DA	3062	1/1	0.14	-	65,65,65,65	0
54	MG	DA	3159	1/1	1.07	-	87,87,87,87	0
54	MG	DA	3122	1/1	0.18	-	87,87,87,87	0
54	MG	DA	3193	1/1	0.55	-	51,51,51,51	0
54	MG	BA	3060	1/1	0.69	-	74,74,74,74	0
54	MG	AA	1730	1/1	0.10	-	49,49,49,49	0
54	MG	DA	3257	1/1	0.21	-	94,94,94,94	0
54	MG	DA	3007	1/1	0.18	-	43,43,43,43	0
54	MG	BB	210	1/1	0.11	-	100,100,100,100	0
54	MG	BA	3045	1/1	0.12	-	80,80,80,80	0
54	MG	DA	3073	1/1	0.12	-	80,80,80,80	0
54	MG	CA	1668	1/1	1.15	-	116,116,116,116	0
54	MG	DA	3098	1/1	0.36	-	71,71,71,71	0
54	MG	BA	3066	1/1	0.48	-	56,56,56,56	0
54	MG	BA	2935	1/1	0.52	-	34,34,34,34	0
54	MG	BA	3029	1/1	0.56	-	63,63,63,63	0
54	MG	DA	3196	1/1	1.06	-	39,39,39,39	0
54	MG	DA	3028	1/1	0.16	-	78,78,78,78	0
54	MG	BB	205	1/1	0.43	-	71,71,71,71	0
54	MG	BA	3190	1/1	0.34	-	115,115,115,115	0
54	MG	BA	3300	1/1	0.47	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1724	1/1	0.25	-	74,74,74,74	0
54	MG	BA	3225	1/1	0.57	-	74,74,74,74	0
54	MG	BA	3069	1/1	0.11	-	109,109,109,109	0
54	MG	BA	3137	1/1	0.53	-	54,54,54,54	0
54	MG	BA	2946	1/1	0.47	-	33,33,33,33	0
54	MG	BA	3117	1/1	0.13	-	77,77,77,77	0
54	MG	DA	3002	1/1	0.44	-	59,59,59,59	0
54	MG	DA	2939	1/1	0.18	-	40,40,40,40	0
54	MG	DA	3219	1/1	0.31	-	67,67,67,67	0
54	MG	DA	2969	1/1	0.21	-	42,42,42,42	0
54	MG	BB	214	1/1	0.22	-	101,101,101,101	0
54	MG	DA	2978	1/1	0.27	-	44,44,44,44	0
54	MG	BA	2923	1/1	0.34	-	29,29,29,29	0
54	MG	AA	1691	1/1	0.36	-	78,78,78,78	0
54	MG	BA	3042	1/1	0.12	-	90,90,90,90	0
54	MG	DA	3065	1/1	0.40	-	56,56,56,56	0
54	MG	BA	3023	1/1	0.56	-	64,64,64,64	0
54	MG	BA	3116	1/1	0.50	-	85,85,85,85	0
54	MG	CA	1639	1/1	0.62	-	66,66,66,66	0
54	MG	BA	2918	1/1	0.35	-	17,17,17,17	0
54	MG	DA	2997	1/1	0.13	-	35,35,35,35	0
54	MG	DA	3107	1/1	0.27	-	67,67,67,67	0
54	MG	DA	2952	1/1	0.35	-	50,50,50,50	0
54	MG	AA	1706	1/1	0.26	-	103,103,103,103	0
54	MG	CA	1740	1/1	0.25	-	117,117,117,117	0
54	MG	BA	3052	1/1	0.24	-	56,56,56,56	0
54	MG	BA	2955	1/1	0.20	-	50,50,50,50	0
54	MG	DA	3169	1/1	0.13	-	112,112,112,112	0
54	MG	DA	2940	1/1	0.70	-	51,51,51,51	0
54	MG	DA	3031	1/1	0.07	-	62,62,62,62	0
54	MG	CA	1710	1/1	0.20	-	119,119,119,119	0
54	MG	BA	3026	1/1	0.41	-	82,82,82,82	0
54	MG	DA	3227	1/1	0.34	-	34,34,34,34	0
54	MG	BA	2901	1/1	0.40	-	23,23,23,23	0
54	MG	DA	3276	1/1	0.20	-	128,128,128,128	0
54	MG	DB	212	1/1	0.17	-	70,70,70,70	0
54	MG	AA	1741	1/1	0.13	-	74,74,74,74	0
54	MG	DA	3205	1/1	0.32	-	48,48,48,48	0
54	MG	AA	1668	1/1	0.13	-	90,90,90,90	0
54	MG	DA	2908	1/1	0.26	-	24,24,24,24	0
54	MG	DA	3312	1/1	0.61	-	66,66,66,66	0
54	MG	DA	3252	1/1	0.11	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
54	MG	CA	1705	1/1	0.20	-	54,54,54,54	0
54	MG	DA	2995	1/1	0.51	-	48,48,48,48	0
54	MG	DA	3020	1/1	0.20	-	63,63,63,63	0
54	MG	DA	3123	1/1	0.07	-	59,59,59,59	0
54	MG	DA	3047	1/1	0.38	-	66,66,66,66	0
54	MG	DA	3281	1/1	0.28	-	73,73,73,73	0
54	MG	DA	3004	1/1	0.32	-	67,67,67,67	0
54	MG	BA	2968	1/1	0.48	-	51,51,51,51	0
54	MG	BA	3249	1/1	0.29	-	37,37,37,37	0
54	MG	DA	3234	1/1	0.12	-	130,130,130,130	0
54	MG	DA	2934	1/1	0.47	-	25,25,25,25	0
54	MG	BA	3022	1/1	0.19	-	77,77,77,77	0
54	MG	AA	1672	1/1	0.62	-	101,101,101,101	0
54	MG	BA	2914	1/1	0.46	-	31,31,31,31	0
54	MG	DA	3109	1/1	0.29	-	54,54,54,54	0
54	MG	DA	2936	1/1	0.40	-	27,27,27,27	0
54	MG	DA	3226	1/1	0.44	-	80,80,80,80	0
54	MG	BA	2910	1/1	0.53	-	27,27,27,27	0
54	MG	CA	1719	1/1	0.10	-	78,78,78,78	0
54	MG	BA	3142	1/1	0.08	-	89,89,89,89	0
54	MG	BA	3302	1/1	0.31	-	121,121,121,121	0
54	MG	BA	3167	1/1	0.11	-	50,50,50,50	0
54	MG	BA	3209	1/1	0.25	-	69,69,69,69	0
54	MG	AA	1631	1/1	0.32	-	70,70,70,70	0
54	MG	DA	2975	1/1	0.07	-	58,58,58,58	0
54	MG	AA	1637	1/1	0.41	-	61,61,61,61	0
54	MG	DA	2944	1/1	0.34	-	35,35,35,35	0
54	MG	DA	3053	1/1	0.25	-	61,61,61,61	0
54	MG	BA	3220	1/1	0.34	-	56,56,56,56	0
54	MG	DA	3189	1/1	0.28	-	37,37,37,37	0
54	MG	BA	3292	1/1	0.21	-	72,72,72,72	0
54	MG	BA	3243	1/1	0.17	-	82,82,82,82	0
54	MG	CA	1676	1/1	0.39	-	82,82,82,82	0
54	MG	BA	3043	1/1	0.34	-	70,70,70,70	0
54	MG	AA	1647	1/1	0.23	-	85,85,85,85	0
54	MG	AA	1735	1/1	0.16	-	104,104,104,104	0
54	MG	DA	2943	1/1	0.43	-	32,32,32,32	0
54	MG	DA	3018	1/1	0.15	-	73,73,73,73	0
54	MG	DA	3284	1/1	0.32	-	134,134,134,134	0
54	MG	AA	1719	1/1	0.27	-	78,78,78,78	0
54	MG	AA	1620	1/1	0.23	-	56,56,56,56	0
54	MG	DA	2991	1/1	0.24	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1697	1/1	0.37	-	80,80,80,80	0
54	MG	AA	1619	1/1	0.20	-	80,80,80,80	0
54	MG	DA	2911	1/1	0.40	-	7,7,7,7	0
54	MG	AA	1756	1/1	0.20	-	106,106,106,106	0
54	MG	BA	3175	1/1	0.22	-	85,85,85,85	0
54	MG	DA	3012	1/1	0.38	-	45,45,45,45	0
54	MG	BA	3266	1/1	0.26	-	98,98,98,98	0
54	MG	DA	2938	1/1	0.30	-	66,66,66,66	0
54	MG	BA	2991	1/1	0.15	-	36,36,36,36	0
54	MG	BA	2979	1/1	0.26	-	40,40,40,40	0
54	MG	DA	3222	1/1	0.55	-	70,70,70,70	0
54	MG	DA	3139	1/1	0.13	-	60,60,60,60	0
54	MG	BA	3257	1/1	0.37	-	64,64,64,64	0
54	MG	DB	204	1/1	0.11	-	75,75,75,75	0
54	MG	DA	3238	1/1	0.27	-	58,58,58,58	0
54	MG	BA	3168	1/1	0.17	-	76,76,76,76	0
54	MG	AA	1685	1/1	0.20	-	106,106,106,106	0
54	MG	BA	2966	1/1	0.12	-	75,75,75,75	0
54	MG	BA	2987	1/1	0.29	-	59,59,59,59	0
54	MG	BA	3264	1/1	0.09	-	116,116,116,116	0
54	MG	BA	2980	1/1	0.24	-	40,40,40,40	0
54	MG	BA	2953	1/1	0.15	-	37,37,37,37	0
54	MG	BA	3004	1/1	1.27	-	74,74,74,74	0
54	MG	CA	1672	1/1	0.35	-	62,62,62,62	0
54	MG	CA	1612	1/1	0.92	-	58,58,58,58	0
54	MG	DA	3106	1/1	0.41	-	67,67,67,67	0
54	MG	DA	3200	1/1	0.12	-	87,87,87,87	0
54	MG	DB	202	1/1	0.65	-	64,64,64,64	0
54	MG	CA	1645	1/1	0.63	-	72,72,72,72	0
54	MG	BB	213	1/1	0.66	-	84,84,84,84	0
54	MG	BA	3179	1/1	0.46	-	19,19,19,19	0
54	MG	DA	3199	1/1	0.70	-	38,38,38,38	0
54	MG	AA	1711	1/1	0.58	-	53,53,53,53	0
54	MG	DA	2985	1/1	0.41	-	48,48,48,48	0
54	MG	DA	3315	1/1	0.17	-	52,52,52,52	0
54	MG	BA	2998	1/1	0.28	-	46,46,46,46	0
54	MG	AV	6302	1/1	0.55	-	121,121,121,121	0
54	MG	CA	1681	1/1	0.50	-	81,81,81,81	0
54	MG	DA	3033	1/1	0.50	-	101,101,101,101	0
54	MG	BA	3248	1/1	0.12	-	77,77,77,77	0
54	MG	CA	1725	1/1	0.19	-	105,105,105,105	0
54	MG	DB	213	1/1	0.48	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3131	1/1	0.27	-	67,67,67,67	0
54	MG	BA	3093	1/1	0.32	-	83,83,83,83	0
54	MG	DA	2970	1/1	0.22	-	67,67,67,67	0
54	MG	AA	1713	1/1	0.32	-	93,93,93,93	0
54	MG	BA	3018	1/1	0.35	-	68,68,68,68	0
54	MG	AA	1755	1/1	0.19	-	103,103,103,103	0
54	MG	DA	3085	1/1	0.13	-	89,89,89,89	0
54	MG	BA	3083	1/1	0.33	-	87,87,87,87	0
54	MG	BA	3143	1/1	0.69	-	84,84,84,84	0
54	MG	DA	3197	1/1	0.37	-	28,28,28,28	0
54	MG	BA	3233	1/1	0.25	-	52,52,52,52	0
54	MG	DA	3188	1/1	0.48	-	9,9,9,9	0
54	MG	BA	3007	1/1	0.17	-	55,55,55,55	0
54	MG	BA	3290	1/1	0.28	-	42,42,42,42	0
54	MG	CA	1647	1/1	0.33	-	77,77,77,77	0
54	MG	AA	1607	1/1	0.21	-	54,54,54,54	0
54	MG	BA	3273	1/1	0.21	-	83,83,83,83	0
54	MG	DA	2998	1/1	0.43	-	68,68,68,68	0
54	MG	DA	3264	1/1	0.24	-	61,61,61,61	0
54	MG	BA	3180	1/1	0.27	-	26,26,26,26	0
54	MG	AA	1634	1/1	0.18	-	70,70,70,70	0
54	MG	BA	2995	1/1	0.19	-	47,47,47,47	0
54	MG	DA	3131	1/1	0.41	-	66,66,66,66	0
54	MG	DA	3216	1/1	0.67	-	46,46,46,46	0
54	MG	CA	1738	1/1	0.47	-	81,81,81,81	0
54	MG	AA	1621	1/1	0.61	-	74,74,74,74	0
54	MG	AA	1612	1/1	0.27	-	64,64,64,64	0
54	MG	BA	2993	1/1	0.24	-	58,58,58,58	0
54	MG	AA	1724	1/1	0.27	-	85,85,85,85	0
54	MG	DA	3255	1/1	0.14	-	101,101,101,101	0
54	MG	DA	2961	1/1	0.14	-	29,29,29,29	0
54	MG	DA	3224	1/1	0.18	-	72,72,72,72	0
54	MG	BA	2976	1/1	0.48	-	70,70,70,70	0
54	MG	DA	3231	1/1	0.71	-	60,60,60,60	0
54	MG	BA	3172	1/1	0.49	-	102,102,102,102	0
54	MG	DA	3153	1/1	0.18	-	85,85,85,85	0
54	MG	CA	1706	1/1	0.52	-	101,101,101,101	0
54	MG	AA	1748	1/1	0.17	-	96,96,96,96	0
54	MG	BA	3297	1/1	0.39	-	67,67,67,67	0
54	MG	BA	3049	1/1	0.18	-	86,86,86,86	0
54	MG	BA	3230	1/1	0.52	-	44,44,44,44	0
54	MG	BA	3288	1/1	0.62	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3021	1/1	0.22	-	60,60,60,60	0
54	MG	DA	3217	1/1	0.16	-	56,56,56,56	0
54	MG	BA	3199	1/1	0.68	-	68,68,68,68	0
54	MG	AA	1661	1/1	0.43	-	65,65,65,65	0
54	MG	DA	3145	1/1	0.43	-	70,70,70,70	0
54	MG	BA	3151	1/1	0.55	-	56,56,56,56	0
54	MG	DA	3302	1/1	0.56	-	77,77,77,77	0
54	MG	DA	3060	1/1	0.16	-	87,87,87,87	0
54	MG	BA	3102	1/1	0.17	-	69,69,69,69	0
54	MG	DA	3301	1/1	0.28	-	80,80,80,80	0
54	MG	BA	3241	1/1	0.25	-	60,60,60,60	0
54	MG	BB	216	1/1	0.23	-	79,79,79,79	0
54	MG	DA	2992	1/1	0.17	-	46,46,46,46	0
54	MG	CA	1700	1/1	0.47	-	65,65,65,65	0
54	MG	DA	3249	1/1	0.40	-	56,56,56,56	0
54	MG	BA	2956	1/1	0.38	-	35,35,35,35	0
54	MG	BA	3229	1/1	0.35	-	62,62,62,62	0
54	MG	DA	3311	1/1	0.12	-	95,95,95,95	0
54	MG	BA	3065	1/1	0.21	-	61,61,61,61	0
54	MG	CA	1626	1/1	0.30	-	65,65,65,65	0
54	MG	BA	3028	1/1	0.58	-	62,62,62,62	0
54	MG	BA	3188	1/1	0.42	-	45,45,45,45	0
54	MG	BA	3269	1/1	0.26	-	63,63,63,63	0
54	MG	CA	1702	1/1	0.71	-	68,68,68,68	0
54	MG	DG	201	1/1	0.49	-	101,101,101,101	0
54	MG	DA	3048	1/1	0.09	-	66,66,66,66	0
54	MG	AA	1657	1/1	0.47	-	101,101,101,101	0
54	MG	BA	3205	1/1	0.27	-	38,38,38,38	0
54	MG	DA	3056	1/1	0.19	-	48,48,48,48	0
54	MG	DA	3029	1/1	0.24	-	70,70,70,70	0
54	MG	AA	1758	1/1	0.11	-	73,73,73,73	0
54	MG	BA	3006	1/1	0.52	-	77,77,77,77	0
54	MG	DA	2984	1/1	0.18	-	66,66,66,66	0
54	MG	BA	2949	1/1	0.20	-	47,47,47,47	0
54	MG	CA	1730	1/1	0.10	-	122,122,122,122	0
54	MG	DA	3331	1/1	0.18	-	52,52,52,52	0
54	MG	CA	1614	1/1	0.43	-	89,89,89,89	0
54	MG	BA	2904	1/1	0.39	-	13,13,13,13	0
54	MG	BA	2943	1/1	0.36	-	42,42,42,42	0
54	MG	DA	3236	1/1	0.53	-	63,63,63,63	0
54	MG	BA	2913	1/1	0.32	-	16,16,16,16	0
54	MG	BB	202	1/1	0.26	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3316	1/1	0.23	-	97,97,97,97	0
54	MG	BA	2909	1/1	0.40	-	24,24,24,24	0
54	MG	CA	1680	1/1	0.33	-	58,58,58,58	0
54	MG	DA	3146	1/1	0.12	-	95,95,95,95	0
54	MG	DA	3067	1/1	0.18	-	63,63,63,63	0
54	MG	BA	2920	1/1	0.36	-	28,28,28,28	0
54	MG	CA	1655	1/1	0.25	-	80,80,80,80	0
54	MG	BA	3296	1/1	0.17	-	47,47,47,47	0
54	MG	BA	3236	1/1	0.23	-	119,119,119,119	0
54	MG	BA	2964	1/1	0.45	-	30,30,30,30	0
54	MG	DA	3072	1/1	0.56	-	73,73,73,73	0
54	MG	DA	3241	1/1	0.54	-	54,54,54,54	0
54	MG	CA	1696	1/1	0.24	-	133,133,133,133	0
54	MG	AA	1703	1/1	0.15	-	83,83,83,83	0
54	MG	AA	1759	1/1	0.08	-	81,81,81,81	0
54	MG	BA	3144	1/1	0.36	-	75,75,75,75	0
54	MG	AA	1615	1/1	0.14	-	42,42,42,42	0
54	MG	DA	3134	1/1	0.18	-	71,71,71,71	0
54	MG	BA	3070	1/1	0.36	-	75,75,75,75	0
54	MG	AA	1644	1/1	0.32	-	53,53,53,53	0
54	MG	BA	3126	1/1	0.13	-	54,54,54,54	0
54	MG	DA	3180	1/1	0.16	-	77,77,77,77	0
54	MG	BA	3262	1/1	0.33	-	60,60,60,60	0
54	MG	DA	2967	1/1	0.34	-	54,54,54,54	0
54	MG	DA	3015	1/1	0.23	-	74,74,74,74	0
54	MG	CA	1684	1/1	0.10	-	117,117,117,117	0
54	MG	DA	3161	1/1	0.30	-	74,74,74,74	0
54	MG	DA	3074	1/1	0.29	-	64,64,64,64	0
54	MG	BA	3170	1/1	0.11	-	64,64,64,64	0
54	MG	DA	3148	1/1	0.21	-	99,99,99,99	0
54	MG	BA	2950	1/1	0.20	-	32,32,32,32	0
54	MG	BA	3124	1/1	0.33	-	89,89,89,89	0
54	MG	DB	203	1/1	0.22	-	82,82,82,82	0
54	MG	DA	3046	1/1	0.08	-	76,76,76,76	0
54	MG	DA	3214	1/1	0.34	-	46,46,46,46	0
54	MG	CA	1662	1/1	0.76	-	86,86,86,86	0
54	MG	DA	2971	1/1	0.34	-	47,47,47,47	0
54	MG	DA	3254	1/1	0.40	-	79,79,79,79	0
54	MG	DA	3156	1/1	0.16	-	78,78,78,78	0
54	MG	CA	1609	1/1	0.24	-	93,93,93,93	0
54	MG	DA	3324	1/1	0.51	-	78,78,78,78	0
54	MG	DB	205	1/1	0.07	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3054	1/1	0.23	-	46,46,46,46	0
54	MG	BA	2975	1/1	0.18	-	37,37,37,37	0
54	MG	AA	1677	1/1	0.50	-	64,64,64,64	0
54	MG	DA	2999	1/1	0.47	-	76,76,76,76	0
54	MG	BA	3291	1/1	0.28	-	68,68,68,68	0
54	MG	BB	208	1/1	0.45	-	109,109,109,109	0
54	MG	BA	3213	1/1	0.32	-	101,101,101,101	0
54	MG	DA	3030	1/1	0.41	-	71,71,71,71	0
54	MG	CA	1607	1/1	0.28	-	52,52,52,52	0
54	MG	DB	211	1/1	0.11	-	109,109,109,109	0
54	MG	BA	3204	1/1	0.35	-	74,74,74,74	0
54	MG	BA	3287	1/1	0.39	-	74,74,74,74	0
54	MG	AA	1624	1/1	0.42	-	67,67,67,67	0
54	MG	AA	1669	1/1	0.34	-	110,110,110,110	0
54	MG	DA	3313	1/1	0.24	-	107,107,107,107	0
54	MG	BA	3271	1/1	0.18	-	91,91,91,91	0
54	MG	BA	3113	1/1	0.26	-	71,71,71,71	0
54	MG	BA	3087	1/1	0.08	-	69,69,69,69	0
54	MG	BA	3110	1/1	0.17	-	86,86,86,86	0
54	MG	DA	2921	1/1	0.36	-	17,17,17,17	0
54	MG	DA	3176	1/1	0.22	-	83,83,83,83	0
54	MG	BA	2972	1/1	0.39	-	49,49,49,49	0
54	MG	BA	3061	1/1	0.24	-	91,91,91,91	0
54	MG	CA	1630	1/1	0.35	-	70,70,70,70	0
54	MG	BA	3307	1/1	0.11	-	68,68,68,68	0
54	MG	BA	3014	1/1	0.19	-	47,47,47,47	0
54	MG	AA	1720	1/1	0.25	-	69,69,69,69	0
54	MG	DA	3003	1/1	0.37	-	41,41,41,41	0
54	MG	DA	3292	1/1	0.38	-	33,33,33,33	0
54	MG	CA	1605	1/1	0.19	-	56,56,56,56	0
54	MG	BA	2929	1/1	0.44	-	37,37,37,37	0
54	MG	DA	3282	1/1	0.13	-	96,96,96,96	0
54	MG	DA	2913	1/1	0.41	-	17,17,17,17	0
54	MG	BA	3278	1/1	0.32	-	115,115,115,115	0
54	MG	DA	3168	1/1	0.47	-	94,94,94,94	0
54	MG	CA	1634	1/1	0.28	-	60,60,60,60	0
54	MG	AA	1702	1/1	1.06	-	94,94,94,94	0
54	MG	AA	1743	1/1	0.49	-	83,83,83,83	0
54	MG	BA	2902	1/1	0.49	-	16,16,16,16	0
54	MG	BA	3058	1/1	0.08	-	114,114,114,114	0
54	MG	CA	1686	1/1	0.23	-	60,60,60,60	0
54	MG	DA	2928	1/1	0.25	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1622	1/1	0.25	-	79,79,79,79	0
54	MG	DA	2926	1/1	0.25	-	43,43,43,43	0
54	MG	DA	3013	1/1	0.29	-	44,44,44,44	0
54	MG	BA	3041	1/1	0.21	-	67,67,67,67	0
54	MG	BA	3192	1/1	0.59	-	52,52,52,52	0
54	MG	DA	3050	1/1	0.09	-	105,105,105,105	0
54	MG	DA	2916	1/1	0.28	-	22,22,22,22	0
54	MG	BA	3001	1/1	0.30	-	59,59,59,59	0
54	MG	CA	1625	1/1	0.09	-	94,94,94,94	0
54	MG	DA	3006	1/1	0.09	-	74,74,74,74	0
54	MG	DA	3043	1/1	0.74	-	70,70,70,70	0
54	MG	DA	3151	1/1	0.36	-	82,82,82,82	0
54	MG	DA	2942	1/1	0.28	-	39,39,39,39	0
54	MG	CA	1688	1/1	0.37	-	99,99,99,99	0
54	MG	DA	3129	1/1	0.26	-	63,63,63,63	0
54	MG	DA	3260	1/1	0.64	-	102,102,102,102	0
54	MG	DA	3149	1/1	0.52	-	74,74,74,74	0
54	MG	BA	3237	1/1	0.17	-	60,60,60,60	0
54	MG	BA	3103	1/1	0.24	-	88,88,88,88	0
54	MG	AA	1613	1/1	0.15	-	47,47,47,47	0
54	MG	CA	1629	1/1	0.16	-	106,106,106,106	0
54	MG	BA	3169	1/1	0.49	-	75,75,75,75	0
54	MG	DA	3009	1/1	0.49	-	49,49,49,49	0
54	MG	BA	2971	1/1	0.41	-	65,65,65,65	0
54	MG	BA	3078	1/1	0.14	-	83,83,83,83	0
54	MG	AA	1667	1/1	0.53	-	61,61,61,61	0
54	MG	DA	3299	1/1	0.22	-	68,68,68,68	0
54	MG	BA	3277	1/1	0.23	-	71,71,71,71	0
54	MG	DA	3248	1/1	0.35	-	75,75,75,75	0
54	MG	DA	3054	1/1	0.17	-	75,75,75,75	0
54	MG	BA	3127	1/1	0.79	-	56,56,56,56	0
54	MG	CA	1623	1/1	0.54	-	99,99,99,99	0
54	MG	AA	1627	1/1	0.11	-	85,85,85,85	0
54	MG	BA	3053	1/1	0.23	-	67,67,67,67	0
54	MG	BA	3027	1/1	0.57	-	62,62,62,62	0
54	MG	CA	1671	1/1	0.22	-	74,74,74,74	0
54	MG	CA	1635	1/1	0.15	-	67,67,67,67	0
54	MG	BA	3270	1/1	0.24	-	61,61,61,61	0
54	MG	BA	3253	1/1	0.47	-	76,76,76,76	0
54	MG	BA	2921	1/1	0.39	-	21,21,21,21	0
54	MG	DA	3132	1/1	0.07	-	70,70,70,70	0
54	MG	BA	2924	1/1	0.48	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3235	1/1	0.11	-	62,62,62,62	0
54	MG	DA	2902	1/1	0.39	-	10,10,10,10	0
54	MG	DA	3322	1/1	0.35	-	95,95,95,95	0
54	MG	DA	2965	1/1	0.49	-	57,57,57,57	0
54	MG	DA	3192	1/1	0.27	-	30,30,30,30	0
54	MG	AA	1763	1/1	0.16	-	96,96,96,96	0
54	MG	DB	216	1/1	0.43	-	88,88,88,88	0
54	MG	BA	3063	1/1	0.22	-	56,56,56,56	0
54	MG	DA	3314	1/1	0.82	-	102,102,102,102	0
54	MG	BA	3030	1/1	0.16	-	57,57,57,57	0
54	MG	BA	2945	1/1	0.29	-	72,72,72,72	0
54	MG	BA	3039	1/1	0.18	-	94,94,94,94	0
54	MG	CA	1685	1/1	0.55	-	106,106,106,106	0
54	MG	BA	3244	1/1	0.74	-	47,47,47,47	0
54	MG	AA	1684	1/1	0.40	-	95,95,95,95	0
54	MG	DA	3011	1/1	0.17	-	99,99,99,99	0
54	MG	BA	3173	1/1	0.40	-	80,80,80,80	0
54	MG	CA	1728	1/1	0.36	-	82,82,82,82	0
54	MG	DA	3096	1/1	0.31	-	40,40,40,40	0
54	MG	DA	2930	1/1	0.21	-	36,36,36,36	0
54	MG	AA	1674	1/1	0.47	-	79,79,79,79	0
54	MG	DA	3268	1/1	0.42	-	81,81,81,81	0
54	MG	BA	3089	1/1	0.32	-	59,59,59,59	0
54	MG	AA	1663	1/1	0.14	-	70,70,70,70	0
55	ZN	CN	101	1/1	0.08	-	144,144,144,144	0
54	MG	BA	3308	1/1	0.52	-	94,94,94,94	0
54	MG	DA	3055	1/1	0.79	-	93,93,93,93	0
54	MG	DA	2935	1/1	0.57	-	30,30,30,30	0
54	MG	AA	1690	1/1	0.08	-	117,117,117,117	0
54	MG	AA	1708	1/1	0.14	-	101,101,101,101	0
54	MG	B2	101	1/1	0.53	-	64,64,64,64	0
54	MG	DA	3179	1/1	0.21	-	68,68,68,68	0
54	MG	AA	1664	1/1	0.56	-	103,103,103,103	0
54	MG	BA	3226	1/1	0.32	-	81,81,81,81	0
54	MG	BA	3282	1/1	0.30	-	62,62,62,62	0
54	MG	BA	3231	1/1	0.17	-	22,22,22,22	0
54	MG	BA	3306	1/1	0.34	-	74,74,74,74	0
54	MG	BK	201	1/1	0.24	-	91,91,91,91	0
54	MG	CA	1638	1/1	0.25	-	65,65,65,65	0
54	MG	BA	2970	1/1	0.59	-	45,45,45,45	0
54	MG	CA	1643	1/1	0.13	-	58,58,58,58	0
54	MG	DA	3150	1/1	0.29	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3294	1/1	0.29	-	61,61,61,61	0
54	MG	DA	2945	1/1	0.65	-	41,41,41,41	0
54	MG	AA	1609	1/1	0.61	-	70,70,70,70	0
54	MG	BA	3216	1/1	0.27	-	65,65,65,65	0
54	MG	BA	3218	1/1	0.68	-	75,75,75,75	0
54	MG	DA	3171	1/1	0.26	-	61,61,61,61	0
54	MG	CA	1695	1/1	0.41	-	80,80,80,80	0
54	MG	CA	1683	1/1	0.38	-	91,91,91,91	0
54	MG	CA	1613	1/1	0.24	-	87,87,87,87	0
54	MG	DA	3228	1/1	0.39	-	51,51,51,51	0
54	MG	AA	1639	1/1	0.35	-	79,79,79,79	0
54	MG	DA	3082	1/1	0.39	-	70,70,70,70	0
54	MG	AA	1643	1/1	0.28	-	70,70,70,70	0
54	MG	CA	1606	1/1	0.12	-	68,68,68,68	0
54	MG	BA	3080	1/1	0.12	-	73,73,73,73	0
54	MG	DA	2947	1/1	0.30	-	40,40,40,40	0
54	MG	BA	3139	1/1	0.27	-	78,78,78,78	0
54	MG	DA	3051	1/1	0.20	-	89,89,89,89	0
54	MG	DA	3041	1/1	0.16	-	51,51,51,51	0
54	MG	BA	3193	1/1	0.39	-	53,53,53,53	0
54	MG	DA	2914	1/1	0.42	-	27,27,27,27	0
54	MG	BA	2986	1/1	0.26	-	67,67,67,67	0
54	MG	AA	1736	1/1	0.10	-	79,79,79,79	0
54	MG	DA	2931	1/1	0.27	-	23,23,23,23	0
54	MG	BA	3163	1/1	0.47	-	72,72,72,72	0
54	MG	DA	3005	1/1	0.31	-	33,33,33,33	0
54	MG	BA	3203	1/1	0.18	-	41,41,41,41	0
54	MG	AA	1605	1/1	0.56	-	42,42,42,42	0
54	MG	BA	3003	1/1	0.31	-	48,48,48,48	0
54	MG	DA	2901	1/1	0.46	-	7,7,7,7	0
54	MG	DA	3059	1/1	0.22	-	67,67,67,67	0
54	MG	DA	3286	1/1	0.24	-	98,98,98,98	0
54	MG	DA	3112	1/1	0.20	-	60,60,60,60	0
54	MG	BA	3081	1/1	0.13	-	65,65,65,65	0
54	MG	DA	3191	1/1	0.49	-	24,24,24,24	0
54	MG	CA	1734	1/1	0.14	-	117,117,117,117	0
54	MG	BA	2957	1/1	0.53	-	35,35,35,35	0
54	MG	AA	1671	1/1	0.14	-	114,114,114,114	0
54	MG	DA	3290	1/1	0.15	-	85,85,85,85	0
54	MG	DA	3212	1/1	0.46	-	78,78,78,78	0
54	MG	BA	3251	1/1	0.10	-	64,64,64,64	0
54	MG	BB	204	1/1	0.11	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	2912	1/1	0.43	-	18,18,18,18	0
54	MG	CA	1604	1/1	0.25	-	59,59,59,59	0
54	MG	DA	3211	1/1	0.23	-	38,38,38,38	0
54	MG	DA	3088	1/1	0.11	-	70,70,70,70	0
54	MG	AA	1749	1/1	0.26	-	90,90,90,90	0
54	MG	DA	3275	1/1	0.18	-	78,78,78,78	0
54	MG	DA	3136	1/1	0.42	-	68,68,68,68	0
54	MG	BA	3111	1/1	0.51	-	46,46,46,46	0
54	MG	DA	2905	1/1	0.36	-	9,9,9,9	0
54	MG	AA	1652	1/1	0.24	-	89,89,89,89	0
54	MG	BA	3238	1/1	0.18	-	91,91,91,91	0
54	MG	BA	3161	1/1	0.25	-	62,62,62,62	0
54	MG	DA	2903	1/1	0.34	-	7,7,7,7	0
54	MG	BA	3260	1/1	0.15	-	62,62,62,62	0
54	MG	DA	3247	1/1	0.23	-	40,40,40,40	0
54	MG	DA	2923	1/1	0.24	-	17,17,17,17	0
54	MG	AA	1721	1/1	0.58	-	66,66,66,66	0
54	MG	BA	3095	1/1	0.13	-	83,83,83,83	0
54	MG	DA	3157	1/1	0.15	-	71,71,71,71	0
54	MG	AA	1717	1/1	0.33	-	81,81,81,81	0
54	MG	DA	3075	1/1	0.15	-	64,64,64,64	0
54	MG	BA	3012	1/1	0.15	-	91,91,91,91	0
54	MG	AA	1726	1/1	0.07	-	108,108,108,108	0
54	MG	DA	3014	1/1	0.40	-	69,69,69,69	0
54	MG	BA	3155	1/1	0.30	-	85,85,85,85	0
54	MG	BA	3034	1/1	0.80	-	102,102,102,102	0
54	MG	DA	2968	1/1	0.33	-	56,56,56,56	0
54	MG	BA	3118	1/1	0.49	-	109,109,109,109	0
54	MG	CA	1732	1/1	0.17	-	73,73,73,73	0
54	MG	DA	3245	1/1	0.49	-	54,54,54,54	0
54	MG	BA	3129	1/1	0.11	-	75,75,75,75	0
54	MG	BA	3294	1/1	0.18	-	64,64,64,64	0
54	MG	DA	3155	1/1	0.07	-	124,124,124,124	0
54	MG	DA	3278	1/1	0.36	-	75,75,75,75	0
54	MG	DA	2974	1/1	0.10	-	46,46,46,46	0
54	MG	BA	3185	1/1	0.24	-	56,56,56,56	0
54	MG	DB	206	1/1	0.35	-	99,99,99,99	0
54	MG	DA	3318	1/1	0.29	-	101,101,101,101	0
54	MG	DA	3288	1/1	0.28	-	78,78,78,78	0
54	MG	BA	2931	1/1	0.54	-	32,32,32,32	0
54	MG	DA	3303	1/1	0.17	-	66,66,66,66	0
54	MG	DA	3038	1/1	0.27	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3013	1/1	0.11	-	90,90,90,90	0
54	MG	DA	3297	1/1	0.39	-	49,49,49,49	0
54	MG	BA	3136	1/1	0.21	-	87,87,87,87	0
54	MG	CA	1637	1/1	0.20	-	112,112,112,112	0
54	MG	BA	3098	1/1	0.18	-	78,78,78,78	0
54	MG	DA	3202	1/1	0.64	-	44,44,44,44	0
54	MG	AA	1617	1/1	0.21	-	77,77,77,77	0
54	MG	BA	2928	1/1	0.39	-	42,42,42,42	0
54	MG	AA	1625	1/1	1.02	-	88,88,88,88	0
54	MG	DA	3172	1/1	0.38	-	81,81,81,81	0
54	MG	DA	2951	1/1	0.20	-	38,38,38,38	0
54	MG	AA	1744	1/1	0.22	-	82,82,82,82	0
54	MG	CA	1677	1/1	0.34	-	85,85,85,85	0
54	MG	BA	2959	1/1	0.39	-	55,55,55,55	0
54	MG	DA	3232	1/1	0.35	-	39,39,39,39	0
54	MG	DA	3325	1/1	0.72	-	92,92,92,92	0
54	MG	DA	3133	1/1	0.14	-	89,89,89,89	0
54	MG	BA	3183	1/1	0.33	-	27,27,27,27	0
54	MG	BA	3281	1/1	0.22	-	84,84,84,84	0
54	MG	BA	3104	1/1	0.33	-	63,63,63,63	0
54	MG	BA	2906	1/1	0.20	-	5,5,5,5	0
54	MG	AA	1632	1/1	0.09	-	68,68,68,68	0
54	MG	DA	3147	1/1	0.14	-	78,78,78,78	0
54	MG	DA	3077	1/1	0.71	-	67,67,67,67	0
54	MG	DA	3022	1/1	0.26	-	60,60,60,60	0
54	MG	AA	1710	1/1	0.27	-	65,65,65,65	0
54	MG	DA	3182	1/1	0.38	-	86,86,86,86	0
54	MG	BA	3181	1/1	0.51	-	22,22,22,22	0
54	MG	BA	2934	1/1	0.42	-	28,28,28,28	0
54	MG	BA	3082	1/1	0.19	-	61,61,61,61	0
54	MG	BA	3265	1/1	0.34	-	80,80,80,80	0
54	MG	BA	3055	1/1	0.20	-	60,60,60,60	0
54	MG	BA	3140	1/1	0.41	-	76,76,76,76	0
54	MG	CA	1674	1/1	0.17	-	74,74,74,74	0
54	MG	DA	2907	1/1	0.46	-	7,7,7,7	0
54	MG	DA	3204	1/1	0.17	-	54,54,54,54	0
54	MG	DA	3321	1/1	0.55	-	30,30,30,30	0
54	MG	DA	3328	1/1	0.07	-	45,45,45,45	0
54	MG	BA	3202	1/1	0.58	-	63,63,63,63	0
54	MG	DA	3035	1/1	0.50	-	77,77,77,77	0
54	MG	CA	1652	1/1	0.46	-	85,85,85,85	0
54	MG	DA	2918	1/1	0.36	-	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1687	1/1	0.33	-	64,64,64,64	0
54	MG	BA	2922	1/1	0.44	-	25,25,25,25	0
54	MG	DA	2909	1/1	0.39	-	5,5,5,5	0
54	MG	AA	1750	1/1	0.28	-	109,109,109,109	0
54	MG	DA	3092	1/1	0.10	-	98,98,98,98	0
54	MG	BA	3032	1/1	0.24	-	59,59,59,59	0
54	MG	BA	3000	1/1	0.17	-	65,65,65,65	0
54	MG	BA	3120	1/1	0.25	-	57,57,57,57	0
54	MG	DA	3130	1/1	0.29	-	82,82,82,82	0
54	MG	DA	2910	1/1	0.28	-	6,6,6,6	0
54	MG	DA	3277	1/1	0.33	-	52,52,52,52	0
54	MG	BA	2919	1/1	0.39	-	24,24,24,24	0
54	MG	DA	3100	1/1	0.44	-	59,59,59,59	0
54	MG	AA	1745	1/1	0.20	-	97,97,97,97	0
54	MG	BA	3177	1/1	0.24	-	93,93,93,93	0
54	MG	BA	3047	1/1	0.37	-	65,65,65,65	0
54	MG	BA	3067	1/1	0.09	-	86,86,86,86	0
54	MG	DA	3319	1/1	0.22	-	83,83,83,83	0
54	MG	DA	2960	1/1	0.34	-	42,42,42,42	0
54	MG	DA	2972	1/1	0.50	-	47,47,47,47	0
54	MG	AA	1747	1/1	0.74	-	75,75,75,75	0
54	MG	DA	3215	1/1	0.45	-	39,39,39,39	0
54	MG	CA	1660	1/1	0.10	-	100,100,100,100	0
54	MG	DA	2948	1/1	0.31	-	52,52,52,52	0
54	MG	DA	2933	1/1	0.46	-	30,30,30,30	0
54	MG	DA	3101	1/1	0.78	-	72,72,72,72	0
54	MG	DA	3280	1/1	0.21	-	84,84,84,84	0
54	MG	DA	3187	1/1	0.22	-	90,90,90,90	0
54	MG	DA	3137	1/1	0.18	-	68,68,68,68	0
54	MG	BA	3305	1/1	0.46	-	103,103,103,103	0
54	MG	BA	3198	1/1	0.23	-	81,81,81,81	0
54	MG	CA	1664	1/1	0.18	-	82,82,82,82	0
54	MG	BA	2926	1/1	0.55	-	31,31,31,31	0
54	MG	DA	3119	1/1	0.69	-	88,88,88,88	0
55	ZN	AD	301	1/1	0.27	-	80,80,80,80	0
54	MG	CA	1617	1/1	0.34	-	90,90,90,90	0
54	MG	DA	3272	1/1	0.37	-	41,41,41,41	0
54	MG	DA	3256	1/1	0.19	-	82,82,82,82	0
54	MG	BA	3211	1/1	0.41	-	59,59,59,59	0
54	MG	DA	2920	1/1	0.41	-	30,30,30,30	0
54	MG	BA	2961	1/1	0.39	-	43,43,43,43	0
54	MG	DA	3253	1/1	0.09	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3083	1/1	0.22	-	67,67,67,67	0
54	MG	DA	2925	1/1	0.44	-	24,24,24,24	0
54	MG	DA	3008	1/1	0.51	-	59,59,59,59	0
54	MG	AA	1737	1/1	0.30	-	86,86,86,86	0
54	MG	DA	3295	1/1	0.26	-	63,63,63,63	0
54	MG	AA	1689	1/1	0.31	-	68,68,68,68	0
54	MG	BA	3010	1/1	0.17	-	37,37,37,37	0
54	MG	BA	2981	1/1	0.16	-	48,48,48,48	0
54	MG	BA	3048	1/1	0.24	-	67,67,67,67	0
54	MG	BA	3035	1/1	0.36	-	44,44,44,44	0
54	MG	BA	3101	1/1	0.50	-	75,75,75,75	0
54	MG	CA	1722	1/1	0.47	-	108,108,108,108	0
54	MG	BA	2969	1/1	0.15	-	37,37,37,37	0
54	MG	BA	2937	1/1	0.33	-	36,36,36,36	0
54	MG	AA	1682	1/1	0.39	-	85,85,85,85	0
54	MG	BA	3122	1/1	0.22	-	101,101,101,101	0
54	MG	AA	1638	1/1	0.45	-	63,63,63,63	0
54	MG	DA	3240	1/1	0.33	-	60,60,60,60	0
54	MG	BA	3239	1/1	0.59	-	82,82,82,82	0
54	MG	DA	2981	1/1	0.30	-	55,55,55,55	0
54	MG	DA	2929	1/1	0.39	-	39,39,39,39	0
54	MG	BA	2974	1/1	0.32	-	45,45,45,45	0
54	MG	D4	101	1/1	0.57	-	55,55,55,55	0
54	MG	DA	3167	1/1	0.12	-	68,68,68,68	0
54	MG	CA	1708	1/1	0.18	-	143,143,143,143	0
54	MG	DA	3184	1/1	0.34	-	117,117,117,117	0
54	MG	DA	3269	1/1	0.55	-	91,91,91,91	0
54	MG	BA	2916	1/1	0.42	-	38,38,38,38	0
54	MG	BA	3005	1/1	0.52	-	69,69,69,69	0
54	MG	DA	2917	1/1	0.27	-	22,22,22,22	0
54	MG	CA	1689	1/1	0.34	-	83,83,83,83	0
54	MG	AA	1650	1/1	0.36	-	103,103,103,103	0
54	MG	DA	2932	1/1	0.52	-	38,38,38,38	0
54	MG	DA	3125	1/1	0.28	-	81,81,81,81	0
54	MG	AA	1727	1/1	0.14	-	100,100,100,100	0
54	MG	AA	1618	1/1	0.10	-	91,91,91,91	0
54	MG	AA	1604	1/1	0.11	-	57,57,57,57	0
54	MG	CA	1733	1/1	0.13	-	72,72,72,72	0
54	MG	AA	1673	1/1	0.46	-	61,61,61,61	0
54	MG	DB	207	1/1	0.32	-	72,72,72,72	0
54	MG	AV	6303	1/1	0.18	-	67,67,67,67	0
54	MG	BA	3149	1/1	0.65	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	2932	1/1	0.31	-	41,41,41,41	0
54	MG	DA	2954	1/1	0.27	-	28,28,28,28	0
54	MG	DA	3207	1/1	0.40	-	42,42,42,42	0
54	MG	AA	1642	1/1	0.56	-	97,97,97,97	0
54	MG	DA	3042	1/1	0.53	-	79,79,79,79	0
54	MG	DA	3097	1/1	0.30	-	94,94,94,94	0
54	MG	CA	1726	1/1	0.35	-	87,87,87,87	0
54	MG	DA	2958	1/1	0.14	-	2,2,2,2	0
54	MG	AA	1659	1/1	0.36	-	51,51,51,51	0
54	MG	BA	3194	1/1	0.51	-	45,45,45,45	0
54	MG	BA	2944	1/1	0.14	-	17,17,17,17	0
54	MG	DA	3027	1/1	0.53	-	53,53,53,53	0
54	MG	CA	1682	1/1	0.20	-	97,97,97,97	0
54	MG	DA	3115	1/1	0.53	-	65,65,65,65	0
54	MG	DA	3261	1/1	0.28	-	73,73,73,73	0
54	MG	BA	3195	1/1	0.15	-	53,53,53,53	0
54	MG	CA	1737	1/1	0.20	-	70,70,70,70	0
54	MG	BA	3217	1/1	0.40	-	111,111,111,111	0
54	MG	BA	2948	1/1	0.69	-	39,39,39,39	0
54	MG	CA	1616	1/1	0.37	-	75,75,75,75	0
54	MG	BA	2973	1/1	0.19	-	61,61,61,61	0
54	MG	AV	6304	1/1	0.45	-	118,118,118,118	0
54	MG	AA	1729	1/1	0.17	-	75,75,75,75	0
54	MG	BA	2989	1/1	0.33	-	53,53,53,53	0
54	MG	AA	1665	1/1	0.26	-	82,82,82,82	0
54	MG	BA	3224	1/1	0.21	-	45,45,45,45	0
54	MG	AA	1739	1/1	0.19	-	129,129,129,129	0
54	MG	DA	3307	1/1	0.35	-	73,73,73,73	0
54	MG	DA	3223	1/1	0.60	-	45,45,45,45	0
54	MG	DA	3244	1/1	0.23	-	87,87,87,87	0
54	MG	DA	3039	1/1	0.33	-	48,48,48,48	0
54	MG	BA	2907	1/1	0.27	-	7,7,7,7	0
54	MG	DA	3239	1/1	0.22	-	42,42,42,42	0
54	MG	CA	1608	1/1	0.11	-	61,61,61,61	0
54	MG	CA	1736	1/1	1.00	-	115,115,115,115	0
54	MG	BA	2978	1/1	0.31	-	59,59,59,59	0
54	MG	BA	2939	1/1	0.49	-	26,26,26,26	0
54	MG	AA	1761	1/1	0.26	-	104,104,104,104	0
54	MG	BA	3286	1/1	0.31	-	67,67,67,67	0
54	MG	BA	2985	1/1	0.52	-	54,54,54,54	0
54	MG	CA	1611	1/1	0.23	-	76,76,76,76	0
54	MG	BA	3130	1/1	0.13	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3258	1/1	0.48	-	72,72,72,72	0
54	MG	BA	3115	1/1	0.38	-	91,91,91,91	0
54	MG	AA	1656	1/1	0.27	-	72,72,72,72	0
54	MG	CA	1707	1/1	0.09	-	104,104,104,104	0
54	MG	DA	3118	1/1	0.29	-	62,62,62,62	0
54	MG	BA	3176	1/1	0.37	-	99,99,99,99	0
54	MG	CA	1704	1/1	0.56	-	108,108,108,108	0
54	MG	CA	1739	1/1	0.11	-	99,99,99,99	0
54	MG	DA	3152	1/1	0.21	-	77,77,77,77	0
54	MG	DA	3068	1/1	0.36	-	72,72,72,72	0
54	MG	AA	1651	1/1	0.45	-	97,97,97,97	0
54	MG	DA	3120	1/1	0.62	-	66,66,66,66	0
54	MG	DA	3334	1/1	0.20	-	72,72,72,72	0
54	MG	DA	3225	1/1	0.07	-	80,80,80,80	0
54	MG	DA	3246	1/1	0.62	-	67,67,67,67	0
54	MG	CA	1628	1/1	0.19	-	100,100,100,100	0
54	MG	DA	2924	1/1	0.48	-	41,41,41,41	0
54	MG	DA	3251	1/1	0.41	-	63,63,63,63	0
54	MG	BA	3056	1/1	0.37	-	62,62,62,62	0
54	MG	DA	3287	1/1	0.39	-	69,69,69,69	0
54	MG	CA	1601	1/1	0.47	-	53,53,53,53	0
54	MG	CA	1618	1/1	0.72	-	63,63,63,63	0
54	MG	DA	3175	1/1	0.14	-	81,81,81,81	0
54	MG	BA	3158	1/1	0.14	-	105,105,105,105	0
54	MG	CA	1693	1/1	0.31	-	65,65,65,65	0
54	MG	BA	3002	1/1	0.33	-	45,45,45,45	0
54	MG	BA	2930	1/1	0.34	-	34,34,34,34	0
54	MG	DA	3164	1/1	0.06	-	88,88,88,88	0
54	MG	DA	3103	1/1	0.45	-	79,79,79,79	0
54	MG	DA	3237	1/1	0.29	-	87,87,87,87	0
54	MG	BA	3215	1/1	0.39	-	68,68,68,68	0
54	MG	AA	1679	1/1	0.38	-	78,78,78,78	0
54	MG	BA	3274	1/1	0.06	-	78,78,78,78	0
54	MG	AA	1614	1/1	0.51	-	85,85,85,85	0
54	MG	DA	2956	1/1	0.30	-	45,45,45,45	0
54	MG	BA	3295	1/1	0.63	-	70,70,70,70	0
54	MG	CA	1653	1/1	0.18	-	84,84,84,84	0
54	MG	DA	3267	1/1	0.30	-	76,76,76,76	0
54	MG	AA	1636	1/1	0.35	-	76,76,76,76	0
54	MG	BA	3279	1/1	0.47	-	77,77,77,77	0
54	MG	BA	3134	1/1	0.23	-	64,64,64,64	0
54	MG	DA	3016	1/1	0.18	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3112	1/1	0.38	-	68,68,68,68	0
54	MG	DA	3181	1/1	0.16	-	106,106,106,106	0
54	MG	AA	1622	1/1	0.88	-	88,88,88,88	0
54	MG	BA	3160	1/1	0.42	-	106,106,106,106	0
54	MG	BA	2990	1/1	0.17	-	54,54,54,54	0
54	MG	CA	1631	1/1	0.20	-	68,68,68,68	0
54	MG	AA	1699	1/1	0.29	-	91,91,91,91	0
54	MG	DA	3335	1/1	0.34	-	90,90,90,90	0
54	MG	BA	3133	1/1	0.27	-	67,67,67,67	0
54	MG	DA	3259	1/1	0.33	-	108,108,108,108	0
54	MG	DA	3309	1/1	0.37	-	30,30,30,30	0
54	MG	DA	2986	1/1	0.19	-	55,55,55,55	0
54	MG	CA	1698	1/1	0.21	-	117,117,117,117	0
54	MG	DA	3242	1/1	0.29	-	96,96,96,96	0
54	MG	BA	3148	1/1	0.34	-	68,68,68,68	0
54	MG	AA	1678	1/1	0.29	-	115,115,115,115	0
54	MG	AA	1662	1/1	0.15	-	53,53,53,53	0
54	MG	DA	3174	1/1	0.52	-	42,42,42,42	0
54	MG	BA	3154	1/1	0.18	-	89,89,89,89	0
54	MG	BA	2996	1/1	0.39	-	54,54,54,54	0
54	MG	BA	3242	1/1	0.34	-	44,44,44,44	0
54	MG	DA	2904	1/1	0.46	-	4,4,4,4	0
54	MG	DA	3021	1/1	0.18	-	67,67,67,67	0
54	MG	DA	3110	1/1	0.30	-	86,86,86,86	0
54	MG	BA	3125	1/1	0.37	-	87,87,87,87	0
54	MG	DA	3271	1/1	0.18	-	97,97,97,97	0
54	MG	CA	1721	1/1	0.24	-	101,101,101,101	0
54	MG	BB	207	1/1	0.12	-	105,105,105,105	0
54	MG	AA	1660	1/1	0.31	-	59,59,59,59	0
54	MG	DA	3140	1/1	0.12	-	67,67,67,67	0
54	MG	AA	1687	1/1	0.09	-	73,73,73,73	0
54	MG	DA	3165	1/1	0.66	-	71,71,71,71	0
54	MG	BB	215	1/1	0.14	-	131,131,131,131	0
54	MG	BA	3156	1/1	0.27	-	80,80,80,80	0
54	MG	BA	3227	1/1	0.17	-	48,48,48,48	0
54	MG	BA	3280	1/1	0.36	-	70,70,70,70	0
54	MG	DA	3158	1/1	0.18	-	59,59,59,59	0
54	MG	DA	3218	1/1	0.44	-	48,48,48,48	0
54	MG	CA	1691	1/1	0.29	-	85,85,85,85	0
54	MG	AA	1694	1/1	0.26	-	129,129,129,129	0
54	MG	DA	3090	1/1	0.20	-	71,71,71,71	0
54	MG	DA	3298	1/1	0.57	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	2960	1/1	0.52	-	40,40,40,40	0
54	MG	AA	1742	1/1	0.33	-	87,87,87,87	0
54	MG	BA	3051	1/1	0.28	-	66,66,66,66	0
54	MG	BA	3071	1/1	0.16	-	72,72,72,72	0
54	MG	DA	3206	1/1	0.33	-	37,37,37,37	0
54	MG	DA	3160	1/1	0.15	-	71,71,71,71	0
54	MG	BA	3044	1/1	0.13	-	64,64,64,64	0
54	MG	AA	1680	1/1	0.15	-	90,90,90,90	0
54	MG	BB	206	1/1	0.23	-	70,70,70,70	0
54	MG	BA	3084	1/1	0.38	-	51,51,51,51	0
54	MG	CA	1692	1/1	0.87	-	78,78,78,78	0
54	MG	DA	2941	1/1	0.22	-	37,37,37,37	0
54	MG	DA	3279	1/1	0.08	-	88,88,88,88	0
54	MG	CA	1720	1/1	0.38	-	63,63,63,63	0
54	MG	CA	1667	1/1	0.12	-	67,67,67,67	0
54	MG	DA	3138	1/1	0.15	-	70,70,70,70	0
54	MG	BA	3016	1/1	0.42	-	60,60,60,60	0
54	MG	BA	3275	1/1	0.93	-	87,87,87,87	0
54	MG	DA	3143	1/1	0.27	-	77,77,77,77	0
54	MG	DA	3262	1/1	0.28	-	82,82,82,82	0
54	MG	BA	3015	1/1	0.37	-	58,58,58,58	0
54	MG	CA	1669	1/1	0.15	-	66,66,66,66	0
54	MG	CA	1690	1/1	0.53	-	61,61,61,61	0
54	MG	AA	1715	1/1	0.38	-	63,63,63,63	0
54	MG	AA	1648	1/1	0.40	-	76,76,76,76	0
54	MG	BA	3009	1/1	0.52	-	87,87,87,87	0
54	MG	DA	3330	1/1	0.63	-	69,69,69,69	0
54	MG	BA	3145	1/1	0.19	-	67,67,67,67	0
54	MG	DA	3296	1/1	0.12	-	104,104,104,104	0
54	MG	BA	3086	1/1	0.27	-	102,102,102,102	0
54	MG	BA	3246	1/1	0.23	-	73,73,73,73	0
54	MG	DA	3317	1/1	0.52	-	97,97,97,97	0
54	MG	AA	1608	1/1	0.38	-	47,47,47,47	0
54	MG	DA	3135	1/1	0.22	-	65,65,65,65	0
54	MG	AA	1695	1/1	0.40	-	83,83,83,83	0
54	MG	DA	3081	1/1	0.09	-	71,71,71,71	0
54	MG	DA	3070	1/1	0.33	-	70,70,70,70	0
54	MG	BA	3210	1/1	0.24	-	48,48,48,48	0
54	MG	CA	1636	1/1	0.38	-	93,93,93,93	0
54	MG	BA	3240	1/1	0.09	-	114,114,114,114	0
54	MG	DA	2989	1/1	0.36	-	45,45,45,45	0
54	MG	DA	3327	1/1	0.35	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3127	1/1	0.44	-	90,90,90,90	0
54	MG	DA	3266	1/1	0.35	-	83,83,83,83	0
54	MG	DA	3243	1/1	0.35	-	72,72,72,72	0
54	MG	DA	3091	1/1	0.32	-	125,125,125,125	0
54	MG	DA	3116	1/1	0.22	-	115,115,115,115	0
54	MG	DA	3163	1/1	0.12	-	83,83,83,83	0
54	MG	BA	3097	1/1	0.29	-	53,53,53,53	0
54	MG	BA	3159	1/1	0.41	-	78,78,78,78	0
54	MG	AA	1675	1/1	0.17	-	77,77,77,77	0
54	MG	AA	1732	1/1	0.24	-	63,63,63,63	0
54	MG	BA	3165	1/1	0.26	-	71,71,71,71	0
54	MG	BA	3261	1/1	0.24	-	53,53,53,53	0
54	MG	AA	1746	1/1	0.25	-	100,100,100,100	0
54	MG	DA	3203	1/1	0.21	-	46,46,46,46	0
54	MG	DA	3032	1/1	0.10	-	49,49,49,49	0
54	MG	DA	2919	1/1	0.30	-	45,45,45,45	0
54	MG	BA	2984	1/1	0.22	-	41,41,41,41	0
54	MG	AA	1635	1/1	0.43	-	68,68,68,68	0
54	MG	DA	2980	1/1	0.23	-	63,63,63,63	0
54	MG	DA	3186	1/1	0.12	-	90,90,90,90	0
54	MG	BA	3064	1/1	0.30	-	40,40,40,40	0
54	MG	AA	1686	1/1	0.17	-	72,72,72,72	0
54	MG	BA	3076	1/1	0.28	-	68,68,68,68	0
54	MG	BA	2992	1/1	0.54	-	70,70,70,70	0
54	MG	AA	1683	1/1	0.16	-	102,102,102,102	0
54	MG	CA	1657	1/1	0.37	-	78,78,78,78	0
54	MG	BA	3062	1/1	0.28	-	76,76,76,76	0
54	MG	DA	2987	1/1	0.43	-	70,70,70,70	0
54	MG	BA	3099	1/1	0.15	-	78,78,78,78	0
54	MG	CA	1624	1/1	0.11	-	66,66,66,66	0
54	MG	CA	1727	1/1	0.26	-	75,75,75,75	0
54	MG	DA	3064	1/1	0.21	-	80,80,80,80	0
54	MG	CA	1627	1/1	0.19	-	67,67,67,67	0
54	MG	BA	3285	1/1	0.28	-	87,87,87,87	0
54	MG	BA	2911	1/1	0.46	-	23,23,23,23	0
54	MG	DA	2957	1/1	0.10	-	63,63,63,63	0
54	MG	DA	3283	1/1	0.30	-	53,53,53,53	0
54	MG	BA	3303	1/1	0.23	-	98,98,98,98	0
54	MG	CA	1697	1/1	0.46	-	74,74,74,74	0
54	MG	BA	3019	1/1	0.70	-	58,58,58,58	0
54	MG	BA	3178	1/1	0.42	-	72,72,72,72	0
55	ZN	AN	101	1/1	0.12	-	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1602	1/1	0.59	-	49,49,49,49	0
54	MG	DA	2977	1/1	0.18	-	47,47,47,47	0
54	MG	BA	2982	1/1	0.29	-	41,41,41,41	0
54	MG	CA	1709	1/1	0.39	-	81,81,81,81	0
54	MG	BA	2925	1/1	0.25	-	29,29,29,29	0
54	MG	BA	3186	1/1	0.34	-	52,52,52,52	0
54	MG	DB	217	1/1	0.11	-	74,74,74,74	0
54	MG	AA	1709	1/1	0.37	-	83,83,83,83	0
54	MG	DA	3114	1/1	0.34	-	83,83,83,83	0
54	MG	BA	3094	1/1	0.70	-	70,70,70,70	0
54	MG	AA	1693	1/1	0.36	-	74,74,74,74	0
54	MG	DA	3170	1/1	0.18	-	80,80,80,80	0
54	MG	DA	3036	1/1	0.29	-	51,51,51,51	0
54	MG	DA	2979	1/1	0.20	-	69,69,69,69	0
54	MG	DA	3108	1/1	0.18	-	50,50,50,50	0
54	MG	DA	3291	1/1	0.44	-	78,78,78,78	0
54	MG	BA	2908	1/1	0.47	-	18,18,18,18	0
54	MG	DA	3336	1/1	0.06	-	89,89,89,89	0
54	MG	DA	3305	1/1	0.13	-	110,110,110,110	0
54	MG	AA	1723	1/1	0.54	-	81,81,81,81	0
54	MG	DA	3213	1/1	0.23	-	66,66,66,66	0
54	MG	CA	1713	1/1	0.15	-	80,80,80,80	0
54	MG	AA	1701	1/1	0.42	-	83,83,83,83	0
54	MG	DA	3166	1/1	0.19	-	87,87,87,87	0
54	MG	CA	1717	1/1	0.28	-	84,84,84,84	0
54	MG	CA	1673	1/1	0.12	-	73,73,73,73	0
54	MG	BA	3164	1/1	0.70	-	88,88,88,88	0
54	MG	DA	3086	1/1	0.76	-	92,92,92,92	0
54	MG	BA	3108	1/1	0.36	-	99,99,99,99	0
54	MG	BA	3011	1/1	0.08	-	83,83,83,83	0
54	MG	BA	2983	1/1	0.40	-	62,62,62,62	0
54	MG	CA	1718	1/1	0.13	-	78,78,78,78	0
54	MG	CA	1610	1/1	0.32	-	77,77,77,77	0
54	MG	BA	2988	1/1	0.37	-	60,60,60,60	0
54	MG	BA	3162	1/1	0.07	-	94,94,94,94	0
54	MG	DA	3113	1/1	0.09	-	71,71,71,71	0
54	MG	AA	1714	1/1	0.34	-	58,58,58,58	0
54	MG	BA	3272	1/1	0.43	-	119,119,119,119	0
54	MG	BA	3068	1/1	0.35	-	59,59,59,59	0
54	MG	DA	3304	1/1	0.32	-	59,59,59,59	0
54	MG	BA	3128	1/1	0.46	-	59,59,59,59	0
54	MG	DA	3044	1/1	0.10	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3254	1/1	0.43	-	81,81,81,81	0
54	MG	CA	1654	1/1	0.17	-	111,111,111,111	0
54	MG	BA	2933	1/1	0.32	-	32,32,32,32	0
54	MG	BA	3150	1/1	0.24	-	79,79,79,79	0
54	MG	AA	1705	1/1	0.19	-	92,92,92,92	0
54	MG	DA	3117	1/1	0.21	-	87,87,87,87	0
54	MG	CA	1701	1/1	0.43	-	112,112,112,112	0
54	MG	DA	2964	1/1	0.20	-	34,34,34,34	0
54	MG	AA	1734	1/1	0.44	-	103,103,103,103	0
54	MG	DA	3190	1/1	0.43	-	27,27,27,27	0
54	MG	BA	3072	1/1	0.46	-	67,67,67,67	0
54	MG	DA	3162	1/1	0.11	-	143,143,143,143	0
54	MG	BA	3146	1/1	0.30	-	83,83,83,83	0
54	MG	BA	3268	1/1	0.82	-	58,58,58,58	0
54	MG	BA	3256	1/1	0.44	-	79,79,79,79	0
54	MG	BA	3171	1/1	0.21	-	68,68,68,68	0
54	MG	DA	3066	1/1	0.45	-	85,85,85,85	0
54	MG	BA	3096	1/1	0.20	-	65,65,65,65	0
54	MG	DA	3126	1/1	0.07	-	77,77,77,77	0
54	MG	DA	3329	1/1	0.80	-	69,69,69,69	0
54	MG	AA	1696	1/1	0.23	-	132,132,132,132	0
54	MG	CA	1641	1/1	0.12	-	85,85,85,85	0
54	MG	BA	3038	1/1	0.19	-	65,65,65,65	0
54	MG	DA	3173	1/1	0.18	-	97,97,97,97	0
54	MG	BA	3207	1/1	0.46	-	94,94,94,94	0
54	MG	BA	3008	1/1	0.16	-	57,57,57,57	0
54	MG	DA	3045	1/1	0.28	-	48,48,48,48	0
54	MG	BA	3234	1/1	0.24	-	61,61,61,61	0
54	MG	DA	3063	1/1	0.27	-	79,79,79,79	0
54	MG	BA	2954	1/1	0.18	-	52,52,52,52	0
54	MG	DA	3198	1/1	0.30	-	26,26,26,26	0
54	MG	CA	1649	1/1	0.27	-	80,80,80,80	0
54	MG	DA	3300	1/1	0.28	-	68,68,68,68	0
54	MG	BA	3196	1/1	0.23	-	51,51,51,51	0
54	MG	DA	3270	1/1	0.42	-	81,81,81,81	0
54	MG	CA	1679	1/1	0.13	-	93,93,93,93	0
54	MG	BA	3147	1/1	0.27	-	72,72,72,72	0
54	MG	BA	3221	1/1	0.35	-	48,48,48,48	0
54	MG	DA	3019	1/1	0.41	-	51,51,51,51	0
54	MG	BA	3031	1/1	0.86	-	87,87,87,87	0
54	MG	BA	3228	1/1	0.12	-	66,66,66,66	0
54	MG	BA	3222	1/1	1.17	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1712	1/1	0.12	-	78,78,78,78	0
54	MG	DA	3265	1/1	0.30	-	120,120,120,120	0
54	MG	AA	1733	1/1	0.25	-	91,91,91,91	0
54	MG	DA	3058	1/1	0.13	-	54,54,54,54	0
54	MG	DA	2963	1/1	0.42	-	53,53,53,53	0
54	MG	BA	3025	1/1	0.34	-	65,65,65,65	0
54	MG	BA	3046	1/1	0.96	-	87,87,87,87	0
54	MG	DA	2953	1/1	0.45	-	58,58,58,58	0
54	MG	DB	201	1/1	0.35	-	63,63,63,63	0
54	MG	BA	3092	1/1	0.17	-	63,63,63,63	0
54	MG	CA	1650	1/1	0.33	-	108,108,108,108	0
54	MG	AA	1606	1/1	0.39	-	53,53,53,53	0
54	MG	BA	2941	1/1	0.60	-	50,50,50,50	0
54	MG	DA	2959	1/1	0.39	-	56,56,56,56	0
54	MG	AA	1688	1/1	0.15	-	68,68,68,68	0
54	MG	AA	1601	1/1	0.46	-	31,31,31,31	0
54	MG	DA	3333	1/1	0.17	-	126,126,126,126	0
54	MG	DA	3229	1/1	0.48	-	64,64,64,64	0
54	MG	DA	3111	1/1	0.39	-	67,67,67,67	0
54	MG	CA	1656	1/1	0.16	-	79,79,79,79	0
54	MG	BA	3258	1/1	0.20	-	104,104,104,104	0
54	MG	DA	2950	1/1	0.23	-	29,29,29,29	0
54	MG	DA	3141	1/1	0.15	-	95,95,95,95	0
54	MG	AA	1725	1/1	0.28	-	72,72,72,72	0
54	MG	AA	1646	1/1	0.30	-	99,99,99,99	0
54	MG	DA	3308	1/1	0.22	-	91,91,91,91	0
54	MG	BA	3298	1/1	0.16	-	74,74,74,74	0
54	MG	BA	2963	1/1	0.21	-	54,54,54,54	0
54	MG	AA	1752	1/1	1.00	-	81,81,81,81	0
54	MG	AA	1623	1/1	0.43	-	93,93,93,93	0
54	MG	DA	2906	1/1	0.40	-	27,27,27,27	0
54	MG	BA	3132	1/1	0.20	-	79,79,79,79	0
54	MG	DA	3201	1/1	0.26	-	72,72,72,72	0
54	MG	CA	1675	1/1	0.32	-	107,107,107,107	0
54	MG	BA	3073	1/1	0.23	-	89,89,89,89	0
54	MG	BA	3109	1/1	0.53	-	90,90,90,90	0
54	MG	DA	2937	1/1	0.54	-	25,25,25,25	0
54	MG	DA	3104	1/1	0.19	-	99,99,99,99	0
54	MG	BA	2999	1/1	0.17	-	45,45,45,45	0
54	MG	BA	3079	1/1	0.47	-	86,86,86,86	0
54	MG	DA	3326	1/1	0.15	-	85,85,85,85	0
54	MG	AA	1762	1/1	0.11	-	155,155,155,155	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1610	1/1	0.31	-	78,78,78,78	0
54	MG	BA	2994	1/1	0.74	-	56,56,56,56	0
54	MG	DA	3177	1/1	0.31	-	62,62,62,62	0
54	MG	BA	3037	1/1	0.13	-	93,93,93,93	0
54	MG	DA	3000	1/1	0.31	-	35,35,35,35	0
54	MG	DA	3285	1/1	0.28	-	113,113,113,113	0
54	MG	BA	3141	1/1	0.20	-	78,78,78,78	0
54	MG	CA	1661	1/1	0.46	-	92,92,92,92	0
54	MG	BA	3184	1/1	0.36	-	42,42,42,42	0
54	MG	BA	3255	1/1	0.23	-	57,57,57,57	0
54	MG	AA	1712	1/1	0.61	-	75,75,75,75	0
54	MG	BA	3187	1/1	0.51	-	40,40,40,40	0
54	MG	AA	1616	1/1	0.21	-	63,63,63,63	0
54	MG	DA	3057	1/1	0.21	-	59,59,59,59	0
54	MG	DB	209	1/1	0.14	-	75,75,75,75	0
54	MG	DA	3332	1/1	0.43	-	60,60,60,60	0
54	MG	AA	1670	1/1	0.15	-	85,85,85,85	0
54	MG	BA	3121	1/1	0.26	-	77,77,77,77	0
54	MG	BA	2942	1/1	0.35	-	22,22,22,22	0
54	MG	BA	3119	1/1	0.29	-	64,64,64,64	0
54	MG	CA	1694	1/1	0.40	-	59,59,59,59	0
54	MG	CA	1678	1/1	0.11	-	107,107,107,107	0
54	MG	CA	1621	1/1	0.41	-	67,67,67,67	0
54	MG	D2	101	1/1	0.25	-	66,66,66,66	0
54	MG	BA	2938	1/1	0.21	-	10,10,10,10	0
54	MG	CA	1729	1/1	0.14	-	98,98,98,98	0
54	MG	BA	2997	1/1	0.34	-	57,57,57,57	0
54	MG	BA	3247	1/1	0.12	-	52,52,52,52	0
54	MG	BA	3105	1/1	0.24	-	60,60,60,60	0
54	MG	CA	1665	1/1	0.23	-	89,89,89,89	0
54	MG	DA	2973	1/1	0.28	-	50,50,50,50	0
54	MG	DB	208	1/1	0.23	-	96,96,96,96	0
54	MG	DA	3080	1/1	0.44	-	69,69,69,69	0
54	MG	BA	3033	1/1	0.19	-	67,67,67,67	0

6.5 Other polymers ⓘ

There are no such residues in this entry.