



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 10, 2025 – 10:12 PM EST

PDB ID : 5J4D
Title : E. coli release factor 1 bound to the 70S ribosome in response to a pseudouridylated stop codon
Authors : Svidritskiy, E.; Korostelev, A.A.
Deposited on : 2016-03-31
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

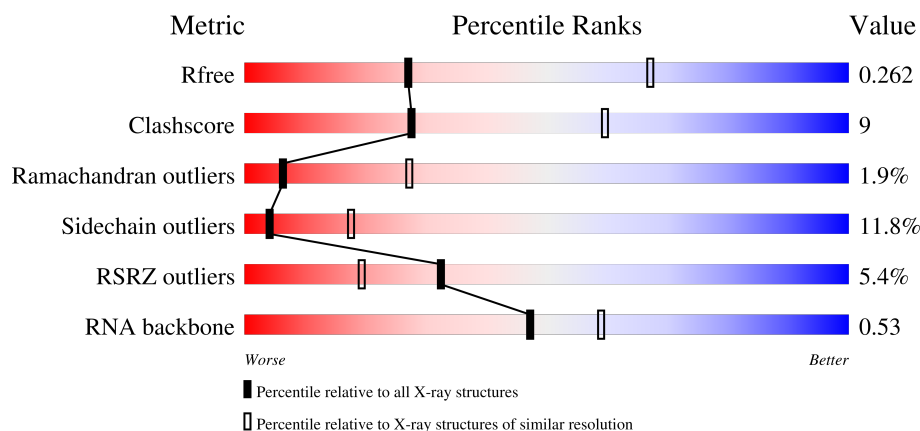
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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







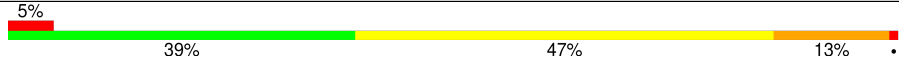
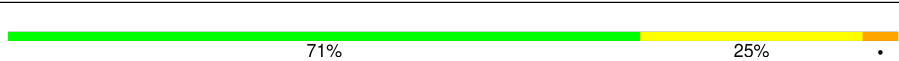
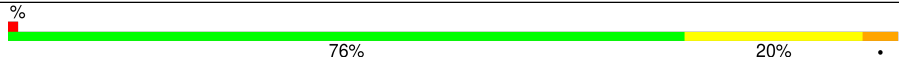
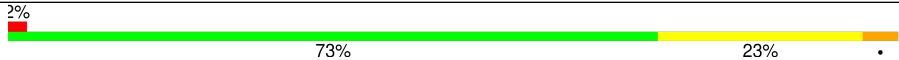
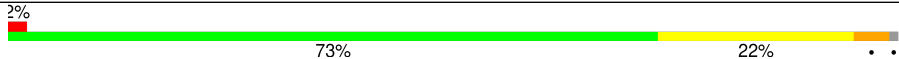
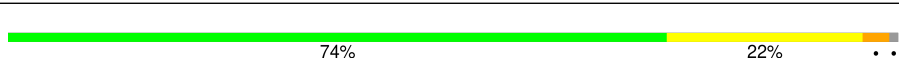
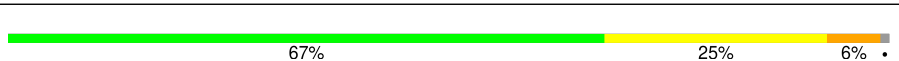
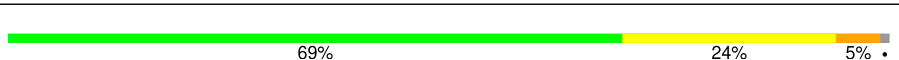


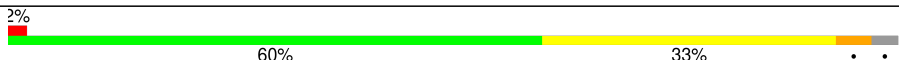
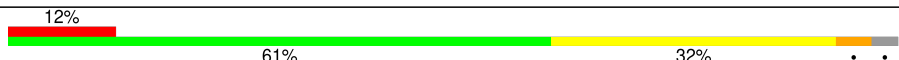


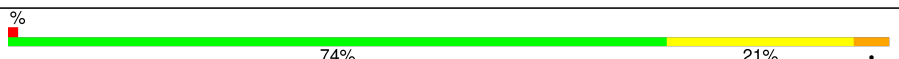

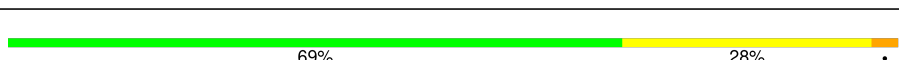
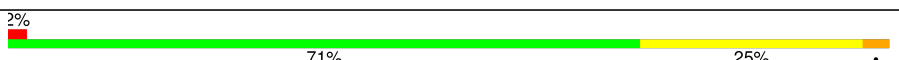
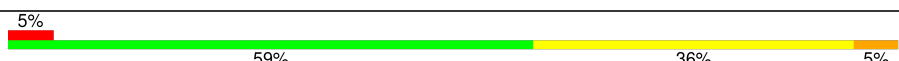
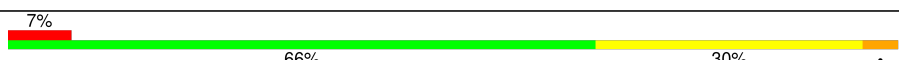
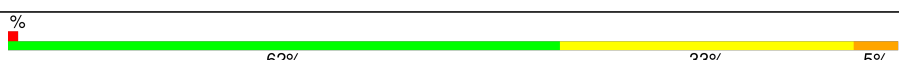
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)
RNA backbone	3690	1021 (3.36-2.84)

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	<div> <div>3%</div> <div>59% 35% 6%</div> </div>
1	FB	1507	<div> <div>3%</div> <div>60% 34% 6%</div> </div>
2	B	2880	<div> <div>2%</div> <div>60% 31% 8%</div> </div>
2	GB	2880	<div> <div>3%</div> <div>62% 30% 7%</div> </div>

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

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

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Mol	Chain	Length	Quality of chain
27	AA	60	
27	FC	60	
28	BA	71	
28	GC	71	
29	CA	60	
29	HC	60	
30	DA	54	
30	IC	54	
31	EA	49	
31	JC	49	
32	FA	65	
32	KC	65	
33	GA	37	
33	LC	37	
34	HA	27	
34	MC	27	
35	JA	368	
35	OC	368	
36	KA	256	
36	PC	256	
37	LA	239	
37	QC	239	
38	MA	209	
38	RC	209	
39	NA	162	

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Mol	Chain	Length	Quality of chain
39	SC	162	
40	OA	101	
40	TC	101	
41	PA	156	
41	UC	156	
42	QA	138	
42	VC	138	
43	RA	128	
43	WC	128	
44	SA	105	
44	XC	105	
45	TA	129	
45	YC	129	
46	UA	132	
46	ZC	132	
47	AD	126	
47	VA	126	
48	BD	61	
48	WA	61	
49	CD	89	
49	XA	89	
50	DD	88	
50	YA	88	
51	ED	105	
51	ZA	105	

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Mol	Chain	Length	Quality of chain
52	AB	88	
52	FD	88	
53	BB	93	
53	GD	93	
54	CB	106	
54	HD	106	
55	DB	27	
55	ID	27	

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	1610	-	-	-	X
56	MG	A	1615	-	-	-	X
56	MG	A	1621	-	-	-	X
56	MG	A	1630	-	-	-	X
56	MG	A	1631	-	-	-	X
56	MG	A	1666	-	-	-	X
56	MG	A	1669	-	-	-	X
56	MG	A	1672	-	-	-	X
56	MG	A	1709	-	-	-	X
56	MG	A	1792	-	-	-	X
56	MG	A	1799	-	-	-	X
56	MG	A	1804	-	-	-	X
56	MG	A	1809	-	-	-	X
56	MG	A	1833	-	-	-	X
56	MG	A	1845	-	-	-	X
56	MG	A	1874	-	-	-	X
56	MG	A	1878	-	-	-	X
56	MG	B	2942	-	-	-	X
56	MG	B	3782	-	-	-	X
56	MG	B	3826	-	-	-	X
56	MG	B	3834	-	-	-	X
56	MG	FB	1615	-	-	-	X
56	MG	FB	1631	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	FB	1633	-	-	-	X
56	MG	FB	1636	-	-	-	X
56	MG	FB	1642	-	-	-	X
56	MG	FB	1686	-	-	-	X
56	MG	FB	1704	-	-	-	X
56	MG	FB	1758	-	-	-	X
56	MG	FB	1766	-	-	-	X
56	MG	FB	1862	-	-	-	X
56	MG	FB	1911	-	-	-	X
56	MG	FB	1917	-	-	-	X
56	MG	FB	1939	-	-	-	X
56	MG	GB	2907	-	-	-	X
56	MG	GB	2921	-	-	-	X
56	MG	GB	2932	-	-	-	X
56	MG	GB	2947	-	-	-	X
56	MG	GB	2951	-	-	-	X
56	MG	GB	2971	-	-	-	X
56	MG	GB	3001	-	-	-	X
56	MG	GB	3016	-	-	-	X
56	MG	GB	3022	-	-	-	X
56	MG	GB	3025	-	-	-	X
56	MG	GB	3117	-	-	-	X
56	MG	GB	3188	-	-	-	X
56	MG	GB	3293	-	-	-	X
56	MG	GB	3376	-	-	-	X
56	MG	GD	101	-	-	-	X
56	MG	HB	207	-	-	-	X
56	MG	HB	221	-	-	-	X
56	MG	MB	203	-	-	-	X
56	MG	RA	202	-	-	-	X
56	MG	RA	203	-	-	-	X
56	MG	SA	201	-	-	-	X
56	MG	WA	101	-	-	-	X

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 300991 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	FB	1507	Total	C	N	O	P	0	0	0
			32394	14424	5998	10465	1507			

- Molecule 2 is a RNA chain called 25S 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	GB	2880	Total	C	N	O	P	0	0	0
			62031	27612	11589	19950	2880			

- 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	HB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			

- Molecule 4 is a RNA chain called tRNA.

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			
4	IA	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			
4	IB	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			
4	NC	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	JB	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	KB	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	LB	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	MB	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	NB	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	OB	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	PB	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	QB	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	RB	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			
14	SB	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	TB	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		0	0	0
			877	553	175	149				
16	UB	110	Total	C	N	O		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	VB	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	WB	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	XB	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	YB	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	ZB	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	AC	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	BC	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	CC	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- 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	DC	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	EC	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	FC	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	GC	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	HC	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	IC	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	JC	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	KC	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	LC	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	MC	11	Total	C	N	O	P	0	0	0
			220	98	44	67	11			

- Molecule 35 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	JA	258	Total	C	N	O	S	0	0	0
			2005	1227	380	390	8			
35	OC	258	Total	C	N	O	S	0	0	0
			2005	1227	380	390	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
JA	361	LEU	-	expression tag	UNP P0A7I0
JA	362	GLU	-	expression tag	UNP P0A7I0
JA	363	HIS	-	expression tag	UNP P0A7I0
JA	364	HIS	-	expression tag	UNP P0A7I0

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Chain	Residue	Modelled	Actual	Comment	Reference
JA	365	HIS	-	expression tag	UNP P0A7I0
JA	366	HIS	-	expression tag	UNP P0A7I0
JA	367	HIS	-	expression tag	UNP P0A7I0
JA	368	HIS	-	expression tag	UNP P0A7I0
OC	361	LEU	-	expression tag	UNP P0A7I0
OC	362	GLU	-	expression tag	UNP P0A7I0
OC	363	HIS	-	expression tag	UNP P0A7I0
OC	364	HIS	-	expression tag	UNP P0A7I0
OC	365	HIS	-	expression tag	UNP P0A7I0
OC	366	HIS	-	expression tag	UNP P0A7I0
OC	367	HIS	-	expression tag	UNP P0A7I0
OC	368	HIS	-	expression tag	UNP P0A7I0

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	KA	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			
36	PC	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	LA	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
37	QC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	MA	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
38	RC	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	NA	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	SC	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	OA	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
40	TC	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	PA	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
41	UC	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	QA	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
42	VC	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	RA	127	Total	C	N	O	0	0	0
			1011	639	198	174			
43	WC	127	Total	C	N	O	0	0	0
			1011	639	198	174			

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	SA	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			
44	XC	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	TA	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			
45	YC	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	UA	122	Total	C	N	O	S	0	0	0
			958	604	193	159	2			
46	ZC	122	Total	C	N	O	S	0	0	0
			958	604	193	159	2			

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	VA	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			
47	AD	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

- Molecule 48 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	WA	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
48	BD	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	XA	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
49	CD	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	YA	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
50	DD	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	ZA	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			
51	ED	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	AB	70	Total	C	N	O	0	0	0
			574	367	112	95			
52	FD	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BB	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
53	GD	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	CB	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
54	HD	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 55 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	DB	24	Total	C	N	O	0	0	0
			208	128	50	30			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	ID	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	A	287	Total	Mg	0	0
			287	287		
56	B	944	Total	Mg	0	0
			944	944		
56	C	44	Total	Mg	0	0
			44	44		
56	D	2	Total	Mg	0	0
			2	2		
56	E	10	Total	Mg	0	0
			10	10		
56	F	15	Total	Mg	0	0
			15	15		
56	G	11	Total	Mg	0	0
			11	11		
56	H	3	Total	Mg	0	0
			3	3		
56	I	7	Total	Mg	0	0
			7	7		
56	J	3	Total	Mg	0	0
			3	3		
56	K	9	Total	Mg	0	0
			9	9		
56	L	5	Total	Mg	0	0
			5	5		
56	M	8	Total	Mg	0	0
			8	8		
56	N	6	Total	Mg	0	0
			6	6		
56	O	3	Total	Mg	0	0
			3	3		
56	P	4	Total	Mg	0	0
			4	4		
56	Q	4	Total	Mg	0	0
			4	4		
56	R	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	S	8	Total 8	Mg 8	0	0
56	T	5	Total 5	Mg 5	0	0
56	U	2	Total 2	Mg 2	0	0
56	W	8	Total 8	Mg 8	0	0
56	X	8	Total 8	Mg 8	0	0
56	Y	5	Total 5	Mg 5	0	0
56	Z	3	Total 3	Mg 3	0	0
56	AA	4	Total 4	Mg 4	0	0
56	BA	3	Total 3	Mg 3	0	0
56	CA	3	Total 3	Mg 3	0	0
56	DA	3	Total 3	Mg 3	0	0
56	EA	2	Total 2	Mg 2	0	0
56	FA	4	Total 4	Mg 4	0	0
56	GA	1	Total 1	Mg 1	0	0
56	HA	2	Total 2	Mg 2	0	0
56	IA	21	Total 21	Mg 21	0	0
56	JA	13	Total 13	Mg 13	0	0
56	KA	4	Total 4	Mg 4	0	0
56	LA	2	Total 2	Mg 2	0	0
56	MA	5	Total 5	Mg 5	0	0
56	NA	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	OA	4	Total 4	Mg 4	0	0
56	PA	3	Total 3	Mg 3	0	0
56	QA	2	Total 2	Mg 2	0	0
56	RA	4	Total 4	Mg 4	0	0
56	SA	3	Total 3	Mg 3	0	0
56	TA	1	Total 1	Mg 1	0	0
56	UA	3	Total 3	Mg 3	0	0
56	VA	3	Total 3	Mg 3	0	0
56	WA	1	Total 1	Mg 1	0	0
56	XA	3	Total 3	Mg 3	0	0
56	YA	1	Total 1	Mg 1	0	0
56	ZA	3	Total 3	Mg 3	0	0
56	BB	1	Total 1	Mg 1	0	0
56	CB	1	Total 1	Mg 1	0	0
56	DB	1	Total 1	Mg 1	0	0
56	FB	349	Total 349	Mg 349	0	0
56	GB	812	Total 812	Mg 812	0	0
56	HB	32	Total 32	Mg 32	0	0
56	IB	5	Total 5	Mg 5	0	0
56	JB	13	Total 13	Mg 13	0	0
56	KB	4	Total 4	Mg 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	LB	5	Total 5	Mg 5	0	0
56	MB	7	Total 7	Mg 7	0	0
56	NB	3	Total 3	Mg 3	0	0
56	OB	2	Total 2	Mg 2	0	0
56	PB	4	Total 4	Mg 4	0	0
56	QB	6	Total 6	Mg 6	0	0
56	RB	6	Total 6	Mg 6	0	0
56	SB	4	Total 4	Mg 4	0	0
56	TB	4	Total 4	Mg 4	0	0
56	UB	1	Total 1	Mg 1	0	0
56	VB	8	Total 8	Mg 8	0	0
56	WB	3	Total 3	Mg 3	0	0
56	XB	4	Total 4	Mg 4	0	0
56	YB	7	Total 7	Mg 7	0	0
56	ZB	1	Total 1	Mg 1	0	0
56	BC	9	Total 9	Mg 9	0	0
56	CC	2	Total 2	Mg 2	0	0
56	DC	3	Total 3	Mg 3	0	0
56	EC	4	Total 4	Mg 4	0	0
56	FC	1	Total 1	Mg 1	0	0
56	GC	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	HC	2	Total 2	Mg 2	0	0
56	KC	5	Total 5	Mg 5	0	0
56	MC	1	Total 1	Mg 1	0	0
56	NC	14	Total 14	Mg 14	0	0
56	OC	7	Total 7	Mg 7	0	0
56	PC	5	Total 5	Mg 5	0	0
56	QC	4	Total 4	Mg 4	0	0
56	RC	11	Total 11	Mg 11	0	0
56	SC	7	Total 7	Mg 7	0	0
56	TC	1	Total 1	Mg 1	0	0
56	UC	2	Total 2	Mg 2	0	0
56	VC	2	Total 2	Mg 2	0	0
56	WC	2	Total 2	Mg 2	0	0
56	XC	2	Total 2	Mg 2	0	0
56	YC	6	Total 6	Mg 6	0	0
56	ZC	2	Total 2	Mg 2	0	0
56	AD	1	Total 1	Mg 1	0	0
56	CD	3	Total 3	Mg 3	0	0
56	DD	1	Total 1	Mg 1	0	0
56	ED	2	Total 2	Mg 2	0	0
56	GD	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	HD	1	Total	Mg	0	0
			1	1		

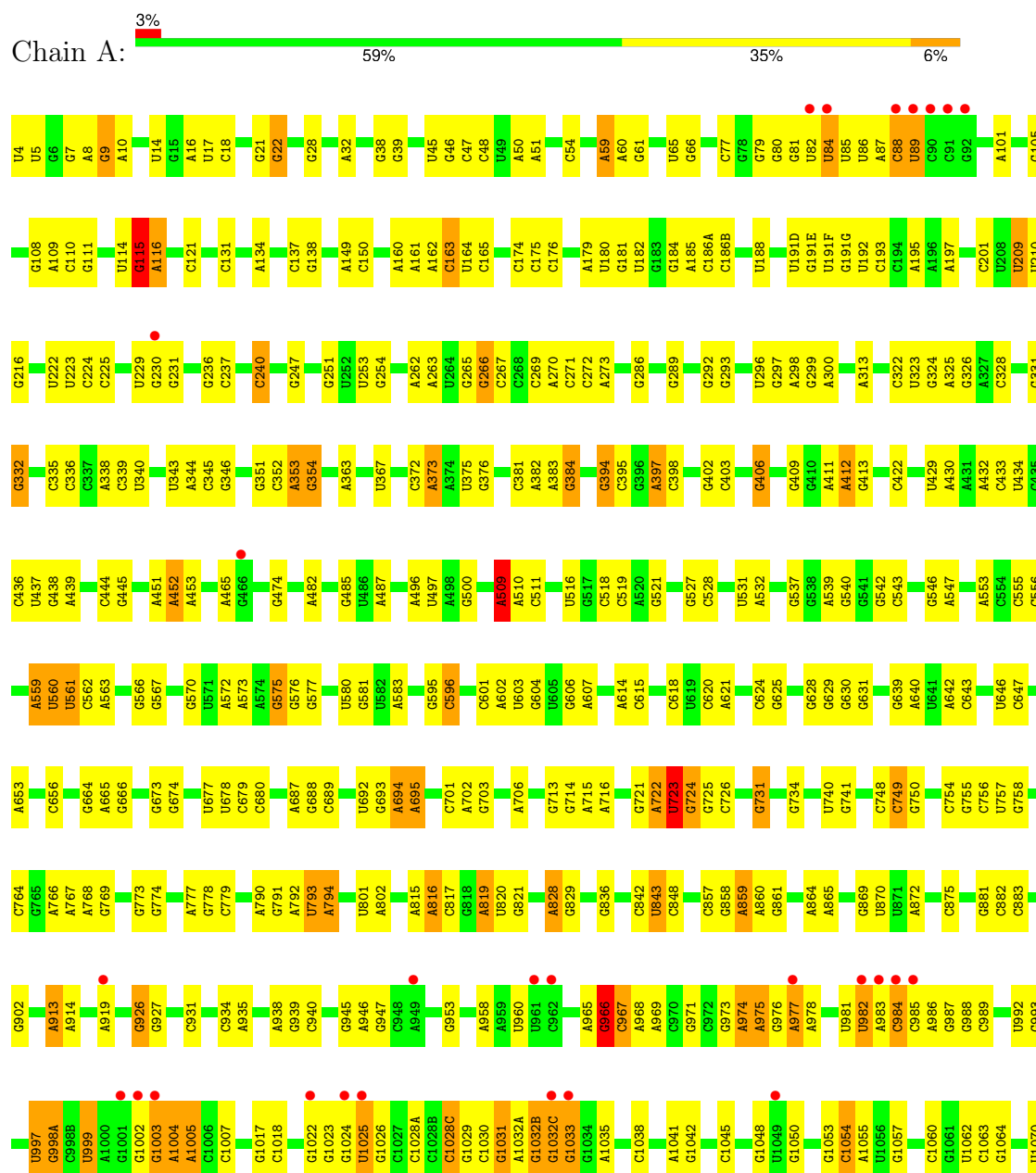
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

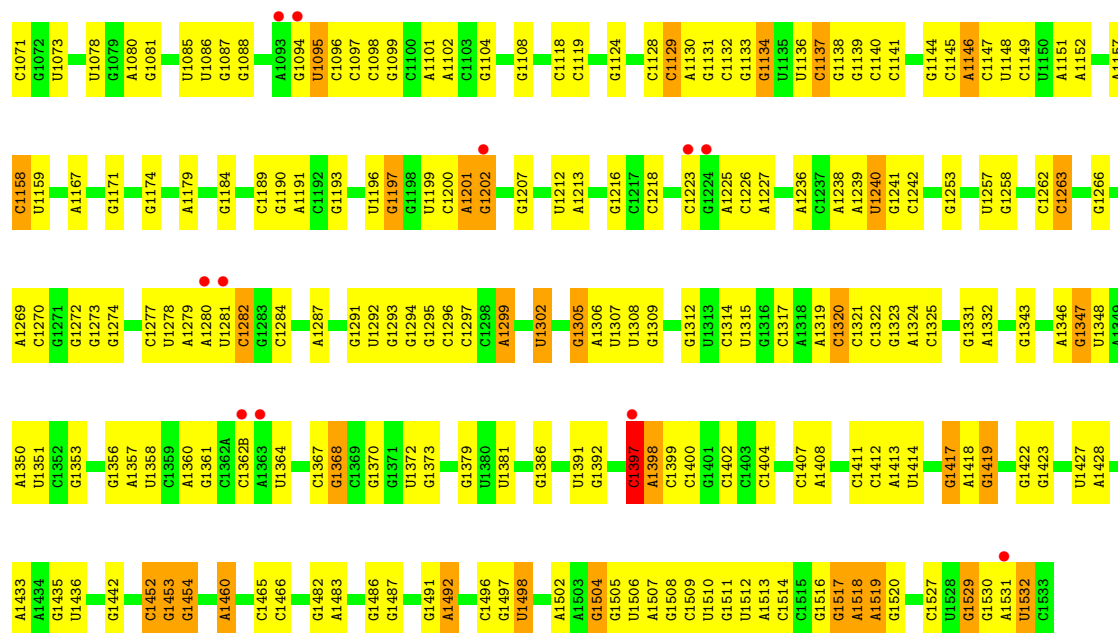
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	V	1	Total	Zn	0	0
			1	1		
57	BA	1	Total	Zn	0	0
			1	1		
57	CA	1	Total	Zn	0	0
			1	1		
57	DA	1	Total	Zn	0	0
			1	1		
57	GA	1	Total	Zn	0	0
			1	1		
57	AC	1	Total	Zn	0	0
			1	1		
57	GC	1	Total	Zn	0	0
			1	1		
57	HC	1	Total	Zn	0	0
			1	1		
57	IC	1	Total	Zn	0	0
			1	1		
57	LC	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

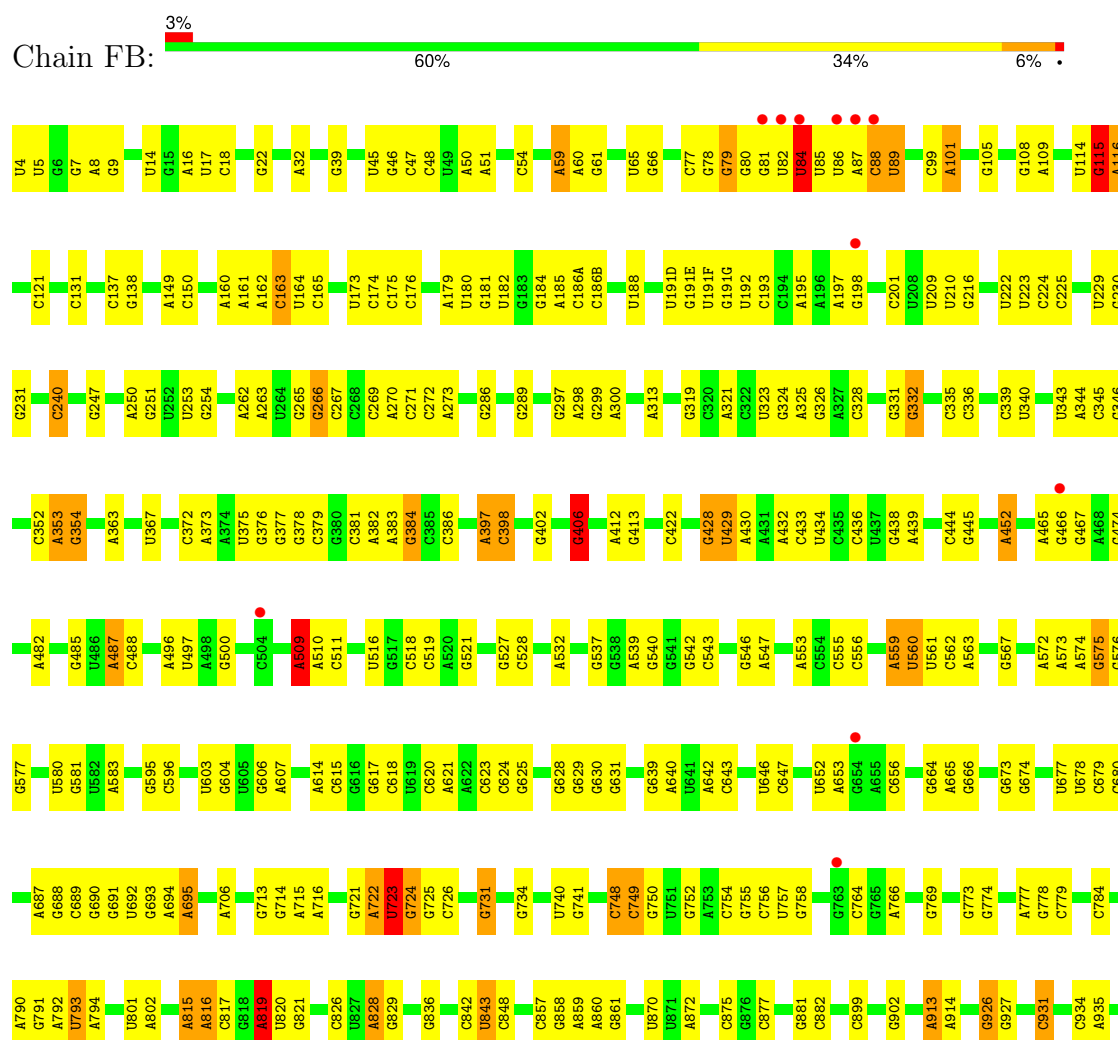
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

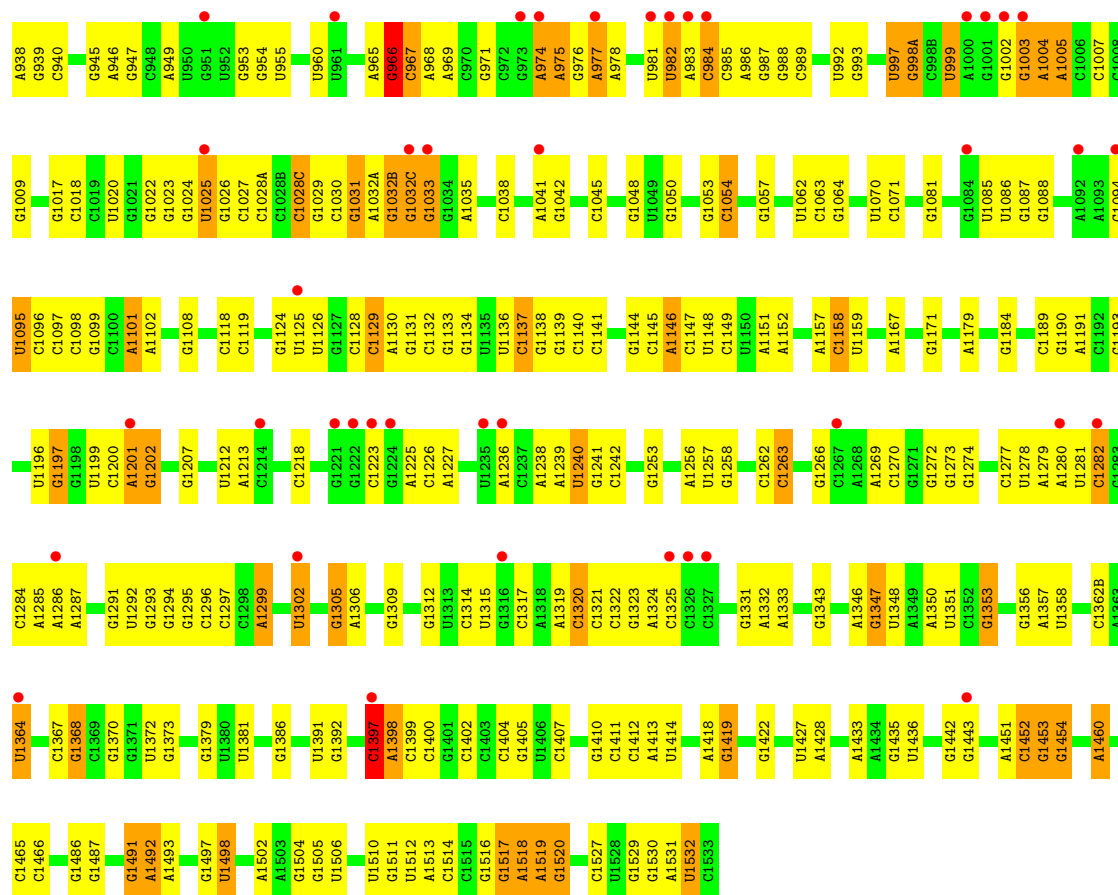
• Molecule 1: 16S ribosomal RNA



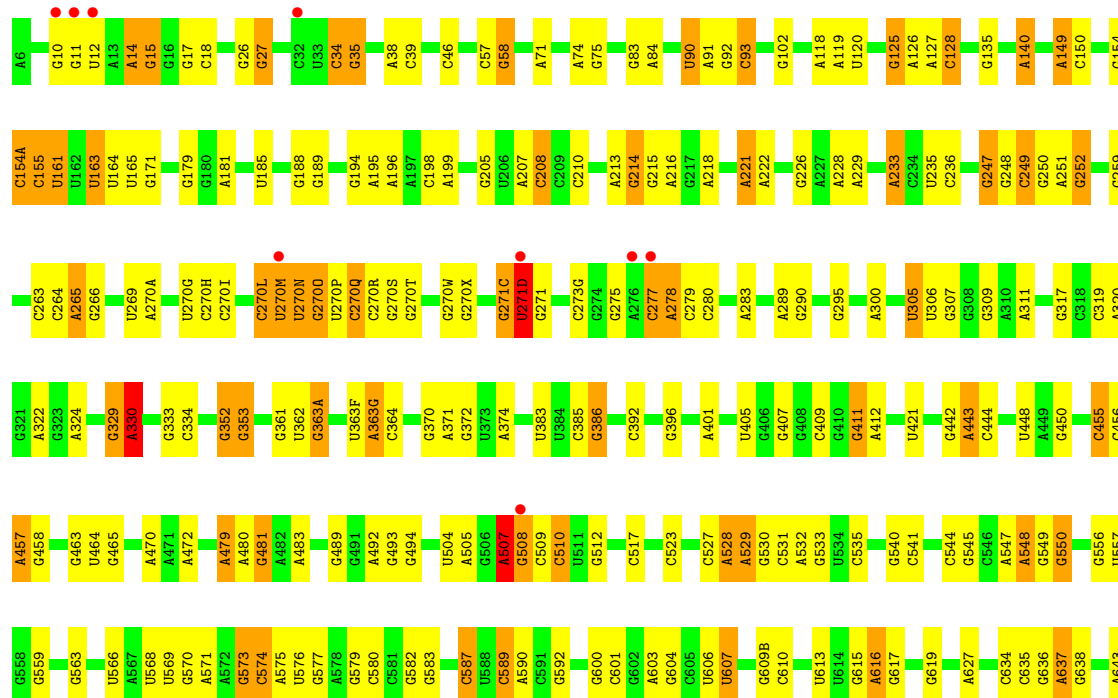


• Molecule 1: 16S ribosomal RNA

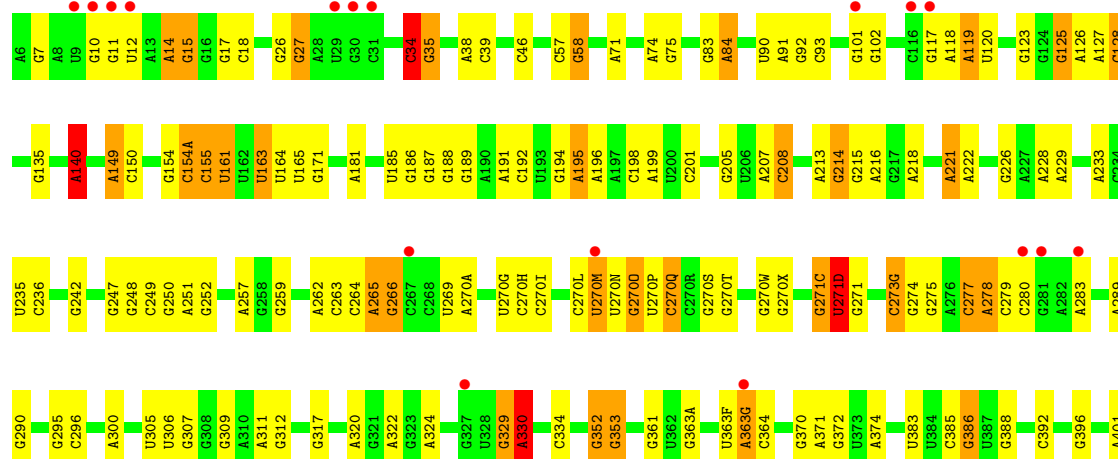




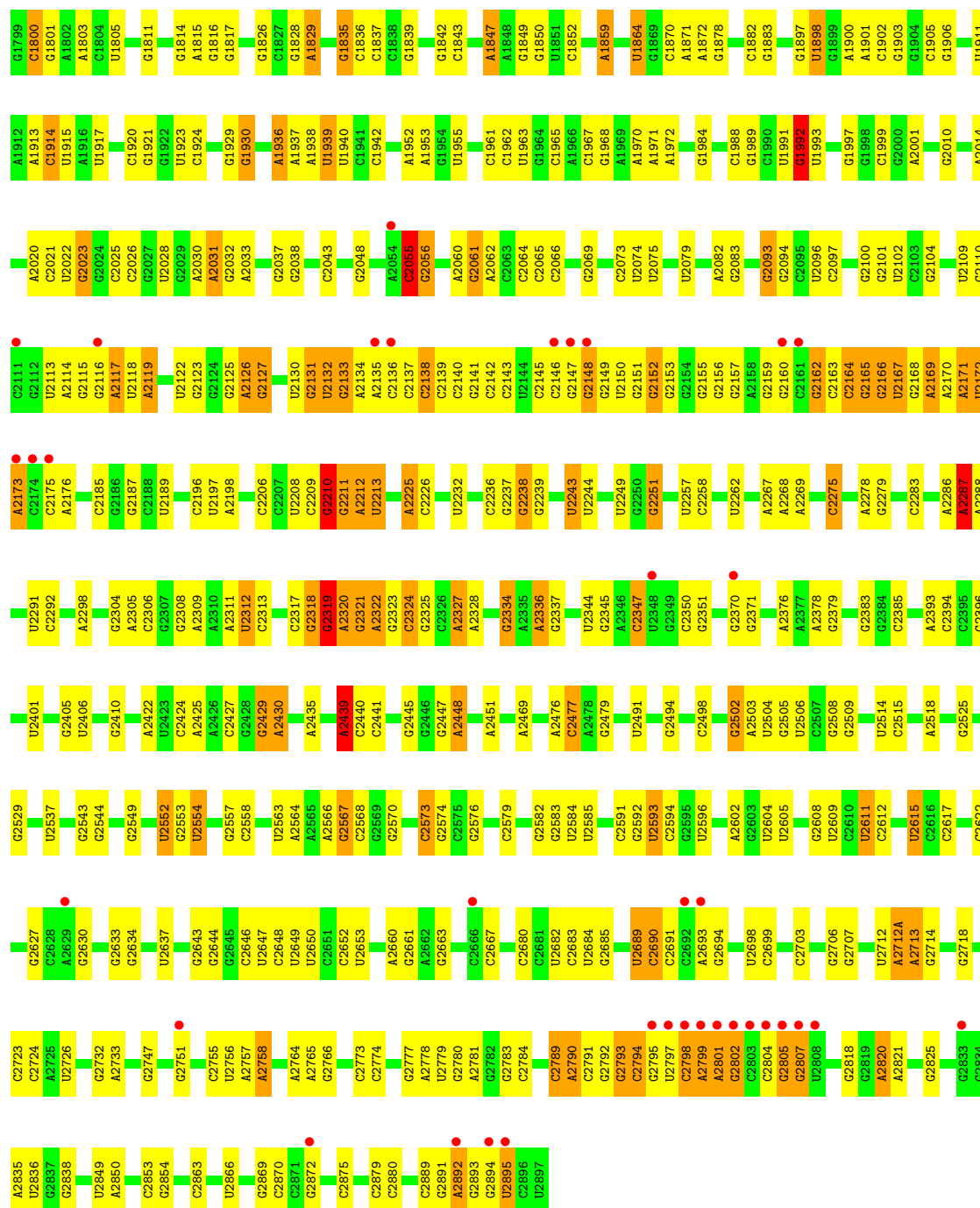
• Molecule 2: 25S ribosomal RNA



G1998	G1999	G2000	A2001	A2005	C2006	A2014	A2015	A2016	A2017	A2018	A2019	A2020	C2021	A2022	G2023	G2024	C2025	C2026	G2027	U2028	A2031	G2032	A2033	C2040	U2041	A2042	C2043	G2048	G2053	A2054	C2055	G2056	A2059	A2060	G2061	A2062	C2063	C2064	C2065	C2066	G2069	C2073	A2077	C2078	U2079	A2082	G2083	G2088	U2089	
G1903	G1904	C1905	G1906	U1911	A1912	A1913	C1914	U1915	A1916	U1917	A1918	A1919	C1920	G1921	G1922	U1923	C1924	G1929	G1930	G1935	A1936	A1937	A1938	U1939	U1940	C1941	C1942	G1948	A1952	A1953	G1954	U1955	C1962	U1963	G1964	C1965	A1966	C1967	G1968	A1969	A1970	A1971	A1972	G1984	C1988	G1989	G1992	U1993	G1997	
A1789	C1790	A1791	U1796	C1797	U1798	G1799	A1800	A1801	A1802	A1803	C1804	U1805	G1811	A1815	C1816	A1821	G1826	A1829	C1837	G1838	G1839	G1842	C1843	A1847	A1848	G1849	G1850	U1851	C1852	A1859	U1864	G1869	C1870	A1871	A1872	G1878	C1882	G1883	C1892	G1897	A1898	G1899	A1900	A1901	C1902					
G1666	G1667	A1668	C1669	U1671	G1674	G1682	C1686	C1687	U1688	A1689	U1692	U1693	C1694	A1698	G1699	A1700	A1701	U1709	C1710	G1728	A1729	U1730	G1731	A1732	G1743	C1754	C1761	A1762	G1763	G1764	C1771	G1772	A1773	G1776	U1777	U1778	U1779	C1781	C1782	A1783	A1784	U1785	A1786	A1787	C1788					
A1558	G1559	A1566	A1567	G1568	A1569	A1570	A1571	C1574	C1575	U1576	C1577	U1578	C1585	A1586	A1587	C1588	C1592	G1593	G1594	G1595	U1602	A1603	A1608	A1609	A1610	A1614	U1621	A1631	U1639	C1640	A1641	G1642	G1647	C1648	G1649	G1650	G1651	A1652	G1653	A1654	C1657	C1658	U1659	C1660	C1663					
G1459	A1460	G1461	G1466	C1467	A1471	A1472	G1478	G1483	A1490	G1491	C1492	A1494	A1495	A1496	U1497	A1508	A1509	A1510	A1511	G1512	C1513	U1516	C1517	G1518	G1519	U1520	G1521	G1522	G1530	C1531	C1532	C1533	G1534	U1535	A1536	C1537	G1538	G1539	G1540	U1541	G1542	A1543	C1544	C1547	C1550	C1551	C1557			
A1359	A1360	G1364	A1365	A1366	A1367	G1368	U1372	A1373	A1379	G1380	G1385	G1388	G1389	U1394	A1395	U1396	U1397	C1398	C1399	A1400	G1401	C1404	U1405	U1406	C1407	C1408	C1409	G1410	G1416	C1417	G1418	A1419	U1420	G1421	C1428	G1429	C1430	U1431	A1434	G1441	G1442	A1444B	G1448	A1449B	U1454					
A1241	G1245	G1246	G1252	A1253	G1256	C1257	C1258	C1261	A1262	U1263	G1264	G1266	G1271	U1272	C1289	C1290	C1291	U1292	C1293	C1297	C1298	C1299	U1300	A1301	G1309	U1313	A1317	C1318	G1332	C1333	A1336	G1339	U1340	U1341	C1345	G1346	G1347	U1357	G1358											
G1131	C1135	G1136	G1139	C1140	U1141	C1142	A1142B	A1143	G1153	G1154	A1155	U1165	C1166	G1170	G1171	G1173	A1174	U1175	A1176	A1177	C1178	C1179	C1180	G1184	C1185	G1186	G1187	G1190	C1201	C1202	G1203	A1204	U1205	A1210	U1211	G1212	A1213	A1214	G1215	G1216	C1217	G1218	A1220	G1235	G1236	G1238				
U1061	G1062	C1063	U1065	U1066	A1067	G1068	A1069	G1071	C1072	A1073	G1074	C1075	C1076	C1077	A1078	C1079	C1080	A1084	A1085	A1086	G1087	A1088	G1089	U1090	G1091	C1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	G1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	G1122	A1126	C1129	A1130
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A777	A782	A783	A784	G785	A788	A789	C790	C791	G792	C796	C797	A800	U803	A804	A805	G806	G807	U811	C812	C813	U814	A816	G717	C825	U826	U827	A829	G830	C831	U832	U833	U847	G848	A849	C855	C856	G857	U858	C859	U860	A861	A862	A863	G864	C865	G771	A774	G775	U871	
A644	C645	A646	G647	G648	U654	A655	G656	U657	C658	C664	C671	C672	C673	G674	C678	G682	G686	G700	G715	A716	G717	G725	G726	C730	G733	G742	G743	U747	A751	C758	G759	G760	A761	A764	G765	G768	G769	G771	A774	G775	G776									



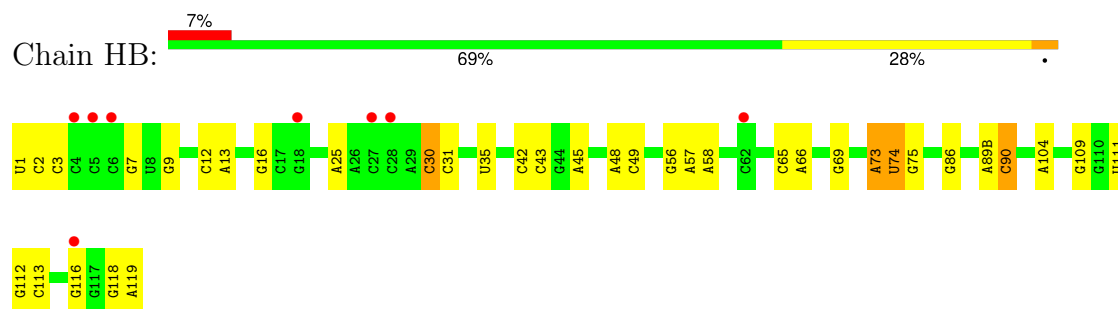




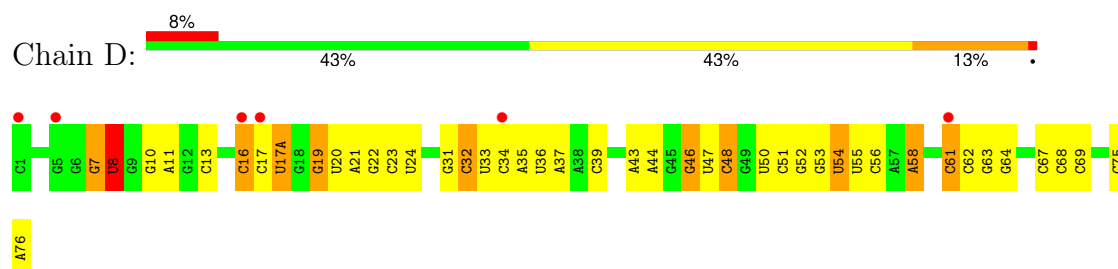
• Molecule 3: 5S ribosomal RNA



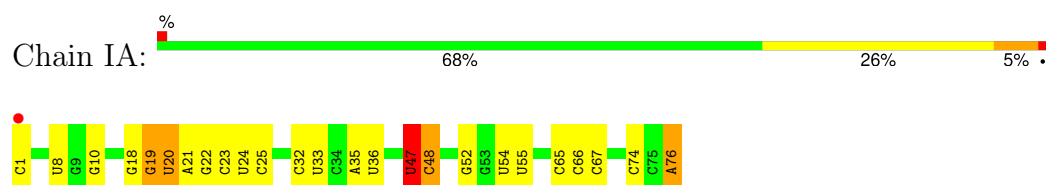
- Molecule 3: 5S ribosomal RNA



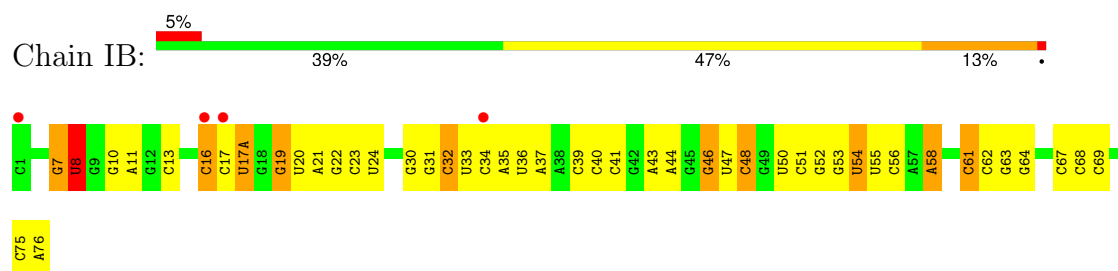
- Molecule 4: tRNA



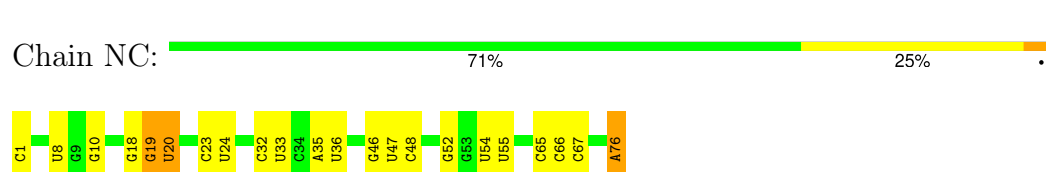
- Molecule 4: tRNA



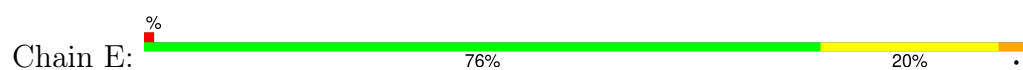
- Molecule 4: tRNA

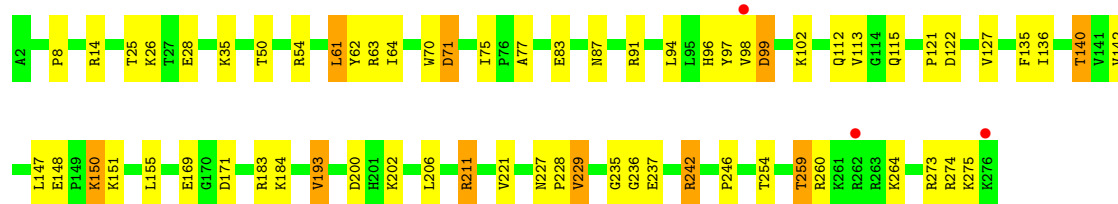


- Molecule 4: tRNA

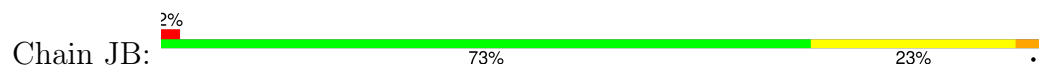


- Molecule 5: 50S ribosomal protein L2

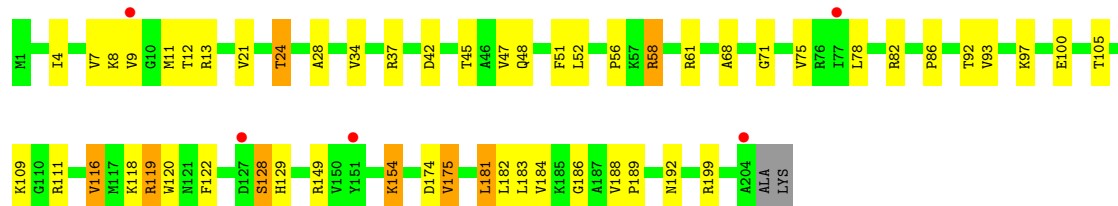




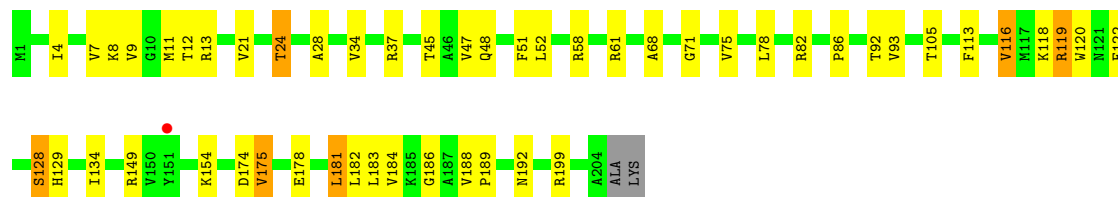
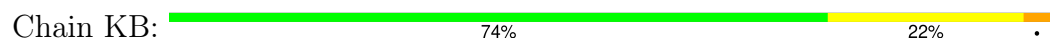
• Molecule 5: 50S ribosomal protein L2



• Molecule 6: 50S ribosomal protein L3

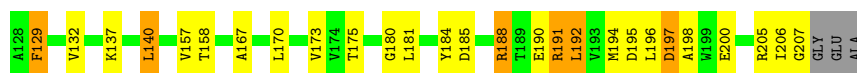


• Molecule 6: 50S ribosomal protein L3



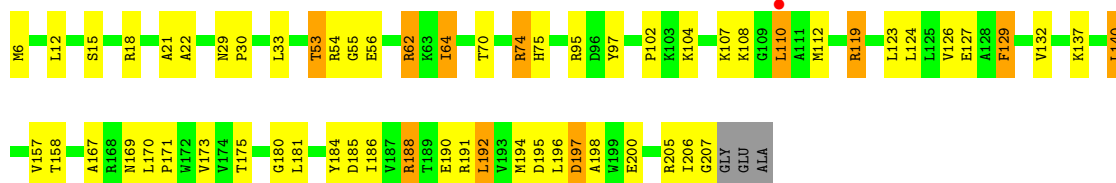
• Molecule 7: 50S ribosomal protein L4





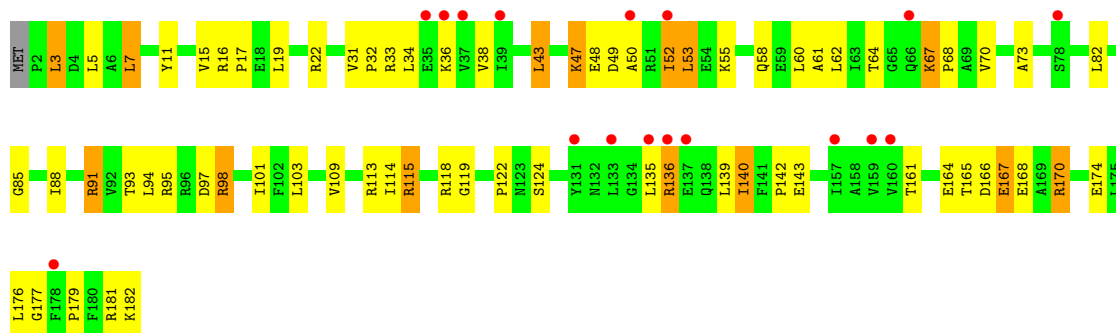
• Molecule 7: 50S ribosomal protein L4

Chain LB: 69% 24% 5% .



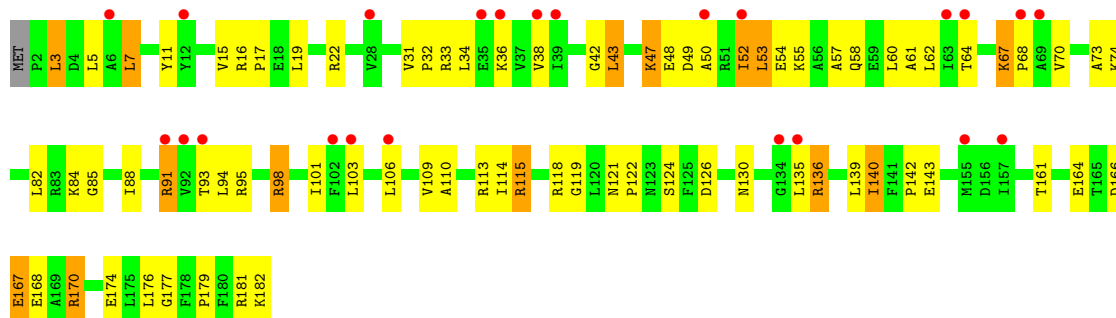
• Molecule 8: 50S ribosomal protein L5

Chain H: 9% 61% 31% 8% .



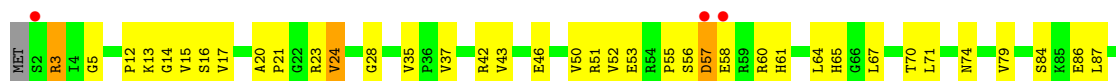
• Molecule 8: 50S ribosomal protein L5

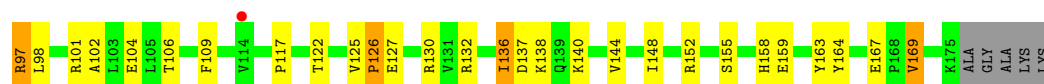
Chain MB: 13% 57% 35% 8% .



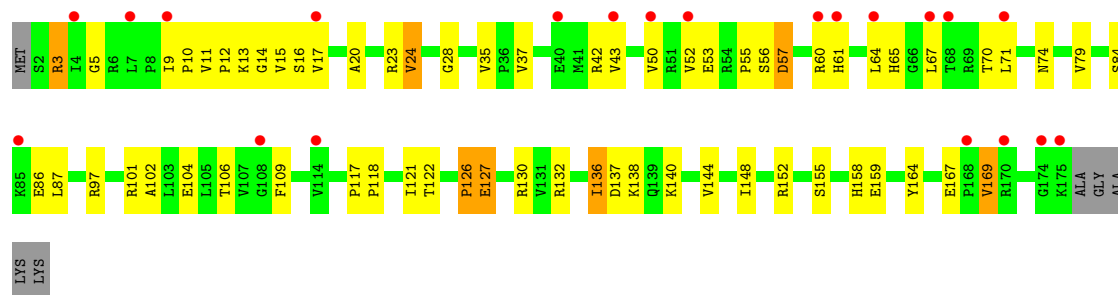
• Molecule 9: 50S ribosomal protein L6

Chain I: 2% 60% 33% . .

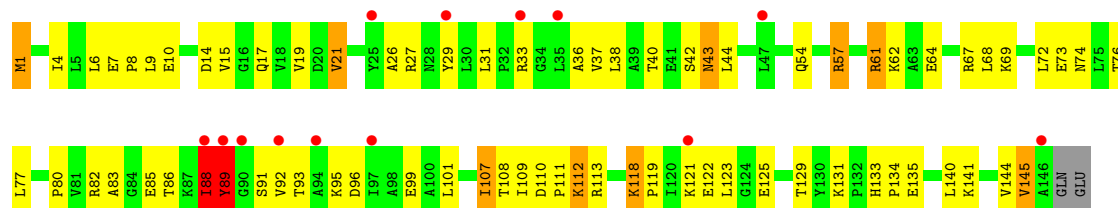




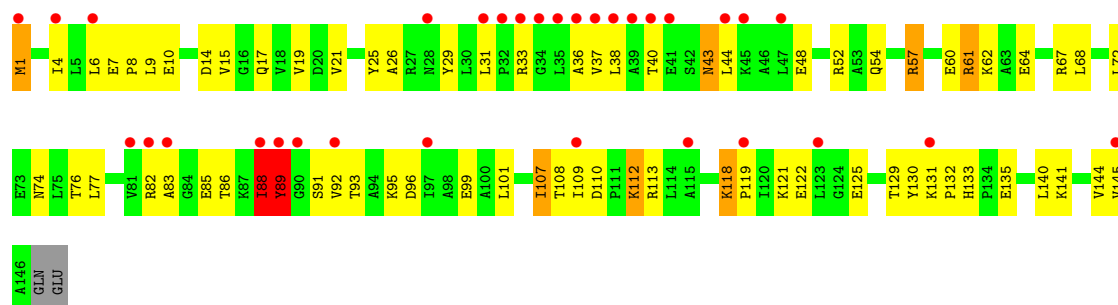
• Molecule 9: 50S ribosomal protein L6



• Molecule 10: 50S ribosomal protein L9



• Molecule 10: 50S ribosomal protein L9

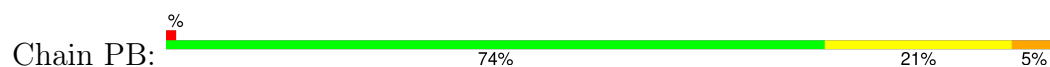


• Molecule 11: 50S ribosomal protein L13





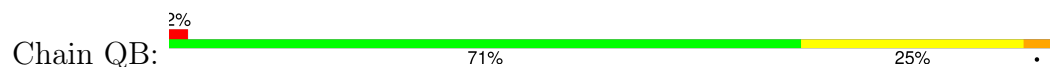
- Molecule 11: 50S ribosomal protein L13



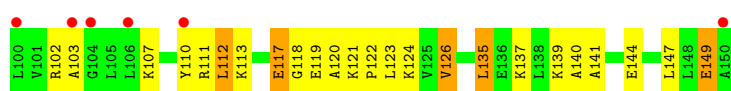
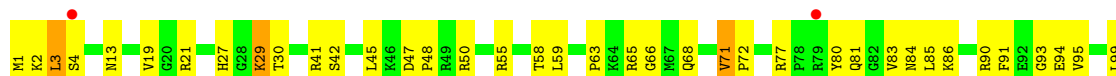
- Molecule 12: 50S ribosomal protein L14



- Molecule 12: 50S ribosomal protein L14

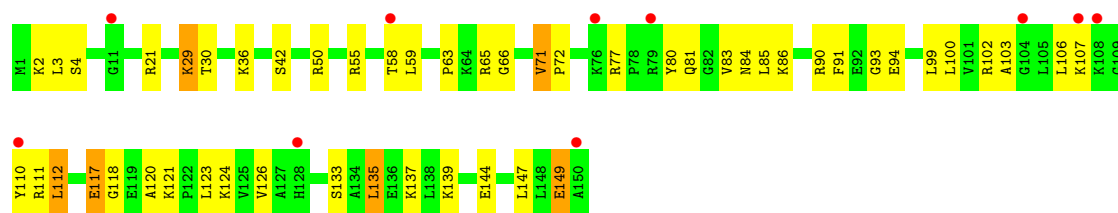


- Molecule 13: 50S ribosomal protein L15

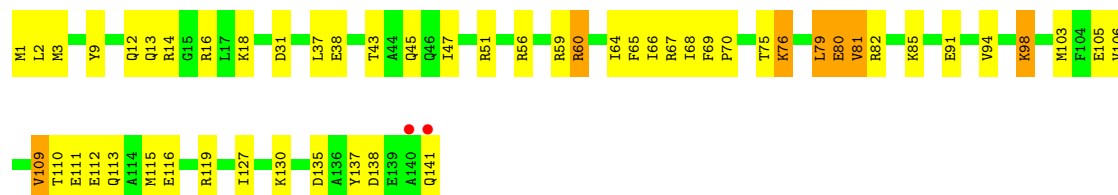


- Molecule 13: 50S ribosomal protein L15

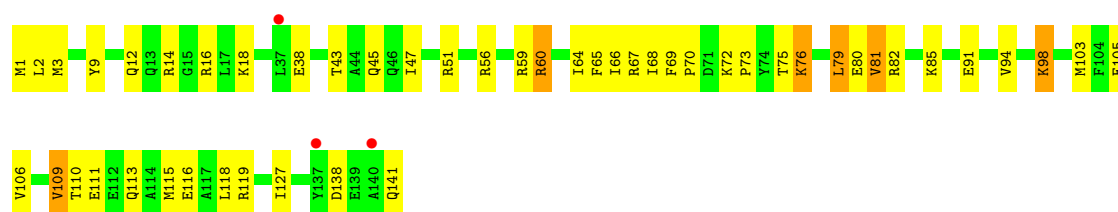




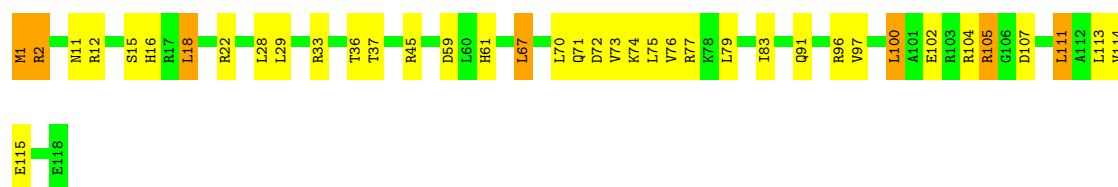
• Molecule 14: 50S ribosomal protein L16



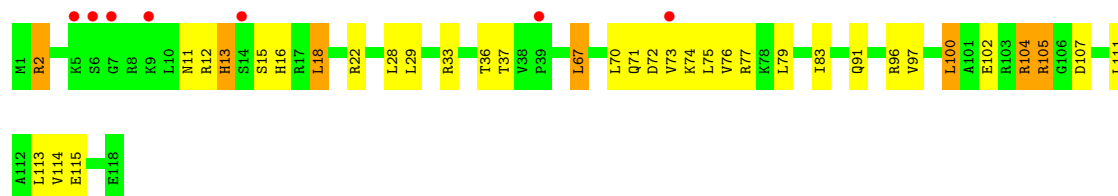
• Molecule 14: 50S ribosomal protein L16



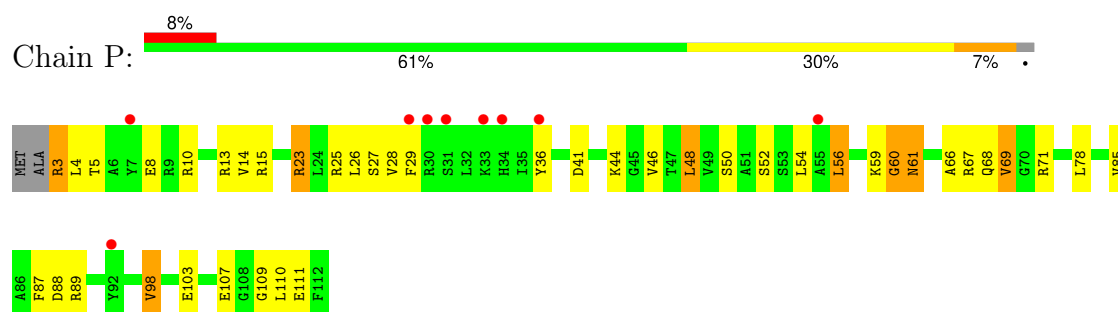
• Molecule 15: 50S ribosomal protein L17



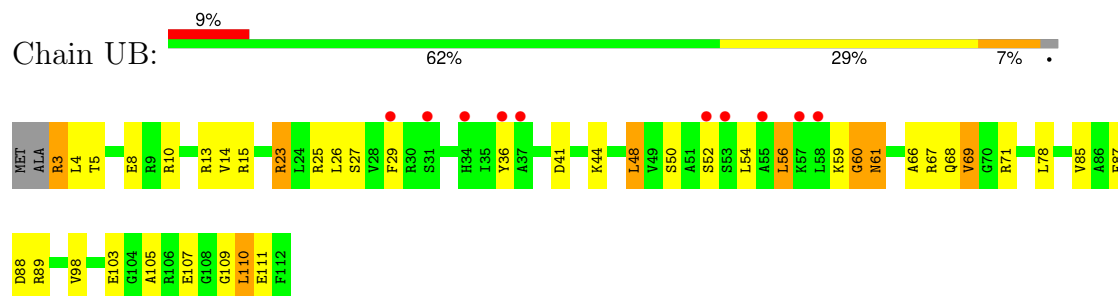
• Molecule 15: 50S ribosomal protein L17



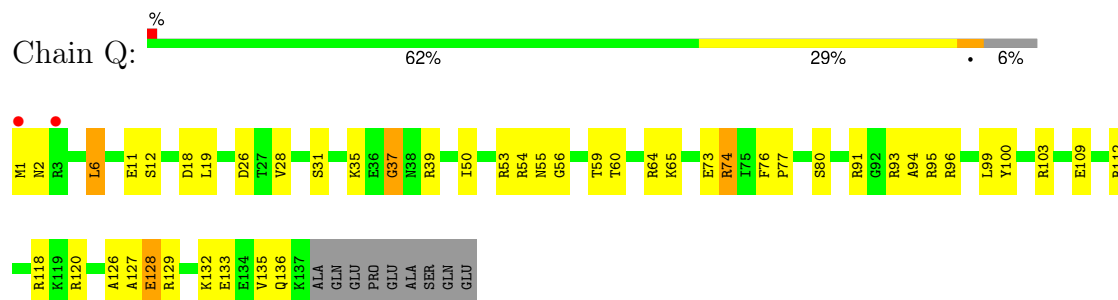
• Molecule 16: 50S ribosomal protein L18



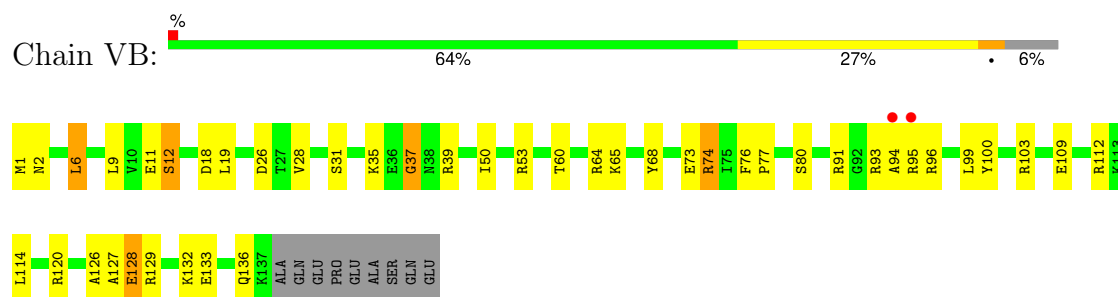
- Molecule 16: 50S ribosomal protein L18



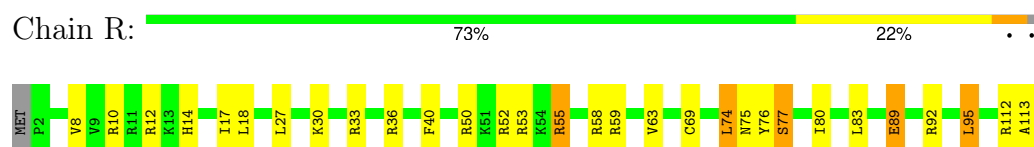
- Molecule 17: 50S ribosomal protein L19



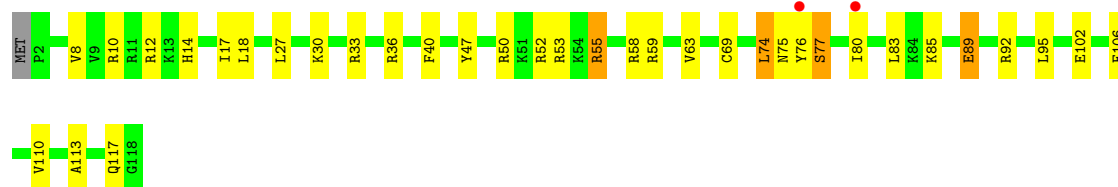
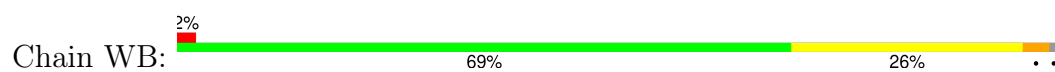
- Molecule 17: 50S ribosomal protein L19



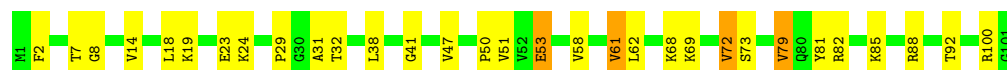
- Molecule 18: 50S ribosomal protein L20



- Molecule 18: 50S ribosomal protein L20



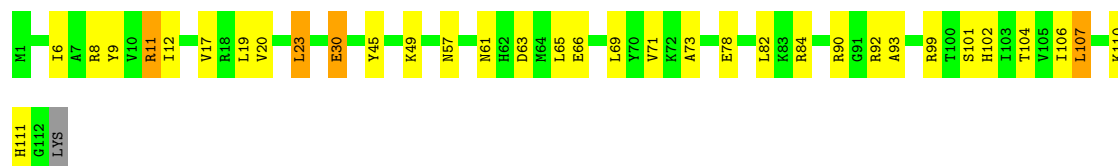
- Molecule 19: 50S ribosomal protein L21



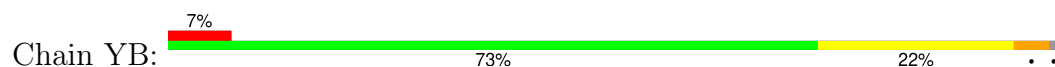
- Molecule 19: 50S ribosomal protein L21



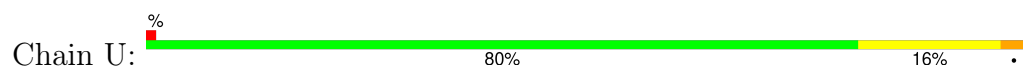
- Molecule 20: 50S ribosomal protein L22

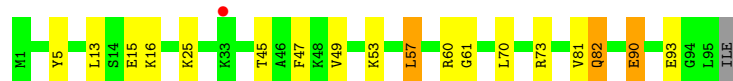


- Molecule 20: 50S ribosomal protein L22

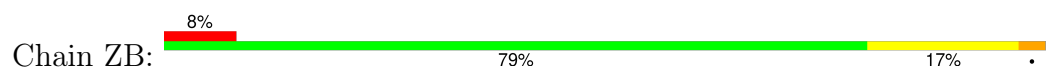


- Molecule 21: 50S ribosomal protein L23

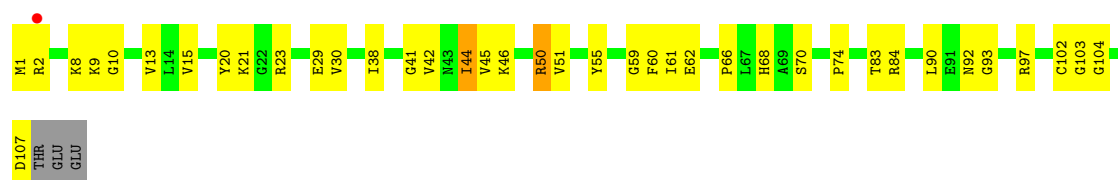




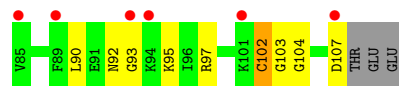
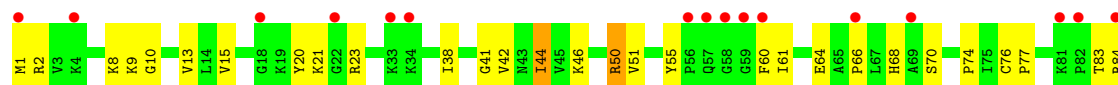
- Molecule 21: 50S ribosomal protein L23



- Molecule 22: 50S ribosomal protein L24



- Molecule 22: 50S ribosomal protein L24

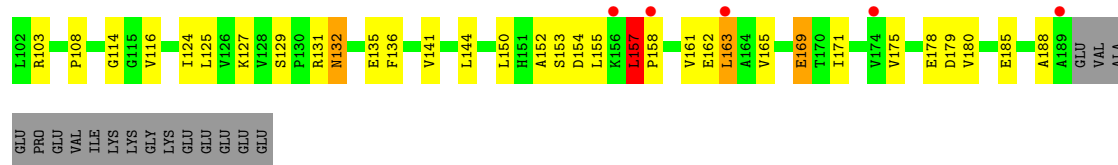


- Molecule 23: 50S ribosomal protein L25

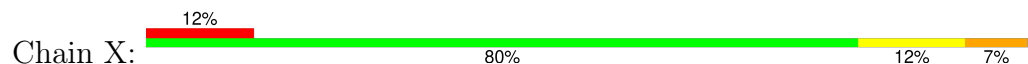


- Molecule 23: 50S ribosomal protein L25

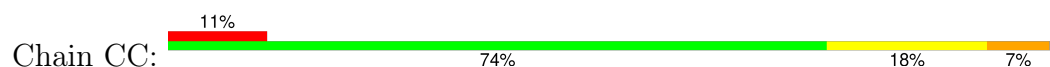




- Molecule 24: 50S ribosomal protein L27



- 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

Chain AA:  70% 25% 5%



- Molecule 27: 50S ribosomal protein L30

Chain FC:  70% 25% 5%



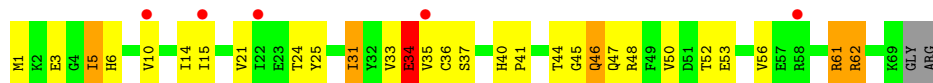
- Molecule 28: 50S ribosomal protein L31

Chain BA:  3% 55% 34% 7% . .




- Molecule 28: 50S ribosomal protein L31

Chain GC:  7% 56% 32% 7% . .




- Molecule 29: 50S ribosomal protein L32

Chain CA:  78% 20% .



- Molecule 29: 50S ribosomal protein L32

Chain HC:  2% 77% 22% .

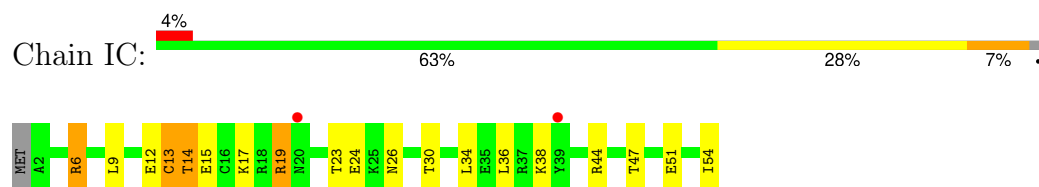


- Molecule 30: 50S ribosomal protein L33

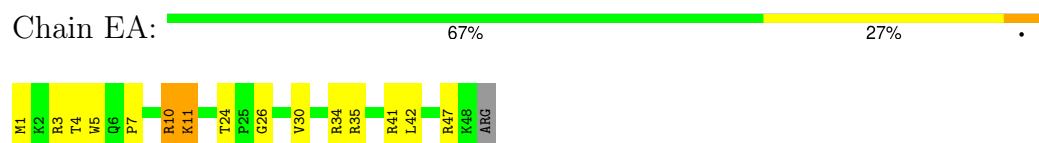
Chain DA:  61% 31% 6% .



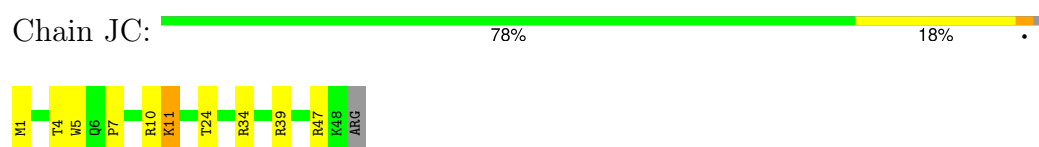
- Molecule 30: 50S ribosomal protein L33



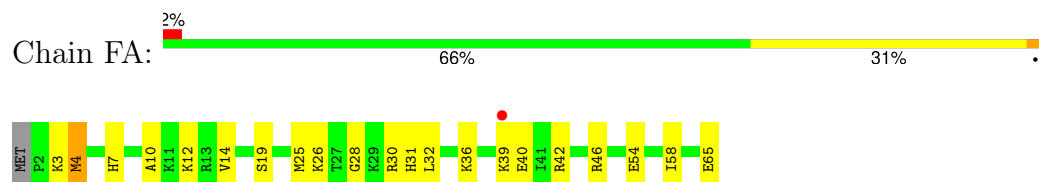
- Molecule 31: 50S ribosomal protein L34



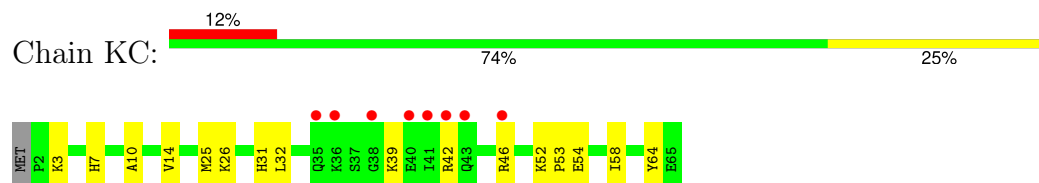
- Molecule 31: 50S ribosomal protein L34



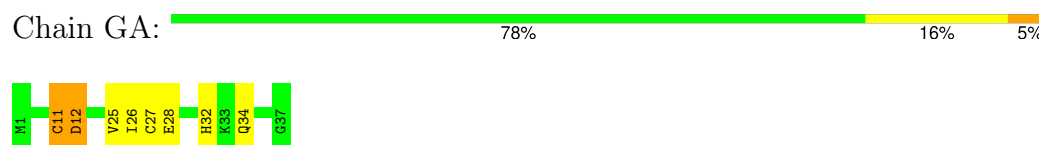
- Molecule 32: 50S ribosomal protein L35



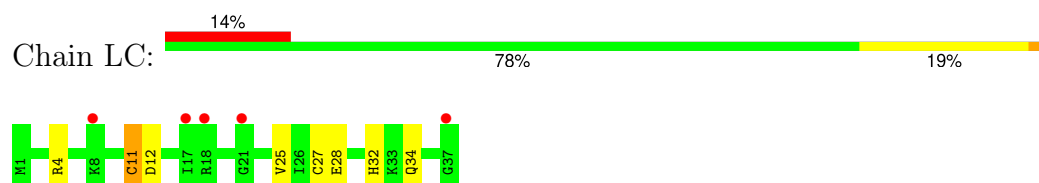
- Molecule 32: 50S ribosomal protein L35



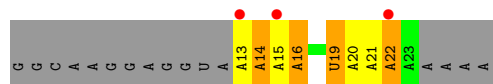
- Molecule 33: 50S ribosomal protein L36



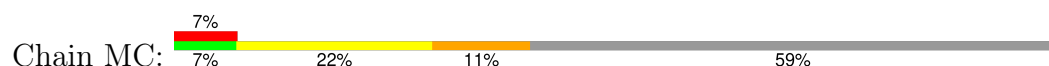
- Molecule 33: 50S ribosomal protein L36



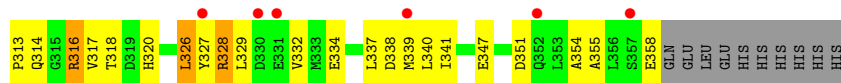
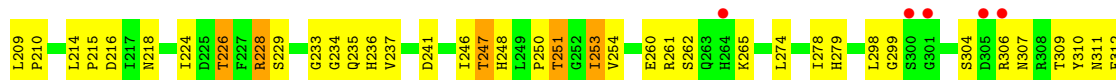
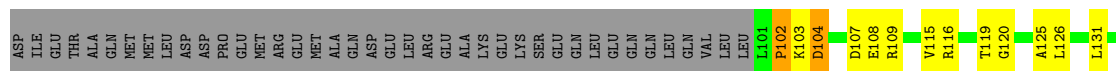
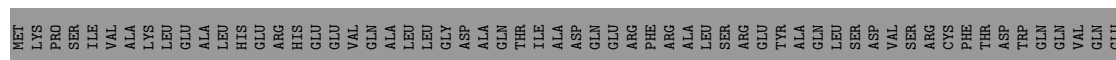
- Molecule 34: mRNA



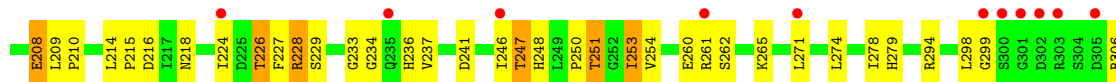
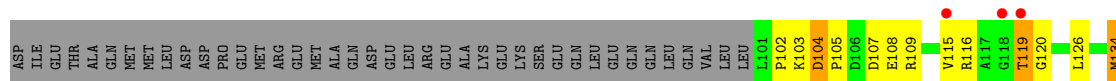
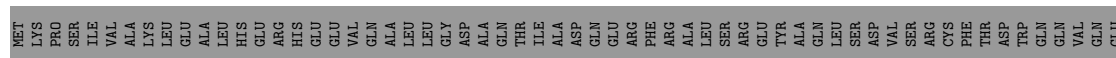
- Molecule 34: mRNA

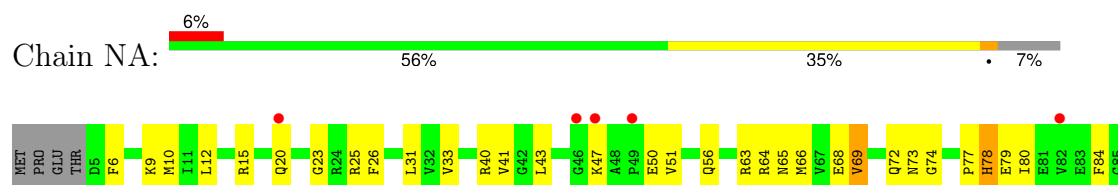


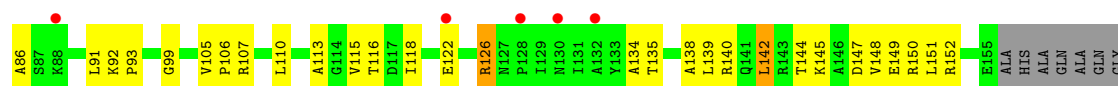
- Molecule 35: Peptide chain release factor 1



- Molecule 35: Peptide chain release factor 1







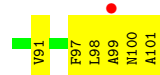
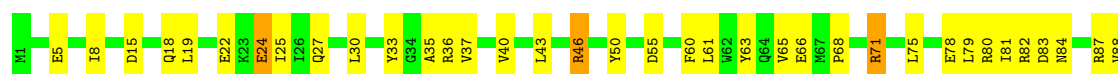
- Molecule 39: 30S ribosomal protein S5



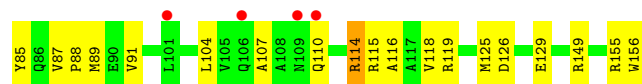
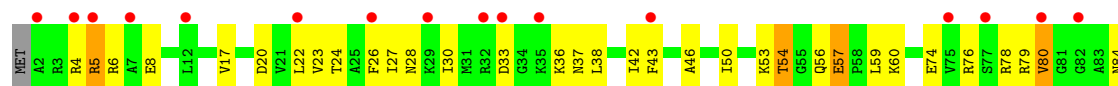
- Molecule 40: 30S ribosomal protein S6



- Molecule 40: 30S ribosomal protein S6



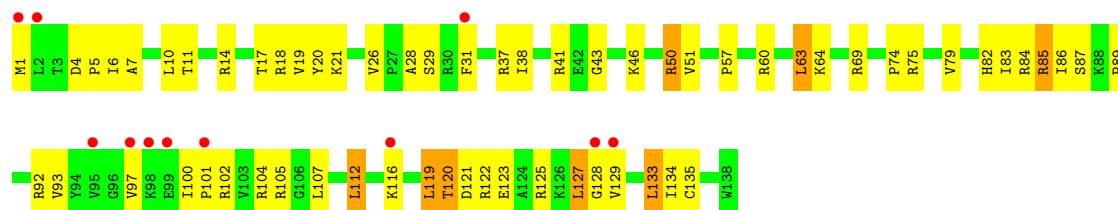
- Molecule 41: 30S ribosomal protein S7



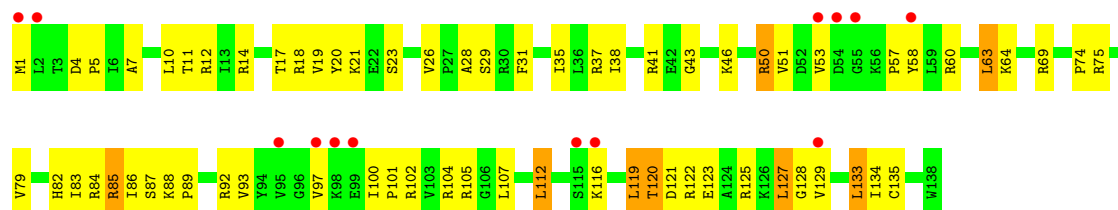
- Molecule 41: 30S ribosomal protein S7



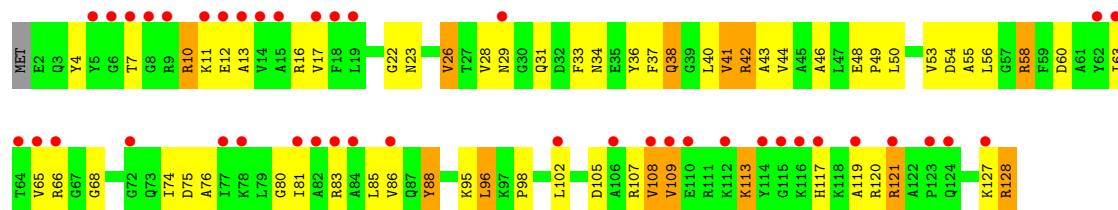
- Molecule 42: 30S ribosomal protein S8



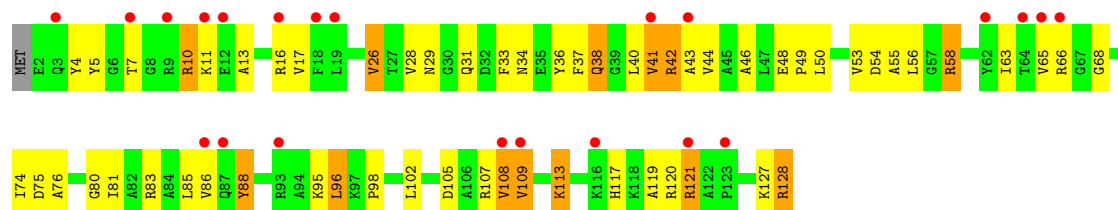
- Molecule 42: 30S ribosomal protein S8



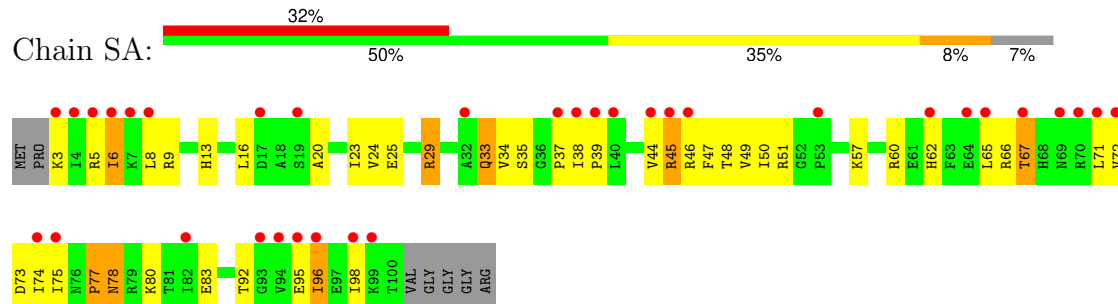
- Molecule 43: 30S ribosomal protein S9



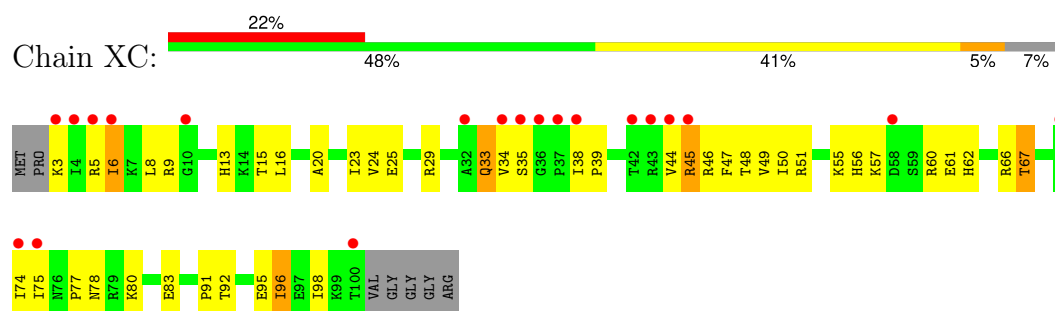
- Molecule 43: 30S ribosomal protein S9



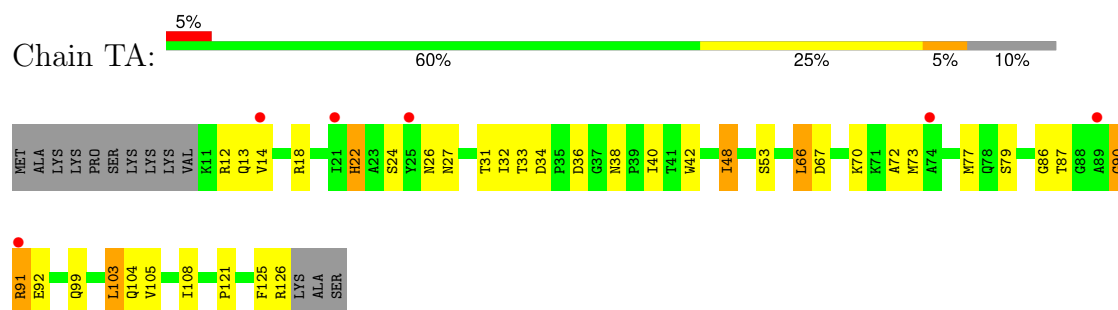
- Molecule 44: 30S ribosomal protein S10



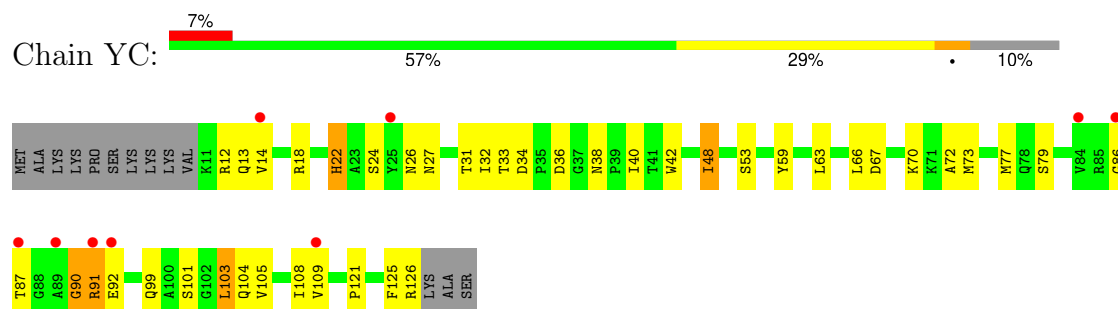
- Molecule 44: 30S ribosomal protein S10



- Molecule 45: 30S ribosomal protein S11

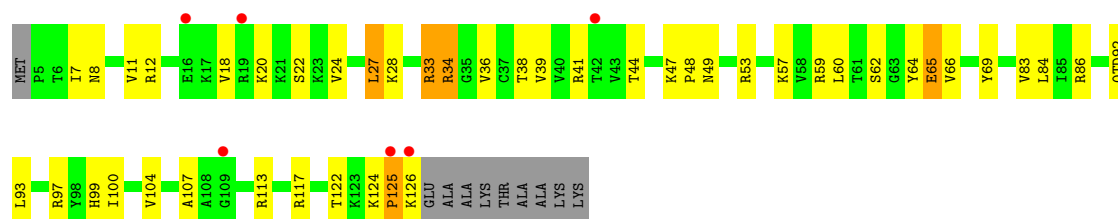


- Molecule 45: 30S ribosomal protein S11

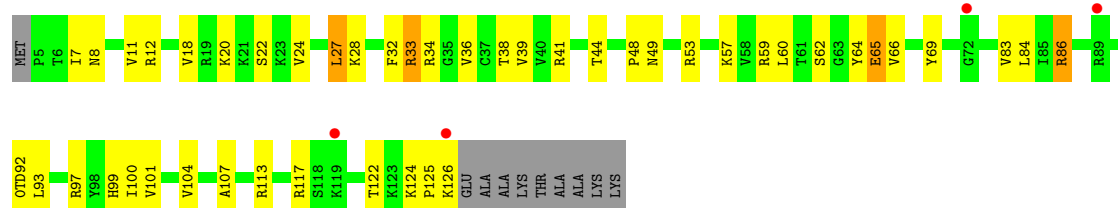


- Molecule 46: 30S ribosomal protein S12

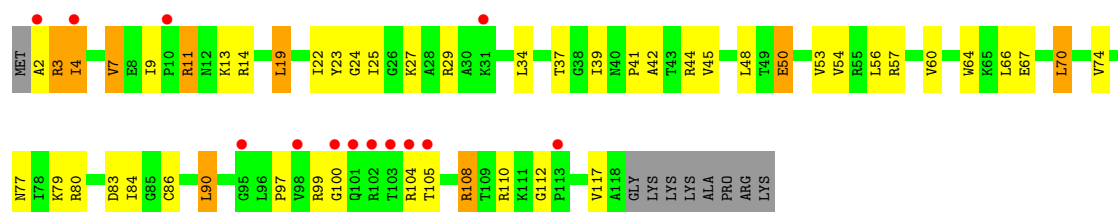




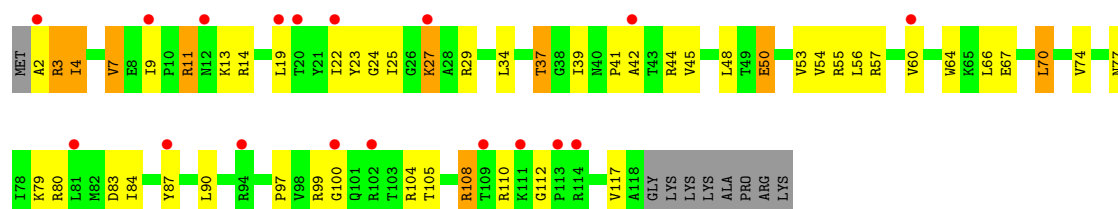
- Molecule 46: 30S ribosomal protein S12



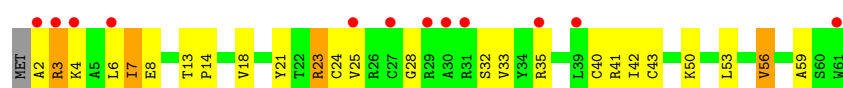
- Molecule 47: 30S ribosomal protein S13



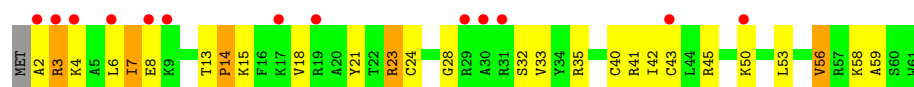
- Molecule 47: 30S ribosomal protein S13



- Molecule 48: 30S ribosomal protein S14 type Z



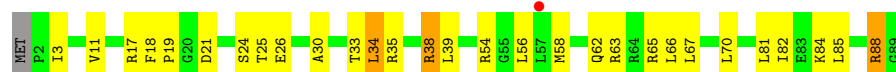
- Molecule 48: 30S ribosomal protein S14 type Z



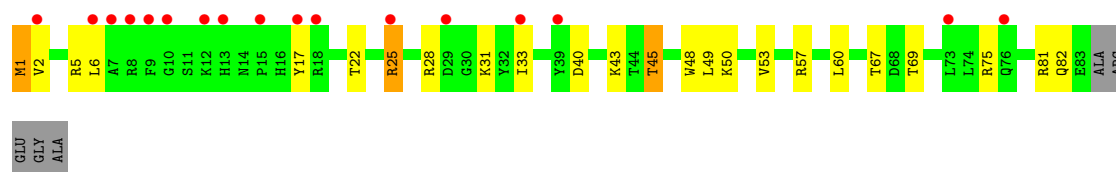
- Molecule 49: 30S ribosomal protein S15



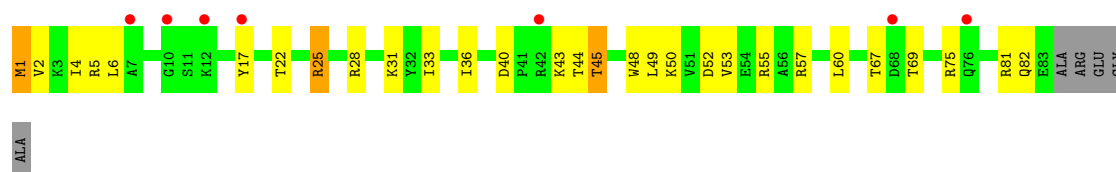
- Molecule 49: 30S ribosomal protein S15



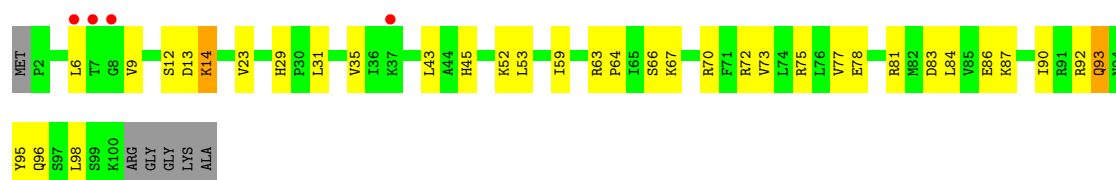
- Molecule 50: 30S ribosomal protein S16



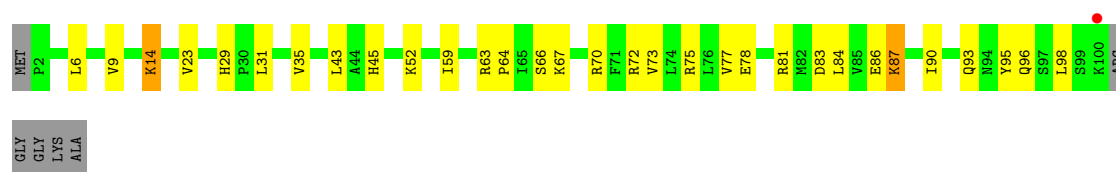
- Molecule 50: 30S ribosomal protein S16



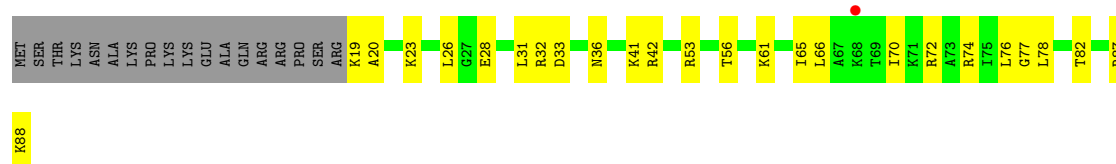
- Molecule 51: 30S ribosomal protein S17



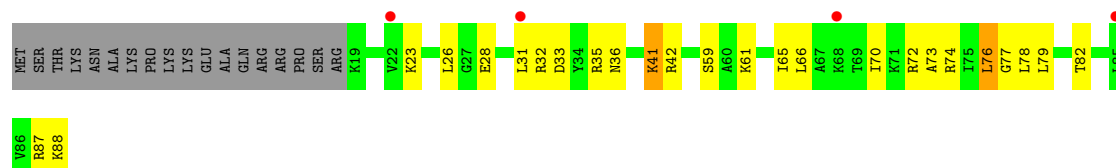
- Molecule 51: 30S ribosomal protein S17



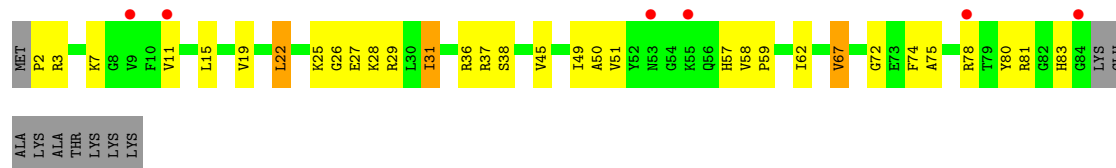
- Molecule 52: 30S ribosomal protein S18



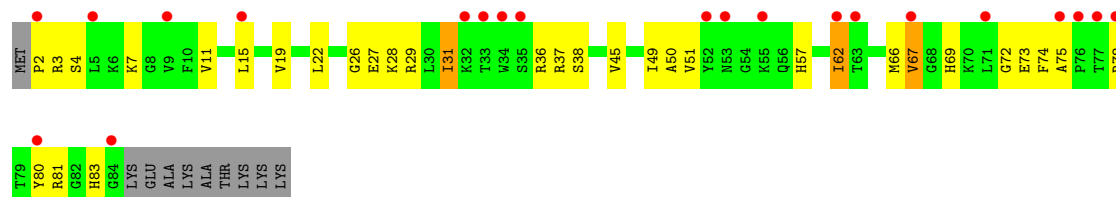
- Molecule 52: 30S ribosomal protein S18



- Molecule 53: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S19



-
- Figure 1 shows a schematic representation of the 24 amino acid residues of the protein. The residues are arranged in a linear sequence from MET to LYS. The residues are color-coded: MET (grey), G2 (yellow), K3 (yellow), G4 (yellow), D5 (yellow), R6 (green), R7 (yellow), T8 (green), R9 (green), R10 (orange), I13 (green), W14 (green), R15 (green), G16 (green), T17 (green), Y18 (green), R22 (yellow), P23 (yellow), R24 (green), K25 (green), LYS (grey), and LYS (grey). Red dots above the residues indicate specific sites of interest.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.54Å 454.40Å 619.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 3.10 49.98 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.98-3.10) 100.0 (49.98-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.221 , 0.256 0.232 , 0.262	Depositor DCC
R_{free} test set	21343 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	74.6	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	300991	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.40% 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: MG, OMG, M2G, 2MU, 0TD, 5MU, 4OC, 7MG, 4SU, PSU, 2MG, 2MA, MA6, ZN, UR3, 5MC

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	0.53	0/35961	0.97	23/56125 (0.0%)
1	FB	0.55	1/35961 (0.0%)	0.99	26/56125 (0.0%)
2	B	0.85	30/69214 (0.0%)	1.22	348/108048 (0.3%)
2	GB	0.70	13/69214 (0.0%)	1.12	225/108048 (0.2%)
3	C	0.59	0/2881	1.00	1/4494 (0.0%)
3	HB	0.49	0/2881	0.92	0/4494
4	D	0.38	0/1744	0.85	1/2719 (0.0%)
4	IA	0.59	0/1744	1.01	2/2719 (0.1%)
4	IB	0.38	0/1744	0.86	1/2719 (0.0%)
4	NC	0.56	0/1744	0.97	1/2719 (0.0%)
5	E	0.66	1/2195 (0.0%)	0.68	0/2955
5	JB	0.55	0/2195	0.63	0/2955
6	F	0.58	0/1596	0.62	0/2153
6	KB	0.50	0/1596	0.60	0/2153
7	G	0.58	0/1621	0.63	0/2194
7	LB	0.49	0/1621	0.59	0/2194
8	H	0.39	0/1496	0.56	1/2013 (0.0%)
8	MB	0.35	0/1496	0.55	1/2013 (0.0%)
9	I	0.48	0/1356	0.57	0/1834
9	NB	0.32	0/1356	0.51	0/1834
10	J	0.45	0/1152	0.57	0/1559
10	OB	0.37	0/1152	0.55	0/1559
11	K	0.55	0/1148	0.59	0/1547
11	PB	0.43	0/1148	0.55	0/1547
12	L	0.55	0/942	0.60	0/1268
12	QB	0.50	0/942	0.57	0/1268
13	M	0.55	0/1162	0.62	0/1544
13	RB	0.47	0/1162	0.60	0/1544
14	N	0.62	2/1142 (0.2%)	0.58	0/1525
14	SB	0.51	0/1142	0.56	0/1525
15	O	0.50	0/982	0.62	0/1312
15	TB	0.43	0/982	0.58	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	P	0.40	0/887	0.53	0/1180
16	UB	0.35	0/887	0.50	0/1180
17	Q	0.47	0/1157	0.56	0/1544
17	VB	0.43	0/1157	0.56	0/1544
18	R	0.58	0/982	0.61	0/1306
18	WB	0.47	0/982	0.54	0/1306
19	S	0.60	0/790	0.62	0/1057
19	XB	0.49	0/790	0.57	0/1057
20	T	0.60	0/901	0.64	0/1209
20	YB	0.52	0/901	0.62	0/1209
21	U	0.62	0/764	0.63	1/1025 (0.1%)
21	ZB	0.50	0/764	0.61	1/1025 (0.1%)
22	AC	0.49	0/827	0.59	0/1103
22	V	0.56	0/827	0.62	0/1103
23	BC	0.38	0/1527	0.52	0/2073
23	W	0.44	0/1527	0.54	0/2073
24	CC	0.48	0/671	0.61	0/892
24	X	0.59	0/671	0.64	0/892
25	DC	0.49	0/768	0.62	0/1021
25	Y	0.58	0/768	0.64	0/1021
26	EC	0.44	0/594	0.52	0/785
26	Z	0.59	0/594	0.57	0/785
27	AA	0.58	0/482	0.59	0/646
27	FC	0.45	0/482	0.58	0/646
28	BA	0.37	0/565	0.48	0/761
28	GC	0.37	0/565	0.48	0/761
29	CA	0.56	0/474	0.64	0/640
29	HC	0.48	0/474	0.59	0/640
30	DA	0.49	0/460	0.59	0/613
30	IC	0.44	0/460	0.55	0/613
31	EA	0.70	0/426	0.69	0/561
31	JC	0.56	0/426	0.62	0/561
32	FA	0.68	0/525	0.59	0/691
32	KC	0.54	0/525	0.57	0/691
33	GA	0.62	0/310	0.64	0/407
33	LC	0.45	0/310	0.58	0/407
34	HA	0.81	0/225	0.90	0/348
34	MC	0.82	0/225	0.87	0/348
35	JA	0.42	0/2037	0.59	0/2746
35	OC	0.38	0/2037	0.58	0/2746
36	KA	0.35	0/1935	0.53	0/2609
36	PC	0.36	0/1935	0.53	0/2609
37	LA	0.33	0/1636	0.47	0/2205

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	QC	0.34	0/1636	0.47	0/2205
38	MA	0.42	1/1733 (0.1%)	0.56	0/2318
38	RC	0.48	1/1733 (0.1%)	0.57	0/2318
39	NA	0.42	0/1171	0.55	0/1576
39	SC	0.47	0/1171	0.55	0/1576
40	OA	0.46	0/856	0.55	0/1154
40	TC	0.42	0/856	0.53	0/1154
41	PA	0.34	0/1276	0.46	0/1709
41	UC	0.33	0/1276	0.47	0/1709
42	QA	0.38	0/1136	0.55	0/1527
42	VC	0.39	0/1136	0.56	0/1527
43	RA	0.32	0/1029	0.47	0/1378
43	WC	0.32	0/1029	0.47	0/1378
44	SA	0.33	0/807	0.50	0/1085
44	XC	0.34	0/807	0.50	0/1085
45	TA	0.43	0/879	0.55	0/1187
45	YC	0.43	0/879	0.55	0/1187
46	UA	0.45	0/963	0.54	0/1287
46	ZC	0.45	0/963	0.54	0/1287
47	AD	0.31	0/943	0.52	0/1265
47	VA	0.32	0/943	0.52	0/1265
48	BD	0.35	0/501	0.50	0/664
48	WA	0.34	0/501	0.49	0/664
49	CD	0.42	0/745	0.53	0/992
49	XA	0.41	0/745	0.53	0/992
50	DD	0.41	0/716	0.52	0/963
50	YA	0.35	0/716	0.49	0/963
51	ED	0.45	0/836	0.53	0/1117
51	ZA	0.43	0/836	0.53	0/1117
52	AB	0.46	0/579	0.57	0/768
52	FD	0.45	0/579	0.57	0/768
53	BB	0.28	0/680	0.51	0/915
53	GD	0.28	0/680	0.51	0/915
54	CB	0.33	0/764	0.52	0/1006
54	HD	0.37	0/764	0.53	0/1006
55	DB	0.32	0/212	0.47	0/277
55	ID	0.31	0/212	0.45	0/277
All	All	0.63	49/322210 (0.0%)	0.98	632/481238 (0.1%)

The worst 5 of 49 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1142(B)	A	N9-C4	-9.19	1.32	1.37
2	B	1762	A	N9-C4	8.08	1.42	1.37
2	B	2249	U	C4-O4	7.73	1.29	1.23
2	B	330	A	N9-C4	-7.25	1.33	1.37
5	E	237	GLU	CG-CD	7.22	1.62	1.51

The worst 5 of 632 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1671	U	N3-C4-O4	12.55	128.19	119.40
2	GB	330	A	C2-N3-C4	-11.88	104.66	110.60
2	GB	2593	U	N3-C4-C5	-11.59	107.65	114.60
2	B	1021	A	C2-N3-C4	-11.37	104.92	110.60
2	GB	1021	A	C2-N3-C4	-10.84	105.18	110.60

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	372	0
1	FB	32394	0	16366	348	0
2	B	62031	0	31273	576	0
2	GB	62031	0	31269	584	0
3	C	2576	0	1305	19	0
3	HB	2576	0	1305	17	0
4	D	1642	0	841	29	0
4	IA	1642	0	841	20	0
4	IB	1642	0	840	30	0
4	NC	1642	0	841	13	0
5	E	2145	0	2234	43	0
5	JB	2145	0	2234	51	0
6	F	1563	0	1629	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	KB	1563	0	1629	33	0
7	G	1586	0	1632	45	0
7	LB	1586	0	1632	40	0
8	H	1471	0	1526	50	0
8	MB	1471	0	1526	53	0
9	I	1330	0	1407	44	0
9	NB	1330	0	1407	42	0
10	J	1137	0	1225	46	0
10	OB	1137	0	1225	42	0
11	K	1121	0	1195	18	0
11	PB	1121	0	1195	22	0
12	L	932	0	994	21	0
12	QB	932	0	993	18	0
13	M	1145	0	1228	51	0
13	RB	1145	0	1228	43	0
14	N	1121	0	1179	40	0
14	SB	1121	0	1179	37	0
15	O	968	0	1032	26	0
15	TB	968	0	1033	26	0
16	P	877	0	938	31	0
16	UB	877	0	938	28	0
17	Q	1143	0	1211	41	0
17	VB	1143	0	1211	44	0
18	R	964	0	1022	20	0
18	WB	964	0	1022	23	0
19	S	779	0	852	12	0
19	XB	779	0	852	14	0
20	T	890	0	951	23	0
20	YB	890	0	951	20	0
21	U	750	0	814	9	0
21	ZB	750	0	814	10	0
22	AC	814	0	904	20	0
22	V	814	0	904	22	0
23	BC	1495	0	1521	38	0
23	W	1495	0	1521	34	0
24	CC	662	0	688	20	0
24	X	662	0	688	18	0
25	DC	761	0	837	23	0
25	Y	761	0	837	24	0
26	EC	592	0	654	15	0
26	Z	592	0	654	16	0
27	AA	477	0	529	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	FC	477	0	529	13	0
28	BA	552	0	537	19	0
28	GC	552	0	537	17	0
29	CA	460	0	480	9	0
29	HC	460	0	480	10	0
30	DA	453	0	473	13	0
30	IC	453	0	473	13	0
31	EA	418	0	467	14	0
31	JC	418	0	467	12	0
32	FA	517	0	582	15	0
32	KC	517	0	582	10	0
33	GA	307	0	335	5	0
33	LC	307	0	335	5	0
34	HA	220	0	108	7	0
34	MC	220	0	108	7	0
35	JA	2005	0	1964	61	0
35	OC	2005	0	1964	59	0
36	KA	1900	0	1951	66	0
36	PC	1900	0	1951	69	0
37	LA	1612	0	1677	50	0
37	QC	1612	0	1676	51	0
38	MA	1703	0	1767	71	0
38	RC	1703	0	1766	66	0
39	NA	1155	0	1213	33	0
39	SC	1155	0	1213	29	0
40	OA	843	0	857	34	0
40	TC	843	0	857	31	0
41	PA	1257	0	1296	29	0
41	UC	1257	0	1296	30	0
42	QA	1116	0	1177	52	0
42	VC	1116	0	1177	55	0
43	RA	1011	0	1043	45	0
43	WC	1011	0	1043	45	0
44	SA	794	0	840	36	0
44	XC	794	0	840	35	0
45	TA	864	0	881	30	0
45	YC	864	0	881	34	0
46	UA	958	0	1047	31	0
46	ZC	958	0	1047	29	0
47	AD	933	0	992	40	0
47	VA	933	0	992	44	0
48	BD	492	0	533	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	WA	492	0	533	20	0
49	CD	734	0	771	21	0
49	XA	734	0	771	22	0
50	DD	700	0	720	19	0
50	YA	700	0	720	15	0
51	ED	823	0	893	18	0
51	ZA	823	0	893	21	0
52	AB	574	0	644	16	0
52	FD	574	0	644	18	0
53	BB	665	0	686	19	0
53	GD	665	0	686	20	0
54	CB	762	0	859	32	0
54	HD	762	0	859	34	0
55	DB	208	0	221	3	0
55	ID	208	0	221	5	0
56	A	287	0	0	0	0
56	AA	4	0	0	0	0
56	AD	1	0	0	0	0
56	B	944	0	0	0	0
56	BA	3	0	0	0	0
56	BB	1	0	0	0	0
56	BC	9	0	0	0	0
56	C	44	0	0	0	0
56	CA	3	0	0	0	0
56	CB	1	0	0	0	0
56	CC	2	0	0	0	0
56	CD	3	0	0	0	0
56	D	2	0	0	0	0
56	DA	3	0	0	0	0
56	DB	1	0	0	0	0
56	DC	3	0	0	0	0
56	DD	1	0	0	0	0
56	E	10	0	0	0	0
56	EA	2	0	0	0	0
56	EC	4	0	0	0	0
56	ED	2	0	0	0	0
56	F	15	0	0	0	0
56	FA	4	0	0	0	0
56	FB	349	0	0	0	0
56	FC	1	0	0	0	0
56	G	11	0	0	0	0
56	GA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	GB	812	0	0	0	0
56	GC	2	0	0	0	0
56	GD	1	0	0	0	0
56	H	3	0	0	0	0
56	HA	2	0	0	0	0
56	HB	32	0	0	0	0
56	HC	2	0	0	0	0
56	HD	1	0	0	0	0
56	I	7	0	0	0	0
56	IA	21	0	0	0	0
56	IB	5	0	0	0	0
56	J	3	0	0	0	0
56	JA	13	0	0	0	0
56	JB	13	0	0	0	0
56	K	9	0	0	0	0
56	KA	4	0	0	0	0
56	KB	4	0	0	0	0
56	KC	5	0	0	0	0
56	L	5	0	0	0	0
56	LA	2	0	0	0	0
56	LB	5	0	0	0	0
56	M	8	0	0	0	0
56	MA	5	0	0	0	0
56	MB	7	0	0	0	0
56	MC	1	0	0	0	0
56	N	6	0	0	0	0
56	NA	3	0	0	0	0
56	NB	3	0	0	0	0
56	NC	14	0	0	0	0
56	O	3	0	0	0	0
56	OA	4	0	0	0	0
56	OB	2	0	0	0	0
56	OC	7	0	0	0	0
56	P	4	0	0	0	0
56	PA	3	0	0	0	0
56	PB	4	0	0	0	0
56	PC	5	0	0	0	0
56	Q	4	0	0	0	0
56	QA	2	0	0	0	0
56	QB	6	0	0	0	0
56	QC	4	0	0	0	0
56	R	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	RA	4	0	0	0	0
56	RB	6	0	0	0	0
56	RC	11	0	0	0	0
56	S	8	0	0	0	0
56	SA	3	0	0	0	0
56	SB	4	0	0	0	0
56	SC	7	0	0	0	0
56	T	5	0	0	0	0
56	TA	1	0	0	0	0
56	TB	4	0	0	0	0
56	TC	1	0	0	0	0
56	U	2	0	0	0	0
56	UA	3	0	0	0	0
56	UB	1	0	0	0	0
56	UC	2	0	0	0	0
56	VA	3	0	0	0	0
56	VB	8	0	0	0	0
56	VC	2	0	0	0	0
56	W	8	0	0	0	0
56	WA	1	0	0	0	0
56	WB	3	0	0	0	0
56	WC	2	0	0	0	0
56	X	8	0	0	0	0
56	XA	3	0	0	0	0
56	XB	4	0	0	0	0
56	XC	2	0	0	0	0
56	Y	5	0	0	0	0
56	YA	1	0	0	0	0
56	YB	7	0	0	0	0
56	YC	6	0	0	0	0
56	Z	3	0	0	0	0
56	ZA	3	0	0	0	0
56	ZB	1	0	0	0	0
56	ZC	2	0	0	0	0
57	AC	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	GA	1	0	0	0	0
57	GC	1	0	0	0	0
57	HC	1	0	0	0	0
57	IC	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	LC	1	0	0	0	0
57	V	1	0	0	0	0
All	All	300991	0	203678	4336	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 9.

The worst 5 of 4336 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)
38:RC:9:CYS:SG	38:RC:18:LYS:NZ	2.06	1.28
38:MA:9:CYS:SG	38:MA:18:LYS:NZ	2.09	1.26
38:MA:18:LYS:NZ	38:MA:26:CYS:SG	2.12	1.20
38:RC:18:LYS:NZ	38:RC:26:CYS:SG	2.15	1.20
42:VC:50:ARG:HB3	42:VC:50:ARG:HH11	1.21	1.03

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%)	252 (92%)	20 (7%)	1 (0%)	30	63
5	JB	273/275 (99%)	250 (92%)	22 (8%)	1 (0%)	30	63
6	F	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	13	42
6	KB	202/206 (98%)	189 (94%)	11 (5%)	2 (1%)	13	42
7	G	200/205 (98%)	184 (92%)	14 (7%)	2 (1%)	13	42
7	LB	200/205 (98%)	182 (91%)	16 (8%)	2 (1%)	13	42
8	H	179/182 (98%)	156 (87%)	19 (11%)	4 (2%)	5	24
8	MB	179/182 (98%)	157 (88%)	18 (10%)	4 (2%)	5	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	172/180 (96%)	155 (90%)	16 (9%)	1 (1%)	22	53
9	NB	172/180 (96%)	155 (90%)	16 (9%)	1 (1%)	22	53
10	J	144/148 (97%)	128 (89%)	12 (8%)	4 (3%)	4	20
10	OB	144/148 (97%)	128 (89%)	12 (8%)	4 (3%)	4	20
11	K	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
11	PB	138/140 (99%)	128 (93%)	10 (7%)	0	100	100
12	L	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	7	30
12	QB	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	16	48
13	M	148/150 (99%)	134 (90%)	13 (9%)	1 (1%)	19	51
13	RB	148/150 (99%)	134 (90%)	13 (9%)	1 (1%)	19	51
14	N	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	19	51
14	SB	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	19	51
15	O	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	7	30
15	TB	116/118 (98%)	108 (93%)	6 (5%)	2 (2%)	7	30
16	P	108/112 (96%)	96 (89%)	10 (9%)	2 (2%)	6	27
16	UB	108/112 (96%)	96 (89%)	10 (9%)	2 (2%)	6	27
17	Q	135/146 (92%)	122 (90%)	10 (7%)	3 (2%)	5	24
17	VB	135/146 (92%)	122 (90%)	11 (8%)	2 (2%)	8	33
18	R	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
18	WB	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
19	S	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	6	26
19	XB	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	13	42
20	T	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
20	YB	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
21	U	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
21	ZB	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
22	AC	105/110 (96%)	93 (89%)	12 (11%)	0	100	100
22	V	105/110 (96%)	95 (90%)	10 (10%)	0	100	100
23	BC	187/206 (91%)	167 (89%)	16 (9%)	4 (2%)	5	25
23	W	187/206 (91%)	167 (89%)	16 (9%)	4 (2%)	5	25
24	CC	82/85 (96%)	75 (92%)	4 (5%)	3 (4%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	X	82/85 (96%)	75 (92%)	4 (5%)	3 (4%)	2	16
25	DC	95/98 (97%)	88 (93%)	6 (6%)	1 (1%)	12	39
25	Y	95/98 (97%)	88 (93%)	5 (5%)	2 (2%)	5	25
26	EC	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%)	54 (93%)	3 (5%)	1 (2%)	7	30
27	FC	58/60 (97%)	53 (91%)	4 (7%)	1 (2%)	7	30
28	BA	67/71 (94%)	45 (67%)	16 (24%)	6 (9%)	0	3
28	GC	67/71 (94%)	45 (67%)	16 (24%)	6 (9%)	0	3
29	CA	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
29	HC	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
30	DA	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
30	IC	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
31	EA	46/49 (94%)	46 (100%)	0	0	100	100
31	JC	46/49 (94%)	46 (100%)	0	0	100	100
32	FA	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
32	KC	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
33	GA	35/37 (95%)	32 (91%)	1 (3%)	2 (6%)	1	8
33	LC	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	3	20
35	JA	256/368 (70%)	215 (84%)	32 (12%)	9 (4%)	3	16
35	OC	256/368 (70%)	218 (85%)	28 (11%)	10 (4%)	2	14
36	KA	232/256 (91%)	191 (82%)	24 (10%)	17 (7%)	1	5
36	PC	232/256 (91%)	190 (82%)	25 (11%)	17 (7%)	1	5
37	LA	204/239 (85%)	181 (89%)	18 (9%)	5 (2%)	4	22
37	QC	204/239 (85%)	179 (88%)	20 (10%)	5 (2%)	4	22
38	MA	206/209 (99%)	184 (89%)	17 (8%)	5 (2%)	5	22
38	RC	206/209 (99%)	182 (88%)	19 (9%)	5 (2%)	5	22
39	NA	149/162 (92%)	132 (89%)	14 (9%)	3 (2%)	6	26
39	SC	149/162 (92%)	132 (89%)	14 (9%)	3 (2%)	6	26
40	OA	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
40	TC	99/101 (98%)	92 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	PA	153/156 (98%)	139 (91%)	9 (6%)	5 (3%)	3	17
41	UC	153/156 (98%)	137 (90%)	11 (7%)	5 (3%)	3	17
42	QA	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
42	VC	136/138 (99%)	124 (91%)	12 (9%)	0	100	100
43	RA	125/128 (98%)	109 (87%)	14 (11%)	2 (2%)	8	31
43	WC	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	16	48
44	SA	96/105 (91%)	81 (84%)	12 (12%)	3 (3%)	3	19
44	XC	96/105 (91%)	81 (84%)	12 (12%)	3 (3%)	3	19
45	TA	114/129 (88%)	103 (90%)	8 (7%)	3 (3%)	4	21
45	YC	114/129 (88%)	104 (91%)	7 (6%)	3 (3%)	4	21
46	UA	119/132 (90%)	104 (87%)	13 (11%)	2 (2%)	7	30
46	ZC	119/132 (90%)	105 (88%)	12 (10%)	2 (2%)	7	30
47	AD	115/126 (91%)	101 (88%)	13 (11%)	1 (1%)	14	45
47	VA	115/126 (91%)	100 (87%)	14 (12%)	1 (1%)	14	45
48	BD	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	17
48	WA	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	17
49	CD	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	11	38
49	XA	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	11	38
50	DD	81/88 (92%)	75 (93%)	6 (7%)	0	100	100
50	YA	81/88 (92%)	75 (93%)	6 (7%)	0	100	100
51	ED	97/105 (92%)	86 (89%)	9 (9%)	2 (2%)	5	25
51	ZA	97/105 (92%)	87 (90%)	8 (8%)	2 (2%)	5	25
52	AB	68/88 (77%)	60 (88%)	7 (10%)	1 (2%)	8	33
52	FD	68/88 (77%)	61 (90%)	5 (7%)	2 (3%)	3	20
53	BB	81/93 (87%)	70 (86%)	7 (9%)	4 (5%)	2	11
53	GD	81/93 (87%)	70 (86%)	7 (9%)	4 (5%)	2	11
54	CB	97/106 (92%)	83 (86%)	9 (9%)	5 (5%)	1	10
54	HD	97/106 (92%)	82 (84%)	10 (10%)	5 (5%)	1	10
55	DB	22/27 (82%)	17 (77%)	4 (18%)	1 (4%)	2	12
55	ID	22/27 (82%)	18 (82%)	3 (14%)	1 (4%)	2	12
All	All	11996/12852 (93%)	10786 (90%)	982 (8%)	228 (2%)	6	27

5 of 228 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	47	LYS
9	I	126	PRO
10	J	92	VAL
14	N	60	ARG
15	O	2	ARG

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%)	196 (90%)	21 (10%)	6	25
5	JB	217/217 (100%)	193 (89%)	24 (11%)	5	20
6	F	165/166 (99%)	150 (91%)	15 (9%)	7	28
6	KB	165/166 (99%)	149 (90%)	16 (10%)	6	25
7	G	161/162 (99%)	137 (85%)	24 (15%)	2	10
7	LB	161/162 (99%)	138 (86%)	23 (14%)	2	11
8	H	154/156 (99%)	132 (86%)	22 (14%)	2	11
8	MB	154/156 (99%)	132 (86%)	22 (14%)	2	11
9	I	144/148 (97%)	130 (90%)	14 (10%)	6	25
9	NB	144/148 (97%)	130 (90%)	14 (10%)	6	25
10	J	122/124 (98%)	95 (78%)	27 (22%)	1	3
10	OB	122/124 (98%)	96 (79%)	26 (21%)	1	4
11	K	119/119 (100%)	103 (87%)	16 (13%)	3	13
11	PB	119/119 (100%)	103 (87%)	16 (13%)	3	13
12	L	100/100 (100%)	90 (90%)	10 (10%)	6	24
12	QB	100/100 (100%)	89 (89%)	11 (11%)	5	21
13	M	116/116 (100%)	103 (89%)	13 (11%)	5	20
13	RB	116/116 (100%)	104 (90%)	12 (10%)	6	22
14	N	111/111 (100%)	100 (90%)	11 (10%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	SB	111/111 (100%)	101 (91%)	10 (9%)	8	29
15	O	101/101 (100%)	89 (88%)	12 (12%)	4	17
15	TB	101/101 (100%)	88 (87%)	13 (13%)	3	15
16	P	87/88 (99%)	73 (84%)	14 (16%)	2	9
16	UB	87/88 (99%)	73 (84%)	14 (16%)	2	9
17	Q	121/128 (94%)	111 (92%)	10 (8%)	9	33
17	VB	121/128 (94%)	112 (93%)	9 (7%)	11	36
18	R	93/94 (99%)	84 (90%)	9 (10%)	6	25
18	WB	93/94 (99%)	84 (90%)	9 (10%)	6	25
19	S	82/82 (100%)	69 (84%)	13 (16%)	2	9
19	XB	82/82 (100%)	69 (84%)	13 (16%)	2	9
20	T	91/92 (99%)	84 (92%)	7 (8%)	10	35
20	YB	91/92 (99%)	84 (92%)	7 (8%)	10	35
21	U	77/78 (99%)	69 (90%)	8 (10%)	5	22
21	ZB	77/78 (99%)	70 (91%)	7 (9%)	7	28
22	AC	87/91 (96%)	77 (88%)	10 (12%)	4	19
22	V	87/91 (96%)	79 (91%)	8 (9%)	7	28
23	BC	163/179 (91%)	144 (88%)	19 (12%)	4	18
23	W	163/179 (91%)	144 (88%)	19 (12%)	4	18
24	CC	66/67 (98%)	60 (91%)	6 (9%)	7	28
24	X	66/67 (98%)	60 (91%)	6 (9%)	7	28
25	DC	81/83 (98%)	72 (89%)	9 (11%)	5	20
25	Y	81/83 (98%)	72 (89%)	9 (11%)	5	20
26	EC	66/67 (98%)	60 (91%)	6 (9%)	7	28
26	Z	66/67 (98%)	60 (91%)	6 (9%)	7	28
27	AA	52/52 (100%)	47 (90%)	5 (10%)	7	26
27	FC	52/52 (100%)	47 (90%)	5 (10%)	7	26
28	BA	59/63 (94%)	52 (88%)	7 (12%)	4	17
28	GC	59/63 (94%)	52 (88%)	7 (12%)	4	17
29	CA	51/52 (98%)	46 (90%)	5 (10%)	6	25
29	HC	51/52 (98%)	46 (90%)	5 (10%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	DA	51/52 (98%)	46 (90%)	5 (10%)	6	25
30	IC	51/52 (98%)	46 (90%)	5 (10%)	6	25
31	EA	41/42 (98%)	35 (85%)	6 (15%)	2	11
31	JC	41/42 (98%)	37 (90%)	4 (10%)	6	25
32	FA	54/55 (98%)	48 (89%)	6 (11%)	5	20
32	KC	54/55 (98%)	50 (93%)	4 (7%)	11	36
33	GA	34/34 (100%)	33 (97%)	1 (3%)	37	65
33	LC	34/34 (100%)	34 (100%)	0	100	100
35	JA	209/308 (68%)	178 (85%)	31 (15%)	2	10
35	OC	209/308 (68%)	177 (85%)	32 (15%)	2	10
36	KA	202/220 (92%)	172 (85%)	30 (15%)	2	10
36	PC	202/220 (92%)	172 (85%)	30 (15%)	2	10
37	LA	160/188 (85%)	141 (88%)	19 (12%)	4	17
37	QC	160/188 (85%)	142 (89%)	18 (11%)	4	20
38	MA	180/181 (99%)	153 (85%)	27 (15%)	2	10
38	RC	180/181 (99%)	152 (84%)	28 (16%)	2	9
39	NA	116/123 (94%)	100 (86%)	16 (14%)	3	13
39	SC	116/123 (94%)	98 (84%)	18 (16%)	2	9
40	OA	90/90 (100%)	81 (90%)	9 (10%)	6	24
40	TC	90/90 (100%)	81 (90%)	9 (10%)	6	24
41	PA	126/127 (99%)	113 (90%)	13 (10%)	6	22
41	UC	126/127 (99%)	112 (89%)	14 (11%)	5	20
42	QA	119/119 (100%)	106 (89%)	13 (11%)	5	21
42	VC	119/119 (100%)	106 (89%)	13 (11%)	5	21
43	RA	98/99 (99%)	81 (83%)	17 (17%)	1	7
43	WC	98/99 (99%)	82 (84%)	16 (16%)	2	8
44	SA	88/92 (96%)	81 (92%)	7 (8%)	10	34
44	XC	88/92 (96%)	81 (92%)	7 (8%)	10	34
45	TA	88/99 (89%)	80 (91%)	8 (9%)	7	28
45	YC	88/99 (89%)	79 (90%)	9 (10%)	6	23
46	UA	102/108 (94%)	90 (88%)	12 (12%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	ZC	102/108 (94%)	91 (89%)	11 (11%)	5	21
47	AD	94/101 (93%)	79 (84%)	15 (16%)	2	9
47	VA	94/101 (93%)	79 (84%)	15 (16%)	2	9
48	BD	49/50 (98%)	41 (84%)	8 (16%)	2	8
48	WA	49/50 (98%)	41 (84%)	8 (16%)	2	8
49	CD	79/80 (99%)	75 (95%)	4 (5%)	20	49
49	XA	79/80 (99%)	75 (95%)	4 (5%)	20	49
50	DD	72/74 (97%)	63 (88%)	9 (12%)	3	15
50	YA	72/74 (97%)	63 (88%)	9 (12%)	3	15
51	ED	94/97 (97%)	86 (92%)	8 (8%)	8	32
51	ZA	94/97 (97%)	85 (90%)	9 (10%)	7	26
52	AB	61/77 (79%)	56 (92%)	5 (8%)	9	33
52	FD	61/77 (79%)	56 (92%)	5 (8%)	9	33
53	BB	72/80 (90%)	63 (88%)	9 (12%)	3	15
53	GD	72/80 (90%)	65 (90%)	7 (10%)	6	25
54	CB	76/82 (93%)	67 (88%)	9 (12%)	4	17
54	HD	76/82 (93%)	68 (90%)	8 (10%)	5	22
55	DB	19/22 (86%)	18 (95%)	1 (5%)	19	48
55	ID	19/22 (86%)	18 (95%)	1 (5%)	19	48
All	All	10120/10672 (95%)	8924 (88%)	1196 (12%)	4	17

5 of 1196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	OC	119	THR
48	BD	7	ILE
35	OC	328	ARG
32	KC	32	LEU
39	SC	64	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
36	PC	94	ASN

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Mol	Chain	Res	Type
45	YC	22	HIS
46	ZC	8	ASN
45	YC	99	GLN
43	RA	3	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1502/1507 (99%)	227 (15%)	11 (0%)
1	FB	1502/1507 (99%)	229 (15%)	11 (0%)
2	B	2876/2880 (99%)	476 (16%)	24 (0%)
2	GB	2876/2880 (99%)	476 (16%)	21 (0%)
3	C	119/120 (99%)	16 (13%)	1 (0%)
3	HB	119/120 (99%)	16 (13%)	1 (0%)
34	HA	9/27 (33%)	4 (44%)	0
34	MC	9/27 (33%)	4 (44%)	0
4	D	76/77 (98%)	15 (19%)	0
4	IA	76/77 (98%)	7 (9%)	1 (1%)
4	IB	76/77 (98%)	15 (19%)	0
4	NC	76/77 (98%)	7 (9%)	1 (1%)
All	All	9316/9376 (99%)	1492 (16%)	71 (0%)

5 of 1492 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	47	C

5 of 71 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	GB	1210	A
2	GB	1396	U
2	GB	2136	C
2	B	1396	U
2	B	1379	A

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

66 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	5MU	B	1915	2	19,22,23	1.98	3 (15%)	27,32,35	2.45	5 (18%)
4	5MU	IB	54	4	19,22,23	2.08	3 (15%)	27,32,35	2.02	8 (29%)
46	0TD	ZC	92	46	8,9,10	2.80	2 (25%)	6,11,13	2.59	3 (50%)
1	PSU	A	516	1	18,21,22	1.52	2 (11%)	21,30,33	1.66	5 (23%)
2	5MU	B	1939	2,56	19,22,23	2.11	2 (10%)	27,32,35	2.51	8 (29%)
4	4SU	D	8	4	18,21,22	5.79	1 (5%)	25,30,33	0.67	0
1	UR3	FB	1498	56,1	19,22,23	1.75	1 (5%)	26,32,35	1.62	3 (11%)
1	5MC	FB	1404	1	19,22,23	2.96	4 (21%)	26,32,35	1.20	2 (7%)
1	MA6	FB	1519	1	19,26,27	1.83	4 (21%)	18,38,41	1.63	3 (16%)
4	5MU	NC	54	4	19,22,23	2.12	3 (15%)	27,32,35	2.07	9 (33%)
4	5MU	IA	54	56,4	19,22,23	2.09	3 (15%)	27,32,35	2.19	10 (37%)
1	7MG	A	527	56,1	23,26,27	2.96	7 (30%)	27,39,42	2.12	9 (33%)
4	5MC	IB	32	4	19,22,23	2.66	5 (26%)	26,32,35	1.04	2 (7%)
1	5MC	A	1404	1	19,22,23	2.75	4 (21%)	26,32,35	1.24	2 (7%)
1	5MC	A	967	1	19,22,23	2.76	5 (26%)	26,32,35	1.10	1 (3%)
2	2MU	GB	2552	2,56	19,22,24	2.55	3 (15%)	25,31,36	2.26	8 (32%)
4	PSU	D	55	4	18,21,22	1.77	3 (16%)	21,30,33	1.61	2 (9%)
1	5MC	FB	1407	1	19,22,23	2.75	4 (21%)	26,32,35	1.06	2 (7%)
2	2MA	GB	2503	2	17,25,26	1.49	2 (11%)	16,37,40	1.87	2 (12%)
2	5MC	GB	1962	2	19,22,23	2.82	5 (26%)	26,32,35	1.09	2 (7%)
2	PSU	B	1911	2	18,21,22	1.66	2 (11%)	21,30,33	1.63	4 (19%)
1	5MC	A	1400	1	19,22,23	2.60	4 (21%)	26,32,35	1.09	2 (7%)
4	5MU	D	54	4	19,22,23	2.08	3 (15%)	27,32,35	2.01	7 (25%)
2	PSU	GB	1917	2	18,21,22	1.76	2 (11%)	21,30,33	1.87	5 (23%)
1	MA6	FB	1518	1	19,26,27	1.94	4 (21%)	18,38,41	2.09	3 (16%)
1	7MG	FB	527	1	23,26,27	2.95	7 (30%)	27,39,42	2.14	10 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4OC	A	1402	1	20,23,24	1.16	2 (10%)	25,32,35	1.04	1 (4%)
2	4OC	GB	1920	2	19,22,24	1.13	1 (5%)	25,31,35	1.07	1 (4%)
1	4OC	FB	1402	56,1	20,23,24	1.07	2 (10%)	25,32,35	1.11	3 (12%)
4	4SU	NC	8	4	18,21,22	5.77	1 (5%)	25,30,33	0.97	1 (4%)
1	2MG	A	1207	1	18,26,27	2.21	3 (16%)	16,38,41	1.60	3 (18%)
2	5MC	GB	1942	2	19,22,23	2.70	4 (21%)	26,32,35	1.47	4 (15%)
34	PSU	MC	19	34,56	18,21,22	1.68	2 (11%)	21,30,33	1.89	7 (33%)
2	2MA	B	2503	2	17,25,26	1.47	2 (11%)	16,37,40	1.44	3 (18%)
2	4OC	B	1920	2,56	19,22,24	1.12	1 (5%)	25,31,35	1.11	1 (4%)
1	MA6	A	1518	1	19,26,27	1.94	4 (21%)	18,38,41	2.20	3 (16%)
4	5MC	IA	32	4	19,22,23	2.53	4 (21%)	26,32,35	1.17	3 (11%)
2	PSU	B	1917	2	18,21,22	1.63	2 (11%)	21,30,33	1.76	5 (23%)
2	2MU	B	2552	2,56	19,22,24	2.68	7 (36%)	25,31,36	2.43	8 (32%)
4	PSU	IA	55	4	18,21,22	1.71	2 (11%)	21,30,33	1.85	4 (19%)
4	4SU	IA	8	4	18,21,22	5.80	1 (5%)	25,30,33	0.94	0
4	PSU	NC	55	4	18,21,22	1.85	3 (16%)	21,30,33	1.69	2 (9%)
2	PSU	GB	1911	2	18,21,22	1.63	2 (11%)	21,30,33	1.89	6 (28%)
1	M2G	A	966	1	20,27,28	2.43	4 (20%)	19,40,43	1.41	4 (21%)
4	5MC	D	32	4	19,22,23	2.71	5 (26%)	26,32,35	0.97	2 (7%)
2	PSU	B	2605	2	18,21,22	1.59	2 (11%)	21,30,33	1.71	4 (19%)
1	PSU	FB	516	1	18,21,22	1.52	2 (11%)	21,30,33	1.60	4 (19%)
46	0TD	UA	92	46	8,9,10	2.32	2 (25%)	6,11,13	2.62	3 (50%)
2	5MU	GB	1915	2	19,22,23	2.10	3 (15%)	27,32,35	2.13	7 (25%)
1	M2G	FB	966	1	20,27,28	2.32	3 (15%)	19,40,43	1.40	5 (26%)
1	UR3	A	1498	56,1	19,22,23	1.73	1 (5%)	26,32,35	1.61	3 (11%)
2	5MU	GB	1939	2,56	19,22,23	2.27	3 (15%)	27,32,35	2.57	7 (25%)
1	MA6	A	1519	1	19,26,27	1.96	4 (21%)	18,38,41	1.84	3 (16%)
1	5MC	A	1407	1	19,22,23	2.64	4 (21%)	26,32,35	1.16	2 (7%)
1	2MG	FB	1207	1	18,26,27	2.20	3 (16%)	16,38,41	1.60	3 (18%)
2	OMG	GB	2251	2,4	19,26,27	2.07	5 (26%)	21,38,41	1.44	5 (23%)
2	OMG	B	2251	2,4	19,26,27	2.13	5 (26%)	21,38,41	1.37	3 (14%)
4	5MC	NC	32	4	19,22,23	2.60	4 (21%)	26,32,35	1.20	3 (11%)
2	5MC	B	1942	2,56	19,22,23	2.81	4 (21%)	26,32,35	1.37	4 (15%)
1	5MC	FB	1400	1	19,22,23	2.53	4 (21%)	26,32,35	1.01	2 (7%)
1	5MC	FB	967	1	19,22,23	2.41	5 (26%)	26,32,35	1.16	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	GB	2605	2	18,21,22	1.58	3 (16%)	21,30,33	1.59	5 (23%)
4	4SU	IB	8	4	18,21,22	5.86	1 (5%)	25,30,33	0.63	0
34	PSU	HA	19	34	18,21,22	1.64	2 (11%)	21,30,33	1.93	6 (28%)
2	5MC	B	1962	2,56	19,22,23	2.83	4 (21%)	26,32,35	1.25	2 (7%)
4	PSU	IB	55	4	18,21,22	1.73	3 (16%)	21,30,33	1.61	3 (14%)

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	5MU	B	1915	2	-	0/7/25/26	0/2/2/2
4	5MU	IB	54	4	-	0/7/25/26	0/2/2/2
46	0TD	ZC	92	46	-	2/7/12/14	-
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
2	5MU	B	1939	2,56	-	0/7/25/26	0/2/2/2
4	4SU	D	8	4	-	0/7/25/26	0/2/2/2
1	UR3	FB	1498	56,1	-	0/7/25/26	0/2/2/2
1	5MC	FB	1404	1	-	0/7/25/26	0/2/2/2
1	MA6	FB	1519	1	-	4/7/29/30	0/3/3/3
4	5MU	NC	54	4	-	0/7/25/26	0/2/2/2
4	5MU	IA	54	56,4	-	0/7/25/26	0/2/2/2
1	7MG	A	527	56,1	-	1/7/37/38	0/3/3/3
4	5MC	IB	32	4	-	0/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
2	2MU	GB	2552	2,56	-	2/9/27/28	0/2/2/2
4	PSU	D	55	4	-	0/7/25/26	0/2/2/2
1	5MC	FB	1407	1	-	0/7/25/26	0/2/2/2
2	2MA	GB	2503	2	-	1/3/25/26	0/3/3/3
2	5MC	GB	1962	2	-	2/7/25/26	0/2/2/2
2	PSU	B	1911	2	-	0/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	1/7/25/26	0/2/2/2
4	5MU	D	54	4	-	0/7/25/26	0/2/2/2
2	PSU	GB	1917	2	-	0/7/25/26	0/2/2/2
1	MA6	FB	1518	1	-	0/7/29/30	0/3/3/3
1	7MG	FB	527	1	-	1/7/37/38	0/3/3/3
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
2	4OC	GB	1920	2	-	0/9/27/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4OC	FB	1402	56,1	-	2/9/29/30	0/2/2/2
4	4SU	NC	8	4	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
2	5MC	GB	1942	2	-	0/7/25/26	0/2/2/2
34	PSU	MC	19	34,56	-	0/7/25/26	0/2/2/2
2	2MA	B	2503	2	-	1/3/25/26	0/3/3/3
2	4OC	B	1920	2,56	-	1/9/27/30	0/2/2/2
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
4	5MC	IA	32	4	-	0/7/25/26	0/2/2/2
2	PSU	B	1917	2	-	0/7/25/26	0/2/2/2
2	2MU	B	2552	2,56	-	2/9/27/28	0/2/2/2
4	PSU	IA	55	4	-	0/7/25/26	0/2/2/2
4	4SU	IA	8	4	-	0/7/25/26	0/2/2/2
4	PSU	NC	55	4	-	0/7/25/26	0/2/2/2
2	PSU	GB	1911	2	-	0/7/25/26	0/2/2/2
1	M2G	A	966	1	-	0/7/29/30	0/3/3/3
4	5MC	D	32	4	-	0/7/25/26	0/2/2/2
2	PSU	B	2605	2	-	0/7/25/26	0/2/2/2
1	PSU	FB	516	1	-	0/7/25/26	0/2/2/2
46	0TD	UA	92	46	-	2/7/12/14	-
2	5MU	GB	1915	2	-	0/7/25/26	0/2/2/2
1	M2G	FB	966	1	-	0/7/29/30	0/3/3/3
1	UR3	A	1498	56,1	-	0/7/25/26	0/2/2/2
2	5MU	GB	1939	2,56	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	4/7/29/30	0/3/3/3
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	2MG	FB	1207	1	-	0/5/27/28	0/3/3/3
2	OMG	GB	2251	2,4	-	1/5/27/28	0/3/3/3
2	OMG	B	2251	2,4	-	1/5/27/28	0/3/3/3
4	5MC	NC	32	4	-	0/7/25/26	0/2/2/2
2	5MC	B	1942	2,56	-	0/7/25/26	0/2/2/2
1	5MC	FB	1400	1	-	1/7/25/26	0/2/2/2
1	5MC	FB	967	1	-	0/7/25/26	0/2/2/2
2	PSU	GB	2605	2	-	0/7/25/26	0/2/2/2
4	4SU	IB	8	4	-	0/7/25/26	0/2/2/2
34	PSU	HA	19	34	-	0/7/25/26	0/2/2/2
2	5MC	B	1962	2,56	-	2/7/25/26	0/2/2/2
4	PSU	IB	55	4	-	0/7/25/26	0/2/2/2

The worst 5 of 207 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	IB	8	4SU	C4-S4	-24.80	1.24	1.68
4	IA	8	4SU	C4-S4	-24.51	1.24	1.68
4	D	8	4SU	C4-S4	-24.49	1.24	1.68
4	NC	8	4SU	C4-S4	-24.42	1.25	1.68
1	FB	1404	5MC	C5-C4	-10.88	1.35	1.44

The worst 5 of 255 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1915	5MU	C5-C4-N3	7.39	121.75	115.32
1	A	1518	MA6	N3-C2-N1	-6.56	119.77	128.67
2	GB	1939	5MU	C4-N3-C2	-6.31	119.06	127.34
2	B	1939	5MU	C4-N3-C2	-6.03	119.44	127.34
2	B	1915	5MU	C4-N3-C2	-5.98	119.50	127.34

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1519	MA6	C5-C6-N6-C10
2	B	2251	OMG	C1'-C2'-O2'-CM2
2	B	2552	2MU	C1'-C2'-O2'-C6'
1	FB	1519	MA6	C5-C6-N6-C10
2	GB	2251	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

25 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	IB	54	5MU	1	0
2	B	1939	5MU	1	0
4	D	8	4SU	3	0
1	FB	1498	UR3	2	0
1	FB	1519	MA6	2	0
4	IB	32	5MC	1	0
1	A	967	5MC	2	0
2	GB	2552	2MU	2	0
4	D	54	5MU	1	0
1	FB	1518	MA6	1	0
34	MC	19	PSU	1	0
2	B	1920	4OC	1	0
1	A	1518	MA6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2552	2MU	2	0
1	A	966	M2G	1	0
4	D	32	5MC	1	0
1	FB	966	M2G	1	0
1	A	1498	UR3	1	0
2	GB	1939	5MU	1	0
1	A	1519	MA6	1	0
2	GB	2251	OMG	1	0
2	B	2251	OMG	1	0
1	FB	967	5MC	2	0
4	IB	8	4SU	3	0
34	HA	19	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2903 ligands modelled in this entry, 2903 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%)	0.10	38 (2%) 58 39	52, 100, 166, 256	0
1	FB	1495/1507 (99%)	0.29	52 (3%) 47 28	57, 88, 151, 209	0
2	B	2869/2880 (99%)	-0.29	65 (2%) 61 42	36, 55, 145, 201	0
2	GB	2869/2880 (99%)	0.17	99 (3%) 47 28	47, 73, 172, 242	0
3	C	120/120 (100%)	0.08	1 (0%) 82 68	63, 83, 96, 117	0
3	HB	120/120 (100%)	0.60	8 (6%) 25 15	80, 111, 128, 144	0
4	D	73/77 (94%)	0.48	6 (8%) 19 11	67, 157, 172, 174	0
4	IA	73/77 (94%)	-0.11	1 (1%) 73 56	52, 84, 91, 100	0
4	IB	73/77 (94%)	0.50	4 (5%) 32 19	79, 164, 182, 186	0
4	NC	73/77 (94%)	-0.18	0 100 100	61, 89, 100, 105	0
5	E	275/275 (100%)	-0.26	3 (1%) 77 61	36, 50, 58, 66	0
5	JB	275/275 (100%)	0.02	5 (1%) 67 49	45, 64, 74, 85	0
6	F	204/206 (99%)	-0.01	5 (2%) 58 39	39, 60, 79, 86	0
6	KB	204/206 (99%)	0.30	1 (0%) 87 75	53, 77, 97, 107	0
7	G	202/205 (98%)	-0.26	0 100 100	34, 59, 78, 86	0
7	LB	202/205 (98%)	0.14	1 (0%) 87 75	50, 78, 91, 101	0
8	H	181/182 (99%)	0.62	17 (9%) 15 9	85, 91, 111, 119	0
8	MB	181/182 (99%)	0.96	23 (12%) 9 5	99, 119, 132, 135	0
9	I	174/180 (96%)	0.05	4 (2%) 61 42	64, 72, 78, 91	0
9	NB	174/180 (96%)	1.24	21 (12%) 10 6	109, 147, 163, 169	0
10	J	146/148 (98%)	0.71	13 (8%) 17 10	64, 96, 111, 113	0
10	OB	146/148 (98%)	1.38	32 (21%) 3 1	86, 120, 129, 130	0
11	K	140/140 (100%)	-0.15	1 (0%) 84 70	44, 56, 75, 77	0
11	PB	140/140 (100%)	0.39	2 (1%) 73 56	64, 82, 99, 103	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
12	L	122/122 (100%)	-0.21	0 100 100	50, 59, 68, 71	0
12	QB	122/122 (100%)	0.01	2 (1%) 70 52	59, 69, 75, 79	0
13	M	150/150 (100%)	0.20	8 (5%) 33 20	36, 64, 87, 90	0
13	RB	150/150 (100%)	0.53	10 (6%) 25 15	50, 79, 105, 107	0
14	N	141/141 (100%)	-0.01	2 (1%) 73 56	48, 59, 72, 80	0
14	SB	141/141 (100%)	0.34	3 (2%) 63 44	63, 82, 97, 103	0
15	O	118/118 (100%)	0.03	0 100 100	47, 60, 73, 78	0
15	TB	118/118 (100%)	0.70	7 (5%) 29 18	62, 76, 83, 87	0
16	P	110/112 (98%)	0.44	9 (8%) 19 11	72, 80, 87, 89	0
16	UB	110/112 (98%)	1.05	10 (9%) 16 9	91, 106, 113, 116	0
17	Q	137/146 (93%)	0.03	2 (1%) 71 54	59, 68, 119, 142	0
17	VB	137/146 (93%)	0.14	2 (1%) 71 54	69, 79, 108, 117	0
18	R	117/118 (99%)	-0.19	0 100 100	39, 52, 63, 67	0
18	WB	117/118 (99%)	0.39	2 (1%) 69 50	55, 77, 90, 93	0
19	S	101/101 (100%)	-0.22	0 100 100	40, 60, 67, 71	0
19	XB	101/101 (100%)	0.30	3 (2%) 52 33	56, 84, 94, 99	0
20	T	112/113 (99%)	-0.29	0 100 100	39, 49, 66, 80	0
20	YB	112/113 (99%)	0.44	8 (7%) 23 14	54, 68, 87, 100	0
21	U	95/96 (98%)	-0.02	1 (1%) 77 61	49, 56, 66, 74	0
21	ZB	95/96 (98%)	0.74	8 (8%) 18 10	71, 84, 95, 97	0
22	AC	107/110 (97%)	1.49	22 (20%) 3 2	82, 90, 101, 103	0
22	V	107/110 (97%)	0.15	1 (0%) 81 66	55, 63, 76, 82	0
23	BC	189/206 (91%)	0.62	11 (5%) 30 18	89, 108, 118, 121	0
23	W	189/206 (91%)	0.28	6 (3%) 50 31	65, 83, 93, 96	0
24	CC	84/85 (98%)	0.75	9 (10%) 12 7	72, 78, 89, 93	0
24	X	84/85 (98%)	0.43	10 (11%) 10 6	52, 59, 72, 77	0
25	DC	97/98 (98%)	0.53	5 (5%) 34 20	56, 73, 108, 115	0
25	Y	97/98 (98%)	0.18	3 (3%) 51 32	43, 56, 88, 95	0
26	EC	70/72 (97%)	1.17	14 (20%) 3 2	88, 95, 103, 107	0
26	Z	70/72 (97%)	0.29	1 (1%) 73 56	57, 63, 68, 77	0
27	AA	60/60 (100%)	0.07	0 100 100	47, 58, 74, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	FC	60/60 (100%)	0.31	0 100 100	69, 78, 88, 92	0
28	BA	69/71 (97%)	0.59	2 (2%) 54 34	119, 124, 142, 145	0
28	GC	69/71 (97%)	0.82	5 (7%) 23 13	135, 143, 153, 154	0
29	CA	59/60 (98%)	-0.17	0 100 100	36, 58, 68, 71	0
29	HC	59/60 (98%)	0.16	1 (1%) 69 50	53, 77, 85, 87	0
30	DA	53/54 (98%)	0.17	0 100 100	61, 66, 69, 70	0
30	IC	53/54 (98%)	0.32	2 (3%) 44 26	74, 82, 85, 87	0
31	EA	48/49 (97%)	-0.15	0 100 100	38, 40, 47, 52	0
31	JC	48/49 (97%)	0.19	0 100 100	53, 57, 64, 71	0
32	FA	64/65 (98%)	0.07	1 (1%) 70 52	43, 49, 58, 59	0
32	KC	64/65 (98%)	0.67	8 (12%) 9 6	58, 65, 74, 74	0
33	GA	37/37 (100%)	0.20	0 100 100	55, 61, 67, 69	0
33	LC	37/37 (100%)	1.08	5 (13%) 8 5	85, 96, 105, 112	0
34	HA	10/27 (37%)	1.32	3 (30%) 1 1	81, 92, 108, 109	0
34	MC	10/27 (37%)	1.01	2 (20%) 3 2	89, 94, 109, 110	0
35	JA	258/368 (70%)	0.44	17 (6%) 26 15	61, 96, 121, 135	0
35	OC	258/368 (70%)	0.75	31 (12%) 10 6	88, 105, 134, 141	0
36	KA	234/256 (91%)	0.73	12 (5%) 34 20	109, 125, 145, 157	0
36	PC	234/256 (91%)	0.74	16 (6%) 25 14	101, 123, 139, 163	0
37	LA	206/239 (86%)	0.58	12 (5%) 30 18	104, 117, 133, 134	0
37	QC	206/239 (86%)	0.84	17 (8%) 19 10	100, 115, 131, 132	0
38	MA	208/209 (99%)	1.06	31 (14%) 7 3	89, 104, 113, 118	0
38	RC	208/209 (99%)	0.52	12 (5%) 30 18	74, 81, 88, 92	0
39	NA	151/162 (93%)	0.79	10 (6%) 26 15	82, 95, 103, 111	0
39	SC	151/162 (93%)	0.47	8 (5%) 33 20	73, 85, 92, 105	0
40	OA	101/101 (100%)	0.27	1 (0%) 79 64	75, 83, 91, 103	0
40	TC	101/101 (100%)	0.35	1 (0%) 79 64	87, 95, 100, 110	0
41	PA	155/156 (99%)	0.86	20 (12%) 9 5	103, 113, 119, 122	0
41	UC	155/156 (99%)	0.74	15 (9%) 15 8	102, 111, 118, 120	0
42	QA	138/138 (100%)	0.72	11 (7%) 20 11	83, 97, 104, 109	0
42	VC	138/138 (100%)	0.50	13 (9%) 15 9	73, 87, 95, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	RA	127/128 (99%)	1.62	42 (33%) 1 0	90, 141, 148, 151	0
43	WC	127/128 (99%)	1.24	22 (17%) 5 3	88, 135, 144, 148	0
44	SA	98/105 (93%)	1.71	34 (34%) 1 0	101, 144, 156, 156	0
44	XC	98/105 (93%)	1.51	23 (23%) 2 1	103, 139, 151, 153	0
45	TA	116/129 (89%)	0.62	6 (5%) 34 20	66, 84, 93, 97	0
45	YC	116/129 (89%)	0.56	9 (7%) 20 11	69, 90, 96, 103	0
46	UA	121/132 (91%)	0.53	6 (4%) 35 21	74, 79, 88, 93	0
46	ZC	121/132 (91%)	0.12	4 (3%) 49 30	67, 73, 80, 84	0
47	AD	117/126 (92%)	1.16	18 (15%) 6 3	98, 137, 141, 143	0
47	VA	117/126 (92%)	0.97	13 (11%) 12 7	94, 125, 130, 131	0
48	BD	60/61 (98%)	1.43	13 (21%) 3 1	108, 116, 133, 134	0
48	WA	60/61 (98%)	1.47	12 (20%) 3 2	110, 119, 127, 128	0
49	CD	88/89 (98%)	0.16	1 (1%) 77 61	70, 86, 94, 96	0
49	XA	88/89 (98%)	0.46	4 (4%) 39 23	66, 85, 94, 96	0
50	DD	83/88 (94%)	0.64	7 (8%) 18 10	73, 80, 94, 111	0
50	YA	83/88 (94%)	1.42	17 (20%) 3 2	96, 109, 126, 143	0
51	ED	99/105 (94%)	0.27	1 (1%) 79 64	69, 81, 87, 90	0
51	ZA	99/105 (94%)	0.46	4 (4%) 43 25	72, 88, 93, 94	0
52	AB	70/88 (79%)	0.25	1 (1%) 73 56	77, 88, 98, 101	0
52	FD	70/88 (79%)	0.42	4 (5%) 30 18	84, 94, 104, 109	0
53	BB	83/93 (89%)	0.97	6 (7%) 23 13	104, 130, 136, 138	0
53	GD	83/93 (89%)	1.50	21 (25%) 2 1	111, 139, 144, 146	0
54	CB	99/106 (93%)	1.66	32 (32%) 1 0	97, 111, 126, 128	0
54	HD	99/106 (93%)	0.92	13 (13%) 8 5	79, 97, 112, 114	0
55	DB	24/27 (88%)	2.73	18 (75%) 0 0	113, 123, 127, 132	0
55	ID	24/27 (88%)	2.17	14 (58%) 0 0	118, 127, 133, 138	0
All	All	21476/22228 (96%)	0.32	1162 (5%) 32 19	34, 82, 143, 256	0

The worst 5 of 1162 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
48	WA	2	ALA	9.5
1	FB	1001	G	8.2

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Mol	Chain	Res	Type	RSRZ
10	OB	83	ALA	7.6
44	XC	73	ASP	7.5
26	EC	1	MET	7.3

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	IB	55	20/21	0.61	0.15	182,183,184,184	0
4	4SU	D	8	20/21	0.62	0.11	163,164,165,165	0
4	5MU	IB	54	21/22	0.68	0.13	180,181,182,183	0
4	PSU	D	55	20/21	0.69	0.11	168,169,171,171	0
4	5MU	D	54	21/22	0.70	0.12	167,167,169,169	0
4	4SU	IB	8	20/21	0.71	0.10	169,170,170,170	0
4	5MC	D	32	21/22	0.75	0.14	139,139,139,139	0
4	5MU	NC	54	21/22	0.84	0.17	97,98,100,100	0
34	PSU	HA	19	20/21	0.85	0.13	87,87,88,88	0
1	PSU	A	516	20/21	0.87	0.11	90,92,95,95	0
1	2MG	A	1207	24/25	0.88	0.10	107,110,114,115	0
4	5MC	IA	32	21/22	0.88	0.12	84,84,85,85	0
4	5MU	IA	54	21/22	0.88	0.16	86,88,90,90	0
4	PSU	IA	55	20/21	0.88	0.13	87,88,90,90	0
1	2MG	FB	1207	24/25	0.88	0.11	108,110,113,114	0
34	PSU	MC	19	20/21	0.88	0.12	91,91,91,91	0
4	5MC	IB	32	21/22	0.89	0.11	147,147,148,148	0
4	PSU	NC	55	20/21	0.89	0.10	97,98,99,99	0
1	PSU	FB	516	20/21	0.90	0.10	83,84,87,87	0
1	5MC	FB	967	21/22	0.90	0.13	88,89,91,92	0
46	0TD	ZC	92	10/11	0.90	0.16	77,78,78,78	0
46	0TD	UA	92	10/11	0.90	0.19	81,81,81,81	0
2	PSU	GB	1911	20/21	0.90	0.11	72,75,76,77	0
1	7MG	FB	527	24/25	0.91	0.12	74,75,76,77	0
2	5MU	B	1915	21/22	0.91	0.09	75,77,79,79	0
4	5MC	NC	32	21/22	0.91	0.11	85,86,86,86	0
1	5MC	A	1400	21/22	0.91	0.12	80,82,85,86	0
1	4OC	A	1402	22/23	0.92	0.11	72,73,75,75	0
4	4SU	IA	8	20/21	0.92	0.10	84,86,86,87	0
1	M2G	FB	966	25/26	0.92	0.12	86,88,90,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PSU	GB	1917	20/21	0.92	0.08	77,79,81,82	0
2	2MA	GB	2503	23/24	0.92	0.12	51,52,53,53	0
2	5MU	GB	1915	21/22	0.93	0.07	88,89,91,92	0
4	4SU	NC	8	20/21	0.93	0.08	89,91,92,92	0
1	5MC	FB	1400	21/22	0.93	0.11	78,80,82,83	0
2	PSU	B	1911	20/21	0.93	0.11	63,65,67,67	0
1	4OC	FB	1402	22/23	0.94	0.10	73,74,75,75	0
2	PSU	B	1917	20/21	0.94	0.08	64,66,68,69	0
2	4OC	GB	1920	21/23	0.94	0.09	70,72,73,74	0
2	2MU	GB	2552	21/23	0.95	0.09	56,57,58,58	0
2	PSU	GB	2605	20/21	0.95	0.09	51,52,52,53	0
1	5MC	A	1404	21/22	0.95	0.09	64,66,67,67	0
1	5MC	FB	1404	21/22	0.95	0.11	65,66,66,66	0
1	UR3	FB	1498	21/22	0.95	0.12	70,70,71,71	0
1	MA6	FB	1519	24/25	0.95	0.10	63,65,66,66	0
2	4OC	B	1920	21/23	0.95	0.10	61,63,64,65	0
2	5MU	B	1939	21/22	0.95	0.11	44,45,46,46	0
1	5MC	A	1407	21/22	0.95	0.10	64,65,67,68	0
1	M2G	A	966	25/26	0.95	0.11	88,90,91,92	0
2	5MC	GB	1942	21/22	0.95	0.09	59,60,61,62	0
2	OMG	GB	2251	24/25	0.95	0.10	57,58,60,60	0
1	7MG	A	527	24/25	0.95	0.10	79,81,83,84	0
1	MA6	A	1519	24/25	0.96	0.09	60,63,64,64	0
1	5MC	A	967	21/22	0.96	0.08	90,91,93,93	0
2	5MU	GB	1939	21/22	0.96	0.11	53,54,54,55	0
1	UR3	A	1498	21/22	0.96	0.09	67,68,69,69	0
2	5MC	GB	1962	21/22	0.96	0.09	58,59,60,61	0
1	5MC	FB	1407	21/22	0.96	0.09	69,70,71,71	0
2	5MC	B	1942	21/22	0.96	0.08	49,50,51,51	0
2	OMG	B	2251	24/25	0.96	0.09	44,44,45,45	0
2	2MA	B	2503	23/24	0.96	0.09	37,38,38,38	0
2	PSU	B	2605	20/21	0.96	0.09	41,42,43,43	0
1	MA6	FB	1518	24/25	0.97	0.10	63,64,66,66	0
2	2MU	B	2552	21/23	0.97	0.09	45,46,47,47	0
1	MA6	A	1518	24/25	0.97	0.08	59,62,63,63	0
2	5MC	B	1962	21/22	0.97	0.07	50,52,53,54	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	B	3443	1/1	-0.68	0.29	176,176,176,176	0
56	MG	GB	3517	1/1	-0.63	0.30	219,219,219,219	0
56	MG	GB	3441	1/1	-0.54	0.30	155,155,155,155	0
56	MG	B	3402	1/1	-0.51	0.33	179,179,179,179	0
56	MG	GB	3293	1/1	-0.50	0.43	190,190,190,190	0
56	MG	B	3782	1/1	-0.48	0.43	175,175,175,175	0
56	MG	B	3798	1/1	-0.41	0.33	157,157,157,157	0
56	MG	B	3721	1/1	-0.36	0.38	147,147,147,147	0
56	MG	B	3669	1/1	-0.35	0.29	146,146,146,146	0
56	MG	GB	3478	1/1	-0.33	0.31	187,187,187,187	0
56	MG	B	3493	1/1	-0.33	0.34	182,182,182,182	0
56	MG	GB	3393	1/1	-0.31	0.26	192,192,192,192	0
56	MG	GB	3449	1/1	-0.31	0.31	197,197,197,197	0
56	MG	IB	104	1/1	-0.30	0.26	163,163,163,163	0
56	MG	GB	3585	1/1	-0.28	0.30	158,158,158,158	0
56	MG	GB	3188	1/1	-0.28	0.44	179,179,179,179	0
56	MG	GB	3472	1/1	-0.24	0.38	189,189,189,189	0
56	MG	B	3496	1/1	-0.24	0.19	167,167,167,167	0
56	MG	GB	3504	1/1	-0.24	0.22	195,195,195,195	0
56	MG	FB	1695	1/1	-0.14	0.38	156,156,156,156	0
56	MG	A	1877	1/1	-0.13	0.22	167,167,167,167	0
56	MG	GC	103	1/1	-0.13	0.34	135,135,135,135	0
56	MG	A	1702	1/1	-0.11	0.29	147,147,147,147	0
56	MG	A	1792	1/1	-0.09	0.41	132,132,132,132	0
56	MG	GB	3663	1/1	-0.08	0.30	206,206,206,206	0
56	MG	GB	3193	1/1	-0.08	0.27	141,141,141,141	0
56	MG	B	3648	1/1	-0.08	0.28	146,146,146,146	0
56	MG	HB	216	1/1	-0.05	0.29	136,136,136,136	0
56	MG	FB	1811	1/1	-0.03	0.28	143,143,143,143	0
56	MG	GB	2947	1/1	-0.02	0.51	109,109,109,109	0
56	MG	A	1804	1/1	-0.02	0.42	136,136,136,136	0
56	MG	GB	3383	1/1	-0.02	0.34	191,191,191,191	0
56	MG	B	3413	1/1	-0.01	0.24	140,140,140,140	0
56	MG	B	3353	1/1	0.00	0.31	173,173,173,173	0
56	MG	A	1870	1/1	0.02	0.23	123,123,123,123	0
56	MG	GB	3209	1/1	0.02	0.26	133,133,133,133	0
56	MG	B	3636	1/1	0.04	0.36	171,171,171,171	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	GB	3261	1/1	0.04	0.19	134,134,134,134	0
56	MG	B	3615	1/1	0.05	0.39	159,159,159,159	0
56	MG	FB	1871	1/1	0.06	0.36	114,114,114,114	0
56	MG	B	3298	1/1	0.07	0.31	168,168,168,168	0
56	MG	FB	1686	1/1	0.09	0.43	124,124,124,124	0
56	MG	A	1765	1/1	0.10	0.26	152,152,152,152	0
56	MG	GB	3586	1/1	0.10	0.28	187,187,187,187	0
56	MG	GB	3229	1/1	0.10	0.34	120,120,120,120	0
56	MG	FB	1876	1/1	0.11	0.20	170,170,170,170	0
56	MG	KA	303	1/1	0.11	0.19	130,130,130,130	0
56	MG	B	3667	1/1	0.12	0.25	145,145,145,145	0
56	MG	A	1760	1/1	0.13	0.36	136,136,136,136	0
56	MG	HB	208	1/1	0.15	0.25	126,126,126,126	0
56	MG	B	3389	1/1	0.16	0.32	124,124,124,124	0
56	MG	FB	1906	1/1	0.16	0.35	136,136,136,136	0
56	MG	GB	3207	1/1	0.16	0.23	126,126,126,126	0
56	MG	GB	3459	1/1	0.16	0.20	140,140,140,140	0
56	MG	FB	1727	1/1	0.16	0.33	141,141,141,141	0
56	MG	GB	3467	1/1	0.17	0.23	120,120,120,120	0
56	MG	FB	1647	1/1	0.18	0.25	143,143,143,143	0
56	MG	FB	1767	1/1	0.20	0.21	121,121,121,121	0
56	MG	A	1731	1/1	0.20	0.23	134,134,134,134	0
56	MG	B	3515	1/1	0.21	0.36	167,167,167,167	0
56	MG	FB	1870	1/1	0.21	0.18	127,127,127,127	0
56	MG	A	1874	1/1	0.23	0.41	126,126,126,126	0
56	MG	IB	103	1/1	0.23	0.14	146,146,146,146	0
56	MG	B	3791	1/1	0.23	0.26	139,139,139,139	0
56	MG	B	3749	1/1	0.23	0.24	130,130,130,130	0
56	MG	GB	3221	1/1	0.24	0.35	164,164,164,164	0
56	MG	A	1642	1/1	0.24	0.37	125,125,125,125	0
56	MG	QC	303	1/1	0.24	0.30	120,120,120,120	0
56	MG	FB	1861	1/1	0.25	0.22	119,119,119,119	0
56	MG	FB	1821	1/1	0.26	0.17	135,135,135,135	0
56	MG	A	1875	1/1	0.26	0.32	126,126,126,126	0
56	MG	XC	201	1/1	0.26	0.39	112,112,112,112	0
56	MG	FB	1786	1/1	0.27	0.27	119,119,119,119	0
56	MG	GB	3286	1/1	0.28	0.37	125,125,125,125	0
56	MG	B	3701	1/1	0.28	0.27	115,115,115,115	0
56	MG	FB	1709	1/1	0.28	0.38	130,130,130,130	0
56	MG	FB	1917	1/1	0.28	0.44	110,110,110,110	0
56	MG	GB	3476	1/1	0.28	0.35	130,130,130,130	0
56	MG	FB	1931	1/1	0.28	0.23	144,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	PC	303	1/1	0.29	0.24	133,133,133,133	0
56	MG	HB	207	1/1	0.30	0.47	107,107,107,107	0
56	MG	A	1845	1/1	0.30	0.45	107,107,107,107	0
56	MG	GB	3314	1/1	0.30	0.28	140,140,140,140	0
56	MG	FB	1826	1/1	0.31	0.20	143,143,143,143	0
56	MG	GB	3001	1/1	0.31	0.45	111,111,111,111	0
56	MG	GB	3139	1/1	0.31	0.33	125,125,125,125	0
56	MG	B	3787	1/1	0.32	0.24	132,132,132,132	0
56	MG	A	1669	1/1	0.32	0.59	114,114,114,114	0
56	MG	B	3685	1/1	0.32	0.34	117,117,117,117	0
56	MG	GB	3356	1/1	0.33	0.14	134,134,134,134	0
56	MG	LA	302	1/1	0.33	0.20	119,119,119,119	0
56	MG	B	3834	1/1	0.33	0.52	165,165,165,165	0
56	MG	GB	3270	1/1	0.33	0.26	97,97,97,97	0
56	MG	FB	1862	1/1	0.34	0.43	118,118,118,118	0
56	MG	OB	202	1/1	0.34	0.17	115,115,115,115	0
56	MG	GB	3230	1/1	0.34	0.30	110,110,110,110	0
56	MG	B	3445	1/1	0.35	0.30	116,116,116,116	0
56	MG	B	3795	1/1	0.35	0.26	151,151,151,151	0
56	MG	PC	302	1/1	0.36	0.32	104,104,104,104	0
56	MG	D	102	1/1	0.36	0.26	153,153,153,153	0
56	MG	GB	3651	1/1	0.37	0.18	130,130,130,130	0
56	MG	GB	3255	1/1	0.38	0.23	100,100,100,100	0
56	MG	FB	1806	1/1	0.38	0.23	135,135,135,135	0
56	MG	A	1882	1/1	0.38	0.33	104,104,104,104	0
56	MG	FB	1919	1/1	0.39	0.27	126,126,126,126	0
56	MG	HB	217	1/1	0.39	0.39	111,111,111,111	0
56	MG	B	3166	1/1	0.39	0.33	93,93,93,93	0
56	MG	B	3818	1/1	0.39	0.23	177,177,177,177	0
56	MG	GB	3465	1/1	0.39	0.24	114,114,114,114	0
56	MG	RA	201	1/1	0.40	0.39	123,123,123,123	0
56	MG	B	3342	1/1	0.42	0.16	115,115,115,115	0
56	MG	FB	1673	1/1	0.42	0.37	113,113,113,113	0
56	MG	SA	201	1/1	0.43	0.53	120,120,120,120	0
56	MG	FB	1792	1/1	0.43	0.20	165,165,165,165	0
56	MG	KA	302	1/1	0.43	0.23	123,123,123,123	0
56	MG	A	1885	1/1	0.44	0.22	135,135,135,135	0
56	MG	OC	407	1/1	0.44	0.19	109,109,109,109	0
56	MG	SC	205	1/1	0.44	0.13	99,99,99,99	0
56	MG	GB	3662	1/1	0.44	0.21	117,117,117,117	0
56	MG	GD	101	1/1	0.44	0.40	99,99,99,99	0
56	MG	B	3606	1/1	0.45	0.26	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	GB	3666	1/1	0.45	0.29	125,125,125,125	0
56	MG	NB	202	1/1	0.45	0.28	120,120,120,120	0
56	MG	GB	3426	1/1	0.45	0.34	117,117,117,117	0
56	MG	HB	221	1/1	0.47	0.42	114,114,114,114	0
56	MG	GC	102	1/1	0.47	0.21	127,127,127,127	0
56	MG	GB	3324	1/1	0.47	0.25	105,105,105,105	0
56	MG	PC	304	1/1	0.47	0.16	135,135,135,135	0
56	MG	B	3411	1/1	0.48	0.18	78,78,78,78	0
56	MG	WA	101	1/1	0.48	0.44	109,109,109,109	0
56	MG	B	3586	1/1	0.48	0.24	116,116,116,116	0
56	MG	A	1746	1/1	0.48	0.26	141,141,141,141	0
56	MG	MC	101	1/1	0.49	0.37	94,94,94,94	0
56	MG	B	3677	1/1	0.49	0.15	149,149,149,149	0
56	MG	BC	306	1/1	0.49	0.13	108,108,108,108	0
56	MG	PC	301	1/1	0.50	0.32	115,115,115,115	0
56	MG	A	1785	1/1	0.50	0.24	107,107,107,107	0
56	MG	MB	204	1/1	0.50	0.24	115,115,115,115	0
56	MG	B	3629	1/1	0.50	0.20	125,125,125,125	0
56	MG	RA	202	1/1	0.51	0.58	117,117,117,117	0
56	MG	FB	1613	1/1	0.51	0.39	80,80,80,80	0
56	MG	FB	1943	1/1	0.51	0.22	105,105,105,105	0
56	MG	FB	1899	1/1	0.52	0.27	86,86,86,86	0
56	MG	NB	201	1/1	0.52	0.39	130,130,130,130	0
56	MG	OC	403	1/1	0.52	0.20	112,112,112,112	0
56	MG	A	1710	1/1	0.53	0.20	135,135,135,135	0
56	MG	NA	201	1/1	0.53	0.33	100,100,100,100	0
56	MG	FB	1663	1/1	0.53	0.23	156,156,156,156	0
56	MG	FB	1925	1/1	0.53	0.11	147,147,147,147	0
56	MG	GB	3086	1/1	0.53	0.30	107,107,107,107	0
56	MG	FB	1631	1/1	0.54	0.46	96,96,96,96	0
56	MG	A	1801	1/1	0.54	0.12	97,97,97,97	0
56	MG	HB	204	1/1	0.54	0.34	91,91,91,91	0
56	MG	B	3707	1/1	0.54	0.14	113,113,113,113	0
56	MG	GB	3632	1/1	0.54	0.20	130,130,130,130	0
56	MG	WC	202	1/1	0.54	0.22	121,121,121,121	0
56	MG	A	1688	1/1	0.54	0.36	82,82,82,82	0
56	MG	FB	1732	1/1	0.54	0.34	105,105,105,105	0
56	MG	FB	1885	1/1	0.55	0.38	115,115,115,115	0
56	MG	GB	3540	1/1	0.55	0.36	115,115,115,115	0
56	MG	A	1824	1/1	0.55	0.24	111,111,111,111	0
56	MG	FB	1791	1/1	0.55	0.29	105,105,105,105	0
56	MG	BC	302	1/1	0.56	0.23	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3485	1/1	0.56	0.22	117,117,117,117	0
56	MG	GB	3059	1/1	0.56	0.39	91,91,91,91	0
56	MG	A	1799	1/1	0.56	0.40	118,118,118,118	0
56	MG	XA	101	1/1	0.56	0.09	86,86,86,86	0
56	MG	A	1613	1/1	0.56	0.18	79,79,79,79	0
56	MG	GB	3445	1/1	0.56	0.21	122,122,122,122	0
56	MG	B	3291	1/1	0.56	0.18	109,109,109,109	0
56	MG	OC	402	1/1	0.57	0.21	110,110,110,110	0
56	MG	FB	1807	1/1	0.57	0.33	97,97,97,97	0
56	MG	FB	1918	1/1	0.57	0.18	92,92,92,92	0
56	MG	VA	203	1/1	0.57	0.39	102,102,102,102	0
56	MG	A	1724	1/1	0.57	0.38	68,68,68,68	0
56	MG	A	1696	1/1	0.57	0.24	157,157,157,157	0
56	MG	HB	210	1/1	0.58	0.21	114,114,114,114	0
56	MG	B	3541	1/1	0.58	0.20	120,120,120,120	0
56	MG	GB	3452	1/1	0.58	0.25	74,74,74,74	0
56	MG	BC	305	1/1	0.58	0.23	110,110,110,110	0
56	MG	BA	104	1/1	0.58	0.20	105,105,105,105	0
56	MG	HB	230	1/1	0.58	0.17	131,131,131,131	0
56	MG	A	1725	1/1	0.58	0.31	114,114,114,114	0
56	MG	GB	3299	1/1	0.58	0.13	134,134,134,134	0
56	MG	GB	2943	1/1	0.58	0.39	92,92,92,92	0
56	MG	GB	3101	1/1	0.58	0.35	115,115,115,115	0
56	MG	A	1864	1/1	0.59	0.15	138,138,138,138	0
56	MG	GB	2945	1/1	0.59	0.31	92,92,92,92	0
56	MG	FB	1915	1/1	0.59	0.16	87,87,87,87	0
56	MG	FB	1741	1/1	0.59	0.26	127,127,127,127	0
56	MG	GB	3357	1/1	0.59	0.17	152,152,152,152	0
56	MG	FB	1697	1/1	0.59	0.37	94,94,94,94	0
56	MG	GB	3607	1/1	0.60	0.25	111,111,111,111	0
56	MG	GB	3220	1/1	0.60	0.25	121,121,121,121	0
56	MG	GB	3420	1/1	0.60	0.33	99,99,99,99	0
56	MG	FB	1678	1/1	0.60	0.25	70,70,70,70	0
56	MG	B	3550	1/1	0.60	0.20	147,147,147,147	0
56	MG	HB	218	1/1	0.60	0.29	116,116,116,116	0
56	MG	A	1621	1/1	0.60	0.42	85,85,85,85	0
56	MG	RA	204	1/1	0.60	0.11	137,137,137,137	0
56	MG	A	1677	1/1	0.61	0.25	105,105,105,105	0
56	MG	GB	3243	1/1	0.61	0.31	93,93,93,93	0
56	MG	A	1737	1/1	0.61	0.24	106,106,106,106	0
56	MG	A	1713	1/1	0.61	0.33	88,88,88,88	0
56	MG	FB	1868	1/1	0.61	0.33	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	GB	3675	1/1	0.61	0.18	134,134,134,134	0
56	MG	GB	3705	1/1	0.61	0.32	104,104,104,104	0
56	MG	UC	201	1/1	0.61	0.29	105,105,105,105	0
56	MG	FB	1939	1/1	0.61	0.45	98,98,98,98	0
56	MG	RA	203	1/1	0.61	0.57	119,119,119,119	0
56	MG	B	3796	1/1	0.61	0.23	113,113,113,113	0
56	MG	HB	222	1/1	0.62	0.24	108,108,108,108	0
56	MG	B	3023	1/1	0.62	0.27	75,75,75,75	0
56	MG	A	1851	1/1	0.62	0.18	117,117,117,117	0
56	MG	JA	412	1/1	0.62	0.14	107,107,107,107	0
56	MG	MB	203	1/1	0.62	0.48	116,116,116,116	0
56	MG	A	1812	1/1	0.62	0.32	128,128,128,128	0
56	MG	HB	206	1/1	0.62	0.29	118,118,118,118	0
56	MG	FB	1724	1/1	0.62	0.21	142,142,142,142	0
56	MG	A	1749	1/1	0.62	0.32	110,110,110,110	0
56	MG	A	1631	1/1	0.62	0.56	98,98,98,98	0
56	MG	C	239	1/1	0.62	0.16	87,87,87,87	0
56	MG	GB	3656	1/1	0.62	0.17	93,93,93,93	0
56	MG	FB	1753	1/1	0.62	0.30	92,92,92,92	0
56	MG	GB	2944	1/1	0.62	0.34	90,90,90,90	0
56	MG	A	1828	1/1	0.63	0.25	106,106,106,106	0
56	MG	W	303	1/1	0.63	0.16	87,87,87,87	0
56	MG	GB	3419	1/1	0.63	0.09	74,74,74,74	0
56	MG	GB	3218	1/1	0.63	0.29	61,61,61,61	0
56	MG	A	1714	1/1	0.63	0.38	97,97,97,97	0
56	MG	FB	1835	1/1	0.63	0.22	104,104,104,104	0
56	MG	VA	202	1/1	0.63	0.28	100,100,100,100	0
56	MG	PA	201	1/1	0.63	0.13	99,99,99,99	0
56	MG	GB	3338	1/1	0.63	0.12	71,71,71,71	0
56	MG	B	3674	1/1	0.63	0.14	131,131,131,131	0
56	MG	D	101	1/1	0.63	0.29	100,100,100,100	0
56	MG	B	3279	1/1	0.64	0.25	75,75,75,75	0
56	MG	GB	3447	1/1	0.64	0.18	199,199,199,199	0
56	MG	GB	3361	1/1	0.64	0.22	91,91,91,91	0
56	MG	B	3405	1/1	0.64	0.17	124,124,124,124	0
56	MG	FB	1896	1/1	0.64	0.16	82,82,82,82	0
56	MG	QC	301	1/1	0.64	0.29	97,97,97,97	0
56	MG	A	1815	1/1	0.64	0.23	108,108,108,108	0
56	MG	HB	203	1/1	0.64	0.27	101,101,101,101	0
56	MG	FB	1720	1/1	0.64	0.23	81,81,81,81	0
56	MG	GB	3626	1/1	0.64	0.19	81,81,81,81	0
56	MG	B	3554	1/1	0.64	0.15	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3574	1/1	0.64	0.15	117,117,117,117	0
56	MG	A	1649	1/1	0.65	0.30	101,101,101,101	0
56	MG	GB	3592	1/1	0.65	0.20	116,116,116,116	0
56	MG	GB	3022	1/1	0.65	0.43	63,63,63,63	0
56	MG	ZA	201	1/1	0.65	0.24	85,85,85,85	0
56	MG	FB	1758	1/1	0.65	0.42	129,129,129,129	0
56	MG	A	1670	1/1	0.65	0.22	122,122,122,122	0
56	MG	BC	307	1/1	0.65	0.23	104,104,104,104	0
56	MG	SA	202	1/1	0.65	0.37	125,125,125,125	0
56	MG	GB	3048	1/1	0.66	0.20	64,64,64,64	0
56	MG	GB	3360	1/1	0.66	0.22	84,84,84,84	0
56	MG	W	304	1/1	0.66	0.20	82,82,82,82	0
56	MG	B	3349	1/1	0.66	0.25	132,132,132,132	0
56	MG	FB	1932	1/1	0.66	0.25	89,89,89,89	0
56	MG	A	1727	1/1	0.66	0.31	92,92,92,92	0
56	MG	GB	3682	1/1	0.66	0.22	77,77,77,77	0
56	MG	GB	3170	1/1	0.66	0.24	77,77,77,77	0
56	MG	B	3378	1/1	0.66	0.20	111,111,111,111	0
56	MG	A	1686	1/1	0.66	0.21	87,87,87,87	0
56	MG	P	201	1/1	0.66	0.12	82,82,82,82	0
56	MG	FB	1717	1/1	0.66	0.36	74,74,74,74	0
56	MG	A	1833	1/1	0.66	0.54	116,116,116,116	0
56	MG	GB	3622	1/1	0.66	0.29	105,105,105,105	0
56	MG	NA	202	1/1	0.66	0.24	101,101,101,101	0
56	MG	FB	1800	1/1	0.66	0.31	92,92,92,92	0
56	MG	GB	3668	1/1	0.67	0.33	68,68,68,68	0
56	MG	YB	203	1/1	0.67	0.20	86,86,86,86	0
56	MG	FB	1902	1/1	0.67	0.17	132,132,132,132	0
56	MG	GB	3219	1/1	0.67	0.26	85,85,85,85	0
56	MG	A	1757	1/1	0.67	0.20	118,118,118,118	0
56	MG	A	1773	1/1	0.67	0.37	88,88,88,88	0
56	MG	GB	3227	1/1	0.67	0.27	95,95,95,95	0
56	MG	GB	3528	1/1	0.67	0.14	79,79,79,79	0
56	MG	B	3283	1/1	0.67	0.25	92,92,92,92	0
56	MG	GB	3571	1/1	0.67	0.16	66,66,66,66	0
56	MG	FB	1864	1/1	0.67	0.21	103,103,103,103	0
56	MG	A	1800	1/1	0.67	0.23	132,132,132,132	0
56	MG	GB	3250	1/1	0.67	0.23	77,77,77,77	0
56	MG	A	1778	1/1	0.67	0.32	104,104,104,104	0
56	MG	GB	3257	1/1	0.67	0.18	86,86,86,86	0
56	MG	FB	1730	1/1	0.67	0.19	78,78,78,78	0
56	MG	C	233	1/1	0.67	0.30	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	QA	202	1/1	0.67	0.18	100,100,100,100	0
56	MG	GB	3654	1/1	0.67	0.19	72,72,72,72	0
56	MG	FB	1891	1/1	0.67	0.17	132,132,132,132	0
56	MG	GB	2940	1/1	0.67	0.31	79,79,79,79	0
56	MG	IA	108	1/1	0.67	0.28	82,82,82,82	0
56	MG	A	1715	1/1	0.67	0.17	102,102,102,102	0
56	MG	A	1740	1/1	0.68	0.20	80,80,80,80	0
56	MG	C	240	1/1	0.68	0.19	75,75,75,75	0
56	MG	FB	1893	1/1	0.68	0.31	86,86,86,86	0
56	MG	UB	201	1/1	0.68	0.28	99,99,99,99	0
56	MG	B	3328	1/1	0.68	0.22	72,72,72,72	0
56	MG	GB	3353	1/1	0.68	0.26	68,68,68,68	0
56	MG	A	1813	1/1	0.68	0.14	89,89,89,89	0
56	MG	B	3792	1/1	0.68	0.18	100,100,100,100	0
56	MG	B	3235	1/1	0.68	0.23	72,72,72,72	0
56	MG	GB	3006	1/1	0.68	0.34	83,83,83,83	0
56	MG	B	3634	1/1	0.68	0.26	106,106,106,106	0
56	MG	GB	3039	1/1	0.68	0.27	52,52,52,52	0
56	MG	GB	3394	1/1	0.68	0.18	77,77,77,77	0
56	MG	A	1745	1/1	0.68	0.25	78,78,78,78	0
56	MG	HB	213	1/1	0.68	0.18	122,122,122,122	0
56	MG	HB	214	1/1	0.68	0.34	107,107,107,107	0
56	MG	GB	3589	1/1	0.68	0.24	94,94,94,94	0
56	MG	FB	1755	1/1	0.68	0.14	70,70,70,70	0
56	MG	GB	3424	1/1	0.68	0.17	128,128,128,128	0
56	MG	GB	3614	1/1	0.68	0.13	139,139,139,139	0
56	MG	A	1668	1/1	0.68	0.39	80,80,80,80	0
56	MG	JA	410	1/1	0.68	0.10	96,96,96,96	0
56	MG	A	1808	1/1	0.68	0.24	94,94,94,94	0
56	MG	C	231	1/1	0.68	0.21	89,89,89,89	0
56	MG	GB	3179	1/1	0.68	0.26	69,69,69,69	0
56	MG	YC	206	1/1	0.68	0.18	88,88,88,88	0
56	MG	B	3758	1/1	0.68	0.20	80,80,80,80	0
56	MG	DA	104	1/1	0.69	0.10	71,71,71,71	0
56	MG	GB	3487	1/1	0.69	0.17	79,79,79,79	0
56	MG	FB	1722	1/1	0.69	0.16	101,101,101,101	0
56	MG	FB	1616	1/1	0.69	0.30	87,87,87,87	0
56	MG	GB	3376	1/1	0.69	0.40	90,90,90,90	0
56	MG	MA	303	1/1	0.69	0.20	101,101,101,101	0
56	MG	EC	103	1/1	0.69	0.16	90,90,90,90	0
56	MG	GB	3385	1/1	0.69	0.26	98,98,98,98	0
56	MG	FB	1633	1/1	0.69	0.45	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	A	1775	1/1	0.69	0.22	96,96,96,96	0
56	MG	JA	408	1/1	0.69	0.25	97,97,97,97	0
56	MG	FB	1748	1/1	0.69	0.22	116,116,116,116	0
56	MG	GB	3603	1/1	0.69	0.18	101,101,101,101	0
56	MG	VA	201	1/1	0.69	0.23	123,123,123,123	0
56	MG	B	3241	1/1	0.69	0.14	77,77,77,77	0
56	MG	PA	202	1/1	0.69	0.22	102,102,102,102	0
56	MG	FB	1869	1/1	0.69	0.23	109,109,109,109	0
56	MG	A	1872	1/1	0.69	0.19	111,111,111,111	0
56	MG	GB	3298	1/1	0.69	0.28	80,80,80,80	0
56	MG	FB	1940	1/1	0.69	0.19	94,94,94,94	0
56	MG	A	1630	1/1	0.69	0.47	88,88,88,88	0
56	MG	GB	2923	1/1	0.69	0.34	62,62,62,62	0
56	MG	XA	102	1/1	0.69	0.19	88,88,88,88	0
56	MG	B	3644	1/1	0.69	0.16	146,146,146,146	0
56	MG	FB	1793	1/1	0.69	0.38	98,98,98,98	0
56	MG	B	3009	1/1	0.70	0.28	72,72,72,72	0
56	MG	A	1831	1/1	0.70	0.27	96,96,96,96	0
56	MG	A	1747	1/1	0.70	0.11	104,104,104,104	0
56	MG	B	3767	1/1	0.70	0.11	60,60,60,60	0
56	MG	GB	3235	1/1	0.70	0.14	57,57,57,57	0
56	MG	BC	304	1/1	0.70	0.26	91,91,91,91	0
56	MG	FB	1681	1/1	0.70	0.29	99,99,99,99	0
56	MG	GB	3531	1/1	0.70	0.21	106,106,106,106	0
56	MG	IB	102	1/1	0.70	0.20	112,112,112,112	0
56	MG	B	3188	1/1	0.70	0.29	74,74,74,74	0
56	MG	A	1816	1/1	0.70	0.22	108,108,108,108	0
56	MG	FB	1643	1/1	0.70	0.33	94,94,94,94	0
56	MG	GB	2971	1/1	0.70	0.53	93,93,93,93	0
56	MG	GB	3423	1/1	0.70	0.24	75,75,75,75	0
56	MG	A	1847	1/1	0.71	0.24	93,93,93,93	0
56	MG	GB	3462	1/1	0.71	0.18	101,101,101,101	0
56	MG	EC	101	1/1	0.71	0.18	95,95,95,95	0
56	MG	FB	1938	1/1	0.71	0.13	104,104,104,104	0
56	MG	A	1610	1/1	0.71	0.42	78,78,78,78	0
56	MG	A	1615	1/1	0.71	0.41	89,89,89,89	0
56	MG	A	1719	1/1	0.71	0.20	101,101,101,101	0
56	MG	GB	3111	1/1	0.71	0.33	66,66,66,66	0
56	MG	H	201	1/1	0.71	0.23	79,79,79,79	0
56	MG	FB	1703	1/1	0.71	0.24	86,86,86,86	0
56	MG	FB	1629	1/1	0.71	0.37	66,66,66,66	0
56	MG	GB	3265	1/1	0.71	0.36	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	2991	1/1	0.71	0.32	56,56,56,56	0
56	MG	B	3567	1/1	0.71	0.19	106,106,106,106	0
56	MG	GB	3701	1/1	0.71	0.19	70,70,70,70	0
56	MG	A	1676	1/1	0.71	0.27	80,80,80,80	0
56	MG	A	1695	1/1	0.71	0.21	71,71,71,71	0
56	MG	GB	2995	1/1	0.71	0.16	58,58,58,58	0
56	MG	FB	1920	1/1	0.71	0.18	70,70,70,70	0
56	MG	B	3778	1/1	0.71	0.23	67,67,67,67	0
56	MG	B	3392	1/1	0.71	0.21	78,78,78,78	0
56	MG	GB	3224	1/1	0.71	0.27	61,61,61,61	0
56	MG	QA	201	1/1	0.72	0.14	106,106,106,106	0
56	MG	IA	109	1/1	0.72	0.11	79,79,79,79	0
56	MG	A	1830	1/1	0.72	0.16	67,67,67,67	0
56	MG	NC	111	1/1	0.72	0.17	87,87,87,87	0
56	MG	GB	3599	1/1	0.72	0.23	101,101,101,101	0
56	MG	GB	3146	1/1	0.72	0.21	67,67,67,67	0
56	MG	A	1803	1/1	0.72	0.17	103,103,103,103	0
56	MG	B	3525	1/1	0.72	0.25	64,64,64,64	0
56	MG	NA	203	1/1	0.72	0.13	98,98,98,98	0
56	MG	A	1722	1/1	0.72	0.26	98,98,98,98	0
56	MG	GB	3498	1/1	0.72	0.14	74,74,74,74	0
56	MG	HB	212	1/1	0.72	0.23	85,85,85,85	0
56	MG	GB	3351	1/1	0.72	0.26	83,83,83,83	0
56	MG	RC	308	1/1	0.72	0.15	83,83,83,83	0
56	MG	RC	310	1/1	0.72	0.26	83,83,83,83	0
56	MG	GB	3202	1/1	0.72	0.21	101,101,101,101	0
56	MG	A	1607	1/1	0.72	0.39	76,76,76,76	0
56	MG	GB	3065	1/1	0.72	0.37	95,95,95,95	0
56	MG	GB	3084	1/1	0.72	0.28	79,79,79,79	0
56	MG	FB	1615	1/1	0.72	0.43	87,87,87,87	0
56	MG	GB	3373	1/1	0.72	0.28	85,85,85,85	0
56	MG	B	3280	1/1	0.73	0.24	87,87,87,87	0
56	MG	B	3540	1/1	0.73	0.12	85,85,85,85	0
56	MG	B	3762	1/1	0.73	0.10	71,71,71,71	0
56	MG	I	204	1/1	0.73	0.12	68,68,68,68	0
56	MG	A	1753	1/1	0.73	0.37	84,84,84,84	0
56	MG	FB	1766	1/1	0.73	0.41	84,84,84,84	0
56	MG	NC	103	1/1	0.73	0.24	84,84,84,84	0
56	MG	B	3547	1/1	0.73	0.14	90,90,90,90	0
56	MG	FB	1779	1/1	0.73	0.16	88,88,88,88	0
56	MG	FB	1704	1/1	0.73	0.46	93,93,93,93	0
56	MG	FB	1628	1/1	0.73	0.35	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	GB	3541	1/1	0.73	0.21	64,64,64,64	0
56	MG	C	208	1/1	0.73	0.30	81,81,81,81	0
56	MG	GB	3689	1/1	0.73	0.19	67,67,67,67	0
56	MG	A	1678	1/1	0.73	0.32	97,97,97,97	0
56	MG	TA	201	1/1	0.73	0.20	92,92,92,92	0
56	MG	B	3039	1/1	0.73	0.30	50,50,50,50	0
56	MG	A	1672	1/1	0.73	0.66	105,105,105,105	0
56	MG	VB	202	1/1	0.73	0.20	80,80,80,80	0
56	MG	WB	203	1/1	0.73	0.15	87,87,87,87	0
56	MG	GB	3596	1/1	0.73	0.39	90,90,90,90	0
56	MG	GB	3358	1/1	0.73	0.11	87,87,87,87	0
56	MG	B	3418	1/1	0.73	0.28	76,76,76,76	0
56	MG	GB	3162	1/1	0.73	0.26	101,101,101,101	0
56	MG	IA	118	1/1	0.73	0.10	67,67,67,67	0
56	MG	GB	3685	1/1	0.74	0.28	70,70,70,70	0
56	MG	GB	2982	1/1	0.74	0.17	67,67,67,67	0
56	MG	A	1849	1/1	0.74	0.37	88,88,88,88	0
56	MG	A	1850	1/1	0.74	0.20	117,117,117,117	0
56	MG	GB	3281	1/1	0.74	0.17	72,72,72,72	0
56	MG	GB	3562	1/1	0.74	0.08	57,57,57,57	0
56	MG	A	1667	1/1	0.74	0.31	82,82,82,82	0
56	MG	A	1852	1/1	0.74	0.25	96,96,96,96	0
56	MG	A	1859	1/1	0.74	0.33	90,90,90,90	0
56	MG	A	1648	1/1	0.74	0.39	100,100,100,100	0
56	MG	HB	211	1/1	0.74	0.28	87,87,87,87	0
56	MG	GB	3300	1/1	0.74	0.13	90,90,90,90	0
56	MG	NC	101	1/1	0.74	0.27	85,85,85,85	0
56	MG	B	3151	1/1	0.74	0.22	55,55,55,55	0
56	MG	GB	3442	1/1	0.74	0.14	194,194,194,194	0
56	MG	HB	215	1/1	0.74	0.23	109,109,109,109	0
56	MG	GB	3317	1/1	0.74	0.19	70,70,70,70	0
56	MG	FB	1740	1/1	0.74	0.20	96,96,96,96	0
56	MG	GB	3328	1/1	0.74	0.23	75,75,75,75	0
56	MG	A	1605	1/1	0.74	0.27	67,67,67,67	0
56	MG	GB	3344	1/1	0.74	0.20	77,77,77,77	0
56	MG	FB	1747	1/1	0.74	0.24	101,101,101,101	0
56	MG	GB	3095	1/1	0.74	0.31	63,63,63,63	0
56	MG	FB	1815	1/1	0.74	0.22	79,79,79,79	0
56	MG	A	1666	1/1	0.74	0.42	80,80,80,80	0
56	MG	GB	3657	1/1	0.74	0.14	101,101,101,101	0
56	MG	GB	3136	1/1	0.74	0.32	71,71,71,71	0
56	MG	A	1679	1/1	0.74	0.23	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	P	202	1/1	0.74	0.11	94,94,94,94	0
56	MG	GB	3362	1/1	0.74	0.24	76,76,76,76	0
56	MG	XC	202	1/1	0.74	0.33	113,113,113,113	0
56	MG	A	1708	1/1	0.74	0.32	79,79,79,79	0
56	MG	AD	201	1/1	0.74	0.11	80,80,80,80	0
56	MG	A	1709	1/1	0.74	0.47	83,83,83,83	0
56	MG	GB	3329	1/1	0.75	0.23	85,85,85,85	0
56	MG	B	3827	1/1	0.75	0.09	64,64,64,64	0
56	MG	GB	3659	1/1	0.75	0.34	80,80,80,80	0
56	MG	AA	104	1/1	0.75	0.16	75,75,75,75	0
56	MG	A	1829	1/1	0.75	0.25	109,109,109,109	0
56	MG	C	201	1/1	0.75	0.23	67,67,67,67	0
56	MG	C	205	1/1	0.75	0.32	68,68,68,68	0
56	MG	A	1744	1/1	0.75	0.14	87,87,87,87	0
56	MG	GB	3489	1/1	0.75	0.22	65,65,65,65	0
56	MG	GB	3030	1/1	0.75	0.39	88,88,88,88	0
56	MG	GB	3033	1/1	0.75	0.28	79,79,79,79	0
56	MG	BC	309	1/1	0.75	0.27	98,98,98,98	0
56	MG	A	1690	1/1	0.75	0.19	94,94,94,94	0
56	MG	GB	3524	1/1	0.75	0.16	83,83,83,83	0
56	MG	FC	101	1/1	0.75	0.14	87,87,87,87	0
56	MG	FB	1726	1/1	0.75	0.36	94,94,94,94	0
56	MG	B	3590	1/1	0.75	0.27	95,95,95,95	0
56	MG	GB	3537	1/1	0.75	0.12	93,93,93,93	0
56	MG	FB	1636	1/1	0.75	0.58	98,98,98,98	0
56	MG	FB	1824	1/1	0.75	0.22	70,70,70,70	0
56	MG	NC	105	1/1	0.75	0.21	94,94,94,94	0
56	MG	GB	3555	1/1	0.75	0.14	72,72,72,72	0
56	MG	FB	1642	1/1	0.75	0.53	104,104,104,104	0
56	MG	GB	3389	1/1	0.75	0.17	74,74,74,74	0
56	MG	GB	3576	1/1	0.75	0.30	70,70,70,70	0
56	MG	B	3273	1/1	0.75	0.34	76,76,76,76	0
56	MG	FB	1848	1/1	0.75	0.35	76,76,76,76	0
56	MG	FB	1646	1/1	0.75	0.28	81,81,81,81	0
56	MG	GB	3117	1/1	0.75	0.41	82,82,82,82	0
56	MG	A	1795	1/1	0.75	0.22	110,110,110,110	0
56	MG	B	3695	1/1	0.75	0.12	71,71,71,71	0
56	MG	GB	3142	1/1	0.75	0.23	50,50,50,50	0
56	MG	HB	226	1/1	0.75	0.24	105,105,105,105	0
56	MG	A	1682	1/1	0.75	0.20	98,98,98,98	0
56	MG	A	1878	1/1	0.75	0.44	101,101,101,101	0
56	MG	B	3719	1/1	0.75	0.23	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3461	1/1	0.75	0.09	56,56,56,56	0
56	MG	MB	202	1/1	0.75	0.25	110,110,110,110	0
56	MG	B	3799	1/1	0.75	0.11	89,89,89,89	0
56	MG	FB	1884	1/1	0.75	0.15	87,87,87,87	0
56	MG	A	1782	1/1	0.75	0.18	130,130,130,130	0
56	MG	A	1685	1/1	0.76	0.15	76,76,76,76	0
56	MG	GB	3535	1/1	0.76	0.19	83,83,83,83	0
56	MG	A	1764	1/1	0.76	0.33	85,85,85,85	0
56	MG	A	1788	1/1	0.76	0.16	76,76,76,76	0
56	MG	GB	3703	1/1	0.76	0.11	70,70,70,70	0
56	MG	B	3807	1/1	0.76	0.19	92,92,92,92	0
56	MG	GB	3706	1/1	0.76	0.25	83,83,83,83	0
56	MG	GB	3554	1/1	0.76	0.17	71,71,71,71	0
56	MG	OA	202	1/1	0.76	0.26	78,78,78,78	0
56	MG	B	3307	1/1	0.76	0.15	81,81,81,81	0
56	MG	B	3214	1/1	0.76	0.27	83,83,83,83	0
56	MG	FB	1644	1/1	0.76	0.21	81,81,81,81	0
56	MG	H	203	1/1	0.76	0.14	89,89,89,89	0
56	MG	A	1789	1/1	0.76	0.19	87,87,87,87	0
56	MG	HC	103	1/1	0.76	0.10	90,90,90,90	0
56	MG	A	1777	1/1	0.76	0.17	91,91,91,91	0
56	MG	FB	1671	1/1	0.76	0.24	87,87,87,87	0
56	MG	FB	1602	1/1	0.76	0.34	66,66,66,66	0
56	MG	FB	1908	1/1	0.76	0.29	65,65,65,65	0
56	MG	FB	1911	1/1	0.76	0.45	110,110,110,110	0
56	MG	FB	1605	1/1	0.76	0.25	70,70,70,70	0
56	MG	B	3010	1/1	0.76	0.35	77,77,77,77	0
56	MG	FB	1837	1/1	0.76	0.35	91,91,91,91	0
56	MG	GB	3038	1/1	0.76	0.18	71,71,71,71	0
56	MG	GB	3223	1/1	0.76	0.09	81,81,81,81	0
56	MG	GB	3648	1/1	0.76	0.14	88,88,88,88	0
56	MG	FB	1843	1/1	0.76	0.09	85,85,85,85	0
56	MG	FB	1614	1/1	0.76	0.24	70,70,70,70	0
56	MG	QC	302	1/1	0.76	0.39	103,103,103,103	0
56	MG	A	1612	1/1	0.76	0.23	54,54,54,54	0
56	MG	KB	301	1/1	0.76	0.36	62,62,62,62	0
56	MG	A	1780	1/1	0.76	0.15	83,83,83,83	0
56	MG	FB	1699	1/1	0.76	0.20	86,86,86,86	0
56	MG	GB	3240	1/1	0.76	0.20	106,106,106,106	0
56	MG	MB	206	1/1	0.76	0.16	127,127,127,127	0
56	MG	FB	1933	1/1	0.76	0.29	126,126,126,126	0
56	MG	GB	3375	1/1	0.76	0.23	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	FB	1936	1/1	0.76	0.27	87,87,87,87	0
56	MG	SB	201	1/1	0.76	0.28	77,77,77,77	0
56	MG	GB	3378	1/1	0.76	0.14	74,74,74,74	0
56	MG	A	1837	1/1	0.77	0.21	124,124,124,124	0
56	MG	F	315	1/1	0.77	0.14	67,67,67,67	0
56	MG	A	1840	1/1	0.77	0.20	65,65,65,65	0
56	MG	B	3627	1/1	0.77	0.12	56,56,56,56	0
56	MG	MA	304	1/1	0.77	0.14	96,96,96,96	0
56	MG	GB	3088	1/1	0.77	0.25	60,60,60,60	0
56	MG	A	1787	1/1	0.77	0.13	77,77,77,77	0
56	MG	FB	1768	1/1	0.77	0.12	80,80,80,80	0
56	MG	B	3815	1/1	0.77	0.14	61,61,61,61	0
56	MG	FB	1872	1/1	0.77	0.12	87,87,87,87	0
56	MG	GB	2921	1/1	0.77	0.52	72,72,72,72	0
56	MG	NC	104	1/1	0.77	0.23	93,93,93,93	0
56	MG	A	1814	1/1	0.77	0.14	92,92,92,92	0
56	MG	B	3823	1/1	0.77	0.06	92,92,92,92	0
56	MG	A	1741	1/1	0.77	0.28	73,73,73,73	0
56	MG	B	3375	1/1	0.77	0.33	79,79,79,79	0
56	MG	OC	405	1/1	0.77	0.22	91,91,91,91	0
56	MG	GB	3674	1/1	0.77	0.12	84,84,84,84	0
56	MG	A	1809	1/1	0.77	0.41	97,97,97,97	0
56	MG	GB	3395	1/1	0.77	0.18	81,81,81,81	0
56	MG	B	3294	1/1	0.77	0.29	75,75,75,75	0
56	MG	MB	207	1/1	0.77	0.20	105,105,105,105	0
56	MG	IA	103	1/1	0.77	0.22	76,76,76,76	0
56	MG	B	3297	1/1	0.77	0.17	50,50,50,50	0
56	MG	A	1717	1/1	0.77	0.30	86,86,86,86	0
56	MG	GB	3425	1/1	0.77	0.28	58,58,58,58	0
56	MG	B	3790	1/1	0.77	0.23	62,62,62,62	0
56	MG	GB	3319	1/1	0.77	0.19	84,84,84,84	0
56	MG	VB	207	1/1	0.77	0.12	83,83,83,83	0
56	MG	UC	202	1/1	0.77	0.23	105,105,105,105	0
56	MG	JA	405	1/1	0.77	0.35	91,91,91,91	0
56	MG	B	3511	1/1	0.77	0.15	65,65,65,65	0
56	MG	FB	1832	1/1	0.77	0.29	76,76,76,76	0
56	MG	B	3593	1/1	0.77	0.08	78,78,78,78	0
56	MG	B	3596	1/1	0.77	0.09	55,55,55,55	0
56	MG	KA	301	1/1	0.77	0.23	118,118,118,118	0
56	MG	B	3826	1/1	0.78	0.43	97,97,97,97	0
56	MG	B	3592	1/1	0.78	0.15	73,73,73,73	0
56	MG	GB	3587	1/1	0.78	0.27	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	FB	1651	1/1	0.78	0.32	90,90,90,90	0
56	MG	GB	3386	1/1	0.78	0.11	76,76,76,76	0
56	MG	FB	1877	1/1	0.78	0.20	80,80,80,80	0
56	MG	B	2967	1/1	0.78	0.35	53,53,53,53	0
56	MG	GB	3602	1/1	0.78	0.17	75,75,75,75	0
56	MG	FB	1664	1/1	0.78	0.24	85,85,85,85	0
56	MG	GB	3604	1/1	0.78	0.28	64,64,64,64	0
56	MG	FB	1888	1/1	0.78	0.31	82,82,82,82	0
56	MG	GB	3611	1/1	0.78	0.12	77,77,77,77	0
56	MG	FB	1769	1/1	0.78	0.23	91,91,91,91	0
56	MG	GB	3025	1/1	0.78	0.40	64,64,64,64	0
56	MG	GB	3238	1/1	0.78	0.29	76,76,76,76	0
56	MG	GB	3630	1/1	0.78	0.22	75,75,75,75	0
56	MG	A	1751	1/1	0.78	0.38	86,86,86,86	0
56	MG	GB	3633	1/1	0.78	0.28	74,74,74,74	0
56	MG	BC	303	1/1	0.78	0.10	106,106,106,106	0
56	MG	IA	117	1/1	0.78	0.20	81,81,81,81	0
56	MG	C	203	1/1	0.78	0.23	79,79,79,79	0
56	MG	B	3490	1/1	0.78	0.10	44,44,44,44	0
56	MG	GB	3041	1/1	0.78	0.20	93,93,93,93	0
56	MG	B	3267	1/1	0.78	0.12	61,61,61,61	0
56	MG	GB	3446	1/1	0.78	0.20	75,75,75,75	0
56	MG	C	212	1/1	0.78	0.19	62,62,62,62	0
56	MG	FB	1803	1/1	0.78	0.31	84,84,84,84	0
56	MG	B	3617	1/1	0.78	0.16	54,54,54,54	0
56	MG	A	1637	1/1	0.78	0.23	67,67,67,67	0
56	MG	B	3376	1/1	0.78	0.13	133,133,133,133	0
56	MG	GB	3092	1/1	0.78	0.31	87,87,87,87	0
56	MG	GB	3676	1/1	0.78	0.18	88,88,88,88	0
56	MG	FB	1814	1/1	0.78	0.14	78,78,78,78	0
56	MG	B	3276	1/1	0.78	0.18	68,68,68,68	0
56	MG	C	244	1/1	0.78	0.12	65,65,65,65	0
56	MG	A	1794	1/1	0.78	0.30	73,73,73,73	0
56	MG	GB	3122	1/1	0.78	0.24	76,76,76,76	0
56	MG	A	1712	1/1	0.78	0.25	76,76,76,76	0
56	MG	A	1819	1/1	0.78	0.23	82,82,82,82	0
56	MG	B	3656	1/1	0.78	0.22	59,59,59,59	0
56	MG	GB	3507	1/1	0.78	0.12	109,109,109,109	0
56	MG	GB	3508	1/1	0.78	0.20	78,78,78,78	0
56	MG	A	1853	1/1	0.78	0.22	99,99,99,99	0
56	MG	GB	3519	1/1	0.78	0.20	85,85,85,85	0
56	MG	A	1687	1/1	0.78	0.24	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3170	1/1	0.78	0.28	62,62,62,62	0
56	MG	B	3172	1/1	0.78	0.24	59,59,59,59	0
56	MG	QC	304	1/1	0.78	0.18	104,104,104,104	0
56	MG	GB	3182	1/1	0.78	0.20	88,88,88,88	0
56	MG	GB	2907	1/1	0.78	0.45	60,60,60,60	0
56	MG	GB	3192	1/1	0.78	0.16	49,49,49,49	0
56	MG	SC	206	1/1	0.78	0.23	93,93,93,93	0
56	MG	B	3432	1/1	0.78	0.22	68,68,68,68	0
56	MG	GB	3549	1/1	0.78	0.35	86,86,86,86	0
56	MG	GB	3553	1/1	0.78	0.10	86,86,86,86	0
56	MG	FB	1637	1/1	0.78	0.34	64,64,64,64	0
56	MG	A	1659	1/1	0.78	0.23	87,87,87,87	0
56	MG	B	2946	1/1	0.78	0.34	72,72,72,72	0
56	MG	GB	3210	1/1	0.78	0.21	77,77,77,77	0
56	MG	B	3704	1/1	0.78	0.11	69,69,69,69	0
56	MG	A	1858	1/1	0.79	0.28	100,100,100,100	0
56	MG	A	1769	1/1	0.79	0.20	85,85,85,85	0
56	MG	GB	3431	1/1	0.79	0.20	76,76,76,76	0
56	MG	FB	1689	1/1	0.79	0.18	66,66,66,66	0
56	MG	GB	3618	1/1	0.79	0.09	109,109,109,109	0
56	MG	ZA	202	1/1	0.79	0.19	87,87,87,87	0
56	MG	NB	203	1/1	0.79	0.20	92,92,92,92	0
56	MG	FB	1696	1/1	0.79	0.29	85,85,85,85	0
56	MG	RB	204	1/1	0.79	0.11	98,98,98,98	0
56	MG	B	3371	1/1	0.79	0.15	133,133,133,133	0
56	MG	GB	3064	1/1	0.79	0.29	72,72,72,72	0
56	MG	B	3056	1/1	0.79	0.15	49,49,49,49	0
56	MG	FB	1702	1/1	0.79	0.17	81,81,81,81	0
56	MG	B	3785	1/1	0.79	0.21	61,61,61,61	0
56	MG	GB	3652	1/1	0.79	0.09	73,73,73,73	0
56	MG	A	1643	1/1	0.79	0.24	70,70,70,70	0
56	MG	GB	3090	1/1	0.79	0.29	67,67,67,67	0
56	MG	FB	1706	1/1	0.79	0.33	69,69,69,69	0
56	MG	P	204	1/1	0.79	0.13	77,77,77,77	0
56	MG	FB	1929	1/1	0.79	0.20	94,94,94,94	0
56	MG	B	2942	1/1	0.79	0.46	58,58,58,58	0
56	MG	FB	1620	1/1	0.79	0.29	67,67,67,67	0
56	MG	GB	3323	1/1	0.79	0.26	71,71,71,71	0
56	MG	A	1634	1/1	0.79	0.28	72,72,72,72	0
56	MG	FB	1723	1/1	0.79	0.30	86,86,86,86	0
56	MG	X	106	1/1	0.79	0.11	63,63,63,63	0
56	MG	FB	1840	1/1	0.79	0.11	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	GB	3511	1/1	0.79	0.28	82,82,82,82	0
56	MG	C	209	1/1	0.79	0.22	62,62,62,62	0
56	MG	GB	3160	1/1	0.79	0.30	89,89,89,89	0
56	MG	BA	103	1/1	0.79	0.08	107,107,107,107	0
56	MG	FB	1853	1/1	0.79	0.17	126,126,126,126	0
56	MG	GB	3530	1/1	0.79	0.14	85,85,85,85	0
56	MG	GB	3711	1/1	0.79	0.16	77,77,77,77	0
56	MG	GB	2914	1/1	0.79	0.40	58,58,58,58	0
56	MG	B	3293	1/1	0.79	0.15	82,82,82,82	0
56	MG	C	222	1/1	0.79	0.11	105,105,105,105	0
56	MG	GB	2932	1/1	0.79	0.51	68,68,68,68	0
56	MG	FB	1733	1/1	0.79	0.30	62,62,62,62	0
56	MG	GB	3369	1/1	0.79	0.18	90,90,90,90	0
56	MG	B	2949	1/1	0.79	0.20	45,45,45,45	0
56	MG	A	1694	1/1	0.79	0.18	90,90,90,90	0
56	MG	C	237	1/1	0.79	0.13	83,83,83,83	0
56	MG	GB	3556	1/1	0.79	0.27	77,77,77,77	0
56	MG	IA	116	1/1	0.79	0.32	84,84,84,84	0
56	MG	A	1743	1/1	0.79	0.15	80,80,80,80	0
56	MG	B	3412	1/1	0.79	0.15	57,57,57,57	0
56	MG	GB	2991	1/1	0.79	0.28	63,63,63,63	0
56	MG	A	1636	1/1	0.79	0.36	82,82,82,82	0
56	MG	A	1768	1/1	0.79	0.28	84,84,84,84	0
56	MG	FB	1668	1/1	0.79	0.30	82,82,82,82	0
56	MG	GB	3007	1/1	0.79	0.34	73,73,73,73	0
56	MG	GB	3016	1/1	0.79	0.42	76,76,76,76	0
56	MG	GB	3597	1/1	0.79	0.14	80,80,80,80	0
56	MG	B	3014	1/1	0.79	0.16	56,56,56,56	0
56	MG	IB	105	1/1	0.79	0.25	117,117,117,117	0
56	MG	F	308	1/1	0.79	0.27	58,58,58,58	0
56	MG	F	311	1/1	0.79	0.07	59,59,59,59	0
56	MG	A	1693	1/1	0.80	0.29	79,79,79,79	0
56	MG	W	302	1/1	0.80	0.10	70,70,70,70	0
56	MG	UA	201	1/1	0.80	0.18	75,75,75,75	0
56	MG	A	1711	1/1	0.80	0.33	95,95,95,95	0
56	MG	GB	3164	1/1	0.80	0.35	46,46,46,46	0
56	MG	GB	2951	1/1	0.80	0.41	71,71,71,71	0
56	MG	B	3398	1/1	0.80	0.23	64,64,64,64	0
56	MG	W	308	1/1	0.80	0.08	73,73,73,73	0
56	MG	GB	3183	1/1	0.80	0.07	61,61,61,61	0
56	MG	GB	2983	1/1	0.80	0.20	69,69,69,69	0
56	MG	FB	1894	1/1	0.80	0.25	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	FB	1804	1/1	0.80	0.26	81,81,81,81	0
56	MG	GB	3194	1/1	0.80	0.15	62,62,62,62	0
56	MG	GB	3197	1/1	0.80	0.17	100,100,100,100	0
56	MG	GB	3529	1/1	0.80	0.17	107,107,107,107	0
56	MG	MA	301	1/1	0.80	0.27	97,97,97,97	0
56	MG	A	1619	1/1	0.80	0.19	61,61,61,61	0
56	MG	GB	3692	1/1	0.80	0.19	81,81,81,81	0
56	MG	FB	1662	1/1	0.80	0.34	66,66,66,66	0
56	MG	A	1611	1/1	0.80	0.24	96,96,96,96	0
56	MG	A	1641	1/1	0.80	0.23	79,79,79,79	0
56	MG	FB	1819	1/1	0.80	0.13	71,71,71,71	0
56	MG	B	3604	1/1	0.80	0.16	60,60,60,60	0
56	MG	A	1776	1/1	0.80	0.23	78,78,78,78	0
56	MG	A	1700	1/1	0.80	0.29	82,82,82,82	0
56	MG	A	1608	1/1	0.80	0.30	55,55,55,55	0
56	MG	FB	1679	1/1	0.80	0.28	81,81,81,81	0
56	MG	A	1868	1/1	0.80	0.14	71,71,71,71	0
56	MG	GB	3567	1/1	0.80	0.12	52,52,52,52	0
56	MG	OC	401	1/1	0.80	0.30	68,68,68,68	0
56	MG	H	202	1/1	0.80	0.10	89,89,89,89	0
56	MG	FB	1687	1/1	0.80	0.22	109,109,109,109	0
56	MG	GB	3578	1/1	0.80	0.15	92,92,92,92	0
56	MG	FB	1688	1/1	0.80	0.20	64,64,64,64	0
56	MG	B	3287	1/1	0.80	0.17	40,40,40,40	0
56	MG	GB	3085	1/1	0.80	0.19	60,60,60,60	0
56	MG	GB	3249	1/1	0.80	0.12	68,68,68,68	0
56	MG	A	1609	1/1	0.80	0.29	55,55,55,55	0
56	MG	GB	3253	1/1	0.80	0.36	76,76,76,76	0
56	MG	JA	404	1/1	0.80	0.16	83,83,83,83	0
56	MG	L	203	1/1	0.80	0.18	71,71,71,71	0
56	MG	FB	1941	1/1	0.80	0.35	89,89,89,89	0
56	MG	FB	1866	1/1	0.80	0.10	94,94,94,94	0
56	MG	GB	3444	1/1	0.80	0.22	78,78,78,78	0
56	MG	A	1606	1/1	0.80	0.26	95,95,95,95	0
56	MG	GB	3278	1/1	0.80	0.31	75,75,75,75	0
56	MG	JB	306	1/1	0.80	0.12	69,69,69,69	0
56	MG	GB	3107	1/1	0.80	0.26	81,81,81,81	0
56	MG	FB	1772	1/1	0.80	0.24	68,68,68,68	0
56	MG	GB	3289	1/1	0.80	0.27	63,63,63,63	0
56	MG	FB	1776	1/1	0.80	0.14	67,67,67,67	0
56	MG	FB	1777	1/1	0.80	0.22	97,97,97,97	0
56	MG	B	3739	1/1	0.80	0.15	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CD	103	1/1	0.80	0.24	84,84,84,84	0
56	MG	FB	1785	1/1	0.80	0.13	87,87,87,87	0
56	MG	GB	2933	1/1	0.81	0.44	63,63,63,63	0
56	MG	A	1763	1/1	0.81	0.29	109,109,109,109	0
56	MG	A	1673	1/1	0.81	0.28	75,75,75,75	0
56	MG	A	1811	1/1	0.81	0.24	76,76,76,76	0
56	MG	HB	227	1/1	0.81	0.10	99,99,99,99	0
56	MG	B	3426	1/1	0.81	0.21	57,57,57,57	0
56	MG	A	1646	1/1	0.81	0.26	74,74,74,74	0
56	MG	FB	1729	1/1	0.81	0.26	72,72,72,72	0
56	MG	B	3609	1/1	0.81	0.13	44,44,44,44	0
56	MG	F	309	1/1	0.81	0.14	38,38,38,38	0
56	MG	B	3433	1/1	0.81	0.17	101,101,101,101	0
56	MG	F	312	1/1	0.81	0.20	77,77,77,77	0
56	MG	A	1856	1/1	0.81	0.27	87,87,87,87	0
56	MG	FB	1742	1/1	0.81	0.38	67,67,67,67	0
56	MG	GB	3409	1/1	0.81	0.16	70,70,70,70	0
56	MG	GB	3410	1/1	0.81	0.36	76,76,76,76	0
56	MG	B	3071	1/1	0.81	0.45	58,58,58,58	0
56	MG	B	3118	1/1	0.81	0.31	96,96,96,96	0
56	MG	FB	1752	1/1	0.81	0.32	96,96,96,96	0
56	MG	A	1718	1/1	0.81	0.25	64,64,64,64	0
56	MG	B	2927	1/1	0.81	0.35	50,50,50,50	0
56	MG	PB	201	1/1	0.81	0.18	93,93,93,93	0
56	MG	GB	3027	1/1	0.81	0.25	74,74,74,74	0
56	MG	GB	3028	1/1	0.81	0.23	71,71,71,71	0
56	MG	GB	3621	1/1	0.81	0.16	64,64,64,64	0
56	MG	GB	3029	1/1	0.81	0.27	75,75,75,75	0
56	MG	GB	3625	1/1	0.81	0.09	78,78,78,78	0
56	MG	I	205	1/1	0.81	0.08	69,69,69,69	0
56	MG	GB	3629	1/1	0.81	0.23	57,57,57,57	0
56	MG	K	206	1/1	0.81	0.10	73,73,73,73	0
56	MG	GB	3245	1/1	0.81	0.28	76,76,76,76	0
56	MG	A	1730	1/1	0.81	0.47	81,81,81,81	0
56	MG	GB	3645	1/1	0.81	0.13	71,71,71,71	0
56	MG	A	1784	1/1	0.81	0.23	85,85,85,85	0
56	MG	A	1866	1/1	0.81	0.17	95,95,95,95	0
56	MG	B	3211	1/1	0.81	0.23	65,65,65,65	0
56	MG	B	3519	1/1	0.81	0.34	50,50,50,50	0
56	MG	EC	102	1/1	0.81	0.14	91,91,91,91	0
56	MG	GB	3655	1/1	0.81	0.12	59,59,59,59	0
56	MG	FB	1677	1/1	0.81	0.33	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	2959	1/1	0.81	0.21	84,84,84,84	0
56	MG	GB	3658	1/1	0.81	0.10	95,95,95,95	0
56	MG	B	2964	1/1	0.81	0.25	55,55,55,55	0
56	MG	GB	3661	1/1	0.81	0.15	66,66,66,66	0
56	MG	GB	3468	1/1	0.81	0.21	86,86,86,86	0
56	MG	B	3683	1/1	0.81	0.17	52,52,52,52	0
56	MG	GB	3474	1/1	0.81	0.20	69,69,69,69	0
56	MG	GB	3475	1/1	0.81	0.21	79,79,79,79	0
56	MG	A	1770	1/1	0.81	0.21	139,139,139,139	0
56	MG	Y	103	1/1	0.81	0.10	74,74,74,74	0
56	MG	GB	3482	1/1	0.81	0.20	77,77,77,77	0
56	MG	B	3688	1/1	0.81	0.08	60,60,60,60	0
56	MG	FB	1798	1/1	0.81	0.41	79,79,79,79	0
56	MG	B	3691	1/1	0.81	0.17	92,92,92,92	0
56	MG	B	3262	1/1	0.81	0.15	45,45,45,45	0
56	MG	GB	3696	1/1	0.81	0.16	72,72,72,72	0
56	MG	GB	3102	1/1	0.81	0.25	50,50,50,50	0
56	MG	B	3391	1/1	0.81	0.10	56,56,56,56	0
56	MG	HA	101	1/1	0.81	0.32	77,77,77,77	0
56	MG	A	1655	1/1	0.81	0.26	66,66,66,66	0
56	MG	GB	3120	1/1	0.81	0.21	79,79,79,79	0
56	MG	HB	202	1/1	0.81	0.20	79,79,79,79	0
56	MG	B	3560	1/1	0.81	0.23	114,114,114,114	0
56	MG	GB	3123	1/1	0.81	0.17	62,62,62,62	0
56	MG	C	214	1/1	0.81	0.13	79,79,79,79	0
56	MG	IA	114	1/1	0.81	0.12	71,71,71,71	0
56	MG	B	2993	1/1	0.81	0.27	47,47,47,47	0
56	MG	GB	3533	1/1	0.81	0.14	93,93,93,93	0
56	MG	B	3000	1/1	0.81	0.20	70,70,70,70	0
56	MG	FB	1822	1/1	0.81	0.28	73,73,73,73	0
56	MG	FB	1714	1/1	0.81	0.26	66,66,66,66	0
56	MG	B	3007	1/1	0.81	0.27	51,51,51,51	0
56	MG	FB	1718	1/1	0.81	0.17	66,66,66,66	0
56	MG	A	1625	1/1	0.81	0.27	66,66,66,66	0
56	MG	FB	1721	1/1	0.81	0.23	76,76,76,76	0
56	MG	HB	209	1/1	0.82	0.11	81,81,81,81	0
56	MG	GB	3083	1/1	0.82	0.26	70,70,70,70	0
56	MG	B	3619	1/1	0.82	0.10	70,70,70,70	0
56	MG	A	1699	1/1	0.82	0.25	92,92,92,92	0
56	MG	FB	1601	1/1	0.82	0.18	88,88,88,88	0
56	MG	JA	401	1/1	0.82	0.28	52,52,52,52	0
56	MG	A	1821	1/1	0.82	0.18	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3499	1/1	0.82	0.13	48,48,48,48	0
56	MG	B	3105	1/1	0.82	0.11	78,78,78,78	0
56	MG	GB	3097	1/1	0.82	0.21	57,57,57,57	0
56	MG	HB	219	1/1	0.82	0.14	94,94,94,94	0
56	MG	B	3113	1/1	0.82	0.17	65,65,65,65	0
56	MG	A	1604	1/1	0.82	0.30	73,73,73,73	0
56	MG	GB	3337	1/1	0.82	0.21	58,58,58,58	0
56	MG	B	3134	1/1	0.82	0.23	56,56,56,56	0
56	MG	HB	228	1/1	0.82	0.24	81,81,81,81	0
56	MG	FB	1624	1/1	0.82	0.31	66,66,66,66	0
56	MG	GB	3558	1/1	0.82	0.07	98,98,98,98	0
56	MG	B	3137	1/1	0.82	0.16	48,48,48,48	0
56	MG	A	1671	1/1	0.82	0.20	94,94,94,94	0
56	MG	GB	3568	1/1	0.82	0.26	66,66,66,66	0
56	MG	FB	1825	1/1	0.82	0.18	86,86,86,86	0
56	MG	KA	304	1/1	0.82	0.25	109,109,109,109	0
56	MG	LB	304	1/1	0.82	0.17	83,83,83,83	0
56	MG	A	1635	1/1	0.82	0.26	104,104,104,104	0
56	MG	GB	3137	1/1	0.82	0.26	66,66,66,66	0
56	MG	GB	2905	1/1	0.82	0.53	62,62,62,62	0
56	MG	A	1716	1/1	0.82	0.22	78,78,78,78	0
56	MG	A	1652	1/1	0.82	0.32	70,70,70,70	0
56	MG	GB	3152	1/1	0.82	0.19	74,74,74,74	0
56	MG	GB	3154	1/1	0.82	0.17	61,61,61,61	0
56	MG	GB	3155	1/1	0.82	0.32	89,89,89,89	0
56	MG	GB	3598	1/1	0.82	0.22	78,78,78,78	0
56	MG	A	1733	1/1	0.82	0.34	100,100,100,100	0
56	MG	MA	305	1/1	0.82	0.20	103,103,103,103	0
56	MG	FB	1846	1/1	0.82	0.16	73,73,73,73	0
56	MG	B	3563	1/1	0.82	0.12	47,47,47,47	0
56	MG	GB	3606	1/1	0.82	0.20	75,75,75,75	0
56	MG	GB	2939	1/1	0.82	0.29	64,64,64,64	0
56	MG	A	1681	1/1	0.82	0.24	69,69,69,69	0
56	MG	XB	202	1/1	0.82	0.15	76,76,76,76	0
56	MG	FB	1859	1/1	0.82	0.17	83,83,83,83	0
56	MG	YB	206	1/1	0.82	0.15	70,70,70,70	0
56	MG	GB	3184	1/1	0.82	0.21	61,61,61,61	0
56	MG	GB	3185	1/1	0.82	0.18	67,67,67,67	0
56	MG	B	3320	1/1	0.82	0.27	64,64,64,64	0
56	MG	B	3212	1/1	0.82	0.24	52,52,52,52	0
56	MG	Q	203	1/1	0.82	0.10	78,78,78,78	0
56	MG	FB	1865	1/1	0.82	0.41	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	GB	2955	1/1	0.82	0.30	69,69,69,69	0
56	MG	GB	2964	1/1	0.82	0.26	59,59,59,59	0
56	MG	B	3339	1/1	0.82	0.11	60,60,60,60	0
56	MG	GB	3635	1/1	0.82	0.21	78,78,78,78	0
56	MG	B	3434	1/1	0.82	0.15	75,75,75,75	0
56	MG	B	3708	1/1	0.82	0.20	71,71,71,71	0
56	MG	GB	2985	1/1	0.82	0.25	58,58,58,58	0
56	MG	B	3436	1/1	0.82	0.11	81,81,81,81	0
56	MG	GB	2993	1/1	0.82	0.12	71,71,71,71	0
56	MG	B	3720	1/1	0.82	0.08	59,59,59,59	0
56	MG	C	211	1/1	0.82	0.28	83,83,83,83	0
56	MG	GB	3004	1/1	0.82	0.26	60,60,60,60	0
56	MG	GB	3451	1/1	0.82	0.12	79,79,79,79	0
56	MG	NC	108	1/1	0.82	0.09	81,81,81,81	0
56	MG	FB	1874	1/1	0.82	0.12	69,69,69,69	0
56	MG	Y	104	1/1	0.82	0.16	71,71,71,71	0
56	MG	GB	3009	1/1	0.82	0.30	62,62,62,62	0
56	MG	A	1887	1/1	0.82	0.37	87,87,87,87	0
56	MG	GB	3237	1/1	0.82	0.25	93,93,93,93	0
56	MG	FB	1878	1/1	0.82	0.20	75,75,75,75	0
56	MG	C	213	1/1	0.82	0.08	72,72,72,72	0
56	MG	FB	1775	1/1	0.82	0.16	83,83,83,83	0
56	MG	B	3738	1/1	0.82	0.14	55,55,55,55	0
56	MG	A	1838	1/1	0.82	0.15	106,106,106,106	0
56	MG	C	225	1/1	0.82	0.14	83,83,83,83	0
56	MG	FB	1782	1/1	0.82	0.23	91,91,91,91	0
56	MG	FB	1895	1/1	0.82	0.12	73,73,73,73	0
56	MG	GB	3488	1/1	0.82	0.19	78,78,78,78	0
56	MG	RC	304	1/1	0.82	0.16	80,80,80,80	0
56	MG	B	3746	1/1	0.82	0.16	68,68,68,68	0
56	MG	GB	3497	1/1	0.82	0.20	59,59,59,59	0
56	MG	B	3457	1/1	0.82	0.09	66,66,66,66	0
56	MG	B	3351	1/1	0.82	0.19	77,77,77,77	0
56	MG	GB	3709	1/1	0.82	0.21	74,74,74,74	0
56	MG	GB	3269	1/1	0.82	0.21	77,77,77,77	0
56	MG	GB	3058	1/1	0.82	0.22	49,49,49,49	0
56	MG	A	1697	1/1	0.82	0.37	78,78,78,78	0
56	MG	A	1844	1/1	0.82	0.22	89,89,89,89	0
56	MG	HB	205	1/1	0.82	0.31	74,74,74,74	0
56	MG	FB	1795	1/1	0.82	0.24	61,61,61,61	0
56	MG	GB	3077	1/1	0.82	0.27	68,68,68,68	0
56	MG	GB	3527	1/1	0.82	0.17	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	GB	3521	1/1	0.83	0.25	76,76,76,76	0
56	MG	A	1738	1/1	0.83	0.18	86,86,86,86	0
56	MG	B	3271	1/1	0.83	0.23	68,68,68,68	0
56	MG	A	1755	1/1	0.83	0.19	71,71,71,71	0
56	MG	GB	3380	1/1	0.83	0.13	57,57,57,57	0
56	MG	A	1706	1/1	0.83	0.34	88,88,88,88	0
56	MG	A	1732	1/1	0.83	0.18	56,56,56,56	0
56	MG	SB	204	1/1	0.83	0.20	81,81,81,81	0
56	MG	TB	204	1/1	0.83	0.35	73,73,73,73	0
56	MG	A	1601	1/1	0.83	0.29	56,56,56,56	0
56	MG	B	2973	1/1	0.83	0.21	41,41,41,41	0
56	MG	VB	203	1/1	0.83	0.16	79,79,79,79	0
56	MG	B	3196	1/1	0.83	0.37	80,80,80,80	0
56	MG	B	3203	1/1	0.83	0.21	57,57,57,57	0
56	MG	IA	106	1/1	0.83	0.22	82,82,82,82	0
56	MG	GB	3548	1/1	0.83	0.14	68,68,68,68	0
56	MG	GB	3121	1/1	0.83	0.29	62,62,62,62	0
56	MG	GB	3683	1/1	0.83	0.15	64,64,64,64	0
56	MG	B	3065	1/1	0.83	0.30	63,63,63,63	0
56	MG	OA	203	1/1	0.83	0.10	62,62,62,62	0
56	MG	FB	1827	1/1	0.83	0.11	71,71,71,71	0
56	MG	B	3487	1/1	0.83	0.12	81,81,81,81	0
56	MG	GB	3260	1/1	0.83	0.16	59,59,59,59	0
56	MG	GB	3000	1/1	0.83	0.24	67,67,67,67	0
56	MG	GB	3704	1/1	0.83	0.13	86,86,86,86	0
56	MG	B	2984	1/1	0.83	0.27	58,58,58,58	0
56	MG	GB	3429	1/1	0.83	0.11	49,49,49,49	0
56	MG	GB	3002	1/1	0.83	0.50	88,88,88,88	0
56	MG	FB	1836	1/1	0.83	0.09	66,66,66,66	0
56	MG	FB	1694	1/1	0.83	0.05	81,81,81,81	0
56	MG	FB	1839	1/1	0.83	0.32	78,78,78,78	0
56	MG	FB	1764	1/1	0.83	0.35	82,82,82,82	0
56	MG	FB	1622	1/1	0.83	0.27	74,74,74,74	0
56	MG	PA	203	1/1	0.83	0.14	92,92,92,92	0
56	MG	GB	3167	1/1	0.83	0.37	82,82,82,82	0
56	MG	B	3296	1/1	0.83	0.12	55,55,55,55	0
56	MG	B	2912	1/1	0.83	0.42	59,59,59,59	0
56	MG	GB	3311	1/1	0.83	0.25	64,64,64,64	0
56	MG	GB	3181	1/1	0.83	0.16	64,64,64,64	0
56	MG	GB	3601	1/1	0.83	0.23	58,58,58,58	0
56	MG	GB	3463	1/1	0.83	0.25	66,66,66,66	0
56	MG	FB	1630	1/1	0.83	0.25	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3218	1/1	0.83	0.13	61,61,61,61	0
56	MG	FB	1632	1/1	0.83	0.37	69,69,69,69	0
56	MG	A	1783	1/1	0.83	0.17	111,111,111,111	0
56	MG	GB	3473	1/1	0.83	0.13	76,76,76,76	0
56	MG	GB	3613	1/1	0.83	0.09	57,57,57,57	0
56	MG	PC	305	1/1	0.83	0.11	96,96,96,96	0
56	MG	FB	1708	1/1	0.83	0.26	73,73,73,73	0
56	MG	P	203	1/1	0.83	0.30	75,75,75,75	0
56	MG	B	3239	1/1	0.83	0.15	64,64,64,64	0
56	MG	FB	1716	1/1	0.83	0.23	82,82,82,82	0
56	MG	FB	1638	1/1	0.83	0.23	60,60,60,60	0
56	MG	GB	2915	1/1	0.83	0.36	52,52,52,52	0
56	MG	GB	2919	1/1	0.83	0.45	66,66,66,66	0
56	MG	B	3616	1/1	0.83	0.11	95,95,95,95	0
56	MG	B	2929	1/1	0.83	0.26	47,47,47,47	0
56	MG	GB	3214	1/1	0.83	0.27	64,64,64,64	0
56	MG	GB	2926	1/1	0.83	0.19	69,69,69,69	0
56	MG	WC	201	1/1	0.83	0.13	121,121,121,121	0
56	MG	A	1620	1/1	0.83	0.22	93,93,93,93	0
56	MG	GB	3647	1/1	0.83	0.16	77,77,77,77	0
56	MG	JA	413	1/1	0.83	0.30	97,97,97,97	0
56	MG	GB	3364	1/1	0.83	0.13	70,70,70,70	0
56	MG	ZC	202	1/1	0.83	0.14	75,75,75,75	0
56	MG	B	3810	1/1	0.83	0.15	59,59,59,59	0
56	MG	GB	3653	1/1	0.83	0.35	78,78,78,78	0
56	MG	ED	202	1/1	0.83	0.32	72,72,72,72	0
56	MG	B	3424	1/1	0.83	0.20	57,57,57,57	0
56	MG	I	202	1/1	0.84	0.23	70,70,70,70	0
56	MG	GB	3280	1/1	0.84	0.20	84,84,84,84	0
56	MG	FB	1905	1/1	0.84	0.28	70,70,70,70	0
56	MG	B	3467	1/1	0.84	0.12	50,50,50,50	0
56	MG	FB	1907	1/1	0.84	0.20	115,115,115,115	0
56	MG	B	2971	1/1	0.84	0.20	51,51,51,51	0
56	MG	I	206	1/1	0.84	0.10	74,74,74,74	0
56	MG	B	3369	1/1	0.84	0.16	69,69,69,69	0
56	MG	A	1881	1/1	0.84	0.17	128,128,128,128	0
56	MG	GB	3308	1/1	0.84	0.13	61,61,61,61	0
56	MG	GB	3087	1/1	0.84	0.38	75,75,75,75	0
56	MG	B	3130	1/1	0.84	0.43	80,80,80,80	0
56	MG	B	3268	1/1	0.84	0.31	70,70,70,70	0
56	MG	HB	224	1/1	0.84	0.09	118,118,118,118	0
56	MG	GB	3544	1/1	0.84	0.15	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	A	1704	1/1	0.84	0.24	65,65,65,65	0
56	MG	FB	1794	1/1	0.84	0.29	85,85,85,85	0
56	MG	B	3136	1/1	0.84	0.17	43,43,43,43	0
56	MG	FB	1684	1/1	0.84	0.31	79,79,79,79	0
56	MG	A	1843	1/1	0.84	0.45	89,89,89,89	0
56	MG	GB	3330	1/1	0.84	0.12	79,79,79,79	0
56	MG	GB	3334	1/1	0.84	0.17	109,109,109,109	0
56	MG	JB	304	1/1	0.84	0.09	76,76,76,76	0
56	MG	JB	305	1/1	0.84	0.13	76,76,76,76	0
56	MG	GB	3103	1/1	0.84	0.15	70,70,70,70	0
56	MG	JB	310	1/1	0.84	0.16	64,64,64,64	0
56	MG	S	207	1/1	0.84	0.25	49,49,49,49	0
56	MG	KB	302	1/1	0.84	0.12	75,75,75,75	0
56	MG	GB	3340	1/1	0.84	0.15	66,66,66,66	0
56	MG	MB	201	1/1	0.84	0.23	111,111,111,111	0
56	MG	FB	1935	1/1	0.84	0.20	71,71,71,71	0
56	MG	GB	3345	1/1	0.84	0.19	68,68,68,68	0
56	MG	GB	3346	1/1	0.84	0.36	66,66,66,66	0
56	MG	MB	205	1/1	0.84	0.14	122,122,122,122	0
56	MG	GB	3582	1/1	0.84	0.16	68,68,68,68	0
56	MG	B	3824	1/1	0.84	0.12	68,68,68,68	0
56	MG	GB	3118	1/1	0.84	0.21	56,56,56,56	0
56	MG	A	1886	1/1	0.84	0.25	78,78,78,78	0
56	MG	B	3152	1/1	0.84	0.27	56,56,56,56	0
56	MG	W	306	1/1	0.84	0.13	77,77,77,77	0
56	MG	B	3539	1/1	0.84	0.14	51,51,51,51	0
56	MG	RB	201	1/1	0.84	0.08	71,71,71,71	0
56	MG	GB	3124	1/1	0.84	0.17	79,79,79,79	0
56	MG	B	3839	1/1	0.84	0.15	50,50,50,50	0
56	MG	FB	1944	1/1	0.84	0.10	78,78,78,78	0
56	MG	TB	203	1/1	0.84	0.15	66,66,66,66	0
56	MG	FB	1946	1/1	0.84	0.17	70,70,70,70	0
56	MG	FB	1948	1/1	0.84	0.30	116,116,116,116	0
56	MG	GB	3143	1/1	0.84	0.23	78,78,78,78	0
56	MG	B	3400	1/1	0.84	0.10	43,43,43,43	0
56	MG	VB	205	1/1	0.84	0.17	70,70,70,70	0
56	MG	FB	1701	1/1	0.84	0.40	68,68,68,68	0
56	MG	WB	202	1/1	0.84	0.20	80,80,80,80	0
56	MG	GB	2913	1/1	0.84	0.22	63,63,63,63	0
56	MG	A	1629	1/1	0.84	0.20	67,67,67,67	0
56	MG	XB	204	1/1	0.84	0.07	97,97,97,97	0
56	MG	YB	201	1/1	0.84	0.33	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	Z	103	1/1	0.84	0.27	74,74,74,74	0
56	MG	A	1790	1/1	0.84	0.14	65,65,65,65	0
56	MG	BA	102	1/1	0.84	0.14	83,83,83,83	0
56	MG	B	2921	1/1	0.84	0.27	42,42,42,42	0
56	MG	A	1684	1/1	0.84	0.16	67,67,67,67	0
56	MG	B	3555	1/1	0.84	0.16	54,54,54,54	0
56	MG	GA	102	1/1	0.84	0.08	67,67,67,67	0
56	MG	B	3189	1/1	0.84	0.20	59,59,59,59	0
56	MG	GB	3411	1/1	0.84	0.11	67,67,67,67	0
56	MG	GB	3414	1/1	0.84	0.22	75,75,75,75	0
56	MG	B	3711	1/1	0.84	0.11	64,64,64,64	0
56	MG	A	1723	1/1	0.84	0.18	79,79,79,79	0
56	MG	GB	3639	1/1	0.84	0.25	71,71,71,71	0
56	MG	C	218	1/1	0.84	0.22	66,66,66,66	0
56	MG	B	3199	1/1	0.84	0.23	55,55,55,55	0
56	MG	B	3571	1/1	0.84	0.18	66,66,66,66	0
56	MG	A	1772	1/1	0.84	0.09	143,143,143,143	0
56	MG	FB	1854	1/1	0.84	0.25	86,86,86,86	0
56	MG	FB	1857	1/1	0.84	0.50	82,82,82,82	0
56	MG	GB	3439	1/1	0.84	0.17	74,74,74,74	0
56	MG	A	1797	1/1	0.84	0.11	90,90,90,90	0
56	MG	NC	106	1/1	0.84	0.14	77,77,77,77	0
56	MG	B	3308	1/1	0.84	0.22	50,50,50,50	0
56	MG	B	3747	1/1	0.84	0.31	74,74,74,74	0
56	MG	FB	1626	1/1	0.84	0.14	72,72,72,72	0
56	MG	A	1656	1/1	0.84	0.45	100,100,100,100	0
56	MG	B	3435	1/1	0.84	0.13	63,63,63,63	0
56	MG	FB	1739	1/1	0.84	0.29	70,70,70,70	0
56	MG	GB	2999	1/1	0.84	0.25	67,67,67,67	0
56	MG	A	1618	1/1	0.84	0.27	80,80,80,80	0
56	MG	B	3440	1/1	0.84	0.12	59,59,59,59	0
56	MG	GB	3672	1/1	0.84	0.26	68,68,68,68	0
56	MG	A	1654	1/1	0.84	0.32	83,83,83,83	0
56	MG	B	3222	1/1	0.84	0.21	50,50,50,50	0
56	MG	FB	1635	1/1	0.84	0.30	78,78,78,78	0
56	MG	B	3447	1/1	0.84	0.22	63,63,63,63	0
56	MG	B	3786	1/1	0.84	0.18	68,68,68,68	0
56	MG	B	3456	1/1	0.84	0.10	50,50,50,50	0
56	MG	RC	302	1/1	0.84	0.34	77,77,77,77	0
56	MG	GB	3018	1/1	0.84	0.32	73,73,73,73	0
56	MG	GB	3020	1/1	0.84	0.23	60,60,60,60	0
56	MG	FB	1880	1/1	0.84	0.21	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	G	3211	1/1	0.84	0.11	60,60,60,60	0
56	MG	B	3073	1/1	0.84	0.28	62,62,62,62	0
56	MG	FB	1887	1/1	0.84	0.23	65,65,65,65	0
56	MG	A	1879	1/1	0.84	0.12	65,65,65,65	0
56	MG	MA	302	1/1	0.84	0.18	105,105,105,105	0
56	MG	GB	3256	1/1	0.84	0.26	72,72,72,72	0
56	MG	GB	3493	1/1	0.84	0.12	62,62,62,62	0
56	MG	B	3465	1/1	0.84	0.14	91,91,91,91	0
56	MG	I	201	1/1	0.84	0.14	77,77,77,77	0
56	MG	FB	1771	1/1	0.84	0.23	83,83,83,83	0
56	MG	GB	3263	1/1	0.84	0.20	77,77,77,77	0
56	MG	FB	1655	1/1	0.84	0.28	63,63,63,63	0
56	MG	FB	1659	1/1	0.84	0.33	69,69,69,69	0
56	MG	FB	1901	1/1	0.84	0.23	75,75,75,75	0
56	MG	GB	3514	1/1	0.85	0.11	67,67,67,67	0
56	MG	B	3573	1/1	0.85	0.13	57,57,57,57	0
56	MG	GB	3062	1/1	0.85	0.35	61,61,61,61	0
56	MG	B	3455	1/1	0.85	0.29	47,47,47,47	0
56	MG	FB	1909	1/1	0.85	0.16	72,72,72,72	0
56	MG	GB	3292	1/1	0.85	0.20	86,86,86,86	0
56	MG	GB	3070	1/1	0.85	0.20	63,63,63,63	0
56	MG	FB	1788	1/1	0.85	0.12	76,76,76,76	0
56	MG	FB	1674	1/1	0.85	0.20	69,69,69,69	0
56	MG	B	3381	1/1	0.85	0.17	77,77,77,77	0
56	MG	B	3384	1/1	0.85	0.10	55,55,55,55	0
56	MG	GB	3309	1/1	0.85	0.32	57,57,57,57	0
56	MG	A	1640	1/1	0.85	0.16	76,76,76,76	0
56	MG	W	305	1/1	0.85	0.09	67,67,67,67	0
56	MG	IB	101	1/1	0.85	0.21	89,89,89,89	0
56	MG	FB	1924	1/1	0.85	0.13	71,71,71,71	0
56	MG	FB	1796	1/1	0.85	0.10	79,79,79,79	0
56	MG	GB	3547	1/1	0.85	0.50	67,67,67,67	0
56	MG	FB	1797	1/1	0.85	0.17	81,81,81,81	0
56	MG	JB	303	1/1	0.85	0.11	71,71,71,71	0
56	MG	B	3390	1/1	0.85	0.13	72,72,72,72	0
56	MG	GB	3550	1/1	0.85	0.22	61,61,61,61	0
56	MG	A	1841	1/1	0.85	0.20	67,67,67,67	0
56	MG	B	3722	1/1	0.85	0.12	44,44,44,44	0
56	MG	B	3599	1/1	0.85	0.16	69,69,69,69	0
56	MG	FB	1805	1/1	0.85	0.27	74,74,74,74	0
56	MG	B	3201	1/1	0.85	0.20	59,59,59,59	0
56	MG	Z	102	1/1	0.85	0.22	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	GB	3339	1/1	0.85	0.10	67,67,67,67	0
56	MG	C	216	1/1	0.85	0.20	80,80,80,80	0
56	MG	B	3486	1/1	0.85	0.17	51,51,51,51	0
56	MG	FB	1942	1/1	0.85	0.13	72,72,72,72	0
56	MG	B	3607	1/1	0.85	0.07	59,59,59,59	0
56	MG	B	3089	1/1	0.85	0.39	67,67,67,67	0
56	MG	GB	3584	1/1	0.85	0.18	71,71,71,71	0
56	MG	C	229	1/1	0.85	0.27	80,80,80,80	0
56	MG	B	3098	1/1	0.85	0.13	46,46,46,46	0
56	MG	GB	3135	1/1	0.85	0.23	61,61,61,61	0
56	MG	A	1822	1/1	0.85	0.24	72,72,72,72	0
56	MG	YA	101	1/1	0.85	0.39	98,98,98,98	0
56	MG	C	236	1/1	0.85	0.29	77,77,77,77	0
56	MG	IA	102	1/1	0.85	0.22	81,81,81,81	0
56	MG	FB	1831	1/1	0.85	0.27	81,81,81,81	0
56	MG	GB	2917	1/1	0.85	0.31	46,46,46,46	0
56	MG	A	1675	1/1	0.85	0.32	74,74,74,74	0
56	MG	A	1771	1/1	0.85	0.12	80,80,80,80	0
56	MG	IA	107	1/1	0.85	0.13	76,76,76,76	0
56	MG	GB	3377	1/1	0.85	0.27	72,72,72,72	0
56	MG	GB	3159	1/1	0.85	0.38	81,81,81,81	0
56	MG	GB	2925	1/1	0.85	0.26	54,54,54,54	0
56	MG	GB	3608	1/1	0.85	0.14	68,68,68,68	0
56	MG	GB	3382	1/1	0.85	0.17	72,72,72,72	0
56	MG	FB	1608	1/1	0.85	0.33	72,72,72,72	0
56	MG	B	3503	1/1	0.85	0.21	77,77,77,77	0
56	MG	B	3505	1/1	0.85	0.08	51,51,51,51	0
56	MG	B	3633	1/1	0.85	0.25	63,63,63,63	0
56	MG	GB	3178	1/1	0.85	0.18	50,50,50,50	0
56	MG	A	1869	1/1	0.85	0.22	79,79,79,79	0
56	MG	F	302	1/1	0.85	0.09	79,79,79,79	0
56	MG	FB	1852	1/1	0.85	0.09	76,76,76,76	0
56	MG	B	3788	1/1	0.85	0.18	56,56,56,56	0
56	MG	IA	121	1/1	0.85	0.09	79,79,79,79	0
56	MG	FB	1855	1/1	0.85	0.14	68,68,68,68	0
56	MG	GB	2952	1/1	0.85	0.29	63,63,63,63	0
56	MG	CC	102	1/1	0.85	0.18	77,77,77,77	0
56	MG	FB	1625	1/1	0.85	0.34	78,78,78,78	0
56	MG	A	1602	1/1	0.85	0.38	69,69,69,69	0
56	MG	JA	403	1/1	0.85	0.22	47,47,47,47	0
56	MG	GB	3196	1/1	0.85	0.21	63,63,63,63	0
56	MG	B	3637	1/1	0.85	0.25	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	2925	1/1	0.85	0.30	52,52,52,52	0
56	MG	GB	3430	1/1	0.85	0.37	75,75,75,75	0
56	MG	B	3423	1/1	0.85	0.13	43,43,43,43	0
56	MG	GB	3432	1/1	0.85	0.30	49,49,49,49	0
56	MG	B	3651	1/1	0.85	0.24	74,74,74,74	0
56	MG	B	3797	1/1	0.85	0.12	60,60,60,60	0
56	MG	B	3335	1/1	0.85	0.13	78,78,78,78	0
56	MG	GB	2997	1/1	0.85	0.27	68,68,68,68	0
56	MG	A	1658	1/1	0.85	0.17	87,87,87,87	0
56	MG	B	3801	1/1	0.85	0.11	74,74,74,74	0
56	MG	A	1639	1/1	0.85	0.19	61,61,61,61	0
56	MG	GB	3448	1/1	0.85	0.24	48,48,48,48	0
56	MG	FB	1639	1/1	0.85	0.21	72,72,72,72	0
56	MG	B	2934	1/1	0.85	0.42	62,62,62,62	0
56	MG	GB	3673	1/1	0.85	0.30	50,50,50,50	0
56	MG	GB	3005	1/1	0.85	0.26	61,61,61,61	0
56	MG	GB	3453	1/1	0.85	0.08	85,85,85,85	0
56	MG	FB	1757	1/1	0.85	0.17	101,101,101,101	0
56	MG	B	3162	1/1	0.85	0.15	43,43,43,43	0
56	MG	B	2937	1/1	0.85	0.34	50,50,50,50	0
56	MG	A	1661	1/1	0.85	0.28	64,64,64,64	0
56	MG	K	209	1/1	0.85	0.07	67,67,67,67	0
56	MG	A	1834	1/1	0.85	0.13	82,82,82,82	0
56	MG	FB	1654	1/1	0.85	0.21	56,56,56,56	0
56	MG	N	203	1/1	0.85	0.06	70,70,70,70	0
56	MG	RC	303	1/1	0.85	0.24	75,75,75,75	0
56	MG	O	203	1/1	0.85	0.18	65,65,65,65	0
56	MG	FB	1773	1/1	0.85	0.40	78,78,78,78	0
56	MG	B	3181	1/1	0.85	0.21	57,57,57,57	0
56	MG	A	1662	1/1	0.85	0.32	95,95,95,95	0
56	MG	GB	3481	1/1	0.85	0.13	64,64,64,64	0
56	MG	A	1664	1/1	0.85	0.24	73,73,73,73	0
56	MG	FB	1667	1/1	0.85	0.20	65,65,65,65	0
56	MG	GB	3259	1/1	0.85	0.18	70,70,70,70	0
56	MG	FB	1780	1/1	0.85	0.17	85,85,85,85	0
56	MG	FB	1904	1/1	0.85	0.14	60,60,60,60	0
56	MG	B	3835	1/1	0.85	0.11	80,80,80,80	0
56	MG	GB	3049	1/1	0.85	0.34	61,61,61,61	0
56	MG	ZC	201	1/1	0.85	0.08	70,70,70,70	0
56	MG	GB	3050	1/1	0.85	0.21	70,70,70,70	0
56	MG	GB	3505	1/1	0.85	0.09	81,81,81,81	0
56	MG	CD	102	1/1	0.85	0.18	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	GB	3051	1/1	0.85	0.35	67,67,67,67	0
56	MG	GB	3272	1/1	0.85	0.19	62,62,62,62	0
56	MG	FB	1783	1/1	0.85	0.29	79,79,79,79	0
56	MG	B	2928	1/1	0.86	0.24	39,39,39,39	0
56	MG	GB	3056	1/1	0.86	0.27	57,57,57,57	0
56	MG	FB	1700	1/1	0.86	0.37	73,73,73,73	0
56	MG	B	3589	1/1	0.86	0.11	60,60,60,60	0
56	MG	GB	3061	1/1	0.86	0.27	62,62,62,62	0
56	MG	B	3169	1/1	0.86	0.17	47,47,47,47	0
56	MG	FB	1923	1/1	0.86	0.27	67,67,67,67	0
56	MG	B	3314	1/1	0.86	0.09	44,44,44,44	0
56	MG	A	1873	1/1	0.86	0.15	80,80,80,80	0
56	MG	FB	1926	1/1	0.86	0.27	85,85,85,85	0
56	MG	GB	3510	1/1	0.86	0.21	73,73,73,73	0
56	MG	GB	3082	1/1	0.86	0.24	53,53,53,53	0
56	MG	B	2963	1/1	0.86	0.23	49,49,49,49	0
56	MG	I	207	1/1	0.86	0.11	70,70,70,70	0
56	MG	J	202	1/1	0.86	0.11	79,79,79,79	0
56	MG	FB	1712	1/1	0.86	0.21	78,78,78,78	0
56	MG	B	3331	1/1	0.86	0.17	49,49,49,49	0
56	MG	HB	225	1/1	0.86	0.20	96,96,96,96	0
56	MG	B	3263	1/1	0.86	0.19	69,69,69,69	0
56	MG	A	1762	1/1	0.86	0.27	93,93,93,93	0
56	MG	B	3421	1/1	0.86	0.12	80,80,80,80	0
56	MG	FB	1719	1/1	0.86	0.18	67,67,67,67	0
56	MG	GB	3096	1/1	0.86	0.26	56,56,56,56	0
56	MG	GB	3312	1/1	0.86	0.21	73,73,73,73	0
56	MG	C	207	1/1	0.86	0.21	57,57,57,57	0
56	MG	GB	3098	1/1	0.86	0.16	68,68,68,68	0
56	MG	FB	1829	1/1	0.86	0.10	69,69,69,69	0
56	MG	B	3732	1/1	0.86	0.13	57,57,57,57	0
56	MG	B	3183	1/1	0.86	0.23	57,57,57,57	0
56	MG	GB	3325	1/1	0.86	0.17	54,54,54,54	0
56	MG	B	3610	1/1	0.86	0.26	73,73,73,73	0
56	MG	B	2965	1/1	0.86	0.24	45,45,45,45	0
56	MG	GB	3115	1/1	0.86	0.24	61,61,61,61	0
56	MG	GB	3331	1/1	0.86	0.14	61,61,61,61	0
56	MG	B	3512	1/1	0.86	0.17	71,71,71,71	0
56	MG	FB	1838	1/1	0.86	0.10	76,76,76,76	0
56	MG	GB	3119	1/1	0.86	0.14	59,59,59,59	0
56	MG	GB	2912	1/1	0.86	0.40	57,57,57,57	0
56	MG	R	202	1/1	0.86	0.18	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	A	1742	1/1	0.86	0.25	66,66,66,66	0
56	MG	FB	1842	1/1	0.86	0.09	73,73,73,73	0
56	MG	U	101	1/1	0.86	0.18	56,56,56,56	0
56	MG	GB	3126	1/1	0.86	0.20	53,53,53,53	0
56	MG	GB	3352	1/1	0.86	0.24	67,67,67,67	0
56	MG	GB	3579	1/1	0.86	0.08	65,65,65,65	0
56	MG	OB	201	1/1	0.86	0.17	102,102,102,102	0
56	MG	W	301	1/1	0.86	0.23	73,73,73,73	0
56	MG	FB	1641	1/1	0.86	0.24	61,61,61,61	0
56	MG	PB	202	1/1	0.86	0.12	89,89,89,89	0
56	MG	QB	201	1/1	0.86	0.24	73,73,73,73	0
56	MG	QB	202	1/1	0.86	0.16	66,66,66,66	0
56	MG	QB	205	1/1	0.86	0.18	68,68,68,68	0
56	MG	FB	1849	1/1	0.86	0.13	65,65,65,65	0
56	MG	FB	1850	1/1	0.86	0.08	89,89,89,89	0
56	MG	GB	3359	1/1	0.86	0.13	77,77,77,77	0
56	MG	GB	3588	1/1	0.86	0.14	69,69,69,69	0
56	MG	FB	1851	1/1	0.86	0.15	70,70,70,70	0
56	MG	FB	1735	1/1	0.86	0.09	85,85,85,85	0
56	MG	GB	3593	1/1	0.86	0.29	53,53,53,53	0
56	MG	B	3518	1/1	0.86	0.27	56,56,56,56	0
56	MG	GB	2934	1/1	0.86	0.28	60,60,60,60	0
56	MG	B	3761	1/1	0.86	0.14	53,53,53,53	0
56	MG	C	219	1/1	0.86	0.33	81,81,81,81	0
56	MG	B	3191	1/1	0.86	0.23	59,59,59,59	0
56	MG	FB	1743	1/1	0.86	0.20	84,84,84,84	0
56	MG	B	3358	1/1	0.86	0.29	96,96,96,96	0
56	MG	FB	1650	1/1	0.86	0.30	66,66,66,66	0
56	MG	GB	2950	1/1	0.86	0.33	60,60,60,60	0
56	MG	FB	1863	1/1	0.86	0.24	72,72,72,72	0
56	MG	GB	3174	1/1	0.86	0.20	64,64,64,64	0
56	MG	YB	207	1/1	0.86	0.12	79,79,79,79	0
56	MG	B	3528	1/1	0.86	0.10	43,43,43,43	0
56	MG	FB	1653	1/1	0.86	0.24	65,65,65,65	0
56	MG	GB	3387	1/1	0.86	0.17	66,66,66,66	0
56	MG	FB	1754	1/1	0.86	0.27	86,86,86,86	0
56	MG	GB	2970	1/1	0.86	0.28	52,52,52,52	0
56	MG	C	230	1/1	0.86	0.23	69,69,69,69	0
56	MG	GB	2973	1/1	0.86	0.22	50,50,50,50	0
56	MG	GB	3405	1/1	0.86	0.19	70,70,70,70	0
56	MG	DC	102	1/1	0.86	0.21	78,78,78,78	0
56	MG	GB	3407	1/1	0.86	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3532	1/1	0.86	0.15	95,95,95,95	0
56	MG	GB	3187	1/1	0.86	0.10	55,55,55,55	0
56	MG	B	3278	1/1	0.86	0.18	54,54,54,54	0
56	MG	GB	3634	1/1	0.86	0.22	63,63,63,63	0
56	MG	GB	3190	1/1	0.86	0.26	71,71,71,71	0
56	MG	B	3012	1/1	0.86	0.26	51,51,51,51	0
56	MG	GB	3640	1/1	0.86	0.16	96,96,96,96	0
56	MG	A	1692	1/1	0.86	0.23	63,63,63,63	0
56	MG	NC	102	1/1	0.86	0.18	65,65,65,65	0
56	MG	B	3018	1/1	0.86	0.28	50,50,50,50	0
56	MG	FB	1665	1/1	0.86	0.39	70,70,70,70	0
56	MG	B	3649	1/1	0.86	0.10	104,104,104,104	0
56	MG	A	1622	1/1	0.86	0.23	73,73,73,73	0
56	MG	FB	1669	1/1	0.86	0.26	67,67,67,67	0
56	MG	FB	1882	1/1	0.86	0.07	77,77,77,77	0
56	MG	NC	112	1/1	0.86	0.26	76,76,76,76	0
56	MG	B	3028	1/1	0.86	0.45	50,50,50,50	0
56	MG	B	2947	1/1	0.86	0.20	40,40,40,40	0
56	MG	GB	3434	1/1	0.86	0.17	63,63,63,63	0
56	MG	GB	3437	1/1	0.86	0.30	70,70,70,70	0
56	MG	B	3454	1/1	0.86	0.12	67,67,67,67	0
56	MG	FB	1676	1/1	0.86	0.19	74,74,74,74	0
56	MG	FB	1889	1/1	0.86	0.18	69,69,69,69	0
56	MG	B	3386	1/1	0.86	0.09	101,101,101,101	0
56	MG	GB	3222	1/1	0.86	0.22	60,60,60,60	0
56	MG	GB	3012	1/1	0.86	0.23	52,52,52,52	0
56	MG	HA	102	1/1	0.86	0.42	69,69,69,69	0
56	MG	GB	3226	1/1	0.86	0.16	67,67,67,67	0
56	MG	B	3675	1/1	0.86	0.16	60,60,60,60	0
56	MG	GB	3450	1/1	0.86	0.20	77,77,77,77	0
56	MG	B	3050	1/1	0.86	0.18	42,42,42,42	0
56	MG	FB	1683	1/1	0.86	0.26	75,75,75,75	0
56	MG	GB	3233	1/1	0.86	0.17	65,65,65,65	0
56	MG	GB	3684	1/1	0.86	0.13	66,66,66,66	0
56	MG	GB	3454	1/1	0.86	0.09	77,77,77,77	0
56	MG	GB	3688	1/1	0.86	0.17	74,74,74,74	0
56	MG	GB	3234	1/1	0.86	0.27	57,57,57,57	0
56	MG	B	3678	1/1	0.86	0.17	57,57,57,57	0
56	MG	FB	1900	1/1	0.86	0.07	56,56,56,56	0
56	MG	GB	3700	1/1	0.86	0.09	61,61,61,61	0
56	MG	B	3217	1/1	0.86	0.19	54,54,54,54	0
56	MG	FB	1790	1/1	0.86	0.15	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	G	3206	1/1	0.86	0.18	58,58,58,58	0
56	MG	B	2986	1/1	0.86	0.18	37,37,37,37	0
56	MG	IA	112	1/1	0.86	0.23	83,83,83,83	0
56	MG	CB	201	1/1	0.86	0.24	94,94,94,94	0
56	MG	B	3064	1/1	0.86	0.25	52,52,52,52	0
56	MG	B	3578	1/1	0.86	0.09	54,54,54,54	0
56	MG	FB	1603	1/1	0.86	0.30	60,60,60,60	0
56	MG	ED	201	1/1	0.86	0.22	83,83,83,83	0
56	MG	FB	1698	1/1	0.86	0.17	82,82,82,82	0
56	MG	GB	3258	1/1	0.86	0.12	74,74,74,74	0
56	MG	B	3484	1/1	0.87	0.12	50,50,50,50	0
56	MG	B	3066	1/1	0.87	0.29	55,55,55,55	0
56	MG	GB	3008	1/1	0.87	0.25	62,62,62,62	0
56	MG	B	3710	1/1	0.87	0.12	69,69,69,69	0
56	MG	HB	231	1/1	0.87	0.27	79,79,79,79	0
56	MG	B	3228	1/1	0.87	0.18	58,58,58,58	0
56	MG	B	3302	1/1	0.87	0.18	54,54,54,54	0
56	MG	B	3230	1/1	0.87	0.12	59,59,59,59	0
56	MG	GB	3564	1/1	0.87	0.21	70,70,70,70	0
56	MG	GB	3366	1/1	0.87	0.15	65,65,65,65	0
56	MG	A	1793	1/1	0.87	0.14	116,116,116,116	0
56	MG	OA	204	1/1	0.87	0.09	82,82,82,82	0
56	MG	GB	3575	1/1	0.87	0.08	72,72,72,72	0
56	MG	FB	1737	1/1	0.87	0.21	61,61,61,61	0
56	MG	JB	308	1/1	0.87	0.11	73,73,73,73	0
56	MG	FB	1927	1/1	0.87	0.25	69,69,69,69	0
56	MG	B	3312	1/1	0.87	0.14	53,53,53,53	0
56	MG	B	3725	1/1	0.87	0.07	53,53,53,53	0
56	MG	A	1827	1/1	0.87	0.17	85,85,85,85	0
56	MG	B	3077	1/1	0.87	0.25	45,45,45,45	0
56	MG	GB	3034	1/1	0.87	0.36	63,63,63,63	0
56	MG	GB	3203	1/1	0.87	0.21	60,60,60,60	0
56	MG	FB	1661	1/1	0.87	0.18	66,66,66,66	0
56	MG	B	3247	1/1	0.87	0.11	62,62,62,62	0
56	MG	FB	1845	1/1	0.87	0.20	74,74,74,74	0
56	MG	GB	3044	1/1	0.87	0.34	57,57,57,57	0
56	MG	X	108	1/1	0.87	0.23	53,53,53,53	0
56	MG	B	3248	1/1	0.87	0.32	84,84,84,84	0
56	MG	GB	3404	1/1	0.87	0.20	64,64,64,64	0
56	MG	B	3180	1/1	0.87	0.22	58,58,58,58	0
56	MG	FB	1666	1/1	0.87	0.27	66,66,66,66	0
56	MG	B	2911	1/1	0.87	0.31	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3752	1/1	0.87	0.07	53,53,53,53	0
56	MG	B	3266	1/1	0.87	0.12	54,54,54,54	0
56	MG	GB	3412	1/1	0.87	0.25	75,75,75,75	0
56	MG	B	3096	1/1	0.87	0.26	54,54,54,54	0
56	MG	FB	1765	1/1	0.87	0.14	77,77,77,77	0
56	MG	GB	2906	1/1	0.87	0.34	53,53,53,53	0
56	MG	GB	3422	1/1	0.87	0.17	64,64,64,64	0
56	MG	A	1728	1/1	0.87	0.30	61,61,61,61	0
56	MG	GB	3068	1/1	0.87	0.16	66,66,66,66	0
56	MG	B	2919	1/1	0.87	0.28	52,52,52,52	0
56	MG	B	3635	1/1	0.87	0.13	56,56,56,56	0
56	MG	GB	3236	1/1	0.87	0.25	74,74,74,74	0
56	MG	GB	3079	1/1	0.87	0.22	62,62,62,62	0
56	MG	B	3780	1/1	0.87	0.16	70,70,70,70	0
56	MG	B	3529	1/1	0.87	0.23	43,43,43,43	0
56	MG	GB	3242	1/1	0.87	0.12	65,65,65,65	0
56	MG	B	2976	1/1	0.87	0.29	44,44,44,44	0
56	MG	GB	3438	1/1	0.87	0.20	52,52,52,52	0
56	MG	B	3638	1/1	0.87	0.26	61,61,61,61	0
56	MG	GB	3248	1/1	0.87	0.21	60,60,60,60	0
56	MG	YB	202	1/1	0.87	0.13	71,71,71,71	0
56	MG	B	3368	1/1	0.87	0.19	57,57,57,57	0
56	MG	YB	204	1/1	0.87	0.13	78,78,78,78	0
56	MG	F	310	1/1	0.87	0.09	69,69,69,69	0
56	MG	B	3115	1/1	0.87	0.12	39,39,39,39	0
56	MG	BC	301	1/1	0.87	0.23	85,85,85,85	0
56	MG	GB	3089	1/1	0.87	0.17	66,66,66,66	0
56	MG	FB	1778	1/1	0.87	0.38	83,83,83,83	0
56	MG	GB	2927	1/1	0.87	0.29	62,62,62,62	0
56	MG	GB	3094	1/1	0.87	0.21	54,54,54,54	0
56	MG	B	3370	1/1	0.87	0.17	64,64,64,64	0
56	MG	A	1616	1/1	0.87	0.25	74,74,74,74	0
56	MG	A	1860	1/1	0.87	0.43	81,81,81,81	0
56	MG	CC	101	1/1	0.87	0.34	66,66,66,66	0
56	MG	FB	1875	1/1	0.87	0.17	72,72,72,72	0
56	MG	G	3207	1/1	0.87	0.13	36,36,36,36	0
56	MG	GB	3457	1/1	0.87	0.16	80,80,80,80	0
56	MG	GB	3266	1/1	0.87	0.15	57,57,57,57	0
56	MG	B	3663	1/1	0.87	0.11	51,51,51,51	0
56	MG	B	3664	1/1	0.87	0.11	54,54,54,54	0
56	MG	GB	3104	1/1	0.87	0.12	65,65,65,65	0
56	MG	FB	1611	1/1	0.87	0.36	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	GB	3109	1/1	0.87	0.22	63,63,63,63	0
56	MG	B	3032	1/1	0.87	0.22	43,43,43,43	0
56	MG	IA	120	1/1	0.87	0.17	85,85,85,85	0
56	MG	B	3668	1/1	0.87	0.08	63,63,63,63	0
56	MG	B	3452	1/1	0.87	0.27	82,82,82,82	0
56	MG	B	3205	1/1	0.87	0.11	68,68,68,68	0
56	MG	GB	3294	1/1	0.87	0.22	64,64,64,64	0
56	MG	GB	2963	1/1	0.87	0.33	59,59,59,59	0
56	MG	B	3561	1/1	0.87	0.21	52,52,52,52	0
56	MG	GB	3486	1/1	0.87	0.23	68,68,68,68	0
56	MG	A	1863	1/1	0.87	0.17	93,93,93,93	0
56	MG	GB	3301	1/1	0.87	0.12	55,55,55,55	0
56	MG	GB	3307	1/1	0.87	0.14	51,51,51,51	0
56	MG	GB	3697	1/1	0.87	0.31	69,69,69,69	0
56	MG	OC	404	1/1	0.87	0.09	97,97,97,97	0
56	MG	GB	3699	1/1	0.87	0.17	57,57,57,57	0
56	MG	B	2962	1/1	0.87	0.30	43,43,43,43	0
56	MG	B	3681	1/1	0.87	0.38	71,71,71,71	0
56	MG	GB	3310	1/1	0.87	0.14	69,69,69,69	0
56	MG	GB	2979	1/1	0.87	0.26	52,52,52,52	0
56	MG	GB	3129	1/1	0.87	0.25	65,65,65,65	0
56	MG	GB	3131	1/1	0.87	0.25	71,71,71,71	0
56	MG	B	3385	1/1	0.87	0.14	59,59,59,59	0
56	MG	GB	3710	1/1	0.87	0.32	61,61,61,61	0
56	MG	FB	1710	1/1	0.87	0.31	67,67,67,67	0
56	MG	B	2998	1/1	0.87	0.21	47,47,47,47	0
56	MG	GB	3138	1/1	0.87	0.37	67,67,67,67	0
56	MG	GB	2986	1/1	0.87	0.34	49,49,49,49	0
56	MG	GB	3518	1/1	0.87	0.19	96,96,96,96	0
56	MG	B	3687	1/1	0.87	0.14	52,52,52,52	0
56	MG	GB	2992	1/1	0.87	0.22	64,64,64,64	0
56	MG	SC	202	1/1	0.87	0.26	92,92,92,92	0
56	MG	SC	204	1/1	0.87	0.17	81,81,81,81	0
56	MG	B	3463	1/1	0.87	0.16	65,65,65,65	0
56	MG	GB	3526	1/1	0.87	0.23	80,80,80,80	0
56	MG	GB	2994	1/1	0.87	0.34	74,74,74,74	0
56	MG	B	3689	1/1	0.87	0.09	50,50,50,50	0
56	MG	VC	201	1/1	0.87	0.50	77,77,77,77	0
56	MG	VC	202	1/1	0.87	0.20	75,75,75,75	0
56	MG	A	1663	1/1	0.87	0.13	63,63,63,63	0
56	MG	GB	2998	1/1	0.87	0.17	55,55,55,55	0
56	MG	LA	301	1/1	0.87	0.27	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	GB	3161	1/1	0.87	0.29	73,73,73,73	0
56	MG	B	3694	1/1	0.87	0.29	54,54,54,54	0
56	MG	B	3004	1/1	0.87	0.31	43,43,43,43	0
56	MG	GB	3165	1/1	0.87	0.29	66,66,66,66	0
56	MG	GB	3347	1/1	0.87	0.23	66,66,66,66	0
56	MG	B	3474	1/1	0.87	0.11	41,41,41,41	0
56	MG	GB	3169	1/1	0.87	0.12	54,54,54,54	0
56	MG	DD	101	1/1	0.87	0.13	71,71,71,71	0
56	MG	HB	223	1/1	0.87	0.18	85,85,85,85	0
56	MG	B	3479	1/1	0.87	0.18	39,39,39,39	0
56	MG	FB	1823	1/1	0.87	0.18	87,87,87,87	0
56	MG	GB	3388	1/1	0.88	0.26	64,64,64,64	0
56	MG	GB	3572	1/1	0.88	0.25	67,67,67,67	0
56	MG	FB	1949	1/1	0.88	0.13	82,82,82,82	0
56	MG	B	3200	1/1	0.88	0.33	66,66,66,66	0
56	MG	GB	3577	1/1	0.88	0.14	91,91,91,91	0
56	MG	JB	302	1/1	0.88	0.15	63,63,63,63	0
56	MG	FB	1649	1/1	0.88	0.32	62,62,62,62	0
56	MG	GB	3067	1/1	0.88	0.15	57,57,57,57	0
56	MG	GB	3399	1/1	0.88	0.14	54,54,54,54	0
56	MG	GB	3583	1/1	0.88	0.27	68,68,68,68	0
56	MG	GB	3403	1/1	0.88	0.43	65,65,65,65	0
56	MG	O	202	1/1	0.88	0.14	70,70,70,70	0
56	MG	JB	313	1/1	0.88	0.12	68,68,68,68	0
56	MG	B	3508	1/1	0.88	0.14	65,65,65,65	0
56	MG	GB	3406	1/1	0.88	0.17	59,59,59,59	0
56	MG	GB	3073	1/1	0.88	0.15	64,64,64,64	0
56	MG	GB	3408	1/1	0.88	0.18	55,55,55,55	0
56	MG	B	3428	1/1	0.88	0.17	48,48,48,48	0
56	MG	A	1836	1/1	0.88	0.20	105,105,105,105	0
56	MG	B	3119	1/1	0.88	0.35	69,69,69,69	0
56	MG	B	3129	1/1	0.88	0.26	54,54,54,54	0
56	MG	A	1689	1/1	0.88	0.08	56,56,56,56	0
56	MG	FB	1760	1/1	0.88	0.40	68,68,68,68	0
56	MG	B	3373	1/1	0.88	0.11	50,50,50,50	0
56	MG	S	203	1/1	0.88	0.16	57,57,57,57	0
56	MG	A	1855	1/1	0.88	0.17	89,89,89,89	0
56	MG	S	208	1/1	0.88	0.14	53,53,53,53	0
56	MG	GB	2928	1/1	0.88	0.51	77,77,77,77	0
56	MG	GB	3091	1/1	0.88	0.28	57,57,57,57	0
56	MG	T	203	1/1	0.88	0.10	58,58,58,58	0
56	MG	B	3038	1/1	0.88	0.21	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	GB	3612	1/1	0.88	0.14	71,71,71,71	0
56	MG	B	3744	1/1	0.88	0.09	48,48,48,48	0
56	MG	A	1626	1/1	0.88	0.38	63,63,63,63	0
56	MG	B	3139	1/1	0.88	0.12	47,47,47,47	0
56	MG	B	3146	1/1	0.88	0.20	48,48,48,48	0
56	MG	B	2983	1/1	0.88	0.21	50,50,50,50	0
56	MG	GB	3623	1/1	0.88	0.14	63,63,63,63	0
56	MG	B	3753	1/1	0.88	0.23	75,75,75,75	0
56	MG	B	3754	1/1	0.88	0.15	57,57,57,57	0
56	MG	X	104	1/1	0.88	0.20	51,51,51,51	0
56	MG	GB	3264	1/1	0.88	0.08	71,71,71,71	0
56	MG	GB	3631	1/1	0.88	0.09	60,60,60,60	0
56	MG	GB	3105	1/1	0.88	0.38	73,73,73,73	0
56	MG	B	3544	1/1	0.88	0.17	85,85,85,85	0
56	MG	A	1823	1/1	0.88	0.13	54,54,54,54	0
56	MG	FB	1881	1/1	0.88	0.27	68,68,68,68	0
56	MG	GB	3114	1/1	0.88	0.29	69,69,69,69	0
56	MG	B	3549	1/1	0.88	0.11	51,51,51,51	0
56	MG	GB	3642	1/1	0.88	0.14	76,76,76,76	0
56	MG	GB	3643	1/1	0.88	0.19	55,55,55,55	0
56	MG	FB	1883	1/1	0.88	0.10	70,70,70,70	0
56	MG	GB	2968	1/1	0.88	0.42	69,69,69,69	0
56	MG	UA	203	1/1	0.88	0.12	74,74,74,74	0
56	MG	ZB	101	1/1	0.88	0.24	78,78,78,78	0
56	MG	GB	3649	1/1	0.88	0.17	70,70,70,70	0
56	MG	B	3763	1/1	0.88	0.11	56,56,56,56	0
56	MG	GB	3455	1/1	0.88	0.14	64,64,64,64	0
56	MG	GB	2972	1/1	0.88	0.31	51,51,51,51	0
56	MG	FB	1886	1/1	0.88	0.17	82,82,82,82	0
56	MG	FB	1787	1/1	0.88	0.32	77,77,77,77	0
56	MG	GB	2980	1/1	0.88	0.17	43,43,43,43	0
56	MG	B	3303	1/1	0.88	0.11	41,41,41,41	0
56	MG	B	3777	1/1	0.88	0.12	50,50,50,50	0
56	MG	GB	3130	1/1	0.88	0.25	60,60,60,60	0
56	MG	GB	3469	1/1	0.88	0.17	65,65,65,65	0
56	MG	A	1754	1/1	0.88	0.43	90,90,90,90	0
56	MG	A	1739	1/1	0.88	0.17	59,59,59,59	0
56	MG	B	3662	1/1	0.88	0.08	65,65,65,65	0
56	MG	B	3559	1/1	0.88	0.18	63,63,63,63	0
56	MG	A	1861	1/1	0.88	0.10	92,92,92,92	0
56	MG	GB	3477	1/1	0.88	0.09	60,60,60,60	0
56	MG	E	310	1/1	0.88	0.09	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	KC	102	1/1	0.88	0.17	61,61,61,61	0
56	MG	B	3395	1/1	0.88	0.12	58,58,58,58	0
56	MG	B	3562	1/1	0.88	0.16	73,73,73,73	0
56	MG	GB	3678	1/1	0.88	0.12	87,87,87,87	0
56	MG	GB	3483	1/1	0.88	0.21	78,78,78,78	0
56	MG	FB	1799	1/1	0.88	0.32	71,71,71,71	0
56	MG	A	1603	1/1	0.88	0.21	78,78,78,78	0
56	MG	B	3470	1/1	0.88	0.14	71,71,71,71	0
56	MG	GB	3686	1/1	0.88	0.47	65,65,65,65	0
56	MG	B	3570	1/1	0.88	0.12	65,65,65,65	0
56	MG	GB	3156	1/1	0.88	0.20	46,46,46,46	0
56	MG	B	3794	1/1	0.88	0.13	60,60,60,60	0
56	MG	FB	1609	1/1	0.88	0.25	64,64,64,64	0
56	MG	A	1650	1/1	0.88	0.13	86,86,86,86	0
56	MG	G	3204	1/1	0.88	0.07	49,49,49,49	0
56	MG	GB	3335	1/1	0.88	0.17	54,54,54,54	0
56	MG	IA	110	1/1	0.88	0.19	83,83,83,83	0
56	MG	B	3323	1/1	0.88	0.24	83,83,83,83	0
56	MG	B	3483	1/1	0.88	0.12	48,48,48,48	0
56	MG	GB	3010	1/1	0.88	0.25	67,67,67,67	0
56	MG	IA	115	1/1	0.88	0.28	73,73,73,73	0
56	MG	A	1865	1/1	0.88	0.21	77,77,77,77	0
56	MG	B	3584	1/1	0.88	0.07	46,46,46,46	0
56	MG	B	3406	1/1	0.88	0.09	55,55,55,55	0
56	MG	HB	201	1/1	0.88	0.49	78,78,78,78	0
56	MG	GB	3021	1/1	0.88	0.22	56,56,56,56	0
56	MG	RC	301	1/1	0.88	0.38	69,69,69,69	0
56	MG	B	3804	1/1	0.88	0.10	51,51,51,51	0
56	MG	A	1761	1/1	0.88	0.23	74,74,74,74	0
56	MG	B	2961	1/1	0.88	0.20	38,38,38,38	0
56	MG	RC	306	1/1	0.88	0.17	81,81,81,81	0
56	MG	B	2904	1/1	0.88	0.28	46,46,46,46	0
56	MG	RC	309	1/1	0.88	0.09	77,77,77,77	0
56	MG	B	3104	1/1	0.88	0.22	70,70,70,70	0
56	MG	SC	201	1/1	0.88	0.39	70,70,70,70	0
56	MG	A	1674	1/1	0.88	0.28	65,65,65,65	0
56	MG	JA	406	1/1	0.88	0.07	87,87,87,87	0
56	MG	GB	3191	1/1	0.88	0.17	68,68,68,68	0
56	MG	FB	1934	1/1	0.88	0.14	82,82,82,82	0
56	MG	SC	207	1/1	0.88	0.20	85,85,85,85	0
56	MG	B	3597	1/1	0.88	0.10	49,49,49,49	0
56	MG	B	3825	1/1	0.88	0.13	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	GB	3040	1/1	0.88	0.31	48,48,48,48	0
56	MG	GB	3372	1/1	0.88	0.18	81,81,81,81	0
56	MG	JA	411	1/1	0.88	0.25	100,100,100,100	0
56	MG	A	1817	1/1	0.88	0.10	66,66,66,66	0
56	MG	GB	3047	1/1	0.88	0.20	59,59,59,59	0
56	MG	B	3501	1/1	0.88	0.12	48,48,48,48	0
56	MG	YC	203	1/1	0.88	0.15	82,82,82,82	0
56	MG	YC	205	1/1	0.88	0.21	66,66,66,66	0
56	MG	L	202	1/1	0.88	0.13	58,58,58,58	0
56	MG	A	1805	1/1	0.88	0.32	87,87,87,87	0
56	MG	GB	3381	1/1	0.88	0.27	66,66,66,66	0
56	MG	FB	1844	1/1	0.88	0.21	81,81,81,81	0
56	MG	GB	3561	1/1	0.88	0.15	68,68,68,68	0
56	MG	M	201	1/1	0.88	0.20	44,44,44,44	0
56	MG	GB	3563	1/1	0.88	0.15	72,72,72,72	0
56	MG	M	204	1/1	0.88	0.14	69,69,69,69	0
56	MG	FB	1947	1/1	0.88	0.18	73,73,73,73	0
56	MG	N	202	1/1	0.88	0.06	71,71,71,71	0
56	MG	B	3419	1/1	0.89	0.12	54,54,54,54	0
56	MG	B	3729	1/1	0.89	0.09	93,93,93,93	0
56	MG	FB	1802	1/1	0.89	0.19	64,64,64,64	0
56	MG	GB	3560	1/1	0.89	0.26	60,60,60,60	0
56	MG	GB	3374	1/1	0.89	0.17	62,62,62,62	0
56	MG	FB	1690	1/1	0.89	0.20	69,69,69,69	0
56	MG	FB	1693	1/1	0.89	0.32	66,66,66,66	0
56	MG	B	3255	1/1	0.89	0.15	48,48,48,48	0
56	MG	GB	3566	1/1	0.89	0.27	66,66,66,66	0
56	MG	B	3514	1/1	0.89	0.09	55,55,55,55	0
56	MG	UA	202	1/1	0.89	0.26	79,79,79,79	0
56	MG	X	101	1/1	0.89	0.27	58,58,58,58	0
56	MG	A	1883	1/1	0.89	0.15	79,79,79,79	0
56	MG	FB	1930	1/1	0.89	0.14	68,68,68,68	0
56	MG	X	105	1/1	0.89	0.17	55,55,55,55	0
56	MG	B	3186	1/1	0.89	0.22	48,48,48,48	0
56	MG	C	224	1/1	0.89	0.15	74,74,74,74	0
56	MG	Y	101	1/1	0.89	0.14	49,49,49,49	0
56	MG	B	3624	1/1	0.89	0.11	66,66,66,66	0
56	MG	LB	303	1/1	0.89	0.23	53,53,53,53	0
56	MG	C	226	1/1	0.89	0.09	89,89,89,89	0
56	MG	Z	101	1/1	0.89	0.20	76,76,76,76	0
56	MG	GB	3053	1/1	0.89	0.13	53,53,53,53	0
56	MG	GB	3055	1/1	0.89	0.23	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	GB	3400	1/1	0.89	0.24	71,71,71,71	0
56	MG	GB	3402	1/1	0.89	0.25	66,66,66,66	0
56	MG	B	3625	1/1	0.89	0.25	58,58,58,58	0
56	MG	B	3341	1/1	0.89	0.25	58,58,58,58	0
56	MG	A	1748	1/1	0.89	0.14	76,76,76,76	0
56	MG	C	232	1/1	0.89	0.08	82,82,82,82	0
56	MG	B	3630	1/1	0.89	0.08	39,39,39,39	0
56	MG	FB	1834	1/1	0.89	0.33	68,68,68,68	0
56	MG	GB	3228	1/1	0.89	0.12	62,62,62,62	0
56	MG	A	1633	1/1	0.89	0.32	86,86,86,86	0
56	MG	B	3003	1/1	0.89	0.23	53,53,53,53	0
56	MG	FA	104	1/1	0.89	0.11	49,49,49,49	0
56	MG	B	3269	1/1	0.89	0.10	52,52,52,52	0
56	MG	B	3356	1/1	0.89	0.18	50,50,50,50	0
56	MG	B	3193	1/1	0.89	0.10	54,54,54,54	0
56	MG	FB	1841	1/1	0.89	0.14	85,85,85,85	0
56	MG	GB	3609	1/1	0.89	0.19	73,73,73,73	0
56	MG	GB	3081	1/1	0.89	0.19	51,51,51,51	0
56	MG	GB	3239	1/1	0.89	0.11	54,54,54,54	0
56	MG	B	3060	1/1	0.89	0.18	53,53,53,53	0
56	MG	B	3773	1/1	0.89	0.10	99,99,99,99	0
56	MG	GB	3617	1/1	0.89	0.23	67,67,67,67	0
56	MG	GB	3427	1/1	0.89	0.17	61,61,61,61	0
56	MG	GB	3619	1/1	0.89	0.09	75,75,75,75	0
56	MG	FB	1618	1/1	0.89	0.43	67,67,67,67	0
56	MG	IA	105	1/1	0.89	0.23	80,80,80,80	0
56	MG	GB	3247	1/1	0.89	0.25	62,62,62,62	0
56	MG	B	3640	1/1	0.89	0.11	53,53,53,53	0
56	MG	FB	1728	1/1	0.89	0.41	81,81,81,81	0
56	MG	FB	1623	1/1	0.89	0.27	53,53,53,53	0
56	MG	GB	3251	1/1	0.89	0.11	55,55,55,55	0
56	MG	B	3441	1/1	0.89	0.23	49,49,49,49	0
56	MG	GB	3440	1/1	0.89	0.14	80,80,80,80	0
56	MG	F	303	1/1	0.89	0.18	71,71,71,71	0
56	MG	B	3645	1/1	0.89	0.12	70,70,70,70	0
56	MG	B	2966	1/1	0.89	0.32	60,60,60,60	0
56	MG	GB	3636	1/1	0.89	0.18	75,75,75,75	0
56	MG	GB	3638	1/1	0.89	0.43	66,66,66,66	0
56	MG	GB	3093	1/1	0.89	0.22	58,58,58,58	0
56	MG	A	1848	1/1	0.89	0.33	70,70,70,70	0
56	MG	B	2969	1/1	0.89	0.29	57,57,57,57	0
56	MG	FB	1856	1/1	0.89	0.12	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3202	1/1	0.89	0.29	64,64,64,64	0
56	MG	GB	2936	1/1	0.89	0.29	54,54,54,54	0
56	MG	A	1698	1/1	0.89	0.34	77,77,77,77	0
56	MG	A	1810	1/1	0.89	0.21	75,75,75,75	0
56	MG	B	3289	1/1	0.89	0.14	38,38,38,38	0
56	MG	FB	1744	1/1	0.89	0.18	55,55,55,55	0
56	MG	A	1657	1/1	0.89	0.49	90,90,90,90	0
56	MG	G	3208	1/1	0.89	0.17	58,58,58,58	0
56	MG	GB	3458	1/1	0.89	0.06	95,95,95,95	0
56	MG	B	3150	1/1	0.89	0.19	53,53,53,53	0
56	MG	A	1820	1/1	0.89	0.26	93,93,93,93	0
56	MG	GB	3282	1/1	0.89	0.11	70,70,70,70	0
56	MG	GB	3283	1/1	0.89	0.21	73,73,73,73	0
56	MG	KC	104	1/1	0.89	0.11	60,60,60,60	0
56	MG	GB	3113	1/1	0.89	0.14	69,69,69,69	0
56	MG	GB	3288	1/1	0.89	0.14	73,73,73,73	0
56	MG	B	3093	1/1	0.89	0.28	54,54,54,54	0
56	MG	GB	3471	1/1	0.89	0.22	64,64,64,64	0
56	MG	B	3387	1/1	0.89	0.23	60,60,60,60	0
56	MG	B	3095	1/1	0.89	0.25	56,56,56,56	0
56	MG	B	3472	1/1	0.89	0.14	55,55,55,55	0
56	MG	NC	107	1/1	0.89	0.08	96,96,96,96	0
56	MG	B	3680	1/1	0.89	0.19	52,52,52,52	0
56	MG	B	3019	1/1	0.89	0.27	51,51,51,51	0
56	MG	B	3806	1/1	0.89	0.11	58,58,58,58	0
56	MG	NC	113	1/1	0.89	0.08	80,80,80,80	0
56	MG	B	3575	1/1	0.89	0.18	69,69,69,69	0
56	MG	GB	3480	1/1	0.89	0.15	70,70,70,70	0
56	MG	GB	3306	1/1	0.89	0.22	57,57,57,57	0
56	MG	B	3299	1/1	0.89	0.15	45,45,45,45	0
56	MG	GB	2974	1/1	0.89	0.23	49,49,49,49	0
56	MG	B	3814	1/1	0.89	0.27	38,38,38,38	0
56	MG	GB	3687	1/1	0.89	0.08	72,72,72,72	0
56	MG	B	3583	1/1	0.89	0.07	73,73,73,73	0
56	MG	B	3817	1/1	0.89	0.09	46,46,46,46	0
56	MG	B	3224	1/1	0.89	0.12	52,52,52,52	0
56	MG	A	1842	1/1	0.89	0.08	67,67,67,67	0
56	MG	GB	3496	1/1	0.89	0.11	70,70,70,70	0
56	MG	B	3101	1/1	0.89	0.32	47,47,47,47	0
56	MG	GB	2987	1/1	0.89	0.19	48,48,48,48	0
56	MG	GB	3499	1/1	0.89	0.17	61,61,61,61	0
56	MG	GB	3702	1/1	0.89	0.08	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	GB	3502	1/1	0.89	0.09	53,53,53,53	0
56	MG	A	1645	1/1	0.89	0.13	75,75,75,75	0
56	MG	B	3591	1/1	0.89	0.22	61,61,61,61	0
56	MG	B	3401	1/1	0.89	0.09	46,46,46,46	0
56	MG	B	3832	1/1	0.89	0.06	59,59,59,59	0
56	MG	B	3833	1/1	0.89	0.18	48,48,48,48	0
56	MG	GB	3151	1/1	0.89	0.20	70,70,70,70	0
56	MG	B	3310	1/1	0.89	0.21	56,56,56,56	0
56	MG	B	3177	1/1	0.89	0.11	47,47,47,47	0
56	MG	FB	1784	1/1	0.89	0.15	60,60,60,60	0
56	MG	B	3178	1/1	0.89	0.22	43,43,43,43	0
56	MG	GB	3157	1/1	0.89	0.14	68,68,68,68	0
56	MG	FB	1898	1/1	0.89	0.13	70,70,70,70	0
56	MG	B	3842	1/1	0.89	0.13	60,60,60,60	0
56	MG	R	201	1/1	0.89	0.12	54,54,54,54	0
56	MG	FB	1675	1/1	0.89	0.37	72,72,72,72	0
56	MG	GB	3163	1/1	0.89	0.15	74,74,74,74	0
56	MG	B	3409	1/1	0.89	0.18	105,105,105,105	0
56	MG	C	202	1/1	0.89	0.29	59,59,59,59	0
56	MG	B	3600	1/1	0.89	0.08	54,54,54,54	0
56	MG	B	3712	1/1	0.89	0.09	59,59,59,59	0
56	MG	GB	3355	1/1	0.89	0.17	69,69,69,69	0
56	MG	YC	204	1/1	0.89	0.15	94,94,94,94	0
56	MG	B	3246	1/1	0.89	0.14	47,47,47,47	0
56	MG	GB	3173	1/1	0.89	0.12	80,80,80,80	0
56	MG	B	3322	1/1	0.89	0.16	46,46,46,46	0
56	MG	GB	3546	1/1	0.89	0.08	63,63,63,63	0
56	MG	HB	220	1/1	0.89	0.14	92,92,92,92	0
56	MG	GB	3177	1/1	0.89	0.34	58,58,58,58	0
56	MG	A	1651	1/1	0.89	0.36	97,97,97,97	0
56	MG	B	3106	1/1	0.89	0.25	58,58,58,58	0
56	MG	GB	3019	1/1	0.89	0.24	49,49,49,49	0
56	MG	FB	1912	1/1	0.89	0.21	73,73,73,73	0
56	MG	B	3723	1/1	0.89	0.11	67,67,67,67	0
56	MG	GB	3267	1/1	0.90	0.24	74,74,74,74	0
56	MG	GB	3066	1/1	0.90	0.26	55,55,55,55	0
56	MG	B	3568	1/1	0.90	0.10	53,53,53,53	0
56	MG	GB	3271	1/1	0.90	0.33	84,84,84,84	0
56	MG	B	3340	1/1	0.90	0.08	62,62,62,62	0
56	MG	GB	3491	1/1	0.90	0.29	55,55,55,55	0
56	MG	B	3698	1/1	0.90	0.10	77,77,77,77	0
56	MG	B	3699	1/1	0.90	0.21	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	FB	1634	1/1	0.90	0.29	80,80,80,80	0
56	MG	A	1786	1/1	0.90	0.23	59,59,59,59	0
56	MG	B	3703	1/1	0.90	0.12	59,59,59,59	0
56	MG	CA	104	1/1	0.90	0.09	65,65,65,65	0
56	MG	DA	103	1/1	0.90	0.07	68,68,68,68	0
56	MG	A	1644	1/1	0.90	0.27	62,62,62,62	0
56	MG	GB	3506	1/1	0.90	0.26	71,71,71,71	0
56	MG	B	3706	1/1	0.90	0.16	50,50,50,50	0
56	MG	B	3449	1/1	0.90	0.19	46,46,46,46	0
56	MG	FB	1789	1/1	0.90	0.10	69,69,69,69	0
56	MG	C	220	1/1	0.90	0.06	83,83,83,83	0
56	MG	GB	3512	1/1	0.90	0.12	67,67,67,67	0
56	MG	B	3345	1/1	0.90	0.18	72,72,72,72	0
56	MG	IA	101	1/1	0.90	0.12	67,67,67,67	0
56	MG	B	3576	1/1	0.90	0.15	69,69,69,69	0
56	MG	FB	1648	1/1	0.90	0.32	57,57,57,57	0
56	MG	B	3453	1/1	0.90	0.15	44,44,44,44	0
56	MG	IA	104	1/1	0.90	0.16	44,44,44,44	0
56	MG	B	3006	1/1	0.90	0.25	53,53,53,53	0
56	MG	B	3716	1/1	0.90	0.18	65,65,65,65	0
56	MG	B	3164	1/1	0.90	0.14	46,46,46,46	0
56	MG	B	3258	1/1	0.90	0.16	49,49,49,49	0
56	MG	B	3354	1/1	0.90	0.09	48,48,48,48	0
56	MG	B	2917	1/1	0.90	0.44	46,46,46,46	0
56	MG	GB	2904	1/1	0.90	0.47	57,57,57,57	0
56	MG	GB	3321	1/1	0.90	0.23	61,61,61,61	0
56	MG	GB	3536	1/1	0.90	0.18	67,67,67,67	0
56	MG	C	234	1/1	0.90	0.07	65,65,65,65	0
56	MG	B	3462	1/1	0.90	0.12	41,41,41,41	0
56	MG	B	3724	1/1	0.90	0.10	48,48,48,48	0
56	MG	B	3167	1/1	0.90	0.12	44,44,44,44	0
56	MG	FB	1810	1/1	0.90	0.24	71,71,71,71	0
56	MG	B	3264	1/1	0.90	0.23	70,70,70,70	0
56	MG	C	242	1/1	0.90	0.08	86,86,86,86	0
56	MG	GB	3332	1/1	0.90	0.12	64,64,64,64	0
56	MG	B	3595	1/1	0.90	0.17	75,75,75,75	0
56	MG	KB	303	1/1	0.90	0.17	79,79,79,79	0
56	MG	LB	302	1/1	0.90	0.26	61,61,61,61	0
56	MG	GB	2918	1/1	0.90	0.34	56,56,56,56	0
56	MG	GB	3336	1/1	0.90	0.14	68,68,68,68	0
56	MG	LB	305	1/1	0.90	0.21	55,55,55,55	0
56	MG	B	3737	1/1	0.90	0.09	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3265	1/1	0.90	0.23	62,62,62,62	0
56	MG	B	3076	1/1	0.90	0.23	45,45,45,45	0
56	MG	B	3008	1/1	0.90	0.26	80,80,80,80	0
56	MG	A	1720	1/1	0.90	0.31	72,72,72,72	0
56	MG	B	3476	1/1	0.90	0.16	67,67,67,67	0
56	MG	B	3748	1/1	0.90	0.20	65,65,65,65	0
56	MG	B	3605	1/1	0.90	0.21	57,57,57,57	0
56	MG	GB	3565	1/1	0.90	0.12	60,60,60,60	0
56	MG	B	2920	1/1	0.90	0.35	44,44,44,44	0
56	MG	B	3270	1/1	0.90	0.21	56,56,56,56	0
56	MG	B	3094	1/1	0.90	0.20	51,51,51,51	0
56	MG	GB	3132	1/1	0.90	0.18	65,65,65,65	0
56	MG	FB	1833	1/1	0.90	0.21	62,62,62,62	0
56	MG	PB	203	1/1	0.90	0.12	91,91,91,91	0
56	MG	PB	204	1/1	0.90	0.06	95,95,95,95	0
56	MG	GB	3574	1/1	0.90	0.07	83,83,83,83	0
56	MG	B	3756	1/1	0.90	0.12	59,59,59,59	0
56	MG	QB	203	1/1	0.90	0.15	69,69,69,69	0
56	MG	GB	2941	1/1	0.90	0.29	53,53,53,53	0
56	MG	FB	1685	1/1	0.90	0.14	61,61,61,61	0
56	MG	A	1802	1/1	0.90	0.29	73,73,73,73	0
56	MG	GB	3140	1/1	0.90	0.25	74,74,74,74	0
56	MG	GB	3580	1/1	0.90	0.14	74,74,74,74	0
56	MG	TB	202	1/1	0.90	0.14	72,72,72,72	0
56	MG	B	3612	1/1	0.90	0.11	59,59,59,59	0
56	MG	GB	2946	1/1	0.90	0.30	52,52,52,52	0
56	MG	B	3614	1/1	0.90	0.16	50,50,50,50	0
56	MG	GB	3367	1/1	0.90	0.24	76,76,76,76	0
56	MG	B	3275	1/1	0.90	0.26	49,49,49,49	0
56	MG	A	1846	1/1	0.90	0.15	57,57,57,57	0
56	MG	FB	1691	1/1	0.90	0.23	74,74,74,74	0
56	MG	VB	208	1/1	0.90	0.11	74,74,74,74	0
56	MG	WB	201	1/1	0.90	0.11	80,80,80,80	0
56	MG	GB	2953	1/1	0.90	0.24	56,56,56,56	0
56	MG	B	3015	1/1	0.90	0.20	49,49,49,49	0
56	MG	GB	2961	1/1	0.90	0.32	64,64,64,64	0
56	MG	GB	2962	1/1	0.90	0.22	61,61,61,61	0
56	MG	B	3099	1/1	0.90	0.17	37,37,37,37	0
56	MG	B	3494	1/1	0.90	0.20	70,70,70,70	0
56	MG	GB	2967	1/1	0.90	0.28	61,61,61,61	0
56	MG	B	3495	1/1	0.90	0.13	46,46,46,46	0
56	MG	YB	205	1/1	0.90	0.12	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3781	1/1	0.90	0.11	69,69,69,69	0
56	MG	B	3100	1/1	0.90	0.27	46,46,46,46	0
56	MG	A	1729	1/1	0.90	0.20	63,63,63,63	0
56	MG	A	1880	1/1	0.90	0.21	77,77,77,77	0
56	MG	B	3192	1/1	0.90	0.31	58,58,58,58	0
56	MG	GB	2976	1/1	0.90	0.27	52,52,52,52	0
56	MG	GB	3391	1/1	0.90	0.20	60,60,60,60	0
56	MG	K	201	1/1	0.90	0.29	58,58,58,58	0
56	MG	K	204	1/1	0.90	0.10	65,65,65,65	0
56	MG	K	205	1/1	0.90	0.10	56,56,56,56	0
56	MG	BC	308	1/1	0.90	0.12	104,104,104,104	0
56	MG	B	3022	1/1	0.90	0.23	45,45,45,45	0
56	MG	K	208	1/1	0.90	0.06	71,71,71,71	0
56	MG	B	3789	1/1	0.90	0.21	46,46,46,46	0
56	MG	B	3396	1/1	0.90	0.23	49,49,49,49	0
56	MG	B	3292	1/1	0.90	0.17	50,50,50,50	0
56	MG	A	1653	1/1	0.90	0.31	74,74,74,74	0
56	MG	B	3024	1/1	0.90	0.15	40,40,40,40	0
56	MG	B	3295	1/1	0.90	0.10	55,55,55,55	0
56	MG	B	3517	1/1	0.90	0.16	53,53,53,53	0
56	MG	GB	3628	1/1	0.90	0.14	73,73,73,73	0
56	MG	GB	2996	1/1	0.90	0.41	57,57,57,57	0
56	MG	O	201	1/1	0.90	0.06	76,76,76,76	0
56	MG	FB	1867	1/1	0.90	0.17	82,82,82,82	0
56	MG	B	3025	1/1	0.90	0.18	47,47,47,47	0
56	MG	B	3116	1/1	0.90	0.11	49,49,49,49	0
56	MG	GB	3415	1/1	0.90	0.26	55,55,55,55	0
56	MG	GB	3417	1/1	0.90	0.08	66,66,66,66	0
56	MG	B	3407	1/1	0.90	0.10	72,72,72,72	0
56	MG	GB	3637	1/1	0.90	0.08	49,49,49,49	0
56	MG	GB	3201	1/1	0.90	0.30	57,57,57,57	0
56	MG	B	3650	1/1	0.90	0.18	58,58,58,58	0
56	MG	GB	3003	1/1	0.90	0.32	55,55,55,55	0
56	MG	NC	110	1/1	0.90	0.16	69,69,69,69	0
56	MG	GB	3205	1/1	0.90	0.31	71,71,71,71	0
56	MG	B	3026	1/1	0.90	0.10	40,40,40,40	0
56	MG	B	3655	1/1	0.90	0.18	46,46,46,46	0
56	MG	Q	202	1/1	0.90	0.17	74,74,74,74	0
56	MG	GB	3212	1/1	0.90	0.30	55,55,55,55	0
56	MG	B	3027	1/1	0.90	0.17	42,42,42,42	0
56	MG	B	3530	1/1	0.90	0.10	58,58,58,58	0
56	MG	B	3120	1/1	0.90	0.34	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	S	202	1/1	0.90	0.12	63,63,63,63	0
56	MG	B	3127	1/1	0.90	0.19	55,55,55,55	0
56	MG	GB	3015	1/1	0.90	0.22	54,54,54,54	0
56	MG	B	3816	1/1	0.90	0.17	60,60,60,60	0
56	MG	ZA	203	1/1	0.90	0.33	91,91,91,91	0
56	MG	B	3306	1/1	0.90	0.07	44,44,44,44	0
56	MG	A	1758	1/1	0.90	0.12	77,77,77,77	0
56	MG	A	1807	1/1	0.90	0.15	87,87,87,87	0
56	MG	B	3131	1/1	0.90	0.20	57,57,57,57	0
56	MG	GB	3023	1/1	0.90	0.32	51,51,51,51	0
56	MG	GB	3231	1/1	0.90	0.14	60,60,60,60	0
56	MG	FB	1604	1/1	0.90	0.44	67,67,67,67	0
56	MG	GB	3026	1/1	0.90	0.17	54,54,54,54	0
56	MG	B	3133	1/1	0.90	0.20	50,50,50,50	0
56	MG	FB	1745	1/1	0.90	0.14	67,67,67,67	0
56	MG	B	3676	1/1	0.90	0.09	55,55,55,55	0
56	MG	A	1759	1/1	0.90	0.33	62,62,62,62	0
56	MG	FB	1610	1/1	0.90	0.34	68,68,68,68	0
56	MG	GB	3679	1/1	0.90	0.13	72,72,72,72	0
56	MG	A	1647	1/1	0.90	0.16	82,82,82,82	0
56	MG	SC	203	1/1	0.90	0.25	85,85,85,85	0
56	MG	FB	1897	1/1	0.90	0.26	67,67,67,67	0
56	MG	B	3226	1/1	0.90	0.22	64,64,64,64	0
56	MG	W	307	1/1	0.90	0.06	87,87,87,87	0
56	MG	GB	3461	1/1	0.90	0.24	76,76,76,76	0
56	MG	B	3557	1/1	0.90	0.13	47,47,47,47	0
56	MG	B	3682	1/1	0.90	0.17	67,67,67,67	0
56	MG	GB	3045	1/1	0.90	0.28	51,51,51,51	0
56	MG	X	103	1/1	0.90	0.38	64,64,64,64	0
56	MG	GB	3695	1/1	0.90	0.16	75,75,75,75	0
56	MG	FB	1761	1/1	0.90	0.13	72,72,72,72	0
56	MG	A	1707	1/1	0.90	0.30	79,79,79,79	0
56	MG	GB	3698	1/1	0.90	0.15	68,68,68,68	0
56	MG	YC	202	1/1	0.90	0.11	81,81,81,81	0
56	MG	GB	3470	1/1	0.90	0.21	73,73,73,73	0
56	MG	FB	1621	1/1	0.90	0.25	74,74,74,74	0
56	MG	A	1628	1/1	0.90	0.37	77,77,77,77	0
56	MG	B	3844	1/1	0.90	0.11	53,53,53,53	0
56	MG	B	2907	1/1	0.90	0.30	41,41,41,41	0
56	MG	FB	1910	1/1	0.90	0.17	78,78,78,78	0
56	MG	B	3334	1/1	0.90	0.10	46,46,46,46	0
56	MG	B	3149	1/1	0.90	0.14	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	GB	3707	1/1	0.90	0.35	42,42,42,42	0
56	MG	FB	1627	1/1	0.90	0.28	75,75,75,75	0
56	MG	FB	1916	1/1	0.90	0.11	73,73,73,73	0
56	MG	B	2960	1/1	0.90	0.16	47,47,47,47	0
56	MG	B	3693	1/1	0.90	0.08	51,51,51,51	0
57	ZN	GC	101	1/1	0.90	0.09	149,149,149,149	0
56	MG	B	3195	1/1	0.91	0.14	52,52,52,52	0
56	MG	B	3521	1/1	0.91	0.16	73,73,73,73	0
56	MG	GB	3262	1/1	0.91	0.17	50,50,50,50	0
56	MG	C	243	1/1	0.91	0.18	57,57,57,57	0
56	MG	B	3690	1/1	0.91	0.19	59,59,59,59	0
56	MG	GB	3116	1/1	0.91	0.25	66,66,66,66	0
56	MG	GB	2978	1/1	0.91	0.24	58,58,58,58	0
56	MG	B	2931	1/1	0.91	0.24	39,39,39,39	0
56	MG	GB	3268	1/1	0.91	0.34	42,42,42,42	0
56	MG	B	3793	1/1	0.91	0.09	81,81,81,81	0
56	MG	E	303	1/1	0.91	0.15	62,62,62,62	0
56	MG	E	308	1/1	0.91	0.23	52,52,52,52	0
56	MG	B	2933	1/1	0.91	0.13	52,52,52,52	0
56	MG	GB	3443	1/1	0.91	0.17	69,69,69,69	0
56	MG	Y	105	1/1	0.91	0.08	52,52,52,52	0
56	MG	B	3608	1/1	0.91	0.14	63,63,63,63	0
56	MG	B	3318	1/1	0.91	0.23	49,49,49,49	0
56	MG	GB	3616	1/1	0.91	0.12	81,81,81,81	0
56	MG	B	3148	1/1	0.91	0.14	67,67,67,67	0
56	MG	AA	103	1/1	0.91	0.16	59,59,59,59	0
56	MG	A	1832	1/1	0.91	0.15	67,67,67,67	0
56	MG	GB	3620	1/1	0.91	0.22	69,69,69,69	0
56	MG	B	3533	1/1	0.91	0.13	60,60,60,60	0
56	MG	GB	3134	1/1	0.91	0.21	61,61,61,61	0
56	MG	B	3800	1/1	0.91	0.10	52,52,52,52	0
56	MG	GB	3624	1/1	0.91	0.16	65,65,65,65	0
56	MG	B	3394	1/1	0.91	0.12	52,52,52,52	0
56	MG	BB	101	1/1	0.91	0.15	127,127,127,127	0
56	MG	GB	3297	1/1	0.91	0.43	67,67,67,67	0
56	MG	SB	202	1/1	0.91	0.27	80,80,80,80	0
56	MG	SB	203	1/1	0.91	0.24	73,73,73,73	0
56	MG	A	1798	1/1	0.91	0.18	70,70,70,70	0
56	MG	FB	1913	1/1	0.91	0.19	72,72,72,72	0
56	MG	FB	1914	1/1	0.91	0.11	63,63,63,63	0
56	MG	B	2938	1/1	0.91	0.26	55,55,55,55	0
56	MG	B	3542	1/1	0.91	0.07	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	GB	3144	1/1	0.91	0.13	57,57,57,57	0
56	MG	B	3809	1/1	0.91	0.20	66,66,66,66	0
56	MG	VB	204	1/1	0.91	0.13	74,74,74,74	0
56	MG	GB	3466	1/1	0.91	0.09	80,80,80,80	0
56	MG	B	3621	1/1	0.91	0.13	49,49,49,49	0
56	MG	G	3210	1/1	0.91	0.17	62,62,62,62	0
56	MG	B	3041	1/1	0.91	0.10	39,39,39,39	0
56	MG	FB	1813	1/1	0.91	0.09	69,69,69,69	0
56	MG	B	3545	1/1	0.91	0.05	74,74,74,74	0
56	MG	GB	3316	1/1	0.91	0.07	73,73,73,73	0
56	MG	B	3207	1/1	0.91	0.08	41,41,41,41	0
56	MG	B	3628	1/1	0.91	0.16	61,61,61,61	0
56	MG	B	3209	1/1	0.91	0.14	51,51,51,51	0
56	MG	B	2940	1/1	0.91	0.14	33,33,33,33	0
56	MG	B	3055	1/1	0.91	0.21	37,37,37,37	0
56	MG	A	1884	1/1	0.91	0.21	60,60,60,60	0
56	MG	FB	1715	1/1	0.91	0.26	82,82,82,82	0
56	MG	B	3216	1/1	0.91	0.22	51,51,51,51	0
56	MG	GB	3166	1/1	0.91	0.22	52,52,52,52	0
56	MG	B	3408	1/1	0.91	0.21	55,55,55,55	0
56	MG	B	3828	1/1	0.91	0.09	66,66,66,66	0
56	MG	B	3478	1/1	0.91	0.12	50,50,50,50	0
56	MG	IA	113	1/1	0.91	0.20	71,71,71,71	0
56	MG	A	1703	1/1	0.91	0.14	61,61,61,61	0
56	MG	B	3481	1/1	0.91	0.07	54,54,54,54	0
56	MG	B	3736	1/1	0.91	0.12	52,52,52,52	0
56	MG	GB	3495	1/1	0.91	0.12	72,72,72,72	0
56	MG	K	207	1/1	0.91	0.16	67,67,67,67	0
56	MG	GB	3180	1/1	0.91	0.32	68,68,68,68	0
56	MG	A	1734	1/1	0.91	0.32	72,72,72,72	0
56	MG	DC	101	1/1	0.91	0.13	60,60,60,60	0
56	MG	B	3564	1/1	0.91	0.08	52,52,52,52	0
56	MG	GB	3501	1/1	0.91	0.10	77,77,77,77	0
56	MG	A	1624	1/1	0.91	0.20	63,63,63,63	0
56	MG	B	3016	1/1	0.91	0.26	76,76,76,76	0
56	MG	GB	3350	1/1	0.91	0.21	61,61,61,61	0
56	MG	L	204	1/1	0.91	0.10	60,60,60,60	0
56	MG	FB	1731	1/1	0.91	0.15	70,70,70,70	0
56	MG	B	3175	1/1	0.91	0.30	60,60,60,60	0
56	MG	GB	3354	1/1	0.91	0.30	81,81,81,81	0
56	MG	B	3017	1/1	0.91	0.23	51,51,51,51	0
56	MG	B	3653	1/1	0.91	0.11	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	FB	1736	1/1	0.91	0.18	58,58,58,58	0
56	MG	GB	3515	1/1	0.91	0.26	76,76,76,76	0
56	MG	GB	3516	1/1	0.91	0.17	63,63,63,63	0
56	MG	GB	3694	1/1	0.91	0.13	61,61,61,61	0
56	MG	GB	2911	1/1	0.91	0.37	45,45,45,45	0
56	MG	B	3572	1/1	0.91	0.26	66,66,66,66	0
56	MG	N	206	1/1	0.91	0.10	69,69,69,69	0
56	MG	B	3125	1/1	0.91	0.34	60,60,60,60	0
56	MG	GB	3199	1/1	0.91	0.17	67,67,67,67	0
56	MG	GB	3054	1/1	0.91	0.24	56,56,56,56	0
56	MG	B	3365	1/1	0.91	0.12	73,73,73,73	0
56	MG	GB	2916	1/1	0.91	0.16	51,51,51,51	0
56	MG	NC	114	1/1	0.91	0.17	64,64,64,64	0
56	MG	FB	1640	1/1	0.91	0.23	64,64,64,64	0
56	MG	B	2955	1/1	0.91	0.14	46,46,46,46	0
56	MG	GB	3060	1/1	0.91	0.24	61,61,61,61	0
56	MG	B	3237	1/1	0.91	0.13	45,45,45,45	0
56	MG	GB	3534	1/1	0.91	0.24	59,59,59,59	0
56	MG	B	3665	1/1	0.91	0.23	56,56,56,56	0
56	MG	B	2956	1/1	0.91	0.33	49,49,49,49	0
56	MG	GB	3217	1/1	0.91	0.13	65,65,65,65	0
56	MG	FB	1645	1/1	0.91	0.17	56,56,56,56	0
56	MG	FB	1749	1/1	0.91	0.13	111,111,111,111	0
56	MG	GB	3543	1/1	0.91	0.11	55,55,55,55	0
56	MG	B	3498	1/1	0.91	0.24	60,60,60,60	0
56	MG	GB	3545	1/1	0.91	0.23	77,77,77,77	0
56	MG	B	2901	1/1	0.91	0.18	49,49,49,49	0
56	MG	GB	3069	1/1	0.91	0.31	59,59,59,59	0
56	MG	GB	3384	1/1	0.91	0.19	63,63,63,63	0
56	MG	B	3500	1/1	0.91	0.07	52,52,52,52	0
56	MG	B	3768	1/1	0.91	0.11	41,41,41,41	0
56	MG	C	221	1/1	0.91	0.23	70,70,70,70	0
56	MG	GB	2935	1/1	0.91	0.18	50,50,50,50	0
56	MG	B	3771	1/1	0.91	0.12	47,47,47,47	0
56	MG	FB	1759	1/1	0.91	0.30	66,66,66,66	0
56	MG	GB	3557	1/1	0.91	0.17	76,76,76,76	0
56	MG	GB	3392	1/1	0.91	0.30	56,56,56,56	0
56	MG	B	3080	1/1	0.91	0.13	66,66,66,66	0
56	MG	B	3774	1/1	0.91	0.12	46,46,46,46	0
56	MG	B	3776	1/1	0.91	0.10	62,62,62,62	0
56	MG	FB	1657	1/1	0.91	0.37	62,62,62,62	0
56	MG	B	3374	1/1	0.91	0.07	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	T	204	1/1	0.91	0.06	56,56,56,56	0
56	MG	TC	201	1/1	0.91	0.07	79,79,79,79	0
56	MG	OA	201	1/1	0.91	0.19	72,72,72,72	0
56	MG	GB	2948	1/1	0.91	0.27	51,51,51,51	0
56	MG	T	205	1/1	0.91	0.09	58,58,58,58	0
56	MG	FB	1770	1/1	0.91	0.26	93,93,93,93	0
56	MG	A	1638	1/1	0.91	0.20	61,61,61,61	0
56	MG	GB	3573	1/1	0.91	0.10	69,69,69,69	0
56	MG	HB	229	1/1	0.91	0.10	100,100,100,100	0
56	MG	B	2995	1/1	0.91	0.16	49,49,49,49	0
56	MG	GB	3244	1/1	0.91	0.17	52,52,52,52	0
56	MG	B	3438	1/1	0.91	0.20	63,63,63,63	0
56	MG	GB	2958	1/1	0.91	0.40	65,65,65,65	0
56	MG	GB	2960	1/1	0.91	0.23	63,63,63,63	0
56	MG	GB	3413	1/1	0.91	0.10	58,58,58,58	0
56	MG	FB	1774	1/1	0.91	0.19	67,67,67,67	0
56	MG	GB	3099	1/1	0.91	0.24	48,48,48,48	0
56	MG	B	3250	1/1	0.91	0.09	42,42,42,42	0
56	MG	GB	3418	1/1	0.91	0.12	58,58,58,58	0
56	MG	B	3135	1/1	0.91	0.14	48,48,48,48	0
56	MG	B	2906	1/1	0.91	0.32	29,29,29,29	0
56	MG	B	3444	1/1	0.91	0.12	52,52,52,52	0
56	MG	FB	1672	1/1	0.91	0.23	60,60,60,60	0
56	MG	C	238	1/1	0.91	0.08	91,91,91,91	0
56	MG	A	1767	1/1	0.91	0.10	77,77,77,77	0
56	MG	B	3666	1/1	0.92	0.20	41,41,41,41	0
56	MG	A	1756	1/1	0.92	0.15	66,66,66,66	0
56	MG	B	2992	1/1	0.92	0.14	38,38,38,38	0
56	MG	A	1665	1/1	0.92	0.31	66,66,66,66	0
56	MG	GB	3363	1/1	0.92	0.12	75,75,75,75	0
56	MG	B	2994	1/1	0.92	0.29	58,58,58,58	0
56	MG	GB	3551	1/1	0.92	0.12	96,96,96,96	0
56	MG	GB	3552	1/1	0.92	0.10	68,68,68,68	0
56	MG	HB	232	1/1	0.92	0.35	84,84,84,84	0
56	MG	B	2958	1/1	0.92	0.33	49,49,49,49	0
56	MG	B	3185	1/1	0.92	0.13	45,45,45,45	0
56	MG	GB	3368	1/1	0.92	0.12	70,70,70,70	0
56	MG	B	3803	1/1	0.92	0.13	58,58,58,58	0
56	MG	GB	3186	1/1	0.92	0.10	63,63,63,63	0
56	MG	B	3361	1/1	0.92	0.15	72,72,72,72	0
56	MG	GB	3559	1/1	0.92	0.17	72,72,72,72	0
56	MG	B	3362	1/1	0.92	0.20	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	GB	3024	1/1	0.92	0.25	57,57,57,57	0
56	MG	B	3679	1/1	0.92	0.13	66,66,66,66	0
56	MG	JB	307	1/1	0.92	0.14	63,63,63,63	0
56	MG	B	3031	1/1	0.92	0.20	54,54,54,54	0
56	MG	JB	309	1/1	0.92	0.14	69,69,69,69	0
56	MG	B	3565	1/1	0.92	0.12	49,49,49,49	0
56	MG	GB	3379	1/1	0.92	0.25	64,64,64,64	0
56	MG	B	3813	1/1	0.92	0.12	52,52,52,52	0
56	MG	B	3566	1/1	0.92	0.16	60,60,60,60	0
56	MG	B	3460	1/1	0.92	0.12	43,43,43,43	0
56	MG	KB	304	1/1	0.92	0.05	82,82,82,82	0
56	MG	GB	3569	1/1	0.92	0.25	55,55,55,55	0
56	MG	GB	3570	1/1	0.92	0.07	82,82,82,82	0
56	MG	B	2923	1/1	0.92	0.27	40,40,40,40	0
56	MG	GB	3200	1/1	0.92	0.43	63,63,63,63	0
56	MG	B	3272	1/1	0.92	0.18	63,63,63,63	0
56	MG	B	3035	1/1	0.92	0.20	63,63,63,63	0
56	MG	FB	1801	1/1	0.92	0.16	75,75,75,75	0
56	MG	B	3820	1/1	0.92	0.11	54,54,54,54	0
56	MG	GB	3206	1/1	0.92	0.16	64,64,64,64	0
56	MG	B	3037	1/1	0.92	0.19	52,52,52,52	0
56	MG	A	1701	1/1	0.92	0.36	56,56,56,56	0
56	MG	B	3468	1/1	0.92	0.12	57,57,57,57	0
56	MG	B	3469	1/1	0.92	0.26	60,60,60,60	0
56	MG	A	1779	1/1	0.92	0.33	82,82,82,82	0
56	MG	GB	3396	1/1	0.92	0.26	71,71,71,71	0
56	MG	B	3577	1/1	0.92	0.07	66,66,66,66	0
56	MG	B	3829	1/1	0.92	0.06	46,46,46,46	0
56	MG	B	3830	1/1	0.92	0.12	60,60,60,60	0
56	MG	FB	1692	1/1	0.92	0.18	67,67,67,67	0
56	MG	A	1627	1/1	0.92	0.39	73,73,73,73	0
56	MG	FB	1817	1/1	0.92	0.24	62,62,62,62	0
56	MG	B	3582	1/1	0.92	0.09	46,46,46,46	0
56	MG	FB	1820	1/1	0.92	0.20	85,85,85,85	0
56	MG	B	3042	1/1	0.92	0.31	53,53,53,53	0
56	MG	QB	206	1/1	0.92	0.14	63,63,63,63	0
56	MG	B	3197	1/1	0.92	0.24	53,53,53,53	0
56	MG	RB	202	1/1	0.92	0.15	77,77,77,77	0
56	MG	RB	203	1/1	0.92	0.28	57,57,57,57	0
56	MG	GB	2901	1/1	0.92	0.17	58,58,58,58	0
56	MG	B	3043	1/1	0.92	0.22	54,54,54,54	0
56	MG	GB	3063	1/1	0.92	0.09	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3288	1/1	0.92	0.09	59,59,59,59	0
56	MG	SA	203	1/1	0.92	0.22	109,109,109,109	0
56	MG	B	3047	1/1	0.92	0.22	42,42,42,42	0
56	MG	GB	3416	1/1	0.92	0.19	61,61,61,61	0
56	MG	GB	2910	1/1	0.92	0.33	48,48,48,48	0
56	MG	S	205	1/1	0.92	0.10	54,54,54,54	0
56	MG	FB	1828	1/1	0.92	0.22	70,70,70,70	0
56	MG	B	3121	1/1	0.92	0.21	43,43,43,43	0
56	MG	B	3049	1/1	0.92	0.29	40,40,40,40	0
56	MG	GB	3075	1/1	0.92	0.22	65,65,65,65	0
56	MG	B	3388	1/1	0.92	0.15	55,55,55,55	0
56	MG	A	1862	1/1	0.92	0.20	60,60,60,60	0
56	MG	GB	3080	1/1	0.92	0.14	58,58,58,58	0
56	MG	C	206	1/1	0.92	0.21	54,54,54,54	0
56	MG	A	1876	1/1	0.92	0.10	83,83,83,83	0
56	MG	U	102	1/1	0.92	0.22	55,55,55,55	0
56	MG	XB	203	1/1	0.92	0.23	79,79,79,79	0
56	MG	A	1614	1/1	0.92	0.31	52,52,52,52	0
56	MG	GB	2922	1/1	0.92	0.40	63,63,63,63	0
56	MG	B	3492	1/1	0.92	0.07	75,75,75,75	0
56	MG	B	3057	1/1	0.92	0.09	61,61,61,61	0
56	MG	B	3132	1/1	0.92	0.23	46,46,46,46	0
56	MG	B	3059	1/1	0.92	0.11	43,43,43,43	0
56	MG	A	1752	1/1	0.92	0.16	67,67,67,67	0
56	MG	B	3301	1/1	0.92	0.12	49,49,49,49	0
56	MG	B	3061	1/1	0.92	0.38	58,58,58,58	0
56	MG	B	3062	1/1	0.92	0.19	40,40,40,40	0
56	MG	B	3063	1/1	0.92	0.17	44,44,44,44	0
56	MG	B	2909	1/1	0.92	0.32	33,33,33,33	0
56	MG	GB	2938	1/1	0.92	0.27	45,45,45,45	0
56	MG	B	3504	1/1	0.92	0.09	45,45,45,45	0
56	MG	B	2910	1/1	0.92	0.22	34,34,34,34	0
56	MG	B	3507	1/1	0.92	0.09	42,42,42,42	0
56	MG	B	3309	1/1	0.92	0.18	56,56,56,56	0
56	MG	C	227	1/1	0.92	0.11	64,64,64,64	0
56	MG	B	3013	1/1	0.92	0.23	50,50,50,50	0
56	MG	B	3311	1/1	0.92	0.10	46,46,46,46	0
56	MG	B	3623	1/1	0.92	0.12	64,64,64,64	0
56	MG	A	1691	1/1	0.92	0.11	61,61,61,61	0
56	MG	GB	3275	1/1	0.92	0.15	61,61,61,61	0
56	MG	GB	3277	1/1	0.92	0.14	54,54,54,54	0
56	MG	GB	2949	1/1	0.92	0.41	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	FB	1858	1/1	0.92	0.06	97,97,97,97	0
56	MG	GB	3112	1/1	0.92	0.13	64,64,64,64	0
56	MG	B	2972	1/1	0.92	0.30	45,45,45,45	0
56	MG	B	3626	1/1	0.92	0.10	54,54,54,54	0
56	MG	KC	101	1/1	0.92	0.20	58,58,58,58	0
56	MG	B	3755	1/1	0.92	0.06	61,61,61,61	0
56	MG	KC	103	1/1	0.92	0.30	64,64,64,64	0
56	MG	FB	1738	1/1	0.92	0.34	69,69,69,69	0
56	MG	B	3315	1/1	0.92	0.16	43,43,43,43	0
56	MG	B	3757	1/1	0.92	0.11	53,53,53,53	0
56	MG	GB	3660	1/1	0.92	0.31	46,46,46,46	0
56	MG	B	3317	1/1	0.92	0.12	55,55,55,55	0
56	MG	B	3075	1/1	0.92	0.17	42,42,42,42	0
56	MG	B	3319	1/1	0.92	0.17	47,47,47,47	0
56	MG	B	2941	1/1	0.92	0.28	49,49,49,49	0
56	MG	GB	3667	1/1	0.92	0.15	54,54,54,54	0
56	MG	GB	2965	1/1	0.92	0.20	54,54,54,54	0
56	MG	NC	109	1/1	0.92	0.06	89,89,89,89	0
56	MG	GB	3669	1/1	0.92	0.17	57,57,57,57	0
56	MG	GB	2966	1/1	0.92	0.31	56,56,56,56	0
56	MG	GB	3125	1/1	0.92	0.23	62,62,62,62	0
56	MG	GB	3302	1/1	0.92	0.18	47,47,47,47	0
56	MG	GB	3303	1/1	0.92	0.15	61,61,61,61	0
56	MG	GB	3304	1/1	0.92	0.34	58,58,58,58	0
56	MG	FA	102	1/1	0.92	0.17	58,58,58,58	0
56	MG	FB	1746	1/1	0.92	0.06	63,63,63,63	0
56	MG	GB	3680	1/1	0.92	0.22	60,60,60,60	0
56	MG	B	3321	1/1	0.92	0.35	60,60,60,60	0
56	MG	B	3159	1/1	0.92	0.20	47,47,47,47	0
56	MG	B	3769	1/1	0.92	0.07	69,69,69,69	0
56	MG	GB	3133	1/1	0.92	0.27	69,69,69,69	0
56	MG	FB	1751	1/1	0.92	0.16	83,83,83,83	0
56	MG	GB	3490	1/1	0.92	0.13	63,63,63,63	0
56	MG	GB	3313	1/1	0.92	0.15	56,56,56,56	0
56	MG	E	301	1/1	0.92	0.13	52,52,52,52	0
56	MG	B	2975	1/1	0.92	0.38	49,49,49,49	0
56	MG	GB	3693	1/1	0.92	0.07	69,69,69,69	0
56	MG	B	3531	1/1	0.92	0.13	42,42,42,42	0
56	MG	B	3163	1/1	0.92	0.12	49,49,49,49	0
56	MG	GB	3320	1/1	0.92	0.13	60,60,60,60	0
56	MG	F	301	1/1	0.92	0.19	46,46,46,46	0
56	MG	GB	3322	1/1	0.92	0.20	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RC	305	1/1	0.92	0.08	75,75,75,75	0
56	MG	GB	2981	1/1	0.92	0.24	50,50,50,50	0
56	MG	A	1680	1/1	0.92	0.33	75,75,75,75	0
56	MG	B	3536	1/1	0.92	0.11	38,38,38,38	0
56	MG	GB	3326	1/1	0.92	0.10	60,60,60,60	0
56	MG	RC	311	1/1	0.92	0.10	78,78,78,78	0
56	MG	GB	3327	1/1	0.92	0.09	76,76,76,76	0
56	MG	F	304	1/1	0.92	0.09	49,49,49,49	0
56	MG	GB	3509	1/1	0.92	0.16	75,75,75,75	0
56	MG	F	305	1/1	0.92	0.17	58,58,58,58	0
56	MG	FB	1762	1/1	0.92	0.17	69,69,69,69	0
56	MG	B	3537	1/1	0.92	0.12	46,46,46,46	0
56	MG	GB	3153	1/1	0.92	0.12	59,59,59,59	0
56	MG	GB	3333	1/1	0.92	0.33	66,66,66,66	0
56	MG	B	3082	1/1	0.92	0.21	44,44,44,44	0
56	MG	FB	1890	1/1	0.92	0.08	60,60,60,60	0
56	MG	B	3087	1/1	0.92	0.24	53,53,53,53	0
56	MG	B	2915	1/1	0.92	0.26	57,57,57,57	0
56	MG	B	3783	1/1	0.92	0.18	50,50,50,50	0
56	MG	B	3437	1/1	0.92	0.08	39,39,39,39	0
56	MG	GB	3525	1/1	0.92	0.11	79,79,79,79	0
56	MG	B	3652	1/1	0.92	0.18	56,56,56,56	0
56	MG	YC	201	1/1	0.92	0.14	68,68,68,68	0
56	MG	G	3205	1/1	0.92	0.08	40,40,40,40	0
56	MG	B	3257	1/1	0.92	0.21	54,54,54,54	0
56	MG	B	3090	1/1	0.92	0.10	53,53,53,53	0
56	MG	A	1867	1/1	0.92	0.14	64,64,64,64	0
56	MG	GB	3349	1/1	0.92	0.21	51,51,51,51	0
56	MG	GB	3532	1/1	0.92	0.12	70,70,70,70	0
56	MG	B	3658	1/1	0.92	0.14	54,54,54,54	0
56	MG	A	1617	1/1	0.92	0.31	59,59,59,59	0
56	MG	B	3347	1/1	0.92	0.20	54,54,54,54	0
56	MG	FB	1656	1/1	0.92	0.31	70,70,70,70	0
56	MG	GB	3171	1/1	0.92	0.18	63,63,63,63	0
56	MG	B	3551	1/1	0.92	0.13	51,51,51,51	0
56	MG	B	3553	1/1	0.92	0.18	59,59,59,59	0
56	MG	GB	3176	1/1	0.92	0.17	51,51,51,51	0
56	MG	FB	1781	1/1	0.92	0.15	90,90,90,90	0
56	MG	L	205	1/1	0.93	0.14	61,61,61,61	0
56	MG	GB	3043	1/1	0.93	0.20	52,52,52,52	0
56	MG	B	3448	1/1	0.93	0.08	58,58,58,58	0
56	MG	GB	3211	1/1	0.93	0.13	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	2981	1/1	0.93	0.20	41,41,41,41	0
56	MG	M	208	1/1	0.93	0.13	44,44,44,44	0
56	MG	N	201	1/1	0.93	0.27	51,51,51,51	0
56	MG	FB	1808	1/1	0.93	0.13	66,66,66,66	0
56	MG	A	1806	1/1	0.93	0.12	56,56,56,56	0
56	MG	B	3535	1/1	0.93	0.09	60,60,60,60	0
56	MG	JB	311	1/1	0.93	0.17	63,63,63,63	0
56	MG	FB	1812	1/1	0.93	0.08	70,70,70,70	0
56	MG	A	1660	1/1	0.93	0.13	60,60,60,60	0
56	MG	B	3379	1/1	0.93	0.19	52,52,52,52	0
56	MG	B	3837	1/1	0.93	0.13	50,50,50,50	0
56	MG	A	1818	1/1	0.93	0.15	65,65,65,65	0
56	MG	B	3840	1/1	0.93	0.18	48,48,48,48	0
56	MG	B	3841	1/1	0.93	0.16	73,73,73,73	0
56	MG	B	3726	1/1	0.93	0.15	50,50,50,50	0
56	MG	GB	2902	1/1	0.93	0.58	51,51,51,51	0
56	MG	B	3383	1/1	0.93	0.13	47,47,47,47	0
56	MG	B	3730	1/1	0.93	0.06	55,55,55,55	0
56	MG	B	2922	1/1	0.93	0.26	51,51,51,51	0
56	MG	B	3733	1/1	0.93	0.07	54,54,54,54	0
56	MG	B	3734	1/1	0.93	0.09	69,69,69,69	0
56	MG	S	201	1/1	0.93	0.15	63,63,63,63	0
56	MG	B	3735	1/1	0.93	0.06	71,71,71,71	0
56	MG	FB	1705	1/1	0.93	0.24	60,60,60,60	0
56	MG	GB	3071	1/1	0.93	0.18	56,56,56,56	0
56	MG	FB	1830	1/1	0.93	0.28	69,69,69,69	0
56	MG	B	3458	1/1	0.93	0.11	41,41,41,41	0
56	MG	GB	3600	1/1	0.93	0.32	52,52,52,52	0
56	MG	GB	3076	1/1	0.93	0.17	59,59,59,59	0
56	MG	S	204	1/1	0.93	0.12	60,60,60,60	0
56	MG	B	3138	1/1	0.93	0.23	63,63,63,63	0
56	MG	B	3260	1/1	0.93	0.21	47,47,47,47	0
56	MG	B	3546	1/1	0.93	0.07	47,47,47,47	0
56	MG	GB	2920	1/1	0.93	0.43	57,57,57,57	0
56	MG	FB	1713	1/1	0.93	0.30	75,75,75,75	0
56	MG	GB	3252	1/1	0.93	0.14	59,59,59,59	0
56	MG	B	3741	1/1	0.93	0.09	47,47,47,47	0
56	MG	B	3742	1/1	0.93	0.13	54,54,54,54	0
56	MG	GB	2924	1/1	0.93	0.30	51,51,51,51	0
56	MG	GB	3433	1/1	0.93	0.09	65,65,65,65	0
56	MG	GB	3615	1/1	0.93	0.20	76,76,76,76	0
56	MG	B	3261	1/1	0.93	0.25	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	GB	3435	1/1	0.93	0.08	53,53,53,53	0
56	MG	B	2939	1/1	0.93	0.33	48,48,48,48	0
56	MG	B	3464	1/1	0.93	0.11	48,48,48,48	0
56	MG	TB	201	1/1	0.93	0.16	66,66,66,66	0
56	MG	B	3143	1/1	0.93	0.12	39,39,39,39	0
56	MG	B	3466	1/1	0.93	0.07	51,51,51,51	0
56	MG	B	3750	1/1	0.93	0.18	57,57,57,57	0
56	MG	A	1825	1/1	0.93	0.12	56,56,56,56	0
56	MG	B	2924	1/1	0.93	0.29	35,35,35,35	0
56	MG	FB	1847	1/1	0.93	0.14	67,67,67,67	0
56	MG	GB	2937	1/1	0.93	0.21	49,49,49,49	0
56	MG	A	1781	1/1	0.93	0.14	95,95,95,95	0
56	MG	FB	1725	1/1	0.93	0.16	68,68,68,68	0
56	MG	B	3646	1/1	0.93	0.11	54,54,54,54	0
56	MG	GB	3100	1/1	0.93	0.15	58,58,58,58	0
56	MG	B	3558	1/1	0.93	0.15	64,64,64,64	0
56	MG	GB	2942	1/1	0.93	0.32	54,54,54,54	0
56	MG	B	2944	1/1	0.93	0.35	44,44,44,44	0
56	MG	GB	3276	1/1	0.93	0.09	79,79,79,79	0
56	MG	B	2926	1/1	0.93	0.32	36,36,36,36	0
56	MG	FB	1607	1/1	0.93	0.35	58,58,58,58	0
56	MG	B	3001	1/1	0.93	0.16	37,37,37,37	0
56	MG	B	3397	1/1	0.93	0.19	52,52,52,52	0
56	MG	GB	3110	1/1	0.93	0.16	72,72,72,72	0
56	MG	GB	3641	1/1	0.93	0.12	64,64,64,64	0
56	MG	B	3477	1/1	0.93	0.07	43,43,43,43	0
56	MG	GB	3285	1/1	0.93	0.20	52,52,52,52	0
56	MG	GB	3644	1/1	0.93	0.10	77,77,77,77	0
56	MG	B	3654	1/1	0.93	0.12	66,66,66,66	0
56	MG	GB	3646	1/1	0.93	0.07	75,75,75,75	0
56	MG	B	3325	1/1	0.93	0.14	53,53,53,53	0
56	MG	FB	1860	1/1	0.93	0.16	89,89,89,89	0
56	MG	B	3204	1/1	0.93	0.07	40,40,40,40	0
56	MG	GB	3650	1/1	0.93	0.13	57,57,57,57	0
56	MG	B	3770	1/1	0.93	0.08	65,65,65,65	0
56	MG	GB	2954	1/1	0.93	0.36	50,50,50,50	0
56	MG	GB	3295	1/1	0.93	0.07	65,65,65,65	0
56	MG	B	3153	1/1	0.93	0.23	42,42,42,42	0
56	MG	B	3660	1/1	0.93	0.10	54,54,54,54	0
56	MG	B	3661	1/1	0.93	0.10	51,51,51,51	0
56	MG	B	3332	1/1	0.93	0.12	65,65,65,65	0
56	MG	DC	103	1/1	0.93	0.18	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3333	1/1	0.93	0.07	78,78,78,78	0
56	MG	B	3154	1/1	0.93	0.15	58,58,58,58	0
56	MG	B	3002	1/1	0.93	0.18	38,38,38,38	0
56	MG	B	3337	1/1	0.93	0.11	46,46,46,46	0
56	MG	GB	3479	1/1	0.93	0.13	66,66,66,66	0
56	MG	B	3488	1/1	0.93	0.09	57,57,57,57	0
56	MG	HC	102	1/1	0.93	0.09	62,62,62,62	0
56	MG	GB	3127	1/1	0.93	0.16	68,68,68,68	0
56	MG	B	3160	1/1	0.93	0.15	60,60,60,60	0
56	MG	DA	102	1/1	0.93	0.22	62,62,62,62	0
56	MG	GB	2969	1/1	0.93	0.17	53,53,53,53	0
56	MG	FB	1750	1/1	0.93	0.34	70,70,70,70	0
56	MG	B	3107	1/1	0.93	0.23	56,56,56,56	0
56	MG	B	3112	1/1	0.93	0.11	49,49,49,49	0
56	MG	B	3215	1/1	0.93	0.26	47,47,47,47	0
56	MG	FB	1879	1/1	0.93	0.16	78,78,78,78	0
56	MG	GB	3677	1/1	0.93	0.24	60,60,60,60	0
56	MG	B	3417	1/1	0.93	0.10	57,57,57,57	0
56	MG	B	3580	1/1	0.93	0.09	58,58,58,58	0
56	MG	B	2970	1/1	0.93	0.20	36,36,36,36	0
56	MG	F	306	1/1	0.93	0.14	60,60,60,60	0
56	MG	B	3067	1/1	0.93	0.34	50,50,50,50	0
56	MG	B	3420	1/1	0.93	0.16	43,43,43,43	0
56	MG	B	3068	1/1	0.93	0.15	43,43,43,43	0
56	MG	B	2914	1/1	0.93	0.26	47,47,47,47	0
56	MG	GB	3149	1/1	0.93	0.25	58,58,58,58	0
56	MG	GB	3150	1/1	0.93	0.08	46,46,46,46	0
56	MG	FB	1763	1/1	0.93	0.18	67,67,67,67	0
56	MG	GB	3690	1/1	0.93	0.11	64,64,64,64	0
56	MG	B	3352	1/1	0.93	0.22	53,53,53,53	0
56	MG	F	314	1/1	0.93	0.23	39,39,39,39	0
56	MG	B	3223	1/1	0.93	0.38	65,65,65,65	0
56	MG	OC	406	1/1	0.93	0.10	70,70,70,70	0
56	MG	FB	1892	1/1	0.93	0.14	68,68,68,68	0
56	MG	B	3072	1/1	0.93	0.06	46,46,46,46	0
56	MG	B	3429	1/1	0.93	0.21	46,46,46,46	0
56	MG	GB	3513	1/1	0.93	0.09	49,49,49,49	0
56	MG	B	3594	1/1	0.93	0.10	56,56,56,56	0
56	MG	IA	111	1/1	0.93	0.19	49,49,49,49	0
56	MG	B	3355	1/1	0.93	0.09	55,55,55,55	0
56	MG	B	3225	1/1	0.93	0.19	46,46,46,46	0
56	MG	G	3209	1/1	0.93	0.23	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	A	1705	1/1	0.93	0.18	66,66,66,66	0
56	MG	GB	3520	1/1	0.93	0.14	73,73,73,73	0
56	MG	GB	3341	1/1	0.93	0.11	54,54,54,54	0
56	MG	GB	3522	1/1	0.93	0.11	71,71,71,71	0
56	MG	B	3598	1/1	0.93	0.09	62,62,62,62	0
56	MG	A	1683	1/1	0.93	0.31	80,80,80,80	0
56	MG	FB	1903	1/1	0.93	0.07	76,76,76,76	0
56	MG	B	3229	1/1	0.93	0.14	45,45,45,45	0
56	MG	B	2918	1/1	0.93	0.29	43,43,43,43	0
56	MG	B	3367	1/1	0.93	0.14	63,63,63,63	0
56	MG	B	3811	1/1	0.93	0.08	48,48,48,48	0
56	MG	I	203	1/1	0.93	0.10	68,68,68,68	0
56	MG	B	3812	1/1	0.93	0.05	62,62,62,62	0
56	MG	B	2932	1/1	0.93	0.24	52,52,52,52	0
56	MG	GB	3014	1/1	0.93	0.30	64,64,64,64	0
56	MG	B	3520	1/1	0.93	0.09	64,64,64,64	0
56	MG	JA	407	1/1	0.93	0.16	61,61,61,61	0
56	MG	GB	3017	1/1	0.93	0.20	56,56,56,56	0
56	MG	GB	3538	1/1	0.93	0.13	58,58,58,58	0
56	MG	B	3705	1/1	0.93	0.12	49,49,49,49	0
56	MG	JA	409	1/1	0.93	0.33	89,89,89,89	0
56	MG	J	201	1/1	0.93	0.09	84,84,84,84	0
56	MG	B	3079	1/1	0.93	0.20	48,48,48,48	0
56	MG	B	3524	1/1	0.93	0.14	48,48,48,48	0
56	MG	FB	1670	1/1	0.93	0.43	74,74,74,74	0
56	MG	K	202	1/1	0.93	0.04	63,63,63,63	0
56	MG	GB	3189	1/1	0.93	0.12	64,64,64,64	0
56	MG	B	2978	1/1	0.93	0.16	44,44,44,44	0
56	MG	B	3611	1/1	0.93	0.10	48,48,48,48	0
56	MG	B	3821	1/1	0.93	0.13	53,53,53,53	0
56	MG	B	2979	1/1	0.93	0.14	43,43,43,43	0
56	MG	B	3244	1/1	0.93	0.24	53,53,53,53	0
56	MG	B	3715	1/1	0.93	0.09	64,64,64,64	0
56	MG	GB	3031	1/1	0.93	0.28	60,60,60,60	0
56	MG	GB	3198	1/1	0.93	0.32	59,59,59,59	0
56	MG	FB	1928	1/1	0.93	0.22	62,62,62,62	0
56	MG	CD	101	1/1	0.93	0.32	77,77,77,77	0
56	MG	L	201	1/1	0.93	0.13	54,54,54,54	0
56	MG	GB	3035	1/1	0.93	0.11	65,65,65,65	0
56	MG	GB	3036	1/1	0.93	0.21	58,58,58,58	0
56	MG	B	2980	1/1	0.93	0.26	54,54,54,54	0
56	MG	GB	3204	1/1	0.93	0.18	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3717	1/1	0.93	0.10	52,52,52,52	0
56	MG	B	3718	1/1	0.93	0.12	54,54,54,54	0
56	MG	C	215	1/1	0.94	0.15	58,58,58,58	0
56	MG	B	3174	1/1	0.94	0.16	42,42,42,42	0
56	MG	B	2903	1/1	0.94	0.38	35,35,35,35	0
56	MG	B	3686	1/1	0.94	0.17	43,43,43,43	0
56	MG	B	3070	1/1	0.94	0.08	47,47,47,47	0
56	MG	RB	206	1/1	0.94	0.12	59,59,59,59	0
56	MG	GB	3523	1/1	0.94	0.20	61,61,61,61	0
56	MG	B	3048	1/1	0.94	0.27	45,45,45,45	0
56	MG	B	3538	1/1	0.94	0.14	57,57,57,57	0
56	MG	B	3779	1/1	0.94	0.09	58,58,58,58	0
56	MG	B	3399	1/1	0.94	0.27	53,53,53,53	0
56	MG	GB	3128	1/1	0.94	0.35	58,58,58,58	0
56	MG	GB	3665	1/1	0.94	0.09	61,61,61,61	0
56	MG	B	3338	1/1	0.94	0.09	47,47,47,47	0
56	MG	A	1835	1/1	0.94	0.08	70,70,70,70	0
56	MG	B	2977	1/1	0.94	0.31	53,53,53,53	0
56	MG	GB	2903	1/1	0.94	0.29	36,36,36,36	0
56	MG	GB	3670	1/1	0.94	0.08	52,52,52,52	0
56	MG	Q	201	1/1	0.94	0.20	62,62,62,62	0
56	MG	B	3182	1/1	0.94	0.29	50,50,50,50	0
56	MG	GB	3401	1/1	0.94	0.10	68,68,68,68	0
56	MG	B	3140	1/1	0.94	0.19	54,54,54,54	0
56	MG	Q	204	1/1	0.94	0.10	74,74,74,74	0
56	MG	B	3344	1/1	0.94	0.31	49,49,49,49	0
56	MG	XB	201	1/1	0.94	0.20	55,55,55,55	0
56	MG	GB	3539	1/1	0.94	0.18	68,68,68,68	0
56	MG	B	3184	1/1	0.94	0.12	46,46,46,46	0
56	MG	B	3702	1/1	0.94	0.14	86,86,86,86	0
56	MG	GB	3681	1/1	0.94	0.09	60,60,60,60	0
56	MG	GB	3542	1/1	0.94	0.09	112,112,112,112	0
56	MG	C	235	1/1	0.94	0.09	73,73,73,73	0
56	MG	B	3618	1/1	0.94	0.14	43,43,43,43	0
56	MG	B	3142	1/1	0.94	0.13	46,46,46,46	0
56	MG	B	3410	1/1	0.94	0.16	49,49,49,49	0
56	MG	GB	3145	1/1	0.94	0.33	65,65,65,65	0
56	MG	B	3074	1/1	0.94	0.22	36,36,36,36	0
56	MG	GB	3147	1/1	0.94	0.09	54,54,54,54	0
56	MG	GB	3279	1/1	0.94	0.20	69,69,69,69	0
56	MG	GB	3691	1/1	0.94	0.10	71,71,71,71	0
56	MG	B	3231	1/1	0.94	0.27	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	C	241	1/1	0.94	0.14	81,81,81,81	0
56	MG	GB	3032	1/1	0.94	0.16	54,54,54,54	0
56	MG	B	3232	1/1	0.94	0.16	57,57,57,57	0
56	MG	B	3709	1/1	0.94	0.13	64,64,64,64	0
56	MG	B	3415	1/1	0.94	0.12	42,42,42,42	0
56	MG	GB	3287	1/1	0.94	0.22	62,62,62,62	0
56	MG	B	3416	1/1	0.94	0.19	37,37,37,37	0
56	MG	B	3187	1/1	0.94	0.10	59,59,59,59	0
56	MG	GB	3291	1/1	0.94	0.12	73,73,73,73	0
56	MG	B	3714	1/1	0.94	0.16	52,52,52,52	0
56	MG	B	3144	1/1	0.94	0.14	40,40,40,40	0
56	MG	GB	3428	1/1	0.94	0.21	59,59,59,59	0
56	MG	E	305	1/1	0.94	0.10	50,50,50,50	0
56	MG	B	3802	1/1	0.94	0.07	77,77,77,77	0
56	MG	GB	3296	1/1	0.94	0.09	65,65,65,65	0
56	MG	GB	3708	1/1	0.94	0.11	71,71,71,71	0
56	MG	GB	2929	1/1	0.94	0.22	46,46,46,46	0
56	MG	GB	2930	1/1	0.94	0.41	64,64,64,64	0
56	MG	GB	3046	1/1	0.94	0.26	55,55,55,55	0
56	MG	B	3238	1/1	0.94	0.10	44,44,44,44	0
56	MG	B	3051	1/1	0.94	0.31	40,40,40,40	0
56	MG	B	3109	1/1	0.94	0.26	53,53,53,53	0
56	MG	KC	105	1/1	0.94	0.22	73,73,73,73	0
56	MG	GB	3168	1/1	0.94	0.28	61,61,61,61	0
56	MG	B	3053	1/1	0.94	0.14	46,46,46,46	0
56	MG	B	3808	1/1	0.94	0.06	50,50,50,50	0
56	MG	GB	3052	1/1	0.94	0.25	55,55,55,55	0
56	MG	B	2948	1/1	0.94	0.23	43,43,43,43	0
56	MG	FB	1682	1/1	0.94	0.31	64,64,64,64	0
56	MG	B	3364	1/1	0.94	0.09	37,37,37,37	0
56	MG	B	3194	1/1	0.94	0.19	53,53,53,53	0
56	MG	GB	3057	1/1	0.94	0.13	44,44,44,44	0
56	MG	B	2916	1/1	0.94	0.28	36,36,36,36	0
56	MG	B	3641	1/1	0.94	0.11	50,50,50,50	0
56	MG	B	3305	1/1	0.94	0.16	49,49,49,49	0
56	MG	B	3569	1/1	0.94	0.09	61,61,61,61	0
56	MG	B	3727	1/1	0.94	0.13	49,49,49,49	0
56	MG	B	3249	1/1	0.94	0.08	43,43,43,43	0
56	MG	G	3203	1/1	0.94	0.17	42,42,42,42	0
56	MG	A	1721	1/1	0.94	0.07	97,97,97,97	0
56	MG	B	3253	1/1	0.94	0.14	53,53,53,53	0
56	MG	GB	3594	1/1	0.94	0.11	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3081	1/1	0.94	0.22	44,44,44,44	0
56	MG	B	3198	1/1	0.94	0.19	47,47,47,47	0
56	MG	A	1766	1/1	0.94	0.08	103,103,103,103	0
56	MG	B	3259	1/1	0.94	0.08	38,38,38,38	0
56	MG	DB	101	1/1	0.94	0.23	119,119,119,119	0
56	MG	GB	3072	1/1	0.94	0.20	49,49,49,49	0
56	MG	B	3156	1/1	0.94	0.19	50,50,50,50	0
56	MG	GB	3074	1/1	0.94	0.21	59,59,59,59	0
56	MG	GB	2956	1/1	0.94	0.25	47,47,47,47	0
56	MG	GB	2957	1/1	0.94	0.32	51,51,51,51	0
56	MG	B	3442	1/1	0.94	0.05	58,58,58,58	0
56	MG	GB	3078	1/1	0.94	0.32	64,64,64,64	0
56	MG	GB	2959	1/1	0.94	0.26	56,56,56,56	0
56	MG	B	3157	1/1	0.94	0.14	44,44,44,44	0
56	MG	B	3657	1/1	0.94	0.14	45,45,45,45	0
56	MG	B	3581	1/1	0.94	0.10	46,46,46,46	0
56	MG	FB	1606	1/1	0.94	0.37	57,57,57,57	0
56	MG	B	2957	1/1	0.94	0.17	45,45,45,45	0
56	MG	B	3382	1/1	0.94	0.17	54,54,54,54	0
56	MG	GB	3208	1/1	0.94	0.10	53,53,53,53	0
56	MG	B	3088	1/1	0.94	0.12	50,50,50,50	0
56	MG	A	1796	1/1	0.94	0.11	61,61,61,61	0
56	MG	B	3836	1/1	0.94	0.24	46,46,46,46	0
56	MG	FB	1711	1/1	0.94	0.16	69,69,69,69	0
56	MG	FB	1612	1/1	0.94	0.30	63,63,63,63	0
56	MG	B	3588	1/1	0.94	0.06	46,46,46,46	0
56	MG	B	3838	1/1	0.94	0.15	54,54,54,54	0
56	MG	B	3005	1/1	0.94	0.25	45,45,45,45	0
56	MG	B	3451	1/1	0.94	0.07	53,53,53,53	0
56	MG	FB	1617	1/1	0.94	0.34	59,59,59,59	0
56	MG	LB	301	1/1	0.94	0.13	60,60,60,60	0
56	MG	FB	1816	1/1	0.94	0.07	75,75,75,75	0
56	MG	GB	3494	1/1	0.94	0.13	67,67,67,67	0
56	MG	B	3206	1/1	0.94	0.16	44,44,44,44	0
56	MG	FB	1619	1/1	0.94	0.35	58,58,58,58	0
56	MG	B	3523	1/1	0.94	0.10	54,54,54,54	0
56	MG	K	203	1/1	0.94	0.13	73,73,73,73	0
56	MG	B	3091	1/1	0.94	0.15	36,36,36,36	0
56	MG	GB	3500	1/1	0.94	0.17	57,57,57,57	0
56	MG	B	3670	1/1	0.94	0.08	52,52,52,52	0
56	MG	B	3040	1/1	0.94	0.21	41,41,41,41	0
56	MG	B	3527	1/1	0.94	0.15	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3760	1/1	0.94	0.13	65,65,65,65	0
56	MG	B	3324	1/1	0.94	0.20	44,44,44,44	0
56	MG	GB	3108	1/1	0.94	0.19	54,54,54,54	0
56	MG	A	1750	1/1	0.94	0.11	80,80,80,80	0
56	MG	A	1857	1/1	0.94	0.12	69,69,69,69	0
56	MG	B	3764	1/1	0.94	0.11	48,48,48,48	0
56	MG	B	2902	1/1	0.94	0.36	35,35,35,35	0
56	MG	IA	119	1/1	0.94	0.05	73,73,73,73	0
56	MG	B	3045	1/1	0.94	0.29	43,43,43,43	0
56	MG	FB	1734	1/1	0.94	0.17	65,65,65,65	0
56	MG	B	3601	1/1	0.94	0.14	53,53,53,53	0
56	MG	B	3603	1/1	0.94	0.14	48,48,48,48	0
57	ZN	BA	101	1/1	0.94	0.11	131,131,131,131	0
56	MG	M	205	1/1	0.94	0.11	45,45,45,45	0
56	MG	B	3069	1/1	0.95	0.21	40,40,40,40	0
56	MG	B	2989	1/1	0.95	0.25	53,53,53,53	0
56	MG	B	3639	1/1	0.95	0.12	46,46,46,46	0
56	MG	B	2990	1/1	0.95	0.22	41,41,41,41	0
56	MG	GB	3421	1/1	0.95	0.08	77,77,77,77	0
56	MG	B	3171	1/1	0.95	0.12	48,48,48,48	0
56	MG	VB	201	1/1	0.95	0.15	74,74,74,74	0
56	MG	FB	1921	1/1	0.95	0.12	78,78,78,78	0
56	MG	FB	1922	1/1	0.95	0.07	83,83,83,83	0
56	MG	B	3097	1/1	0.95	0.36	54,54,54,54	0
56	MG	GB	2975	1/1	0.95	0.35	61,61,61,61	0
56	MG	GB	3305	1/1	0.95	0.28	49,49,49,49	0
56	MG	B	3316	1/1	0.95	0.14	35,35,35,35	0
56	MG	A	1791	1/1	0.95	0.21	59,59,59,59	0
56	MG	B	2913	1/1	0.95	0.28	38,38,38,38	0
56	MG	B	3029	1/1	0.95	0.18	41,41,41,41	0
56	MG	B	3805	1/1	0.95	0.08	54,54,54,54	0
56	MG	GB	3195	1/1	0.95	0.10	52,52,52,52	0
56	MG	A	1726	1/1	0.95	0.19	73,73,73,73	0
56	MG	B	3220	1/1	0.95	0.15	46,46,46,46	0
56	MG	GB	3436	1/1	0.95	0.13	71,71,71,71	0
56	MG	B	3513	1/1	0.95	0.14	53,53,53,53	0
56	MG	B	3221	1/1	0.95	0.13	53,53,53,53	0
56	MG	E	306	1/1	0.95	0.11	51,51,51,51	0
56	MG	GB	2988	1/1	0.95	0.24	50,50,50,50	0
56	MG	GB	2990	1/1	0.95	0.39	63,63,63,63	0
56	MG	E	307	1/1	0.95	0.09	55,55,55,55	0
56	MG	B	3731	1/1	0.95	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3102	1/1	0.95	0.21	46,46,46,46	0
56	MG	FB	1937	1/1	0.95	0.30	65,65,65,65	0
56	MG	B	3516	1/1	0.95	0.16	57,57,57,57	0
56	MG	B	3103	1/1	0.95	0.19	51,51,51,51	0
56	MG	FB	1660	1/1	0.95	0.31	70,70,70,70	0
56	MG	B	2968	1/1	0.95	0.26	53,53,53,53	0
56	MG	B	3585	1/1	0.95	0.15	49,49,49,49	0
56	MG	B	3450	1/1	0.95	0.10	63,63,63,63	0
56	MG	B	3587	1/1	0.95	0.05	62,62,62,62	0
56	MG	GB	3216	1/1	0.95	0.34	60,60,60,60	0
56	MG	FB	1756	1/1	0.95	0.25	68,68,68,68	0
56	MG	B	2950	1/1	0.95	0.22	62,62,62,62	0
56	MG	GB	3581	1/1	0.95	0.12	69,69,69,69	0
56	MG	GB	3712	1/1	0.95	0.06	66,66,66,66	0
56	MG	GB	3456	1/1	0.95	0.21	68,68,68,68	0
56	MG	B	3740	1/1	0.95	0.19	70,70,70,70	0
56	MG	B	3329	1/1	0.95	0.12	47,47,47,47	0
56	MG	B	3330	1/1	0.95	0.09	41,41,41,41	0
56	MG	B	3743	1/1	0.95	0.07	52,52,52,52	0
56	MG	B	3141	1/1	0.95	0.15	44,44,44,44	0
56	MG	B	3277	1/1	0.95	0.10	51,51,51,51	0
56	MG	B	3526	1/1	0.95	0.30	49,49,49,49	0
56	MG	GB	3342	1/1	0.95	0.07	45,45,45,45	0
56	MG	GB	3343	1/1	0.95	0.07	57,57,57,57	0
56	MG	B	3393	1/1	0.95	0.11	46,46,46,46	0
56	MG	GB	3013	1/1	0.95	0.27	56,56,56,56	0
56	MG	B	3078	1/1	0.95	0.17	43,43,43,43	0
56	MG	GB	2908	1/1	0.95	0.32	44,44,44,44	0
56	MG	GB	3348	1/1	0.95	0.12	59,59,59,59	0
56	MG	B	3036	1/1	0.95	0.27	45,45,45,45	0
56	MG	B	3751	1/1	0.95	0.10	48,48,48,48	0
56	MG	B	3671	1/1	0.95	0.15	46,46,46,46	0
56	MG	B	3108	1/1	0.95	0.13	35,35,35,35	0
56	MG	B	2996	1/1	0.95	0.21	38,38,38,38	0
56	MG	GB	3605	1/1	0.95	0.09	61,61,61,61	0
56	MG	FB	1680	1/1	0.95	0.18	87,87,87,87	0
56	MG	AA	101	1/1	0.95	0.24	59,59,59,59	0
56	MG	B	3284	1/1	0.95	0.28	72,72,72,72	0
56	MG	B	3110	1/1	0.95	0.24	48,48,48,48	0
56	MG	GB	3241	1/1	0.95	0.30	74,74,74,74	0
56	MG	B	2997	1/1	0.95	0.25	42,42,42,42	0
56	MG	GB	3484	1/1	0.95	0.09	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	GB	3485	1/1	0.95	0.09	68,68,68,68	0
56	MG	XA	103	1/1	0.95	0.13	72,72,72,72	0
56	MG	B	3602	1/1	0.95	0.07	54,54,54,54	0
56	MG	B	2952	1/1	0.95	0.22	46,46,46,46	0
56	MG	GB	3246	1/1	0.95	0.17	79,79,79,79	0
56	MG	FB	1873	1/1	0.95	0.09	107,107,107,107	0
56	MG	CA	103	1/1	0.95	0.21	49,49,49,49	0
56	MG	B	3290	1/1	0.95	0.20	51,51,51,51	0
56	MG	B	3343	1/1	0.95	0.13	56,56,56,56	0
56	MG	B	3843	1/1	0.95	0.07	49,49,49,49	0
56	MG	GB	3371	1/1	0.95	0.11	56,56,56,56	0
56	MG	B	3084	1/1	0.95	0.28	42,42,42,42	0
56	MG	EA	101	1/1	0.95	0.31	45,45,45,45	0
56	MG	GB	3627	1/1	0.95	0.08	60,60,60,60	0
56	MG	FA	101	1/1	0.95	0.08	54,54,54,54	0
56	MG	B	2953	1/1	0.95	0.23	37,37,37,37	0
56	MG	B	3765	1/1	0.95	0.07	50,50,50,50	0
56	MG	B	3766	1/1	0.95	0.21	42,42,42,42	0
56	MG	B	3346	1/1	0.95	0.13	45,45,45,45	0
56	MG	JB	312	1/1	0.95	0.07	62,62,62,62	0
56	MG	A	1871	1/1	0.95	0.12	85,85,85,85	0
56	MG	B	3543	1/1	0.95	0.07	44,44,44,44	0
56	MG	GB	3148	1/1	0.95	0.31	59,59,59,59	0
56	MG	B	3473	1/1	0.95	0.15	51,51,51,51	0
56	MG	B	3348	1/1	0.95	0.15	55,55,55,55	0
56	MG	B	3772	1/1	0.95	0.12	57,57,57,57	0
56	MG	B	3242	1/1	0.95	0.16	49,49,49,49	0
56	MG	A	1623	1/1	0.95	0.21	67,67,67,67	0
56	MG	B	2974	1/1	0.95	0.18	39,39,39,39	0
56	MG	B	3414	1/1	0.95	0.10	47,47,47,47	0
56	MG	B	2987	1/1	0.95	0.20	34,34,34,34	0
56	MG	GB	3390	1/1	0.95	0.08	47,47,47,47	0
56	MG	C	217	1/1	0.95	0.23	60,60,60,60	0
56	MG	B	3158	1/1	0.95	0.14	50,50,50,50	0
56	MG	GB	3273	1/1	0.95	0.07	54,54,54,54	0
56	MG	B	3122	1/1	0.95	0.27	46,46,46,46	0
56	MG	B	3124	1/1	0.95	0.16	44,44,44,44	0
56	MG	B	3556	1/1	0.95	0.22	45,45,45,45	0
56	MG	GB	3397	1/1	0.95	0.30	60,60,60,60	0
56	MG	M	202	1/1	0.95	0.11	58,58,58,58	0
56	MG	B	3092	1/1	0.95	0.20	44,44,44,44	0
56	MG	C	223	1/1	0.95	0.14	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3254	1/1	0.95	0.13	61,61,61,61	0
56	MG	B	3304	1/1	0.95	0.15	43,43,43,43	0
56	MG	B	3126	1/1	0.95	0.10	43,43,43,43	0
56	MG	GB	3284	1/1	0.95	0.24	64,64,64,64	0
56	MG	B	3256	1/1	0.95	0.10	38,38,38,38	0
56	MG	N	204	1/1	0.95	0.11	61,61,61,61	0
56	MG	C	228	1/1	0.95	0.06	76,76,76,76	0
56	MG	QB	204	1/1	0.95	0.12	65,65,65,65	0
56	MG	B	3366	1/1	0.95	0.17	50,50,50,50	0
56	MG	B	3631	1/1	0.95	0.18	50,50,50,50	0
56	MG	GB	3664	1/1	0.95	0.12	58,58,58,58	0
56	MG	GB	3290	1/1	0.95	0.28	48,48,48,48	0
56	MG	FB	1818	1/1	0.95	0.06	83,83,83,83	0
56	MG	B	2988	1/1	0.95	0.24	38,38,38,38	0
56	MG	B	3165	1/1	0.95	0.13	46,46,46,46	0
56	MG	B	3128	1/1	0.95	0.08	33,33,33,33	0
56	MG	B	3497	1/1	0.95	0.12	52,52,52,52	0
56	MG	GB	3671	1/1	0.95	0.08	82,82,82,82	0
56	MG	B	3425	1/1	0.96	0.17	47,47,47,47	0
56	MG	B	3684	1/1	0.96	0.06	61,61,61,61	0
56	MG	GB	3011	1/1	0.96	0.18	54,54,54,54	0
56	MG	B	2951	1/1	0.96	0.40	43,43,43,43	0
56	MG	B	3210	1/1	0.96	0.14	54,54,54,54	0
56	MG	B	3161	1/1	0.96	0.12	38,38,38,38	0
56	MG	E	302	1/1	0.96	0.17	52,52,52,52	0
56	MG	B	3822	1/1	0.96	0.24	44,44,44,44	0
56	MG	FB	1707	1/1	0.96	0.24	69,69,69,69	0
56	MG	E	304	1/1	0.96	0.11	55,55,55,55	0
56	MG	B	3274	1/1	0.96	0.13	54,54,54,54	0
56	MG	B	3044	1/1	0.96	0.12	40,40,40,40	0
56	MG	B	2908	1/1	0.96	0.22	42,42,42,42	0
56	MG	JA	402	1/1	0.96	0.22	54,54,54,54	0
56	MG	GB	3318	1/1	0.96	0.14	54,54,54,54	0
56	MG	B	3579	1/1	0.96	0.09	47,47,47,47	0
56	MG	E	309	1/1	0.96	0.05	53,53,53,53	0
56	MG	GB	2931	1/1	0.96	0.23	47,47,47,47	0
56	MG	B	3692	1/1	0.96	0.11	51,51,51,51	0
56	MG	B	3759	1/1	0.96	0.11	47,47,47,47	0
56	MG	B	3632	1/1	0.96	0.14	64,64,64,64	0
56	MG	A	1854	1/1	0.96	0.09	75,75,75,75	0
56	MG	EC	104	1/1	0.96	0.18	79,79,79,79	0
56	MG	B	3480	1/1	0.96	0.06	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3696	1/1	0.96	0.12	52,52,52,52	0
56	MG	S	206	1/1	0.96	0.06	57,57,57,57	0
56	MG	FB	1809	1/1	0.96	0.14	63,63,63,63	0
56	MG	B	3697	1/1	0.96	0.09	56,56,56,56	0
56	MG	F	307	1/1	0.96	0.07	70,70,70,70	0
56	MG	GB	3232	1/1	0.96	0.17	61,61,61,61	0
56	MG	B	3030	1/1	0.96	0.29	59,59,59,59	0
56	MG	B	3482	1/1	0.96	0.11	47,47,47,47	0
56	MG	B	3086	1/1	0.96	0.18	43,43,43,43	0
56	MG	B	2954	1/1	0.96	0.19	42,42,42,42	0
56	MG	B	3439	1/1	0.96	0.13	49,49,49,49	0
56	MG	F	313	1/1	0.96	0.22	49,49,49,49	0
56	MG	B	3282	1/1	0.96	0.15	50,50,50,50	0
56	MG	B	3251	1/1	0.96	0.29	53,53,53,53	0
56	MG	G	3202	1/1	0.96	0.21	34,34,34,34	0
56	MG	GB	3141	1/1	0.96	0.20	49,49,49,49	0
56	MG	B	3642	1/1	0.96	0.04	52,52,52,52	0
56	MG	B	3643	1/1	0.96	0.07	56,56,56,56	0
56	MG	B	3252	1/1	0.96	0.10	45,45,45,45	0
56	MG	B	3775	1/1	0.96	0.08	42,42,42,42	0
56	MG	B	3285	1/1	0.96	0.09	42,42,42,42	0
56	MG	B	3357	1/1	0.96	0.07	54,54,54,54	0
56	MG	FB	1652	1/1	0.96	0.44	70,70,70,70	0
56	MG	B	3647	1/1	0.96	0.10	48,48,48,48	0
56	MG	B	3219	1/1	0.96	0.16	43,43,43,43	0
56	MG	B	3446	1/1	0.96	0.06	42,42,42,42	0
56	MG	X	107	1/1	0.96	0.12	72,72,72,72	0
56	MG	B	3360	1/1	0.96	0.07	43,43,43,43	0
56	MG	FB	1658	1/1	0.96	0.08	72,72,72,72	0
56	MG	B	2935	1/1	0.96	0.35	44,44,44,44	0
56	MG	Y	102	1/1	0.96	0.20	54,54,54,54	0
56	MG	C	210	1/1	0.96	0.43	75,75,75,75	0
56	MG	GB	3460	1/1	0.96	0.07	63,63,63,63	0
56	MG	GB	3158	1/1	0.96	0.08	52,52,52,52	0
56	MG	B	3034	1/1	0.96	0.22	55,55,55,55	0
56	MG	B	3548	1/1	0.96	0.05	44,44,44,44	0
56	MG	GB	3464	1/1	0.96	0.11	83,83,83,83	0
56	MG	B	2945	1/1	0.96	0.19	47,47,47,47	0
56	MG	B	2936	1/1	0.96	0.26	34,34,34,34	0
56	MG	B	3326	1/1	0.96	0.18	44,44,44,44	0
56	MG	B	3552	1/1	0.96	0.11	46,46,46,46	0
56	MG	AA	102	1/1	0.96	0.05	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	A	1826	1/1	0.96	0.11	58,58,58,58	0
56	MG	B	3659	1/1	0.96	0.06	52,52,52,52	0
56	MG	B	2905	1/1	0.96	0.14	45,45,45,45	0
56	MG	B	2982	1/1	0.96	0.19	42,42,42,42	0
56	MG	A	1632	1/1	0.96	0.41	65,65,65,65	0
56	MG	CA	102	1/1	0.96	0.20	52,52,52,52	0
56	MG	GB	3274	1/1	0.96	0.30	73,73,73,73	0
56	MG	B	3728	1/1	0.96	0.10	50,50,50,50	0
56	MG	B	3179	1/1	0.96	0.20	47,47,47,47	0
56	MG	B	3155	1/1	0.96	0.10	43,43,43,43	0
56	MG	GB	2984	1/1	0.96	0.27	66,66,66,66	0
56	MG	B	3510	1/1	0.96	0.08	45,45,45,45	0
56	MG	B	3459	1/1	0.96	0.08	46,46,46,46	0
56	MG	RB	205	1/1	0.96	0.14	55,55,55,55	0
56	MG	B	3114	1/1	0.96	0.18	49,49,49,49	0
56	MG	EA	102	1/1	0.96	0.07	44,44,44,44	0
56	MG	GB	2989	1/1	0.96	0.34	59,59,59,59	0
56	MG	FB	1945	1/1	0.96	0.07	68,68,68,68	0
56	MG	GB	3590	1/1	0.96	0.10	76,76,76,76	0
56	MG	GB	3591	1/1	0.96	0.15	71,71,71,71	0
56	MG	A	1735	1/1	0.96	0.30	69,69,69,69	0
56	MG	B	3336	1/1	0.96	0.26	60,60,60,60	0
56	MG	FA	103	1/1	0.96	0.09	48,48,48,48	0
56	MG	GB	3595	1/1	0.96	0.14	74,74,74,74	0
56	MG	B	3613	1/1	0.96	0.22	55,55,55,55	0
56	MG	B	3377	1/1	0.96	0.09	44,44,44,44	0
56	MG	B	3673	1/1	0.96	0.09	50,50,50,50	0
56	MG	B	3233	1/1	0.96	0.16	51,51,51,51	0
56	MG	B	3011	1/1	0.96	0.28	55,55,55,55	0
56	MG	VB	206	1/1	0.96	0.06	69,69,69,69	0
56	MG	B	3380	1/1	0.96	0.09	51,51,51,51	0
56	MG	B	3236	1/1	0.96	0.28	44,44,44,44	0
56	MG	B	3117	1/1	0.96	0.28	48,48,48,48	0
56	MG	M	207	1/1	0.96	0.22	51,51,51,51	0
56	MG	GB	3398	1/1	0.96	0.13	63,63,63,63	0
56	MG	B	3620	1/1	0.96	0.07	50,50,50,50	0
56	MG	B	3745	1/1	0.96	0.10	56,56,56,56	0
56	MG	GB	3503	1/1	0.96	0.15	52,52,52,52	0
56	MG	B	3208	1/1	0.96	0.22	47,47,47,47	0
56	MG	B	3622	1/1	0.96	0.10	55,55,55,55	0
56	MG	HD	201	1/1	0.96	0.11	79,79,79,79	0
56	MG	B	3522	1/1	0.96	0.12	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	N	205	1/1	0.96	0.09	65,65,65,65	0
56	MG	B	2930	1/1	0.97	0.21	34,34,34,34	0
56	MG	B	3475	1/1	0.97	0.23	46,46,46,46	0
56	MG	B	3046	1/1	0.97	0.16	34,34,34,34	0
56	MG	B	3700	1/1	0.97	0.07	46,46,46,46	0
56	MG	B	3243	1/1	0.97	0.14	43,43,43,43	0
56	MG	GB	3042	1/1	0.97	0.29	54,54,54,54	0
56	MG	B	3190	1/1	0.97	0.22	57,57,57,57	0
56	MG	B	3359	1/1	0.97	0.25	63,63,63,63	0
56	MG	B	3245	1/1	0.97	0.19	52,52,52,52	0
56	MG	B	3784	1/1	0.97	0.09	44,44,44,44	0
56	MG	B	2943	1/1	0.97	0.20	37,37,37,37	0
56	MG	GB	3365	1/1	0.97	0.27	60,60,60,60	0
56	MG	GB	3254	1/1	0.97	0.08	62,62,62,62	0
56	MG	B	3176	1/1	0.97	0.16	53,53,53,53	0
56	MG	M	203	1/1	0.97	0.18	43,43,43,43	0
56	MG	B	3058	1/1	0.97	0.37	48,48,48,48	0
56	MG	B	3147	1/1	0.97	0.10	52,52,52,52	0
56	MG	M	206	1/1	0.97	0.24	49,49,49,49	0
56	MG	GB	3315	1/1	0.97	0.05	51,51,51,51	0
56	MG	B	2999	1/1	0.97	0.22	35,35,35,35	0
56	MG	RC	307	1/1	0.97	0.06	85,85,85,85	0
56	MG	B	3831	1/1	0.97	0.15	43,43,43,43	0
56	MG	G	3201	1/1	0.97	0.14	36,36,36,36	0
56	MG	A	1839	1/1	0.97	0.09	85,85,85,85	0
56	MG	GB	3106	1/1	0.97	0.32	66,66,66,66	0
56	MG	B	3672	1/1	0.97	0.09	52,52,52,52	0
56	MG	B	3422	1/1	0.97	0.09	66,66,66,66	0
56	MG	GB	3610	1/1	0.97	0.08	78,78,78,78	0
56	MG	B	3213	1/1	0.97	0.13	48,48,48,48	0
56	MG	B	3489	1/1	0.97	0.17	40,40,40,40	0
56	MG	B	2985	1/1	0.97	0.25	46,46,46,46	0
56	MG	GB	3215	1/1	0.97	0.19	55,55,55,55	0
56	MG	B	3491	1/1	0.97	0.12	48,48,48,48	0
56	MG	B	3085	1/1	0.97	0.05	38,38,38,38	0
56	MG	B	3234	1/1	0.97	0.09	51,51,51,51	0
56	MG	B	3372	1/1	0.97	0.09	40,40,40,40	0
56	MG	B	3300	1/1	0.97	0.21	50,50,50,50	0
56	MG	B	3430	1/1	0.97	0.11	46,46,46,46	0
56	MG	B	3534	1/1	0.97	0.04	45,45,45,45	0
56	MG	B	3431	1/1	0.97	0.07	47,47,47,47	0
56	MG	B	3020	1/1	0.97	0.24	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	GB	3225	1/1	0.97	0.07	65,65,65,65	0
56	MG	B	3111	1/1	0.97	0.17	33,33,33,33	0
56	MG	GB	3172	1/1	0.97	0.15	57,57,57,57	0
56	MG	C	204	1/1	0.97	0.24	54,54,54,54	0
56	MG	B	3052	1/1	0.97	0.24	47,47,47,47	0
56	MG	GB	3175	1/1	0.97	0.09	52,52,52,52	0
56	MG	B	3403	1/1	0.97	0.06	50,50,50,50	0
56	MG	GB	2977	1/1	0.97	0.22	52,52,52,52	0
56	MG	B	3404	1/1	0.97	0.13	47,47,47,47	0
56	MG	B	3350	1/1	0.97	0.06	40,40,40,40	0
56	MG	JB	301	1/1	0.97	0.19	45,45,45,45	0
56	MG	B	3327	1/1	0.97	0.07	43,43,43,43	0
56	MG	J	203	1/1	0.97	0.28	80,80,80,80	0
56	MG	B	3506	1/1	0.97	0.07	46,46,46,46	0
56	MG	A	1774	1/1	0.97	0.06	106,106,106,106	0
56	MG	B	3054	1/1	0.97	0.34	58,58,58,58	0
56	MG	T	202	1/1	0.97	0.08	45,45,45,45	0
56	MG	B	3509	1/1	0.97	0.06	52,52,52,52	0
57	ZN	AC	201	1/1	0.97	0.05	100,100,100,100	0
56	MG	B	3240	1/1	0.97	0.13	51,51,51,51	0
56	MG	B	3281	1/1	0.98	0.20	53,53,53,53	0
56	MG	B	3083	1/1	0.98	0.33	40,40,40,40	0
56	MG	B	3021	1/1	0.98	0.20	43,43,43,43	0
56	MG	GB	3213	1/1	0.98	0.06	59,59,59,59	0
56	MG	B	3502	1/1	0.98	0.07	48,48,48,48	0
56	MG	GB	2909	1/1	0.98	0.33	38,38,38,38	0
56	MG	B	3713	1/1	0.98	0.07	46,46,46,46	0
56	MG	B	3819	1/1	0.98	0.10	56,56,56,56	0
56	MG	B	3427	1/1	0.98	0.05	47,47,47,47	0
56	MG	B	3227	1/1	0.98	0.10	44,44,44,44	0
56	MG	B	3173	1/1	0.98	0.07	40,40,40,40	0
56	MG	B	3363	1/1	0.98	0.06	44,44,44,44	0
56	MG	B	3313	1/1	0.98	0.13	49,49,49,49	0
56	MG	B	3286	1/1	0.98	0.06	41,41,41,41	0
56	MG	B	3168	1/1	0.98	0.10	35,35,35,35	0
56	MG	B	3123	1/1	0.98	0.11	33,33,33,33	0
56	MG	GB	3492	1/1	0.98	0.06	70,70,70,70	0
56	MG	X	102	1/1	0.98	0.20	50,50,50,50	0
56	MG	B	3471	1/1	0.98	0.09	49,49,49,49	0
56	MG	T	201	1/1	0.98	0.13	42,42,42,42	0
56	MG	B	3145	1/1	0.98	0.06	43,43,43,43	0
56	MG	GB	3370	1/1	0.98	0.09	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3033	1/1	0.99	0.30	50,50,50,50	0
57	ZN	CA	101	1/1	0.99	0.03	62,62,62,62	0
57	ZN	DA	101	1/1	0.99	0.02	71,71,71,71	0
57	ZN	GA	101	1/1	0.99	0.03	70,70,70,70	0
56	MG	A	1736	1/1	0.99	0.04	53,53,53,53	0
56	MG	GB	3037	1/1	0.99	0.07	52,52,52,52	0
57	ZN	HC	101	1/1	0.99	0.03	86,86,86,86	0
57	ZN	IC	101	1/1	0.99	0.04	91,91,91,91	0
57	ZN	V	501	1/1	1.00	0.04	72,72,72,72	0
57	ZN	LC	101	1/1	1.00	0.02	97,97,97,97	0

6.5 Other polymers [i](#)

There are no such residues in this entry.