



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 22, 2026 – 09:46 PM UTC

PDB ID : 6BOK / pdb_00006bok
Title : E. coli release factor 1 (containing deletion 302-304) bound to the 70S ribosome
Authors : Svidritskiy, E.; Korostelev, A.A.
Deposited on : 2017-11-20
Resolution : 3.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

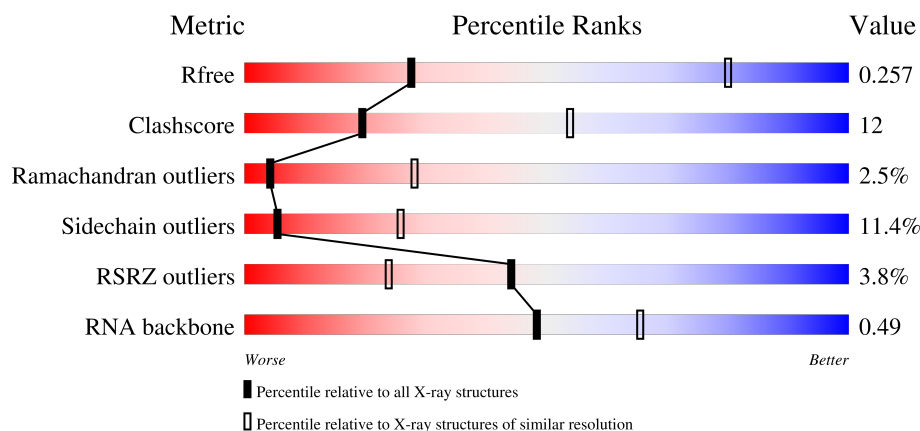
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 Å.

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



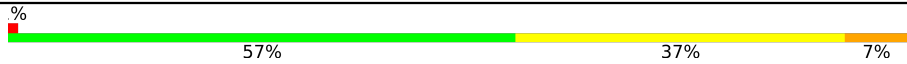
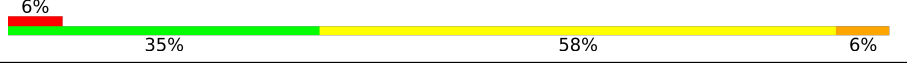
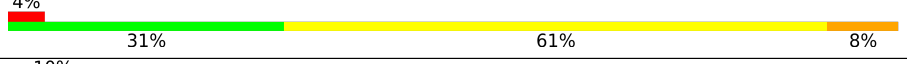
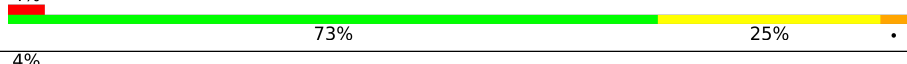
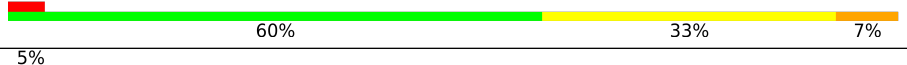
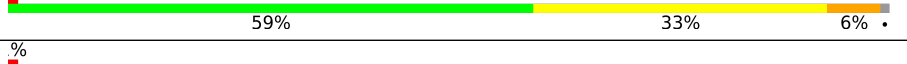
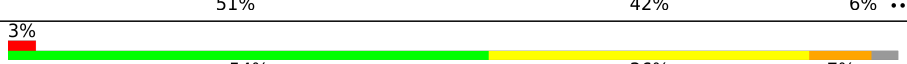
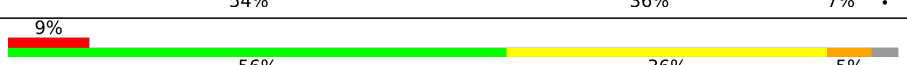
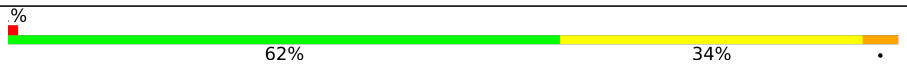
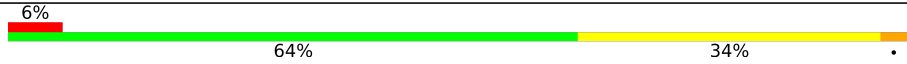
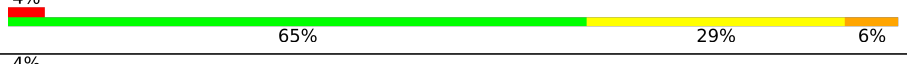
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)
RNA backbone	3983	1006 (4.02-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1507	3% 52% 42% 6%
1	DB	1507	3% 52% 41% 6%
2	B	2880	2% 54% 38% 8%
2	EB	2880	3% 55% 37% 8%

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Mol	Chain	Length	Quality of chain
3	C	120	
3	FB	120	
4	D	77	
4	GB	77	
4	IA	77	
4	LC	77	
5	E	275	
5	HB	275	
6	F	206	
6	IB	206	
7	G	205	
7	JB	205	
8	H	182	
8	KB	182	
9	I	180	
9	LB	180	
10	J	148	
10	MB	148	
11	K	140	
11	NB	140	
12	L	122	
12	OB	122	
13	M	150	
13	PB	150	
14	N	141	

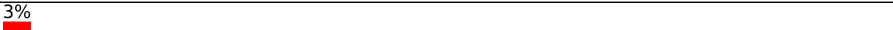
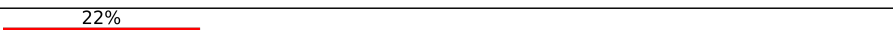
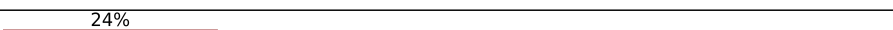
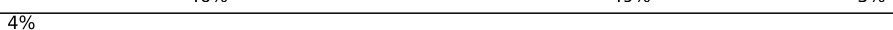
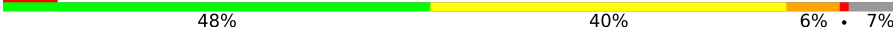
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Mol	Chain	Length	Quality of chain
14	QB	141	
15	O	118	
15	RB	118	
16	P	112	
16	SB	112	
17	Q	146	
17	TB	146	
18	R	118	
18	UB	118	
19	S	101	
19	VB	101	
20	T	113	
20	WB	113	
21	U	96	
21	XB	96	
22	V	110	
22	YB	110	
23	W	206	
23	ZB	206	
24	AC	85	
24	X	85	
25	BC	98	
25	Y	98	
26	CC	72	
26	Z	72	

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Mol	Chain	Length	Quality of chain
27	AA	60	
27	DC	60	
28	BA	71	
28	EC	71	
29	CA	60	
29	FC	60	
30	DA	54	
30	GC	54	
31	EA	49	
31	HC	49	
32	FA	65	
32	IC	65	
33	GA	37	
33	JC	37	
34	HA	27	
34	KC	27	
35	JA	256	
35	MC	256	
36	KA	239	
36	NC	239	
37	LA	209	
37	OC	209	
38	MA	162	
38	PC	162	
39	NA	101	

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Mol	Chain	Length	Quality of chain
39	QC	101	
40	OA	156	
40	RC	156	
41	PA	138	
41	SC	138	
42	QA	128	
42	TC	128	
43	RA	105	
43	UC	105	
44	SA	129	
44	VC	129	
45	TA	132	
45	WC	132	
46	UA	126	
46	XC	126	
47	VA	61	
47	YC	61	
48	WA	89	
48	ZC	89	
49	AD	88	
49	XA	88	
50	BD	105	
50	YA	105	
51	CD	88	
51	ZA	88	

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Mol	Chain	Length	Quality of chain
52	AB	93	
52	DD	93	
53	BB	106	
53	ED	106	
54	CB	27	
54	FD	27	
55	GD	365	
55	HD	365	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	A	1602	-	-	-	X
56	MG	A	1604	-	-	-	X
56	MG	A	1607	-	-	-	X
56	MG	A	1613	-	-	-	X
56	MG	A	1623	-	-	-	X
56	MG	A	1628	-	-	-	X
56	MG	A	1630	-	-	-	X
56	MG	A	1634	-	-	-	X
56	MG	A	1644	-	-	-	X
56	MG	A	1649	-	-	-	X
56	MG	A	1663	-	-	-	X
56	MG	A	1679	-	-	-	X
56	MG	A	1683	-	-	-	X
56	MG	A	1692	-	-	-	X
56	MG	A	1701	-	-	-	X
56	MG	A	1717	-	-	-	X
56	MG	A	1747	-	-	-	X
56	MG	AC	102	-	-	-	X
56	MG	B	2902	-	-	-	X
56	MG	B	2903	-	-	-	X
56	MG	B	2904	-	-	-	X
56	MG	B	2905	-	-	-	X
56	MG	B	2914	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	B	2924	-	-	-	X
56	MG	B	2933	-	-	-	X
56	MG	B	2936	-	-	-	X
56	MG	B	2942	-	-	-	X
56	MG	B	2947	-	-	-	X
56	MG	B	2950	-	-	-	X
56	MG	B	2953	-	-	-	X
56	MG	B	2960	-	-	-	X
56	MG	B	2964	-	-	-	X
56	MG	B	2966	-	-	-	X
56	MG	B	2967	-	-	-	X
56	MG	B	3006	-	-	-	X
56	MG	B	3018	-	-	-	X
56	MG	B	3029	-	-	-	X
56	MG	B	3077	-	-	-	X
56	MG	B	3119	-	-	-	X
56	MG	B	3125	-	-	-	X
56	MG	B	3175	-	-	-	X
56	MG	B	3207	-	-	-	X
56	MG	B	3262	-	-	-	X
56	MG	B	3283	-	-	-	X
56	MG	B	3285	-	-	-	X
56	MG	B	3331	-	-	-	X
56	MG	B	3370	-	-	-	X
56	MG	C	201	-	-	-	X
56	MG	DB	1602	-	-	-	X
56	MG	DB	1603	-	-	-	X
56	MG	DB	1604	-	-	-	X
56	MG	DB	1607	-	-	-	X
56	MG	DB	1608	-	-	-	X
56	MG	DB	1610	-	-	-	X
56	MG	DB	1614	-	-	-	X
56	MG	DB	1615	-	-	-	X
56	MG	DB	1617	-	-	-	X
56	MG	DB	1618	-	-	-	X
56	MG	DB	1622	-	-	-	X
56	MG	DB	1633	-	-	-	X
56	MG	DB	1639	-	-	-	X
56	MG	DB	1699	-	-	-	X
56	MG	DB	1703	-	-	-	X
56	MG	DB	1721	-	-	-	X
56	MG	DB	1738	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	EB	2902	-	-	-	X
56	MG	EB	2903	-	-	-	X
56	MG	EB	2904	-	-	-	X
56	MG	EB	2909	-	-	-	X
56	MG	EB	2911	-	-	-	X
56	MG	EB	2915	-	-	-	X
56	MG	EB	2925	-	-	-	X
56	MG	EB	2935	-	-	-	X
56	MG	EB	2936	-	-	-	X
56	MG	EB	2939	-	-	-	X
56	MG	EB	2945	-	-	-	X
56	MG	EB	2947	-	-	-	X
56	MG	EB	2948	-	-	-	X
56	MG	EB	2950	-	-	-	X
56	MG	EB	2954	-	-	-	X
56	MG	EB	2957	-	-	-	X
56	MG	EB	2960	-	-	-	X
56	MG	EB	2962	-	-	-	X
56	MG	EB	2966	-	-	-	X
56	MG	EB	2971	-	-	-	X
56	MG	EB	2979	-	-	-	X
56	MG	EB	2988	-	-	-	X
56	MG	EB	2996	-	-	-	X
56	MG	EB	3004	-	-	-	X
56	MG	EB	3025	-	-	-	X
56	MG	EB	3035	-	-	-	X
56	MG	EB	3047	-	-	-	X
56	MG	EB	3057	-	-	-	X
56	MG	EB	3103	-	-	-	X
56	MG	EB	3123	-	-	-	X
56	MG	EB	3156	-	-	-	X
56	MG	EB	3246	-	-	-	X
56	MG	FA	101	-	-	-	X
56	MG	FB	201	-	-	-	X
56	MG	FB	205	-	-	-	X
56	MG	GD	401	-	-	-	X
56	MG	HD	401	-	-	-	X
56	MG	IA	105	-	-	-	X
56	MG	IA	107	-	-	-	X
56	MG	JB	301	-	-	-	X
56	MG	LC	103	-	-	-	X
56	MG	VA	101	-	-	-	X

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 299566 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1507	Total	C	N	O	P	0	0	0
			32394	14424	5998	10465	1507			
1	DB	1507	Total	C	N	O	P	0	0	0
			32394	14424	5998	10465	1507			

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	2880	Total	C	N	O	P	0	0	0
			62031	27612	11589	19950	2880			
2	EB	2880	Total	C	N	O	P	0	0	0
			62031	27612	11589	19950	2880			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	154A	C	UNK	conflict	GB 46197919
EB	154A	C	UNK	conflict	GB 46197919

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			
3	FB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			

- Molecule 4 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	77	Total	C	N	O	P S	0	0	0
			1642	734	297	534	76 1			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	IA	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			
4	GB	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			
4	LC	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			
5	HB	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
6	IB	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			
7	JB	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	181	Total	C	N	O	S	0	0	0
			1471	940	267	260	4			
8	KB	181	Total	C	N	O	S	0	0	0
			1471	940	267	260	4			

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
9	LB	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	146	Total	C	N	O	S	0	0	0
			1137	727	201	208	1			
10	MB	146	Total	C	N	O	S	0	0	0
			1137	727	201	208	1			

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
11	NB	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			
12	OB	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
13	PB	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	QB	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
15	RB	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	110	Total	C	N	O	S	0	0	0
			877	553	175	149				
16	SB	110	Total	C	N	O	S	0	0	0
			877	553	175	149				

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			
17	TB	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
18	UB	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
19	VB	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			
20	WB	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
21	XB	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	107	Total	C	N	O	S	0	0	0
			814	523	154	131	6			
22	YB	107	Total	C	N	O	S	0	0	0
			814	523	154	131	6			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	189	Total	C	N	O	S	0	0	0
			1495	953	266	273	3			
23	ZB	189	Total	C	N	O	S	0	0	0
			1495	953	266	273	3			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
24	AC	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	11	ARG	LYS	conflict	UNP Q72HR3

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Chain	Residue	Modelled	Actual	Comment	Reference
AC	11	ARG	LYS	conflict	UNP Q72HR3

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	97	Total	C	N	O	S	0	0	0
			761	478	151	131	1			
25	BC	97	Total	C	N	O	S	0	0	0
			761	478	151	131	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			
26	CC	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	AA	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			
27	DC	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BA	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			
28	EC	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	CA	59	Total	C	N	O	S	0	0	0
			460	290	90	75	5			
29	FC	59	Total	C	N	O	S	0	0	0
			460	290	90	75	5			

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	DA	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
30	GC	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	EA	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
31	HC	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	FA	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
32	IC	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	GA	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
33	JC	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	HA	11	Total	C	N	O	P	0	0	0
			220	98	44	67	11			
34	KC	11	Total	C	N	O	P	0	0	0
			220	98	44	67	11			

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	JA	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			
35	MC	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	KA	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
36	NC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	LA	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
37	OC	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	MA	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
38	PC	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	NA	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
39	QC	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	OA	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RC	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	PA	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
41	SC	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	QA	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				
42	TC	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	RA	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			
43	UC	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	SA	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			
44	VC	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	TA	122	Total	C	N	O	S	0	0	0
			958	604	193	159	2			
45	WC	122	Total	C	N	O	S	0	0	0
			958	604	193	159	2			

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	UA	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			
46	XC	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	VA	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
47	YC	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	WA	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
48	ZC	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	XA	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
49	AD	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	YA	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			
50	BD	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	ZA	70	Total	C	N	O	0	0	0
			574	367	112	95			
51	CD	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	AB	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
52	DD	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BB	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
53	ED	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 54 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	CB	24	Total	C	N	O	0	0	0
			208	128	50	30			
54	FD	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 55 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	GD	255	Total	C	N	O	S	0	0	0
			1980	1214	374	384	8			
55	HD	255	Total	C	N	O	S	0	0	0
			1980	1214	374	384	8			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
GD	?	-	ASP	deletion	UNP B7MKB3
GD	?	-	ARG	deletion	UNP B7MKB3
GD	?	-	SER	deletion	UNP B7MKB3

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Chain	Residue	Modelled	Actual	Comment	Reference
GD	361	LEU	-	expression tag	UNP B7MKB3
GD	362	GLU	-	expression tag	UNP B7MKB3
GD	363	HIS	-	expression tag	UNP B7MKB3
GD	364	HIS	-	expression tag	UNP B7MKB3
GD	365	HIS	-	expression tag	UNP B7MKB3
GD	366	HIS	-	expression tag	UNP B7MKB3
GD	367	HIS	-	expression tag	UNP B7MKB3
GD	368	HIS	-	expression tag	UNP B7MKB3
HD	?	-	ASP	deletion	UNP B7MKB3
HD	?	-	ARG	deletion	UNP B7MKB3
HD	?	-	SER	deletion	UNP B7MKB3
HD	361	LEU	-	expression tag	UNP B7MKB3
HD	362	GLU	-	expression tag	UNP B7MKB3
HD	363	HIS	-	expression tag	UNP B7MKB3
HD	364	HIS	-	expression tag	UNP B7MKB3
HD	365	HIS	-	expression tag	UNP B7MKB3
HD	366	HIS	-	expression tag	UNP B7MKB3
HD	367	HIS	-	expression tag	UNP B7MKB3
HD	368	HIS	-	expression tag	UNP B7MKB3

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	A	160	Total Mg 160 160	0	0
56	B	514	Total Mg 514 514	0	0
56	C	23	Total Mg 23 23	0	0
56	D	6	Total Mg 6 6	0	0
56	E	4	Total Mg 4 4	0	0
56	F	1	Total Mg 1 1	0	0
56	G	4	Total Mg 4 4	0	0
56	H	1	Total Mg 1 1	0	0
56	I	3	Total Mg 3 3	0	0
56	J	5	Total Mg 5 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	K	2	Total 2	Mg 2	0	0
56	L	7	Total 7	Mg 7	0	0
56	M	4	Total 4	Mg 4	0	0
56	N	3	Total 3	Mg 3	0	0
56	O	1	Total 1	Mg 1	0	0
56	P	2	Total 2	Mg 2	0	0
56	Q	3	Total 3	Mg 3	0	0
56	R	4	Total 4	Mg 4	0	0
56	S	3	Total 3	Mg 3	0	0
56	T	2	Total 2	Mg 2	0	0
56	U	2	Total 2	Mg 2	0	0
56	V	5	Total 5	Mg 5	0	0
56	W	12	Total 12	Mg 12	0	0
56	Y	4	Total 4	Mg 4	0	0
56	Z	3	Total 3	Mg 3	0	0
56	CA	1	Total 1	Mg 1	0	0
56	EA	1	Total 1	Mg 1	0	0
56	FA	1	Total 1	Mg 1	0	0
56	HA	1	Total 1	Mg 1	0	0
56	IA	8	Total 8	Mg 8	0	0
56	JA	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	KA	1	Total 1	Mg 1	0	0
56	LA	1	Total 1	Mg 1	0	0
56	MA	3	Total 3	Mg 3	0	0
56	NA	2	Total 2	Mg 2	0	0
56	OA	3	Total 3	Mg 3	0	0
56	PA	2	Total 2	Mg 2	0	0
56	RA	2	Total 2	Mg 2	0	0
56	SA	1	Total 1	Mg 1	0	0
56	TA	3	Total 3	Mg 3	0	0
56	VA	2	Total 2	Mg 2	0	0
56	WA	3	Total 3	Mg 3	0	0
56	YA	2	Total 2	Mg 2	0	0
56	ZA	1	Total 1	Mg 1	0	0
56	AB	1	Total 1	Mg 1	0	0
56	BB	1	Total 1	Mg 1	0	0
56	DB	177	Total 177	Mg 177	0	0
56	EB	395	Total 395	Mg 395	0	0
56	FB	17	Total 17	Mg 17	0	0
56	GB	5	Total 5	Mg 5	0	0
56	HB	8	Total 8	Mg 8	0	0
56	IB	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	JB	2	Total 2	Mg 2	0	0
56	KB	1	Total 1	Mg 1	0	0
56	LB	5	Total 5	Mg 5	0	0
56	MB	2	Total 2	Mg 2	0	0
56	NB	1	Total 1	Mg 1	0	0
56	OB	3	Total 3	Mg 3	0	0
56	PB	2	Total 2	Mg 2	0	0
56	QB	3	Total 3	Mg 3	0	0
56	RB	5	Total 5	Mg 5	0	0
56	SB	1	Total 1	Mg 1	0	0
56	TB	5	Total 5	Mg 5	0	0
56	VB	1	Total 1	Mg 1	0	0
56	WB	3	Total 3	Mg 3	0	0
56	XB	2	Total 2	Mg 2	0	0
56	YB	3	Total 3	Mg 3	0	0
56	ZB	2	Total 2	Mg 2	0	0
56	AC	2	Total 2	Mg 2	0	0
56	BC	1	Total 1	Mg 1	0	0
56	DC	1	Total 1	Mg 1	0	0
56	FC	1	Total 1	Mg 1	0	0
56	HC	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	IC	2	Total 2	Mg 2	0	0
56	JC	1	Total 1	Mg 1	0	0
56	KC	1	Total 1	Mg 1	0	0
56	LC	8	Total 8	Mg 8	0	0
56	MC	3	Total 3	Mg 3	0	0
56	PC	2	Total 2	Mg 2	0	0
56	QC	2	Total 2	Mg 2	0	0
56	RC	2	Total 2	Mg 2	0	0
56	SC	1	Total 1	Mg 1	0	0
56	TC	2	Total 2	Mg 2	0	0
56	UC	1	Total 1	Mg 1	0	0
56	WC	2	Total 2	Mg 2	0	0
56	XC	2	Total 2	Mg 2	0	0
56	YC	1	Total 1	Mg 1	0	0
56	ZC	1	Total 1	Mg 1	0	0
56	AD	1	Total 1	Mg 1	0	0
56	BD	2	Total 2	Mg 2	0	0
56	CD	2	Total 2	Mg 2	0	0
56	ED	1	Total 1	Mg 1	0	0
56	GD	5	Total 5	Mg 5	0	0
56	HD	3	Total 3	Mg 3	0	0

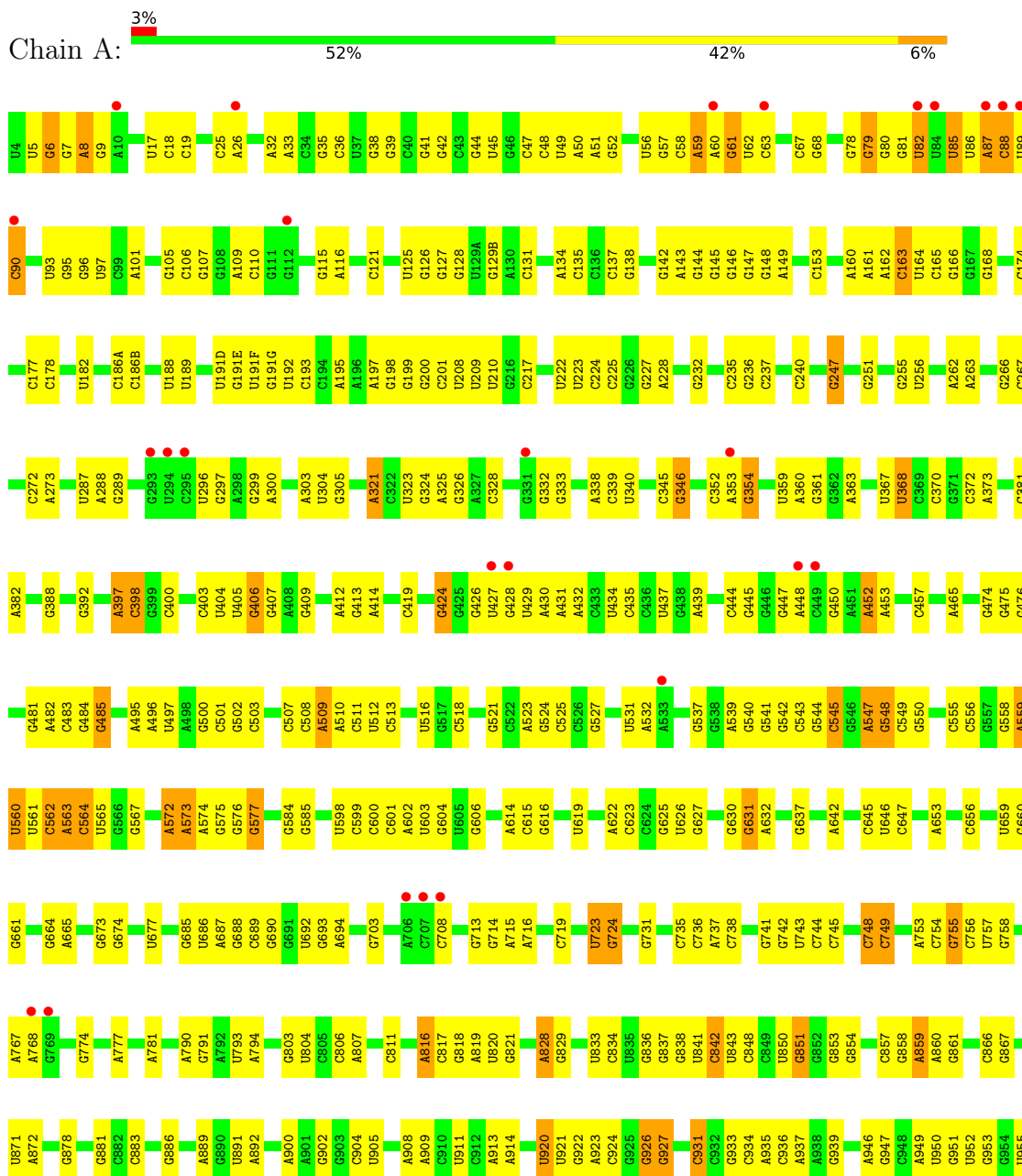
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

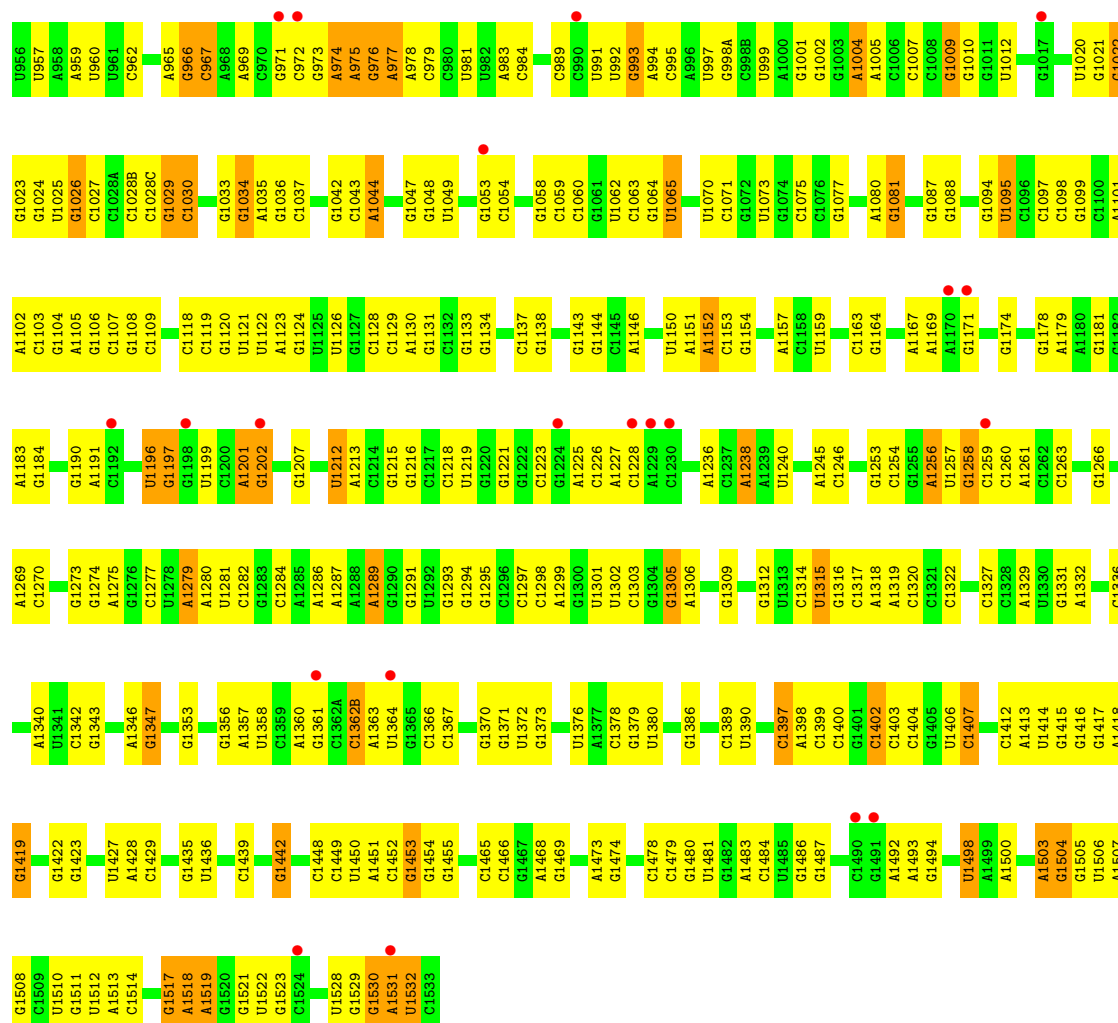
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	V	1	Total 1	Zn 1	0	0
57	BA	1	Total 1	Zn 1	0	0
57	CA	1	Total 1	Zn 1	0	0
57	DA	1	Total 1	Zn 1	0	0
57	GA	1	Total 1	Zn 1	0	0
57	YB	1	Total 1	Zn 1	0	0
57	EC	1	Total 1	Zn 1	0	0
57	FC	1	Total 1	Zn 1	0	0
57	GC	1	Total 1	Zn 1	0	0
57	JC	1	Total 1	Zn 1	0	0

3 Residue-property plots

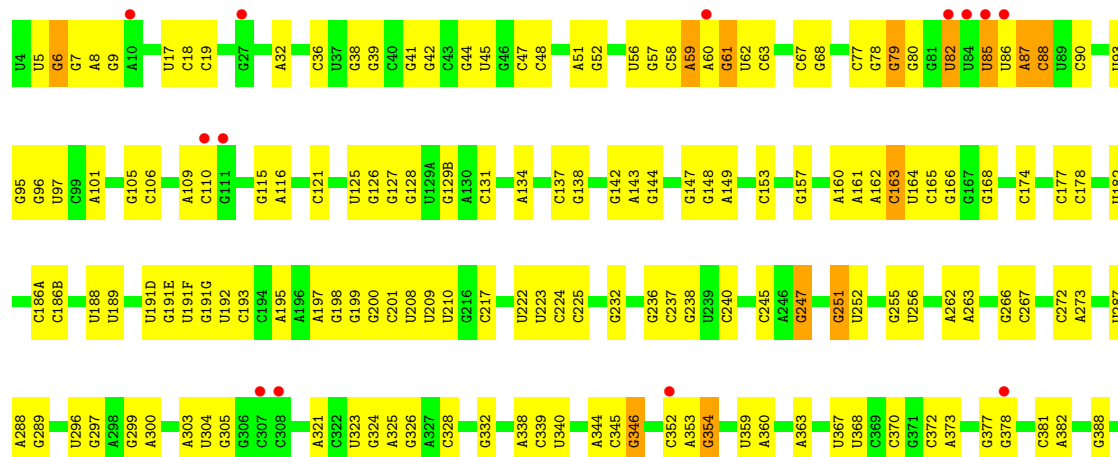
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

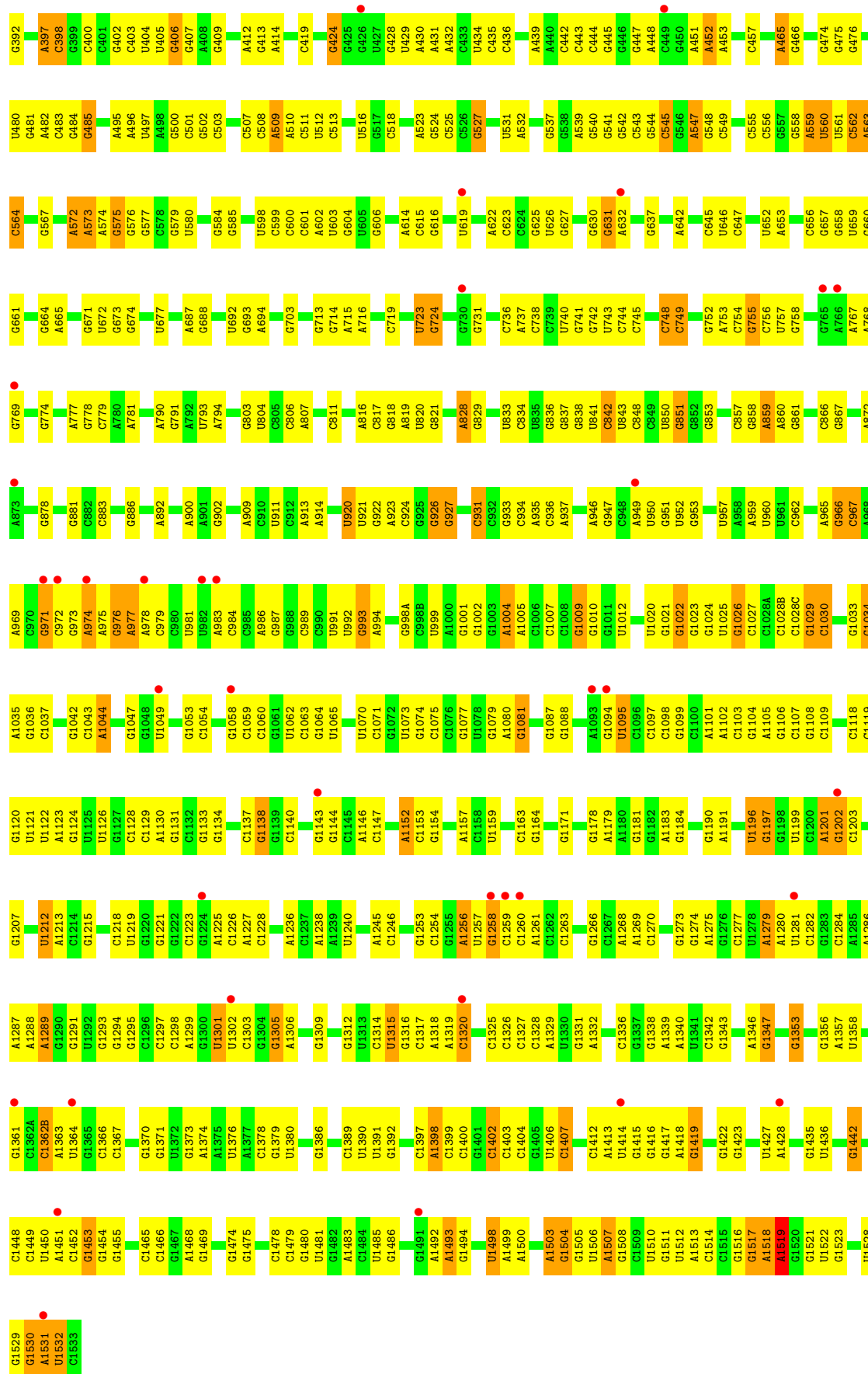
• Molecule 1: 16S ribosomal RNA



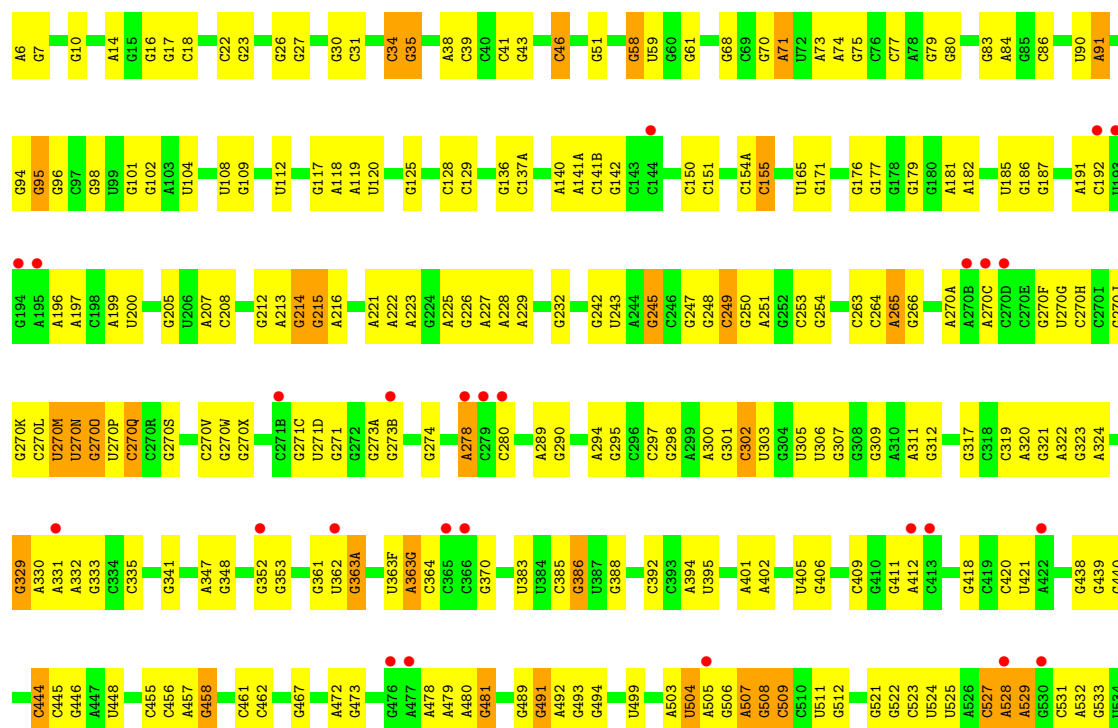
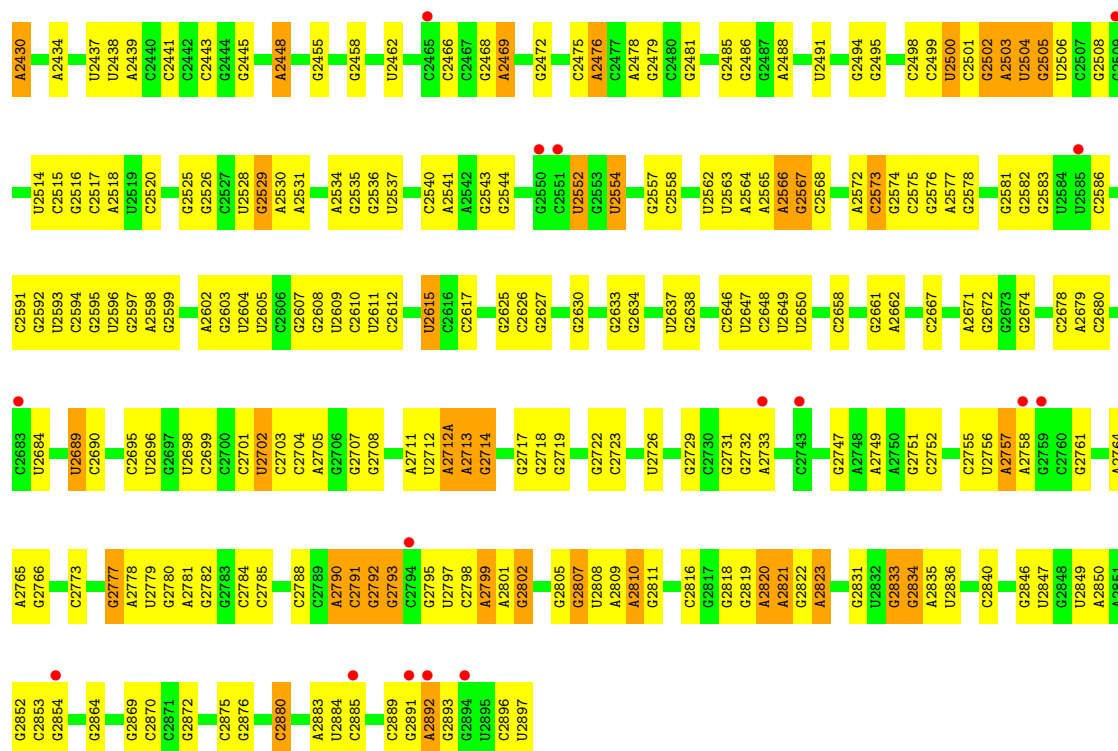


● Molecule 1: 16S ribosomal RNA

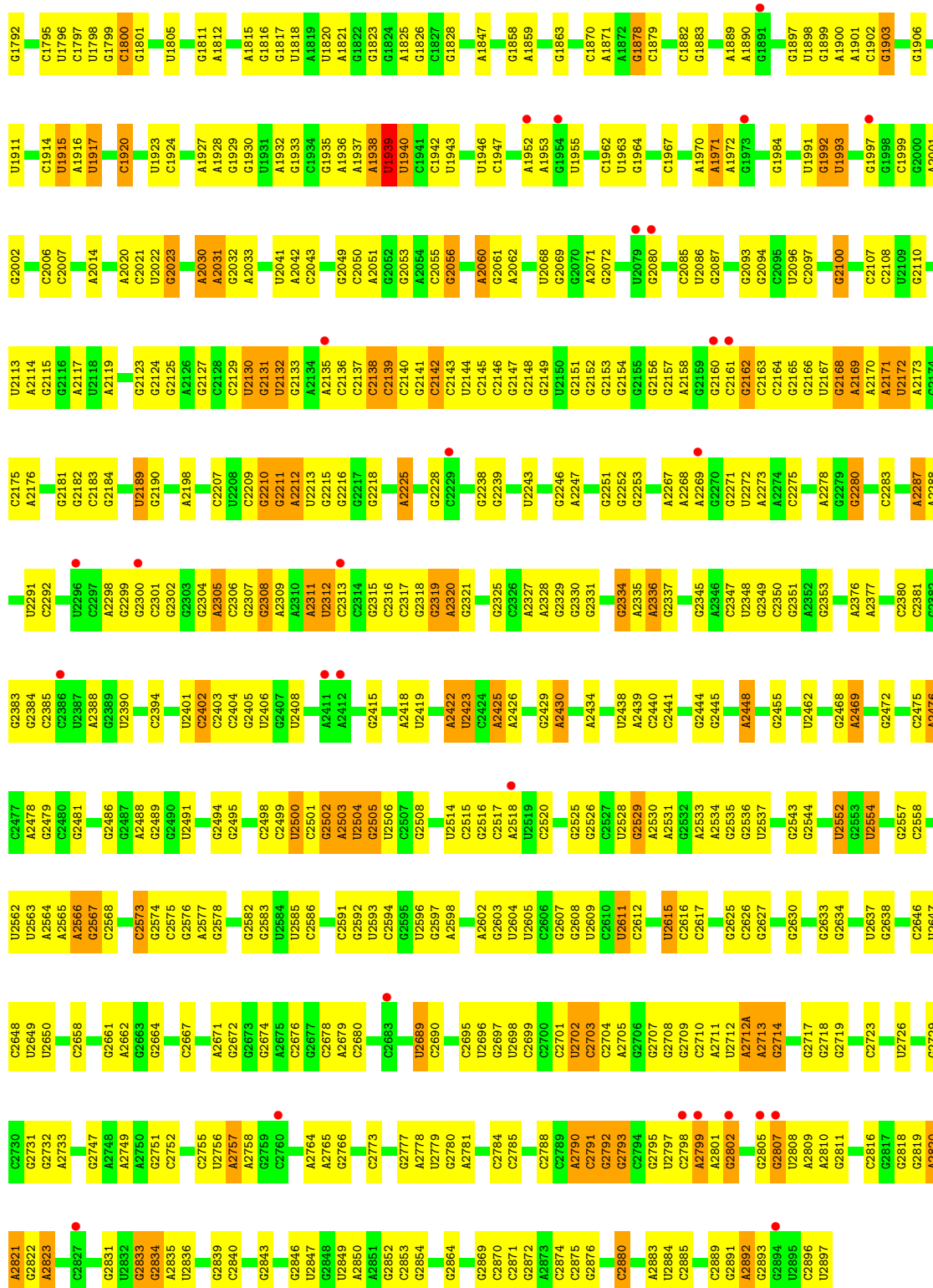




C1180	C1186	C1187	C1188	C1189	C1196	C1202	C1203	C1204	C1205	C1209	C1210	C1211	C1212	C1213	C1214	C1218	C1219	C1220	C1225	C1226	C1227	C1240	C1243	C1246	C1251	C1252	C1253	C1254	C1255	C1256	C1260	C1261	C1264	C1268	C1269	C1270	C1271	C1272	C1273	C1278	C1288	C1291	C1292	C1293	C1299	C1300	C1301	C1302	C1310	C1319	C1320	C1321	C1322	C1326	C1327	C1333	C1334	C1335	C1336	C1339	C1340	C1341	C1342	C1343	C1344	C1345	C1352	C1353	C1354	C1355	C1356	C1357	C1358	C1359	C1360	C1364	C1365	C1366	C1367	C1368	C1372	C1379	C1380	C1384	C1385	C1389	C1392	C1393																			
U1394	U1395	U1396	U1405	U1406	U1407	U1408	U1409	U1410	U1416	U1417	U1418	U1419	U1420	U1421	U1425	U1426	U1427	U1428	U1434	U1437	U1438	U1441	U1444B	U1449B	U1449	U1450	U1454	U1455	U1460	U1461	U1464	U1465	U1466	U1467	U1468	U1469	U1470	U1471	U1477	U1478	U1483	U1484	U1488	U1493	U1594	U1595	U1596	U1597	U1598	U1599	U1602	U1603	U1604	U1605	U1608	U1609	U1610	U1614	U1618	U1625	U1626	U1630B	U1631	U1635	U1636	U1637	U1638	U1639	U1640	U1641	U1642	U1647	U1648	U1651	U1652	U1653	U1654	U1657	U1658	U1659	U1672	U1673	U1674																								
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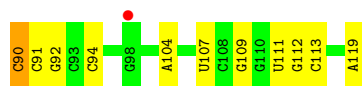
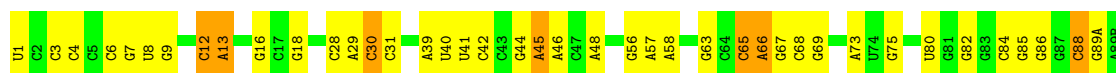


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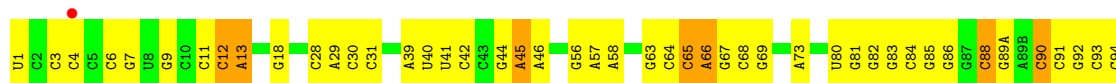


• Molecule 3: 5S ribosomal RNA





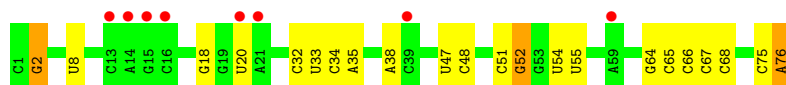
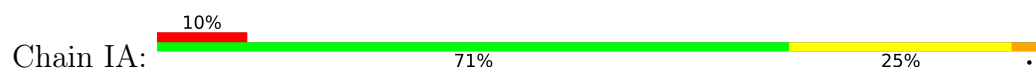
• Molecule 3: 5S ribosomal RNA



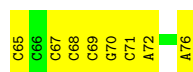
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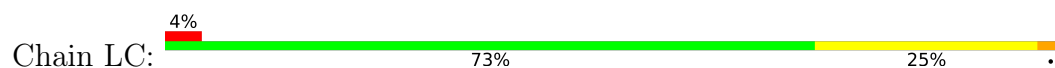
• Molecule 4: 16S ribosomal RNA



• Molecule 4: 16S ribosomal RNA

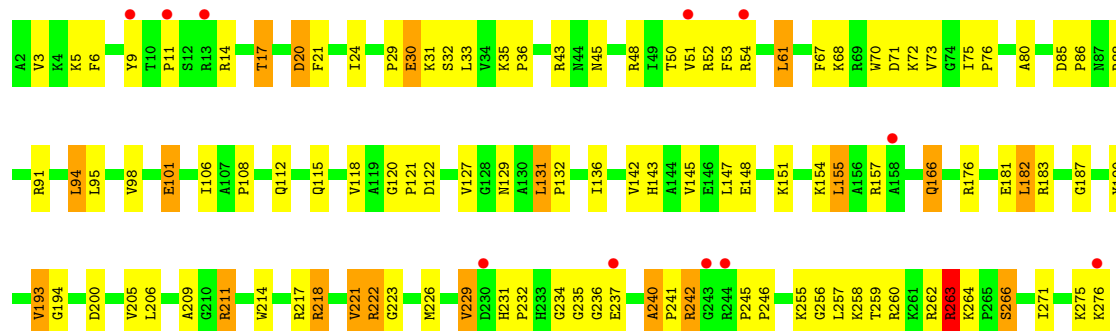


• Molecule 4: 16S ribosomal RNA

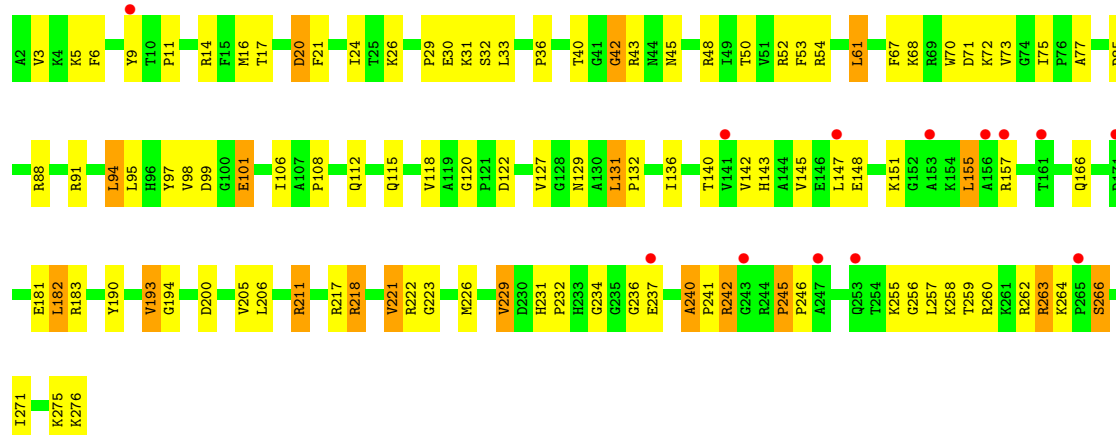




• Molecule 5: 50S ribosomal protein L2



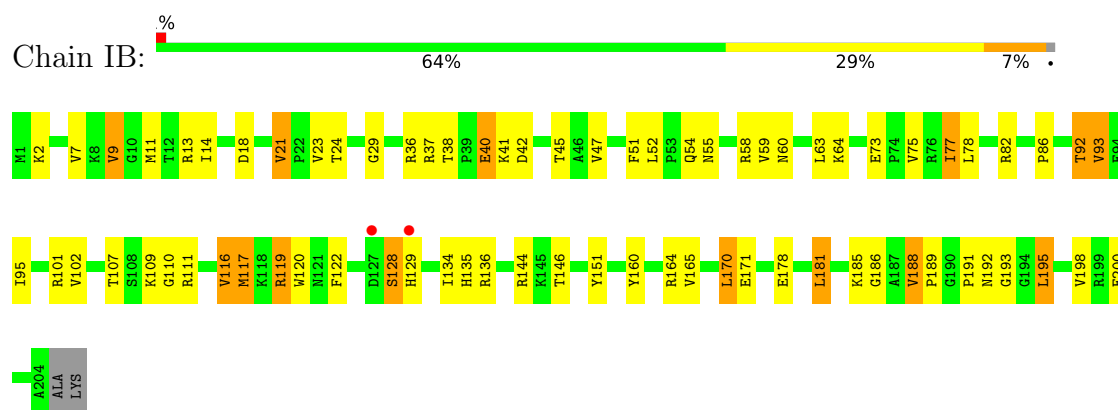
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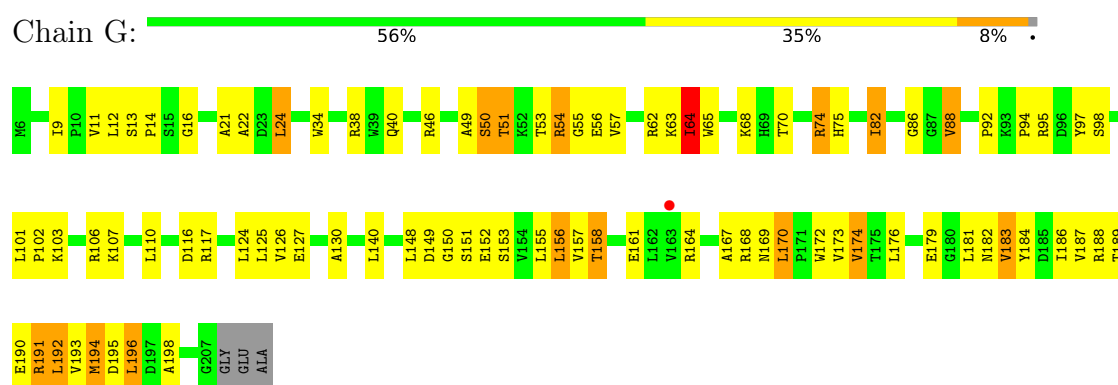
• Molecule 6: 50S ribosomal protein L3



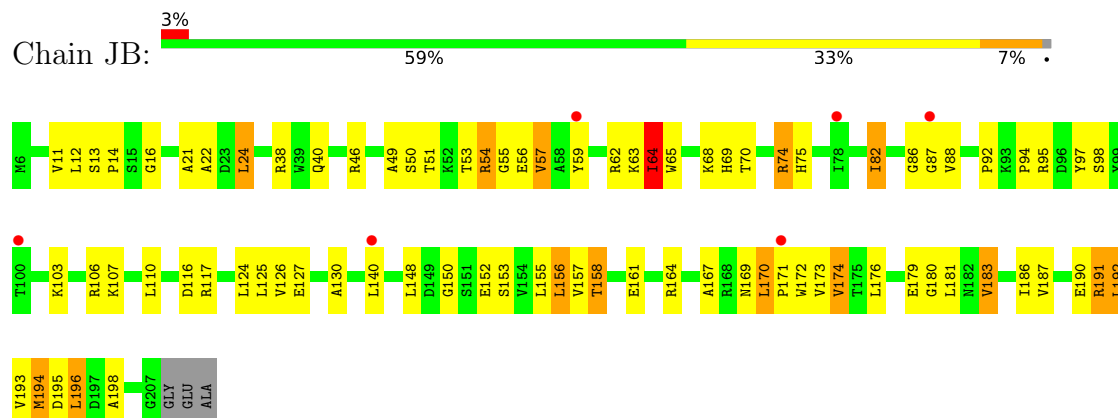
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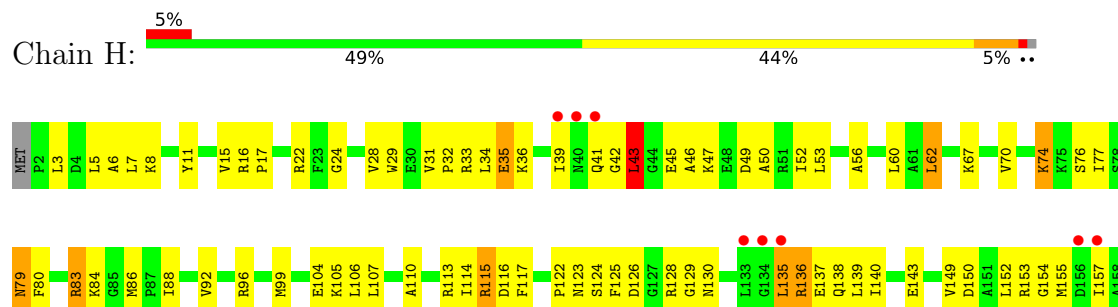
• Molecule 7: 50S ribosomal protein L4



• Molecule 7: 50S ribosomal protein L4

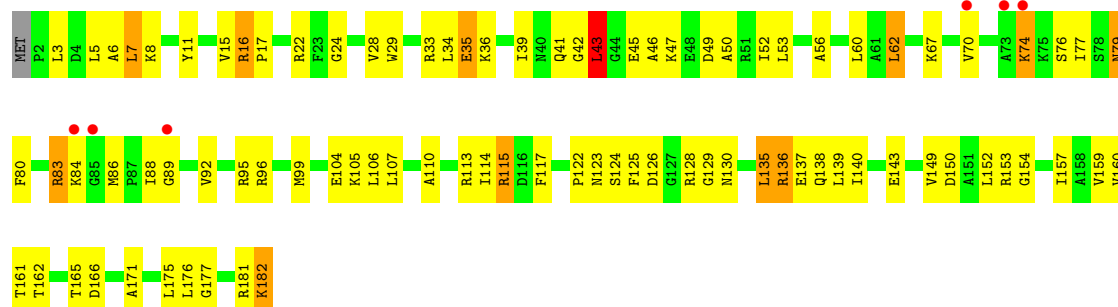


• Molecule 8: 50S ribosomal protein L5

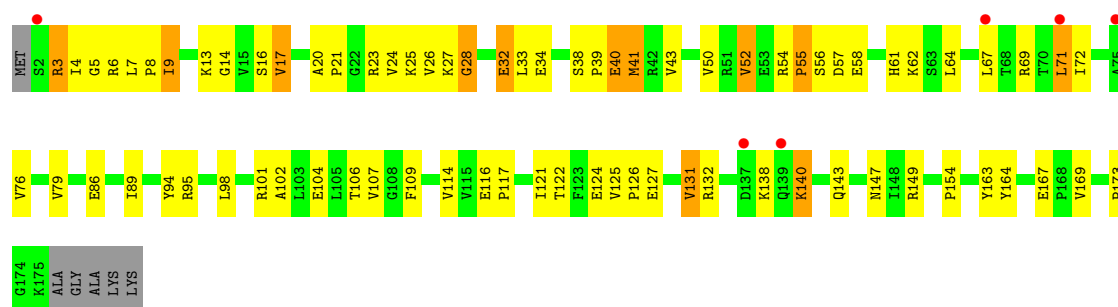




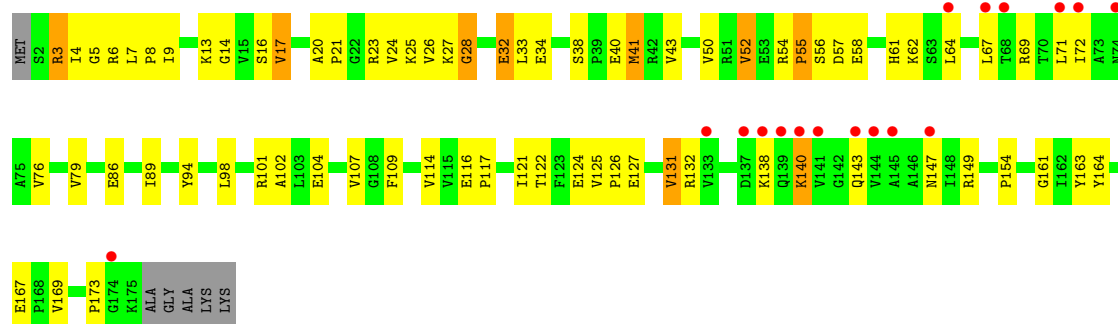
• Molecule 8: 50S ribosomal protein L5



• Molecule 9: 50S ribosomal protein L6

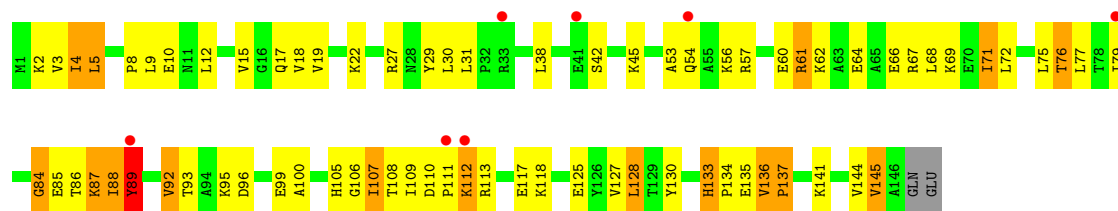


• Molecule 9: 50S ribosomal protein L6

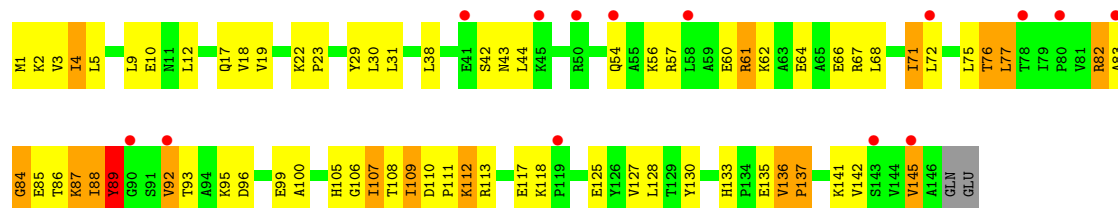


• Molecule 10: 50S ribosomal protein L9

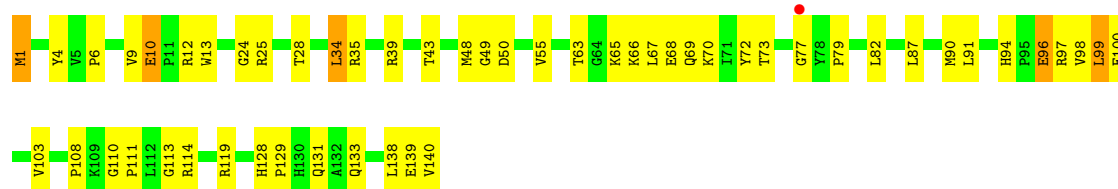




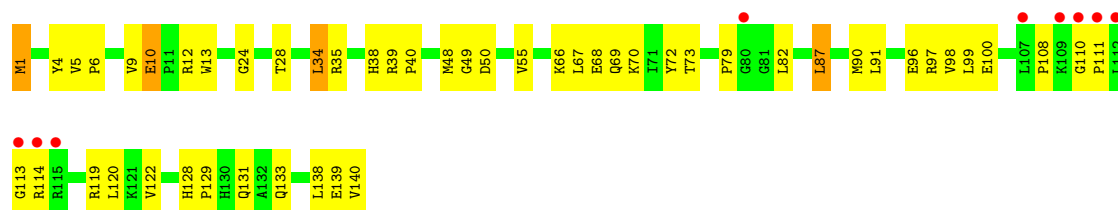
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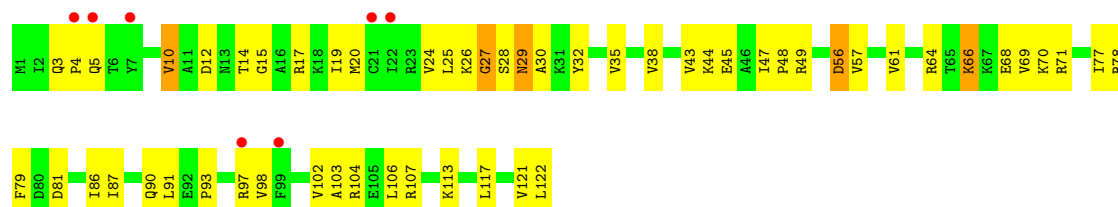
• Molecule 11: 50S ribosomal protein L13



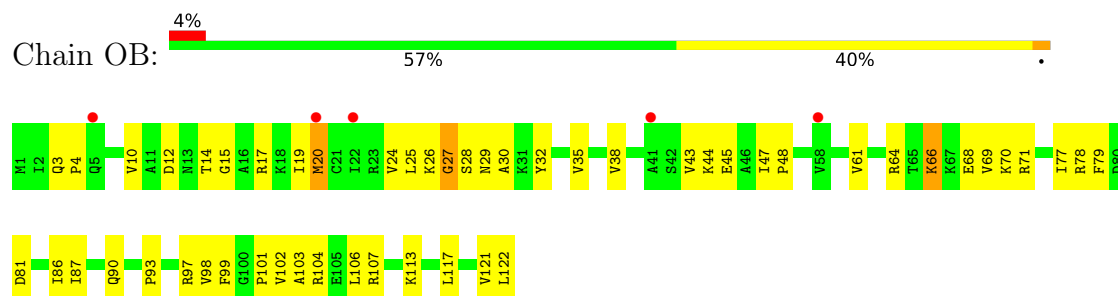
• Molecule 11: 50S ribosomal protein L13



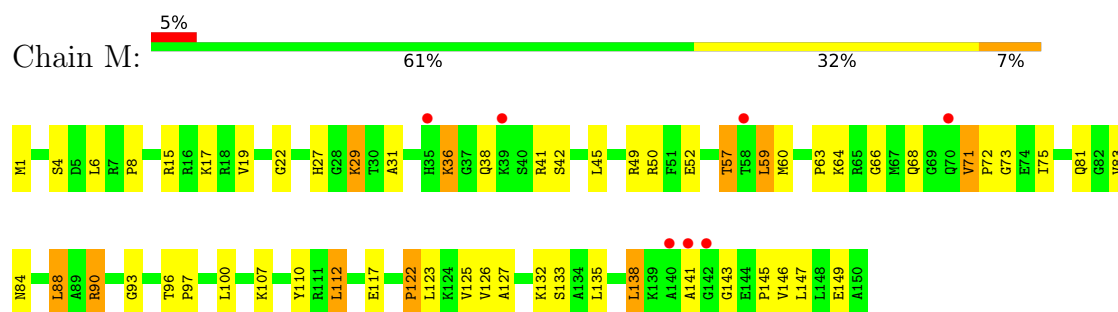
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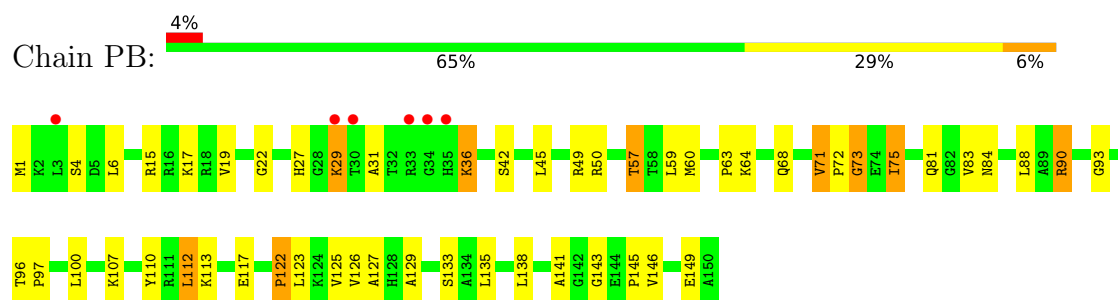
- Molecule 12: 50S ribosomal protein L14



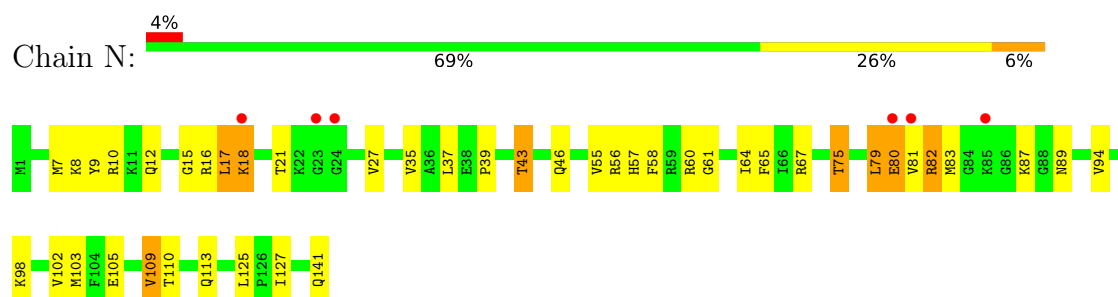
- Molecule 13: 50S ribosomal protein L15



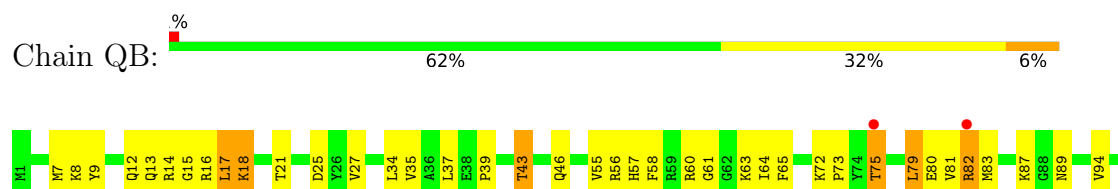
- Molecule 13: 50S ribosomal protein L15



- Molecule 14: 50S ribosomal protein L16

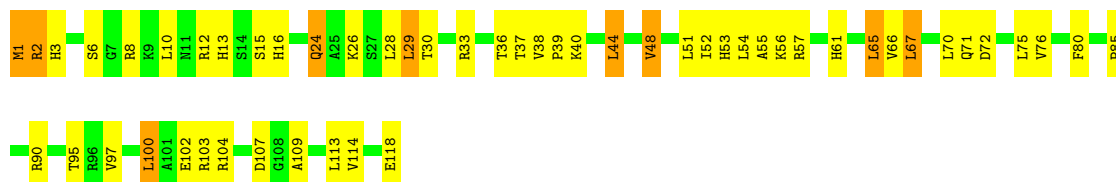


- Molecule 14: 50S ribosomal protein L16





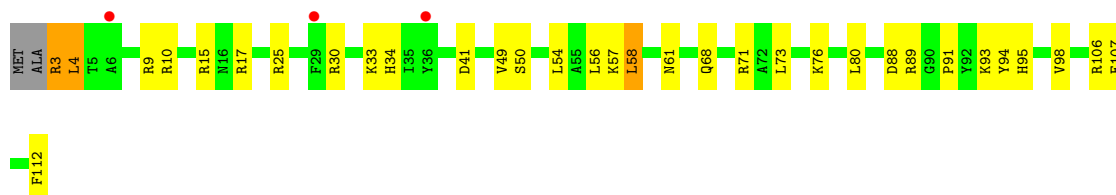
- Molecule 15: 50S ribosomal protein L17



- Molecule 15: 50S ribosomal protein L17



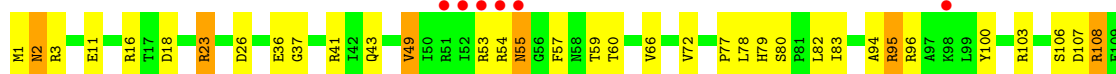
- Molecule 16: 50S ribosomal protein L18



- Molecule 16: 50S ribosomal protein L18

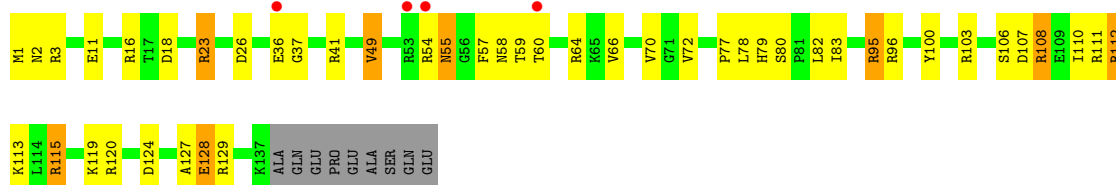


- Molecule 17: 50S ribosomal protein L19

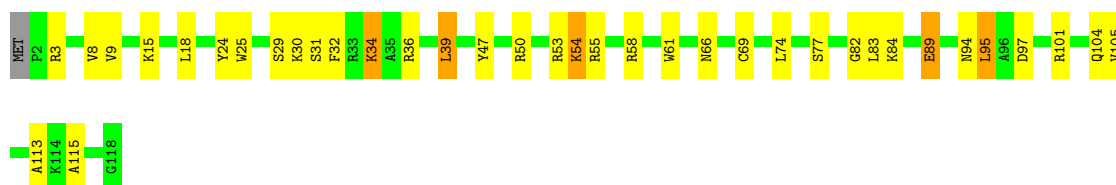




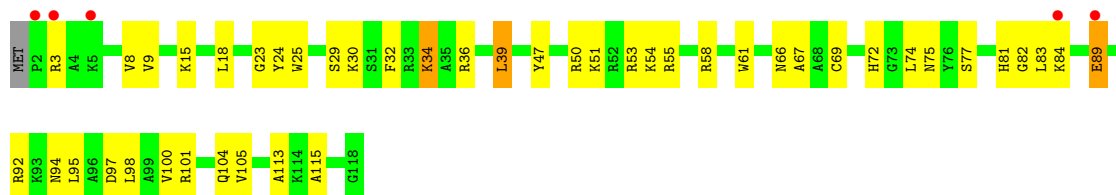
- Molecule 17: 50S ribosomal protein L19



- Molecule 18: 50S ribosomal protein L20



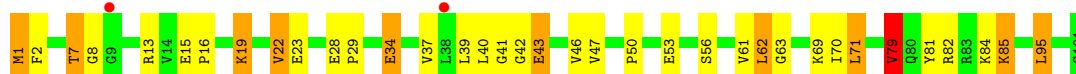
- Molecule 18: 50S ribosomal protein L20



- Molecule 19: 50S ribosomal protein L21

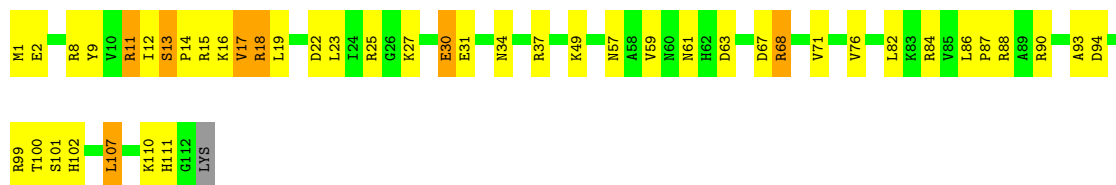


- Molecule 19: 50S ribosomal protein L21



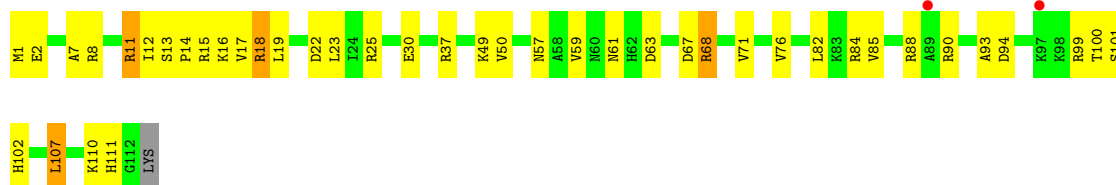
- Molecule 20: 50S ribosomal protein L22

Chain T:  59% 34% 6% .



- Molecule 20: 50S ribosomal protein L22

Chain WB:  2% 62% 34% . .



- Molecule 21: 50S ribosomal protein L23

Chain U:  77% 21% ..



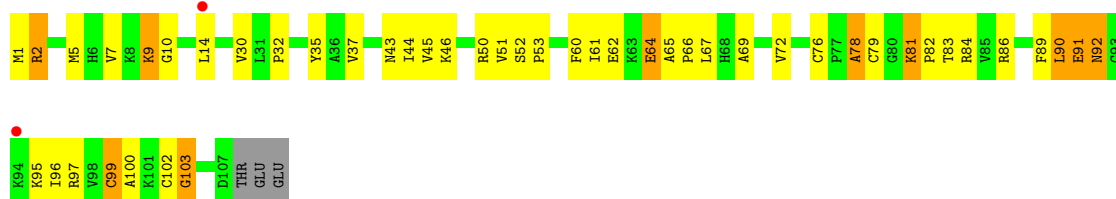
- Molecule 21: 50S ribosomal protein L23

Chain XB:  5% 77% 21% ..



- Molecule 22: 50S ribosomal protein L24

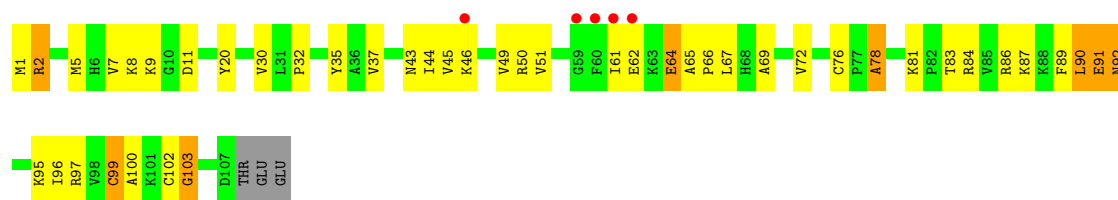
Chain V:  2% 55% 34% 9% .



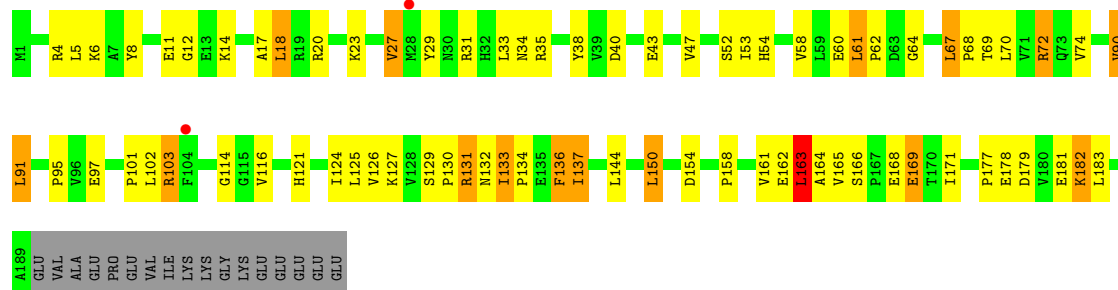
- Molecule 22: 50S ribosomal protein L24

Chain YB:  5% 56% 34% 7% .

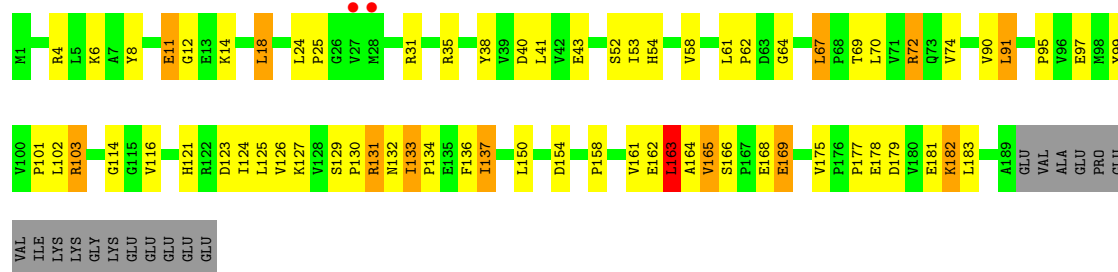




• Molecule 23: 50S ribosomal protein L25



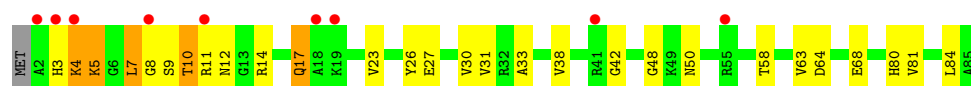
• Molecule 23: 50S ribosomal protein L25



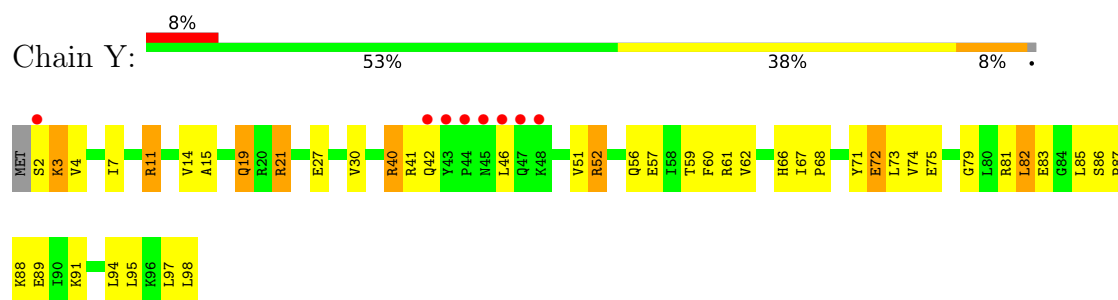
• Molecule 24: 50S ribosomal protein L27



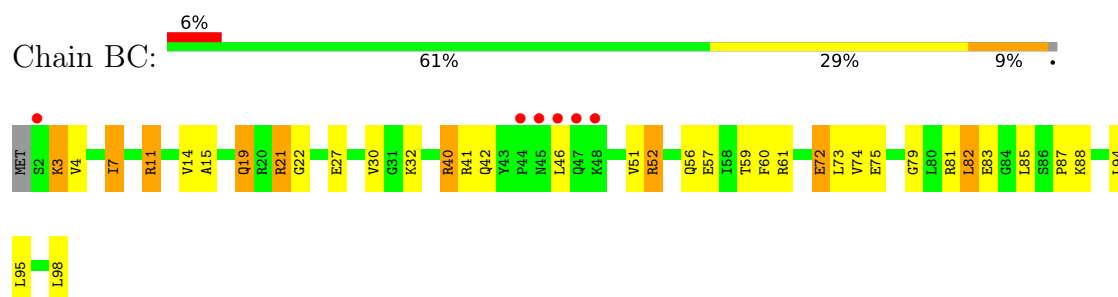
• Molecule 24: 50S ribosomal protein L27



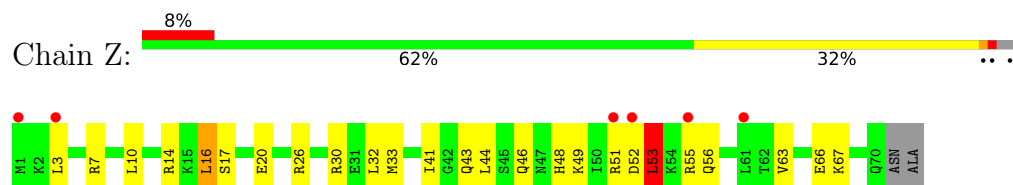
• Molecule 25: 50S ribosomal protein L28



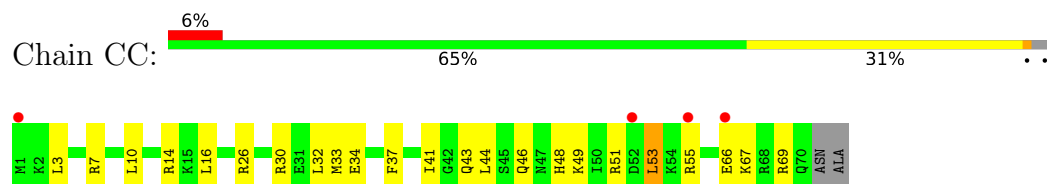
- Molecule 25: 50S ribosomal protein L28



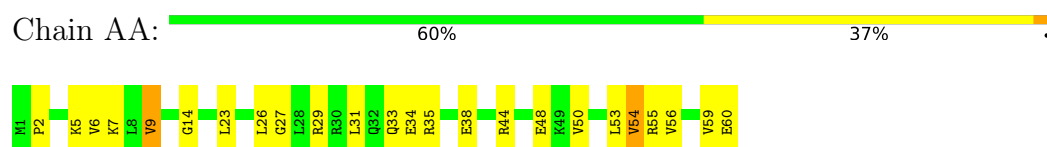
- Molecule 26: 50S ribosomal protein L29



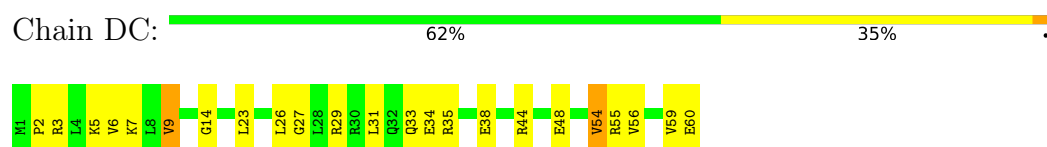
- Molecule 26: 50S ribosomal protein L29



- Molecule 27: 50S ribosomal protein L30



- Molecule 27: 50S ribosomal protein L30



- Molecule 28: 50S ribosomal protein L31

Chain BA:  56% 34% 6% ..



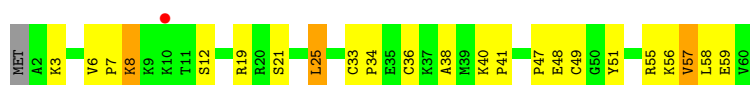
- Molecule 28: 50S ribosomal protein L31

Chain EC:  59% 31% 6% ..



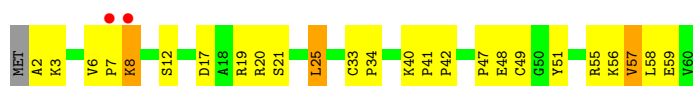
- Molecule 29: 50S ribosomal protein L32

Chain CA:  60% 33% 5% .



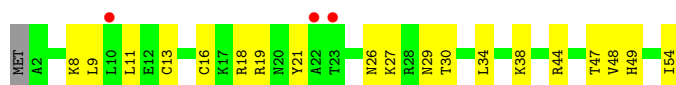
- Molecule 29: 50S ribosomal protein L32

Chain FC:  57% 37% 5% .



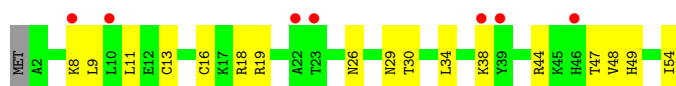
- Molecule 30: 50S ribosomal protein L33

Chain DA:  63% 35% .



- Molecule 30: 50S ribosomal protein L33

Chain GC:  67% 31% .

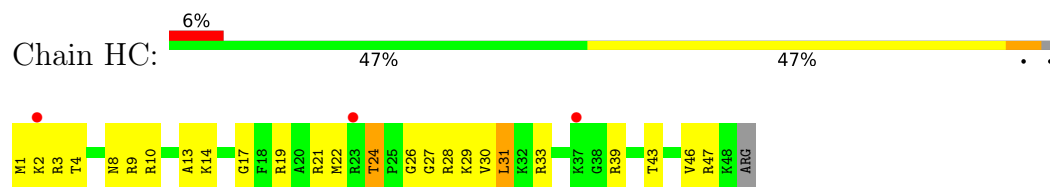


- Molecule 31: 50S ribosomal protein L34

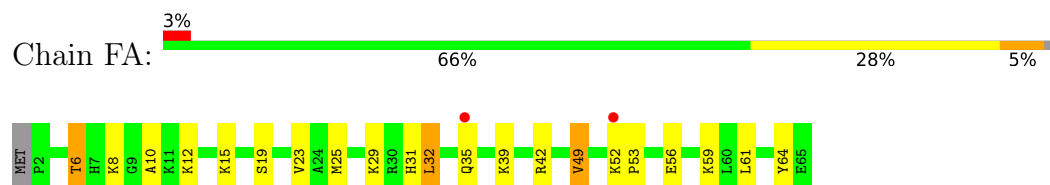
Chain EA:  51% 41% 6% .



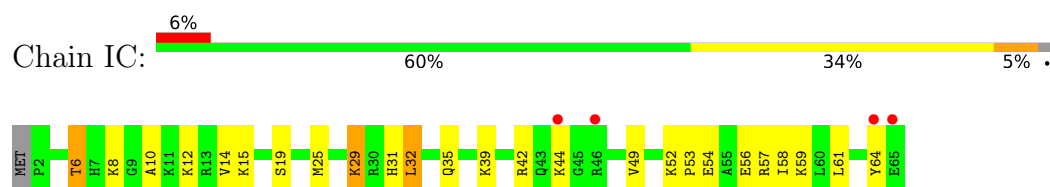
- Molecule 31: 50S ribosomal protein L34



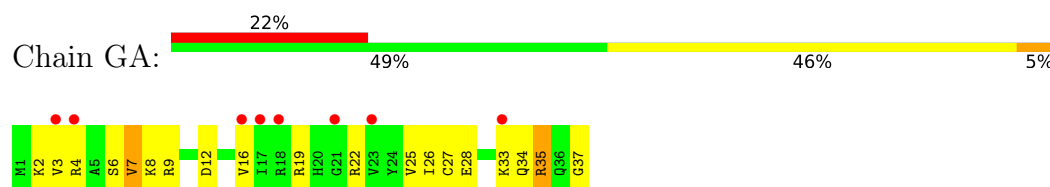
- Molecule 32: 50S ribosomal protein L35



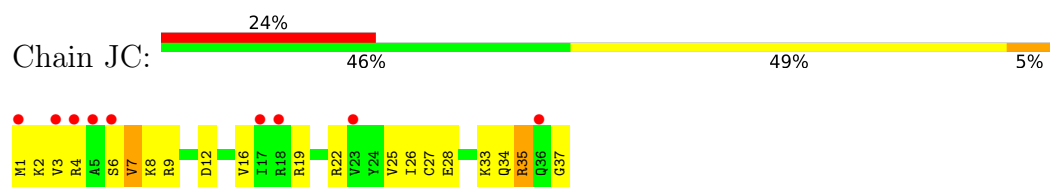
- Molecule 32: 50S ribosomal protein L35



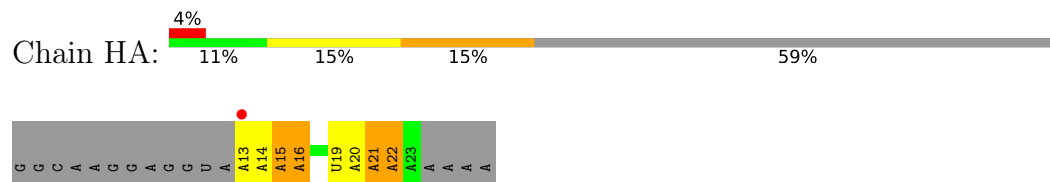
- Molecule 33: 50S ribosomal protein L36



- Molecule 33: 50S ribosomal protein L36

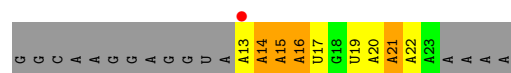


- Molecule 34: mRNA

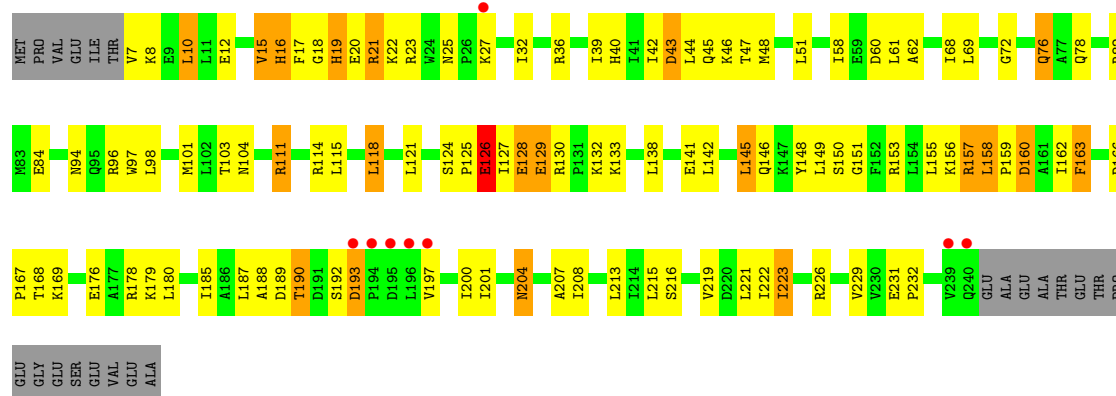


- Molecule 34: mRNA

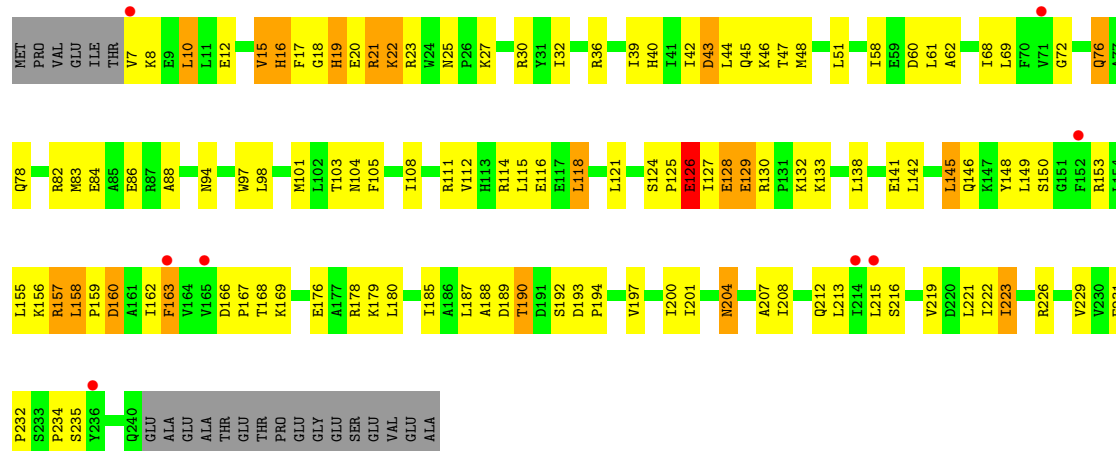




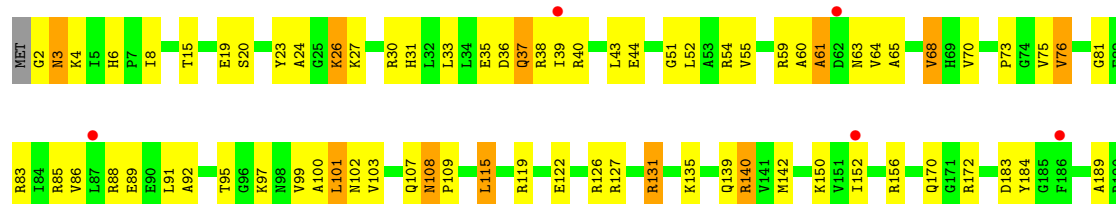
• Molecule 35: 30S ribosomal protein S2

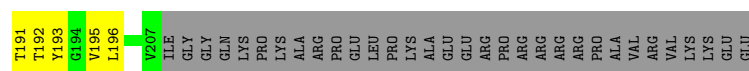


• Molecule 35: 30S ribosomal protein S2

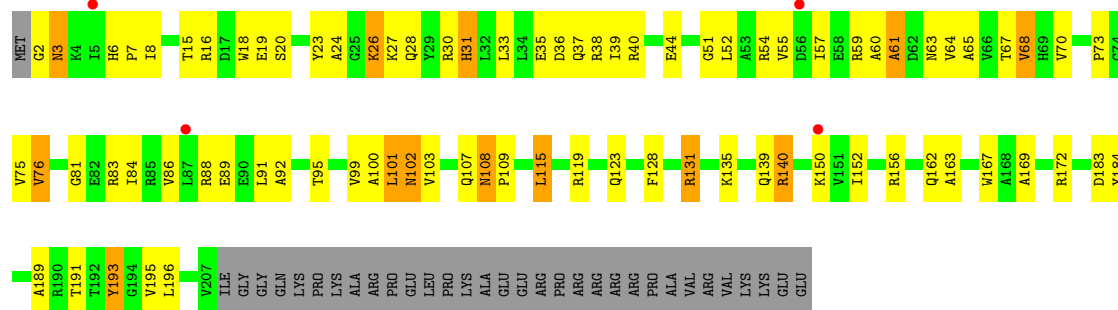


• Molecule 36: 30S ribosomal protein S3

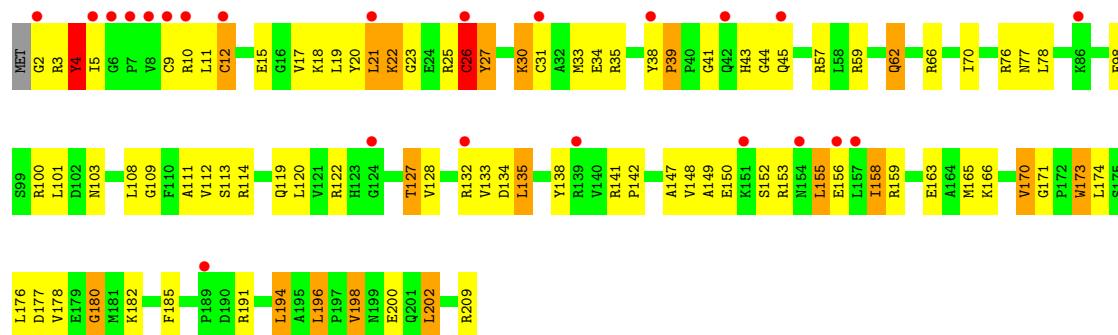




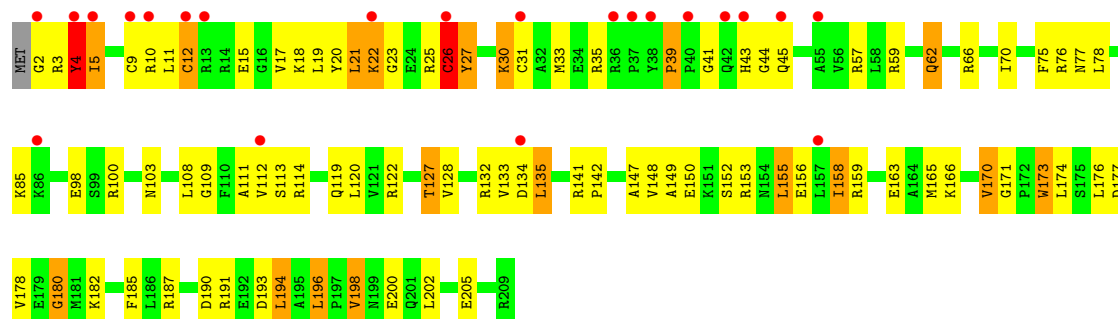
• Molecule 36: 30S ribosomal protein S3



• Molecule 37: 30S ribosomal protein S4

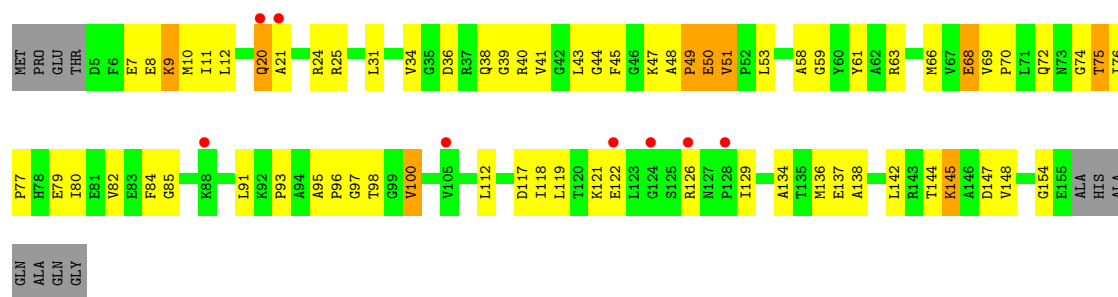


• Molecule 37: 30S ribosomal protein S4

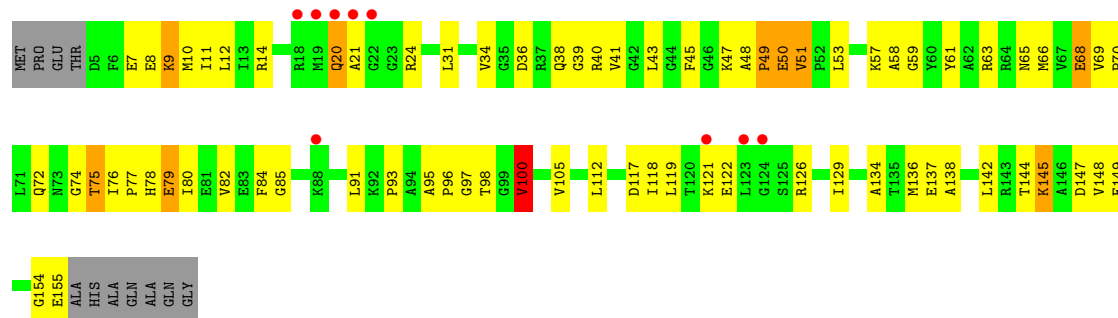


• Molecule 38: 30S ribosomal protein S5

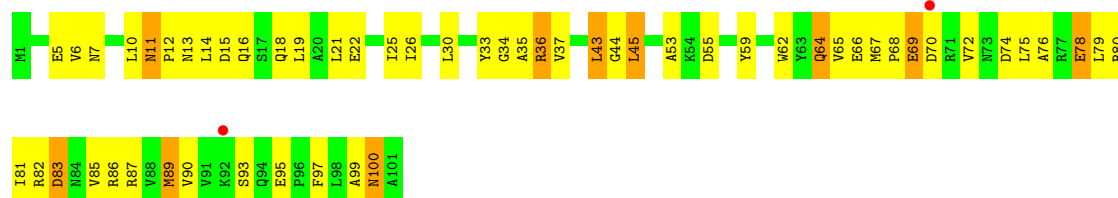




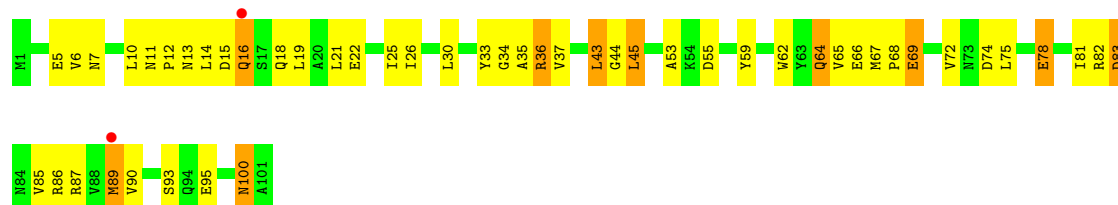
- Molecule 38: 30S ribosomal protein S5



- Molecule 39: 30S ribosomal protein S6

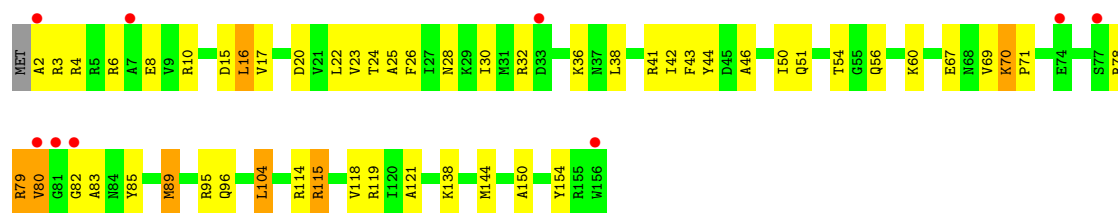


- Molecule 39: 30S ribosomal protein S6

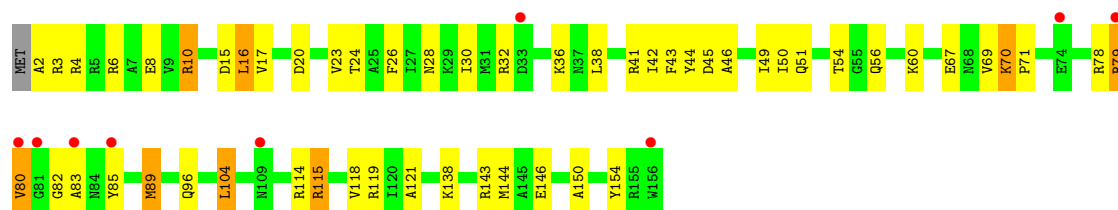


- Molecule 40: 30S ribosomal protein S7

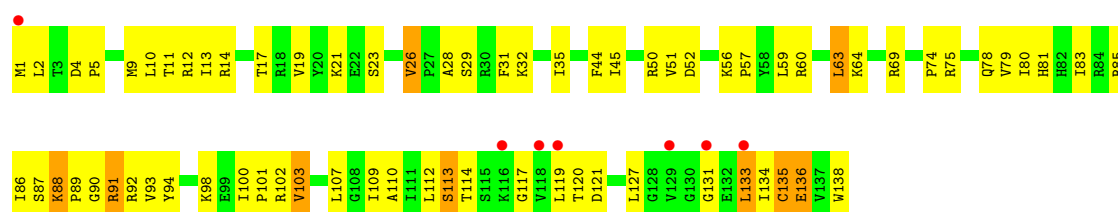




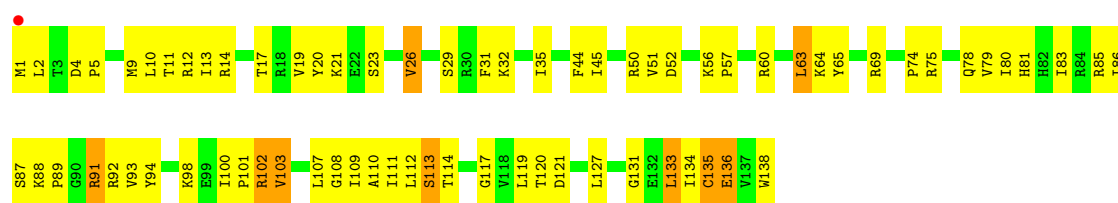
• Molecule 40: 30S ribosomal protein S7



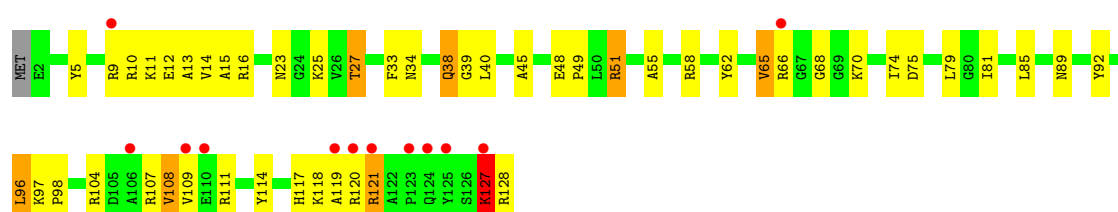
• Molecule 41: 30S ribosomal protein S8



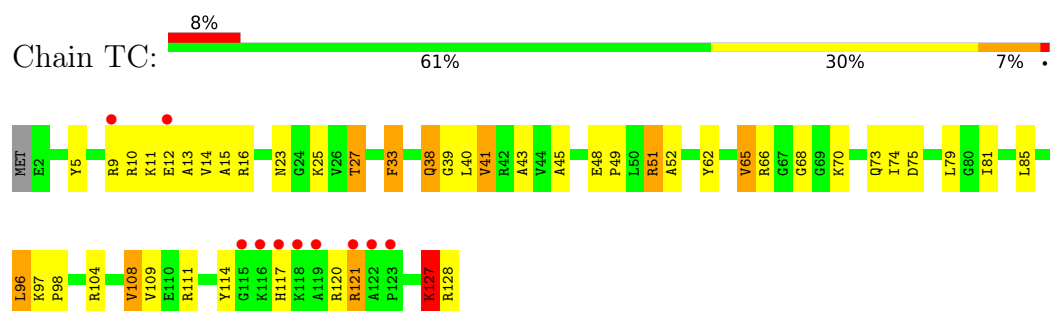
• Molecule 42: 30S ribosomal protein S9



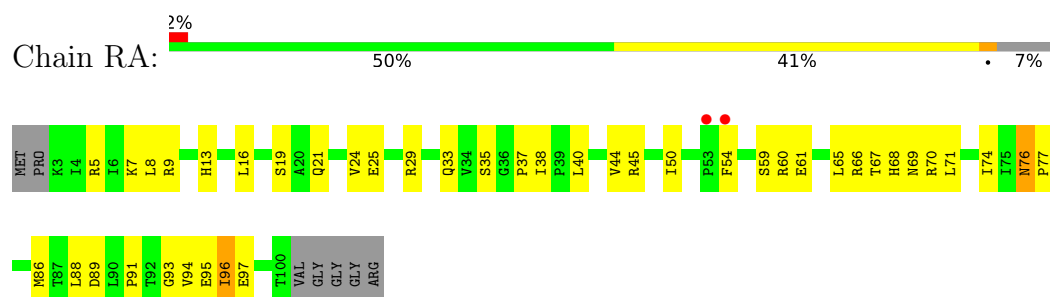
• Molecule 42: 30S ribosomal protein S9



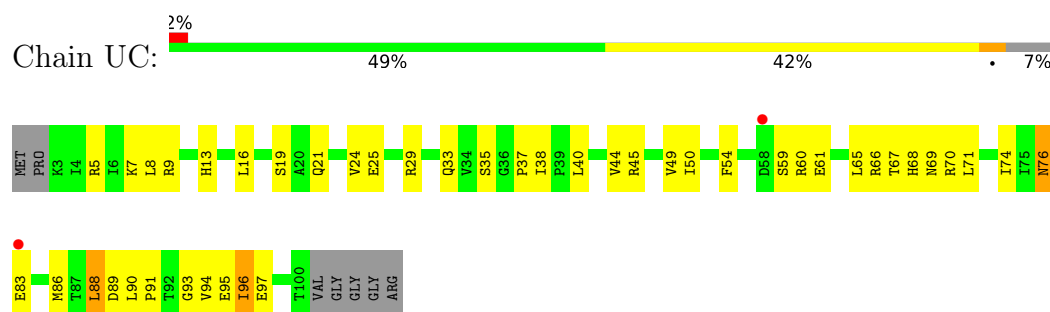
- Molecule 42: 30S ribosomal protein S9



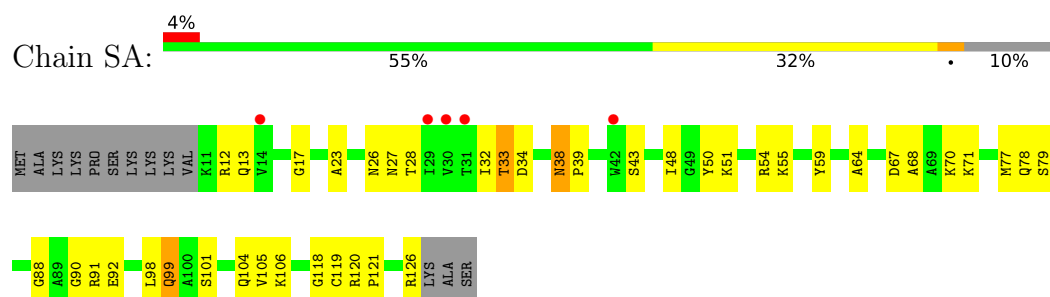
- Molecule 43: 30S ribosomal protein S10



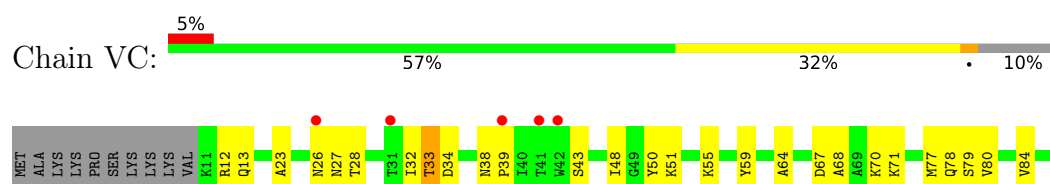
- Molecule 43: 30S ribosomal protein S10



- Molecule 44: 30S ribosomal protein S11

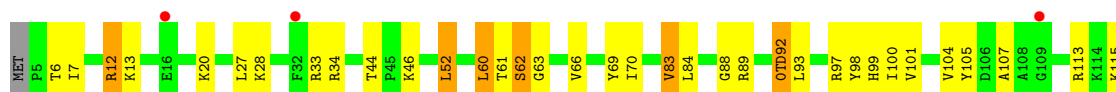


- Molecule 44: 30S ribosomal protein S11

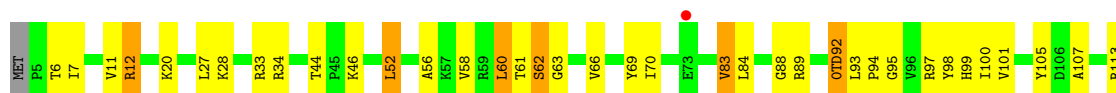




- Molecule 45: 30S ribosomal protein S12



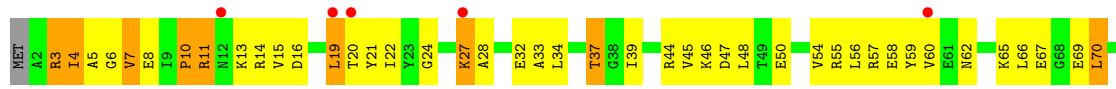
- Molecule 45: 30S ribosomal protein S12



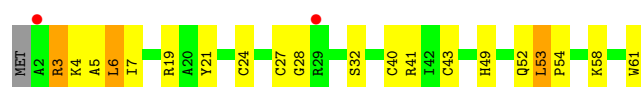
- Molecule 46: 30S ribosomal protein S13



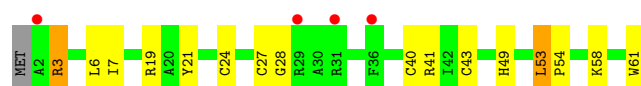
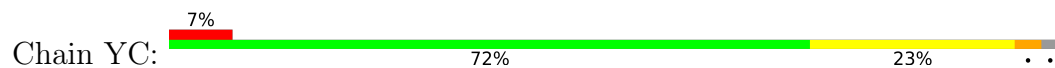
- Molecule 46: 30S ribosomal protein S13



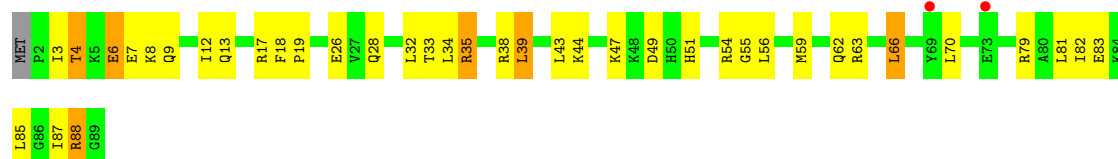
- Molecule 47: 30S ribosomal protein S14 type Z



- Molecule 47: 30S ribosomal protein S14 type Z



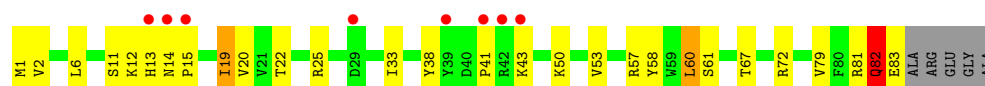
- Molecule 48: 30S ribosomal protein S15



- Molecule 48: 30S ribosomal protein S15



- Molecule 49: 30S ribosomal protein S16

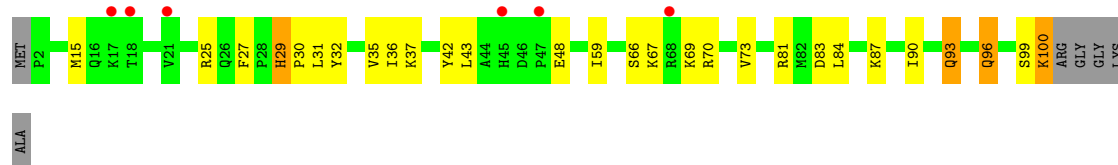


- Molecule 49: 30S ribosomal protein S16



- Molecule 50: 30S ribosomal protein S17





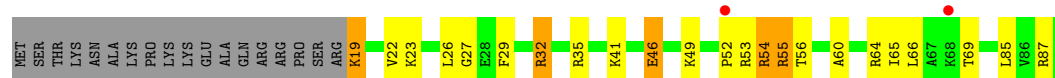
- Molecule 50: 30S ribosomal protein S17



- Molecule 51: 30S ribosomal protein S18



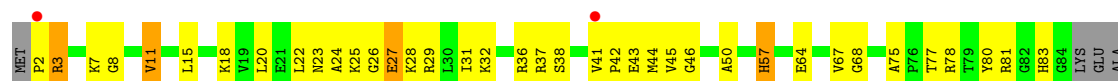
- Molecule 51: 30S ribosomal protein S18



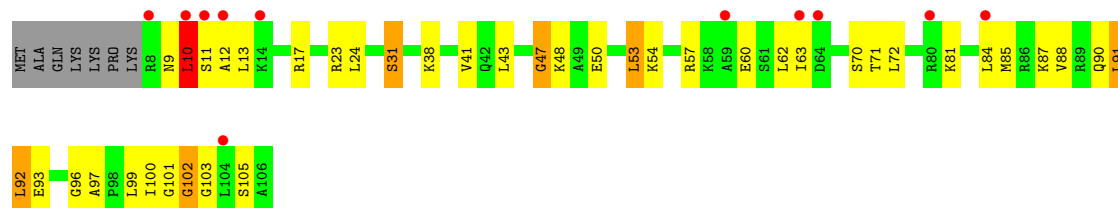
- Molecule 52: 30S ribosomal protein S19

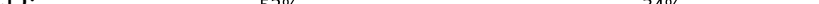


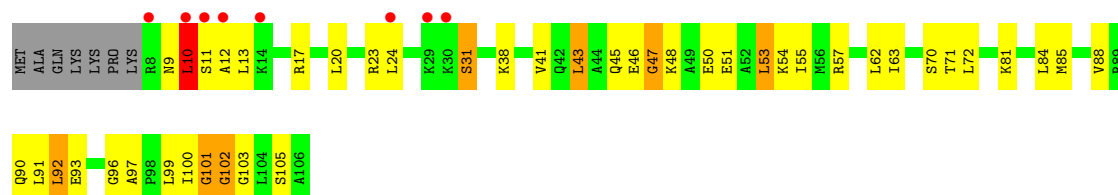
- Molecule 52: 30S ribosomal protein S19

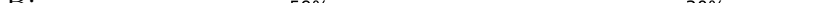


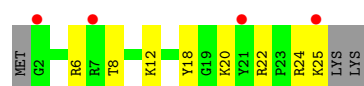
- Molecule 53: 30S ribosomal protein S20

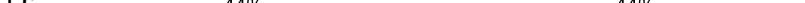


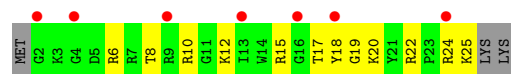
- Chain ED: 

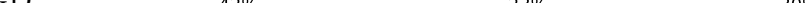


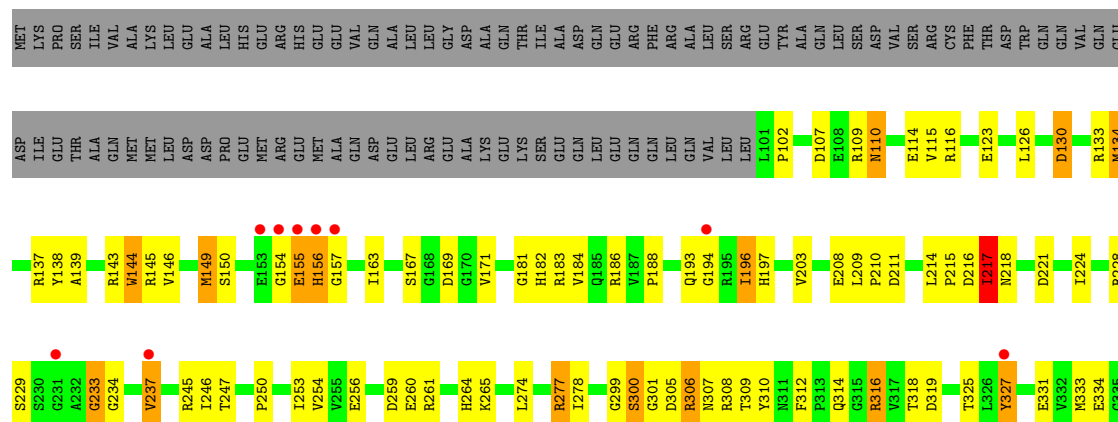
- Chain CB: 



- Chain FD: 

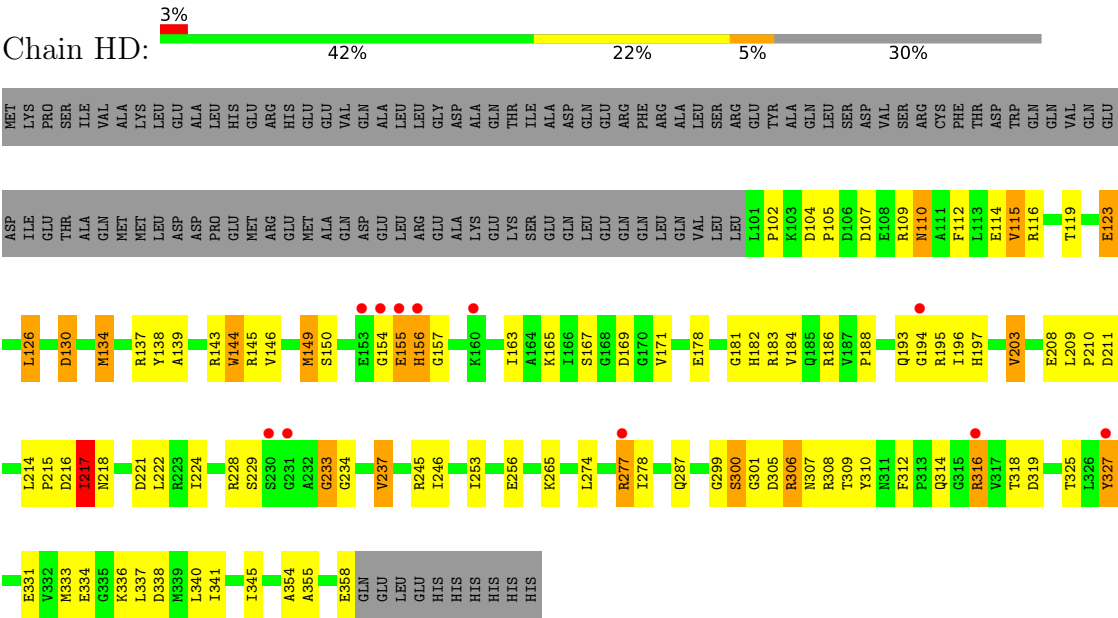


- Chain GD: 





● Molecule 55: Peptide chain release factor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.82Å 450.45Å 615.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.55 50.00 – 3.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-3.55) 99.8 (50.00-3.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.58Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	(Not available) , (Not available) 0.221 , 0.257	Depositor DCC
R_{free} test set	13965 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	124.9	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 83.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	299566	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4OC, 0TD, 2MU, M2G, ZN, 2MG, 2MA, 7MG, PSU, 4SU, 5MC, UR3, 5MU, MG, OMG, MA6

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	A	0.36	0/35961	0.48	0/56125
1	DB	0.37	0/35961	0.49	0/56125
2	B	0.55	0/69214	0.63	2/108048 (0.0%)
2	EB	0.47	0/69214	0.60	2/108048 (0.0%)
3	C	0.38	0/2881	0.49	0/4494
3	FB	0.33	0/2881	0.45	0/4494
4	D	0.29	1/1744 (0.1%)	0.34	0/2719
4	GB	0.30	1/1744 (0.1%)	0.34	0/2719
4	IA	0.42	0/1744	0.51	0/2719
4	LC	0.41	1/1744 (0.1%)	0.50	0/2719
5	E	0.92	0/2195	1.07	7/2955 (0.2%)
5	HB	0.83	0/2195	1.05	5/2955 (0.2%)
6	F	0.78	0/1596	0.98	6/2153 (0.3%)
6	IB	0.71	0/1596	0.96	1/2153 (0.0%)
7	G	0.87	1/1621 (0.1%)	1.00	4/2194 (0.2%)
7	JB	0.77	1/1621 (0.1%)	0.99	3/2194 (0.1%)
8	H	0.54	0/1496	0.86	0/2013
8	KB	0.48	0/1496	0.86	3/2013 (0.1%)
9	I	0.66	0/1356	0.96	5/1834 (0.3%)
9	LB	0.49	0/1356	0.90	4/1834 (0.2%)
10	J	0.64	0/1152	0.90	3/1559 (0.2%)
10	MB	0.63	0/1152	0.91	1/1559 (0.1%)
11	K	0.76	0/1148	1.08	7/1547 (0.5%)
11	NB	0.63	0/1148	1.05	4/1547 (0.3%)
12	L	0.85	0/942	1.00	2/1268 (0.2%)
12	OB	0.82	0/942	1.00	2/1268 (0.2%)
13	M	0.73	0/1162	1.01	2/1544 (0.1%)
13	PB	0.67	0/1162	1.00	3/1544 (0.2%)
14	N	0.81	0/1142	0.98	4/1525 (0.3%)
14	QB	0.75	0/1142	0.95	1/1525 (0.1%)
15	O	0.78	0/982	1.01	0/1312
15	RB	0.71	0/982	0.95	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	P	0.56	0/887	0.87	0/1180
16	SB	0.48	0/887	0.86	2/1180 (0.2%)
17	Q	0.74	0/1157	0.95	0/1544
17	TB	0.69	0/1157	0.94	0/1544
18	R	0.85	0/982	0.97	0/1306
18	UB	0.75	0/982	0.95	0/1306
19	S	0.78	0/790	1.08	3/1057 (0.3%)
19	VB	0.68	0/790	1.01	1/1057 (0.1%)
20	T	0.95	0/901	1.03	2/1209 (0.2%)
20	WB	0.85	0/901	1.00	1/1209 (0.1%)
21	U	0.87	0/764	0.95	0/1025
21	XB	0.74	0/764	0.91	0/1025
22	V	0.80	0/827	0.94	0/1103
22	YB	0.75	0/827	0.94	0/1103
23	W	0.58	0/1527	0.94	1/2073 (0.0%)
23	ZB	0.50	0/1527	0.93	1/2073 (0.0%)
24	AC	0.77	0/671	1.03	2/892 (0.2%)
24	X	0.91	0/671	1.04	2/892 (0.2%)
25	BC	0.81	0/768	1.07	2/1021 (0.2%)
25	Y	0.87	0/768	1.07	5/1021 (0.5%)
26	CC	0.68	0/594	0.93	0/785
26	Z	0.83	0/594	0.98	2/785 (0.3%)
27	AA	0.76	0/482	0.94	0/646
27	DC	0.71	0/482	0.93	0/646
28	BA	0.57	0/565	0.76	1/761 (0.1%)
28	EC	0.55	0/565	0.76	1/761 (0.1%)
29	CA	0.77	0/474	0.91	0/640
29	FC	0.68	0/474	0.93	0/640
30	DA	0.55	0/460	0.82	0/613
30	GC	0.53	0/460	0.81	0/613
31	EA	1.03	0/426	1.16	3/561 (0.5%)
31	HC	0.91	0/426	1.03	0/561
32	FA	0.85	0/525	1.00	0/691
32	IC	0.75	0/525	0.98	0/691
33	GA	0.61	0/310	0.86	0/407
33	JC	0.59	0/310	0.85	0/407
34	HA	0.53	0/247	0.56	0/382
34	KC	0.53	0/247	0.55	0/382
35	JA	0.55	0/1935	0.89	2/2609 (0.1%)
35	MC	0.56	0/1935	0.89	0/2609
36	KA	0.52	0/1636	0.86	0/2205
36	NC	0.51	0/1636	0.86	1/2205 (0.0%)
37	LA	0.59	0/1733	0.93	5/2318 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	OC	0.65	0/1733	0.96	5/2318 (0.2%)
38	MA	0.61	0/1171	0.95	2/1576 (0.1%)
38	PC	0.63	0/1171	0.96	5/1576 (0.3%)
39	NA	0.58	0/856	0.94	4/1154 (0.3%)
39	QC	0.54	0/856	0.92	2/1154 (0.2%)
40	OA	0.54	0/1276	0.82	2/1709 (0.1%)
40	RC	0.54	0/1276	0.82	2/1709 (0.1%)
41	PA	0.56	0/1136	0.94	0/1527
41	SC	0.58	0/1136	0.96	0/1527
42	QA	0.43	0/1029	0.81	0/1378
42	TC	0.42	0/1029	0.79	0/1378
43	RA	0.48	0/807	0.77	0/1085
43	UC	0.48	0/807	0.78	0/1085
44	SA	0.65	0/879	0.96	2/1187 (0.2%)
44	VC	0.64	0/879	0.93	2/1187 (0.2%)
45	TA	0.66	0/963	0.94	0/1287
45	WC	0.68	0/963	0.94	0/1287
46	UA	0.49	0/943	0.87	0/1265
46	XC	0.48	0/943	0.86	0/1265
47	VA	0.47	0/501	0.85	2/664 (0.3%)
47	YC	0.46	0/501	0.88	2/664 (0.3%)
48	WA	0.65	0/745	0.84	0/992
48	ZC	0.67	0/745	0.84	0/992
49	AD	0.59	0/716	0.86	0/963
49	XA	0.54	0/716	0.87	0/963
50	BD	0.60	0/836	0.93	2/1117 (0.2%)
50	YA	0.60	0/836	0.91	2/1117 (0.2%)
51	CD	0.59	0/579	0.85	1/768 (0.1%)
51	ZA	0.62	0/579	0.85	0/768
52	AB	0.45	0/680	0.82	1/915 (0.1%)
52	DD	0.46	0/680	0.80	1/915 (0.1%)
53	BB	0.53	0/764	0.88	2/1006 (0.2%)
53	ED	0.57	0/764	0.92	4/1006 (0.4%)
54	CB	0.43	0/212	0.77	0/277
54	FD	0.45	0/212	0.74	0/277
55	GD	0.65	0/2012	0.88	0/2713
55	HD	0.58	0/2012	0.85	0/2713
All	All	0.53	5/322204 (0.0%)	0.69	151/481240 (0.0%)

All (5) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	64	ILE	CA-CB	-7.75	1.45	1.54
7	JB	64	ILE	CA-CB	-5.46	1.48	1.54
4	LC	8	4SU	O3'-P	5.44	1.61	1.56
4	D	8	4SU	O3'-P	5.09	1.61	1.56
4	GB	8	4SU	O3'-P	5.01	1.61	1.56

The worst 5 of 151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	NB	110	GLY	CA-C-N	9.29	131.46	119.84
11	NB	110	GLY	C-N-CA	9.29	131.46	119.84
11	K	110	GLY	CA-C-N	8.88	130.94	119.84
11	K	110	GLY	C-N-CA	8.88	130.94	119.84
44	SA	38	ASN	CA-C-N	7.73	127.75	119.78

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32394	0	16367	509	0
1	DB	32394	0	16367	494	0
2	B	62031	0	31275	842	0
2	EB	62031	0	31275	810	0
3	C	2576	0	1305	36	0
3	FB	2576	0	1305	36	0
4	D	1642	0	841	26	0
4	GB	1642	0	841	29	0
4	IA	1642	0	841	12	0
4	LC	1642	0	841	10	0
5	E	2145	0	2234	94	0
5	HB	2145	0	2234	84	0
6	F	1563	0	1629	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	IB	1563	0	1629	56	0
7	G	1586	0	1632	66	0
7	JB	1586	0	1632	63	0
8	H	1471	0	1526	69	0
8	KB	1471	0	1526	64	0
9	I	1330	0	1407	56	0
9	LB	1330	0	1407	50	0
10	J	1137	0	1225	51	0
10	MB	1137	0	1225	43	0
11	K	1121	0	1195	35	0
11	NB	1121	0	1195	33	0
12	L	932	0	994	34	0
12	OB	932	0	994	28	0
13	M	1145	0	1228	40	0
13	PB	1145	0	1228	34	0
14	N	1121	0	1179	35	0
14	QB	1121	0	1179	44	0
15	O	968	0	1033	41	0
15	RB	968	0	1033	45	0
16	P	877	0	938	30	0
16	SB	877	0	938	30	0
17	Q	1143	0	1211	37	0
17	TB	1143	0	1211	34	0
18	R	964	0	1022	26	0
18	UB	964	0	1022	31	0
19	S	779	0	852	29	0
19	VB	779	0	852	29	0
20	T	890	0	951	34	0
20	WB	890	0	951	26	0
21	U	750	0	814	14	0
21	XB	750	0	814	15	0
22	V	814	0	907	31	0
22	YB	814	0	907	28	0
23	W	1495	0	1521	52	0
23	ZB	1495	0	1521	50	0
24	AC	662	0	688	22	0
24	X	662	0	688	22	0
25	BC	761	0	837	28	0
25	Y	761	0	837	32	0
26	CC	592	0	654	18	0
26	Z	592	0	654	18	0
27	AA	477	0	529	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	DC	477	0	529	16	0
28	BA	552	0	537	24	0
28	EC	552	0	537	23	0
29	CA	460	0	484	18	0
29	FC	460	0	484	20	0
30	DA	453	0	477	11	0
30	GC	453	0	477	10	0
31	EA	418	0	467	17	0
31	HC	418	0	467	18	0
32	FA	517	0	582	18	0
32	IC	517	0	582	19	0
33	GA	307	0	338	15	0
33	JC	307	0	337	16	0
34	HA	220	0	108	7	0
34	KC	220	0	108	10	0
35	JA	1900	0	1951	71	0
35	MC	1900	0	1951	73	0
36	KA	1612	0	1677	50	0
36	NC	1612	0	1677	49	0
37	LA	1703	0	1765	77	0
37	OC	1703	0	1765	70	0
38	MA	1155	0	1213	46	0
38	PC	1155	0	1213	51	0
39	NA	843	0	857	46	0
39	QC	843	0	857	41	0
40	OA	1257	0	1296	41	0
40	RC	1257	0	1296	45	0
41	PA	1116	0	1177	51	0
41	SC	1116	0	1177	49	0
42	QA	1011	0	1043	43	0
42	TC	1011	0	1043	44	0
43	RA	794	0	840	24	0
43	UC	794	0	840	27	0
44	SA	864	0	881	29	0
44	VC	864	0	881	22	0
45	TA	958	0	1047	31	0
45	WC	958	0	1047	32	0
46	UA	933	0	992	49	0
46	XC	933	0	992	46	0
47	VA	492	0	533	20	0
47	YC	492	0	533	16	0
48	WA	734	0	771	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	ZC	734	0	771	28	0
49	AD	700	0	720	21	0
49	XA	700	0	720	21	0
50	BD	823	0	893	27	0
50	YA	823	0	893	25	0
51	CD	574	0	644	17	0
51	ZA	574	0	644	19	0
52	AB	665	0	686	29	0
52	DD	665	0	686	29	0
53	BB	762	0	859	28	0
53	ED	762	0	859	27	0
54	CB	208	0	221	5	0
54	FD	208	0	221	13	0
55	GD	1980	0	1942	70	0
55	HD	1980	0	1942	66	0
56	A	160	0	0	0	0
56	AB	1	0	0	0	0
56	AC	2	0	0	0	0
56	AD	1	0	0	0	0
56	B	514	0	0	0	0
56	BB	1	0	0	0	0
56	BC	1	0	0	0	0
56	BD	2	0	0	0	0
56	C	23	0	0	0	0
56	CA	1	0	0	0	0
56	CD	2	0	0	0	0
56	D	6	0	0	0	0
56	DB	177	0	0	0	0
56	DC	1	0	0	0	0
56	E	4	0	0	0	0
56	EA	1	0	0	0	0
56	EB	395	0	0	0	0
56	ED	1	0	0	0	0
56	F	1	0	0	0	0
56	FA	1	0	0	0	0
56	FB	17	0	0	0	0
56	FC	1	0	0	0	0
56	G	4	0	0	0	0
56	GB	5	0	0	0	0
56	GD	5	0	0	0	0
56	H	1	0	0	0	0
56	HA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	HB	8	0	0	0	0
56	HC	1	0	0	0	0
56	HD	3	0	0	0	0
56	I	3	0	0	0	0
56	IA	8	0	0	0	0
56	IB	3	0	0	0	0
56	IC	2	0	0	0	0
56	J	5	0	0	0	0
56	JA	3	0	0	0	0
56	JB	2	0	0	0	0
56	JC	1	0	0	0	0
56	K	2	0	0	0	0
56	KA	1	0	0	0	0
56	KB	1	0	0	0	0
56	KC	1	0	0	0	0
56	L	7	0	0	0	0
56	LA	1	0	0	0	0
56	LB	5	0	0	0	0
56	LC	8	0	0	0	0
56	M	4	0	0	0	0
56	MA	3	0	0	0	0
56	MB	2	0	0	0	0
56	MC	3	0	0	0	0
56	N	3	0	0	0	0
56	NA	2	0	0	0	0
56	NB	1	0	0	0	0
56	O	1	0	0	0	0
56	OA	3	0	0	0	0
56	OB	3	0	0	0	0
56	P	2	0	0	0	0
56	PA	2	0	0	0	0
56	PB	2	0	0	0	0
56	PC	2	0	0	0	0
56	Q	3	0	0	0	0
56	QB	3	0	0	0	0
56	QC	2	0	0	0	0
56	R	4	0	0	0	0
56	RA	2	0	0	0	0
56	RB	5	0	0	0	0
56	RC	2	0	0	0	0
56	S	3	0	0	0	0
56	SA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	SB	1	0	0	0	0
56	SC	1	0	0	0	0
56	T	2	0	0	0	0
56	TA	3	0	0	0	0
56	TB	5	0	0	0	0
56	TC	2	0	0	0	0
56	U	2	0	0	0	0
56	UC	1	0	0	0	0
56	V	5	0	0	0	0
56	VA	2	0	0	0	0
56	VB	1	0	0	0	0
56	W	12	0	0	0	0
56	WA	3	0	0	0	0
56	WB	3	0	0	0	0
56	WC	2	0	0	0	0
56	XB	2	0	0	0	0
56	XC	2	0	0	0	0
56	Y	4	0	0	0	0
56	YA	2	0	0	0	0
56	YB	3	0	0	0	0
56	YC	1	0	0	0	0
56	Z	3	0	0	0	0
56	ZA	1	0	0	0	0
56	ZB	2	0	0	0	0
56	ZC	1	0	0	0	0
57	BA	1	0	0	0	0
57	CA	1	0	0	0	0
57	DA	1	0	0	0	0
57	EC	1	0	0	0	0
57	FC	1	0	0	0	0
57	GA	1	0	0	0	0
57	GC	1	0	0	0	0
57	JC	1	0	0	0	0
57	V	1	0	0	0	0
57	YB	1	0	0	0	0
All	All	299566	0	203671	5595	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 5595 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:LA:18:LYS:NZ	37:LA:31:CYS:SG	2.10	1.23
37:OC:18:LYS:NZ	37:OC:31:CYS:SG	2.10	1.23
37:OC:12:CYS:SG	37:OC:18:LYS:NZ	2.24	1.11
10:J:60:GLU:HG3	10:J:61:ARG:HH12	1.11	1.09
10:MB:60:GLU:HG3	10:MB:61:ARG:HH12	1.19	1.05

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	273/275 (99%)	243 (89%)	25 (9%)	5 (2%)	6	34
5	HB	273/275 (99%)	243 (89%)	25 (9%)	5 (2%)	6	34
6	F	202/206 (98%)	180 (89%)	20 (10%)	2 (1%)	12	45
6	IB	202/206 (98%)	181 (90%)	19 (9%)	2 (1%)	12	45
7	G	200/205 (98%)	187 (94%)	9 (4%)	4 (2%)	6	33
7	JB	200/205 (98%)	186 (93%)	10 (5%)	4 (2%)	6	33
8	H	179/182 (98%)	152 (85%)	20 (11%)	7 (4%)	2	20
8	KB	179/182 (98%)	151 (84%)	22 (12%)	6 (3%)	3	23
9	I	172/180 (96%)	155 (90%)	14 (8%)	3 (2%)	7	35
9	LB	172/180 (96%)	154 (90%)	15 (9%)	3 (2%)	7	35
10	J	144/148 (97%)	118 (82%)	17 (12%)	9 (6%)	1	12
10	MB	144/148 (97%)	118 (82%)	16 (11%)	10 (7%)	1	11
11	K	138/140 (99%)	125 (91%)	12 (9%)	1 (1%)	18	51
11	NB	138/140 (99%)	126 (91%)	11 (8%)	1 (1%)	18	51
12	L	120/122 (98%)	106 (88%)	12 (10%)	2 (2%)	7	35
12	OB	120/122 (98%)	106 (88%)	12 (10%)	2 (2%)	7	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	148/150 (99%)	132 (89%)	11 (7%)	5 (3%)	3	23
13	PB	148/150 (99%)	131 (88%)	12 (8%)	5 (3%)	3	23
14	N	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	9	38
14	QB	139/141 (99%)	125 (90%)	12 (9%)	2 (1%)	9	38
15	O	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	7	35
15	RB	116/118 (98%)	107 (92%)	7 (6%)	2 (2%)	7	35
16	P	108/112 (96%)	99 (92%)	7 (6%)	2 (2%)	6	33
16	SB	108/112 (96%)	100 (93%)	6 (6%)	2 (2%)	6	33
17	Q	135/146 (92%)	118 (87%)	12 (9%)	5 (4%)	2	21
17	TB	135/146 (92%)	118 (87%)	13 (10%)	4 (3%)	3	25
18	R	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	14	47
18	UB	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	47
19	S	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	6	33
19	VB	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	6	33
20	T	110/113 (97%)	104 (94%)	4 (4%)	2 (2%)	6	34
20	WB	110/113 (97%)	103 (94%)	5 (4%)	2 (2%)	6	34
21	U	93/96 (97%)	84 (90%)	8 (9%)	1 (1%)	11	43
21	XB	93/96 (97%)	84 (90%)	8 (9%)	1 (1%)	11	43
22	V	105/110 (96%)	89 (85%)	11 (10%)	5 (5%)	2	16
22	YB	105/110 (96%)	91 (87%)	9 (9%)	5 (5%)	2	16
23	W	187/206 (91%)	165 (88%)	21 (11%)	1 (0%)	24	57
23	ZB	187/206 (91%)	165 (88%)	21 (11%)	1 (0%)	24	57
24	AC	82/85 (96%)	70 (85%)	10 (12%)	2 (2%)	4	29
24	X	82/85 (96%)	69 (84%)	11 (13%)	2 (2%)	4	29
25	BC	95/98 (97%)	84 (88%)	10 (10%)	1 (1%)	11	43
25	Y	95/98 (97%)	86 (90%)	8 (8%)	1 (1%)	11	43
26	CC	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
26	Z	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
27	AA	58/60 (97%)	53 (91%)	4 (7%)	1 (2%)	7	35
27	DC	58/60 (97%)	53 (91%)	4 (7%)	1 (2%)	7	35
28	BA	67/71 (94%)	47 (70%)	19 (28%)	1 (2%)	8	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	EC	67/71 (94%)	47 (70%)	20 (30%)	0	100	100
29	CA	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	6	34
29	FC	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	6	34
30	DA	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
30	GC	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
31	EA	46/49 (94%)	46 (100%)	0	0	100	100
31	HC	46/49 (94%)	46 (100%)	0	0	100	100
32	FA	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
32	IC	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
33	GA	35/37 (95%)	27 (77%)	8 (23%)	0	100	100
33	JC	35/37 (95%)	27 (77%)	8 (23%)	0	100	100
35	JA	232/256 (91%)	189 (82%)	29 (12%)	14 (6%)	1	13
35	MC	232/256 (91%)	188 (81%)	30 (13%)	14 (6%)	1	13
36	KA	204/239 (85%)	172 (84%)	24 (12%)	8 (4%)	2	20
36	NC	204/239 (85%)	172 (84%)	24 (12%)	8 (4%)	2	20
37	LA	206/209 (99%)	179 (87%)	20 (10%)	7 (3%)	3	23
37	OC	206/209 (99%)	182 (88%)	16 (8%)	8 (4%)	2	20
38	MA	149/162 (92%)	132 (89%)	11 (7%)	6 (4%)	2	20
38	PC	149/162 (92%)	132 (89%)	10 (7%)	7 (5%)	2	17
39	NA	99/101 (98%)	88 (89%)	9 (9%)	2 (2%)	6	33
39	QC	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	6	33
40	OA	153/156 (98%)	133 (87%)	13 (8%)	7 (5%)	2	17
40	RC	153/156 (98%)	133 (87%)	13 (8%)	7 (5%)	2	17
41	PA	136/138 (99%)	125 (92%)	9 (7%)	2 (2%)	8	37
41	SC	136/138 (99%)	126 (93%)	9 (7%)	1 (1%)	18	51
42	QA	125/128 (98%)	105 (84%)	17 (14%)	3 (2%)	4	29
42	TC	125/128 (98%)	105 (84%)	16 (13%)	4 (3%)	3	24
43	RA	96/105 (91%)	81 (84%)	12 (12%)	3 (3%)	3	25
43	UC	96/105 (91%)	81 (84%)	12 (12%)	3 (3%)	3	25
44	SA	114/129 (88%)	101 (89%)	10 (9%)	3 (3%)	4	27
44	VC	114/129 (88%)	101 (89%)	9 (8%)	4 (4%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	TA	119/132 (90%)	104 (87%)	11 (9%)	4 (3%)	3	23
45	WC	119/132 (90%)	104 (87%)	11 (9%)	4 (3%)	3	23
46	UA	115/126 (91%)	102 (89%)	12 (10%)	1 (1%)	14	47
46	XC	115/126 (91%)	102 (89%)	11 (10%)	2 (2%)	7	35
47	VA	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
47	YC	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
48	WA	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	5	30
48	ZC	86/89 (97%)	81 (94%)	3 (4%)	2 (2%)	5	30
49	AD	81/88 (92%)	73 (90%)	7 (9%)	1 (1%)	10	42
49	XA	81/88 (92%)	73 (90%)	7 (9%)	1 (1%)	10	42
50	BD	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
50	YA	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
51	CD	68/88 (77%)	62 (91%)	5 (7%)	1 (2%)	8	37
51	ZA	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	8	37
52	AB	81/93 (87%)	63 (78%)	14 (17%)	4 (5%)	1	16
52	DD	81/93 (87%)	63 (78%)	14 (17%)	4 (5%)	1	16
53	BB	97/106 (92%)	90 (93%)	3 (3%)	4 (4%)	2	19
53	ED	97/106 (92%)	90 (93%)	3 (3%)	4 (4%)	2	19
54	CB	22/27 (82%)	18 (82%)	4 (18%)	0	100	100
54	FD	22/27 (82%)	18 (82%)	4 (18%)	0	100	100
55	GD	253/365 (69%)	207 (82%)	35 (14%)	11 (4%)	2	18
55	HD	253/365 (69%)	206 (81%)	37 (15%)	10 (4%)	2	20
All	All	11990/12846 (93%)	10568 (88%)	1121 (9%)	301 (2%)	4	28

5 of 301 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	31	LYS
6	F	192	ASN
7	G	21	ALA
7	G	130	ALA
8	H	74	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	
5	E	217/217 (100%)	194 (89%)	23 (11%)	6	28
5	HB	217/217 (100%)	194 (89%)	23 (11%)	6	28
6	F	165/166 (99%)	141 (86%)	24 (14%)	3	18
6	IB	165/166 (99%)	140 (85%)	25 (15%)	3	16
7	G	161/162 (99%)	142 (88%)	19 (12%)	5	25
7	JB	161/162 (99%)	143 (89%)	18 (11%)	6	27
8	H	154/156 (99%)	133 (86%)	21 (14%)	3	20
8	KB	154/156 (99%)	133 (86%)	21 (14%)	3	20
9	I	144/148 (97%)	129 (90%)	15 (10%)	7	29
9	LB	144/148 (97%)	130 (90%)	14 (10%)	8	31
10	J	122/124 (98%)	98 (80%)	24 (20%)	1	8
10	MB	122/124 (98%)	97 (80%)	25 (20%)	1	7
11	K	119/119 (100%)	110 (92%)	9 (8%)	12	38
11	NB	119/119 (100%)	110 (92%)	9 (8%)	12	38
12	L	100/100 (100%)	89 (89%)	11 (11%)	6	27
12	OB	100/100 (100%)	89 (89%)	11 (11%)	6	27
13	M	116/116 (100%)	98 (84%)	18 (16%)	2	16
13	PB	116/116 (100%)	100 (86%)	16 (14%)	3	20
14	N	111/111 (100%)	98 (88%)	13 (12%)	5	25
14	QB	111/111 (100%)	98 (88%)	13 (12%)	5	25
15	O	101/101 (100%)	88 (87%)	13 (13%)	4	22
15	RB	101/101 (100%)	87 (86%)	14 (14%)	3	19
16	P	87/88 (99%)	82 (94%)	5 (6%)	18	46
16	SB	87/88 (99%)	81 (93%)	6 (7%)	14	41
17	Q	121/128 (94%)	112 (93%)	9 (7%)	13	39
17	TB	121/128 (94%)	112 (93%)	9 (7%)	13	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	R	93/94 (99%)	82 (88%)	11 (12%)	5	25
18	UB	93/94 (99%)	82 (88%)	11 (12%)	5	25
19	S	82/82 (100%)	70 (85%)	12 (15%)	3	17
19	VB	82/82 (100%)	70 (85%)	12 (15%)	3	17
20	T	91/92 (99%)	80 (88%)	11 (12%)	5	24
20	WB	91/92 (99%)	81 (89%)	10 (11%)	6	27
21	U	77/78 (99%)	73 (95%)	4 (5%)	21	48
21	XB	77/78 (99%)	73 (95%)	4 (5%)	21	48
22	V	87/91 (96%)	78 (90%)	9 (10%)	7	29
22	YB	87/91 (96%)	76 (87%)	11 (13%)	4	22
23	W	163/179 (91%)	140 (86%)	23 (14%)	3	19
23	ZB	163/179 (91%)	143 (88%)	20 (12%)	4	23
24	AC	66/67 (98%)	56 (85%)	10 (15%)	3	16
24	X	66/67 (98%)	55 (83%)	11 (17%)	2	13
25	BC	81/83 (98%)	66 (82%)	15 (18%)	1	9
25	Y	81/83 (98%)	66 (82%)	15 (18%)	1	9
26	CC	66/67 (98%)	60 (91%)	6 (9%)	9	33
26	Z	66/67 (98%)	60 (91%)	6 (9%)	9	33
27	AA	52/52 (100%)	49 (94%)	3 (6%)	18	45
27	DC	52/52 (100%)	49 (94%)	3 (6%)	18	45
28	BA	59/63 (94%)	51 (86%)	8 (14%)	3	20
28	EC	59/63 (94%)	52 (88%)	7 (12%)	5	24
29	CA	51/52 (98%)	46 (90%)	5 (10%)	7	31
29	FC	51/52 (98%)	46 (90%)	5 (10%)	7	31
30	DA	51/52 (98%)	47 (92%)	4 (8%)	11	37
30	GC	51/52 (98%)	47 (92%)	4 (8%)	11	37
31	EA	41/42 (98%)	35 (85%)	6 (15%)	3	17
31	HC	41/42 (98%)	35 (85%)	6 (15%)	3	17
32	FA	54/55 (98%)	50 (93%)	4 (7%)	13	39
32	IC	54/55 (98%)	50 (93%)	4 (7%)	13	39
33	GA	34/34 (100%)	28 (82%)	6 (18%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	JC	34/34 (100%)	28 (82%)	6 (18%)	2	11
35	JA	202/220 (92%)	177 (88%)	25 (12%)	4	23
35	MC	202/220 (92%)	177 (88%)	25 (12%)	4	23
36	KA	160/188 (85%)	143 (89%)	17 (11%)	6	28
36	NC	160/188 (85%)	141 (88%)	19 (12%)	5	24
37	LA	180/181 (99%)	156 (87%)	24 (13%)	4	21
37	OC	180/181 (99%)	155 (86%)	25 (14%)	3	19
38	MA	116/123 (94%)	100 (86%)	16 (14%)	3	20
38	PC	116/123 (94%)	99 (85%)	17 (15%)	3	17
39	NA	90/90 (100%)	79 (88%)	11 (12%)	5	23
39	QC	90/90 (100%)	79 (88%)	11 (12%)	5	23
40	OA	126/127 (99%)	119 (94%)	7 (6%)	19	46
40	RC	126/127 (99%)	118 (94%)	8 (6%)	16	43
41	PA	119/119 (100%)	103 (87%)	16 (13%)	4	21
41	SC	119/119 (100%)	102 (86%)	17 (14%)	3	18
42	QA	98/99 (99%)	91 (93%)	7 (7%)	13	40
42	TC	98/99 (99%)	90 (92%)	8 (8%)	10	35
43	RA	88/92 (96%)	78 (89%)	10 (11%)	5	26
43	UC	88/92 (96%)	78 (89%)	10 (11%)	5	26
44	SA	88/99 (89%)	83 (94%)	5 (6%)	18	46
44	VC	88/99 (89%)	82 (93%)	6 (7%)	14	41
45	TA	102/108 (94%)	95 (93%)	7 (7%)	14	41
45	WC	102/108 (94%)	95 (93%)	7 (7%)	14	41
46	UA	94/101 (93%)	81 (86%)	13 (14%)	3	20
46	XC	94/101 (93%)	80 (85%)	14 (15%)	3	17
47	VA	49/50 (98%)	46 (94%)	3 (6%)	17	44
47	YC	49/50 (98%)	46 (94%)	3 (6%)	17	44
48	WA	79/80 (99%)	71 (90%)	8 (10%)	7	29
48	ZC	79/80 (99%)	71 (90%)	8 (10%)	7	29
49	AD	72/74 (97%)	63 (88%)	9 (12%)	4	22
49	XA	72/74 (97%)	63 (88%)	9 (12%)	4	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	BD	94/97 (97%)	89 (95%)	5 (5%)	20	47
50	YA	94/97 (97%)	89 (95%)	5 (5%)	20	47
51	CD	61/77 (79%)	55 (90%)	6 (10%)	7	31
51	ZA	61/77 (79%)	55 (90%)	6 (10%)	7	31
52	AB	72/80 (90%)	64 (89%)	8 (11%)	6	27
52	DD	72/80 (90%)	65 (90%)	7 (10%)	8	31
53	BB	76/82 (93%)	69 (91%)	7 (9%)	8	32
53	ED	76/82 (93%)	69 (91%)	7 (9%)	8	32
54	CB	19/22 (86%)	19 (100%)	0	100	100
54	FD	19/22 (86%)	19 (100%)	0	100	100
55	GD	206/305 (68%)	179 (87%)	27 (13%)	4	21
55	HD	206/305 (68%)	177 (86%)	29 (14%)	3	19
All	All	10114/10666 (95%)	8962 (89%)	1152 (11%)	5	26

5 of 1152 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	NC	193	TYR
55	HD	306	ARG
38	PC	9	LYS
36	NC	191	THR
46	XC	11	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 167 such sidechains are listed below:

Mol	Chain	Res	Type
36	NC	110	ASN
45	WC	99	HIS
36	NC	170	GLN
40	RC	86	GLN
50	BD	96	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1505/1507 (99%)	228 (15%)	10 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	DB	1505/1507 (99%)	223 (14%)	10 (0%)
2	B	2879/2880 (99%)	499 (17%)	15 (0%)
2	EB	2879/2880 (99%)	497 (17%)	15 (0%)
3	C	119/120 (99%)	18 (15%)	0
3	FB	119/120 (99%)	17 (14%)	0
34	HA	9/27 (33%)	4 (44%)	1 (11%)
34	KC	9/27 (33%)	4 (44%)	1 (11%)
4	D	76/77 (98%)	13 (17%)	0
4	GB	76/77 (98%)	13 (17%)	0
4	IA	76/77 (98%)	7 (9%)	0
4	LC	76/77 (98%)	7 (9%)	0
All	All	9328/9376 (99%)	1530 (16%)	52 (0%)

5 of 1530 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	6	G
1	A	8	A
1	A	9	G
1	A	32	A

5 of 52 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	DB	560	U
1	DB	1201	A
2	EB	2422	A
1	DB	563	A
1	DB	723	U

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

64 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMG	EB	2251	2,4	23,26,27	1.99	3 (13%)	32,38,41	1.86	8 (25%)
1	2MG	DB	1207	1	23,26,27	2.18	3 (13%)	33,38,41	2.11	12 (36%)
2	5MU	EB	1939	2	19,22,23	2.22	5 (26%)	27,32,35	2.60	8 (29%)
2	PSU	B	1911	2	18,21,22	1.52	2 (11%)	21,30,33	1.71	5 (23%)
2	4OC	EB	1920	2	19,22,24	1.03	1 (5%)	25,31,35	0.84	0
1	5MC	A	1407	1	19,22,23	2.87	4 (21%)	26,32,35	1.24	1 (3%)
2	2MA	B	2503	2	22,25,26	1.70	6 (27%)	32,37,40	2.34	8 (25%)
1	7MG	DB	527	1	23,26,27	2.94	7 (30%)	27,39,42	2.28	9 (33%)
1	M2G	DB	966	1	24,27,28	2.21	3 (12%)	33,40,43	1.80	8 (24%)
2	5MU	EB	1915	2	19,22,23	2.02	3 (15%)	27,32,35	2.31	5 (18%)
4	4SU	LC	8	4	18,21,22	4.70	7 (38%)	25,30,33	6.03	11 (44%)
1	5MC	DB	1404	1	19,22,23	2.61	4 (21%)	26,32,35	1.28	3 (11%)
1	5MC	DB	967	1	19,22,23	2.39	5 (26%)	26,32,35	1.32	3 (11%)
2	PSU	EB	1911	2	18,21,22	1.58	2 (11%)	21,30,33	2.09	6 (28%)
2	5MC	B	1942	2	19,22,23	2.99	4 (21%)	26,32,35	1.38	4 (15%)
1	5MC	DB	1407	1	19,22,23	3.12	4 (21%)	26,32,35	1.17	2 (7%)
1	5MC	A	1404	1	19,22,23	2.78	4 (21%)	26,32,35	1.21	1 (3%)
1	5MC	A	1400	1	19,22,23	2.34	4 (21%)	26,32,35	1.21	4 (15%)
2	5MC	B	1962	2	19,22,23	2.65	4 (21%)	26,32,35	1.29	2 (7%)
1	UR3	A	1498	1	19,22,23	1.79	2 (10%)	26,32,35	1.55	4 (15%)
2	PSU	EB	2605	2	18,21,22	1.48	2 (11%)	21,30,33	1.66	5 (23%)
4	5MC	GB	32	4	19,22,23	2.65	4 (21%)	26,32,35	1.13	3 (11%)
45	0TD	WC	92	45	8,9,10	3.17	2 (25%)	6,11,13	3.11	3 (50%)
1	MA6	DB	1519	1	23,26,27	1.49	3 (13%)	33,38,41	2.00	10 (30%)
1	MA6	DB	1518	1	23,26,27	1.47	4 (17%)	33,38,41	2.07	10 (30%)
45	0TD	TA	92	45	8,9,10	2.60	2 (25%)	6,11,13	3.29	3 (50%)
1	PSU	A	516	1	18,21,22	1.93	3 (16%)	21,30,33	1.47	5 (23%)
1	UR3	DB	1498	1	19,22,23	1.92	1 (5%)	26,32,35	1.42	3 (11%)
2	PSU	B	2605	2	18,21,22	1.59	3 (16%)	21,30,33	1.69	4 (19%)
2	2MA	EB	2503	2	22,25,26	1.70	6 (27%)	32,37,40	2.31	8 (25%)
4	5MU	D	54	4	19,22,23	2.10	3 (15%)	27,32,35	1.99	8 (29%)
4	PSU	LC	55	4	18,21,22	1.90	3 (16%)	21,30,33	1.71	5 (23%)
4	5MC	LC	32	4	19,22,23	2.33	4 (21%)	26,32,35	1.32	3 (11%)
4	PSU	D	55	4	18,21,22	1.76	2 (11%)	21,30,33	1.48	2 (9%)
1	5MC	DB	1400	1	19,22,23	2.45	4 (21%)	26,32,35	1.26	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5MU	B	1915	2	19,22,23	1.95	3 (15%)	27,32,35	2.45	6 (22%)
4	5MC	IA	32	4	19,22,23	2.61	4 (21%)	26,32,35	1.30	3 (11%)
4	PSU	IA	55	4	18,21,22	1.91	2 (11%)	21,30,33	1.87	6 (28%)
2	2MU	EB	2552	2,56	19,22,24	2.56	3 (15%)	25,31,36	2.26	5 (20%)
4	5MU	GB	54	4	19,22,23	2.07	3 (15%)	27,32,35	2.12	8 (29%)
1	5MC	A	967	1	19,22,23	2.52	5 (26%)	26,32,35	1.31	3 (11%)
2	4OC	B	1920	2	19,22,24	1.14	1 (5%)	25,31,35	0.85	1 (4%)
2	PSU	B	1917	2	18,21,22	1.77	3 (16%)	21,30,33	1.84	5 (23%)
4	4SU	GB	8	4	18,21,22	4.63	7 (38%)	25,30,33	6.22	9 (36%)
4	5MU	LC	54	4	19,22,23	2.22	3 (15%)	27,32,35	1.83	7 (25%)
1	4OC	A	1402	1	20,23,24	1.11	2 (10%)	25,32,35	1.30	5 (20%)
2	5MC	EB	1962	2,56	19,22,23	2.61	5 (26%)	26,32,35	1.24	2 (7%)
4	4SU	D	8	4	18,21,22	4.82	7 (38%)	25,30,33	5.36	10 (40%)
2	OMG	B	2251	2,4	23,26,27	2.06	3 (13%)	32,38,41	1.88	10 (31%)
1	2MG	A	1207	1	23,26,27	2.21	3 (13%)	33,38,41	2.02	11 (33%)
1	MA6	A	1518	1	23,26,27	1.45	4 (17%)	33,38,41	2.05	10 (30%)
2	5MU	B	1939	2	19,22,23	2.28	3 (15%)	27,32,35	2.47	8 (29%)
2	2MU	B	2552	2	19,22,24	2.72	5 (26%)	25,31,36	2.18	6 (24%)
4	4SU	IA	8	4	18,21,22	4.77	7 (38%)	25,30,33	5.16	11 (44%)
1	7MG	A	527	1	23,26,27	2.98	7 (30%)	27,39,42	2.09	8 (29%)
1	MA6	A	1519	1	23,26,27	1.53	4 (17%)	33,38,41	1.94	10 (30%)
1	PSU	DB	516	1	18,21,22	1.82	3 (16%)	21,30,33	1.34	3 (14%)
2	PSU	EB	1917	2	18,21,22	1.71	2 (11%)	21,30,33	1.82	6 (28%)
1	M2G	A	966	1	24,27,28	2.22	3 (12%)	33,40,43	1.83	9 (27%)
2	5MC	EB	1942	2	19,22,23	2.95	4 (21%)	26,32,35	1.44	4 (15%)
4	5MU	IA	54	4,56	19,22,23	2.14	3 (15%)	27,32,35	2.22	10 (37%)
4	PSU	GB	55	4	18,21,22	1.65	3 (16%)	21,30,33	1.58	3 (14%)
1	4OC	DB	1402	1	20,23,24	1.07	2 (10%)	25,32,35	1.59	7 (28%)
4	5MC	D	32	4	19,22,23	2.65	4 (21%)	26,32,35	0.97	2 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	EB	2251	2,4	-	1/9/27/28	0/3/3/3
1	2MG	DB	1207	1	-	0/9/27/28	0/3/3/3
2	5MU	EB	1939	2	-	0/7/25/26	0/2/2/2
2	PSU	B	1911	2	-	0/7/25/26	0/2/2/2
2	4OC	EB	1920	2	-	3/9/27/30	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
2	2MA	B	2503	2	-	1/7/25/26	0/3/3/3
1	7MG	DB	527	1	-	2/7/37/38	0/3/3/3
1	M2G	DB	966	1	-	0/11/29/30	0/3/3/3
2	5MU	EB	1915	2	-	0/7/25/26	0/2/2/2
4	4SU	LC	8	4	-	0/7/25/26	0/2/2/2
1	5MC	DB	1404	1	-	0/7/25/26	0/2/2/2
1	5MC	DB	967	1	-	0/7/25/26	0/2/2/2
2	PSU	EB	1911	2	-	0/7/25/26	0/2/2/2
2	5MC	B	1942	2	-	0/7/25/26	0/2/2/2
1	5MC	DB	1407	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	1/7/25/26	0/2/2/2
2	5MC	B	1962	2	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
2	PSU	EB	2605	2	-	0/7/25/26	0/2/2/2
4	5MC	GB	32	4	-	0/7/25/26	0/2/2/2
45	0TD	WC	92	45	-	5/7/12/14	-
1	MA6	DB	1519	1	-	3/11/29/30	0/3/3/3
1	MA6	DB	1518	1	-	1/11/29/30	0/3/3/3
45	0TD	TA	92	45	-	4/7/12/14	-
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	UR3	DB	1498	1	-	0/7/25/26	0/2/2/2
2	PSU	B	2605	2	-	0/7/25/26	0/2/2/2
2	2MA	EB	2503	2	-	1/7/25/26	0/3/3/3
4	5MU	D	54	4	-	0/7/25/26	0/2/2/2
4	PSU	LC	55	4	-	0/7/25/26	0/2/2/2
4	5MC	LC	32	4	-	0/7/25/26	0/2/2/2
4	PSU	D	55	4	-	0/7/25/26	0/2/2/2
1	5MC	DB	1400	1	-	2/7/25/26	0/2/2/2
2	5MU	B	1915	2	-	0/7/25/26	0/2/2/2
4	5MC	IA	32	4	-	0/7/25/26	0/2/2/2
4	PSU	IA	55	4	-	0/7/25/26	0/2/2/2
2	2MU	EB	2552	2,56	-	0/9/27/28	0/2/2/2
4	5MU	GB	54	4	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
2	4OC	B	1920	2	-	4/9/27/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	B	1917	2	-	0/7/25/26	0/2/2/2
4	4SU	GB	8	4	-	2/7/25/26	0/2/2/2
4	5MU	LC	54	4	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
2	5MC	EB	1962	2,56	-	0/7/25/26	0/2/2/2
4	4SU	D	8	4	-	2/7/25/26	0/2/2/2
2	OMG	B	2251	2,4	-	1/9/27/28	0/3/3/3
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
1	MA6	A	1518	1	-	1/11/29/30	0/3/3/3
2	5MU	B	1939	2	-	0/7/25/26	0/2/2/2
2	2MU	B	2552	2	-	0/9/27/28	0/2/2/2
4	4SU	IA	8	4	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	MA6	A	1519	1	-	3/11/29/30	0/3/3/3
1	PSU	DB	516	1	-	0/7/25/26	0/2/2/2
2	PSU	EB	1917	2	-	0/7/25/26	0/2/2/2
1	M2G	A	966	1	-	0/11/29/30	0/3/3/3
2	5MC	EB	1942	2	-	0/7/25/26	0/2/2/2
4	5MU	IA	54	4,56	-	0/7/25/26	0/2/2/2
4	PSU	GB	55	4	-	0/7/25/26	0/2/2/2
1	4OC	DB	1402	1	-	2/9/29/30	0/2/2/2
4	5MC	D	32	4	-	0/7/25/26	0/2/2/2

The worst 5 of 231 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	8	4SU	C4-N3	12.89	1.50	1.37
4	LC	8	4SU	C4-N3	12.62	1.50	1.37
4	IA	8	4SU	C4-N3	12.22	1.50	1.37
4	GB	8	4SU	C4-N3	12.11	1.50	1.37
4	IA	8	4SU	O2-C2	11.93	1.44	1.23

The worst 5 of 368 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	GB	8	4SU	C4-N3-C2	-19.85	108.28	127.31
4	LC	8	4SU	C4-N3-C2	-16.98	111.03	127.31
4	LC	8	4SU	C1'-N1-C2	13.91	142.57	117.59
4	GB	8	4SU	C1'-N1-C2	11.38	138.02	117.59
4	D	8	4SU	C1'-N1-C2	11.26	137.82	117.59

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1518	MA6	C5-C6-N6-C9
1	A	1519	MA6	O4'-C4'-C5'-O5'
2	B	1920	4OC	C1'-C2'-O2'-CM2
2	B	2251	OMG	C1'-C2'-O2'-CM2
45	TA	92	0TD	CA-CB-SB-CSB

There are no ring outliers.

31 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	EB	1939	5MU	1	0
1	A	1407	5MC	1	0
2	B	2503	2MA	3	0
1	DB	527	7MG	1	0
1	DB	966	M2G	1	0
2	EB	1915	5MU	1	0
1	DB	967	5MC	1	0
1	DB	1407	5MC	1	0
1	A	1498	UR3	1	0
45	WC	92	0TD	4	0
1	DB	1519	MA6	1	0
1	DB	1518	MA6	1	0
45	TA	92	0TD	3	0
1	DB	1498	UR3	2	0
2	EB	2503	2MA	3	0
4	D	54	5MU	1	0
4	D	55	PSU	1	0
2	B	1915	5MU	1	0
2	EB	2552	2MU	2	0
4	GB	54	5MU	1	0
1	A	967	5MC	1	0
2	B	1920	4OC	1	0
4	GB	8	4SU	1	0
1	A	1402	4OC	2	0
1	A	1518	MA6	1	0
2	B	1939	5MU	2	0
2	B	2552	2MU	2	0
2	EB	1917	PSU	1	0
1	A	966	M2G	1	0
4	GB	55	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	DB	1402	4OC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1528 ligands modelled in this entry, 1528 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1495/1507 (99%)	0.11	47 (3%) 51 28	94, 141, 205, 274	0
1	DB	1495/1507 (99%)	0.22	49 (3%) 49 27	100, 130, 190, 262	0
2	B	2869/2880 (99%)	0.00	66 (2%) 61 34	77, 97, 192, 252	0
2	EB	2869/2880 (99%)	0.16	82 (2%) 53 29	88, 112, 211, 267	0
3	C	120/120 (100%)	-0.08	1 (0%) 82 58	108, 129, 142, 160	0
3	FB	120/120 (100%)	0.30	3 (2%) 58 33	119, 157, 177, 190	0
4	D	73/77 (94%)	0.37	5 (6%) 23 14	112, 214, 233, 236	0
4	GB	73/77 (94%)	0.39	3 (4%) 41 22	131, 210, 227, 231	0
4	IA	73/77 (94%)	0.35	8 (10%) 10 7	90, 125, 134, 141	0
4	LC	73/77 (94%)	0.11	3 (4%) 41 22	108, 132, 144, 148	0
5	E	275/275 (100%)	0.10	11 (4%) 42 23	79, 88, 98, 107	0
5	HB	275/275 (100%)	0.11	13 (4%) 36 19	86, 102, 112, 122	0
6	F	204/206 (99%)	0.07	2 (0%) 79 54	78, 102, 123, 133	0
6	IB	204/206 (99%)	0.02	2 (0%) 79 54	90, 116, 136, 147	0
7	G	202/205 (98%)	-0.14	1 (0%) 87 66	71, 100, 121, 131	0
7	JB	202/205 (98%)	0.05	6 (2%) 52 29	84, 115, 132, 137	0
8	H	181/182 (99%)	0.15	9 (4%) 34 19	132, 140, 158, 161	0
8	KB	181/182 (99%)	0.25	6 (3%) 49 27	146, 166, 178, 180	0
9	I	174/180 (96%)	0.02	6 (3%) 48 26	112, 121, 128, 139	0
9	LB	174/180 (96%)	0.70	17 (9%) 13 9	158, 192, 207, 212	0
10	J	146/148 (98%)	0.26	7 (4%) 35 19	102, 140, 148, 150	0
10	MB	146/148 (98%)	0.56	14 (9%) 13 9	123, 153, 164, 166	0
11	K	140/140 (100%)	-0.02	1 (0%) 84 61	84, 100, 119, 128	0
11	NB	140/140 (100%)	0.24	9 (6%) 25 15	100, 122, 137, 142	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
12	L	122/122 (100%)	0.03	7 (5%)	29	17	87, 100, 110, 114	0
12	OB	122/122 (100%)	0.05	5 (4%)	41	22	97, 107, 115, 118	0
13	M	150/150 (100%)	0.19	7 (4%)	36	19	76, 106, 131, 135	0
13	PB	150/150 (100%)	0.25	6 (4%)	42	23	93, 118, 148, 150	0
14	N	141/141 (100%)	0.08	6 (4%)	40	21	94, 105, 118, 126	0
14	QB	141/141 (100%)	0.15	2 (1%)	73	45	106, 126, 140, 148	0
15	O	118/118 (100%)	-0.09	0	100	100	87, 101, 114, 120	0
15	RB	118/118 (100%)	-0.03	0	100	100	97, 111, 121, 125	0
16	P	110/112 (98%)	-0.03	3 (2%)	56	31	116, 127, 132, 134	0
16	SB	110/112 (98%)	0.24	1 (0%)	81	56	139, 155, 162, 165	0
17	Q	137/146 (93%)	0.06	6 (4%)	39	21	99, 111, 155, 184	0
17	TB	137/146 (93%)	0.14	4 (2%)	53	29	108, 117, 147, 158	0
18	R	117/118 (99%)	-0.12	0	100	100	78, 95, 108, 111	0
18	UB	117/118 (99%)	0.26	5 (4%)	40	21	92, 116, 131, 137	0
19	S	101/101 (100%)	-0.25	0	100	100	80, 105, 116, 121	0
19	VB	101/101 (100%)	-0.02	2 (1%)	65	37	96, 127, 136, 141	0
20	T	112/113 (99%)	-0.25	0	100	100	77, 90, 113, 123	0
20	WB	112/113 (99%)	-0.10	2 (1%)	67	40	89, 102, 121, 133	0
21	U	95/96 (98%)	-0.07	1 (1%)	78	52	87, 93, 104, 111	0
21	XB	95/96 (98%)	0.24	5 (5%)	32	18	107, 121, 129, 131	0
22	V	107/110 (97%)	0.11	2 (1%)	66	38	97, 106, 122, 125	0
22	YB	107/110 (97%)	0.49	5 (4%)	36	19	114, 124, 143, 146	0
23	W	189/206 (91%)	-0.01	2 (1%)	78	52	111, 129, 139, 142	0
23	ZB	189/206 (91%)	0.04	2 (1%)	78	52	132, 151, 162, 167	0
24	AC	84/85 (98%)	0.64	9 (10%)	11	8	116, 122, 137, 141	0
24	X	84/85 (98%)	0.52	10 (11%)	9	6	100, 105, 124, 130	0
25	BC	97/98 (98%)	0.48	6 (6%)	26	15	92, 116, 142, 154	0
25	Y	97/98 (98%)	0.41	8 (8%)	17	11	82, 99, 125, 135	0
26	CC	70/72 (97%)	0.39	4 (5%)	29	17	126, 133, 136, 139	0
26	Z	70/72 (97%)	0.13	6 (8%)	16	11	95, 101, 106, 112	0
27	AA	60/60 (100%)	-0.24	0	100	100	92, 104, 123, 130	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	DC	60/60 (100%)	-0.01	0 100 100	108, 120, 133, 138	0
28	BA	69/71 (97%)	0.06	0 100 100	162, 179, 201, 205	0
28	EC	69/71 (97%)	0.13	1 (1%) 73 45	189, 197, 207, 209	0
29	CA	59/60 (98%)	0.11	1 (1%) 69 40	79, 106, 122, 126	0
29	FC	59/60 (98%)	0.05	2 (3%) 48 26	88, 116, 131, 133	0
30	DA	53/54 (98%)	0.54	3 (5%) 29 17	161, 165, 168, 169	0
30	GC	53/54 (98%)	0.84	7 (13%) 7 6	188, 192, 195, 195	0
31	EA	48/49 (97%)	0.48	5 (10%) 11 8	72, 77, 87, 89	0
31	HC	48/49 (97%)	0.70	3 (6%) 26 15	89, 92, 102, 107	0
32	FA	64/65 (98%)	0.24	2 (3%) 51 28	83, 94, 110, 118	0
32	IC	64/65 (98%)	0.19	4 (6%) 26 15	98, 109, 127, 132	0
33	GA	37/37 (100%)	1.04	8 (21%) 2 2	154, 154, 155, 155	0
33	JC	37/37 (100%)	1.31	9 (24%) 2 2	167, 167, 167, 167	0
34	HA	11/27 (40%)	0.85	1 (9%) 15 9	120, 128, 144, 147	0
34	KC	11/27 (40%)	0.54	1 (9%) 15 9	124, 129, 145, 145	0
35	JA	234/256 (91%)	0.14	8 (3%) 48 26	148, 164, 183, 190	0
35	MC	234/256 (91%)	0.15	8 (3%) 48 26	139, 159, 176, 188	0
36	KA	206/239 (86%)	0.02	5 (2%) 59 33	143, 156, 173, 176	0
36	NC	206/239 (86%)	0.08	4 (1%) 66 38	142, 155, 172, 176	0
37	LA	208/209 (99%)	0.75	23 (11%) 10 7	132, 148, 157, 161	0
37	OC	208/209 (99%)	0.52	22 (10%) 11 8	117, 128, 135, 139	0
38	MA	151/162 (93%)	0.25	8 (5%) 32 18	125, 138, 145, 157	0
38	PC	151/162 (93%)	0.11	9 (5%) 27 16	114, 125, 133, 144	0
39	NA	101/101 (100%)	-0.07	2 (1%) 65 37	119, 129, 134, 144	0
39	QC	101/101 (100%)	-0.12	2 (1%) 65 37	125, 134, 141, 147	0
40	OA	155/156 (99%)	0.29	9 (5%) 29 16	141, 155, 164, 165	0
40	RC	155/156 (99%)	0.29	9 (5%) 29 16	142, 153, 160, 163	0
41	PA	138/138 (100%)	0.19	7 (5%) 33 18	124, 141, 147, 152	0
41	SC	138/138 (100%)	-0.06	1 (0%) 84 61	116, 129, 137, 140	0
42	QA	127/128 (99%)	0.38	12 (9%) 14 9	134, 179, 187, 189	0
42	TC	127/128 (99%)	0.39	10 (7%) 18 12	145, 173, 181, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	RA	98/105 (93%)	0.38	2 (2%) 65 37	144, 182, 195, 196	0
43	UC	98/105 (93%)	0.33	2 (2%) 65 37	148, 176, 181, 183	0
44	SA	116/129 (89%)	0.18	5 (4%) 40 21	108, 126, 133, 142	0
44	VC	116/129 (89%)	0.19	6 (5%) 33 18	109, 130, 137, 143	0
45	TA	121/132 (91%)	0.23	3 (2%) 58 33	115, 121, 128, 132	0
45	WC	121/132 (91%)	-0.02	3 (2%) 58 33	108, 114, 123, 128	0
46	UA	117/126 (92%)	0.44	11 (9%) 14 9	132, 167, 173, 174	0
46	XC	117/126 (92%)	0.41	11 (9%) 14 9	147, 178, 186, 187	0
47	VA	60/61 (98%)	0.42	2 (3%) 49 27	151, 158, 167, 168	0
47	YC	60/61 (98%)	0.50	4 (6%) 24 14	152, 160, 176, 177	0
48	WA	88/89 (98%)	0.01	2 (2%) 61 34	108, 126, 138, 140	0
48	ZC	88/89 (98%)	-0.17	2 (2%) 61 34	110, 127, 133, 135	0
49	AD	83/88 (94%)	0.23	5 (6%) 27 16	118, 123, 137, 154	0
49	XA	83/88 (94%)	0.71	8 (9%) 13 9	137, 156, 170, 187	0
50	BD	99/105 (94%)	0.30	9 (9%) 15 9	111, 120, 124, 126	0
50	YA	99/105 (94%)	0.35	6 (6%) 27 15	109, 128, 135, 138	0
51	CD	70/88 (79%)	0.06	2 (2%) 53 29	125, 134, 141, 144	0
51	ZA	70/88 (79%)	0.04	4 (5%) 29 17	120, 130, 138, 141	0
52	AB	83/93 (89%)	0.17	2 (2%) 59 33	143, 170, 175, 177	0
52	DD	83/93 (89%)	0.29	2 (2%) 59 33	158, 183, 188, 189	0
53	BB	99/106 (93%)	0.56	11 (11%) 10 7	141, 154, 170, 172	0
53	ED	99/106 (93%)	0.30	8 (8%) 18 11	119, 140, 155, 156	0
54	CB	24/27 (88%)	1.33	4 (16%) 4 4	155, 165, 170, 174	0
54	FD	24/27 (88%)	1.54	7 (29%) 1 1	160, 168, 173, 175	0
55	GD	255/365 (69%)	0.07	9 (3%) 47 26	94, 137, 163, 184	0
55	HD	255/365 (69%)	0.10	11 (4%) 40 21	117, 143, 169, 180	0
All	All	21472/22222 (96%)	0.16	814 (3%) 44 24	71, 124, 185, 274	0

The worst 5 of 814 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	BC	2	SER	10.2
25	Y	2	SER	9.0

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Mol	Chain	Res	Type	RSRZ
24	AC	3	HIS	8.9
24	X	3	HIS	8.5
2	EB	270(C)	A	7.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PSU	D	55	20/21	0.58	0.11	232,233,236,237	0
4	5MU	D	54	21/22	0.63	0.10	229,231,233,234	0
4	4SU	GB	8	20/21	0.68	0.11	215,218,219,219	0
4	PSU	GB	55	20/21	0.71	0.08	226,228,230,231	0
4	5MU	GB	54	21/22	0.72	0.08	225,227,229,229	0
4	4SU	D	8	20/21	0.75	0.10	218,221,222,223	0
4	PSU	IA	55	20/21	0.85	0.10	135,137,138,138	0
45	0TD	TA	92	10/11	0.85	0.26	123,123,124,124	0
4	5MC	D	32	21/22	0.88	0.09	177,177,177,177	0
2	5MU	B	1915	21/22	0.88	0.09	119,120,123,123	0
1	PSU	DB	516	20/21	0.88	0.09	125,126,129,129	0
4	5MU	LC	54	21/22	0.89	0.09	140,141,144,144	0
4	5MC	GB	32	21/22	0.89	0.09	178,178,178,179	0
4	PSU	LC	55	20/21	0.89	0.07	141,142,144,144	0
45	0TD	WC	92	10/11	0.90	0.16	119,120,120,120	0
2	PSU	B	1911	20/21	0.90	0.09	104,107,109,109	0
1	5MC	A	1400	21/22	0.90	0.13	121,123,125,126	0
2	5MU	EB	1939	21/22	0.90	0.17	93,94,95,95	0
4	4SU	IA	8	20/21	0.91	0.20	122,124,125,126	0
2	4OC	EB	1920	21/23	0.91	0.09	112,114,115,116	0
1	2MG	DB	1207	24/25	0.91	0.10	156,157,160,162	0
1	4OC	DB	1402	22/23	0.91	0.10	115,116,117,117	0
4	5MC	LC	32	21/22	0.91	0.11	128,128,129,129	0
2	PSU	EB	1917	20/21	0.91	0.08	117,119,121,122	0
2	OMG	B	2251	24/25	0.92	0.10	83,84,85,86	0
4	5MU	IA	54	21/22	0.92	0.08	134,134,137,138	0
2	5MU	EB	1915	21/22	0.92	0.06	129,131,132,133	0
1	2MG	A	1207	24/25	0.92	0.08	148,150,153,154	0
1	5MC	A	967	21/22	0.92	0.09	130,131,133,134	0
4	5MC	IA	32	21/22	0.92	0.11	126,126,126,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	7MG	DB	527	24/25	0.92	0.11	117,118,119,120	0
2	5MU	B	1939	21/22	0.92	0.13	84,85,86,86	0
1	PSU	A	516	20/21	0.93	0.07	132,134,137,137	0
2	5MC	EB	1942	21/22	0.93	0.08	101,103,104,104	0
2	5MC	EB	1962	21/22	0.93	0.11	98,99,101,102	0
1	5MC	DB	1400	21/22	0.93	0.11	119,121,123,124	0
2	5MC	B	1942	21/22	0.93	0.09	90,92,93,94	0
1	UR3	DB	1498	21/22	0.93	0.14	111,111,112,112	0
2	4OC	B	1920	21/23	0.93	0.10	102,104,106,107	0
4	4SU	LC	8	20/21	0.93	0.13	130,133,134,134	0
1	M2G	DB	966	25/26	0.93	0.10	130,132,134,134	0
1	5MC	DB	967	21/22	0.93	0.08	131,133,135,136	0
2	2MA	EB	2503	23/24	0.94	0.10	88,89,90,90	0
1	4OC	A	1402	22/23	0.94	0.11	115,116,117,117	0
2	PSU	B	1917	20/21	0.94	0.07	107,108,111,112	0
1	5MC	A	1407	21/22	0.94	0.08	104,105,107,108	0
1	MA6	DB	1518	24/25	0.94	0.17	102,104,105,106	0
1	7MG	A	527	24/25	0.94	0.11	122,124,125,126	0
2	2MU	EB	2552	21/23	0.95	0.14	96,97,98,98	0
1	M2G	A	966	25/26	0.95	0.10	129,130,132,132	0
2	5MC	B	1962	21/22	0.95	0.07	92,93,95,97	0
2	PSU	EB	1911	20/21	0.95	0.07	113,116,117,118	0
1	5MC	A	1404	21/22	0.95	0.09	106,107,108,109	0
2	PSU	B	2605	20/21	0.95	0.10	79,81,81,81	0
1	MA6	A	1518	24/25	0.96	0.11	99,102,104,104	0
1	MA6	DB	1519	24/25	0.96	0.13	103,105,106,106	0
2	2MA	B	2503	23/24	0.96	0.08	78,78,79,79	0
1	5MC	DB	1407	21/22	0.96	0.09	107,109,110,110	0
2	OMG	EB	2251	24/25	0.96	0.11	95,96,98,98	0
1	UR3	A	1498	21/22	0.96	0.11	107,108,109,109	0
2	2MU	B	2552	21/23	0.97	0.13	84,86,86,86	0
1	MA6	A	1519	24/25	0.97	0.10	100,102,104,104	0
2	PSU	EB	2605	20/21	0.97	0.08	89,90,91,91	0
1	5MC	DB	1404	21/22	0.97	0.09	107,108,109,109	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	EB	3285	1/1	-0.43	0.20	220,220,220,220	0
56	MG	B	3188	1/1	-0.42	0.36	217,217,217,217	0
56	MG	B	3142	1/1	-0.42	0.20	214,214,214,214	0
56	MG	EB	3189	1/1	-0.41	0.12	241,241,241,241	0
56	MG	EB	3170	1/1	-0.34	0.16	187,187,187,187	0
56	MG	LB	204	1/1	-0.34	0.23	197,197,197,197	0
56	MG	D	105	1/1	-0.31	0.20	208,208,208,208	0
56	MG	A	1688	1/1	-0.27	0.20	167,167,167,167	0
56	MG	A	1746	1/1	-0.25	0.35	173,173,173,173	0
56	MG	DB	1736	1/1	-0.18	0.26	212,212,212,212	0
56	MG	EB	3026	1/1	-0.17	0.14	175,175,175,175	0
56	MG	GB	103	1/1	-0.13	0.24	211,211,211,211	0
56	MG	DB	1729	1/1	-0.11	0.19	159,159,159,159	0
56	MG	B	3391	1/1	-0.09	0.15	240,240,240,240	0
56	MG	RC	201	1/1	-0.09	0.40	142,142,142,142	0
56	MG	EB	3016	1/1	-0.07	0.36	243,243,243,243	0
56	MG	VA	101	1/1	-0.07	0.44	140,140,140,140	0
56	MG	B	3288	1/1	-0.04	0.22	208,208,208,208	0
56	MG	EB	3195	1/1	-0.03	0.22	152,152,152,152	0
56	MG	A	1680	1/1	-0.02	0.38	176,176,176,176	0
56	MG	B	3352	1/1	-0.02	0.21	183,183,183,183	0
56	MG	A	1711	1/1	-0.02	0.37	130,130,130,130	0
56	MG	A	1728	1/1	-0.02	0.20	160,160,160,160	0
56	MG	A	1755	1/1	0.00	0.19	176,176,176,176	0
56	MG	B	3025	1/1	-0.00	0.36	234,234,234,234	0
56	MG	KA	301	1/1	0.00	0.35	157,157,157,157	0
56	MG	DB	1681	1/1	0.01	0.34	149,149,149,149	0
56	MG	GB	102	1/1	0.03	0.14	204,204,204,204	0
56	MG	A	1729	1/1	0.03	0.40	152,152,152,152	0
56	MG	DB	1690	1/1	0.06	0.31	139,139,139,139	0
56	MG	EB	2945	1/1	0.06	0.52	139,139,139,139	0
56	MG	W	302	1/1	0.08	0.38	129,129,129,129	0
56	MG	RA	201	1/1	0.08	0.18	165,165,165,165	0
56	MG	A	1640	1/1	0.09	0.39	134,134,134,134	0
56	MG	B	3392	1/1	0.09	0.18	192,192,192,192	0
56	MG	KB	201	1/1	0.10	0.19	173,173,173,173	0
56	MG	B	3304	1/1	0.11	0.28	237,237,237,237	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	GD	404	1/1	0.13	0.27	135,135,135,135	0
56	MG	B	2960	1/1	0.14	0.58	223,223,223,223	0
56	MG	B	3384	1/1	0.14	0.26	161,161,161,161	0
56	MG	A	1707	1/1	0.16	0.20	163,163,163,163	0
56	MG	W	310	1/1	0.17	0.12	134,134,134,134	0
56	MG	A	1634	1/1	0.17	0.50	134,134,134,134	0
56	MG	B	3315	1/1	0.17	0.13	203,203,203,203	0
56	MG	B	3175	1/1	0.18	0.45	154,154,154,154	0
56	MG	TC	201	1/1	0.19	0.27	177,177,177,177	0
56	MG	EB	3132	1/1	0.19	0.33	140,140,140,140	0
56	MG	DB	1761	1/1	0.20	0.20	152,152,152,152	0
56	MG	DB	1615	1/1	0.20	0.65	122,122,122,122	0
56	MG	DB	1623	1/1	0.21	0.29	121,121,121,121	0
56	MG	GB	101	1/1	0.21	0.22	202,202,202,202	0
56	MG	EB	3177	1/1	0.21	0.21	122,122,122,122	0
56	MG	DB	1703	1/1	0.22	0.45	163,163,163,163	0
56	MG	EB	2982	1/1	0.22	0.39	133,133,133,133	0
56	MG	EB	2944	1/1	0.22	0.25	102,102,102,102	0
56	MG	EB	3050	1/1	0.23	0.37	160,160,160,160	0
56	MG	LB	202	1/1	0.23	0.32	181,181,181,181	0
56	MG	FB	216	1/1	0.23	0.37	141,141,141,141	0
56	MG	Q	202	1/1	0.23	0.22	148,148,148,148	0
56	MG	JA	301	1/1	0.23	0.23	143,143,143,143	0
56	MG	EB	3251	1/1	0.23	0.08	158,158,158,158	0
56	MG	EB	3019	1/1	0.24	0.31	113,113,113,113	0
56	MG	DB	1685	1/1	0.24	0.20	177,177,177,177	0
56	MG	A	1745	1/1	0.25	0.18	219,219,219,219	0
56	MG	GB	105	1/1	0.25	0.25	172,172,172,172	0
56	MG	B	3176	1/1	0.25	0.23	144,144,144,144	0
56	MG	DB	1742	1/1	0.25	0.27	142,142,142,142	0
56	MG	A	1627	1/1	0.26	0.27	127,127,127,127	0
56	MG	A	1742	1/1	0.26	0.24	179,179,179,179	0
56	MG	JC	102	1/1	0.26	0.18	146,146,146,146	0
56	MG	DB	1601	1/1	0.26	0.40	122,122,122,122	0
56	MG	FB	208	1/1	0.26	0.16	171,171,171,171	0
56	MG	B	3022	1/1	0.26	0.27	118,118,118,118	0
56	MG	EB	3259	1/1	0.27	0.24	141,141,141,141	0
56	MG	EB	3067	1/1	0.27	0.17	131,131,131,131	0
56	MG	EB	3102	1/1	0.27	0.21	126,126,126,126	0
56	MG	EB	2936	1/1	0.27	0.49	128,128,128,128	0
56	MG	XC	201	1/1	0.27	0.14	171,171,171,171	0
56	MG	D	102	1/1	0.27	0.15	210,210,210,210	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	3134	1/1	0.28	0.36	129,129,129,129	0
56	MG	DB	1617	1/1	0.28	0.45	136,136,136,136	0
56	MG	A	1618	1/1	0.28	0.34	126,126,126,126	0
56	MG	EB	3014	1/1	0.28	0.21	136,136,136,136	0
56	MG	B	3274	1/1	0.29	0.32	118,118,118,118	0
56	MG	LC	102	1/1	0.29	0.24	124,124,124,124	0
56	MG	EB	2971	1/1	0.31	0.41	112,112,112,112	0
56	MG	B	3124	1/1	0.31	0.22	155,155,155,155	0
56	MG	EB	3120	1/1	0.32	0.39	143,143,143,143	0
56	MG	EB	2911	1/1	0.33	0.53	111,111,111,111	0
56	MG	B	3262	1/1	0.33	0.45	143,143,143,143	0
56	MG	DB	1602	1/1	0.33	0.53	97,97,97,97	0
56	MG	FB	212	1/1	0.33	0.34	160,160,160,160	0
56	MG	B	3282	1/1	0.33	0.25	147,147,147,147	0
56	MG	DB	1712	1/1	0.33	0.18	199,199,199,199	0
56	MG	A	1635	1/1	0.34	0.26	138,138,138,138	0
56	MG	GD	402	1/1	0.34	0.20	124,124,124,124	0
56	MG	B	3287	1/1	0.34	0.25	151,151,151,151	0
56	MG	LA	301	1/1	0.35	0.19	139,139,139,139	0
56	MG	FB	201	1/1	0.35	0.42	117,117,117,117	0
56	MG	MC	301	1/1	0.35	0.23	149,149,149,149	0
56	MG	A	1656	1/1	0.35	0.18	229,229,229,229	0
56	MG	FB	205	1/1	0.36	0.42	143,143,143,143	0
56	MG	EB	2979	1/1	0.36	0.48	111,111,111,111	0
56	MG	A	1705	1/1	0.36	0.38	143,143,143,143	0
56	MG	EB	3266	1/1	0.36	0.24	138,138,138,138	0
56	MG	DB	1645	1/1	0.36	0.29	139,139,139,139	0
56	MG	TB	203	1/1	0.36	0.19	152,152,152,152	0
56	MG	EB	3205	1/1	0.36	0.21	138,138,138,138	0
56	MG	JA	303	1/1	0.37	0.11	161,161,161,161	0
56	MG	DB	1686	1/1	0.37	0.35	124,124,124,124	0
56	MG	A	1675	1/1	0.37	0.30	118,118,118,118	0
56	MG	DB	1648	1/1	0.37	0.16	143,143,143,143	0
56	MG	B	2908	1/1	0.37	0.32	95,95,95,95	0
56	MG	DB	1714	1/1	0.37	0.38	99,99,99,99	0
56	MG	EB	3201	1/1	0.37	0.24	133,133,133,133	0
56	MG	EB	3103	1/1	0.37	0.41	103,103,103,103	0
56	MG	LB	205	1/1	0.37	0.09	197,197,197,197	0
56	MG	A	1752	1/1	0.38	0.34	160,160,160,160	0
56	MG	EB	2995	1/1	0.38	0.30	152,152,152,152	0
56	MG	A	1726	1/1	0.38	0.23	167,167,167,167	0
56	MG	VA	102	1/1	0.38	0.11	159,159,159,159	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	EB	3022	1/1	0.39	0.39	114,114,114,114	0
56	MG	A	1657	1/1	0.39	0.34	164,164,164,164	0
56	MG	B	3119	1/1	0.39	0.45	100,100,100,100	0
56	MG	A	1622	1/1	0.39	0.38	147,147,147,147	0
56	MG	DB	1654	1/1	0.41	0.22	165,165,165,165	0
56	MG	B	2966	1/1	0.41	0.45	106,106,106,106	0
56	MG	A	1633	1/1	0.41	0.21	140,140,140,140	0
56	MG	GD	405	1/1	0.41	0.28	117,117,117,117	0
56	MG	DB	1756	1/1	0.42	0.32	119,119,119,119	0
56	MG	A	1699	1/1	0.42	0.28	143,143,143,143	0
56	MG	DB	1640	1/1	0.42	0.32	121,121,121,121	0
56	MG	P	201	1/1	0.42	0.13	129,129,129,129	0
56	MG	EB	3191	1/1	0.42	0.19	151,151,151,151	0
56	MG	DB	1725	1/1	0.43	0.35	166,166,166,166	0
56	MG	EB	2989	1/1	0.43	0.30	179,179,179,179	0
56	MG	EB	2966	1/1	0.43	0.41	99,99,99,99	0
56	MG	EB	2969	1/1	0.43	0.28	127,127,127,127	0
56	MG	C	206	1/1	0.43	0.30	130,130,130,130	0
56	MG	A	1615	1/1	0.43	0.29	118,118,118,118	0
56	MG	WA	102	1/1	0.44	0.14	124,124,124,124	0
56	MG	A	1647	1/1	0.44	0.39	149,149,149,149	0
56	MG	LC	105	1/1	0.44	0.16	136,136,136,136	0
56	MG	IB	302	1/1	0.44	0.35	95,95,95,95	0
56	MG	A	1659	1/1	0.44	0.16	153,153,153,153	0
56	MG	A	1758	1/1	0.45	0.20	188,188,188,188	0
56	MG	LC	108	1/1	0.45	0.11	125,125,125,125	0
56	MG	D	103	1/1	0.45	0.09	175,175,175,175	0
56	MG	A	1662	1/1	0.45	0.27	154,154,154,154	0
56	MG	A	1649	1/1	0.45	0.48	125,125,125,125	0
56	MG	A	1623	1/1	0.45	0.54	132,132,132,132	0
56	MG	FB	203	1/1	0.45	0.37	125,125,125,125	0
56	MG	A	1661	1/1	0.45	0.37	145,145,145,145	0
56	MG	HB	304	1/1	0.45	0.28	100,100,100,100	0
56	MG	EB	3066	1/1	0.46	0.20	172,172,172,172	0
56	MG	DB	1668	1/1	0.46	0.26	99,99,99,99	0
56	MG	DB	1758	1/1	0.46	0.29	207,207,207,207	0
56	MG	B	3026	1/1	0.46	0.18	116,116,116,116	0
56	MG	A	1644	1/1	0.46	0.40	114,114,114,114	0
56	MG	DB	1610	1/1	0.47	0.82	109,109,109,109	0
56	MG	EB	2951	1/1	0.47	0.26	95,95,95,95	0
56	MG	DB	1684	1/1	0.48	0.27	133,133,133,133	0
56	MG	C	213	1/1	0.48	0.19	139,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	3086	1/1	0.48	0.14	151,151,151,151	0
56	MG	EB	3232	1/1	0.48	0.23	145,145,145,145	0
56	MG	FB	206	1/1	0.48	0.39	124,124,124,124	0
56	MG	EB	3250	1/1	0.48	0.24	134,134,134,134	0
56	MG	DB	1660	1/1	0.48	0.20	131,131,131,131	0
56	MG	UC	201	1/1	0.48	0.35	164,164,164,164	0
56	MG	A	1611	1/1	0.48	0.26	149,149,149,149	0
56	MG	FB	217	1/1	0.48	0.19	139,139,139,139	0
56	MG	B	3123	1/1	0.48	0.33	103,103,103,103	0
56	MG	YB	202	1/1	0.48	0.24	116,116,116,116	0
56	MG	C	212	1/1	0.49	0.24	128,128,128,128	0
56	MG	EB	3181	1/1	0.49	0.39	155,155,155,155	0
56	MG	EB	3049	1/1	0.49	0.27	106,106,106,106	0
56	MG	DB	1718	1/1	0.50	0.28	145,145,145,145	0
56	MG	LB	201	1/1	0.50	0.24	159,159,159,159	0
56	MG	EB	3134	1/1	0.50	0.27	154,154,154,154	0
56	MG	B	2903	1/1	0.50	0.43	107,107,107,107	0
56	MG	LC	106	1/1	0.50	0.12	124,124,124,124	0
56	MG	A	1738	1/1	0.50	0.39	144,144,144,144	0
56	MG	B	2936	1/1	0.50	0.61	94,94,94,94	0
56	MG	A	1636	1/1	0.51	0.25	140,140,140,140	0
56	MG	DB	1621	1/1	0.51	0.32	110,110,110,110	0
56	MG	B	3131	1/1	0.51	0.23	112,112,112,112	0
56	MG	DB	1628	1/1	0.51	0.23	115,115,115,115	0
56	MG	B	3180	1/1	0.51	0.23	179,179,179,179	0
56	MG	B	3404	1/1	0.51	0.23	121,121,121,121	0
56	MG	DB	1691	1/1	0.51	0.19	109,109,109,109	0
56	MG	C	202	1/1	0.51	0.20	106,106,106,106	0
56	MG	DB	1704	1/1	0.51	0.20	127,127,127,127	0
56	MG	DB	1709	1/1	0.51	0.13	107,107,107,107	0
56	MG	DB	1614	1/1	0.51	0.41	94,94,94,94	0
56	MG	EB	3186	1/1	0.51	0.22	124,124,124,124	0
56	MG	LB	203	1/1	0.51	0.21	168,168,168,168	0
56	MG	IA	102	1/1	0.51	0.29	124,124,124,124	0
56	MG	DB	1717	1/1	0.51	0.21	124,124,124,124	0
56	MG	EB	3128	1/1	0.52	0.30	161,161,161,161	0
56	MG	DB	1657	1/1	0.52	0.17	102,102,102,102	0
56	MG	EB	3059	1/1	0.52	0.22	122,122,122,122	0
56	MG	EB	3142	1/1	0.52	0.38	136,136,136,136	0
56	MG	EB	2950	1/1	0.52	0.42	124,124,124,124	0
56	MG	W	303	1/1	0.52	0.20	125,125,125,125	0
56	MG	ZC	101	1/1	0.52	0.10	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	A	1735	1/1	0.52	0.15	131,131,131,131	0
56	MG	EB	2992	1/1	0.52	0.38	91,91,91,91	0
56	MG	DB	1733	1/1	0.52	0.39	127,127,127,127	0
56	MG	A	1701	1/1	0.53	0.45	141,141,141,141	0
56	MG	B	2963	1/1	0.53	0.34	86,86,86,86	0
56	MG	B	3046	1/1	0.53	0.25	126,126,126,126	0
56	MG	DB	1627	1/1	0.53	0.32	104,104,104,104	0
56	MG	JB	302	1/1	0.53	0.12	116,116,116,116	0
56	MG	YA	201	1/1	0.53	0.28	106,106,106,106	0
56	MG	EB	2942	1/1	0.53	0.24	138,138,138,138	0
56	MG	DB	1722	1/1	0.53	0.17	117,117,117,117	0
56	MG	B	2916	1/1	0.53	0.36	93,93,93,93	0
56	MG	B	3246	1/1	0.53	0.15	125,125,125,125	0
56	MG	A	1717	1/1	0.53	0.74	144,144,144,144	0
56	MG	SB	201	1/1	0.53	0.09	149,149,149,149	0
56	MG	OA	201	1/1	0.53	0.24	142,142,142,142	0
56	MG	B	3154	1/1	0.53	0.29	136,136,136,136	0
56	MG	EB	2939	1/1	0.54	0.41	99,99,99,99	0
56	MG	EB	3237	1/1	0.54	0.29	123,123,123,123	0
56	MG	A	1718	1/1	0.54	0.16	171,171,171,171	0
56	MG	BB	201	1/1	0.54	0.25	131,131,131,131	0
56	MG	DB	1721	1/1	0.54	0.41	134,134,134,134	0
56	MG	A	1696	1/1	0.54	0.33	152,152,152,152	0
56	MG	A	1704	1/1	0.54	0.31	137,137,137,137	0
56	MG	B	2968	1/1	0.54	0.33	97,97,97,97	0
56	MG	A	1601	1/1	0.54	0.37	94,94,94,94	0
56	MG	J	202	1/1	0.55	0.26	138,138,138,138	0
56	MG	A	1678	1/1	0.55	0.29	145,145,145,145	0
56	MG	A	1691	1/1	0.55	0.20	113,113,113,113	0
56	MG	EB	2978	1/1	0.55	0.31	103,103,103,103	0
56	MG	DB	1680	1/1	0.55	0.34	137,137,137,137	0
56	MG	D	106	1/1	0.55	0.19	227,227,227,227	0
56	MG	AC	102	1/1	0.55	0.47	98,98,98,98	0
56	MG	EB	2925	1/1	0.56	0.56	88,88,88,88	0
56	MG	B	3063	1/1	0.56	0.30	100,100,100,100	0
56	MG	A	1703	1/1	0.56	0.16	136,136,136,136	0
56	MG	EB	3203	1/1	0.56	0.19	130,130,130,130	0
56	MG	DB	1751	1/1	0.56	0.32	130,130,130,130	0
56	MG	B	3261	1/1	0.56	0.10	187,187,187,187	0
56	MG	FB	213	1/1	0.56	0.29	137,137,137,137	0
56	MG	EB	2988	1/1	0.56	0.41	104,104,104,104	0
56	MG	A	1651	1/1	0.56	0.39	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	A	1613	1/1	0.56	0.48	116,116,116,116	0
56	MG	YC	101	1/1	0.56	0.20	158,158,158,158	0
56	MG	DB	1775	1/1	0.56	0.20	143,143,143,143	0
56	MG	EB	3087	1/1	0.56	0.17	156,156,156,156	0
56	MG	ZB	302	1/1	0.56	0.15	154,154,154,154	0
56	MG	DB	1699	1/1	0.56	0.58	106,106,106,106	0
56	MG	EB	2984	1/1	0.57	0.30	127,127,127,127	0
56	MG	B	3037	1/1	0.57	0.38	102,102,102,102	0
56	MG	A	1679	1/1	0.57	0.56	116,116,116,116	0
56	MG	A	1628	1/1	0.57	0.63	116,116,116,116	0
56	MG	B	3065	1/1	0.57	0.34	98,98,98,98	0
56	MG	B	3218	1/1	0.57	0.11	109,109,109,109	0
56	MG	EB	3275	1/1	0.57	0.40	135,135,135,135	0
56	MG	EB	3135	1/1	0.57	0.13	111,111,111,111	0
56	MG	B	3159	1/1	0.57	0.26	90,90,90,90	0
56	MG	B	3251	1/1	0.57	0.15	154,154,154,154	0
56	MG	DB	1697	1/1	0.58	0.32	105,105,105,105	0
56	MG	B	3145	1/1	0.58	0.39	123,123,123,123	0
56	MG	DB	1740	1/1	0.58	0.12	130,130,130,130	0
56	MG	B	3010	1/1	0.58	0.29	116,116,116,116	0
56	MG	B	2956	1/1	0.58	0.35	99,99,99,99	0
56	MG	AC	101	1/1	0.58	0.22	115,115,115,115	0
56	MG	A	1630	1/1	0.58	0.49	116,116,116,116	0
56	MG	A	1681	1/1	0.58	0.25	169,169,169,169	0
56	MG	EB	2974	1/1	0.58	0.20	114,114,114,114	0
56	MG	DB	1760	1/1	0.58	0.29	102,102,102,102	0
56	MG	B	3031	1/1	0.58	0.30	87,87,87,87	0
56	MG	EB	3082	1/1	0.58	0.38	112,112,112,112	0
56	MG	EB	3084	1/1	0.58	0.32	87,87,87,87	0
56	MG	C	205	1/1	0.58	0.21	114,114,114,114	0
56	MG	A	1721	1/1	0.58	0.20	95,95,95,95	0
56	MG	B	2942	1/1	0.58	0.43	116,116,116,116	0
56	MG	EB	3112	1/1	0.58	0.19	124,124,124,124	0
56	MG	W	304	1/1	0.58	0.26	119,119,119,119	0
56	MG	EB	3260	1/1	0.58	0.29	220,220,220,220	0
56	MG	B	3003	1/1	0.58	0.23	84,84,84,84	0
56	MG	W	311	1/1	0.58	0.11	134,134,134,134	0
56	MG	EB	3011	1/1	0.58	0.14	163,163,163,163	0
56	MG	A	1709	1/1	0.59	0.36	164,164,164,164	0
56	MG	DB	1698	1/1	0.59	0.34	112,112,112,112	0
56	MG	DB	1773	1/1	0.59	0.35	109,109,109,109	0
56	MG	EA	101	1/1	0.59	0.15	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DB	1607	1/1	0.59	0.75	110,110,110,110	0
56	MG	DB	1667	1/1	0.59	0.20	115,115,115,115	0
56	MG	OA	202	1/1	0.59	0.10	135,135,135,135	0
56	MG	EB	3200	1/1	0.59	0.31	111,111,111,111	0
56	MG	DB	1611	1/1	0.59	0.38	101,101,101,101	0
56	MG	B	2944	1/1	0.60	0.31	115,115,115,115	0
56	MG	DB	1620	1/1	0.60	0.38	126,126,126,126	0
56	MG	EB	3035	1/1	0.60	0.60	116,116,116,116	0
56	MG	EB	3138	1/1	0.60	0.09	116,116,116,116	0
56	MG	C	223	1/1	0.60	0.22	132,132,132,132	0
56	MG	EB	2913	1/1	0.60	0.36	89,89,89,89	0
56	MG	B	3137	1/1	0.60	0.25	132,132,132,132	0
56	MG	DB	1670	1/1	0.60	0.36	167,167,167,167	0
56	MG	DB	1606	1/1	0.60	0.23	90,90,90,90	0
56	MG	DB	1705	1/1	0.60	0.27	130,130,130,130	0
56	MG	DB	1707	1/1	0.60	0.17	108,108,108,108	0
56	MG	B	3126	1/1	0.60	0.17	99,99,99,99	0
56	MG	XC	202	1/1	0.60	0.24	157,157,157,157	0
56	MG	EB	3002	1/1	0.60	0.36	116,116,116,116	0
56	MG	B	3302	1/1	0.60	0.19	105,105,105,105	0
56	MG	CD	102	1/1	0.60	0.12	122,122,122,122	0
56	MG	WA	101	1/1	0.60	0.12	126,126,126,126	0
56	MG	B	2967	1/1	0.60	0.41	125,125,125,125	0
56	MG	J	201	1/1	0.60	0.28	134,134,134,134	0
56	MG	HD	402	1/1	0.60	0.20	128,128,128,128	0
56	MG	EB	3047	1/1	0.61	0.43	98,98,98,98	0
56	MG	B	3380	1/1	0.61	0.20	97,97,97,97	0
56	MG	DB	1774	1/1	0.61	0.23	128,128,128,128	0
56	MG	PC	201	1/1	0.61	0.39	106,106,106,106	0
56	MG	A	1694	1/1	0.61	0.12	168,168,168,168	0
56	MG	PA	202	1/1	0.61	0.18	142,142,142,142	0
56	MG	B	3089	1/1	0.61	0.39	86,86,86,86	0
56	MG	EB	3076	1/1	0.61	0.34	116,116,116,116	0
56	MG	EB	3153	1/1	0.61	0.28	103,103,103,103	0
56	MG	EB	3163	1/1	0.61	0.16	144,144,144,144	0
56	MG	TA	201	1/1	0.61	0.16	118,118,118,118	0
56	MG	B	3170	1/1	0.61	0.14	117,117,117,117	0
56	MG	B	3103	1/1	0.61	0.23	90,90,90,90	0
56	MG	DB	1678	1/1	0.61	0.23	106,106,106,106	0
56	MG	A	1692	1/1	0.61	0.77	145,145,145,145	0
56	MG	NA	202	1/1	0.61	0.11	126,126,126,126	0
56	MG	AB	3301	1/1	0.62	0.12	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	W	305	1/1	0.62	0.27	129,129,129,129	0
56	MG	DB	1677	1/1	0.62	0.29	158,158,158,158	0
56	MG	LC	101	1/1	0.62	0.16	132,132,132,132	0
56	MG	B	3219	1/1	0.62	0.34	131,131,131,131	0
56	MG	EB	3235	1/1	0.62	0.14	122,122,122,122	0
56	MG	DB	1626	1/1	0.62	0.22	111,111,111,111	0
56	MG	B	3006	1/1	0.62	0.45	97,97,97,97	0
56	MG	J	204	1/1	0.62	0.11	138,138,138,138	0
56	MG	K	202	1/1	0.62	0.29	105,105,105,105	0
56	MG	QC	201	1/1	0.62	0.36	120,120,120,120	0
56	MG	DB	1641	1/1	0.62	0.29	146,146,146,146	0
56	MG	B	3308	1/1	0.62	0.28	109,109,109,109	0
56	MG	B	3249	1/1	0.62	0.28	149,149,149,149	0
56	MG	EB	3283	1/1	0.62	0.12	166,166,166,166	0
56	MG	DB	1726	1/1	0.62	0.21	135,135,135,135	0
56	MG	DB	1612	1/1	0.62	0.20	112,112,112,112	0
56	MG	B	3347	1/1	0.62	0.12	124,124,124,124	0
56	MG	CD	101	1/1	0.62	0.11	124,124,124,124	0
56	MG	B	2940	1/1	0.62	0.26	88,88,88,88	0
56	MG	A	1645	1/1	0.62	0.35	137,137,137,137	0
56	MG	VB	201	1/1	0.62	0.16	114,114,114,114	0
56	MG	DB	1741	1/1	0.62	0.32	135,135,135,135	0
56	MG	HD	401	1/1	0.62	0.51	97,97,97,97	0
56	MG	EB	3110	1/1	0.62	0.26	120,120,120,120	0
56	MG	B	3150	1/1	0.63	0.24	113,113,113,113	0
56	MG	EB	3149	1/1	0.63	0.27	113,113,113,113	0
56	MG	DB	1770	1/1	0.63	0.26	137,137,137,137	0
56	MG	DB	1639	1/1	0.63	0.71	140,140,140,140	0
56	MG	B	3362	1/1	0.63	0.12	118,118,118,118	0
56	MG	B	3291	1/1	0.63	0.17	142,142,142,142	0
56	MG	B	2947	1/1	0.63	0.49	108,108,108,108	0
56	MG	C	220	1/1	0.63	0.23	122,122,122,122	0
56	MG	A	1654	1/1	0.63	0.18	154,154,154,154	0
56	MG	B	3075	1/1	0.63	0.38	76,76,76,76	0
56	MG	EB	3284	1/1	0.63	0.23	103,103,103,103	0
56	MG	TA	202	1/1	0.63	0.32	114,114,114,114	0
56	MG	DB	1663	1/1	0.63	0.26	96,96,96,96	0
56	MG	B	2929	1/1	0.63	0.34	90,90,90,90	0
56	MG	A	1612	1/1	0.63	0.26	118,118,118,118	0
56	MG	EB	2946	1/1	0.63	0.20	124,124,124,124	0
56	MG	B	3195	1/1	0.64	0.26	115,115,115,115	0
56	MG	IA	104	1/1	0.64	0.26	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	IA	108	1/1	0.64	0.20	130,130,130,130	0
56	MG	B	3213	1/1	0.64	0.13	92,92,92,92	0
56	MG	B	2984	1/1	0.64	0.36	96,96,96,96	0
56	MG	B	3343	1/1	0.64	0.09	106,106,106,106	0
56	MG	EB	3094	1/1	0.64	0.18	110,110,110,110	0
56	MG	B	2933	1/1	0.64	0.40	89,89,89,89	0
56	MG	DB	1603	1/1	0.64	0.43	108,108,108,108	0
56	MG	DB	1604	1/1	0.64	0.42	103,103,103,103	0
56	MG	A	1617	1/1	0.64	0.17	100,100,100,100	0
56	MG	EB	3060	1/1	0.64	0.20	95,95,95,95	0
56	MG	MA	202	1/1	0.65	0.13	129,129,129,129	0
56	MG	EB	3190	1/1	0.65	0.09	111,111,111,111	0
56	MG	A	1629	1/1	0.65	0.32	123,123,123,123	0
56	MG	A	1631	1/1	0.65	0.28	131,131,131,131	0
56	MG	C	216	1/1	0.65	0.24	123,123,123,123	0
56	MG	B	3074	1/1	0.65	0.32	94,94,94,94	0
56	MG	EB	3018	1/1	0.65	0.15	110,110,110,110	0
56	MG	A	1734	1/1	0.65	0.29	110,110,110,110	0
56	MG	EB	3216	1/1	0.65	0.36	129,129,129,129	0
56	MG	W	307	1/1	0.65	0.14	125,125,125,125	0
56	MG	B	2953	1/1	0.65	0.42	107,107,107,107	0
56	MG	WB	202	1/1	0.65	0.18	96,96,96,96	0
56	MG	B	3054	1/1	0.65	0.37	89,89,89,89	0
56	MG	EB	3244	1/1	0.65	0.20	96,96,96,96	0
56	MG	DB	1622	1/1	0.65	0.46	103,103,103,103	0
56	MG	EB	3107	1/1	0.65	0.32	108,108,108,108	0
56	MG	DC	101	1/1	0.65	0.20	112,112,112,112	0
56	MG	EB	3179	1/1	0.65	0.40	121,121,121,121	0
56	MG	MA	201	1/1	0.65	0.38	114,114,114,114	0
56	MG	EB	2993	1/1	0.65	0.19	88,88,88,88	0
56	MG	DB	1636	1/1	0.66	0.26	137,137,137,137	0
56	MG	FB	204	1/1	0.66	0.22	130,130,130,130	0
56	MG	H	201	1/1	0.66	0.11	129,129,129,129	0
56	MG	EB	3086	1/1	0.66	0.25	104,104,104,104	0
56	MG	Q	203	1/1	0.66	0.14	106,106,106,106	0
56	MG	B	3340	1/1	0.66	0.12	89,89,89,89	0
56	MG	B	2921	1/1	0.66	0.34	88,88,88,88	0
56	MG	DB	1646	1/1	0.66	0.24	101,101,101,101	0
56	MG	DB	1682	1/1	0.66	0.12	128,128,128,128	0
56	MG	B	3257	1/1	0.67	0.18	96,96,96,96	0
56	MG	DB	1644	1/1	0.67	0.23	105,105,105,105	0
56	MG	DB	1674	1/1	0.67	0.12	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	2951	1/1	0.67	0.35	111,111,111,111	0
56	MG	S	203	1/1	0.67	0.06	112,112,112,112	0
56	MG	EB	3176	1/1	0.67	0.09	106,106,106,106	0
56	MG	A	1668	1/1	0.67	0.27	126,126,126,126	0
56	MG	A	1602	1/1	0.67	0.43	98,98,98,98	0
56	MG	TB	205	1/1	0.67	0.05	121,121,121,121	0
56	MG	EB	3245	1/1	0.67	0.12	128,128,128,128	0
56	MG	EB	3180	1/1	0.67	0.15	114,114,114,114	0
56	MG	B	3056	1/1	0.67	0.33	117,117,117,117	0
56	MG	EB	2902	1/1	0.67	0.45	89,89,89,89	0
56	MG	DB	1638	1/1	0.67	0.21	103,103,103,103	0
56	MG	B	3314	1/1	0.67	0.14	99,99,99,99	0
56	MG	EB	3271	1/1	0.67	0.09	127,127,127,127	0
56	MG	EB	3079	1/1	0.67	0.28	139,139,139,139	0
56	MG	DB	1664	1/1	0.67	0.13	137,137,137,137	0
56	MG	A	1663	1/1	0.67	0.46	113,113,113,113	0
56	MG	LC	103	1/1	0.67	0.48	126,126,126,126	0
56	MG	A	1610	1/1	0.68	0.33	108,108,108,108	0
56	MG	B	3367	1/1	0.68	0.20	102,102,102,102	0
56	MG	I	201	1/1	0.68	0.15	130,130,130,130	0
56	MG	C	211	1/1	0.68	0.23	119,119,119,119	0
56	MG	EB	3199	1/1	0.68	0.27	117,117,117,117	0
56	MG	W	308	1/1	0.68	0.14	132,132,132,132	0
56	MG	A	1604	1/1	0.68	0.54	105,105,105,105	0
56	MG	FB	214	1/1	0.68	0.34	128,128,128,128	0
56	MG	B	3181	1/1	0.68	0.24	106,106,106,106	0
56	MG	EB	3029	1/1	0.68	0.13	90,90,90,90	0
56	MG	B	3085	1/1	0.68	0.21	106,106,106,106	0
56	MG	DB	1764	1/1	0.68	0.27	110,110,110,110	0
56	MG	SA	201	1/1	0.68	0.16	106,106,106,106	0
56	MG	HA	101	1/1	0.68	0.13	123,123,123,123	0
56	MG	HB	302	1/1	0.68	0.13	120,120,120,120	0
56	MG	EB	3139	1/1	0.68	0.36	103,103,103,103	0
56	MG	EB	3141	1/1	0.68	0.30	96,96,96,96	0
56	MG	EB	3246	1/1	0.68	0.44	105,105,105,105	0
56	MG	EB	3053	1/1	0.68	0.22	113,113,113,113	0
56	MG	DB	1720	1/1	0.68	0.19	143,143,143,143	0
56	MG	B	3163	1/1	0.68	0.18	89,89,89,89	0
56	MG	B	3401	1/1	0.68	0.15	111,111,111,111	0
56	MG	B	3018	1/1	0.68	0.43	88,88,88,88	0
56	MG	B	3407	1/1	0.68	0.08	78,78,78,78	0
56	MG	V	502	1/1	0.68	0.27	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	EB	2935	1/1	0.68	0.45	98,98,98,98	0
56	MG	B	3051	1/1	0.68	0.33	106,106,106,106	0
56	MG	EB	2996	1/1	0.68	0.42	86,86,86,86	0
56	MG	ZA	101	1/1	0.68	0.23	124,124,124,124	0
56	MG	EB	2947	1/1	0.69	0.40	106,106,106,106	0
56	MG	DB	1752	1/1	0.69	0.08	156,156,156,156	0
56	MG	EB	3122	1/1	0.69	0.16	174,174,174,174	0
56	MG	FB	209	1/1	0.69	0.25	132,132,132,132	0
56	MG	A	1698	1/1	0.69	0.20	160,160,160,160	0
56	MG	A	1616	1/1	0.69	0.33	99,99,99,99	0
56	MG	B	3236	1/1	0.69	0.09	122,122,122,122	0
56	MG	EB	3231	1/1	0.69	0.32	119,119,119,119	0
56	MG	DB	1671	1/1	0.69	0.38	112,112,112,112	0
56	MG	B	3077	1/1	0.69	0.41	99,99,99,99	0
56	MG	B	2923	1/1	0.69	0.37	78,78,78,78	0
56	MG	EB	3057	1/1	0.69	0.56	95,95,95,95	0
56	MG	B	3133	1/1	0.69	0.12	169,169,169,169	0
56	MG	B	2928	1/1	0.69	0.24	107,107,107,107	0
56	MG	A	1693	1/1	0.69	0.23	107,107,107,107	0
56	MG	DB	1609	1/1	0.69	0.27	116,116,116,116	0
56	MG	EB	3257	1/1	0.69	0.18	103,103,103,103	0
56	MG	B	3093	1/1	0.69	0.23	120,120,120,120	0
56	MG	C	208	1/1	0.69	0.32	99,99,99,99	0
56	MG	B	3186	1/1	0.69	0.12	109,109,109,109	0
56	MG	EB	2927	1/1	0.69	0.32	90,90,90,90	0
56	MG	IA	103	1/1	0.69	0.31	124,124,124,124	0
56	MG	B	3356	1/1	0.69	0.13	92,92,92,92	0
56	MG	QB	201	1/1	0.69	0.14	99,99,99,99	0
56	MG	A	1706	1/1	0.69	0.21	135,135,135,135	0
56	MG	B	2915	1/1	0.69	0.36	85,85,85,85	0
56	MG	C	217	1/1	0.69	0.15	113,113,113,113	0
56	MG	DB	1700	1/1	0.69	0.20	145,145,145,145	0
56	MG	B	3151	1/1	0.69	0.22	105,105,105,105	0
56	MG	EB	3182	1/1	0.70	0.21	107,107,107,107	0
56	MG	F	301	1/1	0.70	0.27	106,106,106,106	0
56	MG	EB	2972	1/1	0.70	0.18	104,104,104,104	0
56	MG	EB	3072	1/1	0.70	0.37	98,98,98,98	0
56	MG	TB	201	1/1	0.70	0.19	112,112,112,112	0
56	MG	B	3247	1/1	0.70	0.08	146,146,146,146	0
56	MG	EB	2976	1/1	0.70	0.27	113,113,113,113	0
56	MG	OA	203	1/1	0.70	0.14	142,142,142,142	0
56	MG	DB	1631	1/1	0.70	0.25	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	A	1660	1/1	0.70	0.34	125,125,125,125	0
56	MG	A	1732	1/1	0.70	0.34	149,149,149,149	0
56	MG	B	3225	1/1	0.70	0.21	116,116,116,116	0
56	MG	FA	101	1/1	0.70	0.53	111,111,111,111	0
56	MG	A	1710	1/1	0.70	0.27	126,126,126,126	0
56	MG	B	3370	1/1	0.70	0.66	214,214,214,214	0
56	MG	MA	203	1/1	0.70	0.13	143,143,143,143	0
56	MG	EB	2923	1/1	0.70	0.38	97,97,97,97	0
56	MG	EB	3000	1/1	0.70	0.27	114,114,114,114	0
56	MG	B	3216	1/1	0.70	0.15	157,157,157,157	0
56	MG	DB	1693	1/1	0.71	0.20	111,111,111,111	0
56	MG	DB	1694	1/1	0.71	0.28	125,125,125,125	0
56	MG	EB	3289	1/1	0.71	0.24	109,109,109,109	0
56	MG	EB	3290	1/1	0.71	0.08	131,131,131,131	0
56	MG	WB	201	1/1	0.71	0.24	102,102,102,102	0
56	MG	B	3122	1/1	0.71	0.19	90,90,90,90	0
56	MG	DB	1750	1/1	0.71	0.28	116,116,116,116	0
56	MG	B	3234	1/1	0.71	0.13	87,87,87,87	0
56	MG	EB	3106	1/1	0.71	0.14	120,120,120,120	0
56	MG	A	1713	1/1	0.71	0.16	116,116,116,116	0
56	MG	B	3316	1/1	0.71	0.13	151,151,151,151	0
56	MG	B	3244	1/1	0.71	0.11	82,82,82,82	0
56	MG	FB	210	1/1	0.71	0.26	143,143,143,143	0
56	MG	EB	3119	1/1	0.71	0.20	134,134,134,134	0
56	MG	B	2918	1/1	0.71	0.30	76,76,76,76	0
56	MG	A	1603	1/1	0.71	0.35	88,88,88,88	0
56	MG	EB	3207	1/1	0.71	0.10	121,121,121,121	0
56	MG	EB	3123	1/1	0.71	0.43	103,103,103,103	0
56	MG	EB	3038	1/1	0.71	0.20	97,97,97,97	0
56	MG	B	3127	1/1	0.71	0.27	96,96,96,96	0
56	MG	A	1730	1/1	0.71	0.28	119,119,119,119	0
56	MG	B	3132	1/1	0.71	0.39	104,104,104,104	0
56	MG	A	1643	1/1	0.71	0.40	117,117,117,117	0
56	MG	EB	3054	1/1	0.71	0.28	102,102,102,102	0
56	MG	DB	1633	1/1	0.71	0.51	106,106,106,106	0
56	MG	DB	1635	1/1	0.71	0.25	120,120,120,120	0
56	MG	A	1682	1/1	0.71	0.15	191,191,191,191	0
56	MG	A	1723	1/1	0.71	0.29	180,180,180,180	0
56	MG	B	3098	1/1	0.71	0.30	86,86,86,86	0
56	MG	B	3205	1/1	0.71	0.32	82,82,82,82	0
56	MG	GD	401	1/1	0.71	0.41	95,95,95,95	0
56	MG	A	1670	1/1	0.71	0.15	139,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	3110	1/1	0.71	0.38	94,94,94,94	0
56	MG	MB	201	1/1	0.71	0.16	153,153,153,153	0
56	MG	A	1727	1/1	0.71	0.23	106,106,106,106	0
56	MG	B	3152	1/1	0.71	0.21	107,107,107,107	0
56	MG	B	2924	1/1	0.72	0.41	87,87,87,87	0
56	MG	EB	2991	1/1	0.72	0.28	90,90,90,90	0
56	MG	B	2978	1/1	0.72	0.35	78,78,78,78	0
56	MG	I	202	1/1	0.72	0.09	122,122,122,122	0
56	MG	B	2945	1/1	0.72	0.34	82,82,82,82	0
56	MG	EB	2909	1/1	0.72	0.60	88,88,88,88	0
56	MG	B	3317	1/1	0.72	0.25	120,120,120,120	0
56	MG	JB	301	1/1	0.72	0.49	89,89,89,89	0
56	MG	EB	3001	1/1	0.72	0.26	112,112,112,112	0
56	MG	DB	1665	1/1	0.72	0.24	129,129,129,129	0
56	MG	DB	1762	1/1	0.72	0.25	122,122,122,122	0
56	MG	BC	101	1/1	0.72	0.20	116,116,116,116	0
56	MG	FB	211	1/1	0.72	0.15	146,146,146,146	0
56	MG	EB	3133	1/1	0.72	0.23	91,91,91,91	0
56	MG	EB	3225	1/1	0.72	0.16	115,115,115,115	0
56	MG	B	2989	1/1	0.72	0.32	109,109,109,109	0
56	MG	J	205	1/1	0.72	0.13	134,134,134,134	0
56	MG	EB	2960	1/1	0.72	0.49	95,95,95,95	0
56	MG	RB	204	1/1	0.72	0.16	100,100,100,100	0
56	MG	EB	2904	1/1	0.73	0.66	79,79,79,79	0
56	MG	EB	2973	1/1	0.73	0.39	91,91,91,91	0
56	MG	K	201	1/1	0.73	0.14	111,111,111,111	0
56	MG	A	1753	1/1	0.73	0.21	125,125,125,125	0
56	MG	B	3390	1/1	0.73	0.19	124,124,124,124	0
56	MG	EB	2914	1/1	0.73	0.34	94,94,94,94	0
56	MG	B	3258	1/1	0.73	0.22	107,107,107,107	0
56	MG	A	1684	1/1	0.73	0.36	113,113,113,113	0
56	MG	EB	2986	1/1	0.73	0.23	95,95,95,95	0
56	MG	A	1632	1/1	0.73	0.19	124,124,124,124	0
56	MG	EB	2928	1/1	0.73	0.32	95,95,95,95	0
56	MG	DB	1643	1/1	0.73	0.39	109,109,109,109	0
56	MG	B	3036	1/1	0.73	0.38	110,110,110,110	0
56	MG	B	3125	1/1	0.73	0.43	107,107,107,107	0
56	MG	EB	2941	1/1	0.73	0.39	103,103,103,103	0
56	MG	EB	3164	1/1	0.73	0.08	114,114,114,114	0
56	MG	MC	302	1/1	0.73	0.12	138,138,138,138	0
56	MG	EB	3166	1/1	0.73	0.36	113,113,113,113	0
56	MG	B	3283	1/1	0.73	0.43	226,226,226,226	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	EB	3263	1/1	0.73	0.12	133,133,133,133	0
56	MG	C	204	1/1	0.73	0.20	114,114,114,114	0
56	MG	A	1671	1/1	0.73	0.18	131,131,131,131	0
56	MG	B	3187	1/1	0.73	0.17	84,84,84,84	0
56	MG	C	207	1/1	0.73	0.37	127,127,127,127	0
56	MG	DB	1772	1/1	0.73	0.09	109,109,109,109	0
56	MG	B	3099	1/1	0.73	0.27	87,87,87,87	0
56	MG	EB	3105	1/1	0.73	0.20	97,97,97,97	0
56	MG	B	2905	1/1	0.73	0.57	80,80,80,80	0
56	MG	EB	2961	1/1	0.73	0.31	94,94,94,94	0
56	MG	EB	3109	1/1	0.73	0.13	112,112,112,112	0
56	MG	B	2962	1/1	0.73	0.26	83,83,83,83	0
56	MG	TB	204	1/1	0.73	0.14	112,112,112,112	0
56	MG	B	3116	1/1	0.73	0.31	122,122,122,122	0
56	MG	EB	2903	1/1	0.73	0.46	100,100,100,100	0
56	MG	YB	204	1/1	0.74	0.10	118,118,118,118	0
56	MG	EB	3240	1/1	0.74	0.08	155,155,155,155	0
56	MG	EB	3085	1/1	0.74	0.26	117,117,117,117	0
56	MG	NA	201	1/1	0.74	0.16	129,129,129,129	0
56	MG	A	1676	1/1	0.74	0.38	127,127,127,127	0
56	MG	EB	2924	1/1	0.74	0.33	89,89,89,89	0
56	MG	DB	1666	1/1	0.74	0.27	108,108,108,108	0
56	MG	B	3100	1/1	0.74	0.33	97,97,97,97	0
56	MG	B	3053	1/1	0.74	0.38	101,101,101,101	0
56	MG	EB	2930	1/1	0.74	0.39	84,84,84,84	0
56	MG	EB	3262	1/1	0.74	0.10	112,112,112,112	0
56	MG	A	1614	1/1	0.74	0.21	108,108,108,108	0
56	MG	DB	1766	1/1	0.74	0.31	122,122,122,122	0
56	MG	DB	1767	1/1	0.74	0.10	106,106,106,106	0
56	MG	B	3178	1/1	0.74	0.13	140,140,140,140	0
56	MG	DB	1673	1/1	0.74	0.27	105,105,105,105	0
56	MG	A	1605	1/1	0.74	0.29	103,103,103,103	0
56	MG	B	2986	1/1	0.74	0.40	81,81,81,81	0
56	MG	B	3228	1/1	0.74	0.14	119,119,119,119	0
56	MG	A	1743	1/1	0.74	0.12	174,174,174,174	0
56	MG	EB	2948	1/1	0.74	0.48	123,123,123,123	0
56	MG	QB	203	1/1	0.74	0.09	103,103,103,103	0
56	MG	TA	203	1/1	0.74	0.07	113,113,113,113	0
56	MG	DB	1749	1/1	0.74	0.17	113,113,113,113	0
56	MG	EB	3068	1/1	0.74	0.29	92,92,92,92	0
56	MG	B	3024	1/1	0.74	0.29	85,85,85,85	0
56	MG	EB	3074	1/1	0.74	0.20	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	EB	3230	1/1	0.74	0.09	100,100,100,100	0
56	MG	E	301	1/1	0.74	0.28	71,71,71,71	0
56	MG	EB	3004	1/1	0.74	0.45	102,102,102,102	0
56	MG	B	3160	1/1	0.74	0.19	92,92,92,92	0
56	MG	EB	3012	1/1	0.74	0.33	90,90,90,90	0
56	MG	HD	403	1/1	0.74	0.14	129,129,129,129	0
56	MG	DB	1669	1/1	0.75	0.26	154,154,154,154	0
56	MG	EB	3021	1/1	0.75	0.18	111,111,111,111	0
56	MG	B	2971	1/1	0.75	0.15	82,82,82,82	0
56	MG	EB	3156	1/1	0.75	0.59	109,109,109,109	0
56	MG	EB	2933	1/1	0.75	0.29	95,95,95,95	0
56	MG	XB	102	1/1	0.75	0.14	124,124,124,124	0
56	MG	B	3138	1/1	0.75	0.35	106,106,106,106	0
56	MG	B	2904	1/1	0.75	0.45	74,74,74,74	0
56	MG	B	3335	1/1	0.75	0.10	128,128,128,128	0
56	MG	DB	1732	1/1	0.75	0.17	147,147,147,147	0
56	MG	EB	2910	1/1	0.75	0.37	87,87,87,87	0
56	MG	BD	202	1/1	0.75	0.08	108,108,108,108	0
56	MG	DB	1708	1/1	0.75	0.20	106,106,106,106	0
56	MG	DB	1692	1/1	0.75	0.11	137,137,137,137	0
56	MG	OB	202	1/1	0.75	0.14	100,100,100,100	0
56	MG	B	3078	1/1	0.75	0.28	89,89,89,89	0
56	MG	Y	104	1/1	0.75	0.08	101,101,101,101	0
56	MG	B	3275	1/1	0.75	0.13	116,116,116,116	0
56	MG	EB	3287	1/1	0.75	0.32	110,110,110,110	0
56	MG	B	3083	1/1	0.75	0.33	100,100,100,100	0
56	MG	B	2959	1/1	0.75	0.19	78,78,78,78	0
56	MG	A	1712	1/1	0.76	0.15	125,125,125,125	0
56	MG	Y	103	1/1	0.76	0.20	115,115,115,115	0
56	MG	EB	2915	1/1	0.76	0.57	96,96,96,96	0
56	MG	NB	201	1/1	0.76	0.18	115,115,115,115	0
56	MG	LC	107	1/1	0.76	0.10	110,110,110,110	0
56	MG	EB	2954	1/1	0.76	0.66	103,103,103,103	0
56	MG	L	207	1/1	0.76	0.17	101,101,101,101	0
56	MG	B	3184	1/1	0.76	0.28	116,116,116,116	0
56	MG	EB	2962	1/1	0.76	0.55	114,114,114,114	0
56	MG	PC	202	1/1	0.76	0.21	123,123,123,123	0
56	MG	DB	1618	1/1	0.76	0.57	101,101,101,101	0
56	MG	C	210	1/1	0.76	0.12	123,123,123,123	0
56	MG	EB	3121	1/1	0.76	0.23	116,116,116,116	0
56	MG	DB	1731	1/1	0.76	0.22	133,133,133,133	0
56	MG	E	302	1/1	0.76	0.16	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	3276	1/1	0.76	0.13	83,83,83,83	0
56	MG	EB	3073	1/1	0.76	0.20	105,105,105,105	0
56	MG	B	3033	1/1	0.76	0.23	101,101,101,101	0
56	MG	AD	101	1/1	0.76	0.34	108,108,108,108	0
56	MG	DB	1649	1/1	0.76	0.34	106,106,106,106	0
56	MG	B	2952	1/1	0.76	0.29	78,78,78,78	0
56	MG	A	1697	1/1	0.76	0.39	104,104,104,104	0
56	MG	C	201	1/1	0.76	0.41	94,94,94,94	0
56	MG	B	3165	1/1	0.76	0.17	75,75,75,75	0
56	MG	B	3325	1/1	0.76	0.26	113,113,113,113	0
56	MG	B	3331	1/1	0.76	0.43	105,105,105,105	0
56	MG	B	3273	1/1	0.76	0.12	104,104,104,104	0
56	MG	EB	3044	1/1	0.76	0.14	118,118,118,118	0
56	MG	EB	3159	1/1	0.76	0.10	104,104,104,104	0
56	MG	B	3040	1/1	0.77	0.14	79,79,79,79	0
56	MG	B	3326	1/1	0.77	0.07	94,94,94,94	0
56	MG	A	1607	1/1	0.77	0.54	92,92,92,92	0
56	MG	B	3214	1/1	0.77	0.12	79,79,79,79	0
56	MG	A	1667	1/1	0.77	0.23	105,105,105,105	0
56	MG	B	3114	1/1	0.77	0.21	86,86,86,86	0
56	MG	EB	2929	1/1	0.77	0.29	98,98,98,98	0
56	MG	IA	105	1/1	0.77	0.43	116,116,116,116	0
56	MG	B	2902	1/1	0.77	0.53	61,61,61,61	0
56	MG	EB	2983	1/1	0.77	0.28	88,88,88,88	0
56	MG	U	102	1/1	0.77	0.05	102,102,102,102	0
56	MG	EB	3187	1/1	0.77	0.18	134,134,134,134	0
56	MG	EB	3278	1/1	0.77	0.22	106,106,106,106	0
56	MG	EB	3281	1/1	0.77	0.17	95,95,95,95	0
56	MG	JA	302	1/1	0.77	0.20	146,146,146,146	0
56	MG	B	3118	1/1	0.77	0.21	96,96,96,96	0
56	MG	B	2906	1/1	0.77	0.38	78,78,78,78	0
56	MG	QC	202	1/1	0.77	0.19	124,124,124,124	0
56	MG	B	3357	1/1	0.77	0.13	88,88,88,88	0
56	MG	B	3266	1/1	0.77	0.09	149,149,149,149	0
56	MG	B	3309	1/1	0.77	0.20	111,111,111,111	0
56	MG	DB	1734	1/1	0.77	0.13	121,121,121,121	0
56	MG	B	3369	1/1	0.77	0.09	89,89,89,89	0
56	MG	EB	2998	1/1	0.77	0.23	86,86,86,86	0
56	MG	B	3268	1/1	0.77	0.08	94,94,94,94	0
56	MG	EB	2907	1/1	0.77	0.36	97,97,97,97	0
56	MG	BD	201	1/1	0.77	0.08	122,122,122,122	0
56	MG	FB	207	1/1	0.77	0.15	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	EB	2908	1/1	0.77	0.27	88,88,88,88	0
56	MG	B	3096	1/1	0.77	0.28	111,111,111,111	0
56	MG	EB	3077	1/1	0.77	0.20	133,133,133,133	0
56	MG	J	203	1/1	0.77	0.20	104,104,104,104	0
56	MG	DB	1746	1/1	0.77	0.32	104,104,104,104	0
56	MG	B	2964	1/1	0.77	0.56	88,88,88,88	0
56	MG	B	3082	1/1	0.77	0.27	90,90,90,90	0
56	MG	ZB	301	1/1	0.77	0.21	137,137,137,137	0
56	MG	EB	3160	1/1	0.77	0.25	108,108,108,108	0
56	MG	EB	3043	1/1	0.78	0.17	119,119,119,119	0
56	MG	B	3029	1/1	0.78	0.45	85,85,85,85	0
56	MG	A	1683	1/1	0.78	0.51	106,106,106,106	0
56	MG	B	3267	1/1	0.78	0.13	112,112,112,112	0
56	MG	B	3139	1/1	0.78	0.18	97,97,97,97	0
56	MG	B	3305	1/1	0.78	0.08	120,120,120,120	0
56	MG	B	3032	1/1	0.78	0.24	87,87,87,87	0
56	MG	IA	107	1/1	0.78	0.42	108,108,108,108	0
56	MG	EB	2957	1/1	0.78	0.41	91,91,91,91	0
56	MG	EB	3219	1/1	0.78	0.32	105,105,105,105	0
56	MG	B	3248	1/1	0.78	0.33	103,103,103,103	0
56	MG	IC	102	1/1	0.78	0.12	105,105,105,105	0
56	MG	B	3408	1/1	0.78	0.19	119,119,119,119	0
56	MG	DB	1616	1/1	0.78	0.27	100,100,100,100	0
56	MG	W	306	1/1	0.78	0.17	122,122,122,122	0
56	MG	EB	3070	1/1	0.78	0.17	104,104,104,104	0
56	MG	EB	3010	1/1	0.78	0.20	84,84,84,84	0
56	MG	EB	3239	1/1	0.78	0.20	123,123,123,123	0
56	MG	A	1759	1/1	0.78	0.17	176,176,176,176	0
56	MG	B	2950	1/1	0.78	0.41	92,92,92,92	0
56	MG	W	309	1/1	0.78	0.20	121,121,121,121	0
56	MG	EB	3152	1/1	0.78	0.23	106,106,106,106	0
56	MG	A	1642	1/1	0.78	0.19	106,106,106,106	0
56	MG	IB	303	1/1	0.78	0.10	112,112,112,112	0
56	MG	D	104	1/1	0.78	0.14	131,131,131,131	0
56	MG	EB	3256	1/1	0.78	0.08	106,106,106,106	0
56	MG	DB	1661	1/1	0.78	0.28	97,97,97,97	0
56	MG	EB	3083	1/1	0.78	0.29	106,106,106,106	0
56	MG	TC	202	1/1	0.78	0.09	156,156,156,156	0
56	MG	DB	1624	1/1	0.78	0.35	111,111,111,111	0
56	MG	B	3193	1/1	0.78	0.25	81,81,81,81	0
56	MG	EB	3025	1/1	0.78	0.85	103,103,103,103	0
56	MG	B	3285	1/1	0.78	0.61	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	Z	103	1/1	0.78	0.05	92,92,92,92	0
56	MG	EB	3098	1/1	0.78	0.36	102,102,102,102	0
56	MG	EB	3101	1/1	0.78	0.19	96,96,96,96	0
56	MG	EB	3279	1/1	0.78	0.38	95,95,95,95	0
56	MG	EB	3030	1/1	0.78	0.22	110,110,110,110	0
56	MG	RB	203	1/1	0.78	0.38	114,114,114,114	0
56	MG	B	3111	1/1	0.78	0.19	84,84,84,84	0
56	MG	EB	3104	1/1	0.78	0.30	103,103,103,103	0
56	MG	EB	3036	1/1	0.78	0.30	102,102,102,102	0
56	MG	EB	3286	1/1	0.78	0.26	123,123,123,123	0
56	MG	EB	3037	1/1	0.78	0.22	95,95,95,95	0
56	MG	DB	1738	1/1	0.78	0.42	108,108,108,108	0
56	MG	EB	3108	1/1	0.78	0.33	127,127,127,127	0
56	MG	DB	1652	1/1	0.79	0.36	122,122,122,122	0
56	MG	B	3284	1/1	0.79	0.26	79,79,79,79	0
56	MG	EB	3078	1/1	0.79	0.24	110,110,110,110	0
56	MG	B	3378	1/1	0.79	0.26	101,101,101,101	0
56	MG	B	3233	1/1	0.79	0.34	95,95,95,95	0
56	MG	EB	2990	1/1	0.79	0.26	75,75,75,75	0
56	MG	DB	1605	1/1	0.79	0.26	106,106,106,106	0
56	MG	A	1722	1/1	0.79	0.12	96,96,96,96	0
56	MG	DB	1724	1/1	0.79	0.34	107,107,107,107	0
56	MG	RC	202	1/1	0.79	0.22	152,152,152,152	0
56	MG	B	2930	1/1	0.79	0.31	78,78,78,78	0
56	MG	EB	3092	1/1	0.79	0.25	108,108,108,108	0
56	MG	A	1747	1/1	0.79	0.94	150,150,150,150	0
56	MG	WC	201	1/1	0.79	0.11	96,96,96,96	0
56	MG	A	1665	1/1	0.79	0.19	115,115,115,115	0
56	MG	EB	2999	1/1	0.79	0.21	101,101,101,101	0
56	MG	B	3394	1/1	0.79	0.32	107,107,107,107	0
56	MG	EB	2968	1/1	0.79	0.23	112,112,112,112	0
56	MG	B	2948	1/1	0.79	0.33	93,93,93,93	0
56	MG	DB	1613	1/1	0.79	0.35	97,97,97,97	0
56	MG	B	3346	1/1	0.79	0.10	85,85,85,85	0
56	MG	B	3220	1/1	0.79	0.08	88,88,88,88	0
56	MG	A	1725	1/1	0.79	0.09	119,119,119,119	0
56	MG	EB	2975	1/1	0.79	0.36	105,105,105,105	0
56	MG	KC	101	1/1	0.79	0.21	113,113,113,113	0
56	MG	B	3227	1/1	0.79	0.31	83,83,83,83	0
56	MG	B	3313	1/1	0.79	0.18	133,133,133,133	0
56	MG	B	3277	1/1	0.79	0.17	106,106,106,106	0
56	MG	B	3207	1/1	0.79	0.48	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	3232	1/1	0.79	0.19	83,83,83,83	0
56	MG	EB	3088	1/1	0.80	0.35	97,97,97,97	0
56	MG	B	3318	1/1	0.80	0.15	95,95,95,95	0
56	MG	B	3320	1/1	0.80	0.14	85,85,85,85	0
56	MG	EB	3183	1/1	0.80	0.34	119,119,119,119	0
56	MG	B	3027	1/1	0.80	0.22	95,95,95,95	0
56	MG	EB	3023	1/1	0.80	0.26	101,101,101,101	0
56	MG	RA	202	1/1	0.80	0.18	152,152,152,152	0
56	MG	B	2910	1/1	0.80	0.41	83,83,83,83	0
56	MG	B	3280	1/1	0.80	0.22	94,94,94,94	0
56	MG	B	2911	1/1	0.80	0.17	61,61,61,61	0
56	MG	EB	3197	1/1	0.80	0.36	94,94,94,94	0
56	MG	IC	101	1/1	0.80	0.22	108,108,108,108	0
56	MG	B	3002	1/1	0.80	0.53	85,85,85,85	0
56	MG	B	3208	1/1	0.80	0.10	118,118,118,118	0
56	MG	B	3076	1/1	0.80	0.16	88,88,88,88	0
56	MG	B	2914	1/1	0.80	0.41	93,93,93,93	0
56	MG	A	1736	1/1	0.80	0.14	148,148,148,148	0
56	MG	DB	1629	1/1	0.80	0.25	100,100,100,100	0
56	MG	EB	3113	1/1	0.80	0.43	114,114,114,114	0
56	MG	WA	103	1/1	0.80	0.17	126,126,126,126	0
56	MG	A	1702	1/1	0.80	0.22	115,115,115,115	0
56	MG	YA	202	1/1	0.80	0.14	128,128,128,128	0
56	MG	EB	3052	1/1	0.80	0.37	106,106,106,106	0
56	MG	L	201	1/1	0.80	0.21	99,99,99,99	0
56	MG	HB	301	1/1	0.80	0.24	103,103,103,103	0
56	MG	DB	1739	1/1	0.80	0.23	113,113,113,113	0
56	MG	EB	3236	1/1	0.80	0.14	103,103,103,103	0
56	MG	B	3292	1/1	0.80	0.10	107,107,107,107	0
56	MG	DB	1689	1/1	0.80	0.21	111,111,111,111	0
56	MG	O	201	1/1	0.80	0.28	93,93,93,93	0
56	MG	SC	201	1/1	0.80	0.19	124,124,124,124	0
56	MG	DB	1743	1/1	0.80	0.13	104,104,104,104	0
56	MG	EB	2931	1/1	0.80	0.23	80,80,80,80	0
56	MG	B	3296	1/1	0.80	0.15	101,101,101,101	0
56	MG	B	3364	1/1	0.80	0.20	95,95,95,95	0
56	MG	EB	3071	1/1	0.80	0.36	100,100,100,100	0
56	MG	EB	3146	1/1	0.80	0.18	99,99,99,99	0
56	MG	B	3177	1/1	0.80	0.11	92,92,92,92	0
56	MG	B	3015	1/1	0.80	0.29	71,71,71,71	0
56	MG	T	201	1/1	0.80	0.15	94,94,94,94	0
56	MG	B	3263	1/1	0.80	0.17	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	A	1672	1/1	0.80	0.23	137,137,137,137	0
56	MG	DB	1608	1/1	0.80	0.40	94,94,94,94	0
56	MG	A	1669	1/1	0.80	0.26	93,93,93,93	0
56	MG	B	3148	1/1	0.80	0.39	103,103,103,103	0
56	MG	B	3269	1/1	0.80	0.40	110,110,110,110	0
56	MG	EB	3169	1/1	0.80	0.32	87,87,87,87	0
56	MG	B	2976	1/1	0.80	0.43	96,96,96,96	0
56	MG	A	1626	1/1	0.80	0.27	122,122,122,122	0
56	MG	DB	1769	1/1	0.80	0.14	92,92,92,92	0
56	MG	A	1625	1/1	0.80	0.12	137,137,137,137	0
56	MG	B	3055	1/1	0.81	0.28	82,82,82,82	0
56	MG	A	1748	1/1	0.81	0.08	97,97,97,97	0
56	MG	B	3298	1/1	0.81	0.15	96,96,96,96	0
56	MG	EB	2981	1/1	0.81	0.21	97,97,97,97	0
56	MG	EB	3089	1/1	0.81	0.26	109,109,109,109	0
56	MG	DB	1710	1/1	0.81	0.22	136,136,136,136	0
56	MG	B	3155	1/1	0.81	0.19	101,101,101,101	0
56	MG	EB	3097	1/1	0.81	0.14	87,87,87,87	0
56	MG	EB	3247	1/1	0.81	0.27	156,156,156,156	0
56	MG	EB	3249	1/1	0.81	0.33	137,137,137,137	0
56	MG	B	3061	1/1	0.81	0.35	109,109,109,109	0
56	MG	DB	1715	1/1	0.81	0.42	107,107,107,107	0
56	MG	EB	3254	1/1	0.81	0.15	123,123,123,123	0
56	MG	HB	306	1/1	0.81	0.15	108,108,108,108	0
56	MG	HB	307	1/1	0.81	0.14	102,102,102,102	0
56	MG	HB	308	1/1	0.81	0.14	108,108,108,108	0
56	MG	B	3231	1/1	0.81	0.28	91,91,91,91	0
56	MG	B	3363	1/1	0.81	0.56	229,229,229,229	0
56	MG	B	3062	1/1	0.81	0.26	86,86,86,86	0
56	MG	A	1749	1/1	0.81	0.15	95,95,95,95	0
56	MG	EB	2943	1/1	0.81	0.38	93,93,93,93	0
56	MG	B	3197	1/1	0.81	0.07	116,116,116,116	0
56	MG	DB	1683	1/1	0.81	0.28	109,109,109,109	0
56	MG	B	3199	1/1	0.81	0.40	98,98,98,98	0
56	MG	IA	101	1/1	0.81	0.17	119,119,119,119	0
56	MG	B	3373	1/1	0.81	0.08	109,109,109,109	0
56	MG	B	3374	1/1	0.81	0.38	102,102,102,102	0
56	MG	EB	3116	1/1	0.81	0.30	93,93,93,93	0
56	MG	DB	1650	1/1	0.81	0.35	103,103,103,103	0
56	MG	WC	202	1/1	0.81	0.15	121,121,121,121	0
56	MG	B	3238	1/1	0.81	0.41	93,93,93,93	0
56	MG	B	3239	1/1	0.81	0.11	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	3242	1/1	0.81	0.37	89,89,89,89	0
56	MG	A	1658	1/1	0.81	0.40	109,109,109,109	0
56	MG	B	2958	1/1	0.81	0.29	80,80,80,80	0
56	MG	B	3140	1/1	0.81	0.18	84,84,84,84	0
56	MG	A	1652	1/1	0.81	0.34	123,123,123,123	0
56	MG	FB	202	1/1	0.81	0.15	135,135,135,135	0
56	MG	A	1689	1/1	0.81	0.29	105,105,105,105	0
56	MG	DB	1701	1/1	0.81	0.10	119,119,119,119	0
56	MG	EB	2917	1/1	0.81	0.34	89,89,89,89	0
56	MG	EB	3221	1/1	0.81	0.39	103,103,103,103	0
56	MG	EB	3081	1/1	0.81	0.24	81,81,81,81	0
56	MG	A	1715	1/1	0.81	0.13	137,137,137,137	0
56	MG	A	1646	1/1	0.81	0.22	117,117,117,117	0
56	MG	B	3106	1/1	0.81	0.19	103,103,103,103	0
56	MG	B	3200	1/1	0.82	0.14	111,111,111,111	0
56	MG	HC	101	1/1	0.82	0.14	102,102,102,102	0
56	MG	B	2922	1/1	0.82	0.32	74,74,74,74	0
56	MG	B	3005	1/1	0.82	0.14	72,72,72,72	0
56	MG	B	2912	1/1	0.82	0.20	86,86,86,86	0
56	MG	C	214	1/1	0.82	0.17	97,97,97,97	0
56	MG	EB	3005	1/1	0.82	0.28	99,99,99,99	0
56	MG	EB	3009	1/1	0.82	0.18	93,93,93,93	0
56	MG	EB	2965	1/1	0.82	0.30	84,84,84,84	0
56	MG	EB	3273	1/1	0.82	0.13	88,88,88,88	0
56	MG	A	1641	1/1	0.82	0.36	107,107,107,107	0
56	MG	EB	2922	1/1	0.82	0.37	79,79,79,79	0
56	MG	EB	3075	1/1	0.82	0.18	95,95,95,95	0
56	MG	EB	3280	1/1	0.82	0.11	105,105,105,105	0
56	MG	A	1638	1/1	0.82	0.24	102,102,102,102	0
56	MG	DB	1757	1/1	0.82	0.34	106,106,106,106	0
56	MG	A	1666	1/1	0.82	0.26	105,105,105,105	0
56	MG	B	3217	1/1	0.82	0.23	93,93,93,93	0
56	MG	B	2988	1/1	0.82	0.33	87,87,87,87	0
56	MG	MB	202	1/1	0.82	0.16	148,148,148,148	0
56	MG	B	3038	1/1	0.82	0.19	80,80,80,80	0
56	MG	EB	3213	1/1	0.82	0.30	103,103,103,103	0
56	MG	OB	203	1/1	0.82	0.07	95,95,95,95	0
56	MG	B	3395	1/1	0.82	0.19	99,99,99,99	0
56	MG	DB	1765	1/1	0.82	0.14	122,122,122,122	0
56	MG	T	202	1/1	0.82	0.24	98,98,98,98	0
56	MG	EB	2934	1/1	0.82	0.64	86,86,86,86	0
56	MG	EB	3148	1/1	0.82	0.15	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	3147	1/1	0.82	0.20	94,94,94,94	0
56	MG	DB	1728	1/1	0.82	0.09	99,99,99,99	0
56	MG	B	3097	1/1	0.82	0.45	99,99,99,99	0
56	MG	EB	2985	1/1	0.82	0.22	91,91,91,91	0
56	MG	B	3226	1/1	0.82	0.17	90,90,90,90	0
56	MG	A	1637	1/1	0.82	0.40	92,92,92,92	0
56	MG	B	3043	1/1	0.82	0.41	85,85,85,85	0
56	MG	G	302	1/1	0.82	0.41	73,73,73,73	0
56	MG	B	3001	1/1	0.82	0.28	88,88,88,88	0
56	MG	EB	3168	1/1	0.82	0.32	88,88,88,88	0
56	MG	B	3101	1/1	0.82	0.32	95,95,95,95	0
56	MG	B	3130	1/1	0.82	0.23	82,82,82,82	0
56	MG	B	3272	1/1	0.82	0.29	104,104,104,104	0
56	MG	A	1731	1/1	0.82	0.25	102,102,102,102	0
56	MG	B	3105	1/1	0.82	0.20	83,83,83,83	0
57	ZN	BA	101	1/1	0.82	0.17	180,180,180,180	0
56	MG	EB	3143	1/1	0.83	0.34	89,89,89,89	0
56	MG	EB	3091	1/1	0.83	0.10	97,97,97,97	0
56	MG	EB	3209	1/1	0.83	0.29	97,97,97,97	0
56	MG	EB	2958	1/1	0.83	0.31	78,78,78,78	0
56	MG	EB	2959	1/1	0.83	0.24	99,99,99,99	0
56	MG	DB	1730	1/1	0.83	0.07	108,108,108,108	0
56	MG	B	3128	1/1	0.83	0.28	94,94,94,94	0
56	MG	EB	3223	1/1	0.83	0.09	97,97,97,97	0
56	MG	B	2993	1/1	0.83	0.23	86,86,86,86	0
56	MG	EB	3226	1/1	0.83	0.36	102,102,102,102	0
56	MG	B	2926	1/1	0.83	0.32	74,74,74,74	0
56	MG	DB	1679	1/1	0.83	0.20	134,134,134,134	0
56	MG	DB	1768	1/1	0.83	0.24	104,104,104,104	0
56	MG	B	3167	1/1	0.83	0.28	100,100,100,100	0
56	MG	QB	202	1/1	0.83	0.11	103,103,103,103	0
56	MG	EB	3006	1/1	0.83	0.56	103,103,103,103	0
56	MG	DB	1737	1/1	0.83	0.31	110,110,110,110	0
56	MG	B	3190	1/1	0.83	0.27	88,88,88,88	0
56	MG	B	3286	1/1	0.83	0.11	95,95,95,95	0
56	MG	EB	3173	1/1	0.83	0.19	103,103,103,103	0
56	MG	B	3008	1/1	0.83	0.38	96,96,96,96	0
56	MG	B	3243	1/1	0.83	0.15	97,97,97,97	0
56	MG	EB	2901	1/1	0.83	0.38	79,79,79,79	0
56	MG	EB	2977	1/1	0.83	0.20	120,120,120,120	0
56	MG	B	3172	1/1	0.83	0.40	97,97,97,97	0
56	MG	EB	2940	1/1	0.83	0.31	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	EB	3253	1/1	0.83	0.31	120,120,120,120	0
56	MG	DB	1630	1/1	0.83	0.21	105,105,105,105	0
56	MG	B	3107	1/1	0.83	0.24	96,96,96,96	0
56	MG	B	3108	1/1	0.83	0.13	124,124,124,124	0
56	MG	B	3330	1/1	0.83	0.09	88,88,88,88	0
56	MG	A	1685	1/1	0.83	0.39	149,149,149,149	0
56	MG	A	1621	1/1	0.83	0.20	115,115,115,115	0
56	MG	B	3113	1/1	0.83	0.25	96,96,96,96	0
56	MG	B	3383	1/1	0.83	0.20	114,114,114,114	0
56	MG	R	202	1/1	0.83	0.21	101,101,101,101	0
56	MG	CA	102	1/1	0.83	0.23	81,81,81,81	0
56	MG	B	3017	1/1	0.83	0.54	84,84,84,84	0
56	MG	EB	2918	1/1	0.83	0.35	92,92,92,92	0
57	ZN	EC	101	1/1	0.83	0.11	199,199,199,199	0
56	MG	EB	3117	1/1	0.84	0.23	92,92,92,92	0
56	MG	DB	1672	1/1	0.84	0.29	104,104,104,104	0
56	MG	L	203	1/1	0.84	0.20	104,104,104,104	0
56	MG	B	2927	1/1	0.84	0.36	87,87,87,87	0
56	MG	B	3179	1/1	0.84	0.10	106,106,106,106	0
56	MG	B	2917	1/1	0.84	0.41	79,79,79,79	0
56	MG	EB	3125	1/1	0.84	0.19	96,96,96,96	0
56	MG	DB	1771	1/1	0.84	0.09	106,106,106,106	0
56	MG	B	3094	1/1	0.84	0.18	87,87,87,87	0
56	MG	A	1733	1/1	0.84	0.17	91,91,91,91	0
56	MG	FC	102	1/1	0.84	0.12	101,101,101,101	0
56	MG	B	3386	1/1	0.84	0.13	108,108,108,108	0
56	MG	B	3156	1/1	0.84	0.17	92,92,92,92	0
56	MG	B	2920	1/1	0.84	0.19	82,82,82,82	0
56	MG	EB	3003	1/1	0.84	0.39	86,86,86,86	0
56	MG	B	3224	1/1	0.84	0.08	93,93,93,93	0
56	MG	B	3338	1/1	0.84	0.22	119,119,119,119	0
56	MG	A	1724	1/1	0.84	0.18	122,122,122,122	0
56	MG	V	503	1/1	0.84	0.07	99,99,99,99	0
56	MG	W	301	1/1	0.84	0.10	107,107,107,107	0
56	MG	B	2994	1/1	0.84	0.29	75,75,75,75	0
56	MG	B	3191	1/1	0.84	0.12	81,81,81,81	0
56	MG	B	3192	1/1	0.84	0.20	123,123,123,123	0
56	MG	B	3348	1/1	0.84	0.12	98,98,98,98	0
56	MG	EB	3158	1/1	0.84	0.14	105,105,105,105	0
56	MG	B	3229	1/1	0.84	0.16	112,112,112,112	0
56	MG	IB	301	1/1	0.84	0.18	88,88,88,88	0
56	MG	A	1653	1/1	0.84	0.27	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DB	1656	1/1	0.84	0.21	105,105,105,105	0
56	MG	EB	2970	1/1	0.84	0.20	90,90,90,90	0
56	MG	EB	3090	1/1	0.84	0.21	86,86,86,86	0
56	MG	B	2938	1/1	0.84	0.17	86,86,86,86	0
56	MG	EB	2919	1/1	0.84	0.51	80,80,80,80	0
56	MG	EB	2921	1/1	0.84	0.28	77,77,77,77	0
56	MG	DB	1748	1/1	0.84	0.17	121,121,121,121	0
56	MG	EB	3174	1/1	0.84	0.33	98,98,98,98	0
56	MG	PA	201	1/1	0.84	0.10	129,129,129,129	0
56	MG	EB	3099	1/1	0.84	0.32	103,103,103,103	0
56	MG	I	203	1/1	0.84	0.08	111,111,111,111	0
56	MG	DB	1662	1/1	0.84	0.36	108,108,108,108	0
56	MG	A	1695	1/1	0.84	0.17	105,105,105,105	0
56	MG	B	3271	1/1	0.84	0.09	100,100,100,100	0
56	MG	EB	3042	1/1	0.84	0.26	113,113,113,113	0
56	MG	Y	102	1/1	0.84	0.09	79,79,79,79	0
56	MG	B	3171	1/1	0.84	0.41	81,81,81,81	0
56	MG	EB	3188	1/1	0.84	0.16	89,89,89,89	0
56	MG	ED	201	1/1	0.84	0.31	122,122,122,122	0
56	MG	A	1751	1/1	0.84	0.06	116,116,116,116	0
56	MG	EB	2932	1/1	0.84	0.45	80,80,80,80	0
56	MG	C	209	1/1	0.84	0.14	96,96,96,96	0
56	MG	TB	202	1/1	0.84	0.06	111,111,111,111	0
56	MG	B	2977	1/1	0.84	0.27	83,83,83,83	0
56	MG	A	1760	1/1	0.84	0.34	101,101,101,101	0
56	MG	EB	3114	1/1	0.84	0.11	135,135,135,135	0
56	MG	EB	3291	1/1	0.84	0.23	90,90,90,90	0
57	ZN	YB	201	1/1	0.84	0.25	147,147,147,147	0
56	MG	B	3058	1/1	0.84	0.59	89,89,89,89	0
56	MG	B	3311	1/1	0.85	0.17	87,87,87,87	0
56	MG	DB	1776	1/1	0.85	0.12	94,94,94,94	0
56	MG	B	2934	1/1	0.85	0.33	82,82,82,82	0
56	MG	EB	3115	1/1	0.85	0.24	106,106,106,106	0
56	MG	IA	106	1/1	0.85	0.06	112,112,112,112	0
56	MG	A	1740	1/1	0.85	0.36	129,129,129,129	0
56	MG	B	2979	1/1	0.85	0.45	86,86,86,86	0
56	MG	EB	3020	1/1	0.85	0.20	90,90,90,90	0
56	MG	B	3166	1/1	0.85	0.12	105,105,105,105	0
56	MG	DB	1619	1/1	0.85	0.35	86,86,86,86	0
56	MG	EB	3269	1/1	0.85	0.12	103,103,103,103	0
56	MG	B	3021	1/1	0.85	0.45	93,93,93,93	0
56	MG	EB	3080	1/1	0.85	0.29	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	C	218	1/1	0.85	0.21	123,123,123,123	0
56	MG	EB	3130	1/1	0.85	0.28	97,97,97,97	0
56	MG	B	2957	1/1	0.85	0.22	81,81,81,81	0
56	MG	B	3361	1/1	0.85	0.15	95,95,95,95	0
56	MG	B	3004	1/1	0.85	0.38	80,80,80,80	0
56	MG	EB	3034	1/1	0.85	0.34	106,106,106,106	0
56	MG	B	3297	1/1	0.85	0.15	100,100,100,100	0
56	MG	EB	2916	1/1	0.85	0.41	78,78,78,78	0
56	MG	OB	201	1/1	0.85	0.19	96,96,96,96	0
56	MG	M	201	1/1	0.85	0.19	77,77,77,77	0
56	MG	N	202	1/1	0.85	0.17	96,96,96,96	0
56	MG	EB	3215	1/1	0.85	0.96	119,119,119,119	0
56	MG	A	1608	1/1	0.85	0.26	82,82,82,82	0
56	MG	DB	1763	1/1	0.85	0.04	120,120,120,120	0
56	MG	EB	3295	1/1	0.85	0.10	109,109,109,109	0
56	MG	B	3365	1/1	0.85	0.17	82,82,82,82	0
56	MG	EB	3093	1/1	0.85	0.13	115,115,115,115	0
56	MG	EB	3151	1/1	0.85	0.09	119,119,119,119	0
56	MG	DB	1696	1/1	0.85	0.27	105,105,105,105	0
56	MG	B	3327	1/1	0.85	0.21	92,92,92,92	0
56	MG	EB	2963	1/1	0.85	0.18	85,85,85,85	0
56	MG	EB	3051	1/1	0.85	0.27	95,95,95,95	0
56	MG	EB	3100	1/1	0.85	0.28	92,92,92,92	0
56	MG	A	1650	1/1	0.85	0.39	108,108,108,108	0
56	MG	B	3045	1/1	0.85	0.28	84,84,84,84	0
56	MG	B	3332	1/1	0.85	0.12	102,102,102,102	0
56	MG	DB	1735	1/1	0.85	0.17	101,101,101,101	0
56	MG	EB	3242	1/1	0.85	0.31	103,103,103,103	0
56	MG	A	1624	1/1	0.85	0.30	111,111,111,111	0
56	MG	B	3158	1/1	0.85	0.11	92,92,92,92	0
56	MG	EB	3065	1/1	0.85	0.12	92,92,92,92	0
56	MG	EB	3008	1/1	0.85	0.17	92,92,92,92	0
56	MG	B	3339	1/1	0.85	0.23	98,98,98,98	0
56	MG	A	1739	1/1	0.85	0.06	151,151,151,151	0
56	MG	PB	202	1/1	0.86	0.43	103,103,103,103	0
56	MG	A	1690	1/1	0.86	0.06	111,111,111,111	0
56	MG	EB	3013	1/1	0.86	0.28	81,81,81,81	0
56	MG	C	219	1/1	0.86	0.24	131,131,131,131	0
56	MG	EB	3261	1/1	0.86	0.05	115,115,115,115	0
56	MG	B	2972	1/1	0.86	0.24	72,72,72,72	0
56	MG	DB	1723	1/1	0.86	0.13	102,102,102,102	0
56	MG	B	3095	1/1	0.86	0.33	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	3376	1/1	0.86	0.52	92,92,92,92	0
56	MG	B	2925	1/1	0.86	0.29	73,73,73,73	0
56	MG	EB	3272	1/1	0.86	0.35	128,128,128,128	0
56	MG	A	1720	1/1	0.86	0.20	110,110,110,110	0
56	MG	A	1744	1/1	0.86	0.13	118,118,118,118	0
56	MG	A	1639	1/1	0.86	0.26	95,95,95,95	0
56	MG	B	3034	1/1	0.86	0.29	109,109,109,109	0
56	MG	B	3068	1/1	0.86	0.23	82,82,82,82	0
56	MG	B	3071	1/1	0.86	0.19	90,90,90,90	0
56	MG	YB	203	1/1	0.86	0.17	130,130,130,130	0
56	MG	EB	3032	1/1	0.86	0.25	95,95,95,95	0
56	MG	B	2981	1/1	0.86	0.28	82,82,82,82	0
56	MG	G	304	1/1	0.86	0.14	80,80,80,80	0
56	MG	B	3209	1/1	0.86	0.25	97,97,97,97	0
56	MG	DB	1632	1/1	0.86	0.72	110,110,110,110	0
56	MG	W	312	1/1	0.86	0.07	126,126,126,126	0
56	MG	EB	3039	1/1	0.86	0.36	102,102,102,102	0
56	MG	B	3334	1/1	0.86	0.31	87,87,87,87	0
56	MG	EB	3292	1/1	0.86	0.10	91,91,91,91	0
56	MG	B	3136	1/1	0.86	0.10	91,91,91,91	0
56	MG	B	2907	1/1	0.86	0.16	79,79,79,79	0
56	MG	B	3289	1/1	0.86	0.17	93,93,93,93	0
56	MG	EB	3111	1/1	0.86	0.16	127,127,127,127	0
56	MG	B	3250	1/1	0.86	0.10	96,96,96,96	0
56	MG	B	3410	1/1	0.86	0.14	127,127,127,127	0
56	MG	DB	1642	1/1	0.86	0.21	92,92,92,92	0
56	MG	B	3411	1/1	0.86	0.11	83,83,83,83	0
56	MG	B	3341	1/1	0.86	0.08	94,94,94,94	0
56	MG	A	1677	1/1	0.86	0.17	115,115,115,115	0
56	MG	B	3295	1/1	0.86	0.10	90,90,90,90	0
56	MG	DB	1754	1/1	0.86	0.25	129,129,129,129	0
56	MG	DB	1647	1/1	0.86	0.14	123,123,123,123	0
56	MG	EB	3217	1/1	0.86	0.18	93,93,93,93	0
56	MG	EB	3218	1/1	0.86	0.23	92,92,92,92	0
56	MG	EB	3061	1/1	0.86	0.27	86,86,86,86	0
56	MG	EB	3062	1/1	0.86	0.12	89,89,89,89	0
56	MG	EB	3222	1/1	0.86	0.26	92,92,92,92	0
56	MG	EB	3064	1/1	0.86	0.24	91,91,91,91	0
56	MG	A	1687	1/1	0.86	0.06	167,167,167,167	0
56	MG	GB	104	1/1	0.86	0.13	152,152,152,152	0
56	MG	B	3019	1/1	0.86	0.17	83,83,83,83	0
56	MG	EB	3229	1/1	0.86	0.11	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	EB	2994	1/1	0.86	0.37	87,87,87,87	0
56	MG	B	3079	1/1	0.86	0.17	86,86,86,86	0
56	MG	EB	3069	1/1	0.86	0.19	86,86,86,86	0
56	MG	EB	3234	1/1	0.86	0.12	168,168,168,168	0
56	MG	EB	2937	1/1	0.86	0.43	95,95,95,95	0
56	MG	DB	1651	1/1	0.86	0.23	107,107,107,107	0
56	MG	B	3020	1/1	0.86	0.44	91,91,91,91	0
56	MG	EB	3238	1/1	0.86	0.32	100,100,100,100	0
56	MG	EB	3140	1/1	0.86	0.20	124,124,124,124	0
56	MG	M	204	1/1	0.86	0.31	88,88,88,88	0
56	MG	EB	3241	1/1	0.86	0.21	102,102,102,102	0
56	MG	B	3303	1/1	0.86	0.26	91,91,91,91	0
56	MG	A	1655	1/1	0.86	0.39	96,96,96,96	0
56	MG	EB	3144	1/1	0.86	0.14	106,106,106,106	0
56	MG	B	2935	1/1	0.86	0.39	79,79,79,79	0
56	MG	A	1664	1/1	0.86	0.42	105,105,105,105	0
56	MG	DB	1713	1/1	0.86	0.28	143,143,143,143	0
56	MG	B	2969	1/1	0.86	0.23	83,83,83,83	0
56	MG	B	3091	1/1	0.86	0.25	86,86,86,86	0
56	MG	B	3312	1/1	0.86	0.18	80,80,80,80	0
56	MG	B	3153	1/1	0.86	0.06	165,165,165,165	0
56	MG	DB	1719	1/1	0.86	0.09	113,113,113,113	0
56	MG	EB	3033	1/1	0.87	0.38	103,103,103,103	0
56	MG	A	1609	1/1	0.87	0.20	74,74,74,74	0
56	MG	A	1756	1/1	0.87	0.07	170,170,170,170	0
56	MG	A	1648	1/1	0.87	0.13	139,139,139,139	0
56	MG	EB	2956	1/1	0.87	0.38	92,92,92,92	0
56	MG	EB	3184	1/1	0.87	0.10	120,120,120,120	0
56	MG	A	1620	1/1	0.87	0.34	98,98,98,98	0
56	MG	B	3300	1/1	0.87	0.12	117,117,117,117	0
56	MG	EB	3129	1/1	0.87	0.20	80,80,80,80	0
56	MG	DB	1637	1/1	0.87	0.39	106,106,106,106	0
56	MG	B	2939	1/1	0.87	0.16	76,76,76,76	0
56	MG	B	3007	1/1	0.87	0.29	88,88,88,88	0
56	MG	EB	3046	1/1	0.87	0.29	104,104,104,104	0
56	MG	EB	3196	1/1	0.87	0.14	100,100,100,100	0
56	MG	B	3144	1/1	0.87	0.12	100,100,100,100	0
56	MG	EB	3198	1/1	0.87	0.36	92,92,92,92	0
56	MG	EB	3136	1/1	0.87	0.09	96,96,96,96	0
56	MG	EB	2926	1/1	0.87	0.52	101,101,101,101	0
56	MG	EB	3270	1/1	0.87	0.23	89,89,89,89	0
56	MG	MC	303	1/1	0.87	0.07	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	3049	1/1	0.87	0.14	73,73,73,73	0
56	MG	B	3161	1/1	0.87	0.19	81,81,81,81	0
56	MG	B	3201	1/1	0.87	0.11	87,87,87,87	0
56	MG	B	3203	1/1	0.87	0.19	82,82,82,82	0
56	MG	EB	3096	1/1	0.87	0.24	96,96,96,96	0
56	MG	EB	3210	1/1	0.87	0.36	103,103,103,103	0
56	MG	DB	1675	1/1	0.87	0.20	110,110,110,110	0
56	MG	EB	3214	1/1	0.87	0.07	128,128,128,128	0
56	MG	EB	3145	1/1	0.87	0.10	95,95,95,95	0
56	MG	DB	1676	1/1	0.87	0.18	120,120,120,120	0
56	MG	B	3254	1/1	0.87	0.23	102,102,102,102	0
56	MG	B	2996	1/1	0.87	0.35	75,75,75,75	0
56	MG	B	3230	1/1	0.87	0.10	93,93,93,93	0
56	MG	DB	1745	1/1	0.87	0.25	102,102,102,102	0
56	MG	EB	3063	1/1	0.87	0.23	109,109,109,109	0
56	MG	B	3259	1/1	0.87	0.28	85,85,85,85	0
56	MG	EB	3015	1/1	0.87	0.12	94,94,94,94	0
56	MG	EB	2938	1/1	0.87	0.34	90,90,90,90	0
56	MG	B	3354	1/1	0.87	0.13	103,103,103,103	0
56	MG	EB	2905	1/1	0.87	0.33	78,78,78,78	0
56	MG	B	3182	1/1	0.87	0.27	98,98,98,98	0
56	MG	EB	3165	1/1	0.87	0.15	88,88,88,88	0
56	MG	B	3398	1/1	0.87	0.19	89,89,89,89	0
56	MG	B	3023	1/1	0.87	0.24	79,79,79,79	0
56	MG	L	202	1/1	0.87	0.43	91,91,91,91	0
56	MG	B	3072	1/1	0.87	0.30	88,88,88,88	0
56	MG	EB	3172	1/1	0.87	0.47	120,120,120,120	0
56	MG	D	101	1/1	0.87	0.10	123,123,123,123	0
56	MG	B	3210	1/1	0.87	0.21	87,87,87,87	0
56	MG	B	2985	1/1	0.87	0.25	89,89,89,89	0
56	MG	EB	2949	1/1	0.87	0.38	93,93,93,93	0
56	MG	EB	3243	1/1	0.87	0.12	106,106,106,106	0
56	MG	R	201	1/1	0.88	0.27	100,100,100,100	0
56	MG	EB	3162	1/1	0.88	0.10	87,87,87,87	0
56	MG	B	2946	1/1	0.88	0.28	84,84,84,84	0
56	MG	B	3013	1/1	0.88	0.25	84,84,84,84	0
56	MG	B	3264	1/1	0.88	0.18	97,97,97,97	0
56	MG	B	3265	1/1	0.88	0.16	85,85,85,85	0
56	MG	B	3385	1/1	0.88	0.12	83,83,83,83	0
56	MG	EB	3224	1/1	0.88	0.22	93,93,93,93	0
56	MG	EB	2952	1/1	0.88	0.21	94,94,94,94	0
56	MG	EB	2953	1/1	0.88	0.30	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	EB	3227	1/1	0.88	0.34	109,109,109,109	0
56	MG	DB	1653	1/1	0.88	0.17	95,95,95,95	0
56	MG	EB	2920	1/1	0.88	0.61	87,87,87,87	0
56	MG	DB	1688	1/1	0.88	0.11	113,113,113,113	0
56	MG	EB	3175	1/1	0.88	0.07	106,106,106,106	0
56	MG	EB	2997	1/1	0.88	0.29	85,85,85,85	0
56	MG	B	3042	1/1	0.88	0.44	87,87,87,87	0
56	MG	EB	3293	1/1	0.88	0.14	85,85,85,85	0
56	MG	B	3057	1/1	0.88	0.44	76,76,76,76	0
56	MG	DB	1625	1/1	0.88	0.17	87,87,87,87	0
56	MG	B	3290	1/1	0.88	0.09	90,90,90,90	0
56	MG	B	3115	1/1	0.88	0.26	114,114,114,114	0
56	MG	RB	202	1/1	0.88	0.11	98,98,98,98	0
56	MG	EB	3048	1/1	0.88	0.14	88,88,88,88	0
56	MG	B	3135	1/1	0.88	0.11	66,66,66,66	0
56	MG	DB	1695	1/1	0.88	0.15	109,109,109,109	0
56	MG	B	3294	1/1	0.88	0.12	92,92,92,92	0
56	MG	B	3358	1/1	0.88	0.25	83,83,83,83	0
56	MG	B	3322	1/1	0.88	0.12	90,90,90,90	0
56	MG	A	1757	1/1	0.88	0.07	99,99,99,99	0
56	MG	B	3059	1/1	0.88	0.10	74,74,74,74	0
56	MG	B	2995	1/1	0.88	0.44	84,84,84,84	0
56	MG	A	1741	1/1	0.88	0.10	86,86,86,86	0
56	MG	B	3035	1/1	0.88	0.20	78,78,78,78	0
56	MG	B	2949	1/1	0.88	0.41	82,82,82,82	0
56	MG	N	201	1/1	0.88	0.08	111,111,111,111	0
56	MG	B	3052	1/1	0.88	0.24	78,78,78,78	0
56	MG	EB	3017	1/1	0.88	0.18	93,93,93,93	0
56	MG	B	3069	1/1	0.88	0.13	79,79,79,79	0
56	MG	Z	101	1/1	0.88	0.23	97,97,97,97	0
56	MG	B	2992	1/1	0.88	0.43	80,80,80,80	0
56	MG	EB	3154	1/1	0.88	0.07	114,114,114,114	0
56	MG	P	202	1/1	0.88	0.14	126,126,126,126	0
56	MG	EB	3157	1/1	0.88	0.34	88,88,88,88	0
56	MG	B	3092	1/1	0.88	0.21	86,86,86,86	0
56	MG	G	301	1/1	0.88	0.32	89,89,89,89	0
56	MG	B	3299	1/1	0.89	0.12	103,103,103,103	0
56	MG	EB	3206	1/1	0.89	0.16	93,93,93,93	0
56	MG	B	2991	1/1	0.89	0.30	84,84,84,84	0
56	MG	B	3194	1/1	0.89	0.06	110,110,110,110	0
56	MG	EB	3155	1/1	0.89	0.17	108,108,108,108	0
56	MG	B	2955	1/1	0.89	0.37	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	A	1606	1/1	0.89	0.47	99,99,99,99	0
56	MG	L	204	1/1	0.89	0.12	104,104,104,104	0
56	MG	Y	101	1/1	0.89	0.34	88,88,88,88	0
56	MG	EB	2980	1/1	0.89	0.34	82,82,82,82	0
56	MG	LC	104	1/1	0.89	0.15	101,101,101,101	0
56	MG	EB	3161	1/1	0.89	0.10	78,78,78,78	0
56	MG	B	2943	1/1	0.89	0.19	77,77,77,77	0
56	MG	B	3306	1/1	0.89	0.14	82,82,82,82	0
56	MG	B	3041	1/1	0.89	0.36	81,81,81,81	0
56	MG	EB	3024	1/1	0.89	0.23	100,100,100,100	0
56	MG	A	1754	1/1	0.89	0.18	112,112,112,112	0
56	MG	Z	102	1/1	0.89	0.04	95,95,95,95	0
56	MG	B	3129	1/1	0.89	0.09	106,106,106,106	0
56	MG	N	203	1/1	0.89	0.11	113,113,113,113	0
56	MG	B	3255	1/1	0.89	0.08	89,89,89,89	0
56	MG	EB	3288	1/1	0.89	0.11	111,111,111,111	0
56	MG	B	3256	1/1	0.89	0.45	94,94,94,94	0
56	MG	B	3183	1/1	0.89	0.15	85,85,85,85	0
56	MG	PB	201	1/1	0.89	0.22	99,99,99,99	0
56	MG	Q	201	1/1	0.89	0.13	115,115,115,115	0
56	MG	EB	3233	1/1	0.89	0.21	83,83,83,83	0
56	MG	EB	3124	1/1	0.89	0.35	115,115,115,115	0
56	MG	B	3406	1/1	0.89	0.29	86,86,86,86	0
56	MG	B	3206	1/1	0.89	0.07	105,105,105,105	0
56	MG	B	2901	1/1	0.89	0.39	60,60,60,60	0
56	MG	DB	1753	1/1	0.89	0.24	119,119,119,119	0
56	MG	B	3185	1/1	0.89	0.13	82,82,82,82	0
56	MG	B	3073	1/1	0.89	0.17	87,87,87,87	0
56	MG	B	3319	1/1	0.89	0.09	80,80,80,80	0
56	MG	B	2998	1/1	0.89	0.18	66,66,66,66	0
56	MG	DB	1759	1/1	0.89	0.12	102,102,102,102	0
56	MG	B	3212	1/1	0.89	0.18	95,95,95,95	0
56	MG	B	3366	1/1	0.89	0.18	108,108,108,108	0
56	MG	B	3237	1/1	0.89	0.27	73,73,73,73	0
56	MG	V	504	1/1	0.89	0.17	101,101,101,101	0
56	MG	EB	3095	1/1	0.89	0.28	110,110,110,110	0
56	MG	B	2999	1/1	0.89	0.28	68,68,68,68	0
56	MG	EB	3007	1/1	0.89	0.29	89,89,89,89	0
56	MG	B	3120	1/1	0.89	0.25	80,80,80,80	0
56	MG	B	3328	1/1	0.89	0.15	93,93,93,93	0
56	MG	EB	3255	1/1	0.89	0.20	108,108,108,108	0
56	MG	B	3240	1/1	0.89	0.16	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	3121	1/1	0.89	0.19	95,95,95,95	0
56	MG	B	2990	1/1	0.89	0.29	72,72,72,72	0
56	MG	B	3080	1/1	0.90	0.24	99,99,99,99	0
56	MG	RB	205	1/1	0.90	0.21	95,95,95,95	0
56	MG	EB	3041	1/1	0.90	0.18	90,90,90,90	0
56	MG	DB	1711	1/1	0.90	0.27	115,115,115,115	0
56	MG	DB	1687	1/1	0.90	0.13	96,96,96,96	0
56	MG	M	202	1/1	0.90	0.16	87,87,87,87	0
56	MG	EB	3167	1/1	0.90	0.23	103,103,103,103	0
56	MG	EB	3045	1/1	0.90	0.31	84,84,84,84	0
56	MG	A	1719	1/1	0.90	0.19	126,126,126,126	0
56	MG	V	505	1/1	0.90	0.15	113,113,113,113	0
56	MG	B	3109	1/1	0.90	0.40	86,86,86,86	0
56	MG	EB	3211	1/1	0.90	0.20	100,100,100,100	0
56	MG	B	3143	1/1	0.90	0.26	83,83,83,83	0
56	MG	B	3396	1/1	0.90	0.15	101,101,101,101	0
56	MG	B	3245	1/1	0.90	0.16	85,85,85,85	0
56	MG	B	3399	1/1	0.90	0.36	89,89,89,89	0
56	MG	EB	3294	1/1	0.90	0.16	117,117,117,117	0
56	MG	B	3011	1/1	0.90	0.09	91,91,91,91	0
56	MG	B	3202	1/1	0.90	0.26	74,74,74,74	0
56	MG	B	3012	1/1	0.90	0.33	98,98,98,98	0
56	MG	EB	3058	1/1	0.90	0.32	102,102,102,102	0
56	MG	B	3164	1/1	0.90	0.39	91,91,91,91	0
56	MG	B	3368	1/1	0.90	0.16	90,90,90,90	0
56	MG	DB	1727	1/1	0.90	0.23	108,108,108,108	0
56	MG	EB	3031	1/1	0.90	0.19	95,95,95,95	0
56	MG	E	303	1/1	0.90	0.08	104,104,104,104	0
56	MG	R	203	1/1	0.90	0.48	84,84,84,84	0
56	MG	R	204	1/1	0.90	0.33	86,86,86,86	0
56	MG	E	304	1/1	0.90	0.09	92,92,92,92	0
56	MG	B	3389	1/1	0.90	0.09	98,98,98,98	0
56	MG	EB	3193	1/1	0.90	0.19	106,106,106,106	0
56	MG	A	1750	1/1	0.90	0.17	130,130,130,130	0
56	MG	EB	3126	1/1	0.90	0.10	82,82,82,82	0
56	MG	B	3412	1/1	0.90	0.15	91,91,91,91	0
56	MG	EB	3277	1/1	0.90	0.16	91,91,91,91	0
56	MG	EB	3028	1/1	0.91	0.32	95,95,95,95	0
56	MG	B	3009	1/1	0.91	0.13	81,81,81,81	0
56	MG	B	2961	1/1	0.91	0.24	77,77,77,77	0
56	MG	B	2980	1/1	0.91	0.24	75,75,75,75	0
56	MG	EB	2955	1/1	0.91	0.27	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	3090	1/1	0.91	0.16	85,85,85,85	0
56	MG	B	3402	1/1	0.91	0.20	109,109,109,109	0
56	MG	B	3353	1/1	0.91	0.07	93,93,93,93	0
56	MG	B	3067	1/1	0.91	0.15	71,71,71,71	0
56	MG	B	3222	1/1	0.91	0.11	96,96,96,96	0
56	MG	B	3223	1/1	0.91	0.19	82,82,82,82	0
56	MG	B	3279	1/1	0.91	0.14	79,79,79,79	0
56	MG	EB	3118	1/1	0.91	0.08	102,102,102,102	0
56	MG	B	3050	1/1	0.91	0.13	87,87,87,87	0
56	MG	B	3281	1/1	0.91	0.09	88,88,88,88	0
56	MG	DB	1744	1/1	0.91	0.12	126,126,126,126	0
56	MG	B	3414	1/1	0.91	0.15	93,93,93,93	0
56	MG	B	3387	1/1	0.91	0.28	87,87,87,87	0
56	MG	B	3336	1/1	0.91	0.14	86,86,86,86	0
56	MG	EB	3185	1/1	0.91	0.20	101,101,101,101	0
56	MG	EB	3220	1/1	0.91	0.09	107,107,107,107	0
56	MG	HB	303	1/1	0.91	0.37	94,94,94,94	0
56	MG	GD	403	1/1	0.91	0.07	95,95,95,95	0
56	MG	A	1674	1/1	0.91	0.06	98,98,98,98	0
56	MG	B	2970	1/1	0.91	0.44	72,72,72,72	0
56	MG	EB	3127	1/1	0.91	0.15	99,99,99,99	0
56	MG	B	3060	1/1	0.91	0.36	95,95,95,95	0
56	MG	DB	1658	1/1	0.91	0.19	109,109,109,109	0
57	ZN	V	501	1/1	0.91	0.15	130,130,130,130	0
56	MG	S	202	1/1	0.91	0.08	105,105,105,105	0
56	MG	B	2941	1/1	0.91	0.29	79,79,79,79	0
56	MG	B	3270	1/1	0.91	0.07	81,81,81,81	0
56	MG	B	3349	1/1	0.92	0.28	81,81,81,81	0
56	MG	B	3252	1/1	0.92	0.25	90,90,90,90	0
56	MG	B	3379	1/1	0.92	0.12	104,104,104,104	0
56	MG	DB	1716	1/1	0.92	0.08	119,119,119,119	0
56	MG	B	3087	1/1	0.92	0.18	83,83,83,83	0
56	MG	B	3382	1/1	0.92	0.05	92,92,92,92	0
56	MG	B	3413	1/1	0.92	0.09	98,98,98,98	0
56	MG	EB	3258	1/1	0.92	0.15	90,90,90,90	0
56	MG	B	3307	1/1	0.92	0.12	86,86,86,86	0
56	MG	B	3355	1/1	0.92	0.11	81,81,81,81	0
56	MG	EB	3040	1/1	0.92	0.47	115,115,115,115	0
56	MG	B	3221	1/1	0.92	0.17	89,89,89,89	0
56	MG	B	3141	1/1	0.92	0.33	89,89,89,89	0
56	MG	EB	3265	1/1	0.92	0.10	98,98,98,98	0
56	MG	B	2913	1/1	0.92	0.51	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	A	1708	1/1	0.92	0.14	89,89,89,89	0
56	MG	B	2919	1/1	0.92	0.19	74,74,74,74	0
56	MG	B	3044	1/1	0.92	0.16	69,69,69,69	0
56	MG	EB	2906	1/1	0.92	0.51	79,79,79,79	0
56	MG	B	3066	1/1	0.92	0.29	77,77,77,77	0
56	MG	A	1737	1/1	0.92	0.07	97,97,97,97	0
56	MG	FB	215	1/1	0.92	0.09	135,135,135,135	0
56	MG	B	2931	1/1	0.92	0.34	74,74,74,74	0
56	MG	B	3198	1/1	0.92	0.07	107,107,107,107	0
56	MG	EB	3208	1/1	0.92	0.44	99,99,99,99	0
56	MG	B	3047	1/1	0.92	0.38	88,88,88,88	0
56	MG	B	3345	1/1	0.92	0.10	82,82,82,82	0
56	MG	B	3048	1/1	0.92	0.21	80,80,80,80	0
56	MG	EB	3056	1/1	0.92	0.25	87,87,87,87	0
56	MG	B	3371	1/1	0.92	0.66	80,80,80,80	0
56	MG	B	3403	1/1	0.92	0.19	101,101,101,101	0
56	MG	A	1700	1/1	0.92	0.21	96,96,96,96	0
56	MG	B	2983	1/1	0.92	0.24	71,71,71,71	0
56	MG	B	3196	1/1	0.93	0.06	158,158,158,158	0
56	MG	EB	2964	1/1	0.93	0.12	98,98,98,98	0
56	MG	DB	1655	1/1	0.93	0.24	116,116,116,116	0
56	MG	B	3323	1/1	0.93	0.13	83,83,83,83	0
56	MG	EB	3202	1/1	0.93	0.07	89,89,89,89	0
56	MG	B	3324	1/1	0.93	0.08	94,94,94,94	0
56	MG	B	3301	1/1	0.93	0.20	101,101,101,101	0
56	MG	DB	1659	1/1	0.93	0.13	106,106,106,106	0
56	MG	B	3211	1/1	0.93	0.11	81,81,81,81	0
56	MG	B	3168	1/1	0.93	0.20	79,79,79,79	0
56	MG	B	3388	1/1	0.93	0.14	93,93,93,93	0
56	MG	B	2982	1/1	0.93	0.29	96,96,96,96	0
56	MG	B	3359	1/1	0.93	0.10	79,79,79,79	0
56	MG	EB	3212	1/1	0.93	0.14	100,100,100,100	0
56	MG	RB	201	1/1	0.93	0.16	105,105,105,105	0
56	MG	B	3329	1/1	0.93	0.13	105,105,105,105	0
56	MG	B	2937	1/1	0.93	0.38	81,81,81,81	0
56	MG	B	3215	1/1	0.93	0.07	156,156,156,156	0
56	MG	B	3039	1/1	0.93	0.12	83,83,83,83	0
56	MG	B	3088	1/1	0.93	0.48	88,88,88,88	0
56	MG	DB	1634	1/1	0.93	0.19	99,99,99,99	0
56	MG	B	3397	1/1	0.93	0.16	85,85,85,85	0
56	MG	B	2954	1/1	0.93	0.25	67,67,67,67	0
56	MG	B	3310	1/1	0.93	0.18	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	EB	3267	1/1	0.93	0.14	82,82,82,82	0
56	MG	EB	3178	1/1	0.93	0.47	90,90,90,90	0
56	MG	V	506	1/1	0.93	0.09	119,119,119,119	0
56	MG	B	3400	1/1	0.93	0.42	83,83,83,83	0
56	MG	WB	203	1/1	0.93	0.19	82,82,82,82	0
56	MG	A	1716	1/1	0.93	0.14	95,95,95,95	0
56	MG	B	3235	1/1	0.93	0.33	82,82,82,82	0
56	MG	C	222	1/1	0.93	0.07	119,119,119,119	0
56	MG	EB	3276	1/1	0.93	0.21	121,121,121,121	0
56	MG	L	205	1/1	0.93	0.07	110,110,110,110	0
56	MG	B	3253	1/1	0.93	0.46	98,98,98,98	0
56	MG	B	2974	1/1	0.93	0.52	68,68,68,68	0
56	MG	B	3405	1/1	0.93	0.17	120,120,120,120	0
56	MG	M	203	1/1	0.93	0.20	84,84,84,84	0
56	MG	B	3102	1/1	0.93	0.40	84,84,84,84	0
56	MG	EB	3150	1/1	0.93	0.23	88,88,88,88	0
56	MG	B	3081	1/1	0.93	0.18	76,76,76,76	0
56	MG	B	3064	1/1	0.93	0.22	89,89,89,89	0
56	MG	B	2965	1/1	0.93	0.38	86,86,86,86	0
56	MG	B	3278	1/1	0.93	0.15	83,83,83,83	0
56	MG	B	3241	1/1	0.93	0.35	92,92,92,92	0
56	MG	A	1686	1/1	0.94	0.09	116,116,116,116	0
56	MG	B	2987	1/1	0.94	0.46	82,82,82,82	0
56	MG	B	2975	1/1	0.94	0.25	72,72,72,72	0
56	MG	B	3070	1/1	0.94	0.09	72,72,72,72	0
56	MG	B	3344	1/1	0.94	0.13	93,93,93,93	0
56	MG	B	3409	1/1	0.94	0.07	89,89,89,89	0
56	MG	EB	3264	1/1	0.94	0.09	93,93,93,93	0
56	MG	B	3377	1/1	0.94	0.13	93,93,93,93	0
56	MG	B	3000	1/1	0.94	0.17	76,76,76,76	0
56	MG	C	215	1/1	0.94	0.05	123,123,123,123	0
56	MG	XB	101	1/1	0.94	0.11	119,119,119,119	0
56	MG	B	3117	1/1	0.94	0.17	92,92,92,92	0
56	MG	A	1673	1/1	0.94	0.13	153,153,153,153	0
56	MG	B	2973	1/1	0.94	0.48	80,80,80,80	0
56	MG	EB	3248	1/1	0.94	0.12	100,100,100,100	0
56	MG	EB	3228	1/1	0.94	0.11	111,111,111,111	0
56	MG	L	206	1/1	0.94	0.08	97,97,97,97	0
56	MG	B	3204	1/1	0.94	0.14	76,76,76,76	0
56	MG	B	3351	1/1	0.94	0.06	99,99,99,99	0
56	MG	EB	3171	1/1	0.94	0.24	93,93,93,93	0
56	MG	B	3260	1/1	0.94	0.12	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	3173	1/1	0.94	0.08	74,74,74,74	0
56	MG	B	3174	1/1	0.94	0.18	96,96,96,96	0
56	MG	EB	3282	1/1	0.94	0.10	95,95,95,95	0
56	MG	B	3084	1/1	0.95	0.04	89,89,89,89	0
56	MG	B	3393	1/1	0.95	0.09	99,99,99,99	0
56	MG	B	3189	1/1	0.95	0.11	96,96,96,96	0
56	MG	B	3337	1/1	0.95	0.17	101,101,101,101	0
56	MG	B	3016	1/1	0.95	0.47	81,81,81,81	0
56	MG	EB	3204	1/1	0.95	0.13	92,92,92,92	0
56	MG	B	3146	1/1	0.95	0.44	81,81,81,81	0
56	MG	B	3030	1/1	0.95	0.20	76,76,76,76	0
56	MG	B	3112	1/1	0.95	0.18	84,84,84,84	0
56	MG	B	3342	1/1	0.95	0.18	80,80,80,80	0
56	MG	B	2932	1/1	0.95	0.23	73,73,73,73	0
56	MG	C	221	1/1	0.95	0.11	121,121,121,121	0
56	MG	EB	3027	1/1	0.95	0.12	95,95,95,95	0
56	MG	S	201	1/1	0.95	0.20	98,98,98,98	0
56	MG	B	3014	1/1	0.95	0.27	78,78,78,78	0
56	MG	EB	3131	1/1	0.95	0.12	97,97,97,97	0
56	MG	B	3333	1/1	0.95	0.13	91,91,91,91	0
56	MG	EB	2912	1/1	0.95	0.30	76,76,76,76	0
56	MG	B	3372	1/1	0.95	0.10	76,76,76,76	0
56	MG	DB	1702	1/1	0.95	0.10	111,111,111,111	0
56	MG	A	1619	1/1	0.95	0.27	100,100,100,100	0
56	MG	U	101	1/1	0.95	0.13	85,85,85,85	0
56	MG	EB	2987	1/1	0.95	0.22	82,82,82,82	0
56	MG	DB	1747	1/1	0.95	0.11	106,106,106,106	0
56	MG	B	3360	1/1	0.95	0.05	78,78,78,78	0
56	MG	DB	1706	1/1	0.95	0.11	111,111,111,111	0
56	MG	EB	3252	1/1	0.95	0.12	99,99,99,99	0
56	MG	B	3375	1/1	0.95	0.11	79,79,79,79	0
57	ZN	FC	101	1/1	0.95	0.06	142,142,142,142	0
56	MG	HB	305	1/1	0.96	0.14	96,96,96,96	0
56	MG	EB	3137	1/1	0.96	0.39	91,91,91,91	0
56	MG	B	3169	1/1	0.96	0.29	82,82,82,82	0
56	MG	B	2909	1/1	0.96	0.24	74,74,74,74	0
56	MG	A	1714	1/1	0.96	0.59	115,115,115,115	0
56	MG	EB	3192	1/1	0.96	0.12	88,88,88,88	0
56	MG	B	2997	1/1	0.96	0.27	75,75,75,75	0
56	MG	EB	3194	1/1	0.96	0.15	89,89,89,89	0
56	MG	B	3321	1/1	0.96	0.19	88,88,88,88	0
56	MG	B	3293	1/1	0.96	0.06	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	3104	1/1	0.96	0.10	76,76,76,76	0
56	MG	B	3028	1/1	0.96	0.11	72,72,72,72	0
56	MG	DB	1777	1/1	0.96	0.10	110,110,110,110	0
57	ZN	GC	101	1/1	0.96	0.09	156,156,156,156	0
56	MG	B	3381	1/1	0.97	0.11	80,80,80,80	0
56	MG	EB	3268	1/1	0.97	0.09	94,94,94,94	0
56	MG	B	3162	1/1	0.97	0.27	88,88,88,88	0
56	MG	B	3157	1/1	0.97	0.21	77,77,77,77	0
57	ZN	CA	101	1/1	0.97	0.03	134,134,134,134	0
56	MG	G	303	1/1	0.97	0.09	75,75,75,75	0
56	MG	DB	1755	1/1	0.97	0.04	142,142,142,142	0
56	MG	EB	3055	1/1	0.97	0.14	80,80,80,80	0
56	MG	EB	3274	1/1	0.97	0.20	100,100,100,100	0
57	ZN	DA	101	1/1	0.98	0.05	141,141,141,141	0
56	MG	EB	2967	1/1	0.98	0.32	86,86,86,86	0
56	MG	B	3149	1/1	0.98	0.09	92,92,92,92	0
56	MG	B	3350	1/1	0.98	0.10	79,79,79,79	0
56	MG	C	203	1/1	0.98	0.06	125,125,125,125	0
57	ZN	JC	101	1/1	0.98	0.05	159,159,159,159	0
57	ZN	GA	101	1/1	0.99	0.02	132,132,132,132	0
56	MG	EB	3147	1/1	0.99	0.03	165,165,165,165	0

6.5 Other polymers

There are no such residues in this entry.