



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 12:02 PM UTC

PDB ID : 6BOH / pdb_00006boh
Title : Antibiotic blasticidin S and E. coli release factor 1 (containing deletion 302-304) bound to the 70S ribosome
Authors : Svidritskiy, E.; Korostelev, A.A.
Deposited on : 2017-11-20
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

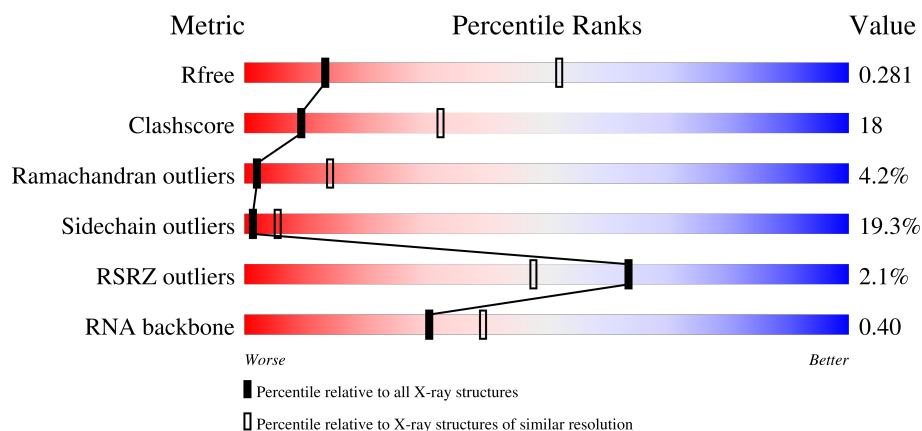
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



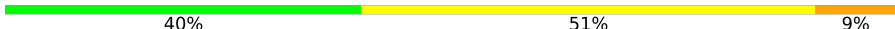
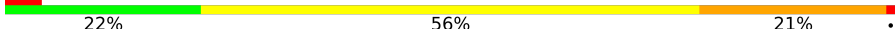
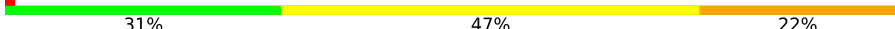
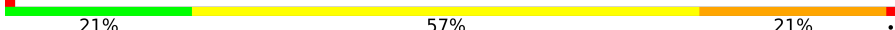
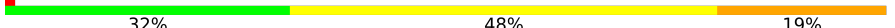
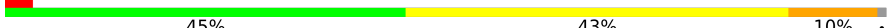
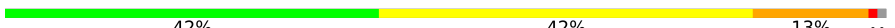
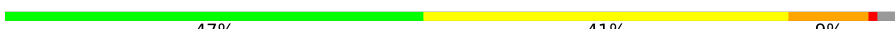
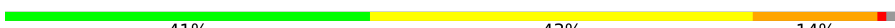
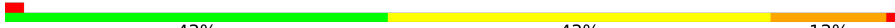
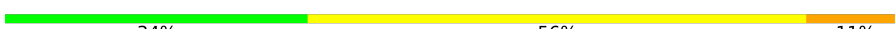
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

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	35% 50% 14%
1	FB	1507	36% 50% 14%
2	B	2880	40% 46% 14%
2	GB	2880	41% 44% 14%

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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	365	
35	KA	365	
35	OC	365	
35	PC	365	
36	LA	256	
36	QC	256	
37	MA	239	
37	RC	239	
38	NA	209	

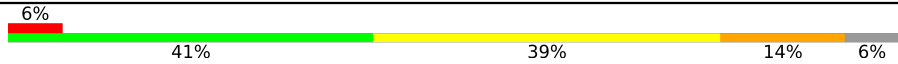
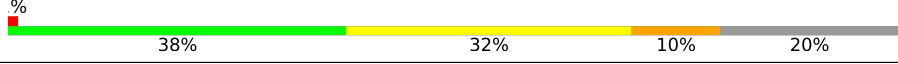
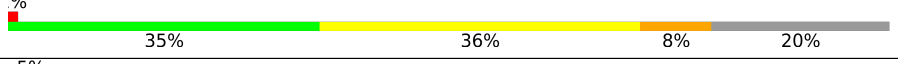
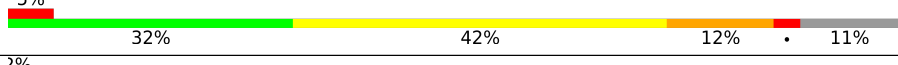
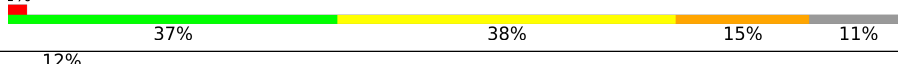
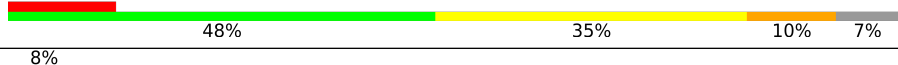
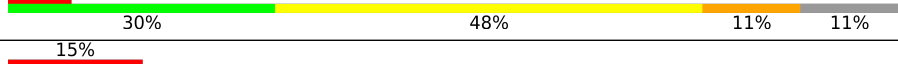
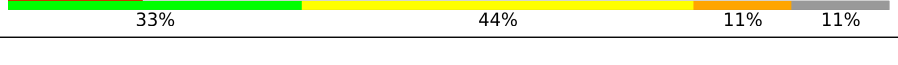
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Mol	Chain	Length	Quality of chain
38	SC	209	
39	OA	162	
39	TC	162	
40	PA	101	
40	UC	101	
41	QA	156	
41	VC	156	
42	RA	138	
42	WC	138	
43	SA	128	
43	XC	128	
44	TA	105	
44	YC	105	
45	UA	129	
45	ZC	129	
46	AD	132	
46	VA	132	
47	BD	126	
47	WA	126	
48	CD	61	
48	XA	61	
49	DD	89	
49	YA	89	
50	ED	88	
50	ZA	88	

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Mol	Chain	Length	Quality of chain
51	AB	105	
51	FD	105	
52	BB	88	
52	GD	88	
53	CB	93	
53	HD	93	
54	DB	106	
54	ID	106	
55	EB	27	
55	JD	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	1642	-	-	-	X
56	MG	A	1645	-	-	-	X
56	MG	A	1721	-	-	-	X
56	MG	B	9007	-	-	-	X
56	MG	B	9021	-	-	-	X
56	MG	B	9050	-	-	-	X
56	MG	C	201	-	-	-	X
56	MG	CC	101	-	-	-	X
56	MG	FB	1604	-	-	-	X
56	MG	FB	1618	-	-	-	X
56	MG	FB	1638	-	-	-	X
56	MG	FB	1643	-	-	-	X
56	MG	GB	9004	-	-	-	X
56	MG	GB	9012	-	-	-	X
56	MG	GB	9020	-	-	-	X
56	MG	GB	9022	-	-	-	X
56	MG	GB	9047	-	-	-	X
56	MG	GB	9108	-	-	-	X
56	MG	HB	201	-	-	-	X

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 298186 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 23S ribosomal RNA.

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	97	Total	C	N	O	S	0	0	0
			761	478	151	131	1			
25	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			
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	110	Total 850	C 525	N 157	O 164	S 4	0	0	0
35	KA	55	Total 455	C 281	N 83	O 89	S 2	0	0	0
35	OC	110	Total 850	C 525	N 157	O 164	S 4	0	0	0
35	PC	55	Total 455	C 281	N 83	O 89	S 2	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
JA	?	-	ASP	deletion	UNP B7MKB3
JA	?	-	ARG	deletion	UNP B7MKB3
JA	?	-	SER	deletion	UNP B7MKB3
JA	358	LEU	-	expression tag	UNP B7MKB3
JA	359	GLU	-	expression tag	UNP B7MKB3
JA	360	HIS	-	expression tag	UNP B7MKB3
JA	361	HIS	-	expression tag	UNP B7MKB3
JA	362	HIS	-	expression tag	UNP B7MKB3
JA	363	HIS	-	expression tag	UNP B7MKB3
JA	364	HIS	-	expression tag	UNP B7MKB3
JA	365	HIS	-	expression tag	UNP B7MKB3
KA	?	-	ASP	deletion	UNP B7MKB3
KA	?	-	ARG	deletion	UNP B7MKB3
KA	?	-	SER	deletion	UNP B7MKB3
KA	361	LEU	-	expression tag	UNP B7MKB3
KA	362	GLU	-	expression tag	UNP B7MKB3
KA	363	HIS	-	expression tag	UNP B7MKB3
KA	364	HIS	-	expression tag	UNP B7MKB3
KA	365	HIS	-	expression tag	UNP B7MKB3
KA	366	HIS	-	expression tag	UNP B7MKB3
KA	367	HIS	-	expression tag	UNP B7MKB3
KA	368	HIS	-	expression tag	UNP B7MKB3
OC	?	-	ASP	deletion	UNP B7MKB3
OC	?	-	ARG	deletion	UNP B7MKB3
OC	?	-	SER	deletion	UNP B7MKB3
OC	358	LEU	-	expression tag	UNP B7MKB3
OC	359	GLU	-	expression tag	UNP B7MKB3
OC	360	HIS	-	expression tag	UNP B7MKB3
OC	361	HIS	-	expression tag	UNP B7MKB3
OC	362	HIS	-	expression tag	UNP B7MKB3
OC	363	HIS	-	expression tag	UNP B7MKB3

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	LA	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			
36	QC	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	MA	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
37	RC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 38 is a protein called 50S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	NA	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
38	SC	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	OA	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
39	TC	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	PA	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
40	UC	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	QA	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
41	VC	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	RA	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
42	WC	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	SA	127	Total	C	N	O	0	0	0
			1011	639	198	174			
43	XC	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	TA	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	YC	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	UA	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			
45	ZC	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	VA	122	Total	C	N	O	S	0	0	0
			958	604	193	159	2			
46	AD	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	WA	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			
47	BD	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	XA	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
48	CD	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	YA	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
49	DD	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	ZA	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
50	ED	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	AB	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			
51	FD	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	BB	70	Total	C	N	O	0	0	0
			574	367	112	95			
52	GD	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	CB	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
53	HD	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	DB	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
54	ID	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	EB	24	Total	C	N	O	0	0	0
			208	128	50	30			
55	JD	24	Total	C	N	O	0	0	0
			208	128	50	30			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	A	183	Total	Mg	0	0
			183	183		
56	B	433	Total	Mg	0	0
			433	433		
56	C	22	Total	Mg	0	0
			22	22		
56	D	5	Total	Mg	0	0
			5	5		
56	E	6	Total	Mg	0	0
			6	6		
56	F	4	Total	Mg	0	0
			4	4		
56	G	2	Total	Mg	0	0
			2	2		
56	H	2	Total	Mg	0	0
			2	2		
56	J	1	Total	Mg	0	0
			1	1		
56	K	4	Total	Mg	0	0
			4	4		
56	L	3	Total	Mg	0	0
			3	3		
56	M	3	Total	Mg	0	0
			3	3		
56	O	2	Total	Mg	0	0
			2	2		
56	Q	1	Total	Mg	0	0
			1	1		
56	R	1	Total	Mg	0	0
			1	1		
56	S	1	Total	Mg	0	0
			1	1		
56	T	2	Total	Mg	0	0
			2	2		
56	U	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	V	2	Total 2	Mg 2	0	0
56	Y	3	Total 3	Mg 3	0	0
56	Z	1	Total 1	Mg 1	0	0
56	AA	1	Total 1	Mg 1	0	0
56	CA	1	Total 1	Mg 1	0	0
56	EA	1	Total 1	Mg 1	0	0
56	FA	1	Total 1	Mg 1	0	0
56	HA	3	Total 3	Mg 3	0	0
56	IA	9	Total 9	Mg 9	0	0
56	JA	1	Total 1	Mg 1	0	0
56	LA	1	Total 1	Mg 1	0	0
56	MA	6	Total 6	Mg 6	0	0
56	NA	2	Total 2	Mg 2	0	0
56	OA	4	Total 4	Mg 4	0	0
56	PA	3	Total 3	Mg 3	0	0
56	QA	1	Total 1	Mg 1	0	0
56	SA	1	Total 1	Mg 1	0	0
56	UA	1	Total 1	Mg 1	0	0
56	VA	2	Total 2	Mg 2	0	0
56	YA	3	Total 3	Mg 3	0	0
56	AB	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BB	1	Total 1	Mg 1	0	0
56	CB	1	Total 1	Mg 1	0	0
56	FB	194	Total 194	Mg 194	0	0
56	GB	402	Total 402	Mg 402	0	0
56	HB	20	Total 20	Mg 20	0	0
56	IB	2	Total 2	Mg 2	0	0
56	JB	5	Total 5	Mg 5	0	0
56	KB	2	Total 2	Mg 2	0	0
56	LB	4	Total 4	Mg 4	0	0
56	NB	1	Total 1	Mg 1	0	0
56	OB	1	Total 1	Mg 1	0	0
56	PB	2	Total 2	Mg 2	0	0
56	QB	2	Total 2	Mg 2	0	0
56	RB	3	Total 3	Mg 3	0	0
56	SB	2	Total 2	Mg 2	0	0
56	TB	1	Total 1	Mg 1	0	0
56	UB	4	Total 4	Mg 4	0	0
56	VB	3	Total 3	Mg 3	0	0
56	XB	2	Total 2	Mg 2	0	0
56	ZB	2	Total 2	Mg 2	0	0
56	AC	1	Total 1	Mg 1	0	0

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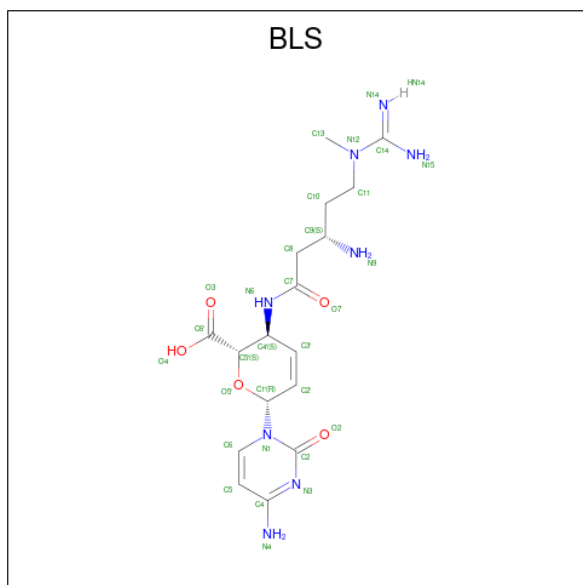
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BC	1	Total 1	Mg 1	0	0
56	CC	1	Total 1	Mg 1	0	0
56	DC	1	Total 1	Mg 1	0	0
56	GC	1	Total 1	Mg 1	0	0
56	IC	1	Total 1	Mg 1	0	0
56	JC	1	Total 1	Mg 1	0	0
56	KC	1	Total 1	Mg 1	0	0
56	MC	3	Total 3	Mg 3	0	0
56	NC	10	Total 10	Mg 10	0	0
56	OC	1	Total 1	Mg 1	0	0
56	PC	1	Total 1	Mg 1	0	0
56	QC	3	Total 3	Mg 3	0	0
56	RC	2	Total 2	Mg 2	0	0
56	SC	4	Total 4	Mg 4	0	0
56	TC	3	Total 3	Mg 3	0	0
56	UC	3	Total 3	Mg 3	0	0
56	VC	1	Total 1	Mg 1	0	0
56	WC	1	Total 1	Mg 1	0	0
56	ZC	1	Total 1	Mg 1	0	0
56	AD	4	Total 4	Mg 4	0	0
56	BD	1	Total 1	Mg 1	0	0

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

- Molecule 57 is BLASTICIDIN S (CCD ID: BLS) (formula: $C_{17}H_{26}N_8O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	B	1	Total	C	N	O	0	0
			30	17	8	5		
57	GB	1	Total	C	N	O	0	0
			30	17	8	5		

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	V	1	Total	Zn	0	0
			1	1		
58	BA	1	Total	Zn	0	0
			1	1		
58	CA	1	Total	Zn	0	0
			1	1		
58	DA	1	Total	Zn	0	0
			1	1		

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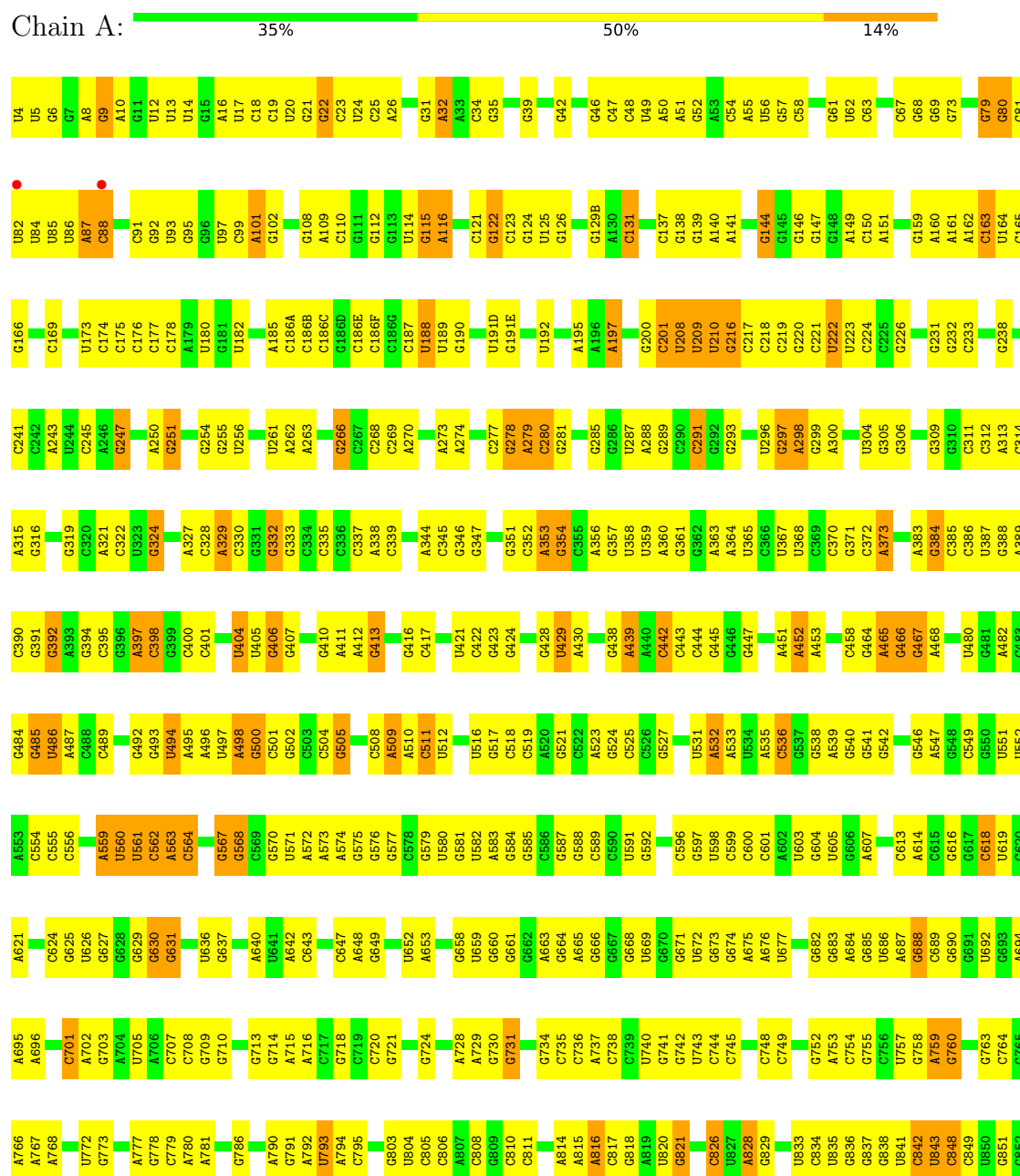
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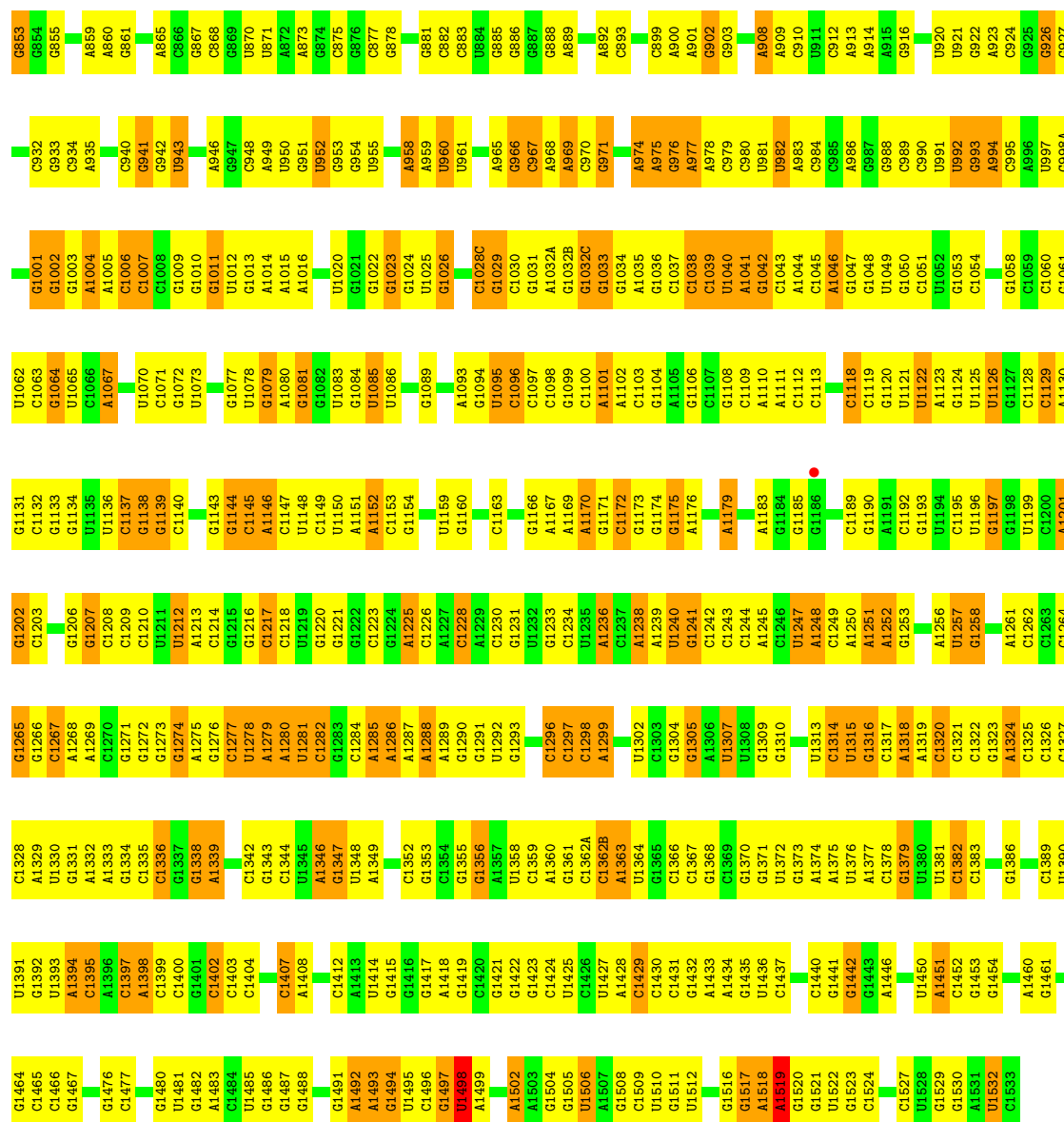
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	GA	1	Total 1	Zn 1	0	0
58	AC	1	Total 1	Zn 1	0	0
58	GC	1	Total 1	Zn 1	0	0
58	HC	1	Total 1	Zn 1	0	0
58	IC	1	Total 1	Zn 1	0	0
58	LC	1	Total 1	Zn 1	0	0

3 Residue-property plots

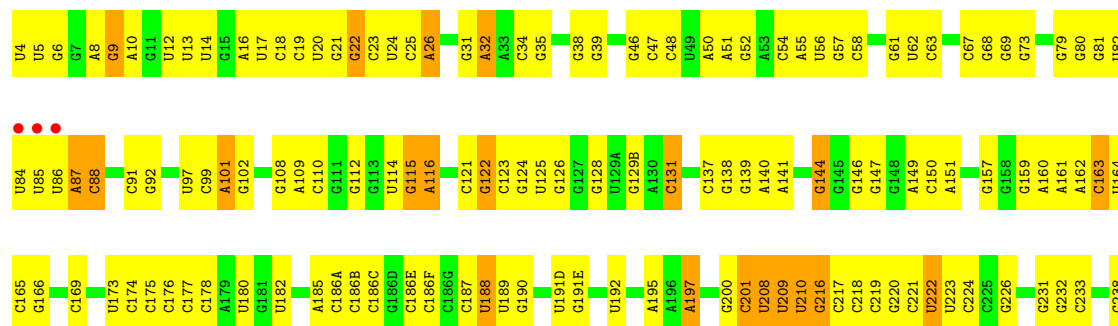
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S ribosomal RNA

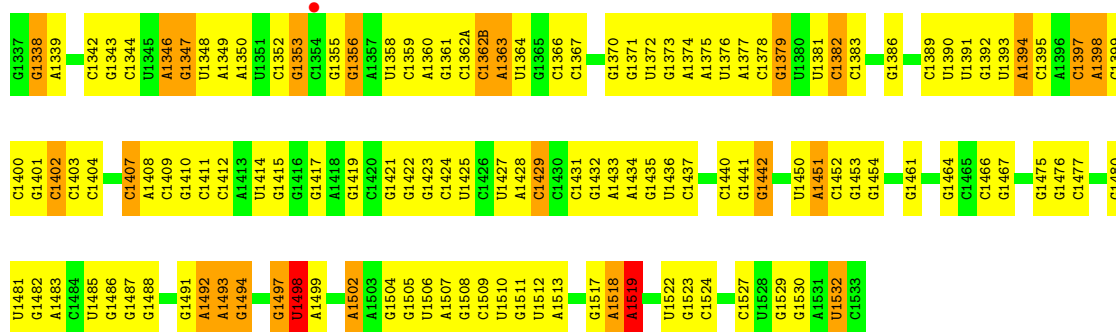




• Molecule 1: 16S ribosomal RNA

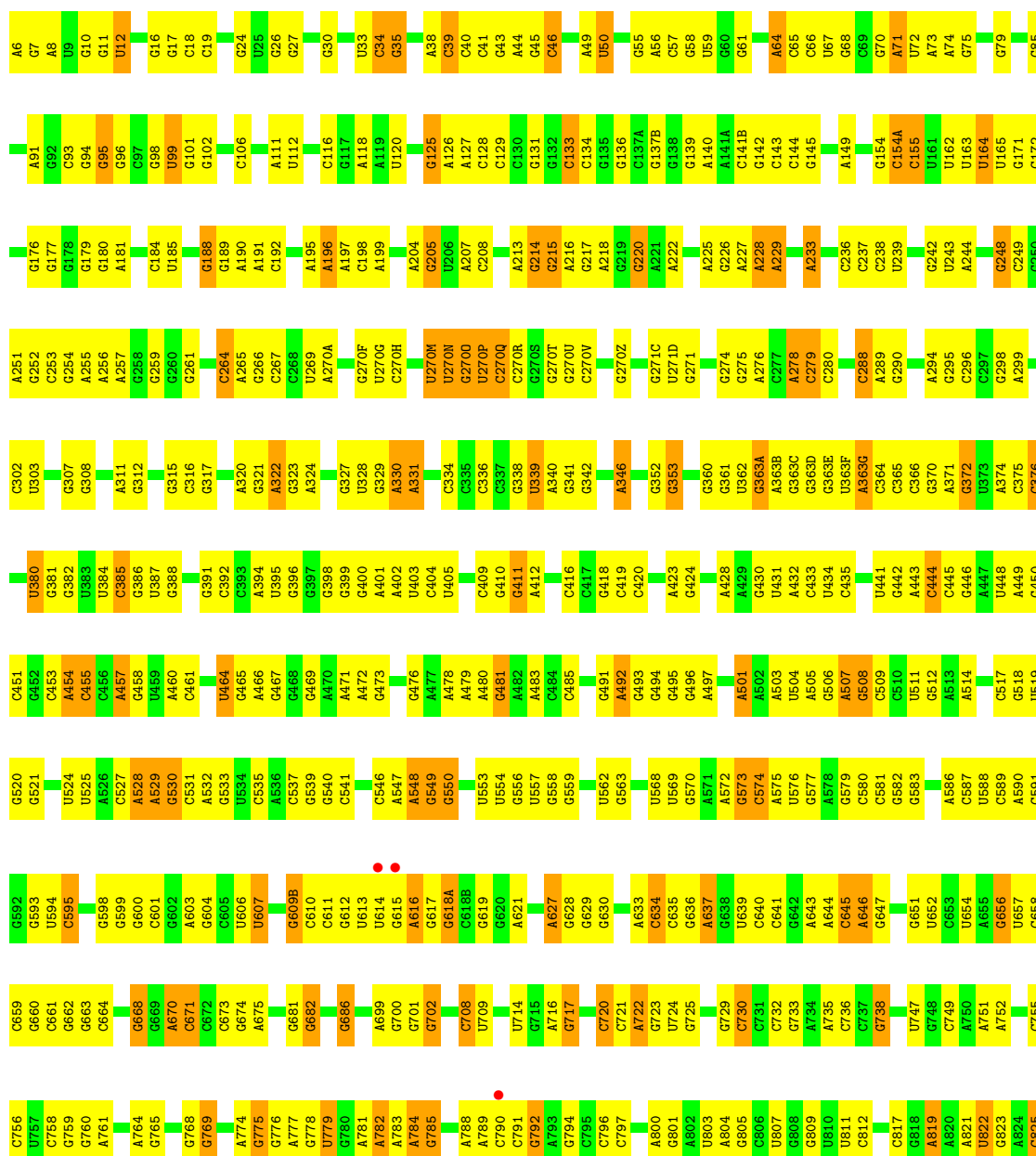




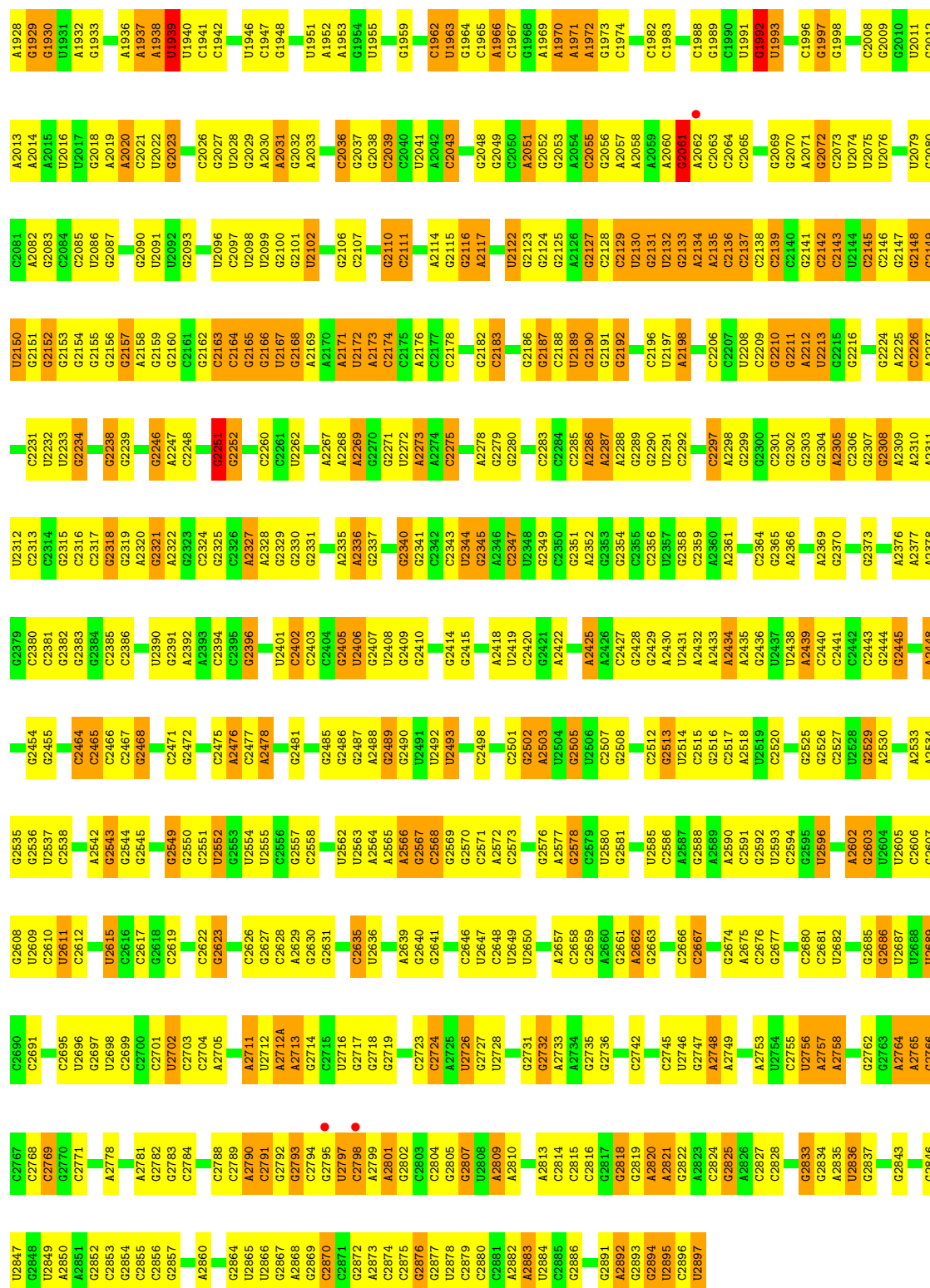


• Molecule 2: 23S ribosomal RNA

Chain B: 40% 46% 14%

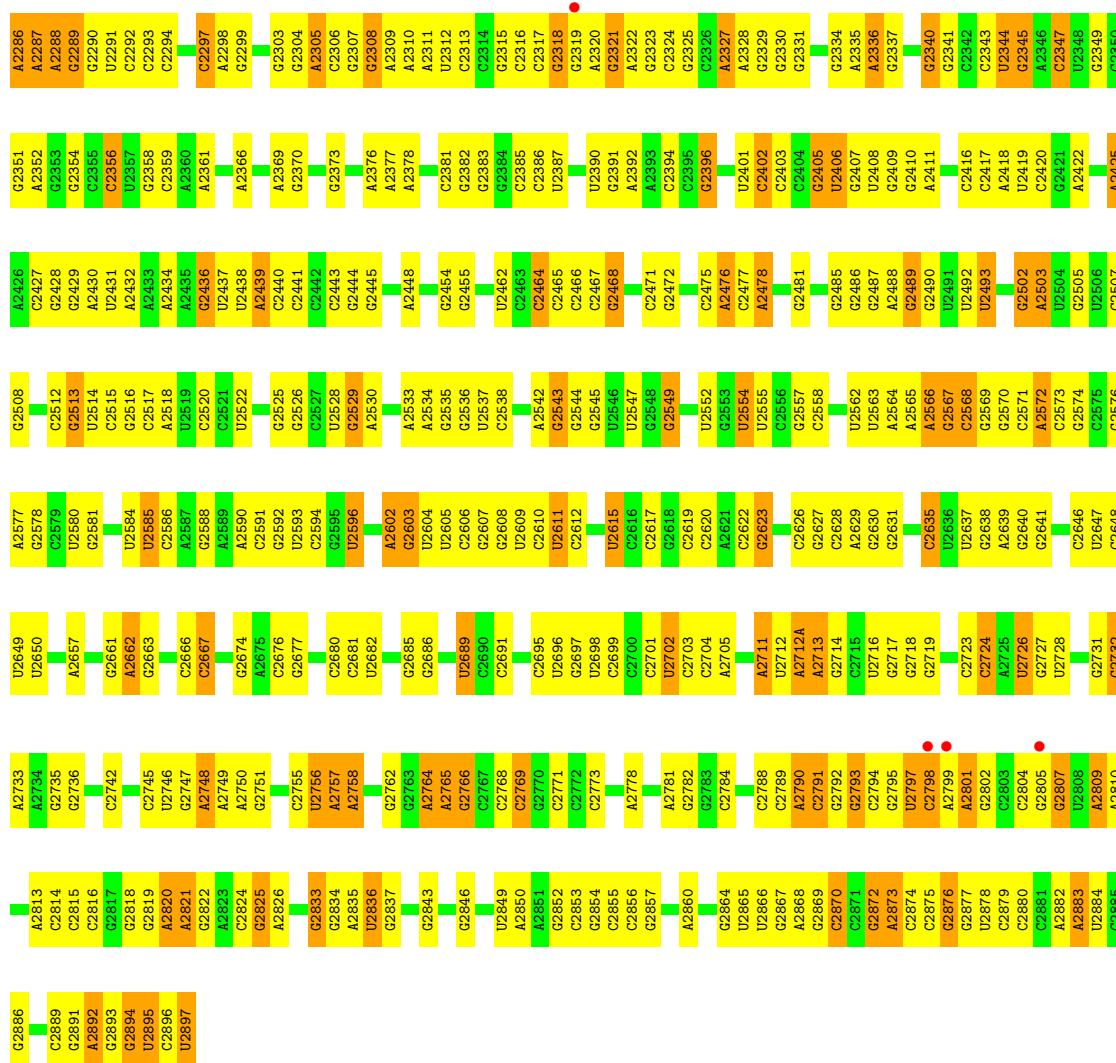


U1833	G1753	G1642	G1561	G1492	G1413	U1340	A1254	U1175	G1100	C1040	C971	C893	U826
U1834	C1754	G1643	G1566	C1493	G1414	U1341	U1255	G1176	U1101	C1041	C972	C894	U827
G1835	G1644	C1644	A1567	A1494	U1415	A1342	G1256	A1177	C1102	G1042	G972	U895	A828
G1846	G1757	C1648	A1568	A1496	G1416	G1345	C1257	C1178	A1103	G1043	A973	A896	A829
A1847	G1758	G1649	A1569	U1497	C1417	C1346	C1258	C1179	C1104	G1044	C974A	C897	G830
A1848	A1759	A1654	A1570	G1500	A1419	G1347	G1259	C1180	U1105	A1045	C974B	G898	G831
G1849	A1760	G1657	A1571	G1501	G1423	U1352	G1264	C1181	G1106	A1046	G975	A899	G832
G1850	C1761	C1658	A1572	U1503	G1424	A1285	A1265	A1182	U1107	G1047	C976	A900	U833
G1851	A1762	G1659	U1573	C1504	G1425	A1353	G1266	G1183	U1108	A1048	G977	A901	C834
G1855	G1763	G1666	U1578	U1505	G1426	A1354	U1267	C1184	C1109	C1049	G978	C902	A835
G1859	G1764	G1667	A1579	C1506	G1427	G1355	A1268	G1186	A1111	G1051	A980	C903	U839
A1859	C1771	A1689	G1581	C1508	G1428	G1356	A1269	G1187	G1112	C1052	G806	U840	U841
G1860	G1772	C1670	C1582	A1508	C1429	U1357	C1270	U1188	U1113	C1053	A983	U907	A841
G1861	A1773	G1671	A1509	A1509	G1430	G1358	G1271	A1189	G1114	A1054	C986	A910	C844
G1862	C1774	C1672	A1585	A1511	C1431	A1360	A1272	G1190	G1108	G1055	C987	A911	G845
U1775	U1775	G1673	A1586	G1512	C1432	A1361	U1273	G1191	C1116	G1056	A990	G914	C846
G1863	G1776	G1674	A1587	C1515	U1433	G1364	A1274	G1203	G1117	A1057	A991	U847	U848
G1864	C1675	C1675	C1588	U1516	U1434	A1365	A1275	G1204	C1118	G1058	C992	C915	A849
G1869	U1779	U1680	C1589	G1517	C1437	A1366	A1278	U1205	G1122	U1060	G993	G916	A848
C1870	G1681	G1681	U1590	G1518	U1438	A1367	A1286	U1206	G1129	U1061	C994	A917	C850
A1871	A1784	G1682	G1591	G1519	A1439	G1374	A1287	C1207	U1130	G1062	C995	A918	U851
A1872	A1785	G1683	C1592	G1520	G1440	A1372	U1288	A1210	A1126	G1063	A996	G919	G852
C1880	A1786	G1684	G1593	G1521	G1441	A1373	C1289	U1211	A1128	U1065	C997	G921	G853
C1881	A1787	C1685	G1594	G1524	G1442	G1375	C1290	U1212	U1129	U1066	C998	G922	G854
C1882	C1686	G1686	C1595	G1525	G1443	C1376	G1289	A1213	A1139	A1067	U999	U922	G855
G1883	G1687	C1687	C1598	G1526	A1444B	G1377	C1291	A1214	U1136	G1068	C924	C925	C856
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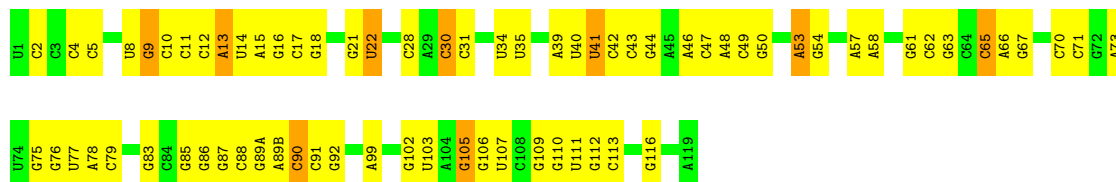


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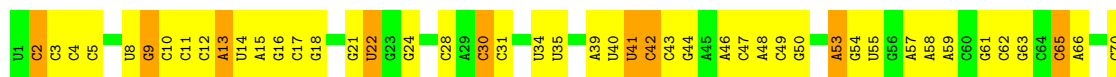
• Molecule 3: 5S ribosomal RNA

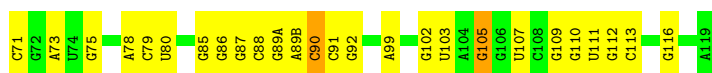
Chain C: 40% 52% 8%



• Molecule 3: 5S ribosomal RNA

Chain HB: 40% 51% 9%

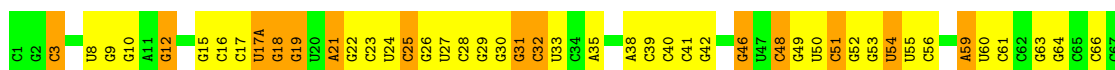




• Molecule 4: tRNA



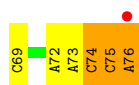
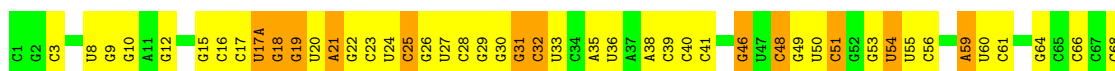
• Molecule 4: tRNA



• Molecule 4: tRNA

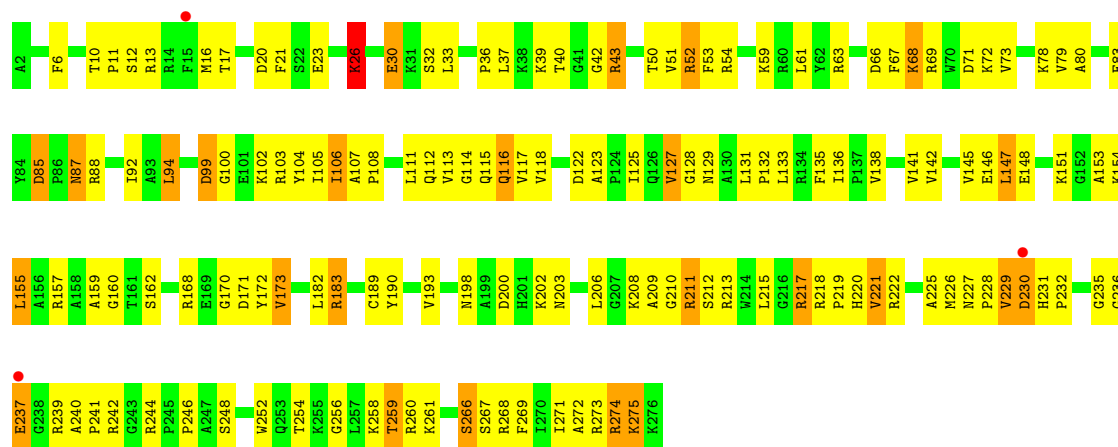


• Molecule 4: tRNA

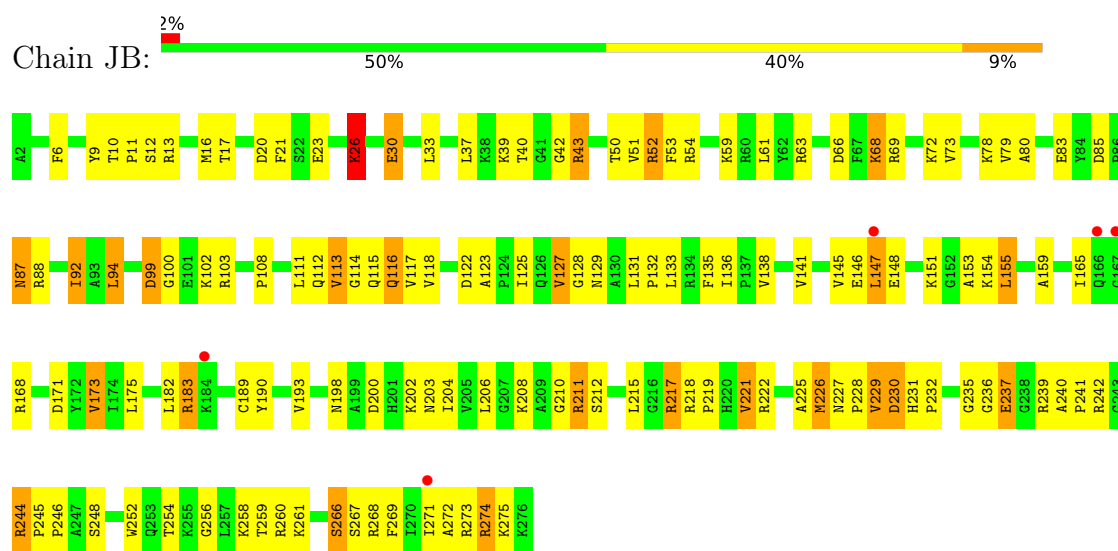


• Molecule 5: 50S ribosomal protein L2

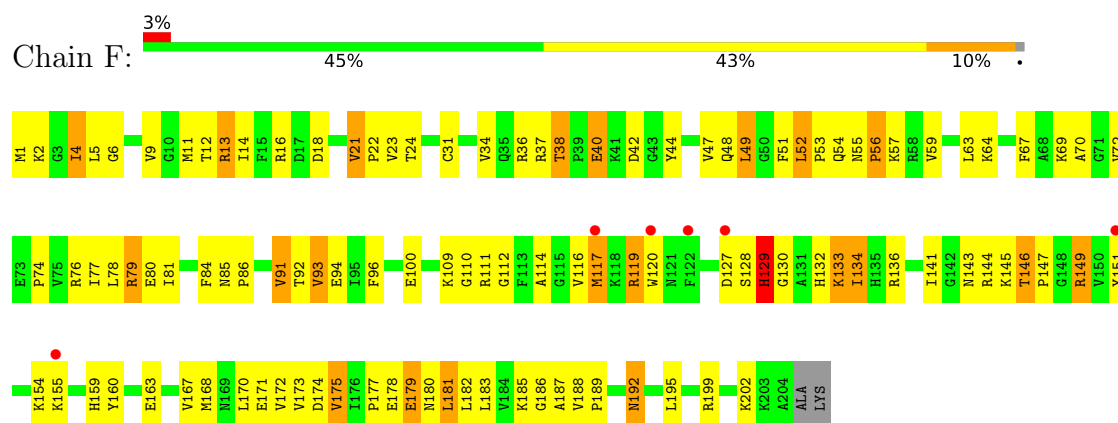




• Molecule 5: 50S ribosomal protein L2

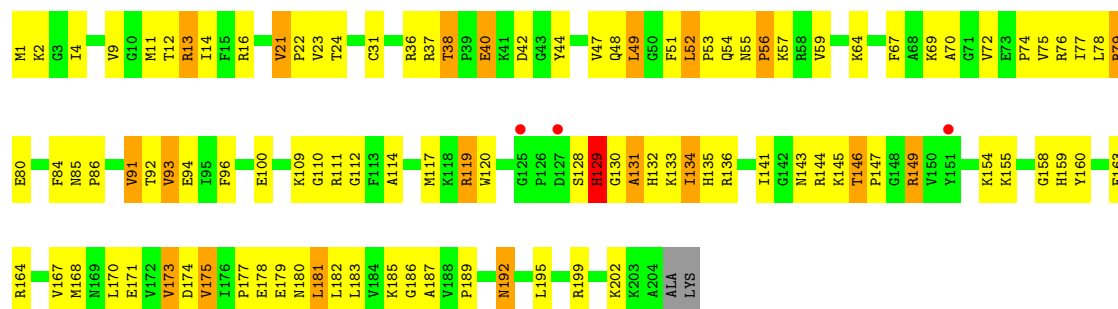


• Molecule 6: 50S ribosomal protein L3



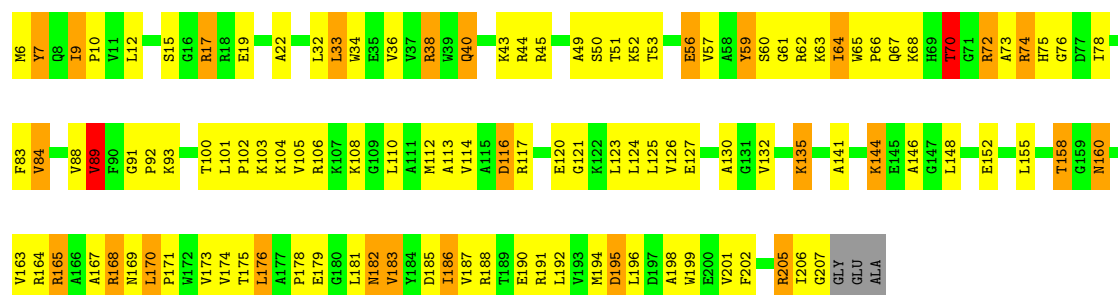
• Molecule 6: 50S ribosomal protein L3





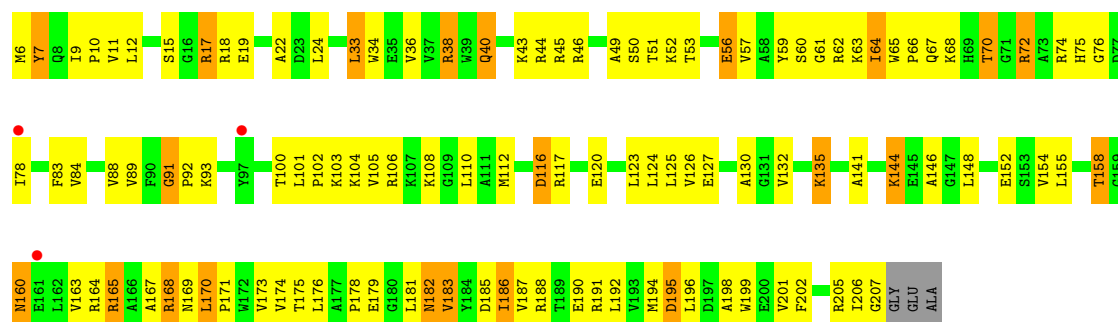
• Molecule 7: 50S ribosomal protein L4

Chain G: 42% 42% 13% ..



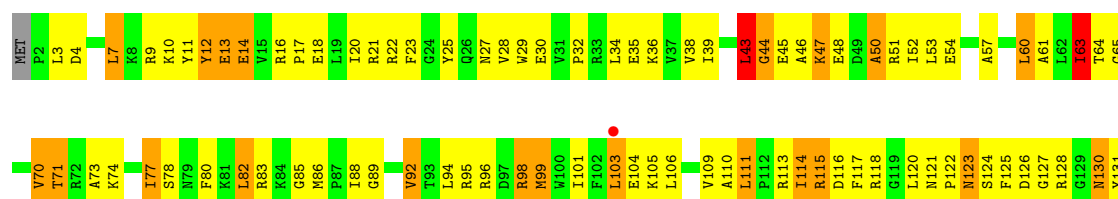
• Molecule 7: 50S ribosomal protein L4

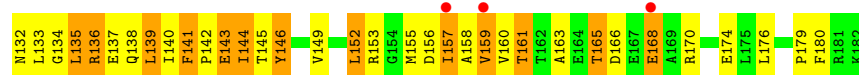
Chain LB: 42% 45% 11% .



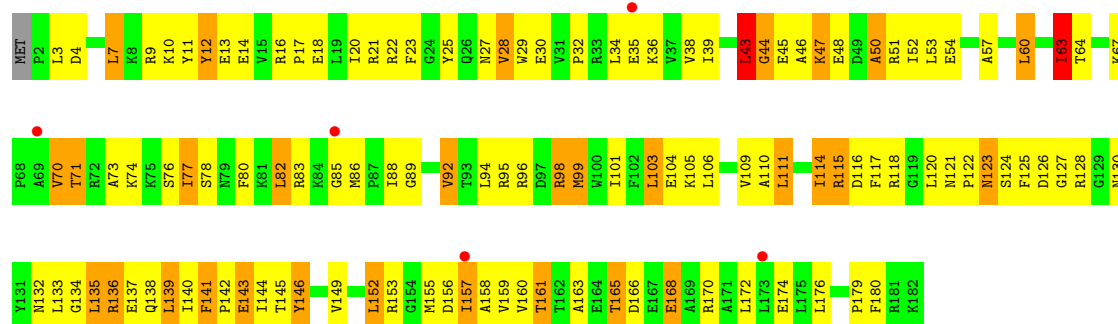
• Molecule 8: 50S ribosomal protein L5

Chain H: 32% 47% 19% ..

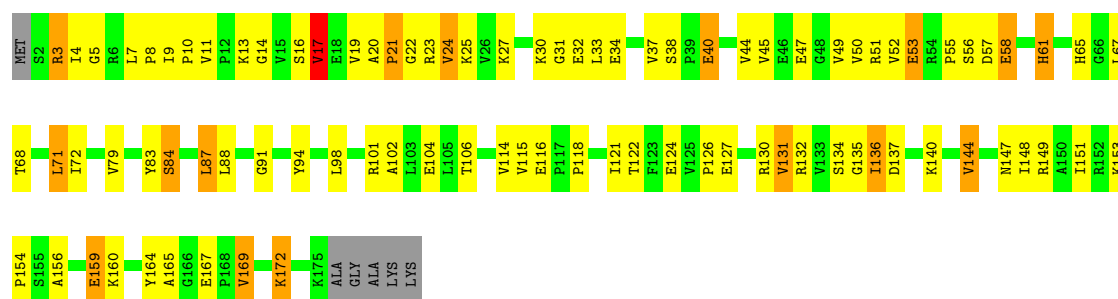




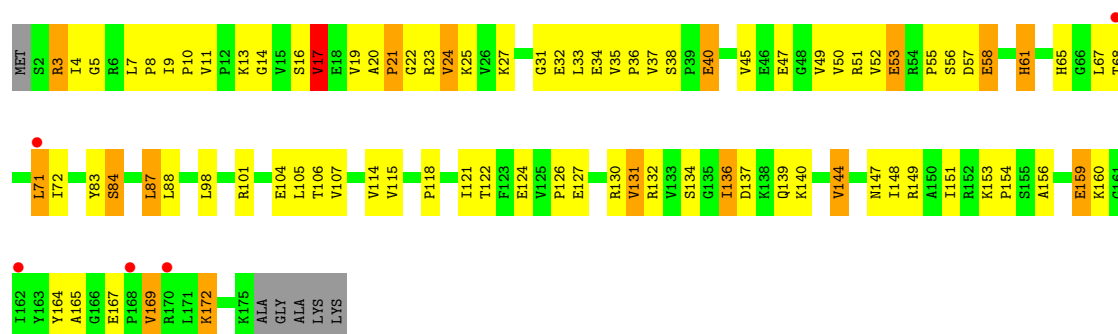
• Molecule 8: 50S ribosomal protein L5



• Molecule 9: 50S ribosomal protein L6

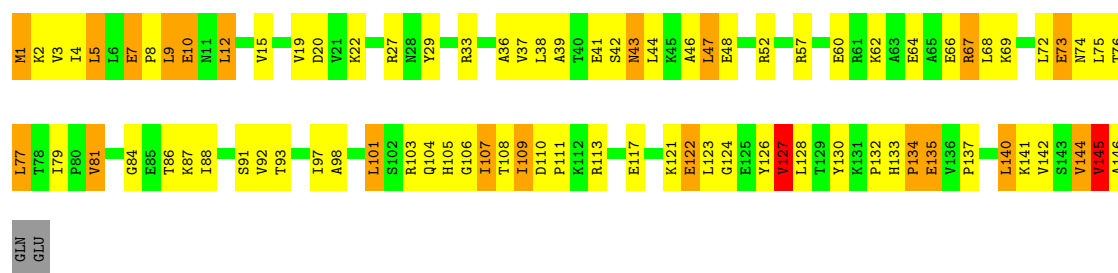


• Molecule 9: 50S ribosomal protein L6

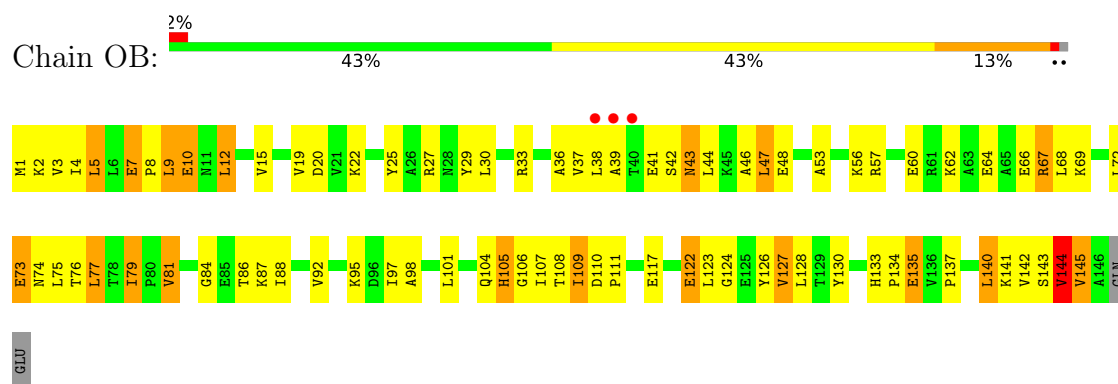


• Molecule 10: 50S ribosomal protein L9

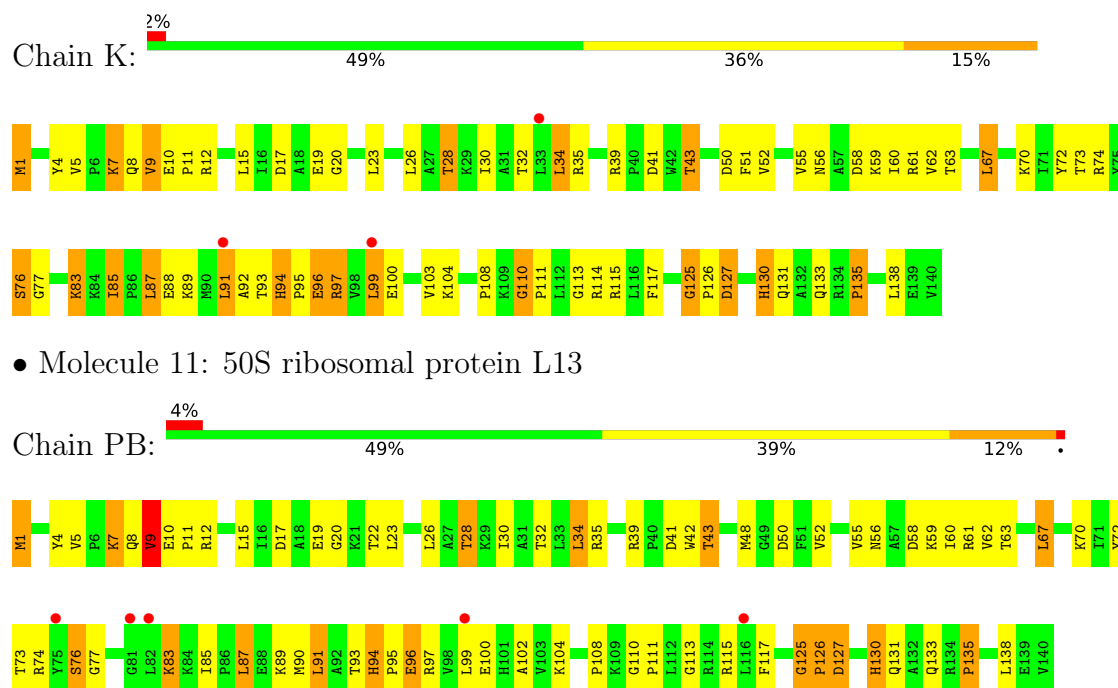




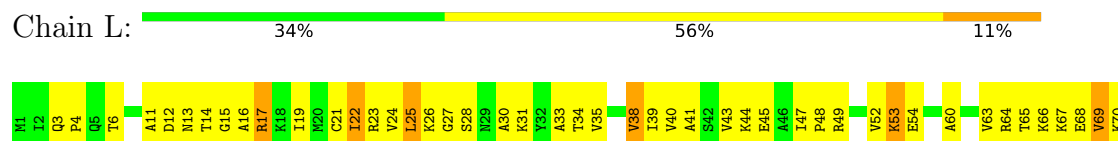
• Molecule 10: 50S ribosomal protein L9



• Molecule 11: 50S ribosomal protein L13

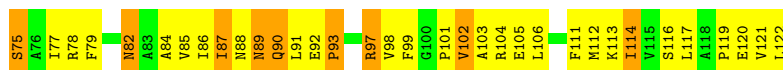
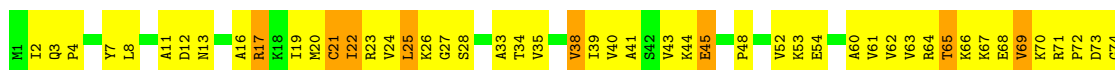


• Molecule 12: 50S ribosomal protein L14





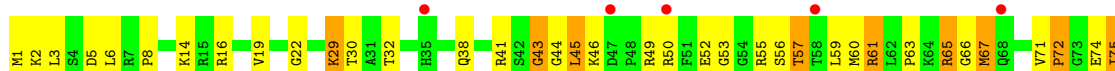
- Molecule 12: 50S ribosomal protein L14



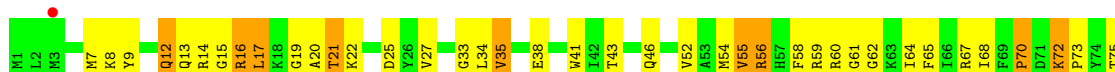
- Molecule 13: 50S ribosomal protein L15



- Molecule 13: 50S ribosomal protein L15



- Molecule 14: 50S ribosomal protein L16

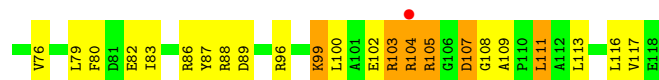
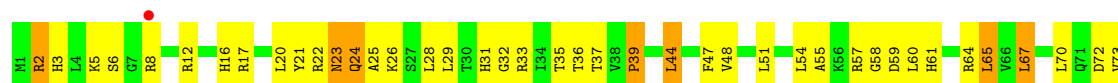


- Molecule 14: 50S ribosomal protein L16

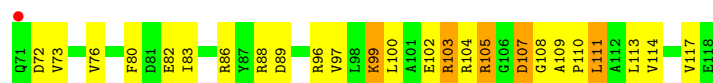
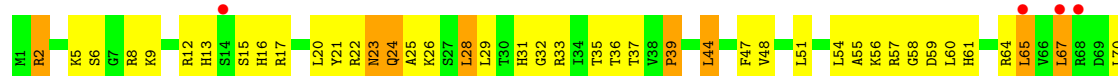
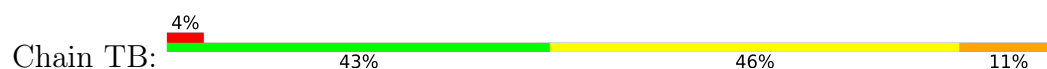




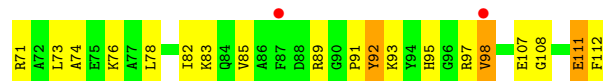
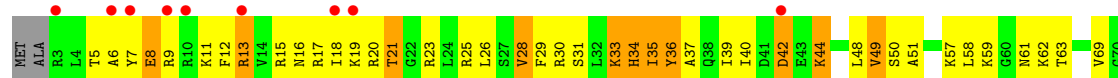
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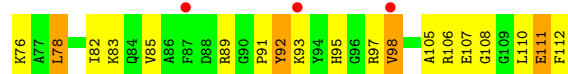
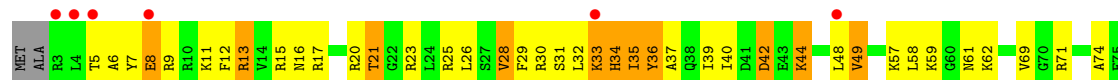
• Molecule 15: 50S ribosomal protein L17



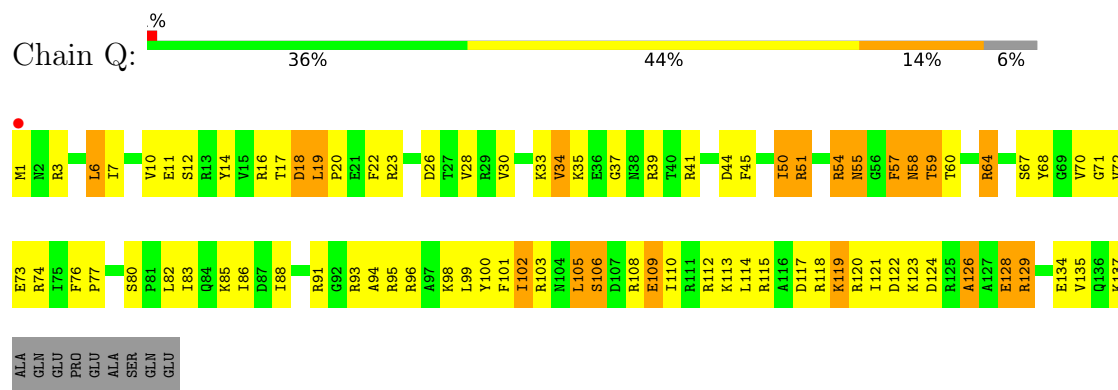
• Molecule 16: 50S ribosomal protein L18



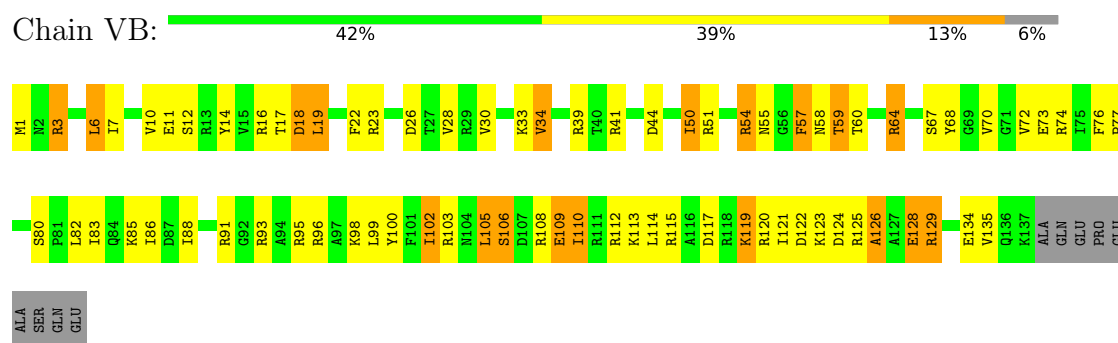
• Molecule 16: 50S ribosomal protein L18



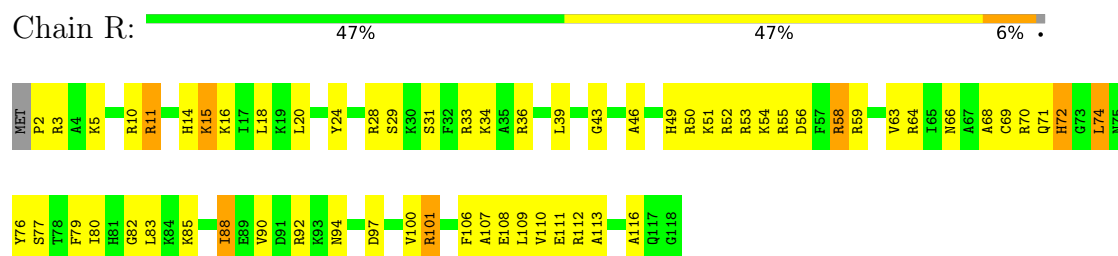
- Molecule 17: 50S ribosomal protein L19



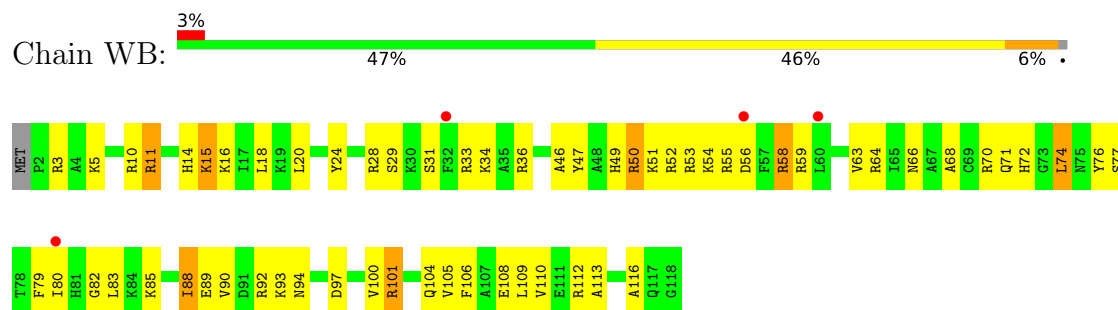
- Molecule 17: 50S ribosomal protein L19



- Molecule 18: 50S ribosomal protein L20

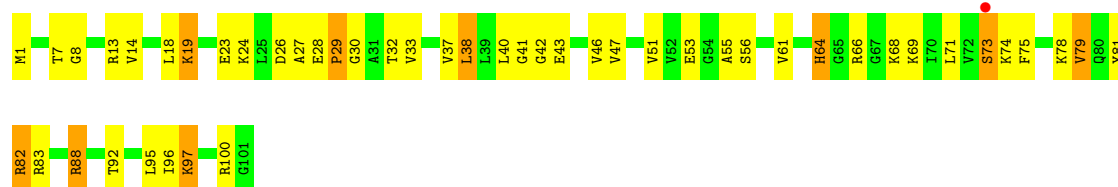


- Molecule 18: 50S ribosomal protein L20

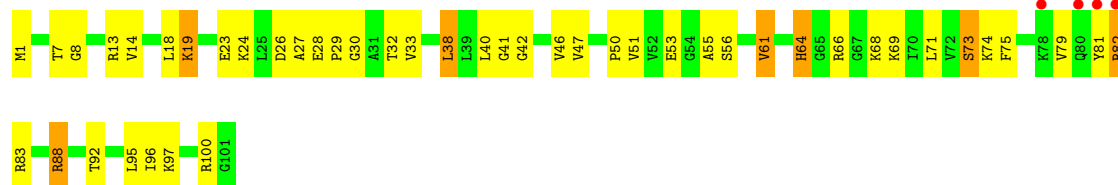


- Molecule 19: 50S ribosomal protein L21

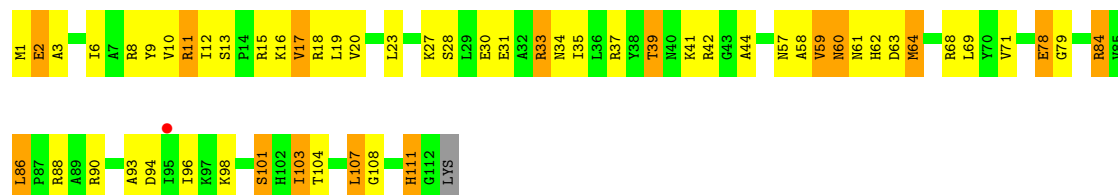




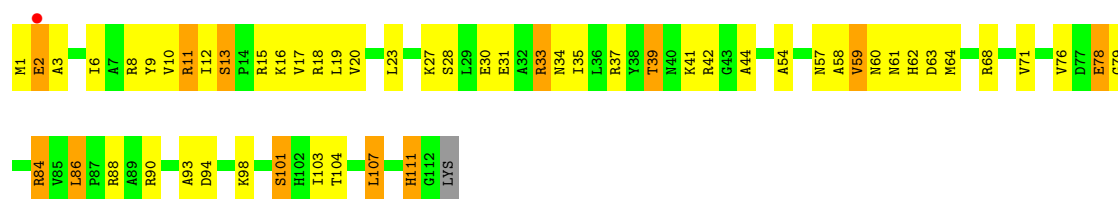
- Molecule 19: 50S ribosomal protein L21



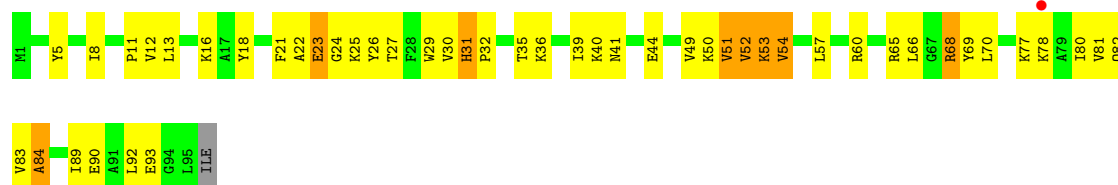
- Molecule 20: 50S ribosomal protein L22



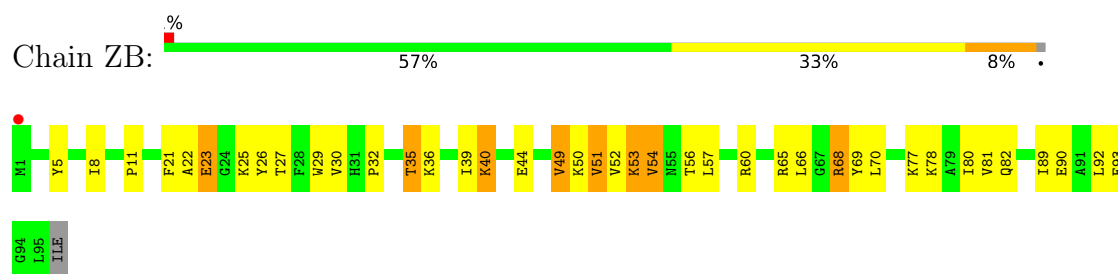
- Molecule 20: 50S ribosomal protein L22



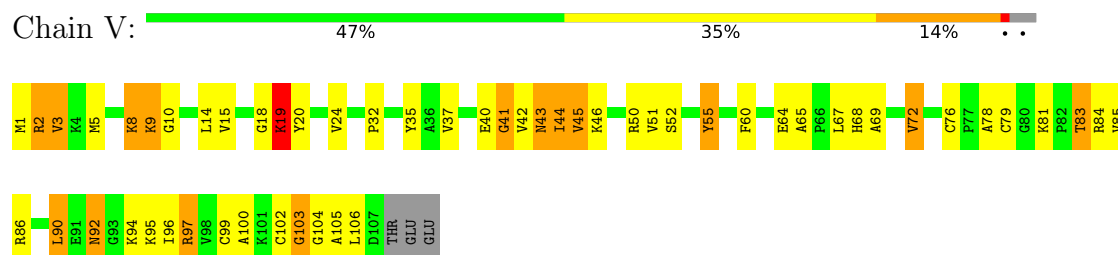
- Molecule 21: 50S ribosomal protein L23



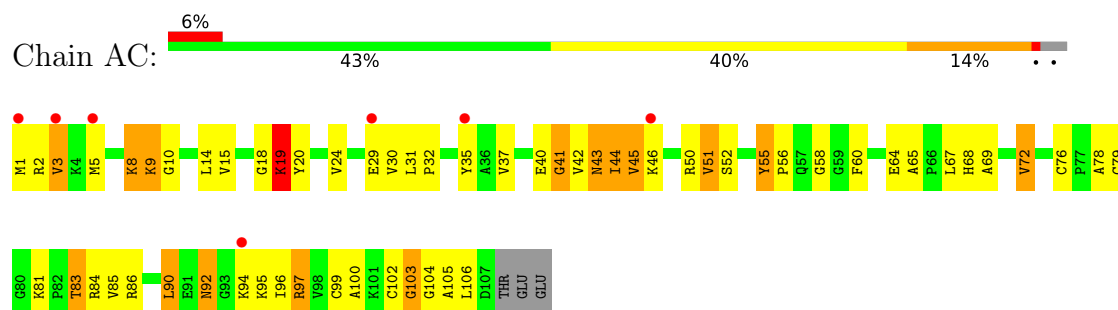
- Molecule 21: 50S ribosomal protein L23



- Molecule 22: 50S ribosomal protein L24



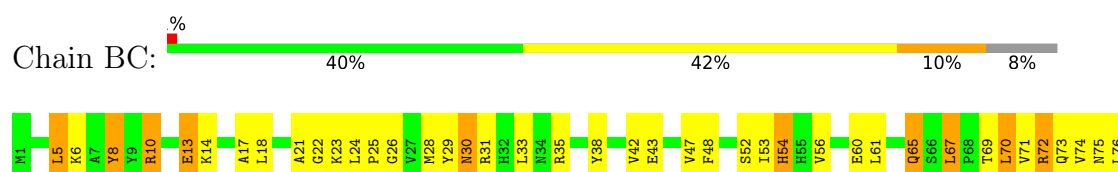
- Molecule 22: 50S ribosomal protein L24

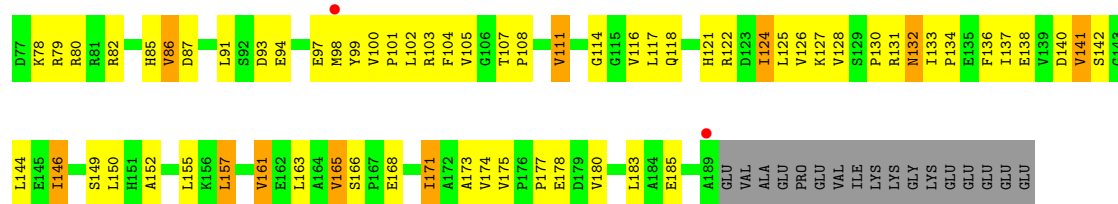


- Molecule 23: 50S ribosomal protein L25

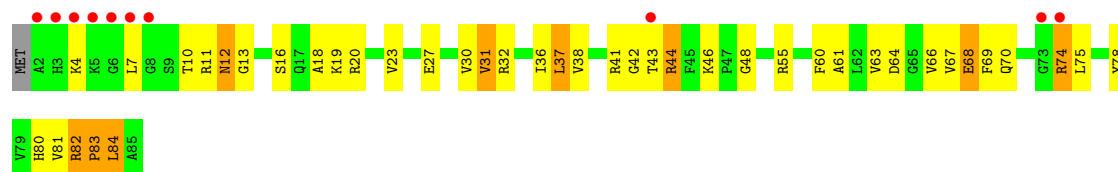


- Molecule 23: 50S ribosomal protein L25

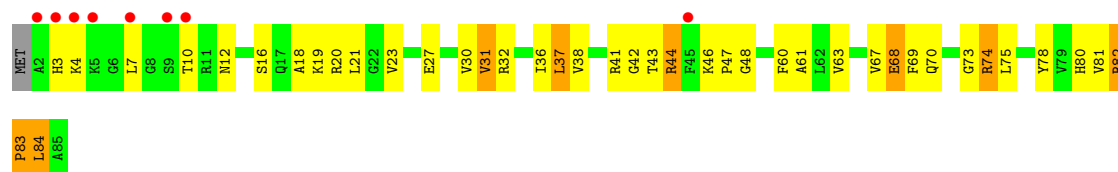




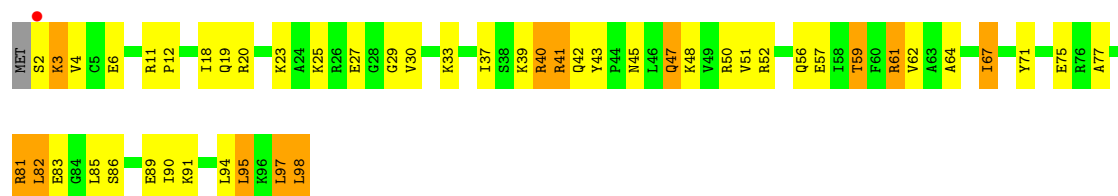
• Molecule 24: 50S ribosomal protein L27



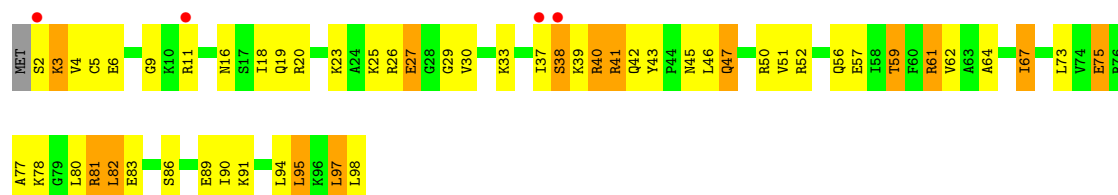
• Molecule 24: 50S ribosomal protein L27



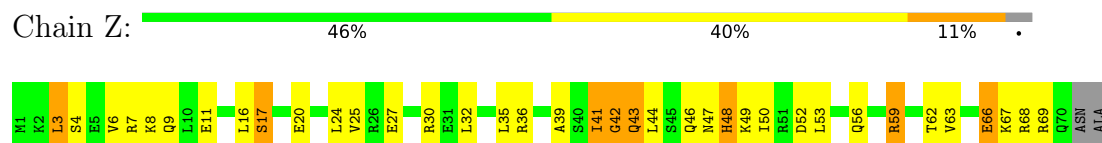
• Molecule 25: 50S ribosomal protein L28



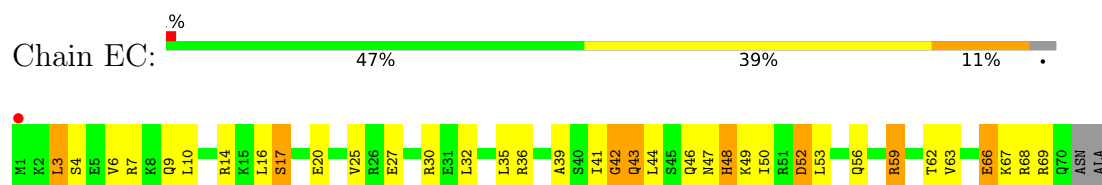
• Molecule 25: 50S ribosomal protein L28



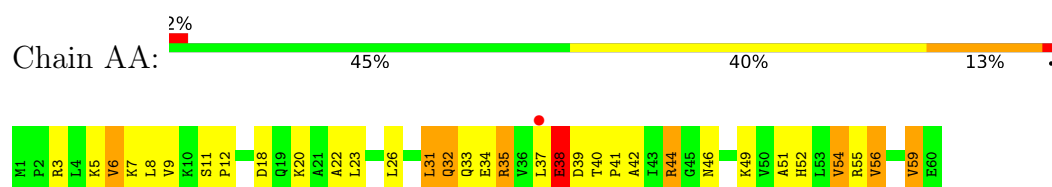
• Molecule 26: 50S ribosomal protein L29



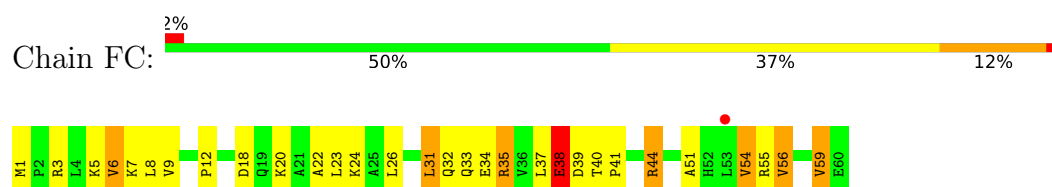
- Molecule 26: 50S ribosomal protein L29



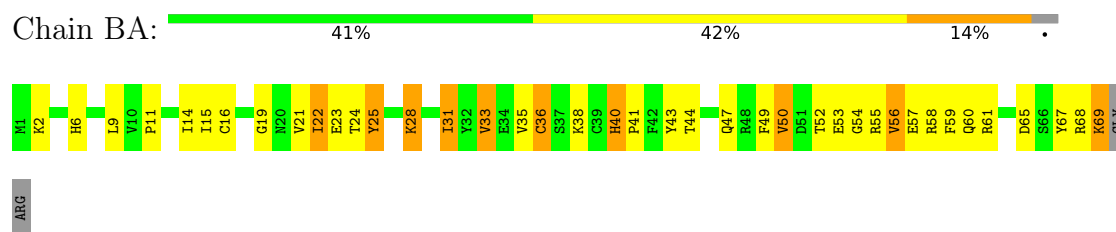
- Molecule 27: 50S ribosomal protein L30



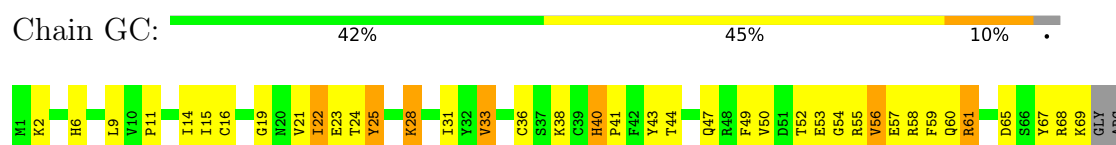
- Molecule 27: 50S ribosomal protein L30



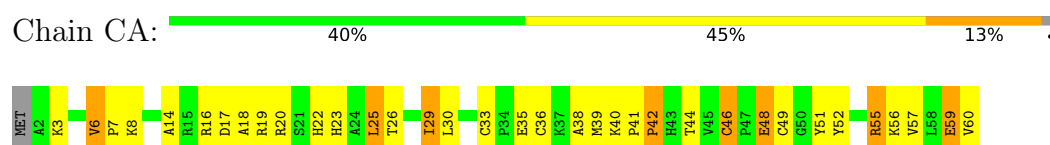
- Molecule 28: 50S ribosomal protein L31



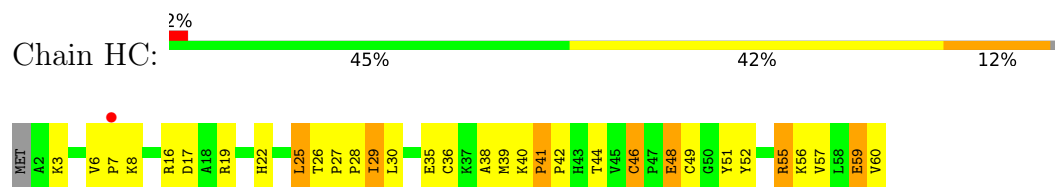
- Molecule 28: 50S ribosomal protein L31



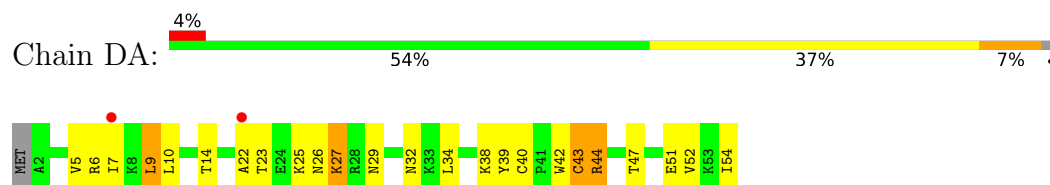
- Molecule 29: 50S ribosomal protein L32



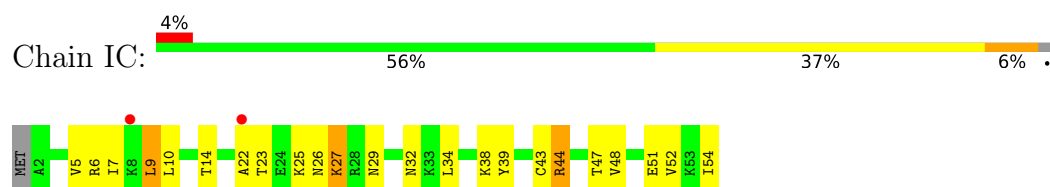
- Molecule 29: 50S ribosomal protein L32



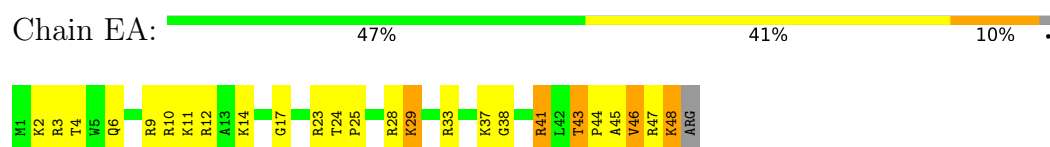
- Molecule 30: 50S ribosomal protein L33



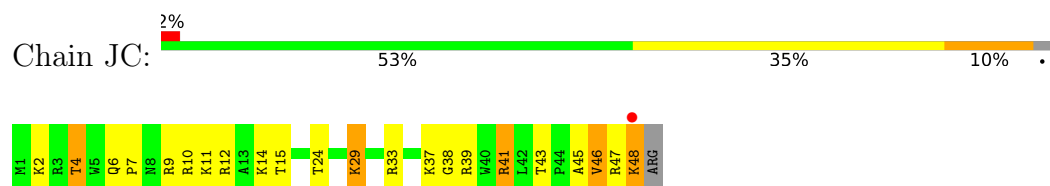
- Molecule 30: 50S ribosomal protein L33



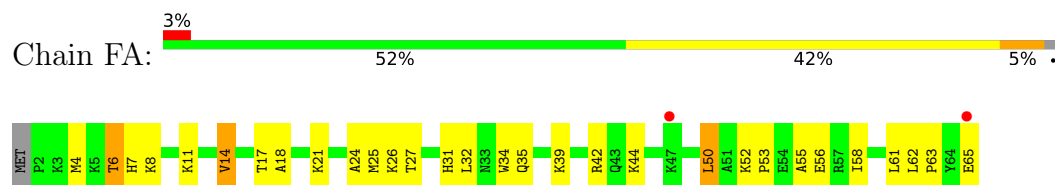
- Molecule 31: 50S ribosomal protein L34



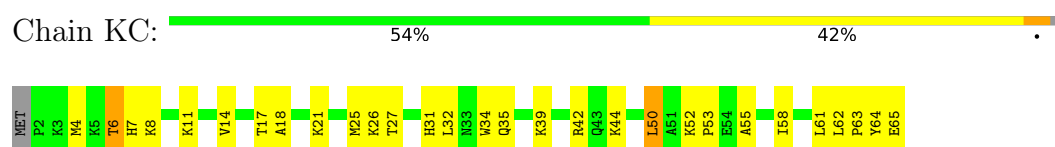
- Molecule 31: 50S ribosomal protein L34



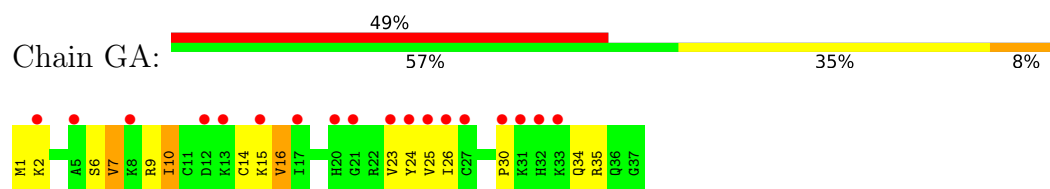
- Molecule 32: 50S ribosomal protein L35



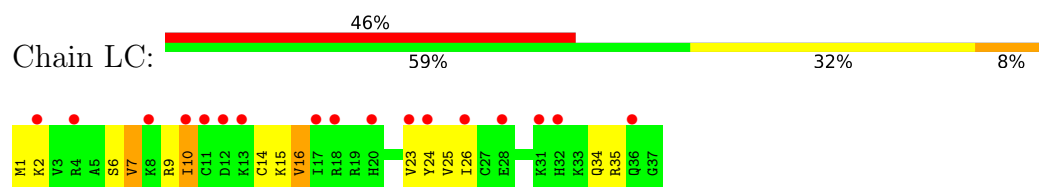
- Molecule 32: 50S ribosomal protein L35



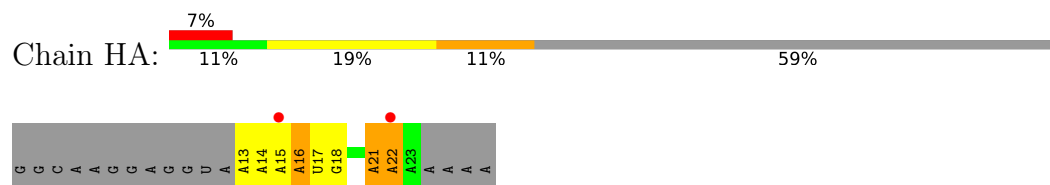
- Molecule 33: 50S ribosomal protein L36



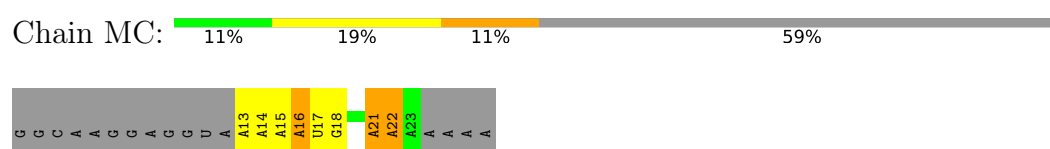
- Molecule 33: 50S ribosomal protein L36



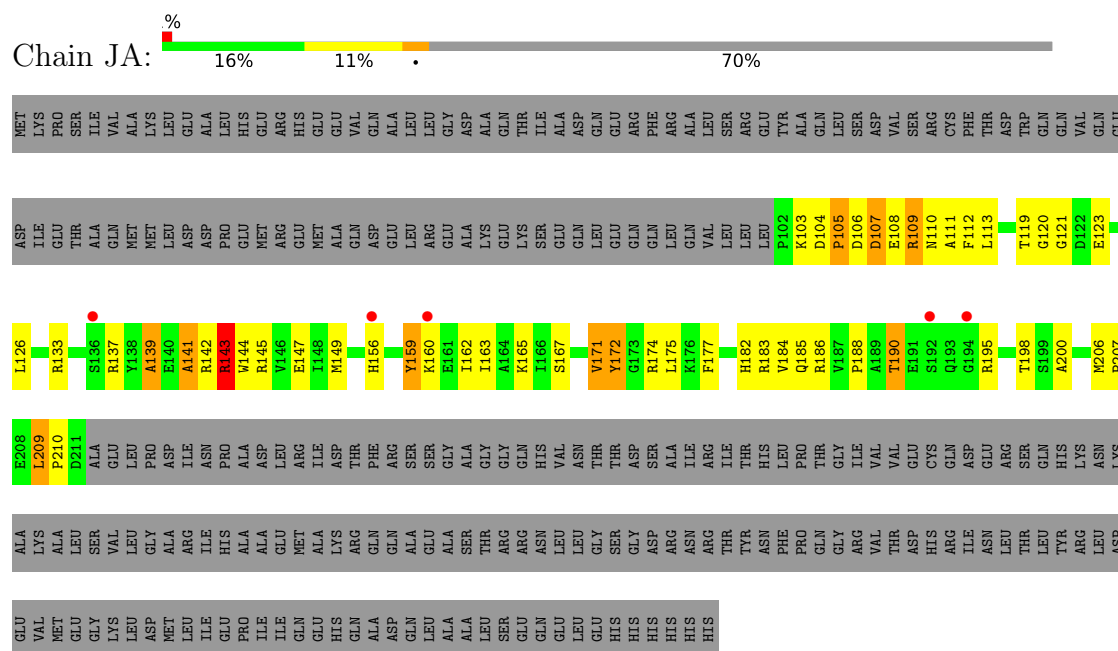
- Molecule 34: mRNA



- Molecule 34: mRNA



- Molecule 35: Peptide chain release factor 1



- Molecule 35: Peptide chain release factor 1

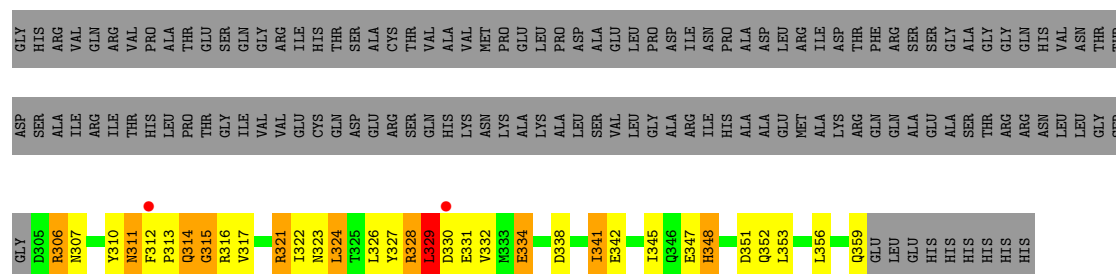
[illegible]

Chain OC:

GLU	ALA	E208	E123	ASP	MET
VAL	LYS	L209	L126	ILE	LYS
MET	ALA	P210	L126	GLU	PRO
GLU	LEU	D211	L133	THR	THR
GLY	SER	ALA	R137	ALA	ILE
LYS	VAL	GLU	R137	GLN	VAL
LEU	LEU	LEU	Y138	MET	ALA
ASP	GLY	PRO	Y138	MET	LYS
MET	ALA	ASP	A139	ASP	LYS
LEU	ARG	ILE	E140	LEU	GLU
ILE	ILE	ASN	A141	ASP	ALA
GLU	HIS	PRO	R142	PRO	LEU
PRO	ALA	ALA	R143	GLU	HIS
ILE	ALA	ASP	W144	MET	GLU
ILE	GLU	LEU	R145	ARG	GLU
GLN	MET	ARG	V146	GLU	HIS
GLU	ALA	ILE	E147	MET	GLU
HIS	LYS	ASP	T148	ALA	GLU
GLN	ARG	THR	M149	GLN	VAL
ALA	GLN	PHE	H156	ASP	GLN
ASP	GLN	ARG	H156	GLU	ALA
GLN	ALA	SER	Y159	ARG	LEU
LEU	GLU	SER	K160	GLU	GLY
ALA	ALA	GLY	E161	ALA	ASP
LEU	THR	GLY	I162	LYS	ALA
SER	ARG	GLY	I163	GLN	ALA
GLU	ARG	GLN	A164	LYS	THR
GLN	ASN	HIS	K165	SER	ILE
LEU	LEU	VAL	I166	GLU	ALA
GLU	LEU	ASN	S167	GLN	ASP
GLU	GLY	THR		LEU	GLN
HIS	SER	THR	V171	GLU	LEU
HIS	GLY	ASP	Y172	GLN	ARG
HIS	ASP	SER	G173	GLN	PHE
HIS	ARG	ALA	R174	LEU	ARG
HIS	ASN	ILE	L175	GLN	ALA
HIS	ARG	ARG	K176	VAL	LEU
HIS	THR	ILE	F177	SER	LEU
	TVR	THR		LEU	ARG
	ASN	HIS	H182	LEU	GLU
	PHE	LEU	R183	P182	TYR
	PRO	PRO	V184	K103	ALA
	GLN	THR	Q185	D104	GLN
	GLY	GLY	R186	P105	LEU
	VAL	ILE	V187	D106	SER
	VAL	VAL	P188	D107	ASP
	THR	VAL	A189	E108	VAL
	ASP	GLU	T190	R109	SER
	HIS	CYS	G194	M110	ARG
	ARG	GLN	R195	A111	CYS
	ILE	ASP	R196	F112	PHE
	ASN	GLU	I196	L113	THR
	LEU	ARG	H197		ASP
	THR	SER	T198		TRP
	LEU	GLN	S199		GLN
	TVR	HIS	A200	T119	VAL
	ARG	LYS		G120	GLN
	LEU	ASN	M206	G121	GLU
	ASP	LYS	D207	E122	

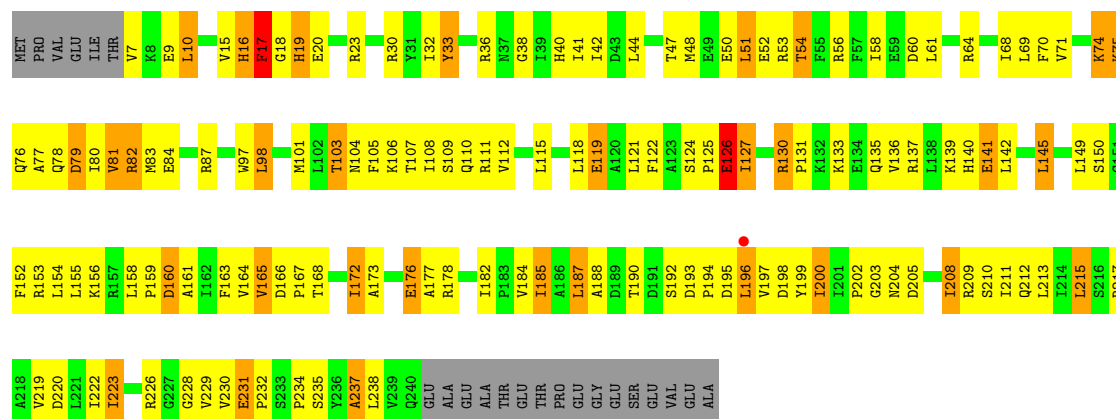
Chain PC: %

GLY	ASP	MET
ASP	ILE	LYS
GLU	GLU	PRO
ALA	THR	SER
LEU	ALA	ILE
PHE	GLN	VAL
ALA	MET	ALA
GLY	MET	LYS
ASP	LEU	LEU
LEU	ASP	GLU
PHE	ASP	ALA
ARG	PRO	LEU
MET	GLU	HIS
THR	MET	GLU
SER	ARG	ARG
ARG	GLU	HIS
THR	MET	GLU
ALA	ALA	GLU
GLU	GLN	VAL
ALA	ASP	GLN
ALA	GLU	ALA
ARG	LEU	LEU
ARG	ARG	LEU
THR	GLU	GLY
ARG	ALA	ASP
VAL	LYS	ALA
GLU	GLN	GLN
ILE	LYS	THR
MET	SER	ILE
THR	GLU	ALA
SER	GLN	ASP
ALA	LEU	GLN
GLY	VAL	LEU
THR	LEU	SER
LYS	LEU	ARG
GLU	LEU	GLU
ILE	PRO	TYR
ILE	LYS	ALA
ALA	ASP	GLN
LYS	PRO	LEU
ILE	ASP	SER
SER	ASP	ASP
GLY	GLU	VAL
ASP	ARG	SER
GLY	ASN	ARG
VAL	ALA	CYS
THR	PHE	THR
GLY	LEU	THR
ARG	GLU	ASP
LEU	VAL	TRP
LYS	ARG	GLN
PHE	ALA	GLN
GLU	GLY	VAL
SER	THR	GLN
Y	GLY	GLN



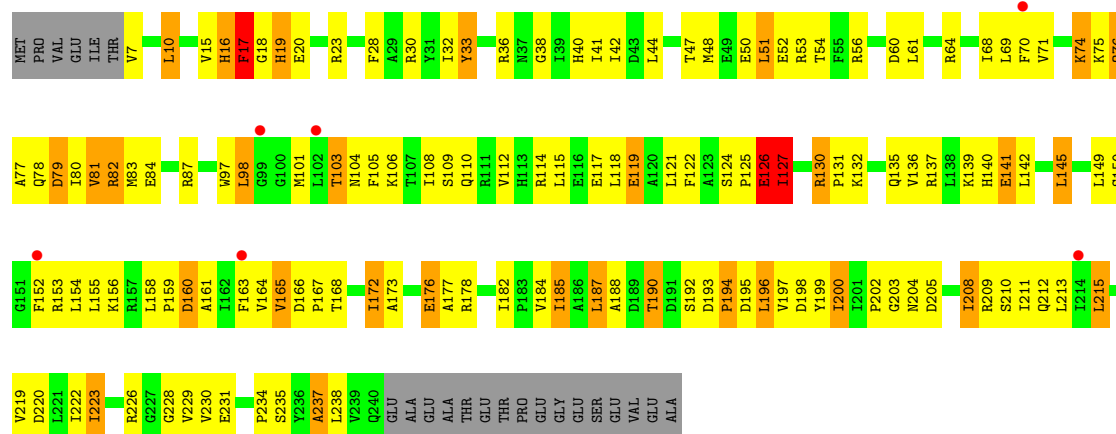
• Molecule 36: 30S ribosomal protein S2

Chain LA: 36% 43% 12% 9%



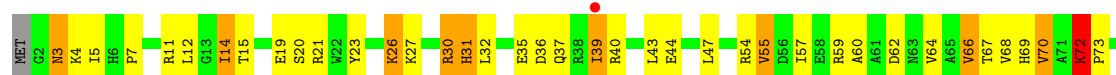
• Molecule 36: 30S ribosomal protein S2

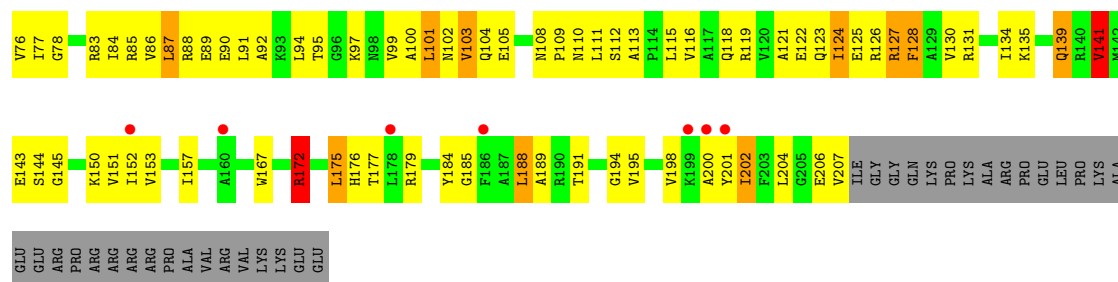
Chain QC: 2% 37% 42% 12% 9%



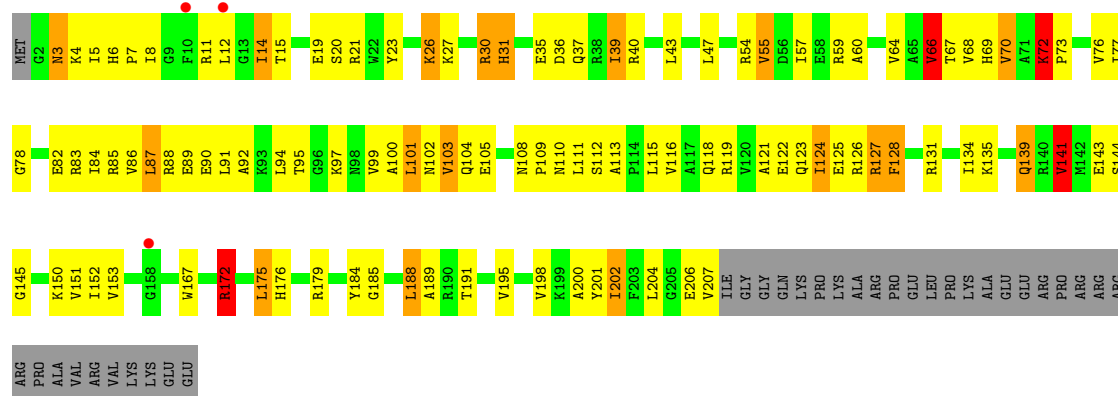
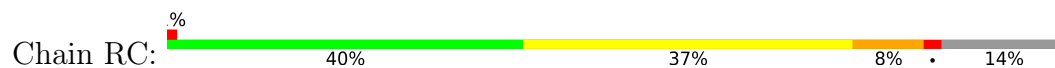
• Molecule 37: 30S ribosomal protein S3

Chain MA: 3% 38% 38% 8% 14%

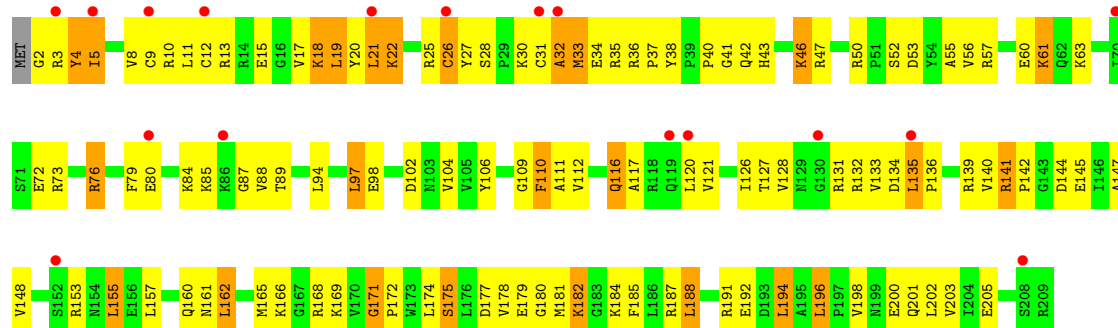
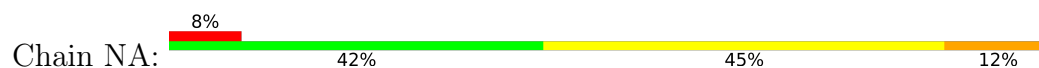




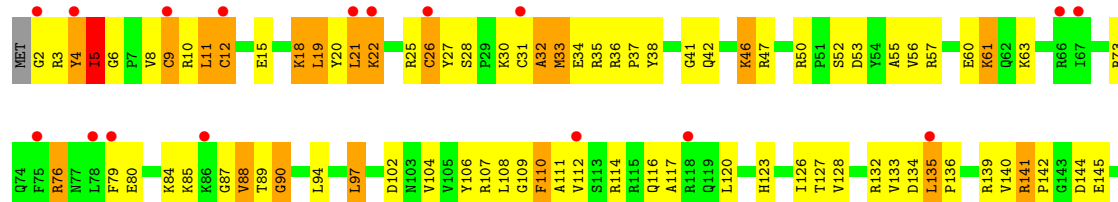
• Molecule 37: 30S ribosomal protein S3

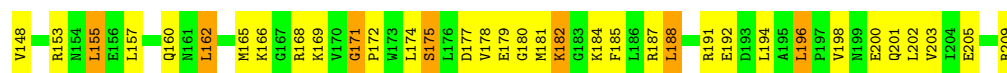


• Molecule 38: 50S ribosomal protein S4

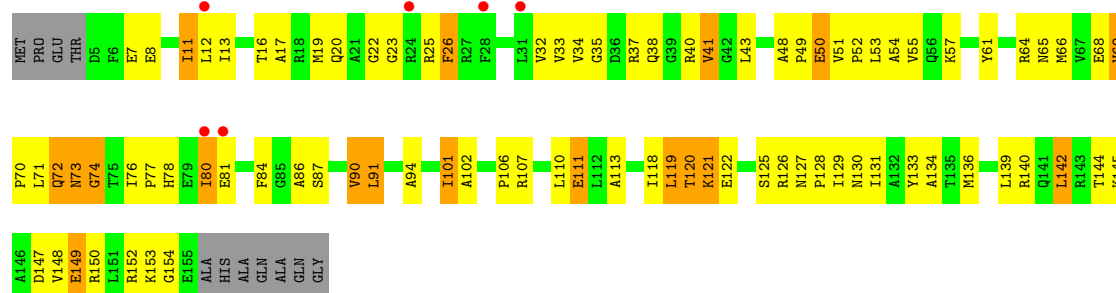


• Molecule 38: 50S ribosomal protein S4

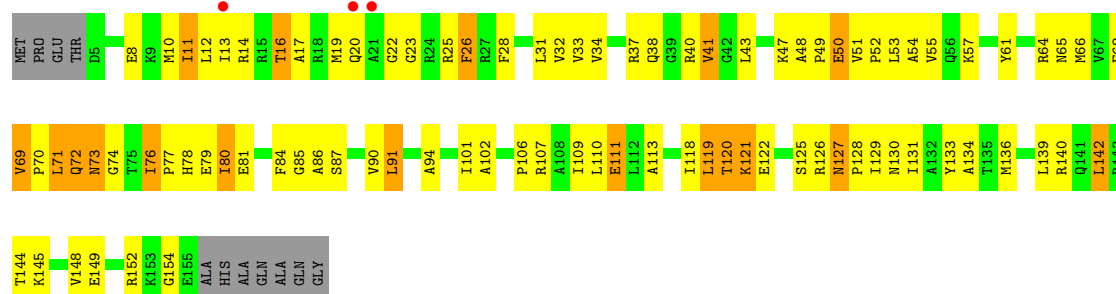




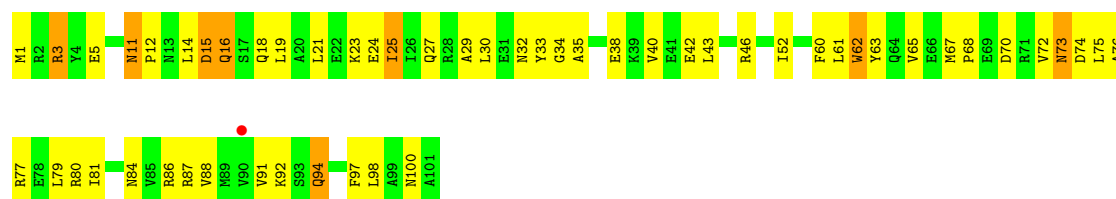
• Molecule 39: 30S ribosomal protein S5



• Molecule 39: 30S ribosomal protein S5



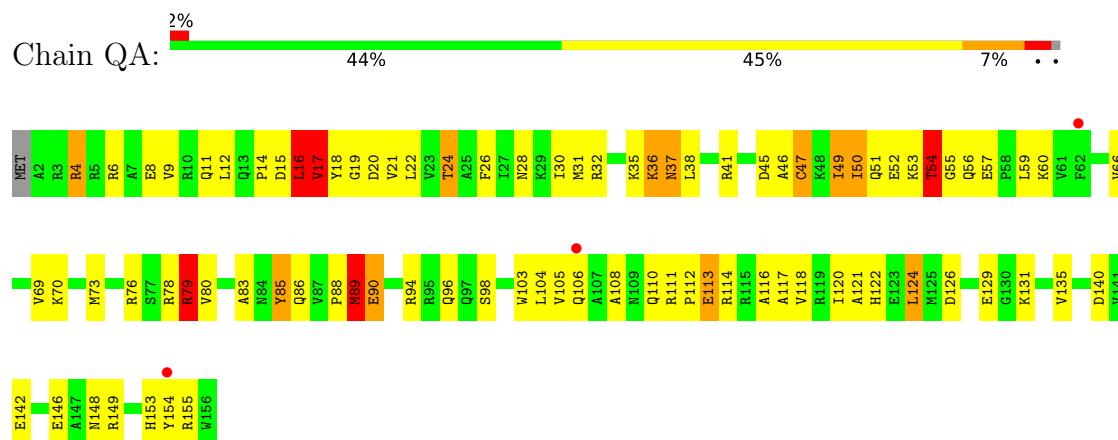
• Molecule 40: 30S ribosomal protein S6



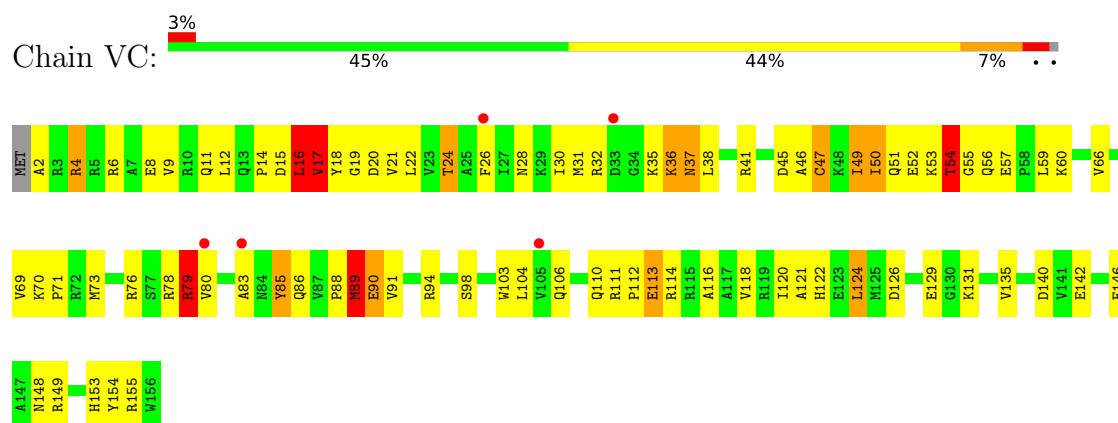
• Molecule 40: 30S ribosomal protein S6



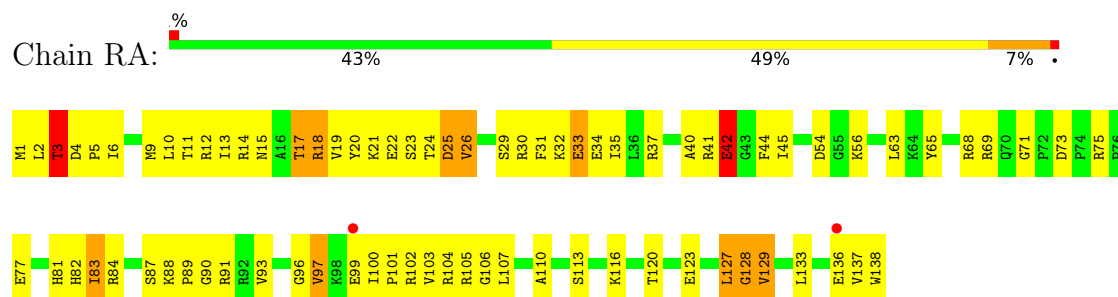
- Molecule 41: 30S ribosomal protein S7



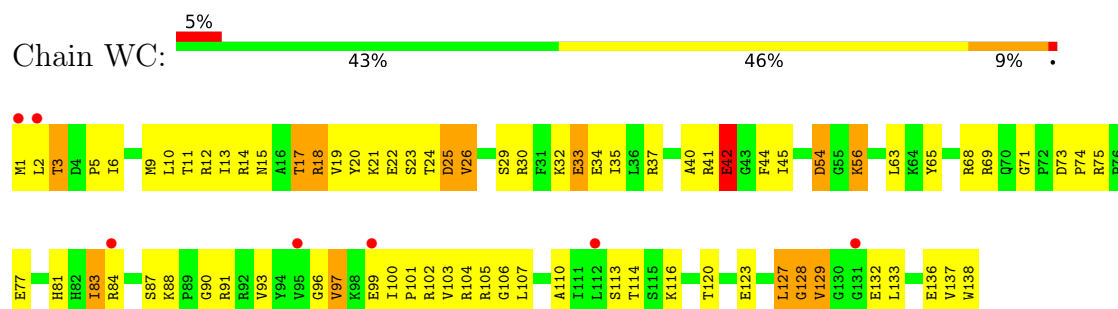
- Molecule 41: 30S ribosomal protein S7



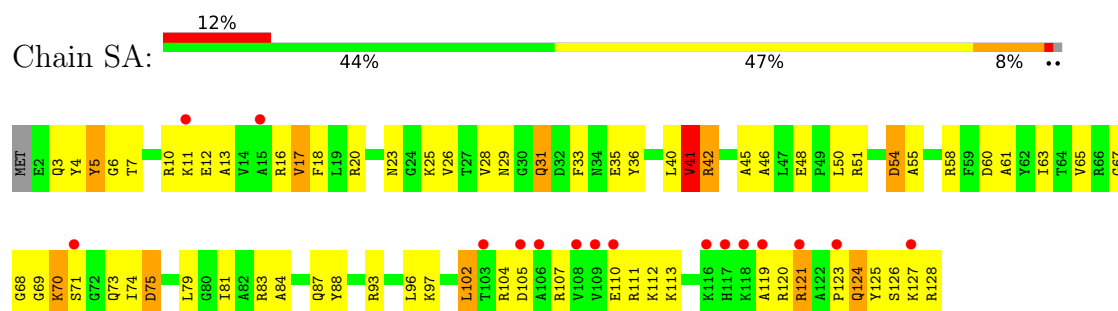
- Molecule 42: 30S ribosomal protein S8



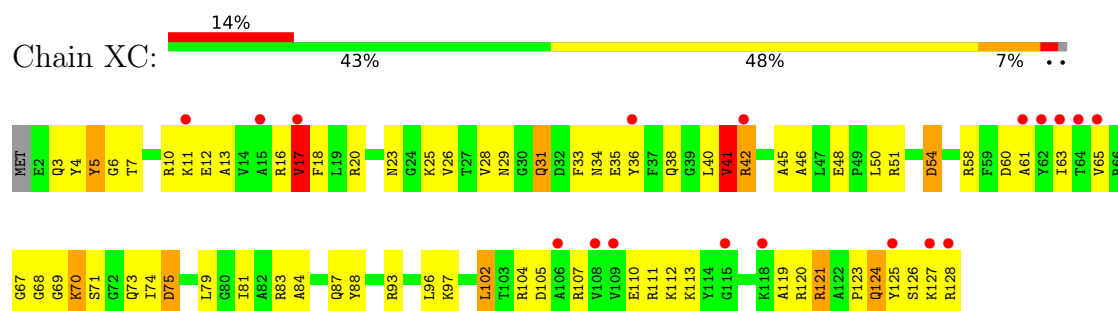
- Molecule 42: 30S ribosomal protein S8



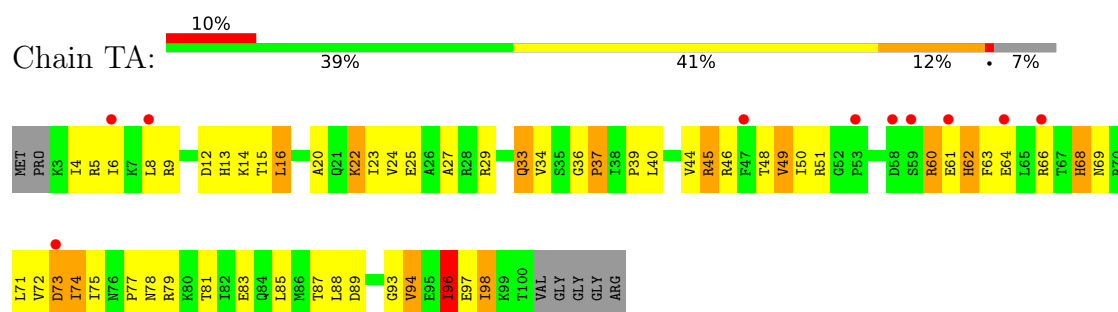
- Molecule 43: 30S ribosomal protein S9



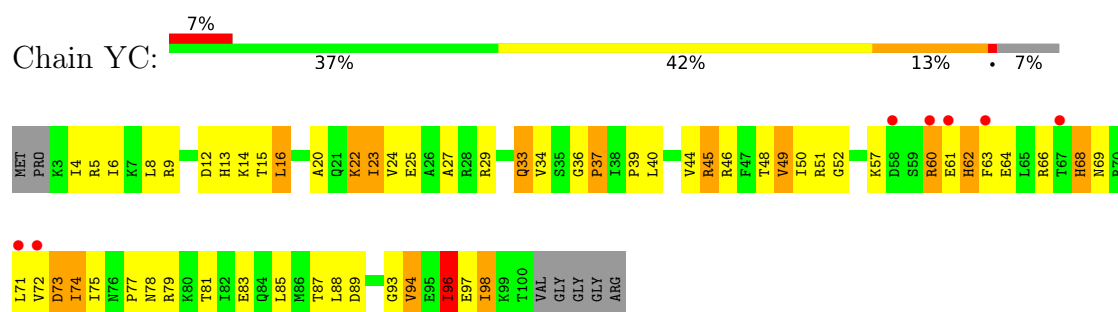
- Molecule 43: 30S ribosomal protein S9



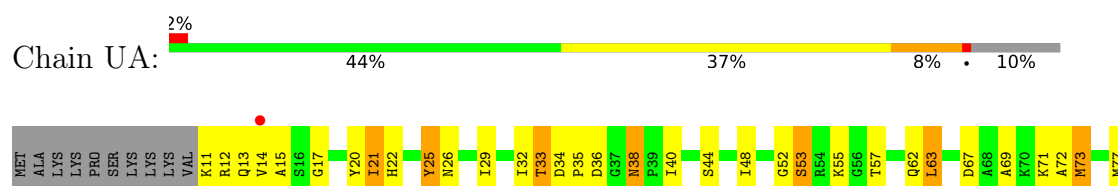
- Molecule 44: 30S ribosomal protein S10



- Molecule 44: 30S ribosomal protein S10

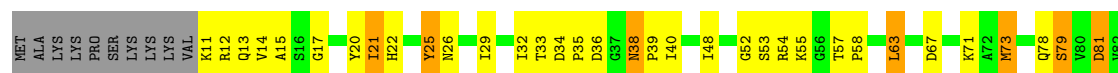
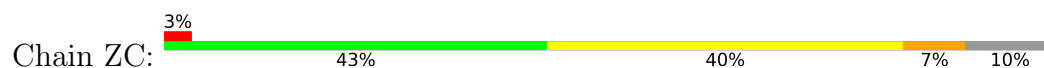


- Molecule 45: 30S ribosomal protein S11

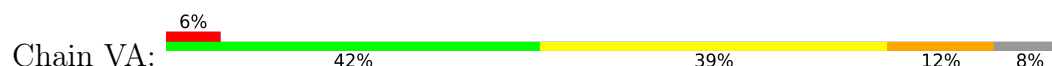




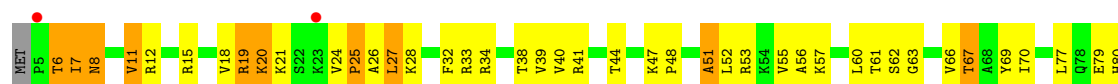
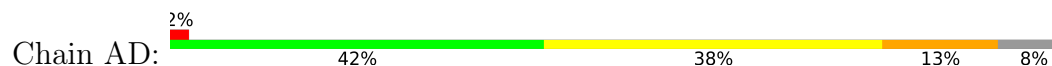
- Molecule 45: 30S ribosomal protein S11



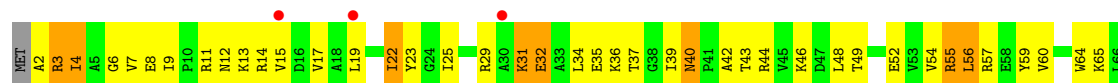
- Molecule 46: 30S ribosomal protein S12



- Molecule 46: 30S ribosomal protein S12

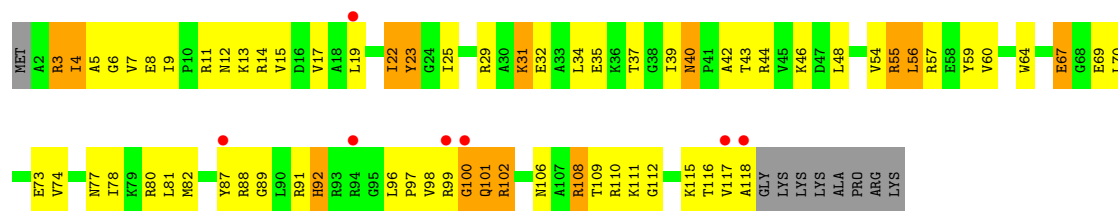


- Molecule 47: 30S ribosomal protein S13



- Molecule 47: 30S ribosomal protein S13

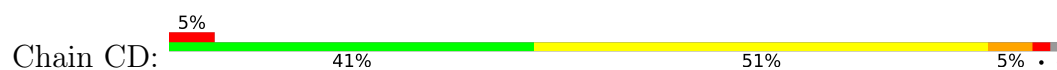




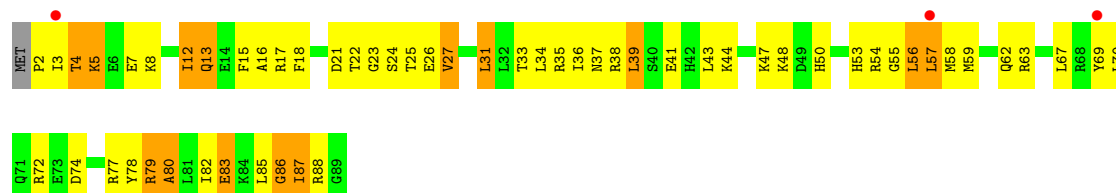
- Molecule 48: 30S ribosomal protein S14 type Z



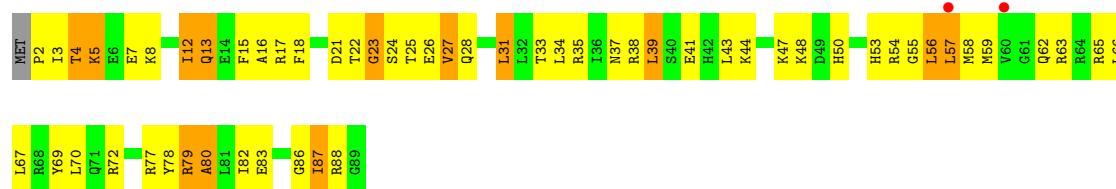
- Molecule 48: 30S ribosomal protein S14 type Z



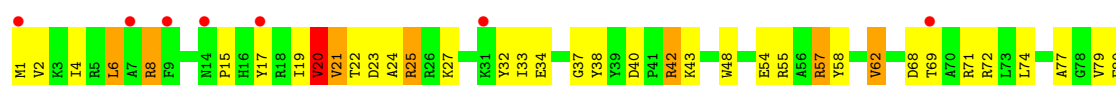
- Molecule 49: 30S ribosomal protein S15



- Molecule 49: 30S ribosomal protein S15



- Molecule 50: 30S ribosomal protein S16

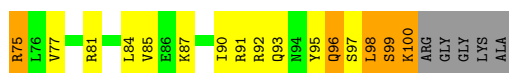
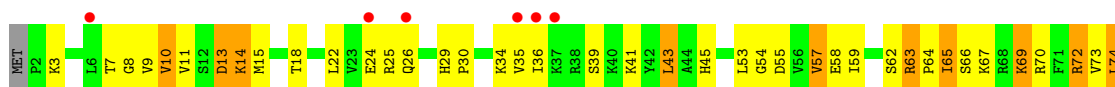
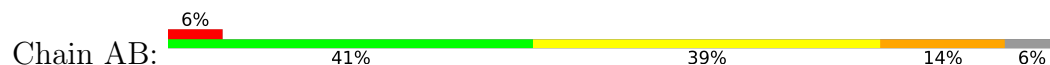




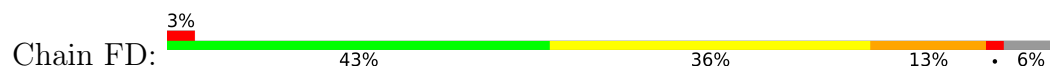
• Molecule 50: 30S ribosomal protein S16



• Molecule 51: 30S ribosomal protein S17



• Molecule 51: 30S ribosomal protein S17

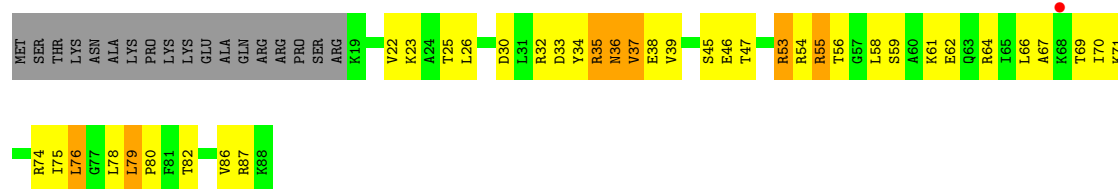


• Molecule 52: 30S ribosomal protein S18

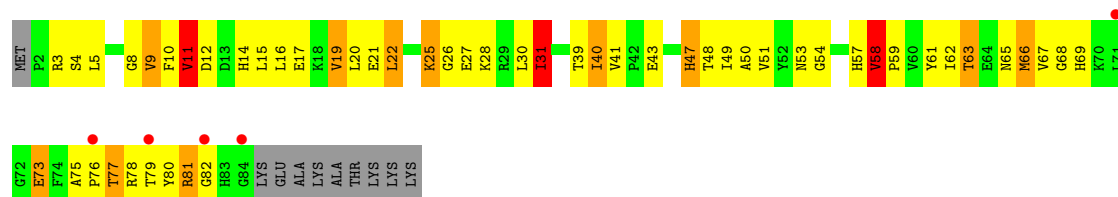


• Molecule 52: 30S ribosomal protein S18

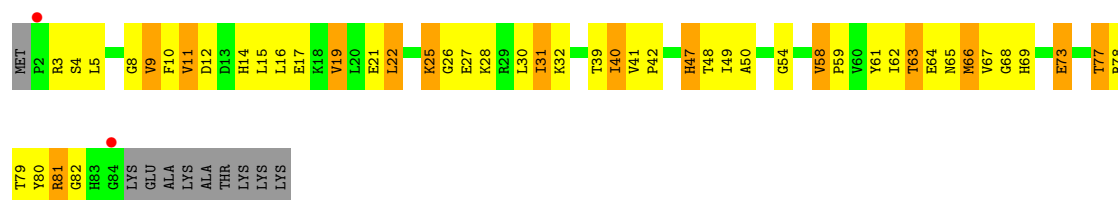




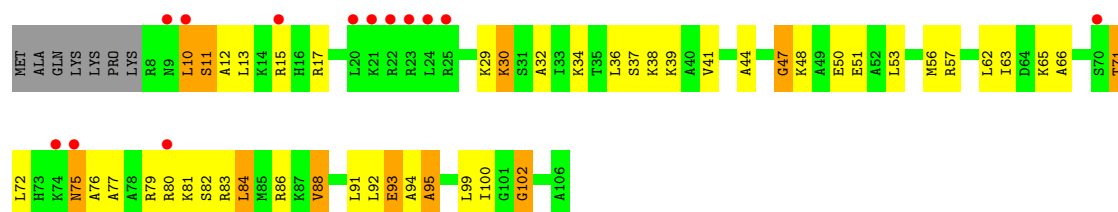
- Molecule 53: 30S ribosomal protein S19



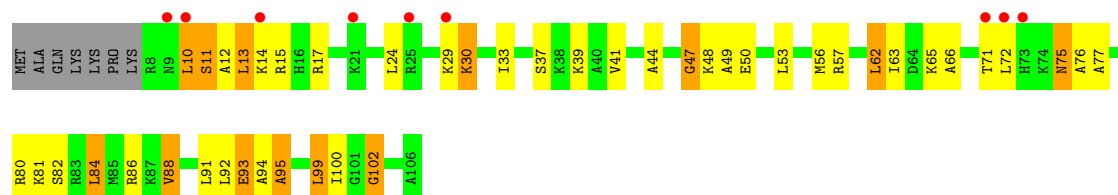
- Molecule 53: 30S ribosomal protein S19



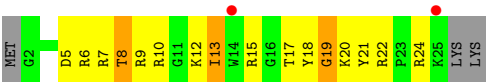
- Molecule 54: 30S ribosomal protein S20



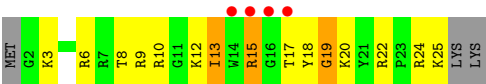
- Molecule 54: 30S ribosomal protein S20



- Molecule 55: 30S ribosomal protein Thx



• Molecule 55: 30S ribosomal protein Thx



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.86Å 450.69Å 615.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.40 50.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.40) 100.0 (50.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 3.41Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	(Not available) , (Not available) 0.243 , 0.281	Depositor DCC
R_{free} test set	7928 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	120.8	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	298186	wwPDB-VP
Average B, all atoms (Å ²)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: ZN, 4OC, 0TD, 2MU, UR3, 2MG, 4SU, MG, OMG, MA6, M2G, BLS, 5MU, 2MA, PSU, 5MC, 7MG

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	0.33	1/35961 (0.0%)	0.47	0/56125
1	FB	0.33	0/35961	0.47	0/56125
2	B	0.50	0/69214	0.61	3/108048 (0.0%)
2	GB	0.45	0/69214	0.58	1/108048 (0.0%)
3	C	0.31	0/2881	0.47	0/4494
3	HB	0.28	0/2881	0.45	0/4494
4	D	0.27	1/1744 (0.1%)	0.37	0/2719
4	IA	0.35	1/1744 (0.1%)	0.44	0/2719
4	IB	0.25	1/1744 (0.1%)	0.36	0/2719
4	NC	0.30	0/1744	0.42	0/2719
5	E	0.96	3/2195 (0.1%)	1.16	9/2955 (0.3%)
5	JB	0.76	0/2195	1.10	6/2955 (0.2%)
6	F	0.68	0/1596	1.04	8/2153 (0.4%)
6	KB	0.71	0/1596	1.04	5/2153 (0.2%)
7	G	0.78	2/1621 (0.1%)	1.09	11/2194 (0.5%)
7	LB	0.66	0/1621	1.04	9/2194 (0.4%)
8	H	0.47	0/1496	0.93	4/2013 (0.2%)
8	MB	0.45	0/1496	0.92	4/2013 (0.2%)
9	I	0.55	0/1356	0.94	7/1834 (0.4%)
9	NB	0.45	0/1356	0.91	6/1834 (0.3%)
10	J	0.58	0/1152	0.94	0/1559
10	OB	0.56	0/1152	0.95	4/1559 (0.3%)
11	K	0.58	0/1148	1.05	7/1547 (0.5%)
11	PB	0.54	0/1148	1.03	8/1547 (0.5%)
12	L	0.71	0/942	1.01	1/1268 (0.1%)
12	QB	0.77	0/942	1.03	1/1268 (0.1%)
13	M	0.68	0/1162	1.01	1/1544 (0.1%)
13	RB	0.60	0/1162	0.98	3/1544 (0.2%)
14	N	0.65	0/1142	0.97	5/1525 (0.3%)
14	SB	0.60	0/1142	0.93	2/1525 (0.1%)
15	O	0.67	0/982	0.96	2/1312 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	TB	0.71	0/982	0.97	1/1312 (0.1%)
16	P	0.53	0/887	0.86	0/1180
16	UB	0.46	0/887	0.85	0/1180
17	Q	0.59	0/1157	0.91	0/1544
17	VB	0.66	0/1157	0.93	0/1544
18	R	0.70	0/982	0.90	0/1306
18	WB	0.62	0/982	0.89	1/1306 (0.1%)
19	S	0.61	0/790	0.92	1/1057 (0.1%)
19	XB	0.51	0/790	0.88	0/1057
20	T	0.82	0/901	1.00	1/1209 (0.1%)
20	YB	0.78	0/901	0.99	3/1209 (0.2%)
21	U	0.84	0/764	1.02	2/1025 (0.2%)
21	ZB	0.71	0/764	0.92	0/1025
22	AC	0.61	0/827	0.94	1/1103 (0.1%)
22	V	0.70	0/827	0.95	0/1103
23	BC	0.51	0/1527	0.89	3/2073 (0.1%)
23	W	0.55	0/1527	0.90	3/2073 (0.1%)
24	CC	0.61	0/671	1.00	3/892 (0.3%)
24	X	0.67	0/671	1.04	3/892 (0.3%)
25	DC	0.69	0/768	1.02	3/1021 (0.3%)
25	Y	0.74	0/768	1.02	3/1021 (0.3%)
26	EC	0.59	0/594	0.93	0/785
26	Z	0.74	0/594	0.98	0/785
27	AA	0.61	0/482	0.98	2/646 (0.3%)
27	FC	0.56	0/482	0.94	0/646
28	BA	0.51	0/565	0.94	2/761 (0.3%)
28	GC	0.48	0/565	0.93	2/761 (0.3%)
29	CA	0.70	0/474	1.05	2/640 (0.3%)
29	HC	0.70	0/474	1.05	4/640 (0.6%)
30	DA	0.45	0/460	0.82	0/613
30	IC	0.43	0/460	0.79	0/613
31	EA	1.04	0/426	1.08	2/561 (0.4%)
31	JC	0.84	0/426	1.00	0/561
32	FA	0.71	0/525	0.93	1/691 (0.1%)
32	KC	0.65	0/525	0.91	0/691
33	GA	0.59	0/310	0.97	1/407 (0.2%)
33	LC	0.63	0/310	0.98	1/407 (0.2%)
34	HA	0.42	0/247	0.47	0/382
34	MC	0.39	0/247	0.46	0/382
35	JA	0.50	0/867	0.85	1/1165 (0.1%)
35	KA	0.49	0/461	0.86	2/622 (0.3%)
35	OC	0.46	0/867	0.85	1/1165 (0.1%)
35	PC	0.46	0/461	0.83	0/622

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
36	LA	0.50	0/1935	0.95	6/2609 (0.2%)
36	QC	0.45	0/1935	0.92	6/2609 (0.2%)
37	MA	0.47	0/1636	0.88	4/2205 (0.2%)
37	RC	0.45	0/1636	0.87	4/2205 (0.2%)
38	NA	0.53	0/1733	0.91	3/2318 (0.1%)
38	SC	0.60	0/1733	0.93	4/2318 (0.2%)
39	OA	0.55	0/1171	0.97	1/1576 (0.1%)
39	TC	0.53	0/1171	0.97	3/1576 (0.2%)
40	PA	0.59	0/856	0.97	3/1154 (0.3%)
40	UC	0.51	0/856	0.96	3/1154 (0.3%)
41	QA	0.49	0/1276	0.86	2/1709 (0.1%)
41	VC	0.46	0/1276	0.85	2/1709 (0.1%)
42	RA	0.47	0/1136	0.88	0/1527
42	WC	0.47	0/1136	0.88	0/1527
43	SA	0.45	0/1029	0.89	0/1378
43	XC	0.42	0/1029	0.88	1/1378 (0.1%)
44	TA	0.49	0/807	0.98	5/1085 (0.5%)
44	YC	0.47	0/807	0.99	8/1085 (0.7%)
45	UA	0.64	0/879	0.98	4/1187 (0.3%)
45	ZC	0.55	0/879	0.95	3/1187 (0.3%)
46	AD	0.64	0/963	0.95	2/1287 (0.2%)
46	VA	0.60	0/963	0.93	2/1287 (0.2%)
47	BD	0.44	0/943	0.84	0/1265
47	WA	0.47	0/943	0.84	0/1265
48	CD	0.39	0/501	0.84	2/664 (0.3%)
48	XA	0.42	0/501	0.87	2/664 (0.3%)
49	DD	0.54	0/745	0.85	0/992
49	YA	0.62	0/745	0.88	0/992
50	ED	0.52	0/716	0.91	1/963 (0.1%)
50	ZA	0.45	0/716	0.89	3/963 (0.3%)
51	AB	0.54	0/836	0.85	0/1117
51	FD	0.54	0/836	0.87	1/1117 (0.1%)
52	BB	0.53	0/579	0.84	0/768
52	GD	0.49	0/579	0.83	0/768
53	CB	0.42	0/680	0.83	2/915 (0.2%)
53	HD	0.42	0/680	0.83	0/915
54	DB	0.48	0/764	0.88	1/1006 (0.1%)
54	ID	0.54	0/764	0.88	1/1006 (0.1%)
55	EB	0.39	0/212	0.76	0/277
55	JD	0.38	0/212	0.73	0/277
All	All	0.48	9/320836 (0.0%)	0.68	235/479388 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
21	U	0	1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	237	GLU	CG-CD	6.19	1.67	1.52
7	G	89	VAL	CA-CB	-5.81	1.47	1.54
5	E	85	ASP	CA-C	-5.64	1.47	1.52
4	IB	8	4SU	O3'-P	5.31	1.61	1.56
7	G	84	VAL	CA-CB	-5.17	1.47	1.54

The worst 5 of 235 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	53	GLY	N-CA-C	-9.72	101.15	115.63
11	PB	125	GLY	CA-C-N	9.50	131.72	119.84
11	PB	125	GLY	C-N-CA	9.50	131.72	119.84
13	RB	53	GLY	N-CA-C	-9.24	101.86	115.63
11	K	125	GLY	CA-C-N	9.17	131.31	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	U	84	ALA	Peptide

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	831	0
1	FB	32394	0	16367	823	0
2	B	62031	0	31273	1294	0
2	GB	62031	0	31275	1276	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2576	0	1305	62	0
3	HB	2576	0	1305	64	0
4	D	1642	0	841	45	0
4	IA	1642	0	841	41	0
4	IB	1642	0	841	46	0
4	NC	1642	0	841	40	0
5	E	2145	0	2234	116	0
5	JB	2145	0	2234	107	0
6	F	1563	0	1629	92	0
6	KB	1563	0	1629	89	0
7	G	1586	0	1632	114	0
7	LB	1586	0	1632	108	0
8	H	1471	0	1526	92	0
8	MB	1471	0	1526	89	1
9	I	1330	0	1407	64	0
9	NB	1330	0	1407	59	0
10	J	1137	0	1225	56	0
10	OB	1137	0	1225	56	0
11	K	1121	0	1195	57	0
11	PB	1121	0	1195	56	0
12	L	932	0	994	77	0
12	QB	932	0	994	74	0
13	M	1145	0	1228	58	0
13	RB	1145	0	1228	48	0
14	N	1121	0	1179	65	0
14	SB	1121	0	1179	62	0
15	O	968	0	1033	36	0
15	TB	968	0	1033	41	0
16	P	877	0	938	49	0
16	UB	877	0	938	48	0
17	Q	1143	0	1211	81	0
17	VB	1143	0	1211	66	0
18	R	964	0	1022	61	0
18	WB	964	0	1022	54	0
19	S	779	0	852	29	0
19	XB	779	0	852	27	0
20	T	890	0	951	42	0
20	YB	890	0	951	43	0
21	U	750	0	814	40	0
21	ZB	750	0	814	37	0
22	AC	814	0	907	41	0
22	V	814	0	907	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	BC	1495	0	1521	82	0
23	W	1495	0	1521	93	0
24	CC	662	0	688	40	0
24	X	662	0	688	37	0
25	DC	761	0	837	52	0
25	Y	761	0	837	48	0
26	EC	592	0	654	32	0
26	Z	592	0	654	32	0
27	AA	477	0	529	27	0
27	FC	477	0	529	24	0
28	BA	552	0	537	31	0
28	GC	552	0	537	30	0
29	CA	460	0	481	32	0
29	HC	460	0	482	30	0
30	DA	453	0	477	15	0
30	IC	453	0	477	13	0
31	EA	418	0	467	24	0
31	JC	418	0	467	30	0
32	FA	517	0	582	34	0
32	KC	517	0	582	30	0
33	GA	307	0	337	11	0
33	LC	307	0	337	9	0
34	HA	220	0	108	9	0
34	MC	220	0	108	10	0
35	JA	850	0	816	38	0
35	KA	455	0	444	25	0
35	OC	850	0	816	39	0
35	PC	455	0	444	27	0
36	LA	1900	0	1951	101	0
36	QC	1900	0	1951	95	0
37	MA	1612	0	1677	94	0
37	RC	1612	0	1677	81	0
38	NA	1703	0	1767	98	0
38	SC	1703	0	1767	97	0
39	OA	1155	0	1213	66	0
39	TC	1155	0	1213	74	0
40	PA	843	0	857	40	0
40	UC	843	0	857	41	0
41	QA	1257	0	1296	62	0
41	VC	1257	0	1296	62	0
42	RA	1116	0	1177	64	0
42	WC	1116	0	1177	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	SA	1011	0	1043	62	0
43	XC	1011	0	1043	60	0
44	TA	794	0	840	37	0
44	YC	794	0	840	40	0
45	UA	864	0	881	42	0
45	ZC	864	0	881	48	0
46	AD	958	0	1047	54	0
46	VA	958	0	1047	55	0
47	BD	933	0	992	64	0
47	WA	933	0	992	66	0
48	CD	492	0	533	36	0
48	XA	492	0	533	38	0
49	DD	734	0	771	44	0
49	YA	734	0	771	42	0
50	ED	700	0	720	33	0
50	ZA	700	0	720	28	0
51	AB	823	0	893	42	0
51	FD	823	0	893	43	0
52	BB	574	0	644	37	0
52	GD	574	0	644	34	0
53	CB	665	0	686	42	0
53	HD	665	0	686	43	0
54	DB	762	0	859	43	0
54	ID	762	0	859	43	0
55	EB	208	0	221	16	0
55	JD	208	0	221	16	0
56	A	183	0	0	0	0
56	AA	1	0	0	0	0
56	AB	2	0	0	0	0
56	AC	1	0	0	0	0
56	AD	4	0	0	0	0
56	B	433	0	0	0	0
56	BB	1	0	0	0	0
56	BC	1	0	0	0	0
56	BD	1	0	0	0	0
56	C	22	0	0	0	0
56	CA	1	0	0	0	0
56	CB	1	0	0	0	0
56	CC	1	0	0	0	0
56	D	5	0	0	0	0
56	DC	1	0	0	0	0
56	DD	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	E	6	0	0	0	0
56	EA	1	0	0	0	0
56	ED	1	0	0	0	0
56	F	4	0	0	0	0
56	FA	1	0	0	0	0
56	FB	194	0	0	0	0
56	G	2	0	0	0	0
56	GB	402	0	0	0	0
56	GC	1	0	0	0	0
56	H	2	0	0	0	0
56	HA	3	0	0	0	0
56	HB	20	0	0	0	0
56	HD	1	0	0	0	0
56	IA	9	0	0	0	0
56	IB	2	0	0	0	0
56	IC	1	0	0	0	0
56	J	1	0	0	0	0
56	JA	1	0	0	0	0
56	JB	5	0	0	0	0
56	JC	1	0	0	0	0
56	K	4	0	0	0	0
56	KB	2	0	0	0	0
56	KC	1	0	0	0	0
56	L	3	0	0	0	0
56	LA	1	0	0	0	0
56	LB	4	0	0	0	0
56	M	3	0	0	0	0
56	MA	6	0	0	0	0
56	MC	3	0	0	0	0
56	NA	2	0	0	0	0
56	NB	1	0	0	0	0
56	NC	10	0	0	0	0
56	O	2	0	0	0	0
56	OA	4	0	0	0	0
56	OB	1	0	0	0	0
56	OC	1	0	0	0	0
56	PA	3	0	0	0	0
56	PB	2	0	0	0	0
56	PC	1	0	0	0	0
56	Q	1	0	0	0	0
56	QA	1	0	0	0	0
56	QB	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	QC	3	0	0	0	0
56	R	1	0	0	0	0
56	RB	3	0	0	0	0
56	RC	2	0	0	0	0
56	S	1	0	0	0	0
56	SA	1	0	0	0	0
56	SB	2	0	0	0	0
56	SC	4	0	0	0	0
56	T	2	0	0	0	0
56	TB	1	0	0	0	0
56	TC	3	0	0	0	0
56	U	1	0	0	0	0
56	UA	1	0	0	0	0
56	UB	4	0	0	0	0
56	UC	3	0	0	0	0
56	V	2	0	0	0	0
56	VA	2	0	0	0	0
56	VB	3	0	0	0	0
56	VC	1	0	0	0	0
56	WC	1	0	0	0	0
56	XB	2	0	0	0	0
56	Y	3	0	0	0	0
56	YA	3	0	0	0	0
56	Z	1	0	0	0	0
56	ZB	2	0	0	0	0
56	ZC	1	0	0	0	0
57	B	30	0	24	4	0
57	GB	30	0	24	7	0
58	AC	1	0	0	0	0
58	BA	1	0	0	0	0
58	CA	1	0	0	0	0
58	DA	1	0	0	0	0
58	GA	1	0	0	0	0
58	GC	1	0	0	0	0
58	HC	1	0	0	0	0
58	IC	1	0	0	0	0
58	LC	1	0	0	0	0
58	V	1	0	0	0	0
All	All	298186	0	202351	8614	1

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 18.

The worst 5 of 8614 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:SC:18:LYS:NZ	38:SC:26:CYS:SG	2.02	1.33
38:SC:18:LYS:NZ	38:SC:31:CYS:SG	2.07	1.27
38:NA:18:LYS:NZ	38:NA:26:CYS:SG	2.09	1.26
3:C:90:C:OP2	14:N:16:ARG:NH1	1.77	1.18
1:FB:9:G:OP2	39:TC:121:LYS:NZ	1.76	1.16

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:1412:A:O2'	8:MB:9:ARG:NH1[1_655]	1.99	0.21

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	273/275 (99%)	243 (89%)	24 (9%)	6 (2%)	5	24
5	JB	273/275 (99%)	245 (90%)	22 (8%)	6 (2%)	5	24
6	F	202/206 (98%)	166 (82%)	28 (14%)	8 (4%)	2	15
6	KB	202/206 (98%)	167 (83%)	29 (14%)	6 (3%)	3	18
7	G	200/205 (98%)	173 (86%)	24 (12%)	3 (2%)	8	30
7	LB	200/205 (98%)	172 (86%)	25 (12%)	3 (2%)	8	30
8	H	179/182 (98%)	134 (75%)	37 (21%)	8 (4%)	2	12
8	MB	179/182 (98%)	134 (75%)	37 (21%)	8 (4%)	2	12
9	I	172/180 (96%)	134 (78%)	32 (19%)	6 (4%)	3	16
9	NB	172/180 (96%)	134 (78%)	32 (19%)	6 (4%)	3	16
10	J	144/148 (97%)	111 (77%)	23 (16%)	10 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	OB	144/148 (97%)	111 (77%)	24 (17%)	9 (6%)	1	7
11	K	138/140 (99%)	115 (83%)	17 (12%)	6 (4%)	2	13
11	PB	138/140 (99%)	118 (86%)	15 (11%)	5 (4%)	2	16
12	L	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	16	44
12	QB	120/122 (98%)	108 (90%)	9 (8%)	3 (2%)	4	21
13	M	148/150 (99%)	126 (85%)	12 (8%)	10 (7%)	1	6
13	RB	148/150 (99%)	124 (84%)	14 (10%)	10 (7%)	1	6
14	N	139/141 (99%)	120 (86%)	17 (12%)	2 (1%)	9	31
14	SB	139/141 (99%)	121 (87%)	15 (11%)	3 (2%)	5	24
15	O	116/118 (98%)	99 (85%)	12 (10%)	5 (4%)	2	13
15	TB	116/118 (98%)	97 (84%)	13 (11%)	6 (5%)	1	10
16	P	108/112 (96%)	82 (76%)	23 (21%)	3 (3%)	4	19
16	UB	108/112 (96%)	83 (77%)	22 (20%)	3 (3%)	4	19
17	Q	135/146 (92%)	118 (87%)	13 (10%)	4 (3%)	3	18
17	VB	135/146 (92%)	117 (87%)	15 (11%)	3 (2%)	5	24
18	R	115/118 (98%)	106 (92%)	9 (8%)	0	100	100
18	WB	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	14	42
19	S	99/101 (98%)	85 (86%)	10 (10%)	4 (4%)	2	15
19	XB	99/101 (98%)	84 (85%)	12 (12%)	3 (3%)	3	18
20	T	110/113 (97%)	97 (88%)	11 (10%)	2 (2%)	6	26
20	YB	110/113 (97%)	98 (89%)	12 (11%)	0	100	100
21	U	93/96 (97%)	83 (89%)	8 (9%)	2 (2%)	5	24
21	ZB	93/96 (97%)	85 (91%)	6 (6%)	2 (2%)	5	24
22	AC	105/110 (96%)	83 (79%)	16 (15%)	6 (6%)	1	9
22	V	105/110 (96%)	83 (79%)	14 (13%)	8 (8%)	1	5
23	BC	187/206 (91%)	137 (73%)	43 (23%)	7 (4%)	2	16
23	W	187/206 (91%)	139 (74%)	41 (22%)	7 (4%)	2	16
24	CC	82/85 (96%)	70 (85%)	8 (10%)	4 (5%)	1	11
24	X	82/85 (96%)	71 (87%)	8 (10%)	3 (4%)	2	16
25	DC	95/98 (97%)	87 (92%)	7 (7%)	1 (1%)	11	38
25	Y	95/98 (97%)	86 (90%)	8 (8%)	1 (1%)	11	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	EC	68/72 (94%)	61 (90%)	4 (6%)	3 (4%)	2	13
26	Z	68/72 (94%)	59 (87%)	6 (9%)	3 (4%)	2	13
27	AA	58/60 (97%)	44 (76%)	12 (21%)	2 (3%)	3	17
27	FC	58/60 (97%)	45 (78%)	11 (19%)	2 (3%)	3	17
28	BA	67/71 (94%)	43 (64%)	16 (24%)	8 (12%)	0	2
28	GC	67/71 (94%)	44 (66%)	15 (22%)	8 (12%)	0	2
29	CA	57/60 (95%)	50 (88%)	6 (10%)	1 (2%)	6	26
29	HC	57/60 (95%)	49 (86%)	8 (14%)	0	100	100
30	DA	51/54 (94%)	42 (82%)	8 (16%)	1 (2%)	6	25
30	IC	51/54 (94%)	42 (82%)	8 (16%)	1 (2%)	6	25
31	EA	46/49 (94%)	41 (89%)	5 (11%)	0	100	100
31	JC	46/49 (94%)	38 (83%)	8 (17%)	0	100	100
32	FA	62/65 (95%)	53 (86%)	9 (14%)	0	100	100
32	KC	62/65 (95%)	53 (86%)	9 (14%)	0	100	100
33	GA	35/37 (95%)	24 (69%)	8 (23%)	3 (9%)	0	4
33	LC	35/37 (95%)	24 (69%)	8 (23%)	3 (9%)	0	4
35	JA	108/365 (30%)	84 (78%)	18 (17%)	6 (6%)	1	9
35	KA	53/365 (14%)	31 (58%)	13 (24%)	9 (17%)	0	0
35	OC	108/365 (30%)	83 (77%)	19 (18%)	6 (6%)	1	9
35	PC	53/365 (14%)	31 (58%)	14 (26%)	8 (15%)	0	0
36	LA	232/256 (91%)	176 (76%)	40 (17%)	16 (7%)	1	6
36	QC	232/256 (91%)	174 (75%)	41 (18%)	17 (7%)	1	5
37	MA	204/239 (85%)	166 (81%)	28 (14%)	10 (5%)	1	11
37	RC	204/239 (85%)	167 (82%)	25 (12%)	12 (6%)	1	8
38	NA	206/209 (99%)	162 (79%)	35 (17%)	9 (4%)	2	13
38	SC	206/209 (99%)	158 (77%)	39 (19%)	9 (4%)	2	13
39	OA	149/162 (92%)	126 (85%)	19 (13%)	4 (3%)	4	20
39	TC	149/162 (92%)	124 (83%)	20 (13%)	5 (3%)	3	17
40	PA	99/101 (98%)	81 (82%)	14 (14%)	4 (4%)	2	15
40	UC	99/101 (98%)	82 (83%)	13 (13%)	4 (4%)	2	15
41	QA	153/156 (98%)	121 (79%)	24 (16%)	8 (5%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	VC	153/156 (98%)	121 (79%)	24 (16%)	8 (5%)	1	10
42	RA	136/138 (99%)	106 (78%)	25 (18%)	5 (4%)	2	16
42	WC	136/138 (99%)	106 (78%)	25 (18%)	5 (4%)	2	16
43	SA	125/128 (98%)	91 (73%)	28 (22%)	6 (5%)	2	11
43	XC	125/128 (98%)	93 (74%)	25 (20%)	7 (6%)	1	9
44	TA	96/105 (91%)	72 (75%)	15 (16%)	9 (9%)	0	3
44	YC	96/105 (91%)	75 (78%)	12 (12%)	9 (9%)	0	3
45	UA	114/129 (88%)	87 (76%)	23 (20%)	4 (4%)	3	16
45	ZC	114/129 (88%)	87 (76%)	24 (21%)	3 (3%)	4	21
46	AD	119/132 (90%)	91 (76%)	20 (17%)	8 (7%)	1	6
46	VA	119/132 (90%)	89 (75%)	22 (18%)	8 (7%)	1	6
47	BD	115/126 (91%)	90 (78%)	18 (16%)	7 (6%)	1	7
47	WA	115/126 (91%)	91 (79%)	18 (16%)	6 (5%)	1	10
48	CD	58/61 (95%)	45 (78%)	12 (21%)	1 (2%)	7	28
48	XA	58/61 (95%)	44 (76%)	13 (22%)	1 (2%)	7	28
49	DD	86/89 (97%)	67 (78%)	16 (19%)	3 (4%)	3	16
49	YA	86/89 (97%)	68 (79%)	14 (16%)	4 (5%)	2	12
50	ED	81/88 (92%)	72 (89%)	8 (10%)	1 (1%)	10	35
50	ZA	81/88 (92%)	71 (88%)	9 (11%)	1 (1%)	10	35
51	AB	97/105 (92%)	78 (80%)	15 (16%)	4 (4%)	2	15
51	FD	97/105 (92%)	81 (84%)	11 (11%)	5 (5%)	1	10
52	BB	68/88 (77%)	63 (93%)	4 (6%)	1 (2%)	8	30
52	GD	68/88 (77%)	61 (90%)	5 (7%)	2 (3%)	3	19
53	CB	81/93 (87%)	58 (72%)	16 (20%)	7 (9%)	0	4
53	HD	81/93 (87%)	58 (72%)	17 (21%)	6 (7%)	1	5
54	DB	97/106 (92%)	79 (81%)	11 (11%)	7 (7%)	1	5
54	ID	97/106 (92%)	79 (81%)	12 (12%)	6 (6%)	1	7
55	EB	22/27 (82%)	18 (82%)	2 (9%)	2 (9%)	0	3
55	JD	22/27 (82%)	18 (82%)	2 (9%)	2 (9%)	0	3
All	All	11806/13576 (87%)	9599 (81%)	1713 (14%)	494 (4%)	2	14

5 of 494 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	122	ASP
7	G	130	ALA
8	H	12	TYR
8	H	43	LEU
8	H	47	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	217/217 (100%)	173 (80%)	44 (20%)	1	4
5	JB	217/217 (100%)	175 (81%)	42 (19%)	1	5
6	F	165/166 (99%)	137 (83%)	28 (17%)	2	9
6	KB	165/166 (99%)	137 (83%)	28 (17%)	2	9
7	G	161/162 (99%)	128 (80%)	33 (20%)	1	4
7	LB	161/162 (99%)	130 (81%)	31 (19%)	1	5
8	H	154/156 (99%)	114 (74%)	40 (26%)	0	1
8	MB	154/156 (99%)	114 (74%)	40 (26%)	0	1
9	I	144/148 (97%)	120 (83%)	24 (17%)	2	9
9	NB	144/148 (97%)	120 (83%)	24 (17%)	2	9
10	J	122/124 (98%)	94 (77%)	28 (23%)	1	2
10	OB	122/124 (98%)	93 (76%)	29 (24%)	1	2
11	K	119/119 (100%)	94 (79%)	25 (21%)	1	4
11	PB	119/119 (100%)	92 (77%)	27 (23%)	1	3
12	L	100/100 (100%)	86 (86%)	14 (14%)	3	13
12	QB	100/100 (100%)	82 (82%)	18 (18%)	2	7
13	M	116/116 (100%)	87 (75%)	29 (25%)	0	1
13	RB	116/116 (100%)	87 (75%)	29 (25%)	0	1
14	N	111/111 (100%)	92 (83%)	19 (17%)	2	9
14	SB	111/111 (100%)	92 (83%)	19 (17%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	101/101 (100%)	82 (81%)	19 (19%)	1	6
15	TB	101/101 (100%)	81 (80%)	20 (20%)	1	5
16	P	87/88 (99%)	68 (78%)	19 (22%)	1	3
16	UB	87/88 (99%)	69 (79%)	18 (21%)	1	4
17	Q	121/128 (94%)	94 (78%)	27 (22%)	1	3
17	VB	121/128 (94%)	92 (76%)	29 (24%)	1	2
18	R	93/94 (99%)	81 (87%)	12 (13%)	4	16
18	WB	93/94 (99%)	81 (87%)	12 (13%)	4	16
19	S	82/82 (100%)	62 (76%)	20 (24%)	1	2
19	XB	82/82 (100%)	63 (77%)	19 (23%)	1	2
20	T	91/92 (99%)	74 (81%)	17 (19%)	1	6
20	YB	91/92 (99%)	76 (84%)	15 (16%)	2	10
21	U	77/78 (99%)	68 (88%)	9 (12%)	5	20
21	ZB	77/78 (99%)	67 (87%)	10 (13%)	4	16
22	AC	87/91 (96%)	67 (77%)	20 (23%)	1	2
22	V	87/91 (96%)	67 (77%)	20 (23%)	1	2
23	BC	163/179 (91%)	131 (80%)	32 (20%)	1	5
23	W	163/179 (91%)	130 (80%)	33 (20%)	1	4
24	CC	66/67 (98%)	54 (82%)	12 (18%)	2	7
24	X	66/67 (98%)	53 (80%)	13 (20%)	1	5
25	DC	81/83 (98%)	65 (80%)	16 (20%)	1	5
25	Y	81/83 (98%)	67 (83%)	14 (17%)	2	8
26	EC	66/67 (98%)	56 (85%)	10 (15%)	3	10
26	Z	66/67 (98%)	55 (83%)	11 (17%)	2	9
27	AA	52/52 (100%)	40 (77%)	12 (23%)	1	2
27	FC	52/52 (100%)	39 (75%)	13 (25%)	0	1
28	BA	59/63 (94%)	45 (76%)	14 (24%)	1	2
28	GC	59/63 (94%)	46 (78%)	13 (22%)	1	3
29	CA	51/52 (98%)	42 (82%)	9 (18%)	2	8
29	HC	51/52 (98%)	44 (86%)	7 (14%)	3	14
30	DA	51/52 (98%)	40 (78%)	11 (22%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	IC	51/52 (98%)	39 (76%)	12 (24%)	1	2
31	EA	41/42 (98%)	32 (78%)	9 (22%)	1	3
31	JC	41/42 (98%)	33 (80%)	8 (20%)	1	5
32	FA	54/55 (98%)	48 (89%)	6 (11%)	6	21
32	KC	54/55 (98%)	48 (89%)	6 (11%)	6	21
33	GA	34/34 (100%)	31 (91%)	3 (9%)	9	31
33	LC	34/34 (100%)	31 (91%)	3 (9%)	9	31
35	JA	85/305 (28%)	70 (82%)	15 (18%)	2	8
35	KA	50/305 (16%)	39 (78%)	11 (22%)	1	3
35	OC	85/305 (28%)	70 (82%)	15 (18%)	2	8
35	PC	50/305 (16%)	39 (78%)	11 (22%)	1	3
36	LA	202/220 (92%)	153 (76%)	49 (24%)	1	2
36	QC	202/220 (92%)	153 (76%)	49 (24%)	1	2
37	MA	160/188 (85%)	137 (86%)	23 (14%)	3	13
37	RC	160/188 (85%)	137 (86%)	23 (14%)	3	13
38	NA	180/181 (99%)	145 (81%)	35 (19%)	1	5
38	SC	180/181 (99%)	144 (80%)	36 (20%)	1	4
39	OA	116/123 (94%)	90 (78%)	26 (22%)	1	3
39	TC	116/123 (94%)	91 (78%)	25 (22%)	1	3
40	PA	90/90 (100%)	77 (86%)	13 (14%)	3	13
40	UC	90/90 (100%)	77 (86%)	13 (14%)	3	13
41	QA	126/127 (99%)	101 (80%)	25 (20%)	1	5
41	VC	126/127 (99%)	101 (80%)	25 (20%)	1	5
42	RA	119/119 (100%)	104 (87%)	15 (13%)	4	18
42	WC	119/119 (100%)	104 (87%)	15 (13%)	4	18
43	SA	98/99 (99%)	82 (84%)	16 (16%)	2	10
43	XC	98/99 (99%)	82 (84%)	16 (16%)	2	10
44	TA	88/92 (96%)	69 (78%)	19 (22%)	1	3
44	YC	88/92 (96%)	69 (78%)	19 (22%)	1	3
45	UA	88/99 (89%)	74 (84%)	14 (16%)	2	10
45	ZC	88/99 (89%)	74 (84%)	14 (16%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	AD	102/108 (94%)	83 (81%)	19 (19%)	1	6
46	VA	102/108 (94%)	84 (82%)	18 (18%)	2	8
47	BD	94/101 (93%)	73 (78%)	21 (22%)	1	3
47	WA	94/101 (93%)	73 (78%)	21 (22%)	1	3
48	CD	49/50 (98%)	41 (84%)	8 (16%)	2	10
48	XA	49/50 (98%)	41 (84%)	8 (16%)	2	10
49	DD	79/80 (99%)	61 (77%)	18 (23%)	1	3
49	YA	79/80 (99%)	61 (77%)	18 (23%)	1	3
50	ED	72/74 (97%)	58 (81%)	14 (19%)	1	5
50	ZA	72/74 (97%)	57 (79%)	15 (21%)	1	4
51	AB	94/97 (97%)	74 (79%)	20 (21%)	1	3
51	FD	94/97 (97%)	74 (79%)	20 (21%)	1	3
52	BB	61/77 (79%)	49 (80%)	12 (20%)	1	5
52	GD	61/77 (79%)	50 (82%)	11 (18%)	2	7
53	CB	72/80 (90%)	56 (78%)	16 (22%)	1	3
53	HD	72/80 (90%)	57 (79%)	15 (21%)	1	4
54	DB	76/82 (93%)	68 (90%)	8 (10%)	6	23
54	ID	76/82 (93%)	68 (90%)	8 (10%)	6	23
55	EB	19/22 (86%)	15 (79%)	4 (21%)	1	3
55	JD	19/22 (86%)	15 (79%)	4 (21%)	1	3
All	All	9972/11276 (88%)	8048 (81%)	1924 (19%)	1	5

5 of 1924 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	BB	37	VAL
45	ZC	12	ARG
10	OB	101	LEU
44	YC	13	HIS
52	GD	55	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
33	LC	36	GLN
47	BD	101	GLN
35	PC	311	ASN
41	VC	64	GLN
53	HD	57	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1505/1507 (99%)	349 (23%)	12 (0%)
1	FB	1505/1507 (99%)	345 (22%)	12 (0%)
2	B	2879/2880 (99%)	657 (22%)	22 (0%)
2	GB	2879/2880 (99%)	657 (22%)	22 (0%)
3	C	119/120 (99%)	19 (15%)	0
3	HB	119/120 (99%)	20 (16%)	0
34	HA	9/27 (33%)	3 (33%)	0
34	MC	9/27 (33%)	3 (33%)	0
4	D	76/77 (98%)	27 (35%)	0
4	IA	76/77 (98%)	20 (26%)	0
4	IB	76/77 (98%)	26 (34%)	0
4	NC	76/77 (98%)	19 (25%)	0
All	All	9328/9376 (99%)	2145 (22%)	68 (0%)

5 of 2145 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	13	U
1	A	22	G
1	A	26	A
1	A	31	G

5 of 68 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	GB	1558	A
2	GB	1939	5MU
2	GB	2439	A
2	B	1608	A
2	B	1558	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	5MC	FB	967	1	19,22,23	2.54	5 (26%)	26,32,35	1.40	5 (19%)
2	PSU	GB	1911	2	18,21,22	1.59	3 (16%)	21,30,33	2.19	7 (33%)
2	2MA	B	2503	2	22,25,26	1.72	5 (22%)	32,37,40	1.95	6 (18%)
2	PSU	B	1911	2	18,21,22	1.35	1 (5%)	21,30,33	2.13	7 (33%)
1	2MG	A	1207	1	23,26,27	2.22	4 (17%)	33,38,41	2.14	11 (33%)
4	PSU	IB	55	4	18,21,22	1.66	2 (11%)	21,30,33	1.74	5 (23%)
1	MA6	A	1519	1	23,26,27	1.43	3 (13%)	33,38,41	2.04	10 (30%)
1	5MC	FB	1404	1	19,22,23	3.02	4 (21%)	26,32,35	1.14	2 (7%)
4	4SU	IA	8	4	18,21,22	4.94	7 (38%)	25,30,33	5.95	10 (40%)
1	MA6	FB	1519	1	23,26,27	1.67	4 (17%)	33,38,41	2.07	12 (36%)
1	5MC	A	1404	1	19,22,23	2.84	5 (26%)	26,32,35	1.27	5 (19%)
4	PSU	D	55	4	18,21,22	1.69	2 (11%)	21,30,33	1.76	5 (23%)
2	2MA	GB	2503	2	22,25,26	1.66	4 (18%)	32,37,40	2.03	7 (21%)
4	4SU	D	8	4	18,21,22	4.71	7 (38%)	25,30,33	5.99	10 (40%)
1	5MC	A	1407	1	19,22,23	2.71	4 (21%)	26,32,35	1.17	3 (11%)
1	MA6	A	1518	1	23,26,27	1.62	4 (17%)	33,38,41	2.19	12 (36%)
1	MA6	FB	1518	1	23,26,27	1.55	4 (17%)	33,38,41	2.19	12 (36%)
2	2MU	GB	2552	2	19,22,24	2.54	5 (26%)	25,31,36	2.31	7 (28%)
4	5MC	NC	32	4	19,22,23	2.64	4 (21%)	26,32,35	1.08	2 (7%)
2	4OC	B	1920	56,2	19,22,24	1.13	1 (5%)	25,31,35	1.55	2 (8%)
1	7MG	A	527	1	23,26,27	3.02	7 (30%)	27,39,42	2.18	8 (29%)
1	5MC	FB	1407	1	19,22,23	2.56	4 (21%)	26,32,35	1.11	3 (11%)
2	PSU	GB	2605	2	18,21,22	1.72	3 (16%)	21,30,33	2.34	6 (28%)
1	PSU	FB	516	1	18,21,22	1.78	3 (16%)	21,30,33	1.40	3 (14%)
1	PSU	A	516	1	18,21,22	1.61	3 (16%)	21,30,33	1.44	2 (9%)
46	0TD	VA	92	46	8,9,10	2.40	2 (25%)	6,11,13	3.17	4 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	M2G	A	966	1	24,27,28	2.21	4 (16%)	33,40,43	1.93	8 (24%)
1	5MC	FB	1400	1	19,22,23	2.66	5 (26%)	26,32,35	1.16	2 (7%)
1	5MC	A	1400	1	19,22,23	2.61	5 (26%)	26,32,35	1.34	4 (15%)
1	4OC	A	1402	1	20,23,24	1.08	2 (10%)	25,32,35	1.20	1 (4%)
2	5MU	GB	1915	2	19,22,23	2.01	3 (15%)	27,32,35	2.19	8 (29%)
2	5MC	GB	1942	2	19,22,23	2.35	4 (21%)	26,32,35	1.55	3 (11%)
1	5MC	A	967	1	19,22,23	2.47	5 (26%)	26,32,35	1.43	4 (15%)
2	5MC	B	1962	2	19,22,23	2.82	5 (26%)	26,32,35	1.48	4 (15%)
2	PSU	B	2605	2	18,21,22	1.53	2 (11%)	21,30,33	2.13	5 (23%)
4	5MC	IB	32	4	19,22,23	2.50	4 (21%)	26,32,35	1.10	2 (7%)
2	OMG	B	2251	2	23,26,27	2.02	3 (13%)	32,38,41	2.11	10 (31%)
4	PSU	NC	55	4	18,21,22	1.72	2 (11%)	21,30,33	1.82	4 (19%)
2	4OC	GB	1920	2	19,22,24	1.07	1 (5%)	25,31,35	1.46	1 (4%)
4	4SU	NC	8	4	18,21,22	4.65	7 (38%)	25,30,33	6.26	10 (40%)
2	2MU	B	2552	2	19,22,24	2.69	6 (31%)	25,31,36	2.27	7 (28%)
4	5MU	IB	54	4	19,22,23	2.06	3 (15%)	27,32,35	2.12	7 (25%)
1	2MG	FB	1207	1	23,26,27	2.20	3 (13%)	33,38,41	2.05	11 (33%)
2	PSU	GB	1917	2	18,21,22	1.81	2 (11%)	21,30,33	1.83	5 (23%)
4	5MC	IA	32	4	19,22,23	2.69	4 (21%)	26,32,35	0.98	2 (7%)
2	5MU	B	1915	2	19,22,23	2.01	3 (15%)	27,32,35	2.30	9 (33%)
4	4SU	IB	8	4	18,21,22	4.57	7 (38%)	25,30,33	5.95	11 (44%)
2	5MC	B	1942	2	19,22,23	2.57	4 (21%)	26,32,35	1.41	3 (11%)
2	5MC	GB	1962	2	19,22,23	2.50	5 (26%)	26,32,35	1.36	2 (7%)
4	5MC	D	32	4	19,22,23	2.69	4 (21%)	26,32,35	1.11	3 (11%)
4	PSU	IA	55	4	18,21,22	1.64	2 (11%)	21,30,33	1.88	4 (19%)
1	4OC	FB	1402	1	20,23,24	1.02	2 (10%)	25,32,35	1.30	2 (8%)
1	UR3	FB	1498	1	19,22,23	1.80	1 (5%)	26,32,35	1.51	3 (11%)
1	UR3	A	1498	1	19,22,23	1.78	1 (5%)	26,32,35	1.43	2 (7%)
4	5MU	D	54	4	19,22,23	2.09	3 (15%)	27,32,35	2.11	6 (22%)
1	7MG	FB	527	1	23,26,27	3.15	7 (30%)	27,39,42	2.29	8 (29%)
4	5MU	NC	54	4	19,22,23	2.09	3 (15%)	27,32,35	2.03	7 (25%)
2	5MU	GB	1939	2	19,22,23	2.24	4 (21%)	27,32,35	2.43	8 (29%)
2	PSU	B	1917	2	18,21,22	1.77	2 (11%)	21,30,33	1.79	4 (19%)
4	5MU	IA	54	4	19,22,23	2.07	3 (15%)	27,32,35	2.05	8 (29%)
2	OMG	GB	2251	2	23,26,27	1.98	3 (13%)	32,38,41	2.08	9 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	M2G	FB	966	1	24,27,28	2.20	4 (16%)	33,40,43	1.88	8 (24%)
46	0TD	AD	92	46	8,9,10	1.98	2 (25%)	6,11,13	3.12	4 (66%)
2	5MU	B	1939	2	19,22,23	2.08	4 (21%)	27,32,35	2.60	8 (29%)

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
1	5MC	FB	967	1	-	0/7/25/26	0/2/2/2
2	PSU	GB	1911	2	-	0/7/25/26	0/2/2/2
2	2MA	B	2503	2	-	1/7/25/26	0/3/3/3
2	PSU	B	1911	2	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
4	PSU	IB	55	4	-	1/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	4/11/29/30	0/3/3/3
1	5MC	FB	1404	1	-	0/7/25/26	0/2/2/2
4	4SU	IA	8	4	-	2/7/25/26	0/2/2/2
1	MA6	FB	1519	1	-	4/11/29/30	0/3/3/3
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
4	PSU	D	55	4	-	1/7/25/26	0/2/2/2
2	2MA	GB	2503	2	-	1/7/25/26	0/3/3/3
4	4SU	D	8	4	-	1/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	3/11/29/30	0/3/3/3
1	MA6	FB	1518	1	-	3/11/29/30	0/3/3/3
2	2MU	GB	2552	2	-	1/9/27/28	0/2/2/2
4	5MC	NC	32	4	-	0/7/25/26	0/2/2/2
2	4OC	B	1920	56,2	-	1/9/27/30	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	5MC	FB	1407	1	-	0/7/25/26	0/2/2/2
2	PSU	GB	2605	2	-	0/7/25/26	0/2/2/2
1	PSU	FB	516	1	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
46	0TD	VA	92	46	-	3/7/12/14	-
1	M2G	A	966	1	-	0/11/29/30	0/3/3/3
1	5MC	FB	1400	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	1/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5MU	GB	1915	2	-	0/7/25/26	0/2/2/2
2	5MC	GB	1942	2	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
2	5MC	B	1962	2	-	2/7/25/26	0/2/2/2
2	PSU	B	2605	2	-	0/7/25/26	0/2/2/2
4	5MC	IB	32	4	-	0/7/25/26	0/2/2/2
2	OMG	B	2251	2	-	3/9/27/28	0/3/3/3
4	PSU	NC	55	4	-	1/7/25/26	0/2/2/2
2	4OC	GB	1920	2	-	1/9/27/30	0/2/2/2
4	4SU	NC	8	4	-	2/7/25/26	0/2/2/2
2	2MU	B	2552	2	-	1/9/27/28	0/2/2/2
4	5MU	IB	54	4	-	0/7/25/26	0/2/2/2
1	2MG	FB	1207	1	-	0/9/27/28	0/3/3/3
2	PSU	GB	1917	2	-	1/7/25/26	0/2/2/2
4	5MC	IA	32	4	-	0/7/25/26	0/2/2/2
2	5MU	B	1915	2	-	0/7/25/26	0/2/2/2
4	4SU	IB	8	4	-	1/7/25/26	0/2/2/2
2	5MC	B	1942	2	-	0/7/25/26	0/2/2/2
2	5MC	GB	1962	2	-	2/7/25/26	0/2/2/2
4	5MC	D	32	4	-	0/7/25/26	0/2/2/2
4	PSU	IA	55	4	-	2/7/25/26	0/2/2/2
1	4OC	FB	1402	1	-	2/9/29/30	0/2/2/2
1	UR3	FB	1498	1	-	2/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	2/7/25/26	0/2/2/2
4	5MU	D	54	4	-	0/7/25/26	0/2/2/2
1	7MG	FB	527	1	-	2/7/37/38	0/3/3/3
4	5MU	NC	54	4	-	0/7/25/26	0/2/2/2
2	5MU	GB	1939	2	-	0/7/25/26	0/2/2/2
2	PSU	B	1917	2	-	0/7/25/26	0/2/2/2
4	5MU	IA	54	4	-	0/7/25/26	0/2/2/2
2	OMG	GB	2251	2	-	3/9/27/28	0/3/3/3
1	M2G	FB	966	1	-	0/11/29/30	0/3/3/3
46	0TD	AD	92	46	-	2/7/12/14	-
2	5MU	B	1939	2	-	1/7/25/26	0/2/2/2

The worst 5 of 234 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	IA	8	4SU	C4-N3	13.44	1.51	1.37
4	D	8	4SU	C4-N3	12.49	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	NC	8	4SU	C4-N3	12.20	1.50	1.37
4	IB	8	4SU	C4-N3	11.78	1.49	1.37
4	IA	8	4SU	O2-C2	11.75	1.43	1.23

The worst 5 of 373 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	IB	8	4SU	S4-C4-N3	-15.25	104.25	120.20
4	NC	8	4SU	C4-N3-C2	-15.06	112.88	127.31
4	IA	8	4SU	C4-N3-C2	-14.45	113.47	127.31
4	IB	8	4SU	C5-C4-S4	-13.95	108.37	124.31
4	D	8	4SU	C4-N3-C2	-13.80	114.09	127.31

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1402	4OC	C1'-C2'-O2'-CM2
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	1518	MA6	C5-C6-N6-C9
1	A	1519	MA6	O4'-C4'-C5'-O5'
2	B	1920	4OC	C3'-C2'-O2'-CM2

There are no ring outliers.

37 monomers are involved in 69 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	FB	967	5MC	4	0
2	B	2503	2MA	2	0
1	A	1207	2MG	3	0
1	A	1519	MA6	1	0
1	FB	1519	MA6	1	0
2	GB	2503	2MA	2	0
4	D	8	4SU	3	0
1	A	1407	5MC	1	0
1	A	1518	MA6	1	0
1	FB	1518	MA6	1	0
4	NC	32	5MC	2	0
2	B	1920	4OC	4	0
1	FB	1407	5MC	1	0
46	VA	92	0TD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	966	M2G	2	0
1	A	1402	4OC	1	0
2	GB	1942	5MC	1	0
1	A	967	5MC	4	0
2	B	1962	5MC	1	0
2	B	2251	OMG	3	0
2	GB	1920	4OC	1	0
2	B	2552	2MU	1	0
1	FB	1207	2MG	3	0
2	GB	1917	PSU	2	0
4	IA	32	5MC	3	0
4	IB	8	4SU	2	0
2	GB	1962	5MC	1	0
1	FB	1402	4OC	2	0
1	FB	1498	UR3	3	0
1	A	1498	UR3	2	0
4	NC	54	5MU	2	0
2	GB	1939	5MU	2	0
4	IA	54	5MU	2	0
2	GB	2251	OMG	3	0
1	FB	966	M2G	1	0
46	AD	92	0TD	1	0
2	B	1939	5MU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1440 ligands modelled in this entry, 1438 are monoatomic - leaving 2 for Mogul analysis.

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
57	BLS	B	9001	-	30,31,31	3.19	12 (40%)	30,43,43	2.36	6 (20%)
57	BLS	GB	9001	-	30,31,31	3.14	11 (36%)	30,43,43	1.97	8 (26%)

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
57	BLS	B	9001	-	-	6/25/38/38	0/2/2/2
57	BLS	GB	9001	-	-	7/25/38/38	0/2/2/2

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	B	9001	BLS	C14-N12	9.09	1.54	1.35
57	GB	9001	BLS	C14-N12	8.65	1.53	1.35
57	GB	9001	BLS	C7-N6	7.71	1.50	1.34
57	B	9001	BLS	C7-N6	6.83	1.48	1.34
57	B	9001	BLS	C4-N4	5.82	1.48	1.33

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	B	9001	BLS	C1'-C2'-C3'	-9.47	110.80	122.45
57	GB	9001	BLS	C1'-C2'-C3'	-7.62	113.08	122.45
57	B	9001	BLS	N15-C14-N12	3.71	122.71	118.64
57	B	9001	BLS	O4-C6'-O3	3.27	131.49	124.08
57	B	9001	BLS	O3-C6'-C5'	-3.17	109.36	120.81

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

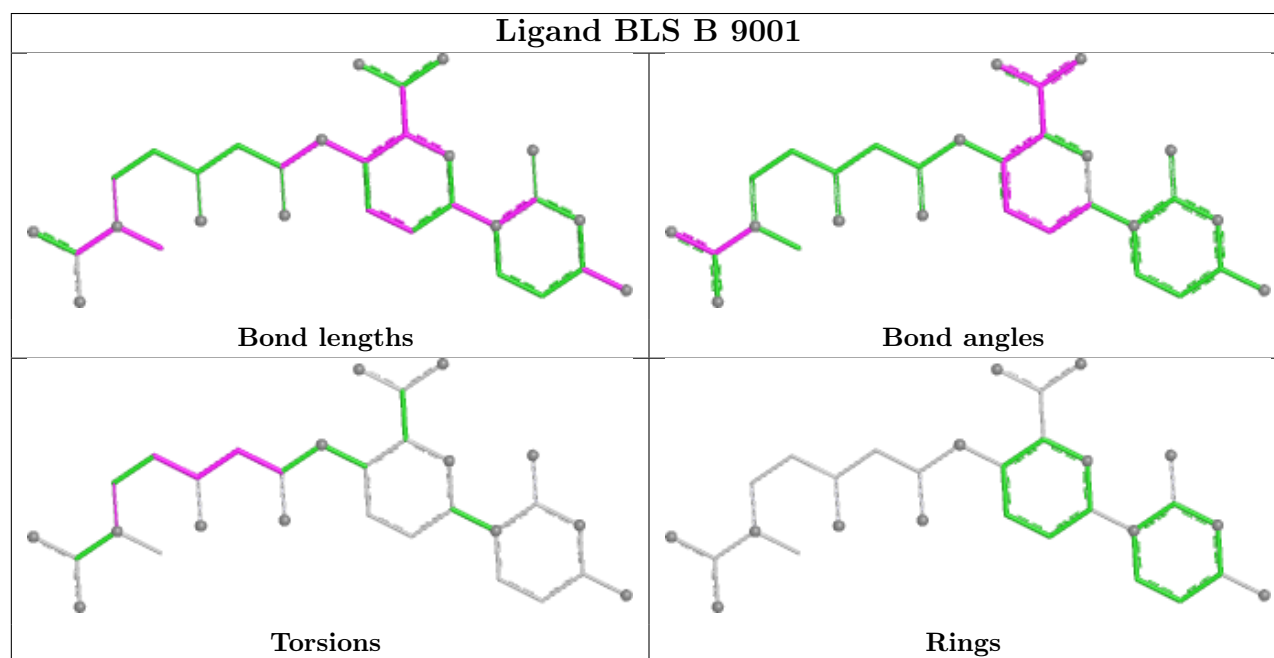
Mol	Chain	Res	Type	Atoms
57	B	9001	BLS	C11-C10-C9-C8
57	B	9001	BLS	C11-C10-C9-N9
57	B	9001	BLS	C10-C11-N12-C13
57	B	9001	BLS	C10-C11-N12-C14
57	GB	9001	BLS	C11-C10-C9-C8

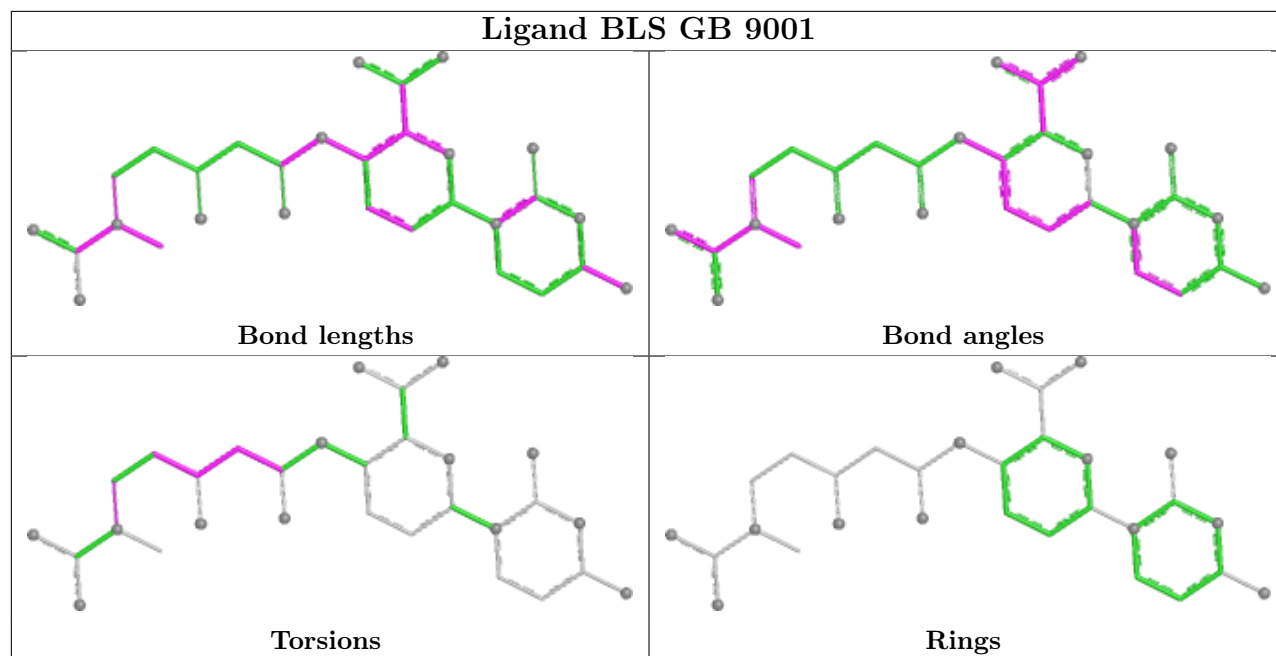
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	B	9001	BLS	4	0
57	GB	9001	BLS	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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%)	-0.69	3 (0%) 91 87	92, 150, 224, 269	0
1	FB	1495/1507 (99%)	-0.48	6 (0%) 88 81	99, 138, 232, 276	0
2	B	2869/2880 (99%)	-0.73	9 (0%) 90 84	73, 105, 203, 272	0
2	GB	2869/2880 (99%)	-0.60	7 (0%) 91 87	81, 114, 229, 316	0
3	C	120/120 (100%)	-0.74	0 100 100	129, 165, 182, 187	0
3	HB	120/120 (100%)	-0.35	0 100 100	139, 177, 198, 207	0
4	D	73/77 (94%)	-0.49	3 (4%) 41 29	135, 221, 238, 244	0
4	IA	73/77 (94%)	-0.45	1 (1%) 73 59	130, 161, 182, 190	0
4	IB	73/77 (94%)	-0.30	1 (1%) 73 59	158, 256, 274, 283	0
4	NC	73/77 (94%)	-0.39	1 (1%) 73 59	148, 189, 217, 220	0
5	E	275/275 (100%)	-0.24	3 (1%) 78 65	69, 83, 95, 102	0
5	JB	275/275 (100%)	0.02	5 (1%) 67 53	84, 104, 121, 128	0
6	F	204/206 (99%)	-0.09	6 (2%) 53 39	82, 119, 139, 147	0
6	KB	204/206 (99%)	-0.03	3 (1%) 72 57	81, 107, 132, 144	0
7	G	202/205 (98%)	-0.30	0 100 100	77, 107, 121, 133	0
7	LB	202/205 (98%)	-0.10	3 (1%) 72 57	82, 126, 141, 150	0
8	H	181/182 (99%)	0.09	4 (2%) 62 47	165, 174, 184, 186	0
8	MB	181/182 (99%)	0.06	5 (2%) 55 41	181, 188, 199, 202	0
9	I	174/180 (96%)	-0.14	0 100 100	116, 131, 138, 155	0
9	NB	174/180 (96%)	0.14	5 (2%) 53 39	149, 188, 215, 222	0
10	J	146/148 (98%)	-0.24	0 100 100	107, 130, 149, 153	0
10	OB	146/148 (98%)	-0.06	3 (2%) 63 48	124, 155, 159, 161	0
11	K	140/140 (100%)	0.10	3 (2%) 63 48	100, 121, 133, 138	0
11	PB	140/140 (100%)	0.21	5 (3%) 46 33	100, 129, 143, 147	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
12	L	122/122 (100%)	-0.20	0 100 100	94, 108, 119, 123	0
12	QB	122/122 (100%)	-0.28	0 100 100	88, 96, 103, 107	0
13	M	150/150 (100%)	0.10	3 (2%) 65 49	82, 110, 137, 139	0
13	RB	150/150 (100%)	0.13	5 (3%) 49 36	104, 124, 140, 142	0
14	N	141/141 (100%)	0.15	1 (0%) 84 73	100, 123, 140, 148	0
14	SB	141/141 (100%)	0.20	5 (3%) 47 34	106, 137, 154, 160	0
15	O	118/118 (100%)	0.10	2 (1%) 69 54	93, 111, 126, 130	0
15	TB	118/118 (100%)	0.24	5 (4%) 40 29	90, 106, 116, 121	0
16	P	110/112 (98%)	0.54	11 (10%) 12 12	147, 157, 163, 164	0
16	UB	110/112 (98%)	0.42	9 (8%) 17 16	153, 169, 181, 188	0
17	Q	137/146 (93%)	-0.07	1 (0%) 84 73	111, 125, 174, 192	0
17	VB	137/146 (93%)	-0.33	0 100 100	93, 108, 139, 148	0
18	R	117/118 (99%)	0.04	0 100 100	83, 116, 131, 132	0
18	WB	117/118 (99%)	0.05	4 (3%) 48 35	98, 129, 143, 146	0
19	S	101/101 (100%)	-0.20	1 (0%) 79 66	86, 126, 132, 136	0
19	XB	101/101 (100%)	-0.21	4 (3%) 42 30	96, 141, 148, 150	0
20	T	112/113 (99%)	-0.28	1 (0%) 81 68	78, 97, 113, 122	0
20	YB	112/113 (99%)	-0.05	1 (0%) 81 68	83, 101, 121, 127	0
21	U	95/96 (98%)	-0.10	1 (1%) 78 65	86, 92, 102, 109	0
21	ZB	95/96 (98%)	0.17	1 (1%) 78 65	109, 120, 129, 135	0
22	AC	107/110 (97%)	0.36	7 (6%) 25 20	120, 125, 139, 143	0
22	V	107/110 (97%)	-0.25	0 100 100	101, 108, 120, 126	0
23	BC	189/206 (91%)	-0.04	2 (1%) 78 65	143, 165, 176, 180	0
23	W	189/206 (91%)	-0.10	0 100 100	131, 152, 162, 164	0
24	CC	84/85 (98%)	0.49	8 (9%) 14 13	128, 134, 146, 154	0
24	X	84/85 (98%)	0.55	10 (11%) 9 10	119, 125, 139, 146	0
25	DC	97/98 (98%)	0.20	4 (4%) 41 29	94, 114, 137, 145	0
25	Y	97/98 (98%)	0.09	1 (1%) 79 66	83, 105, 132, 140	0
26	EC	70/72 (97%)	0.05	1 (1%) 73 59	123, 129, 136, 138	0
26	Z	70/72 (97%)	-0.23	0 100 100	95, 101, 107, 116	0
27	AA	60/60 (100%)	-0.06	1 (1%) 69 54	104, 117, 128, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	FC	60/60 (100%)	0.13	1 (1%) 69 54	118, 131, 141, 142	0
28	BA	69/71 (97%)	-0.29	0 100 100	186, 191, 204, 206	0
28	GC	69/71 (97%)	-0.18	0 100 100	200, 207, 212, 213	0
29	CA	59/60 (98%)	-0.20	0 100 100	90, 115, 125, 130	0
29	HC	59/60 (98%)	-0.36	1 (1%) 69 54	81, 113, 123, 124	0
30	DA	53/54 (98%)	0.20	2 (3%) 44 31	184, 184, 185, 185	0
30	IC	53/54 (98%)	0.49	2 (3%) 44 31	207, 213, 217, 219	0
31	EA	48/49 (97%)	-0.25	0 100 100	72, 77, 83, 88	0
31	JC	48/49 (97%)	0.13	1 (2%) 63 48	89, 91, 100, 110	0
32	FA	64/65 (98%)	0.46	2 (3%) 51 38	93, 102, 119, 127	0
32	KC	64/65 (98%)	0.34	0 100 100	101, 112, 128, 135	0
33	GA	37/37 (100%)	2.05	18 (48%) 0 1	185, 186, 188, 188	0
33	LC	37/37 (100%)	1.93	17 (45%) 0 1	187, 189, 190, 191	0
34	HA	11/27 (40%)	0.61	2 (18%) 3 5	127, 142, 152, 153	0
34	MC	11/27 (40%)	0.02	0 100 100	143, 154, 164, 168	0
35	JA	110/365 (30%)	-0.04	5 (4%) 38 28	158, 176, 196, 210	0
35	KA	55/365 (15%)	-0.04	1 (1%) 67 53	172, 187, 214, 219	0
35	OC	110/365 (30%)	0.05	3 (2%) 56 42	186, 196, 207, 214	0
35	PC	55/365 (15%)	-0.06	2 (3%) 46 33	195, 202, 215, 219	0
36	LA	234/256 (91%)	-0.17	1 (0%) 88 81	148, 161, 170, 174	0
36	QC	234/256 (91%)	-0.00	6 (2%) 57 42	167, 184, 197, 202	0
37	MA	206/239 (86%)	-0.12	8 (3%) 43 31	153, 163, 175, 182	0
37	RC	206/239 (86%)	-0.08	3 (1%) 72 57	159, 177, 193, 200	0
38	NA	208/209 (99%)	0.53	17 (8%) 17 16	135, 159, 171, 177	0
38	SC	208/209 (99%)	0.22	17 (8%) 17 16	117, 126, 133, 137	0
39	OA	151/162 (93%)	0.01	6 (3%) 42 30	128, 140, 147, 155	0
39	TC	151/162 (93%)	-0.09	3 (1%) 65 49	124, 140, 150, 152	0
40	PA	101/101 (100%)	-0.22	1 (0%) 79 66	119, 128, 134, 146	0
40	UC	101/101 (100%)	-0.25	0 100 100	141, 149, 156, 163	0
41	QA	155/156 (99%)	-0.03	3 (1%) 66 51	146, 168, 177, 181	0
41	VC	155/156 (99%)	0.18	5 (3%) 50 37	167, 185, 197, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
42	RA	138/138 (100%)	-0.04	2 (1%) 73 59	130, 145, 149, 153	0
42	WC	138/138 (100%)	0.22	7 (5%) 33 25	128, 144, 156, 163	0
43	SA	127/128 (99%)	0.57	16 (12%) 8 9	167, 190, 195, 199	0
43	XC	127/128 (99%)	0.65	18 (14%) 6 8	176, 212, 221, 227	0
44	TA	98/105 (93%)	0.51	10 (10%) 12 12	166, 189, 198, 201	0
44	YC	98/105 (93%)	0.56	7 (7%) 22 18	176, 197, 211, 213	0
45	UA	116/129 (89%)	-0.07	3 (2%) 57 42	104, 128, 135, 139	0
45	ZC	116/129 (89%)	-0.02	4 (3%) 48 35	126, 154, 160, 162	0
46	AD	121/132 (91%)	0.07	2 (1%) 69 54	109, 116, 124, 136	0
46	VA	121/132 (91%)	0.27	8 (6%) 24 19	115, 124, 134, 139	0
47	BD	117/126 (92%)	0.32	7 (5%) 27 21	179, 210, 214, 215	0
47	WA	117/126 (92%)	0.17	8 (6%) 23 19	161, 193, 196, 198	0
48	CD	60/61 (98%)	0.73	3 (5%) 34 25	180, 189, 208, 209	0
48	XA	60/61 (98%)	0.55	4 (6%) 24 19	164, 171, 193, 194	0
49	DD	88/89 (98%)	0.04	2 (2%) 61 46	126, 142, 153, 155	0
49	YA	88/89 (98%)	-0.04	3 (3%) 48 35	106, 126, 136, 137	0
50	ED	83/88 (94%)	0.19	3 (3%) 46 33	112, 120, 133, 148	0
50	ZA	83/88 (94%)	0.33	7 (8%) 17 15	150, 160, 174, 183	0
51	AB	99/105 (94%)	0.16	6 (6%) 27 21	116, 138, 144, 148	0
51	FD	99/105 (94%)	-0.05	3 (3%) 52 39	115, 124, 130, 132	0
52	BB	70/88 (79%)	-0.34	1 (1%) 73 59	119, 132, 140, 147	0
52	GD	70/88 (79%)	0.02	1 (1%) 73 59	145, 156, 163, 165	0
53	CB	83/93 (89%)	0.48	5 (6%) 27 21	171, 198, 201, 203	0
53	HD	83/93 (89%)	0.33	2 (2%) 59 45	179, 212, 217, 221	0
54	DB	99/106 (93%)	0.64	13 (13%) 7 8	152, 164, 174, 175	0
54	ID	99/106 (93%)	0.35	9 (9%) 15 14	115, 133, 145, 146	0
55	EB	24/27 (88%)	0.91	2 (8%) 17 15	179, 189, 195, 198	0
55	JD	24/27 (88%)	1.11	4 (16%) 4 6	202, 210, 219, 223	0
All	All	21292/22952 (92%)	-0.23	452 (2%) 63 48	69, 131, 210, 316	0

The worst 5 of 452 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
38	NA	120	LEU	7.3
24	X	4	LYS	6.7
42	WC	1	MET	6.2
49	DD	57	LEU	5.9
33	LC	12	ASP	5.9

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

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	4SU	D	8	20/21	0.63	0.09	223,225,227,227	0
4	PSU	D	55	20/21	0.66	0.07	239,243,246,247	0
4	PSU	IB	55	20/21	0.68	0.08	276,281,283,284	0
4	5MU	IB	54	21/22	0.73	0.09	275,277,280,281	0
4	5MU	D	54	21/22	0.74	0.07	237,240,244,246	0
4	PSU	NC	55	20/21	0.75	0.08	211,216,222,223	0
4	4SU	IA	8	20/21	0.78	0.08	158,160,162,163	0
4	5MC	IB	32	21/22	0.79	0.10	204,204,204,204	0
2	PSU	GB	1911	20/21	0.81	0.09	127,133,134,135	0
4	4SU	IB	8	20/21	0.81	0.09	254,257,259,260	0
4	4SU	NC	8	20/21	0.82	0.07	185,190,192,193	0
2	5MU	B	1915	21/22	0.84	0.06	129,131,133,134	0
4	5MC	D	32	21/22	0.86	0.07	212,212,212,212	0
4	5MC	NC	32	21/22	0.87	0.10	156,157,157,157	0
1	5MC	FB	967	21/22	0.87	0.12	160,163,166,168	0
1	PSU	A	516	20/21	0.87	0.07	139,142,145,146	0
2	5MU	GB	1915	21/22	0.88	0.05	143,146,149,150	0
4	5MU	NC	54	21/22	0.88	0.10	213,217,223,226	0
1	2MG	FB	1207	24/25	0.88	0.08	171,174,176,178	0
4	PSU	IA	55	20/21	0.88	0.07	185,189,193,195	0
2	5MU	B	1939	21/22	0.88	0.11	83,84,84,84	0
4	5MU	IA	54	21/22	0.88	0.07	184,188,192,194	0
1	PSU	FB	516	20/21	0.89	0.06	132,134,138,138	0
2	OMG	GB	2251	24/25	0.90	0.11	95,97,100,100	0
2	4OC	GB	1920	21/23	0.90	0.11	123,127,129,131	0
1	5MC	A	967	21/22	0.91	0.09	139,142,145,147	0
4	5MC	IA	32	21/22	0.91	0.10	138,139,139,139	0
1	4OC	A	1402	22/23	0.92	0.11	117,118,120,120	0
1	4OC	FB	1402	22/23	0.92	0.09	134,136,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	5MC	B	1942	21/22	0.92	0.07	90,92,93,94	0
2	5MC	B	1962	21/22	0.92	0.10	90,92,94,95	0
2	PSU	GB	1917	20/21	0.92	0.06	129,132,136,137	0
2	PSU	B	1911	20/21	0.92	0.06	113,117,119,120	0
2	5MU	GB	1939	21/22	0.92	0.10	86,88,89,89	0
1	2MG	A	1207	24/25	0.92	0.08	163,164,166,167	0
1	5MC	A	1400	21/22	0.93	0.10	125,127,130,132	0
2	5MC	GB	1962	21/22	0.93	0.08	93,96,98,99	0
2	2MA	B	2503	23/24	0.93	0.11	76,78,79,80	0
2	2MA	GB	2503	23/24	0.93	0.13	83,84,86,86	0
46	0TD	AD	92	10/11	0.93	0.20	122,122,123,123	0
1	5MC	FB	1400	21/22	0.93	0.13	141,145,148,150	0
2	PSU	B	1917	20/21	0.93	0.06	111,113,117,118	0
1	UR3	FB	1498	21/22	0.94	0.14	130,130,132,132	0
2	4OC	B	1920	21/23	0.94	0.08	106,109,111,113	0
1	7MG	FB	527	24/25	0.94	0.09	122,124,126,127	0
2	5MC	GB	1942	21/22	0.94	0.06	90,93,94,95	0
1	5MC	FB	1404	21/22	0.95	0.09	123,125,126,126	0
1	UR3	A	1498	21/22	0.95	0.09	109,109,110,110	0
2	PSU	GB	2605	20/21	0.95	0.07	85,85,86,87	0
1	M2G	FB	966	25/26	0.95	0.14	157,160,164,165	0
1	M2G	A	966	25/26	0.96	0.09	137,140,143,144	0
1	5MC	FB	1407	21/22	0.96	0.08	121,124,125,126	0
2	OMG	B	2251	24/25	0.96	0.07	87,89,92,92	0
1	7MG	A	527	24/25	0.96	0.09	125,127,129,130	0
2	2MU	B	2552	21/23	0.96	0.10	86,87,88,89	0
2	2MU	GB	2552	21/23	0.96	0.06	86,87,88,89	0
2	PSU	B	2605	20/21	0.96	0.07	78,79,80,81	0
1	MA6	A	1518	24/25	0.96	0.10	98,102,104,104	0
1	5MC	A	1404	21/22	0.97	0.07	105,107,108,108	0
1	MA6	FB	1519	24/25	0.97	0.12	117,121,123,123	0
1	5MC	A	1407	21/22	0.97	0.06	108,110,112,112	0
46	0TD	VA	92	10/11	0.97	0.12	125,126,126,126	0
1	MA6	A	1519	24/25	0.97	0.11	98,101,103,103	0
1	MA6	FB	1518	24/25	0.98	0.09	116,119,122,123	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	GB	9272	1/1	-0.53	0.25	194,194,194,194	0
56	MG	FB	1638	1/1	-0.51	0.51	198,198,198,198	0
56	MG	B	9072	1/1	-0.39	0.18	248,248,248,248	0
56	MG	GB	9320	1/1	-0.32	0.15	223,223,223,223	0
56	MG	FB	1612	1/1	-0.31	0.26	201,201,201,201	0
56	MG	FB	1644	1/1	-0.30	0.19	239,239,239,239	0
56	MG	B	9207	1/1	-0.29	0.24	185,185,185,185	0
56	MG	HB	208	1/1	-0.28	0.32	177,177,177,177	0
56	MG	FB	1765	1/1	-0.22	0.15	234,234,234,234	0
56	MG	A	1747	1/1	-0.21	0.18	215,215,215,215	0
56	MG	GB	9298	1/1	-0.21	0.20	250,250,250,250	0
56	MG	B	9378	1/1	-0.19	0.20	254,254,254,254	0
56	MG	IB	101	1/1	-0.19	0.14	243,243,243,243	0
56	MG	GB	9247	1/1	-0.16	0.11	278,278,278,278	0
56	MG	GB	9136	1/1	-0.16	0.23	154,154,154,154	0
56	MG	A	1764	1/1	-0.14	0.30	204,204,204,204	0
56	MG	A	1778	1/1	-0.14	0.23	156,156,156,156	0
56	MG	A	1620	1/1	-0.11	0.31	201,201,201,201	0
56	MG	A	1634	1/1	-0.10	0.29	165,165,165,165	0
56	MG	FB	1646	1/1	-0.10	0.30	170,170,170,170	0
56	MG	FB	1705	1/1	-0.07	0.18	200,200,200,200	0
56	MG	A	1641	1/1	-0.07	0.23	154,154,154,154	0
56	MG	A	1650	1/1	-0.07	0.34	170,170,170,170	0
56	MG	A	1652	1/1	-0.05	0.18	232,232,232,232	0
56	MG	B	9305	1/1	-0.05	0.28	207,207,207,207	0
56	MG	A	1686	1/1	-0.04	0.38	169,169,169,169	0
56	MG	A	1660	1/1	-0.03	0.19	252,252,252,252	0
56	MG	GC	102	1/1	-0.02	0.21	205,205,205,205	0
56	MG	GB	9278	1/1	-0.01	0.27	149,149,149,149	0
56	MG	GB	9391	1/1	0.00	0.18	172,172,172,172	0
56	MG	GB	9118	1/1	-0.00	0.17	144,144,144,144	0
56	MG	H	202	1/1	0.01	0.14	161,161,161,161	0
56	MG	B	9285	1/1	0.01	0.17	164,164,164,164	0
56	MG	B	9157	1/1	0.02	0.33	128,128,128,128	0
56	MG	HB	209	1/1	0.02	0.22	183,183,183,183	0
56	MG	A	1653	1/1	0.03	0.12	260,260,260,260	0
56	MG	GB	9117	1/1	0.03	0.32	160,160,160,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	IA	102	1/1	0.04	0.32	162,162,162,162	0
56	MG	GB	9066	1/1	0.05	0.25	176,176,176,176	0
56	MG	HB	215	1/1	0.05	0.14	189,189,189,189	0
56	MG	C	213	1/1	0.06	0.24	156,156,156,156	0
56	MG	A	1642	1/1	0.07	0.42	143,143,143,143	0
56	MG	HB	220	1/1	0.07	0.18	159,159,159,159	0
56	MG	GB	9269	1/1	0.08	0.17	146,146,146,146	0
56	MG	GB	9121	1/1	0.08	0.24	186,186,186,186	0
56	MG	GB	9106	1/1	0.09	0.24	142,142,142,142	0
56	MG	FB	1601	1/1	0.09	0.37	117,117,117,117	0
56	MG	A	1638	1/1	0.09	0.17	188,188,188,188	0
56	MG	GB	9167	1/1	0.10	0.24	166,166,166,166	0
56	MG	HB	202	1/1	0.10	0.30	149,149,149,149	0
56	MG	FB	1643	1/1	0.11	0.45	138,138,138,138	0
56	MG	HB	204	1/1	0.11	0.33	138,138,138,138	0
56	MG	FB	1671	1/1	0.11	0.15	255,255,255,255	0
56	MG	IA	101	1/1	0.11	0.35	152,152,152,152	0
56	MG	HB	205	1/1	0.12	0.36	140,140,140,140	0
56	MG	NA	301	1/1	0.14	0.30	159,159,159,159	0
56	MG	FB	1623	1/1	0.14	0.31	136,136,136,136	0
56	MG	HB	201	1/1	0.15	0.43	130,130,130,130	0
56	MG	NA	302	1/1	0.15	0.12	163,163,163,163	0
56	MG	A	1635	1/1	0.16	0.29	168,168,168,168	0
56	MG	FB	1710	1/1	0.16	0.17	155,155,155,155	0
56	MG	A	1664	1/1	0.16	0.21	172,172,172,172	0
56	MG	SB	201	1/1	0.16	0.29	143,143,143,143	0
56	MG	GB	9057	1/1	0.16	0.26	145,145,145,145	0
56	MG	GB	9052	1/1	0.17	0.27	132,132,132,132	0
56	MG	GB	9208	1/1	0.17	0.14	210,210,210,210	0
56	MG	A	1644	1/1	0.17	0.24	159,159,159,159	0
56	MG	GB	9301	1/1	0.17	0.25	252,252,252,252	0
56	MG	GB	9306	1/1	0.17	0.17	151,151,151,151	0
56	MG	GB	9139	1/1	0.17	0.22	166,166,166,166	0
56	MG	FB	1634	1/1	0.18	0.35	128,128,128,128	0
56	MG	GB	9224	1/1	0.18	0.19	152,152,152,152	0
56	MG	GB	9335	1/1	0.19	0.21	141,141,141,141	0
56	MG	A	1631	1/1	0.20	0.29	142,142,142,142	0
56	MG	A	1657	1/1	0.21	0.25	155,155,155,155	0
56	MG	NB	201	1/1	0.21	0.16	189,189,189,189	0
56	MG	FB	1665	1/1	0.21	0.23	188,188,188,188	0
56	MG	A	1717	1/1	0.21	0.29	154,154,154,154	0
56	MG	FB	1730	1/1	0.22	0.19	167,167,167,167	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	GB	9195	1/1	0.22	0.10	172,172,172,172	0
56	MG	HB	210	1/1	0.22	0.26	166,166,166,166	0
56	MG	B	9256	1/1	0.23	0.25	157,157,157,157	0
56	MG	B	9302	1/1	0.23	0.19	167,167,167,167	0
56	MG	FB	1615	1/1	0.23	0.17	209,209,209,209	0
56	MG	A	1742	1/1	0.24	0.14	160,160,160,160	0
56	MG	FB	1684	1/1	0.24	0.17	140,140,140,140	0
56	MG	A	1760	1/1	0.25	0.16	178,178,178,178	0
56	MG	B	9399	1/1	0.25	0.22	175,175,175,175	0
56	MG	A	1714	1/1	0.25	0.19	111,111,111,111	0
56	MG	RC	302	1/1	0.25	0.16	161,161,161,161	0
56	MG	C	201	1/1	0.26	0.43	132,132,132,132	0
56	MG	FB	1630	1/1	0.26	0.31	128,128,128,128	0
56	MG	A	1643	1/1	0.26	0.35	170,170,170,170	0
56	MG	FB	1716	1/1	0.27	0.39	197,197,197,197	0
56	MG	A	1618	1/1	0.28	0.38	141,141,141,141	0
56	MG	A	1782	1/1	0.28	0.15	159,159,159,159	0
56	MG	NC	101	1/1	0.28	0.22	189,189,189,189	0
56	MG	FB	1662	1/1	0.28	0.28	139,139,139,139	0
56	MG	GB	9181	1/1	0.29	0.23	135,135,135,135	0
56	MG	GB	9373	1/1	0.29	0.17	157,157,157,157	0
56	MG	A	1674	1/1	0.30	0.30	133,133,133,133	0
56	MG	FB	1675	1/1	0.30	0.29	197,197,197,197	0
56	MG	IA	108	1/1	0.30	0.11	165,165,165,165	0
56	MG	B	9024	1/1	0.31	0.30	120,120,120,120	0
56	MG	D	102	1/1	0.31	0.18	185,185,185,185	0
56	MG	IB	102	1/1	0.31	0.09	246,246,246,246	0
56	MG	GB	9383	1/1	0.31	0.16	137,137,137,137	0
56	MG	LB	302	1/1	0.32	0.12	137,137,137,137	0
56	MG	FB	1720	1/1	0.32	0.19	164,164,164,164	0
56	MG	A	1640	1/1	0.33	0.23	140,140,140,140	0
56	MG	FB	1780	1/1	0.33	0.16	184,184,184,184	0
56	MG	A	1683	1/1	0.33	0.17	166,166,166,166	0
56	MG	FB	1653	1/1	0.34	0.30	146,146,146,146	0
56	MG	FB	1686	1/1	0.34	0.23	139,139,139,139	0
56	MG	TC	201	1/1	0.34	0.37	120,120,120,120	0
56	MG	A	1719	1/1	0.35	0.28	170,170,170,170	0
56	MG	FB	1635	1/1	0.35	0.18	151,151,151,151	0
56	MG	FB	1659	1/1	0.35	0.22	122,122,122,122	0
56	MG	A	1692	1/1	0.35	0.31	149,149,149,149	0
56	MG	GB	9028	1/1	0.35	0.28	112,112,112,112	0
56	MG	B	9174	1/1	0.35	0.35	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9066	1/1	0.35	0.23	130,130,130,130	0
56	MG	GB	9288	1/1	0.36	0.23	202,202,202,202	0
56	MG	A	1672	1/1	0.36	0.17	158,158,158,158	0
56	MG	GB	9027	1/1	0.36	0.25	140,140,140,140	0
56	MG	GB	9078	1/1	0.36	0.21	185,185,185,185	0
56	MG	GB	9228	1/1	0.36	0.19	226,226,226,226	0
56	MG	GB	9093	1/1	0.36	0.25	116,116,116,116	0
56	MG	GB	9166	1/1	0.36	0.20	129,129,129,129	0
56	MG	D	103	1/1	0.36	0.20	147,147,147,147	0
56	MG	A	1639	1/1	0.36	0.15	166,166,166,166	0
56	MG	FB	1691	1/1	0.37	0.18	144,144,144,144	0
56	MG	A	1622	1/1	0.37	0.30	125,125,125,125	0
56	MG	GB	9024	1/1	0.37	0.22	151,151,151,151	0
56	MG	FB	1756	1/1	0.38	0.14	123,123,123,123	0
56	MG	B	9119	1/1	0.38	0.33	114,114,114,114	0
56	MG	FB	1648	1/1	0.38	0.32	108,108,108,108	0
56	MG	A	1612	1/1	0.38	0.37	125,125,125,125	0
56	MG	LA	5800	1/1	0.38	0.20	163,163,163,163	0
56	MG	GB	9381	1/1	0.38	0.17	132,132,132,132	0
56	MG	HB	207	1/1	0.38	0.31	146,146,146,146	0
56	MG	FB	1651	1/1	0.39	0.20	186,186,186,186	0
56	MG	A	1602	1/1	0.39	0.34	124,124,124,124	0
56	MG	MC	101	1/1	0.39	0.38	130,130,130,130	0
56	MG	B	9280	1/1	0.39	0.18	183,183,183,183	0
56	MG	FB	1708	1/1	0.39	0.15	152,152,152,152	0
56	MG	QA	201	1/1	0.39	0.34	144,144,144,144	0
56	MG	C	215	1/1	0.40	0.10	137,137,137,137	0
56	MG	A	1739	1/1	0.40	0.20	161,161,161,161	0
56	MG	GB	9183	1/1	0.40	0.20	169,169,169,169	0
56	MG	NC	102	1/1	0.40	0.14	165,165,165,165	0
56	MG	B	9183	1/1	0.40	0.18	172,172,172,172	0
56	MG	UB	204	1/1	0.40	0.18	161,161,161,161	0
56	MG	HB	217	1/1	0.41	0.24	135,135,135,135	0
56	MG	A	1677	1/1	0.41	0.13	237,237,237,237	0
56	MG	A	1617	1/1	0.41	0.20	193,193,193,193	0
56	MG	B	9237	1/1	0.41	0.16	165,165,165,165	0
56	MG	GB	9132	1/1	0.41	0.29	151,151,151,151	0
56	MG	GB	9337	1/1	0.41	0.20	147,147,147,147	0
56	MG	FB	1751	1/1	0.41	0.15	174,174,174,174	0
56	MG	B	9177	1/1	0.42	0.28	126,126,126,126	0
56	MG	A	1721	1/1	0.42	0.44	169,169,169,169	0
56	MG	B	9201	1/1	0.42	0.17	159,159,159,159	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9282	1/1	0.42	0.15	153,153,153,153	0
56	MG	A	1685	1/1	0.42	0.13	154,154,154,154	0
56	MG	FB	1622	1/1	0.43	0.25	128,128,128,128	0
56	MG	FB	1633	1/1	0.43	0.18	153,153,153,153	0
56	MG	GB	9238	1/1	0.43	0.34	120,120,120,120	0
56	MG	IA	104	1/1	0.43	0.14	140,140,140,140	0
56	MG	GB	9257	1/1	0.43	0.19	124,124,124,124	0
56	MG	GB	9018	1/1	0.43	0.24	136,136,136,136	0
56	MG	FB	1688	1/1	0.43	0.27	137,137,137,137	0
56	MG	B	9392	1/1	0.44	0.17	140,140,140,140	0
56	MG	FB	1777	1/1	0.44	0.32	135,135,135,135	0
56	MG	A	1656	1/1	0.44	0.18	161,161,161,161	0
56	MG	GB	9229	1/1	0.44	0.17	135,135,135,135	0
56	MG	GB	9140	1/1	0.44	0.23	102,102,102,102	0
56	MG	JA	401	1/1	0.44	0.10	169,169,169,169	0
56	MG	B	9131	1/1	0.44	0.23	92,92,92,92	0
56	MG	FB	1618	1/1	0.44	0.49	111,111,111,111	0
56	MG	A	1702	1/1	0.44	0.15	211,211,211,211	0
56	MG	B	9116	1/1	0.44	0.25	127,127,127,127	0
56	MG	GB	9205	1/1	0.44	0.13	158,158,158,158	0
56	MG	GB	9115	1/1	0.45	0.28	109,109,109,109	0
56	MG	GB	9248	1/1	0.45	0.12	158,158,158,158	0
56	MG	XB	202	1/1	0.45	0.14	140,140,140,140	0
56	MG	B	9042	1/1	0.45	0.33	120,120,120,120	0
56	MG	GB	9017	1/1	0.45	0.19	132,132,132,132	0
56	MG	B	9139	1/1	0.45	0.24	147,147,147,147	0
56	MG	GB	9174	1/1	0.45	0.19	136,136,136,136	0
56	MG	B	9088	1/1	0.45	0.35	108,108,108,108	0
56	MG	GB	9114	1/1	0.45	0.22	134,134,134,134	0
56	MG	B	9036	1/1	0.46	0.22	75,75,75,75	0
56	MG	B	9111	1/1	0.46	0.27	104,104,104,104	0
56	MG	FB	1641	1/1	0.46	0.28	131,131,131,131	0
56	MG	GB	9398	1/1	0.46	0.17	165,165,165,165	0
56	MG	BD	201	1/1	0.46	0.11	182,182,182,182	0
56	MG	GB	9350	1/1	0.47	0.11	143,143,143,143	0
56	MG	GB	9354	1/1	0.47	0.15	164,164,164,164	0
56	MG	GB	9097	1/1	0.47	0.24	134,134,134,134	0
56	MG	A	1689	1/1	0.47	0.17	184,184,184,184	0
56	MG	GB	9303	1/1	0.48	0.16	165,165,165,165	0
56	MG	B	9135	1/1	0.48	0.21	142,142,142,142	0
56	MG	FB	1624	1/1	0.48	0.19	136,136,136,136	0
56	MG	FB	1699	1/1	0.48	0.25	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	FB	1642	1/1	0.48	0.17	121,121,121,121	0
56	MG	GB	9041	1/1	0.48	0.33	111,111,111,111	0
56	MG	HB	214	1/1	0.48	0.16	163,163,163,163	0
56	MG	MA	304	1/1	0.48	0.15	165,165,165,165	0
56	MG	B	9102	1/1	0.49	0.28	107,107,107,107	0
56	MG	FB	1732	1/1	0.49	0.13	164,164,164,164	0
56	MG	FB	1680	1/1	0.49	0.16	139,139,139,139	0
56	MG	B	9144	1/1	0.49	0.24	117,117,117,117	0
56	MG	FB	1757	1/1	0.49	0.18	170,170,170,170	0
56	MG	HB	211	1/1	0.49	0.26	147,147,147,147	0
56	MG	FB	1627	1/1	0.49	0.19	123,123,123,123	0
56	MG	GB	9235	1/1	0.49	0.19	156,156,156,156	0
56	MG	FB	1772	1/1	0.49	0.26	165,165,165,165	0
56	MG	NC	109	1/1	0.49	0.24	157,157,157,157	0
56	MG	A	1713	1/1	0.49	0.21	151,151,151,151	0
56	MG	B	9311	1/1	0.49	0.17	136,136,136,136	0
56	MG	GB	9256	1/1	0.49	0.19	138,138,138,138	0
56	MG	IA	109	1/1	0.50	0.12	140,140,140,140	0
56	MG	B	9324	1/1	0.50	0.17	182,182,182,182	0
56	MG	B	9233	1/1	0.50	0.19	207,207,207,207	0
56	MG	GB	9295	1/1	0.50	0.12	182,182,182,182	0
56	MG	GB	9390	1/1	0.50	0.13	238,238,238,238	0
56	MG	CB	101	1/1	0.50	0.16	191,191,191,191	0
56	MG	B	9385	1/1	0.50	0.16	173,173,173,173	0
56	MG	MC	102	1/1	0.51	0.18	145,145,145,145	0
56	MG	HB	216	1/1	0.51	0.10	184,184,184,184	0
56	MG	B	9349	1/1	0.51	0.13	163,163,163,163	0
56	MG	A	1762	1/1	0.51	0.13	153,153,153,153	0
56	MG	GB	9200	1/1	0.51	0.16	152,152,152,152	0
56	MG	GB	9034	1/1	0.51	0.24	139,139,139,139	0
56	MG	A	1609	1/1	0.51	0.30	112,112,112,112	0
56	MG	C	214	1/1	0.52	0.14	170,170,170,170	0
56	MG	A	1754	1/1	0.52	0.11	201,201,201,201	0
56	MG	C	219	1/1	0.52	0.15	155,155,155,155	0
56	MG	FB	1606	1/1	0.52	0.21	137,137,137,137	0
56	MG	GB	9077	1/1	0.52	0.35	84,84,84,84	0
56	MG	GB	9386	1/1	0.52	0.20	135,135,135,135	0
56	MG	GB	9013	1/1	0.52	0.29	111,111,111,111	0
56	MG	A	1671	1/1	0.52	0.35	114,114,114,114	0
56	MG	A	1748	1/1	0.52	0.19	116,116,116,116	0
56	MG	A	1751	1/1	0.52	0.18	159,159,159,159	0
56	MG	FB	1752	1/1	0.52	0.23	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	SC	302	1/1	0.52	0.28	129,129,129,129	0
56	MG	B	9138	1/1	0.52	0.15	158,158,158,158	0
56	MG	A	1768	1/1	0.52	0.11	151,151,151,151	0
56	MG	B	9277	1/1	0.53	0.19	131,131,131,131	0
56	MG	FB	1702	1/1	0.53	0.23	171,171,171,171	0
56	MG	A	1722	1/1	0.53	0.24	132,132,132,132	0
56	MG	B	9382	1/1	0.53	0.09	135,135,135,135	0
56	MG	FB	1604	1/1	0.53	0.45	103,103,103,103	0
56	MG	HB	203	1/1	0.53	0.28	137,137,137,137	0
56	MG	OA	201	1/1	0.53	0.34	118,118,118,118	0
56	MG	GB	9033	1/1	0.54	0.27	131,131,131,131	0
56	MG	B	9057	1/1	0.54	0.29	85,85,85,85	0
56	MG	B	9199	1/1	0.54	0.17	94,94,94,94	0
56	MG	GB	9313	1/1	0.54	0.10	127,127,127,127	0
56	MG	A	1720	1/1	0.54	0.26	126,126,126,126	0
56	MG	FB	1762	1/1	0.54	0.09	256,256,256,256	0
56	MG	GB	9212	1/1	0.54	0.12	210,210,210,210	0
56	MG	A	1687	1/1	0.54	0.12	247,247,247,247	0
56	MG	GB	9169	1/1	0.54	0.16	142,142,142,142	0
56	MG	A	1636	1/1	0.54	0.23	138,138,138,138	0
56	MG	GB	9234	1/1	0.54	0.19	132,132,132,132	0
56	MG	VC	201	1/1	0.54	0.10	145,145,145,145	0
56	MG	C	218	1/1	0.54	0.12	166,166,166,166	0
56	MG	V	502	1/1	0.55	0.16	109,109,109,109	0
56	MG	B	9222	1/1	0.55	0.29	126,126,126,126	0
56	MG	B	9238	1/1	0.55	0.21	95,95,95,95	0
56	MG	FB	1735	1/1	0.55	0.18	131,131,131,131	0
56	MG	IA	103	1/1	0.55	0.17	149,149,149,149	0
56	MG	B	9430	1/1	0.55	0.15	159,159,159,159	0
56	MG	GB	9275	1/1	0.55	0.25	149,149,149,149	0
56	MG	FB	1714	1/1	0.55	0.17	202,202,202,202	0
56	MG	GB	9055	1/1	0.55	0.25	123,123,123,123	0
56	MG	B	9190	1/1	0.55	0.18	110,110,110,110	0
56	MG	GB	9019	1/1	0.55	0.20	130,130,130,130	0
56	MG	GB	9184	1/1	0.55	0.26	130,130,130,130	0
56	MG	GB	9262	1/1	0.56	0.25	119,119,119,119	0
56	MG	FB	1728	1/1	0.56	0.17	139,139,139,139	0
56	MG	GB	9158	1/1	0.56	0.28	136,136,136,136	0
56	MG	LB	303	1/1	0.56	0.19	123,123,123,123	0
56	MG	B	9396	1/1	0.56	0.17	120,120,120,120	0
56	MG	OB	201	1/1	0.56	0.18	148,148,148,148	0
56	MG	GB	9043	1/1	0.56	0.24	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	GB	9137	1/1	0.56	0.32	134,134,134,134	0
56	MG	FB	1725	1/1	0.56	0.12	138,138,138,138	0
56	MG	GB	9297	1/1	0.56	0.15	132,132,132,132	0
56	MG	GB	9355	1/1	0.57	0.15	131,131,131,131	0
56	MG	B	9351	1/1	0.57	0.13	147,147,147,147	0
56	MG	GB	9138	1/1	0.57	0.33	122,122,122,122	0
56	MG	B	9219	1/1	0.57	0.18	138,138,138,138	0
56	MG	FB	1791	1/1	0.57	0.12	138,138,138,138	0
56	MG	GB	9325	1/1	0.57	0.17	105,105,105,105	0
56	MG	B	9330	1/1	0.57	0.21	125,125,125,125	0
56	MG	FB	1672	1/1	0.57	0.31	131,131,131,131	0
56	MG	GB	9401	1/1	0.57	0.23	106,106,106,106	0
56	MG	GB	9230	1/1	0.57	0.25	137,137,137,137	0
56	MG	B	9321	1/1	0.57	0.13	132,132,132,132	0
56	MG	B	9109	1/1	0.58	0.22	70,70,70,70	0
56	MG	GB	9128	1/1	0.58	0.21	136,136,136,136	0
56	MG	A	1770	1/1	0.58	0.13	163,163,163,163	0
56	MG	UB	201	1/1	0.58	0.14	149,149,149,149	0
56	MG	A	1624	1/1	0.58	0.20	144,144,144,144	0
56	MG	B	9303	1/1	0.58	0.25	120,120,120,120	0
56	MG	FB	1697	1/1	0.58	0.16	149,149,149,149	0
56	MG	A	1758	1/1	0.58	0.10	98,98,98,98	0
56	MG	GB	9095	1/1	0.58	0.37	108,108,108,108	0
56	MG	GB	9152	1/1	0.58	0.21	119,119,119,119	0
56	MG	B	9243	1/1	0.58	0.13	153,153,153,153	0
56	MG	GB	9035	1/1	0.58	0.22	104,104,104,104	0
56	MG	GB	9112	1/1	0.58	0.18	139,139,139,139	0
56	MG	B	9098	1/1	0.58	0.25	114,114,114,114	0
56	MG	B	9013	1/1	0.58	0.22	96,96,96,96	0
56	MG	GB	9051	1/1	0.58	0.33	106,106,106,106	0
56	MG	B	9220	1/1	0.58	0.19	112,112,112,112	0
56	MG	B	9156	1/1	0.59	0.17	145,145,145,145	0
56	MG	GB	9116	1/1	0.59	0.20	124,124,124,124	0
56	MG	GB	9172	1/1	0.59	0.17	135,135,135,135	0
56	MG	B	9267	1/1	0.59	0.11	164,164,164,164	0
56	MG	GB	9331	1/1	0.59	0.09	143,143,143,143	0
56	MG	B	9327	1/1	0.59	0.19	139,139,139,139	0
56	MG	A	1623	1/1	0.59	0.28	119,119,119,119	0
56	MG	GB	9127	1/1	0.59	0.18	119,119,119,119	0
56	MG	B	9112	1/1	0.59	0.22	138,138,138,138	0
56	MG	UA	201	1/1	0.59	0.09	139,139,139,139	0
56	MG	VA	201	1/1	0.59	0.10	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9428	1/1	0.59	0.15	138,138,138,138	0
56	MG	B	9307	1/1	0.59	0.14	142,142,142,142	0
56	MG	GB	9103	1/1	0.59	0.20	126,126,126,126	0
56	MG	H	201	1/1	0.59	0.23	146,146,146,146	0
56	MG	GB	9108	1/1	0.59	0.47	116,116,116,116	0
56	MG	FB	1731	1/1	0.59	0.18	156,156,156,156	0
56	MG	A	1715	1/1	0.59	0.21	121,121,121,121	0
56	MG	GB	9123	1/1	0.60	0.27	109,109,109,109	0
56	MG	B	9235	1/1	0.60	0.12	165,165,165,165	0
56	MG	FB	1605	1/1	0.60	0.37	103,103,103,103	0
56	MG	GB	9207	1/1	0.60	0.23	119,119,119,119	0
56	MG	GB	9075	1/1	0.60	0.20	129,129,129,129	0
56	MG	B	9105	1/1	0.60	0.32	111,111,111,111	0
56	MG	A	1693	1/1	0.60	0.11	154,154,154,154	0
56	MG	A	1780	1/1	0.60	0.17	163,163,163,163	0
56	MG	J	201	1/1	0.60	0.13	157,157,157,157	0
56	MG	GB	9026	1/1	0.60	0.26	88,88,88,88	0
56	MG	FB	1620	1/1	0.60	0.18	126,126,126,126	0
56	MG	A	1745	1/1	0.60	0.14	172,172,172,172	0
56	MG	B	9260	1/1	0.60	0.24	103,103,103,103	0
56	MG	B	9043	1/1	0.60	0.24	95,95,95,95	0
56	MG	FB	1658	1/1	0.60	0.37	119,119,119,119	0
56	MG	FB	1706	1/1	0.60	0.26	117,117,117,117	0
56	MG	A	1756	1/1	0.60	0.19	102,102,102,102	0
56	MG	B	9234	1/1	0.60	0.18	130,130,130,130	0
56	MG	IA	107	1/1	0.60	0.13	109,109,109,109	0
56	MG	GB	9375	1/1	0.60	0.09	152,152,152,152	0
56	MG	C	221	1/1	0.60	0.22	157,157,157,157	0
56	MG	B	9015	1/1	0.61	0.29	84,84,84,84	0
56	MG	A	1699	1/1	0.61	0.18	136,136,136,136	0
56	MG	FB	1613	1/1	0.61	0.37	105,105,105,105	0
56	MG	GB	9146	1/1	0.61	0.16	116,116,116,116	0
56	MG	GB	9151	1/1	0.61	0.23	104,104,104,104	0
56	MG	FB	1744	1/1	0.61	0.17	135,135,135,135	0
56	MG	A	1738	1/1	0.61	0.20	127,127,127,127	0
56	MG	GB	9022	1/1	0.61	0.41	99,99,99,99	0
56	MG	B	9284	1/1	0.61	0.17	128,128,128,128	0
56	MG	GB	9385	1/1	0.61	0.19	105,105,105,105	0
56	MG	SA	201	1/1	0.61	0.13	169,169,169,169	0
56	MG	B	9418	1/1	0.61	0.19	111,111,111,111	0
56	MG	B	9076	1/1	0.61	0.22	104,104,104,104	0
56	MG	B	9080	1/1	0.61	0.26	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	A	1665	1/1	0.61	0.18	134,134,134,134	0
56	MG	A	1606	1/1	0.61	0.20	109,109,109,109	0
56	MG	B	9045	1/1	0.61	0.40	105,105,105,105	0
56	MG	HD	101	1/1	0.61	0.22	150,150,150,150	0
56	MG	GB	9349	1/1	0.62	0.12	134,134,134,134	0
56	MG	FB	1614	1/1	0.62	0.32	125,125,125,125	0
56	MG	A	1604	1/1	0.62	0.20	125,125,125,125	0
56	MG	A	1729	1/1	0.62	0.17	141,141,141,141	0
56	MG	GB	9119	1/1	0.62	0.34	126,126,126,126	0
56	MG	B	9171	1/1	0.62	0.17	150,150,150,150	0
56	MG	A	1663	1/1	0.62	0.20	135,135,135,135	0
56	MG	B	9084	1/1	0.62	0.25	101,101,101,101	0
56	MG	GB	9308	1/1	0.62	0.30	102,102,102,102	0
56	MG	B	9025	1/1	0.62	0.40	87,87,87,87	0
56	MG	GB	9067	1/1	0.62	0.19	105,105,105,105	0
56	MG	GB	9113	1/1	0.62	0.24	99,99,99,99	0
56	MG	GB	9328	1/1	0.62	0.10	152,152,152,152	0
56	MG	A	1613	1/1	0.62	0.33	121,121,121,121	0
56	MG	GB	9038	1/1	0.62	0.30	98,98,98,98	0
56	MG	GB	9279	1/1	0.62	0.12	140,140,140,140	0
56	MG	GB	9343	1/1	0.62	0.09	133,133,133,133	0
56	MG	B	9101	1/1	0.63	0.19	102,102,102,102	0
56	MG	B	9265	1/1	0.63	0.13	136,136,136,136	0
56	MG	GB	9395	1/1	0.63	0.09	158,158,158,158	0
56	MG	B	9310	1/1	0.63	0.08	162,162,162,162	0
56	MG	A	1776	1/1	0.63	0.23	144,144,144,144	0
56	MG	QC	302	1/1	0.63	0.19	143,143,143,143	0
56	MG	B	9289	1/1	0.63	0.23	138,138,138,138	0
56	MG	B	9254	1/1	0.63	0.13	188,188,188,188	0
56	MG	C	208	1/1	0.63	0.15	164,164,164,164	0
56	MG	A	1783	1/1	0.63	0.16	160,160,160,160	0
56	MG	HB	219	1/1	0.63	0.17	141,141,141,141	0
56	MG	GB	9246	1/1	0.63	0.13	133,133,133,133	0
56	MG	MC	103	1/1	0.64	0.20	140,140,140,140	0
56	MG	FB	1723	1/1	0.64	0.25	181,181,181,181	0
56	MG	B	9129	1/1	0.64	0.21	108,108,108,108	0
56	MG	GB	9010	1/1	0.64	0.30	92,92,92,92	0
56	MG	YA	101	1/1	0.64	0.23	126,126,126,126	0
56	MG	A	1707	1/1	0.64	0.23	164,164,164,164	0
56	MG	FB	1637	1/1	0.64	0.36	109,109,109,109	0
56	MG	B	9180	1/1	0.64	0.15	178,178,178,178	0
56	MG	B	9023	1/1	0.64	0.32	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9186	1/1	0.64	0.17	116,116,116,116	0
56	MG	GB	9083	1/1	0.64	0.23	125,125,125,125	0
56	MG	A	1726	1/1	0.65	0.14	140,140,140,140	0
56	MG	GB	9039	1/1	0.65	0.29	130,130,130,130	0
56	MG	GB	9090	1/1	0.65	0.25	129,129,129,129	0
56	MG	C	207	1/1	0.65	0.12	152,152,152,152	0
56	MG	FB	1645	1/1	0.65	0.17	144,144,144,144	0
56	MG	GB	9044	1/1	0.65	0.23	119,119,119,119	0
56	MG	FB	1603	1/1	0.65	0.29	118,118,118,118	0
56	MG	FB	1771	1/1	0.65	0.17	138,138,138,138	0
56	MG	B	9055	1/1	0.65	0.18	127,127,127,127	0
56	MG	GB	9109	1/1	0.65	0.17	111,111,111,111	0
56	MG	GB	9190	1/1	0.65	0.23	112,112,112,112	0
56	MG	FB	1650	1/1	0.65	0.26	135,135,135,135	0
56	MG	B	9423	1/1	0.65	0.25	117,117,117,117	0
56	MG	GB	9392	1/1	0.65	0.20	147,147,147,147	0
56	MG	B	9373	1/1	0.65	0.14	160,160,160,160	0
56	MG	F	303	1/1	0.65	0.12	131,131,131,131	0
56	MG	GB	9270	1/1	0.65	0.17	123,123,123,123	0
56	MG	GB	9271	1/1	0.65	0.29	126,126,126,126	0
56	MG	A	1688	1/1	0.65	0.13	170,170,170,170	0
56	MG	JB	303	1/1	0.66	0.10	102,102,102,102	0
56	MG	A	1666	1/1	0.66	0.25	123,123,123,123	0
56	MG	GB	9092	1/1	0.66	0.22	110,110,110,110	0
56	MG	FB	1703	1/1	0.66	0.17	116,116,116,116	0
56	MG	A	1605	1/1	0.66	0.25	119,119,119,119	0
56	MG	A	1727	1/1	0.66	0.18	161,161,161,161	0
56	MG	GB	9129	1/1	0.66	0.09	103,103,103,103	0
56	MG	FB	1673	1/1	0.66	0.21	133,133,133,133	0
56	MG	FB	1647	1/1	0.66	0.23	136,136,136,136	0
56	MG	C	203	1/1	0.66	0.17	161,161,161,161	0
56	MG	GB	9201	1/1	0.66	0.23	107,107,107,107	0
56	MG	GB	9203	1/1	0.66	0.17	100,100,100,100	0
56	MG	FB	1617	1/1	0.66	0.26	110,110,110,110	0
56	MG	GB	9110	1/1	0.66	0.17	98,98,98,98	0
56	MG	FB	1685	1/1	0.66	0.13	141,141,141,141	0
56	MG	D	101	1/1	0.66	0.13	231,231,231,231	0
56	MG	GB	9380	1/1	0.66	0.11	120,120,120,120	0
56	MG	B	9232	1/1	0.66	0.22	111,111,111,111	0
56	MG	B	9038	1/1	0.66	0.31	85,85,85,85	0
56	MG	GB	9153	1/1	0.66	0.15	110,110,110,110	0
56	MG	A	1718	1/1	0.66	0.20	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	A	1755	1/1	0.66	0.25	110,110,110,110	0
56	MG	GB	9084	1/1	0.66	0.26	111,111,111,111	0
56	MG	A	1700	1/1	0.67	0.14	97,97,97,97	0
56	MG	A	1781	1/1	0.67	0.12	149,149,149,149	0
56	MG	GB	9227	1/1	0.67	0.25	116,116,116,116	0
56	MG	B	9052	1/1	0.67	0.26	114,114,114,114	0
56	MG	A	1698	1/1	0.67	0.13	171,171,171,171	0
56	MG	FB	1781	1/1	0.67	0.39	179,179,179,179	0
56	MG	NC	105	1/1	0.67	0.05	174,174,174,174	0
56	MG	O	202	1/1	0.67	0.28	102,102,102,102	0
56	MG	PC	401	1/1	0.67	0.15	167,167,167,167	0
56	MG	FB	1759	1/1	0.67	0.30	134,134,134,134	0
56	MG	FB	1639	1/1	0.67	0.16	123,123,123,123	0
56	MG	GB	9244	1/1	0.67	0.20	132,132,132,132	0
56	MG	GB	9060	1/1	0.67	0.24	124,124,124,124	0
56	MG	A	1645	1/1	0.67	0.42	131,131,131,131	0
56	MG	FB	1767	1/1	0.67	0.15	137,137,137,137	0
56	MG	GB	9254	1/1	0.67	0.10	109,109,109,109	0
56	MG	GB	9185	1/1	0.68	0.16	120,120,120,120	0
56	MG	SB	202	1/1	0.68	0.21	137,137,137,137	0
56	MG	GB	9290	1/1	0.68	0.15	146,146,146,146	0
56	MG	UB	202	1/1	0.68	0.35	164,164,164,164	0
56	MG	B	9044	1/1	0.68	0.36	73,73,73,73	0
56	MG	GB	9243	1/1	0.68	0.15	127,127,127,127	0
56	MG	GB	9149	1/1	0.68	0.10	108,108,108,108	0
56	MG	A	1676	1/1	0.68	0.26	133,133,133,133	0
56	MG	GB	9104	1/1	0.68	0.18	103,103,103,103	0
56	MG	FB	1670	1/1	0.68	0.18	197,197,197,197	0
56	MG	GB	9155	1/1	0.68	0.15	150,150,150,150	0
56	MG	B	9078	1/1	0.68	0.24	88,88,88,88	0
56	MG	GB	9040	1/1	0.68	0.25	113,113,113,113	0
56	MG	GB	9020	1/1	0.68	0.48	94,94,94,94	0
56	MG	GB	9218	1/1	0.68	0.15	108,108,108,108	0
56	MG	B	9210	1/1	0.68	0.17	133,133,133,133	0
56	MG	C	209	1/1	0.68	0.29	130,130,130,130	0
56	MG	OA	204	1/1	0.68	0.10	134,134,134,134	0
56	MG	A	1690	1/1	0.68	0.32	105,105,105,105	0
56	MG	B	9140	1/1	0.68	0.21	111,111,111,111	0
56	MG	WC	201	1/1	0.68	0.11	134,134,134,134	0
56	MG	FB	1729	1/1	0.68	0.19	134,134,134,134	0
56	MG	PB	201	1/1	0.68	0.10	134,134,134,134	0
56	MG	G	301	1/1	0.69	0.15	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	A	1710	1/1	0.69	0.29	148,148,148,148	0
56	MG	FB	1640	1/1	0.69	0.16	103,103,103,103	0
56	MG	B	9182	1/1	0.69	0.11	116,116,116,116	0
56	MG	B	9308	1/1	0.69	0.10	125,125,125,125	0
56	MG	K	204	1/1	0.69	0.11	133,133,133,133	0
56	MG	C	211	1/1	0.69	0.14	149,149,149,149	0
56	MG	GB	9240	1/1	0.69	0.13	113,113,113,113	0
56	MG	GB	9319	1/1	0.69	0.27	104,104,104,104	0
56	MG	LB	304	1/1	0.69	0.12	127,127,127,127	0
56	MG	A	1759	1/1	0.69	0.40	175,175,175,175	0
56	MG	GB	9321	1/1	0.69	0.13	147,147,147,147	0
56	MG	MA	301	1/1	0.69	0.16	152,152,152,152	0
56	MG	FB	1727	1/1	0.69	0.23	119,119,119,119	0
56	MG	GB	9388	1/1	0.69	0.18	108,108,108,108	0
56	MG	HB	213	1/1	0.69	0.06	187,187,187,187	0
56	MG	A	1763	1/1	0.69	0.11	104,104,104,104	0
56	MG	B	9224	1/1	0.69	0.17	120,120,120,120	0
56	MG	C	202	1/1	0.70	0.29	126,126,126,126	0
56	MG	AB	201	1/1	0.70	0.15	135,135,135,135	0
56	MG	B	9258	1/1	0.70	0.10	109,109,109,109	0
56	MG	GB	9015	1/1	0.70	0.24	86,86,86,86	0
56	MG	A	1704	1/1	0.70	0.15	106,106,106,106	0
56	MG	A	1607	1/1	0.70	0.28	122,122,122,122	0
56	MG	BC	301	1/1	0.70	0.20	136,136,136,136	0
56	MG	GB	9088	1/1	0.70	0.21	115,115,115,115	0
56	MG	FB	1766	1/1	0.70	0.29	110,110,110,110	0
56	MG	GB	9304	1/1	0.70	0.17	102,102,102,102	0
56	MG	GB	9091	1/1	0.70	0.20	107,107,107,107	0
56	MG	K	201	1/1	0.70	0.08	128,128,128,128	0
56	MG	GB	9310	1/1	0.70	0.21	124,124,124,124	0
56	MG	A	1777	1/1	0.70	0.18	152,152,152,152	0
56	MG	A	1696	1/1	0.70	0.10	106,106,106,106	0
56	MG	FB	1776	1/1	0.70	0.11	214,214,214,214	0
56	MG	GB	9220	1/1	0.70	0.21	122,122,122,122	0
56	MG	GB	9168	1/1	0.70	0.15	115,115,115,115	0
56	MG	GB	9056	1/1	0.70	0.25	93,93,93,93	0
56	MG	GB	9400	1/1	0.70	0.09	150,150,150,150	0
56	MG	FB	1607	1/1	0.70	0.33	99,99,99,99	0
56	MG	B	9092	1/1	0.70	0.13	140,140,140,140	0
56	MG	A	1658	1/1	0.70	0.31	177,177,177,177	0
56	MG	GB	9339	1/1	0.70	0.24	102,102,102,102	0
56	MG	FB	1753	1/1	0.71	0.22	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	GB	9225	1/1	0.71	0.12	93,93,93,93	0
56	MG	MA	306	1/1	0.71	0.11	149,149,149,149	0
56	MG	A	1734	1/1	0.71	0.16	143,143,143,143	0
56	MG	B	9213	1/1	0.71	0.20	105,105,105,105	0
56	MG	C	204	1/1	0.71	0.27	113,113,113,113	0
56	MG	GB	9120	1/1	0.71	0.11	101,101,101,101	0
56	MG	B	9115	1/1	0.71	0.27	119,119,119,119	0
56	MG	A	1728	1/1	0.71	0.07	183,183,183,183	0
56	MG	GB	9107	1/1	0.71	0.14	88,88,88,88	0
56	MG	GB	9280	1/1	0.71	0.16	104,104,104,104	0
56	MG	A	1630	1/1	0.71	0.30	112,112,112,112	0
56	MG	SC	304	1/1	0.71	0.11	116,116,116,116	0
56	MG	B	9429	1/1	0.71	0.16	100,100,100,100	0
56	MG	FB	1737	1/1	0.71	0.11	114,114,114,114	0
56	MG	FB	1609	1/1	0.71	0.38	110,110,110,110	0
56	MG	ZC	201	1/1	0.71	0.28	126,126,126,126	0
56	MG	B	9121	1/1	0.71	0.22	142,142,142,142	0
56	MG	B	9335	1/1	0.71	0.13	126,126,126,126	0
56	MG	GB	9125	1/1	0.72	0.26	89,89,89,89	0
56	MG	A	1669	1/1	0.72	0.16	132,132,132,132	0
56	MG	GB	9377	1/1	0.72	0.39	114,114,114,114	0
56	MG	A	1749	1/1	0.72	0.10	129,129,129,129	0
56	MG	GB	9021	1/1	0.72	0.37	109,109,109,109	0
56	MG	FB	1663	1/1	0.72	0.14	110,110,110,110	0
56	MG	GB	9133	1/1	0.72	0.23	107,107,107,107	0
56	MG	PA	201	1/1	0.72	0.07	109,109,109,109	0
56	MG	RB	202	1/1	0.72	0.10	134,134,134,134	0
56	MG	A	1633	1/1	0.72	0.30	112,112,112,112	0
56	MG	GB	9219	1/1	0.72	0.16	143,143,143,143	0
56	MG	GB	9296	1/1	0.72	0.14	133,133,133,133	0
56	MG	D	104	1/1	0.72	0.12	131,131,131,131	0
56	MG	B	9338	1/1	0.72	0.39	112,112,112,112	0
56	MG	FB	1616	1/1	0.72	0.40	108,108,108,108	0
56	MG	B	9348	1/1	0.72	0.12	151,151,151,151	0
56	MG	FB	1770	1/1	0.72	0.12	133,133,133,133	0
56	MG	FB	1678	1/1	0.72	0.24	115,115,115,115	0
56	MG	B	9062	1/1	0.72	0.19	109,109,109,109	0
56	MG	FB	1774	1/1	0.72	0.23	118,118,118,118	0
56	MG	YA	102	1/1	0.72	0.16	134,134,134,134	0
56	MG	A	1732	1/1	0.72	0.22	139,139,139,139	0
56	MG	B	9125	1/1	0.72	0.32	100,100,100,100	0
56	MG	NC	107	1/1	0.72	0.19	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	NC	108	1/1	0.72	0.13	136,136,136,136	0
56	MG	GB	9241	1/1	0.72	0.26	113,113,113,113	0
56	MG	C	217	1/1	0.72	0.13	140,140,140,140	0
56	MG	B	9314	1/1	0.72	0.15	131,131,131,131	0
56	MG	GB	9004	1/1	0.72	0.40	88,88,88,88	0
56	MG	GB	9007	1/1	0.72	0.28	75,75,75,75	0
56	MG	GB	9008	1/1	0.72	0.28	83,83,83,83	0
56	MG	FB	1696	1/1	0.72	0.18	191,191,191,191	0
56	MG	GB	9061	1/1	0.72	0.16	108,108,108,108	0
56	MG	B	9212	1/1	0.72	0.21	108,108,108,108	0
56	MG	FB	1738	1/1	0.72	0.23	143,143,143,143	0
56	MG	B	9050	1/1	0.72	0.44	105,105,105,105	0
56	MG	Y	102	1/1	0.72	0.09	126,126,126,126	0
56	MG	A	1682	1/1	0.73	0.18	136,136,136,136	0
56	MG	B	9269	1/1	0.73	0.12	153,153,153,153	0
56	MG	FB	1660	1/1	0.73	0.32	102,102,102,102	0
56	MG	GB	9089	1/1	0.73	0.30	113,113,113,113	0
56	MG	RB	201	1/1	0.73	0.25	87,87,87,87	0
56	MG	B	9272	1/1	0.73	0.16	116,116,116,116	0
56	MG	GB	9175	1/1	0.73	0.18	92,92,92,92	0
56	MG	GB	9176	1/1	0.73	0.19	104,104,104,104	0
56	MG	Z	101	1/1	0.73	0.20	105,105,105,105	0
56	MG	B	9375	1/1	0.73	0.07	95,95,95,95	0
56	MG	B	9100	1/1	0.73	0.17	100,100,100,100	0
56	MG	A	1648	1/1	0.73	0.13	130,130,130,130	0
56	MG	GB	9188	1/1	0.73	0.22	90,90,90,90	0
56	MG	A	1603	1/1	0.73	0.24	102,102,102,102	0
56	MG	GB	9323	1/1	0.73	0.23	98,98,98,98	0
56	MG	GB	9250	1/1	0.73	0.20	132,132,132,132	0
56	MG	GB	9102	1/1	0.73	0.26	81,81,81,81	0
56	MG	GB	9197	1/1	0.73	0.18	91,91,91,91	0
56	MG	IA	105	1/1	0.73	0.24	135,135,135,135	0
56	MG	GB	9259	1/1	0.73	0.16	91,91,91,91	0
56	MG	D	105	1/1	0.73	0.09	129,129,129,129	0
56	MG	HB	212	1/1	0.73	0.30	130,130,130,130	0
56	MG	GB	9054	1/1	0.73	0.31	105,105,105,105	0
56	MG	FB	1677	1/1	0.73	0.21	119,119,119,119	0
56	MG	B	9253	1/1	0.73	0.12	107,107,107,107	0
56	MG	FB	1724	1/1	0.73	0.34	162,162,162,162	0
56	MG	A	1725	1/1	0.73	0.30	126,126,126,126	0
56	MG	GB	9368	1/1	0.73	0.07	139,139,139,139	0
56	MG	B	9064	1/1	0.73	0.20	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9401	1/1	0.73	0.07	139,139,139,139	0
56	MG	A	1730	1/1	0.73	0.15	115,115,115,115	0
56	MG	B	9067	1/1	0.73	0.19	89,89,89,89	0
56	MG	B	9136	1/1	0.73	0.17	121,121,121,121	0
56	MG	GB	9030	1/1	0.73	0.33	80,80,80,80	0
56	MG	B	9054	1/1	0.74	0.27	115,115,115,115	0
56	MG	GB	9063	1/1	0.74	0.18	115,115,115,115	0
56	MG	B	9262	1/1	0.74	0.23	110,110,110,110	0
56	MG	B	9347	1/1	0.74	0.09	115,115,115,115	0
56	MG	FB	1666	1/1	0.74	0.13	128,128,128,128	0
56	MG	GB	9076	1/1	0.74	0.18	104,104,104,104	0
56	MG	A	1668	1/1	0.74	0.14	147,147,147,147	0
56	MG	FB	1682	1/1	0.74	0.17	130,130,130,130	0
56	MG	A	1701	1/1	0.74	0.20	160,160,160,160	0
56	MG	GB	9191	1/1	0.74	0.17	116,116,116,116	0
56	MG	B	9383	1/1	0.74	0.18	116,116,116,116	0
56	MG	A	1675	1/1	0.75	0.20	96,96,96,96	0
56	MG	B	9376	1/1	0.75	0.17	94,94,94,94	0
56	MG	GB	9287	1/1	0.75	0.07	164,164,164,164	0
56	MG	B	9193	1/1	0.75	0.23	96,96,96,96	0
56	MG	MA	303	1/1	0.75	0.10	139,139,139,139	0
56	MG	AA	101	1/1	0.75	0.20	106,106,106,106	0
56	MG	B	9037	1/1	0.75	0.24	89,89,89,89	0
56	MG	B	9169	1/1	0.75	0.24	110,110,110,110	0
56	MG	B	9204	1/1	0.75	0.22	113,113,113,113	0
56	MG	B	9241	1/1	0.75	0.08	118,118,118,118	0
56	MG	GB	9182	1/1	0.75	0.17	125,125,125,125	0
56	MG	GB	9130	1/1	0.75	0.21	116,116,116,116	0
56	MG	FB	1692	1/1	0.75	0.17	129,129,129,129	0
56	MG	A	1737	1/1	0.75	0.20	131,131,131,131	0
56	MG	GB	9309	1/1	0.75	0.11	109,109,109,109	0
56	MG	GB	9135	1/1	0.75	0.24	105,105,105,105	0
56	MG	GB	9311	1/1	0.75	0.12	132,132,132,132	0
56	MG	GB	9058	1/1	0.75	0.29	117,117,117,117	0
56	MG	B	9301	1/1	0.75	0.11	119,119,119,119	0
56	MG	FB	1625	1/1	0.75	0.23	99,99,99,99	0
56	MG	A	1649	1/1	0.75	0.19	88,88,88,88	0
56	MG	FB	1629	1/1	0.75	0.12	101,101,101,101	0
56	MG	GB	9324	1/1	0.75	0.11	153,153,153,153	0
56	MG	NC	106	1/1	0.75	0.17	108,108,108,108	0
56	MG	FB	1674	1/1	0.75	0.25	107,107,107,107	0
56	MG	GB	9326	1/1	0.75	0.11	180,180,180,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	GB	9147	1/1	0.75	0.28	114,114,114,114	0
56	MG	GB	9329	1/1	0.75	0.16	91,91,91,91	0
56	MG	GB	9072	1/1	0.75	0.16	113,113,113,113	0
56	MG	GB	9263	1/1	0.75	0.12	148,148,148,148	0
56	MG	B	9417	1/1	0.75	0.14	113,113,113,113	0
56	MG	FB	1707	1/1	0.75	0.35	113,113,113,113	0
56	MG	FB	1782	1/1	0.75	0.17	175,175,175,175	0
56	MG	FB	1790	1/1	0.75	0.10	138,138,138,138	0
56	MG	GB	9157	1/1	0.75	0.09	143,143,143,143	0
56	MG	GB	9276	1/1	0.75	0.18	94,94,94,94	0
56	MG	FB	1745	1/1	0.75	0.22	138,138,138,138	0
56	MG	GB	9360	1/1	0.75	0.14	101,101,101,101	0
56	MG	GB	9268	1/1	0.76	0.17	109,109,109,109	0
56	MG	MA	302	1/1	0.76	0.11	157,157,157,157	0
56	MG	B	9248	1/1	0.76	0.22	104,104,104,104	0
56	MG	CC	101	1/1	0.76	0.52	111,111,111,111	0
56	MG	DC	101	1/1	0.76	0.20	122,122,122,122	0
56	MG	B	9058	1/1	0.76	0.17	151,151,151,151	0
56	MG	GB	9086	1/1	0.76	0.13	123,123,123,123	0
56	MG	GB	9053	1/1	0.76	0.36	88,88,88,88	0
56	MG	FB	1783	1/1	0.76	0.14	160,160,160,160	0
56	MG	FB	1788	1/1	0.76	0.11	127,127,127,127	0
56	MG	B	9334	1/1	0.76	0.21	91,91,91,91	0
56	MG	B	9221	1/1	0.76	0.15	161,161,161,161	0
56	MG	B	9419	1/1	0.76	0.10	102,102,102,102	0
56	MG	GB	9031	1/1	0.76	0.32	96,96,96,96	0
56	MG	B	9181	1/1	0.76	0.12	97,97,97,97	0
56	MG	GB	9292	1/1	0.76	0.21	122,122,122,122	0
56	MG	GB	9293	1/1	0.76	0.10	90,90,90,90	0
56	MG	GB	9101	1/1	0.76	0.27	84,84,84,84	0
56	MG	A	1628	1/1	0.76	0.19	101,101,101,101	0
56	MG	FB	1695	1/1	0.76	0.24	118,118,118,118	0
56	MG	B	9319	1/1	0.76	0.08	110,110,110,110	0
56	MG	GB	9068	1/1	0.76	0.25	100,100,100,100	0
56	MG	TC	202	1/1	0.76	0.14	135,135,135,135	0
56	MG	B	9175	1/1	0.76	0.19	102,102,102,102	0
56	MG	HB	206	1/1	0.76	0.18	141,141,141,141	0
56	MG	E	306	1/1	0.76	0.07	88,88,88,88	0
56	MG	A	1616	1/1	0.76	0.25	101,101,101,101	0
56	MG	FB	1778	1/1	0.76	0.12	121,121,121,121	0
56	MG	GB	9316	1/1	0.77	0.12	157,157,157,157	0
56	MG	B	9007	1/1	0.77	0.52	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9402	1/1	0.77	0.20	104,104,104,104	0
56	MG	GB	9080	1/1	0.77	0.29	84,84,84,84	0
56	MG	B	9206	1/1	0.77	0.19	96,96,96,96	0
56	MG	GB	9154	1/1	0.77	0.25	114,114,114,114	0
56	MG	B	9239	1/1	0.77	0.16	86,86,86,86	0
56	MG	GB	9215	1/1	0.77	0.20	145,145,145,145	0
56	MG	B	9133	1/1	0.77	0.18	89,89,89,89	0
56	MG	B	9134	1/1	0.77	0.23	80,80,80,80	0
56	MG	B	9245	1/1	0.77	0.40	103,103,103,103	0
56	MG	A	1654	1/1	0.77	0.25	98,98,98,98	0
56	MG	A	1706	1/1	0.77	0.11	147,147,147,147	0
56	MG	A	1752	1/1	0.77	0.24	112,112,112,112	0
56	MG	GB	9126	1/1	0.77	0.20	109,109,109,109	0
56	MG	A	1615	1/1	0.77	0.29	101,101,101,101	0
56	MG	A	1614	1/1	0.77	0.23	116,116,116,116	0
56	MG	GB	9231	1/1	0.77	0.16	96,96,96,96	0
56	MG	FB	1690	1/1	0.77	0.21	107,107,107,107	0
56	MG	GB	9178	1/1	0.77	0.16	115,115,115,115	0
56	MG	GB	9364	1/1	0.77	0.14	122,122,122,122	0
56	MG	GB	9180	1/1	0.77	0.34	104,104,104,104	0
56	MG	B	9032	1/1	0.77	0.29	73,73,73,73	0
56	MG	QC	301	1/1	0.77	0.19	133,133,133,133	0
56	MG	C	205	1/1	0.77	0.17	101,101,101,101	0
56	MG	A	1711	1/1	0.77	0.21	110,110,110,110	0
56	MG	B	9230	1/1	0.77	0.15	129,129,129,129	0
56	MG	GB	9105	1/1	0.77	0.20	116,116,116,116	0
56	MG	FB	1733	1/1	0.77	0.08	92,92,92,92	0
56	MG	B	9192	1/1	0.77	0.13	132,132,132,132	0
56	MG	UC	202	1/1	0.77	0.11	138,138,138,138	0
56	MG	FB	1736	1/1	0.77	0.16	120,120,120,120	0
56	MG	B	9127	1/1	0.77	0.34	104,104,104,104	0
56	MG	B	9158	1/1	0.77	0.20	90,90,90,90	0
56	MG	A	1712	1/1	0.77	0.11	198,198,198,198	0
56	MG	QB	201	1/1	0.77	0.26	104,104,104,104	0
56	MG	A	1740	1/1	0.78	0.19	108,108,108,108	0
56	MG	FB	1657	1/1	0.78	0.17	166,166,166,166	0
56	MG	GB	9150	1/1	0.78	0.25	143,143,143,143	0
56	MG	B	9231	1/1	0.78	0.13	85,85,85,85	0
56	MG	B	9061	1/1	0.78	0.27	104,104,104,104	0
56	MG	B	9403	1/1	0.78	0.16	132,132,132,132	0
56	MG	A	1691	1/1	0.78	0.08	145,145,145,145	0
56	MG	FB	1722	1/1	0.78	0.17	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9368	1/1	0.78	0.21	92,92,92,92	0
56	MG	B	9194	1/1	0.78	0.09	151,151,151,151	0
56	MG	FB	1794	1/1	0.78	0.20	125,125,125,125	0
56	MG	B	9075	1/1	0.78	0.31	106,106,106,106	0
56	MG	GB	9253	1/1	0.78	0.22	104,104,104,104	0
56	MG	FB	1693	1/1	0.78	0.17	160,160,160,160	0
56	MG	B	9288	1/1	0.78	0.12	153,153,153,153	0
56	MG	SC	301	1/1	0.78	0.25	102,102,102,102	0
56	MG	B	9104	1/1	0.78	0.14	78,78,78,78	0
56	MG	SC	303	1/1	0.78	0.08	114,114,114,114	0
56	MG	B	9380	1/1	0.78	0.18	100,100,100,100	0
56	MG	B	9291	1/1	0.78	0.12	77,77,77,77	0
56	MG	B	9203	1/1	0.78	0.13	128,128,128,128	0
56	MG	GB	9177	1/1	0.78	0.27	124,124,124,124	0
56	MG	UC	203	1/1	0.78	0.08	120,120,120,120	0
56	MG	GB	9111	1/1	0.78	0.25	102,102,102,102	0
56	MG	GB	9047	1/1	0.78	0.48	99,99,99,99	0
56	MG	B	9040	1/1	0.78	0.36	98,98,98,98	0
56	MG	B	9142	1/1	0.78	0.18	116,116,116,116	0
56	MG	B	9229	1/1	0.78	0.14	100,100,100,100	0
56	MG	GB	9374	1/1	0.79	0.27	117,117,117,117	0
56	MG	B	9316	1/1	0.79	0.11	126,126,126,126	0
56	MG	GB	9267	1/1	0.79	0.10	118,118,118,118	0
56	MG	B	9151	1/1	0.79	0.16	95,95,95,95	0
56	MG	B	9355	1/1	0.79	0.07	158,158,158,158	0
56	MG	B	9367	1/1	0.79	0.12	102,102,102,102	0
56	MG	B	9021	1/1	0.79	0.43	79,79,79,79	0
56	MG	B	9073	1/1	0.79	0.20	79,79,79,79	0
56	MG	FB	1619	1/1	0.79	0.19	125,125,125,125	0
56	MG	A	1621	1/1	0.79	0.17	105,105,105,105	0
56	MG	FB	1621	1/1	0.79	0.32	97,97,97,97	0
56	MG	FB	1679	1/1	0.79	0.08	244,244,244,244	0
56	MG	B	9255	1/1	0.79	0.16	100,100,100,100	0
56	MG	B	9422	1/1	0.79	0.11	148,148,148,148	0
56	MG	B	9161	1/1	0.79	0.22	94,94,94,94	0
56	MG	GB	9012	1/1	0.79	0.44	77,77,77,77	0
56	MG	B	9071	1/1	0.79	0.20	85,85,85,85	0
56	MG	B	9124	1/1	0.79	0.26	94,94,94,94	0
56	MG	GB	9294	1/1	0.79	0.16	131,131,131,131	0
56	MG	B	9345	1/1	0.79	0.10	85,85,85,85	0
56	MG	FB	1726	1/1	0.79	0.19	107,107,107,107	0
56	MG	MA	305	1/1	0.79	0.08	156,156,156,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	C	220	1/1	0.79	0.14	161,161,161,161	0
56	MG	GB	9096	1/1	0.79	0.24	114,114,114,114	0
56	MG	B	9431	1/1	0.79	0.11	89,89,89,89	0
56	MG	B	9089	1/1	0.79	0.14	126,126,126,126	0
56	MG	FB	1636	1/1	0.79	0.24	103,103,103,103	0
56	MG	B	9150	1/1	0.79	0.15	101,101,101,101	0
56	MG	A	1750	1/1	0.80	0.15	157,157,157,157	0
56	MG	GB	9025	1/1	0.80	0.30	88,88,88,88	0
56	MG	B	9149	1/1	0.80	0.19	104,104,104,104	0
56	MG	FB	1704	1/1	0.80	0.24	129,129,129,129	0
56	MG	A	1667	1/1	0.80	0.38	112,112,112,112	0
56	MG	B	9122	1/1	0.80	0.18	106,106,106,106	0
56	MG	IC	102	1/1	0.80	0.21	131,131,131,131	0
56	MG	FB	1741	1/1	0.80	0.22	106,106,106,106	0
56	MG	B	9200	1/1	0.80	0.15	109,109,109,109	0
56	MG	FB	1628	1/1	0.80	0.23	98,98,98,98	0
56	MG	B	9155	1/1	0.80	0.10	97,97,97,97	0
56	MG	GB	9194	1/1	0.80	0.07	119,119,119,119	0
56	MG	FB	1792	1/1	0.80	0.11	134,134,134,134	0
56	MG	GB	9371	1/1	0.80	0.13	92,92,92,92	0
56	MG	B	9056	1/1	0.80	0.39	94,94,94,94	0
56	MG	FB	1683	1/1	0.80	0.19	104,104,104,104	0
56	MG	FB	1611	1/1	0.80	0.26	112,112,112,112	0
56	MG	IA	106	1/1	0.80	0.10	135,135,135,135	0
56	MG	B	9276	1/1	0.80	0.28	105,105,105,105	0
56	MG	GB	9206	1/1	0.80	0.24	113,113,113,113	0
56	MG	GB	9011	1/1	0.80	0.27	88,88,88,88	0
56	MG	GB	9261	1/1	0.80	0.22	104,104,104,104	0
56	MG	A	1695	1/1	0.80	0.26	101,101,101,101	0
56	MG	A	1766	1/1	0.80	0.21	133,133,133,133	0
56	MG	GB	9213	1/1	0.80	0.13	92,92,92,92	0
56	MG	B	9083	1/1	0.80	0.27	100,100,100,100	0
56	MG	B	9188	1/1	0.80	0.20	95,95,95,95	0
56	MG	B	9393	1/1	0.80	0.10	98,98,98,98	0
56	MG	GB	9397	1/1	0.80	0.16	104,104,104,104	0
56	MG	FB	1668	1/1	0.80	0.28	105,105,105,105	0
56	MG	B	9020	1/1	0.80	0.26	83,83,83,83	0
56	MG	AB	202	1/1	0.80	0.12	133,133,133,133	0
56	MG	AD	201	1/1	0.80	0.20	97,97,97,97	0
56	MG	GB	9131	1/1	0.80	0.21	90,90,90,90	0
56	MG	B	9352	1/1	0.80	0.12	121,121,121,121	0
56	MG	GB	9032	1/1	0.81	0.33	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	FB	1739	1/1	0.81	0.17	115,115,115,115	0
56	MG	GB	9249	1/1	0.81	0.07	107,107,107,107	0
56	MG	GB	9389	1/1	0.81	0.23	107,107,107,107	0
56	MG	A	1757	1/1	0.81	0.09	169,169,169,169	0
56	MG	FB	1701	1/1	0.81	0.23	114,114,114,114	0
56	MG	GB	9330	1/1	0.81	0.12	95,95,95,95	0
56	MG	LB	301	1/1	0.81	0.06	118,118,118,118	0
56	MG	B	9304	1/1	0.81	0.08	86,86,86,86	0
56	MG	GB	9098	1/1	0.81	0.11	122,122,122,122	0
56	MG	B	9432	1/1	0.81	0.24	119,119,119,119	0
56	MG	A	1694	1/1	0.81	0.19	100,100,100,100	0
56	MG	B	9342	1/1	0.81	0.24	104,104,104,104	0
56	MG	FB	1689	1/1	0.81	0.32	109,109,109,109	0
56	MG	FB	1632	1/1	0.81	0.18	104,104,104,104	0
56	MG	FB	1785	1/1	0.81	0.19	123,123,123,123	0
56	MG	A	1697	1/1	0.81	0.14	135,135,135,135	0
56	MG	FB	1760	1/1	0.81	0.08	112,112,112,112	0
56	MG	GB	9164	1/1	0.81	0.28	85,85,85,85	0
56	MG	B	9346	1/1	0.81	0.08	109,109,109,109	0
56	MG	TC	203	1/1	0.81	0.09	134,134,134,134	0
56	MG	B	9099	1/1	0.81	0.27	83,83,83,83	0
56	MG	FB	1664	1/1	0.81	0.16	98,98,98,98	0
56	MG	FB	1718	1/1	0.81	0.13	133,133,133,133	0
56	MG	B	9117	1/1	0.81	0.28	79,79,79,79	0
56	MG	GB	9173	1/1	0.81	0.09	108,108,108,108	0
56	MG	A	1601	1/1	0.81	0.32	75,75,75,75	0
56	MG	GB	9322	1/1	0.81	0.12	112,112,112,112	0
56	MG	ED	101	1/1	0.81	0.10	120,120,120,120	0
56	MG	GB	9286	1/1	0.81	0.27	105,105,105,105	0
56	MG	B	9070	1/1	0.82	0.10	83,83,83,83	0
56	MG	FB	1709	1/1	0.82	0.12	116,116,116,116	0
56	MG	B	9146	1/1	0.82	0.25	78,78,78,78	0
56	MG	FB	1754	1/1	0.82	0.14	155,155,155,155	0
56	MG	FB	1713	1/1	0.82	0.11	163,163,163,163	0
56	MG	GB	9100	1/1	0.82	0.28	112,112,112,112	0
56	MG	B	9270	1/1	0.82	0.14	93,93,93,93	0
56	MG	B	9086	1/1	0.82	0.31	93,93,93,93	0
56	MG	GB	9314	1/1	0.82	0.33	98,98,98,98	0
56	MG	A	1679	1/1	0.82	0.11	125,125,125,125	0
56	MG	FB	1652	1/1	0.82	0.13	111,111,111,111	0
56	MG	GB	9143	1/1	0.82	0.15	94,94,94,94	0
56	MG	A	1743	1/1	0.82	0.17	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9320	1/1	0.82	0.18	86,86,86,86	0
56	MG	FB	1687	1/1	0.82	0.15	116,116,116,116	0
56	MG	A	1610	1/1	0.82	0.15	152,152,152,152	0
56	MG	B	9215	1/1	0.82	0.14	92,92,92,92	0
56	MG	A	1673	1/1	0.82	0.14	121,121,121,121	0
56	MG	FB	1661	1/1	0.82	0.14	90,90,90,90	0
56	MG	GB	9071	1/1	0.82	0.29	105,105,105,105	0
56	MG	B	9004	1/1	0.82	0.34	70,70,70,70	0
56	MG	A	1647	1/1	0.82	0.24	127,127,127,127	0
56	MG	B	9159	1/1	0.82	0.10	163,163,163,163	0
56	MG	NC	110	1/1	0.82	0.28	100,100,100,100	0
56	MG	GB	9162	1/1	0.82	0.09	97,97,97,97	0
56	MG	B	9389	1/1	0.82	0.16	112,112,112,112	0
56	MG	B	9120	1/1	0.82	0.33	91,91,91,91	0
56	MG	B	9162	1/1	0.82	0.10	85,85,85,85	0
56	MG	GB	9081	1/1	0.82	0.22	97,97,97,97	0
56	MG	B	9167	1/1	0.82	0.21	95,95,95,95	0
56	MG	B	9079	1/1	0.82	0.10	73,73,73,73	0
56	MG	GB	9289	1/1	0.82	0.12	95,95,95,95	0
56	MG	GB	9363	1/1	0.82	0.29	97,97,97,97	0
56	MG	GB	9122	1/1	0.82	0.15	88,88,88,88	0
56	MG	B	9009	1/1	0.82	0.29	82,82,82,82	0
56	MG	UC	201	1/1	0.82	0.14	130,130,130,130	0
56	MG	JB	305	1/1	0.82	0.15	112,112,112,112	0
56	MG	GB	9232	1/1	0.82	0.16	106,106,106,106	0
56	MG	B	9069	1/1	0.82	0.20	111,111,111,111	0
56	MG	B	9266	1/1	0.82	0.12	82,82,82,82	0
56	MG	GB	9237	1/1	0.82	0.14	117,117,117,117	0
56	MG	B	9411	1/1	0.82	0.08	139,139,139,139	0
56	MG	FB	1793	1/1	0.82	0.07	138,138,138,138	0
56	MG	GB	9300	1/1	0.82	0.23	107,107,107,107	0
56	MG	B	9350	1/1	0.82	0.16	115,115,115,115	0
56	MG	B	9030	1/1	0.83	0.41	87,87,87,87	0
56	MG	B	9259	1/1	0.83	0.13	100,100,100,100	0
56	MG	B	9049	1/1	0.83	0.27	69,69,69,69	0
56	MG	B	9068	1/1	0.83	0.29	93,93,93,93	0
56	MG	F	301	1/1	0.83	0.09	114,114,114,114	0
56	MG	B	9264	1/1	0.83	0.07	98,98,98,98	0
56	MG	B	9359	1/1	0.83	0.12	78,78,78,78	0
56	MG	GB	9366	1/1	0.83	0.09	92,92,92,92	0
56	MG	GB	9170	1/1	0.83	0.15	101,101,101,101	0
56	MG	GB	9216	1/1	0.83	0.28	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9362	1/1	0.83	0.11	97,97,97,97	0
56	MG	B	9095	1/1	0.83	0.17	99,99,99,99	0
56	MG	FB	1654	1/1	0.83	0.18	111,111,111,111	0
56	MG	B	9018	1/1	0.83	0.23	82,82,82,82	0
56	MG	B	9114	1/1	0.83	0.18	88,88,88,88	0
56	MG	FB	1784	1/1	0.83	0.11	137,137,137,137	0
56	MG	K	202	1/1	0.83	0.10	105,105,105,105	0
56	MG	FB	1787	1/1	0.83	0.08	127,127,127,127	0
56	MG	QC	303	1/1	0.83	0.20	155,155,155,155	0
56	MG	GB	9274	1/1	0.83	0.30	103,103,103,103	0
56	MG	GB	9387	1/1	0.83	0.14	131,131,131,131	0
56	MG	FB	1715	1/1	0.83	0.19	121,121,121,121	0
56	MG	B	9244	1/1	0.83	0.23	101,101,101,101	0
56	MG	L	203	1/1	0.83	0.09	89,89,89,89	0
56	MG	B	9336	1/1	0.83	0.05	94,94,94,94	0
56	MG	B	9060	1/1	0.83	0.32	91,91,91,91	0
56	MG	GB	9285	1/1	0.83	0.20	108,108,108,108	0
56	MG	B	9130	1/1	0.83	0.15	115,115,115,115	0
56	MG	B	9033	1/1	0.83	0.29	78,78,78,78	0
56	MG	B	9211	1/1	0.83	0.09	169,169,169,169	0
56	MG	FB	1761	1/1	0.83	0.17	125,125,125,125	0
56	MG	A	1632	1/1	0.83	0.39	89,89,89,89	0
56	MG	B	9017	1/1	0.83	0.25	78,78,78,78	0
56	MG	GB	9048	1/1	0.83	0.26	92,92,92,92	0
56	MG	AD	202	1/1	0.83	0.23	103,103,103,103	0
56	MG	VB	201	1/1	0.83	0.14	105,105,105,105	0
56	MG	B	9434	1/1	0.83	0.12	133,133,133,133	0
56	MG	GB	9348	1/1	0.83	0.08	112,112,112,112	0
56	MG	FB	1681	1/1	0.84	0.13	126,126,126,126	0
56	MG	FB	1626	1/1	0.84	0.42	103,103,103,103	0
56	MG	GB	9141	1/1	0.84	0.20	101,101,101,101	0
56	MG	FB	1712	1/1	0.84	0.07	111,111,111,111	0
56	MG	B	9197	1/1	0.84	0.23	73,73,73,73	0
56	MG	GB	9074	1/1	0.84	0.25	101,101,101,101	0
56	MG	B	9328	1/1	0.84	0.08	105,105,105,105	0
56	MG	B	9209	1/1	0.84	0.17	90,90,90,90	0
56	MG	B	9331	1/1	0.84	0.07	118,118,118,118	0
56	MG	B	9356	1/1	0.84	0.10	96,96,96,96	0
56	MG	B	9433	1/1	0.84	0.13	99,99,99,99	0
56	MG	B	9290	1/1	0.84	0.27	107,107,107,107	0
56	MG	GB	9358	1/1	0.84	0.09	94,94,94,94	0
56	MG	GB	9252	1/1	0.84	0.19	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	GB	9361	1/1	0.84	0.14	86,86,86,86	0
56	MG	R	201	1/1	0.84	0.09	119,119,119,119	0
56	MG	C	222	1/1	0.84	0.13	164,164,164,164	0
56	MG	B	9014	1/1	0.84	0.23	60,60,60,60	0
56	MG	GB	9367	1/1	0.84	0.11	118,118,118,118	0
56	MG	GB	9087	1/1	0.84	0.19	81,81,81,81	0
56	MG	GB	9258	1/1	0.84	0.18	104,104,104,104	0
56	MG	FB	1763	1/1	0.84	0.08	108,108,108,108	0
56	MG	B	9296	1/1	0.84	0.12	84,84,84,84	0
56	MG	B	9315	1/1	0.84	0.23	91,91,91,91	0
56	MG	GB	9049	1/1	0.84	0.15	79,79,79,79	0
56	MG	EA	101	1/1	0.84	0.13	85,85,85,85	0
56	MG	GB	9014	1/1	0.84	0.28	88,88,88,88	0
56	MG	GB	9382	1/1	0.84	0.29	107,107,107,107	0
56	MG	HA	101	1/1	0.84	0.18	129,129,129,129	0
56	MG	GB	9318	1/1	0.84	0.07	112,112,112,112	0
56	MG	PA	203	1/1	0.84	0.10	127,127,127,127	0
56	MG	B	9372	1/1	0.84	0.09	102,102,102,102	0
56	MG	A	1746	1/1	0.84	0.14	116,116,116,116	0
56	MG	E	303	1/1	0.84	0.15	76,76,76,76	0
56	MG	B	9077	1/1	0.84	0.13	74,74,74,74	0
56	MG	B	9113	1/1	0.84	0.15	98,98,98,98	0
56	MG	A	1637	1/1	0.84	0.20	102,102,102,102	0
56	MG	B	9323	1/1	0.84	0.09	68,68,68,68	0
56	MG	GB	9327	1/1	0.84	0.11	171,171,171,171	0
56	MG	UB	203	1/1	0.84	0.08	130,130,130,130	0
56	MG	B	9005	1/1	0.84	0.34	79,79,79,79	0
56	MG	B	9195	1/1	0.85	0.08	85,85,85,85	0
56	MG	A	1627	1/1	0.85	0.21	101,101,101,101	0
56	MG	B	9406	1/1	0.85	0.10	130,130,130,130	0
56	MG	B	9143	1/1	0.85	0.23	102,102,102,102	0
56	MG	A	1731	1/1	0.85	0.10	130,130,130,130	0
56	MG	B	9082	1/1	0.85	0.23	98,98,98,98	0
56	MG	B	9148	1/1	0.85	0.26	99,99,99,99	0
56	MG	GB	9036	1/1	0.85	0.22	85,85,85,85	0
56	MG	B	9029	1/1	0.85	0.32	81,81,81,81	0
56	MG	FB	1631	1/1	0.85	0.21	104,104,104,104	0
56	MG	GB	9134	1/1	0.85	0.15	111,111,111,111	0
56	MG	FB	1700	1/1	0.85	0.15	120,120,120,120	0
56	MG	B	9074	1/1	0.85	0.14	109,109,109,109	0
56	MG	GB	9192	1/1	0.85	0.18	123,123,123,123	0
56	MG	B	9370	1/1	0.85	0.08	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	FB	1602	1/1	0.85	0.40	87,87,87,87	0
56	MG	GB	9196	1/1	0.85	0.09	82,82,82,82	0
56	MG	GB	9046	1/1	0.85	0.24	91,91,91,91	0
56	MG	FB	1669	1/1	0.85	0.23	105,105,105,105	0
56	MG	B	9329	1/1	0.85	0.12	91,91,91,91	0
56	MG	GB	9402	1/1	0.85	0.12	122,122,122,122	0
56	MG	FB	1748	1/1	0.85	0.09	119,119,119,119	0
56	MG	GB	9002	1/1	0.85	0.56	75,75,75,75	0
56	MG	A	1735	1/1	0.85	0.12	106,106,106,106	0
56	MG	GB	9006	1/1	0.85	0.50	87,87,87,87	0
56	MG	B	9152	1/1	0.85	0.13	89,89,89,89	0
56	MG	B	9118	1/1	0.85	0.24	117,117,117,117	0
56	MG	GB	9332	1/1	0.85	0.07	102,102,102,102	0
56	MG	GB	9334	1/1	0.85	0.31	89,89,89,89	0
56	MG	B	9103	1/1	0.85	0.13	87,87,87,87	0
56	MG	B	9059	1/1	0.85	0.24	95,95,95,95	0
56	MG	B	9337	1/1	0.85	0.08	96,96,96,96	0
56	MG	RC	301	1/1	0.85	0.10	151,151,151,151	0
56	MG	B	9268	1/1	0.85	0.18	94,94,94,94	0
56	MG	GB	9345	1/1	0.85	0.27	106,106,106,106	0
56	MG	B	9240	1/1	0.85	0.05	88,88,88,88	0
56	MG	GB	9283	1/1	0.85	0.31	99,99,99,99	0
56	MG	B	9388	1/1	0.85	0.13	100,100,100,100	0
56	MG	GB	9160	1/1	0.85	0.15	97,97,97,97	0
56	MG	A	1765	1/1	0.85	0.08	134,134,134,134	0
56	MG	GB	9357	1/1	0.85	0.07	125,125,125,125	0
56	MG	FB	1717	1/1	0.85	0.08	129,129,129,129	0
56	MG	GB	9165	1/1	0.85	0.22	83,83,83,83	0
56	MG	B	9391	1/1	0.85	0.14	121,121,121,121	0
56	MG	B	9309	1/1	0.85	0.09	159,159,159,159	0
56	MG	KB	302	1/1	0.85	0.14	99,99,99,99	0
56	MG	B	9271	1/1	0.85	0.10	76,76,76,76	0
56	MG	B	9006	1/1	0.85	0.27	61,61,61,61	0
56	MG	B	9094	1/1	0.85	0.21	93,93,93,93	0
56	MG	S	201	1/1	0.85	0.07	111,111,111,111	0
56	MG	FB	1773	1/1	0.85	0.13	106,106,106,106	0
56	MG	B	9141	1/1	0.85	0.20	130,130,130,130	0
56	MG	B	9176	1/1	0.86	0.21	90,90,90,90	0
56	MG	AC	202	1/1	0.86	0.21	124,124,124,124	0
56	MG	A	1744	1/1	0.86	0.16	123,123,123,123	0
56	MG	A	1655	1/1	0.86	0.15	232,232,232,232	0
56	MG	B	9387	1/1	0.86	0.13	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	GB	9359	1/1	0.86	0.12	123,123,123,123	0
56	MG	B	9294	1/1	0.86	0.15	82,82,82,82	0
56	MG	B	9106	1/1	0.86	0.14	72,72,72,72	0
56	MG	YA	103	1/1	0.86	0.13	125,125,125,125	0
56	MG	B	9317	1/1	0.86	0.04	137,137,137,137	0
56	MG	GB	9312	1/1	0.86	0.21	93,93,93,93	0
56	MG	K	203	1/1	0.86	0.06	130,130,130,130	0
56	MG	FB	1649	1/1	0.86	0.29	119,119,119,119	0
56	MG	GB	9222	1/1	0.86	0.26	93,93,93,93	0
56	MG	B	9145	1/1	0.86	0.13	78,78,78,78	0
56	MG	A	1646	1/1	0.86	0.17	120,120,120,120	0
56	MG	GB	9179	1/1	0.86	0.20	87,87,87,87	0
56	MG	B	9343	1/1	0.86	0.23	110,110,110,110	0
56	MG	GB	9144	1/1	0.86	0.14	80,80,80,80	0
56	MG	B	9397	1/1	0.86	0.12	96,96,96,96	0
56	MG	JB	302	1/1	0.86	0.09	117,117,117,117	0
56	MG	A	1774	1/1	0.86	0.04	176,176,176,176	0
56	MG	GB	9148	1/1	0.86	0.20	86,86,86,86	0
56	MG	T	202	1/1	0.86	0.10	105,105,105,105	0
56	MG	A	1684	1/1	0.86	0.08	111,111,111,111	0
56	MG	GB	9189	1/1	0.86	0.10	154,154,154,154	0
56	MG	B	9046	1/1	0.86	0.26	70,70,70,70	0
56	MG	FB	1608	1/1	0.86	0.28	86,86,86,86	0
56	MG	FB	1749	1/1	0.86	0.16	110,110,110,110	0
56	MG	GB	9242	1/1	0.86	0.10	122,122,122,122	0
56	MG	B	9087	1/1	0.86	0.14	80,80,80,80	0
56	MG	GB	9393	1/1	0.86	0.07	84,84,84,84	0
56	MG	GB	9394	1/1	0.86	0.09	88,88,88,88	0
56	MG	B	9002	1/1	0.86	0.54	64,64,64,64	0
56	MG	GB	9094	1/1	0.86	0.39	89,89,89,89	0
56	MG	CA	102	1/1	0.86	0.04	116,116,116,116	0
56	MG	TB	201	1/1	0.86	0.28	101,101,101,101	0
56	MG	GB	9199	1/1	0.86	0.15	98,98,98,98	0
56	MG	C	206	1/1	0.86	0.15	149,149,149,149	0
56	MG	A	1709	1/1	0.86	0.15	107,107,107,107	0
56	MG	GB	9029	1/1	0.86	0.21	71,71,71,71	0
56	MG	B	9381	1/1	0.86	0.20	84,84,84,84	0
56	MG	B	9208	1/1	0.87	0.08	104,104,104,104	0
56	MG	FB	1610	1/1	0.87	0.37	87,87,87,87	0
56	MG	B	9107	1/1	0.87	0.17	91,91,91,91	0
56	MG	GB	9045	1/1	0.87	0.11	89,89,89,89	0
56	MG	GB	9369	1/1	0.87	0.18	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	FB	1698	1/1	0.87	0.08	120,120,120,120	0
56	MG	B	9384	1/1	0.87	0.09	98,98,98,98	0
56	MG	U	101	1/1	0.87	0.07	91,91,91,91	0
56	MG	A	1771	1/1	0.87	0.18	99,99,99,99	0
56	MG	A	1779	1/1	0.87	0.08	152,152,152,152	0
56	MG	B	9249	1/1	0.87	0.11	123,123,123,123	0
56	MG	GB	9239	1/1	0.87	0.15	96,96,96,96	0
56	MG	B	9028	1/1	0.87	0.36	90,90,90,90	0
56	MG	B	9363	1/1	0.87	0.17	103,103,103,103	0
56	MG	B	9364	1/1	0.87	0.11	95,95,95,95	0
56	MG	GB	9163	1/1	0.87	0.10	94,94,94,94	0
56	MG	A	1716	1/1	0.87	0.20	112,112,112,112	0
56	MG	FB	1740	1/1	0.87	0.08	156,156,156,156	0
56	MG	B	9295	1/1	0.87	0.06	108,108,108,108	0
56	MG	B	9369	1/1	0.87	0.17	90,90,90,90	0
56	MG	A	1775	1/1	0.87	0.05	208,208,208,208	0
56	MG	B	9400	1/1	0.87	0.07	136,136,136,136	0
56	MG	GB	9341	1/1	0.87	0.21	96,96,96,96	0
56	MG	F	304	1/1	0.87	0.06	119,119,119,119	0
56	MG	GB	9211	1/1	0.87	0.16	123,123,123,123	0
56	MG	GB	9346	1/1	0.87	0.08	118,118,118,118	0
56	MG	B	9184	1/1	0.87	0.24	77,77,77,77	0
56	MG	A	1733	1/1	0.87	0.07	143,143,143,143	0
56	MG	GB	9214	1/1	0.87	0.06	99,99,99,99	0
56	MG	GB	9352	1/1	0.87	0.11	85,85,85,85	0
56	MG	A	1678	1/1	0.87	0.10	97,97,97,97	0
56	MG	B	9011	1/1	0.87	0.36	61,61,61,61	0
56	MG	B	9407	1/1	0.87	0.12	114,114,114,114	0
56	MG	B	9408	1/1	0.87	0.22	85,85,85,85	0
56	MG	B	9326	1/1	0.87	0.08	79,79,79,79	0
56	MG	B	9414	1/1	0.87	0.15	77,77,77,77	0
56	MG	ZB	102	1/1	0.87	0.05	100,100,100,100	0
56	MG	DD	101	1/1	0.87	0.15	144,144,144,144	0
56	MG	B	9281	1/1	0.87	0.22	87,87,87,87	0
56	MG	B	9012	1/1	0.87	0.33	70,70,70,70	0
56	MG	XB	201	1/1	0.88	0.12	117,117,117,117	0
56	MG	B	9110	1/1	0.88	0.29	71,71,71,71	0
56	MG	GB	9353	1/1	0.88	0.28	100,100,100,100	0
56	MG	GB	9251	1/1	0.88	0.26	87,87,87,87	0
56	MG	B	9413	1/1	0.88	0.09	100,100,100,100	0
56	MG	A	1723	1/1	0.88	0.13	170,170,170,170	0
56	MG	B	9166	1/1	0.88	0.14	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	GB	9255	1/1	0.88	0.08	107,107,107,107	0
56	MG	B	9225	1/1	0.88	0.12	147,147,147,147	0
56	MG	B	9228	1/1	0.88	0.11	76,76,76,76	0
56	MG	GB	9362	1/1	0.88	0.11	147,147,147,147	0
56	MG	GB	9016	1/1	0.88	0.26	98,98,98,98	0
56	MG	L	202	1/1	0.88	0.05	117,117,117,117	0
56	MG	B	9081	1/1	0.88	0.14	98,98,98,98	0
56	MG	NC	104	1/1	0.88	0.14	134,134,134,134	0
56	MG	GB	9217	1/1	0.88	0.07	141,141,141,141	0
56	MG	B	9357	1/1	0.88	0.11	94,94,94,94	0
56	MG	Q	201	1/1	0.88	0.14	121,121,121,121	0
56	MG	B	9273	1/1	0.88	0.13	130,130,130,130	0
56	MG	FB	1734	1/1	0.88	0.13	109,109,109,109	0
56	MG	B	9091	1/1	0.88	0.21	78,78,78,78	0
56	MG	A	1662	1/1	0.88	0.11	105,105,105,105	0
56	MG	GB	9065	1/1	0.88	0.35	81,81,81,81	0
56	MG	B	9093	1/1	0.88	0.15	95,95,95,95	0
56	MG	JB	304	1/1	0.88	0.18	101,101,101,101	0
56	MG	OA	203	1/1	0.88	0.12	123,123,123,123	0
56	MG	A	1659	1/1	0.88	0.17	124,124,124,124	0
56	MG	B	9031	1/1	0.88	0.34	78,78,78,78	0
56	MG	B	9283	1/1	0.88	0.21	105,105,105,105	0
56	MG	GB	9233	1/1	0.88	0.13	83,83,83,83	0
56	MG	B	9313	1/1	0.88	0.09	91,91,91,91	0
56	MG	E	302	1/1	0.88	0.15	97,97,97,97	0
56	MG	A	1608	1/1	0.88	0.22	96,96,96,96	0
56	MG	B	9236	1/1	0.88	0.11	77,77,77,77	0
56	MG	FB	1750	1/1	0.88	0.16	105,105,105,105	0
56	MG	B	9179	1/1	0.88	0.09	158,158,158,158	0
56	MG	GB	9338	1/1	0.88	0.05	136,136,136,136	0
56	MG	F	302	1/1	0.88	0.07	119,119,119,119	0
56	MG	B	9404	1/1	0.88	0.08	157,157,157,157	0
56	MG	B	9198	1/1	0.88	0.14	92,92,92,92	0
56	MG	FB	1655	1/1	0.88	0.24	103,103,103,103	0
56	MG	B	9132	1/1	0.88	0.12	93,93,93,93	0
56	MG	AD	204	1/1	0.88	0.07	96,96,96,96	0
56	MG	GB	9202	1/1	0.88	0.09	86,86,86,86	0
56	MG	FB	1721	1/1	0.88	0.09	118,118,118,118	0
56	MG	A	1705	1/1	0.88	0.19	105,105,105,105	0
56	MG	VB	203	1/1	0.88	0.14	112,112,112,112	0
56	MG	GB	9023	1/1	0.89	0.35	79,79,79,79	0
56	MG	OA	202	1/1	0.89	0.09	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	JC	101	1/1	0.89	0.13	87,87,87,87	0
56	MG	HB	218	1/1	0.89	0.13	129,129,129,129	0
56	MG	GB	9333	1/1	0.89	0.13	82,82,82,82	0
56	MG	B	9398	1/1	0.89	0.06	96,96,96,96	0
56	MG	HA	103	1/1	0.89	0.22	111,111,111,111	0
56	MG	B	9223	1/1	0.89	0.14	74,74,74,74	0
56	MG	NC	103	1/1	0.89	0.19	112,112,112,112	0
56	MG	B	9178	1/1	0.89	0.07	125,125,125,125	0
56	MG	FB	1764	1/1	0.89	0.23	136,136,136,136	0
56	MG	B	9165	1/1	0.89	0.08	104,104,104,104	0
56	MG	A	1626	1/1	0.89	0.24	98,98,98,98	0
56	MG	B	9263	1/1	0.89	0.14	77,77,77,77	0
56	MG	GB	9062	1/1	0.89	0.12	110,110,110,110	0
56	MG	GB	9347	1/1	0.89	0.07	126,126,126,126	0
56	MG	GB	9265	1/1	0.89	0.15	106,106,106,106	0
56	MG	GB	9159	1/1	0.89	0.25	94,94,94,94	0
56	MG	B	9016	1/1	0.89	0.28	79,79,79,79	0
56	MG	B	9053	1/1	0.89	0.15	84,84,84,84	0
56	MG	A	1670	1/1	0.89	0.07	91,91,91,91	0
56	MG	B	9358	1/1	0.89	0.10	121,121,121,121	0
56	MG	QB	202	1/1	0.89	0.10	100,100,100,100	0
56	MG	B	9008	1/1	0.89	0.25	61,61,61,61	0
56	MG	GB	9273	1/1	0.89	0.09	96,96,96,96	0
56	MG	GB	9403	1/1	0.89	0.10	89,89,89,89	0
56	MG	A	1619	1/1	0.89	0.27	82,82,82,82	0
56	MG	GB	9317	1/1	0.89	0.11	116,116,116,116	0
56	MG	B	9252	1/1	0.89	0.13	98,98,98,98	0
56	MG	B	9187	1/1	0.89	0.25	101,101,101,101	0
56	MG	GB	9042	1/1	0.89	0.24	78,78,78,78	0
56	MG	B	9154	1/1	0.89	0.36	76,76,76,76	0
56	MG	Y	101	1/1	0.89	0.14	97,97,97,97	0
56	MG	VB	202	1/1	0.89	0.12	97,97,97,97	0
56	MG	GB	9282	1/1	0.89	0.11	107,107,107,107	0
56	MG	C	210	1/1	0.89	0.12	125,125,125,125	0
56	MG	B	9189	1/1	0.89	0.29	102,102,102,102	0
56	MG	B	9297	1/1	0.89	0.13	100,100,100,100	0
56	MG	GB	9142	1/1	0.89	0.18	96,96,96,96	0
56	MG	B	9164	1/1	0.89	0.24	90,90,90,90	0
56	MG	B	9257	1/1	0.89	0.20	92,92,92,92	0
56	MG	GB	9050	1/1	0.89	0.22	76,76,76,76	0
56	MG	L	201	1/1	0.90	0.10	114,114,114,114	0
56	MG	GB	9264	1/1	0.90	0.09	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9191	1/1	0.90	0.19	90,90,90,90	0
56	MG	B	9298	1/1	0.90	0.13	92,92,92,92	0
56	MG	M	203	1/1	0.90	0.21	82,82,82,82	0
56	MG	B	9322	1/1	0.90	0.06	85,85,85,85	0
56	MG	GB	9226	1/1	0.90	0.09	91,91,91,91	0
56	MG	A	1767	1/1	0.90	0.14	93,93,93,93	0
56	MG	GB	9069	1/1	0.90	0.29	82,82,82,82	0
56	MG	A	1611	1/1	0.90	0.26	84,84,84,84	0
56	MG	A	1625	1/1	0.90	0.11	94,94,94,94	0
56	MG	FB	1694	1/1	0.90	0.08	143,143,143,143	0
56	MG	GB	9187	1/1	0.90	0.36	92,92,92,92	0
56	MG	T	201	1/1	0.90	0.07	101,101,101,101	0
56	MG	A	1736	1/1	0.90	0.07	169,169,169,169	0
56	MG	B	9196	1/1	0.90	0.09	93,93,93,93	0
56	MG	FB	1667	1/1	0.90	0.19	103,103,103,103	0
56	MG	GB	9079	1/1	0.90	0.20	86,86,86,86	0
56	MG	A	1772	1/1	0.90	0.09	91,91,91,91	0
56	MG	V	503	1/1	0.90	0.05	93,93,93,93	0
56	MG	GB	9082	1/1	0.90	0.27	105,105,105,105	0
56	MG	B	9185	1/1	0.90	0.10	61,61,61,61	0
56	MG	B	9287	1/1	0.90	0.14	82,82,82,82	0
56	MG	GB	9336	1/1	0.90	0.16	121,121,121,121	0
56	MG	Y	103	1/1	0.90	0.11	101,101,101,101	0
56	MG	B	9251	1/1	0.90	0.20	106,106,106,106	0
56	MG	PB	202	1/1	0.90	0.05	127,127,127,127	0
56	MG	A	1773	1/1	0.90	0.12	116,116,116,116	0
56	MG	B	9218	1/1	0.90	0.09	78,78,78,78	0
56	MG	GB	9342	1/1	0.90	0.08	111,111,111,111	0
56	MG	B	9126	1/1	0.90	0.32	116,116,116,116	0
56	MG	B	9292	1/1	0.90	0.08	98,98,98,98	0
56	MG	HA	102	1/1	0.90	0.35	133,133,133,133	0
56	MG	B	9426	1/1	0.90	0.07	99,99,99,99	0
56	MG	GB	9209	1/1	0.90	0.14	89,89,89,89	0
56	MG	C	216	1/1	0.90	0.08	167,167,167,167	0
56	MG	B	9341	1/1	0.90	0.07	121,121,121,121	0
56	MG	GB	9351	1/1	0.90	0.16	113,113,113,113	0
56	MG	B	9026	1/1	0.90	0.26	92,92,92,92	0
56	MG	GB	9171	1/1	0.90	0.23	88,88,88,88	0
56	MG	AD	203	1/1	0.90	0.08	99,99,99,99	0
56	MG	GB	9059	1/1	0.90	0.30	91,91,91,91	0
56	MG	B	9108	1/1	0.90	0.16	84,84,84,84	0
56	MG	GB	9356	1/1	0.90	0.16	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	GB	9099	1/1	0.90	0.12	93,93,93,93	0
56	MG	B	9063	1/1	0.90	0.19	90,90,90,90	0
56	MG	B	9318	1/1	0.91	0.10	137,137,137,137	0
56	MG	B	9286	1/1	0.91	0.07	84,84,84,84	0
56	MG	A	1708	1/1	0.91	0.06	134,134,134,134	0
56	MG	B	9405	1/1	0.91	0.11	103,103,103,103	0
56	MG	KB	301	1/1	0.91	0.44	90,90,90,90	0
56	MG	B	9361	1/1	0.91	0.10	91,91,91,91	0
56	MG	FA	101	1/1	0.91	0.14	98,98,98,98	0
56	MG	B	9090	1/1	0.91	0.17	77,77,77,77	0
56	MG	B	9250	1/1	0.91	0.20	99,99,99,99	0
56	MG	B	9274	1/1	0.91	0.05	84,84,84,84	0
56	MG	GB	9210	1/1	0.91	0.14	99,99,99,99	0
56	MG	GB	9245	1/1	0.91	0.08	107,107,107,107	0
56	MG	GB	9399	1/1	0.91	0.19	129,129,129,129	0
56	MG	GB	9281	1/1	0.91	0.14	97,97,97,97	0
56	MG	GB	9145	1/1	0.91	0.13	101,101,101,101	0
56	MG	B	9153	1/1	0.91	0.20	66,66,66,66	0
56	MG	O	201	1/1	0.91	0.26	83,83,83,83	0
56	MG	GB	9064	1/1	0.91	0.19	80,80,80,80	0
56	MG	FB	1779	1/1	0.91	0.09	115,115,115,115	0
56	MG	B	9010	1/1	0.91	0.31	69,69,69,69	0
56	MG	B	9293	1/1	0.91	0.21	94,94,94,94	0
56	MG	B	9217	1/1	0.91	0.12	98,98,98,98	0
56	MG	GB	9291	1/1	0.91	0.09	124,124,124,124	0
56	MG	GB	9124	1/1	0.91	0.14	104,104,104,104	0
56	MG	FB	1755	1/1	0.91	0.16	104,104,104,104	0
56	MG	GB	9070	1/1	0.91	0.27	81,81,81,81	0
56	MG	GB	9372	1/1	0.91	0.06	101,101,101,101	0
56	MG	GB	9156	1/1	0.91	0.23	86,86,86,86	0
56	MG	B	9395	1/1	0.91	0.23	76,76,76,76	0
56	MG	A	1661	1/1	0.91	0.09	103,103,103,103	0
56	MG	GB	9073	1/1	0.91	0.16	77,77,77,77	0
56	MG	GB	9378	1/1	0.91	0.07	134,134,134,134	0
56	MG	A	1761	1/1	0.91	0.10	106,106,106,106	0
56	MG	B	9424	1/1	0.91	0.09	112,112,112,112	0
56	MG	B	9048	1/1	0.91	0.19	70,70,70,70	0
56	MG	B	9333	1/1	0.91	0.10	85,85,85,85	0
56	MG	GB	9384	1/1	0.91	0.13	131,131,131,131	0
56	MG	B	9168	1/1	0.91	0.16	91,91,91,91	0
56	MG	B	9022	1/1	0.91	0.24	78,78,78,78	0
56	MG	A	1680	1/1	0.92	0.17	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9227	1/1	0.92	0.13	93,93,93,93	0
56	MG	GB	9085	1/1	0.92	0.15	97,97,97,97	0
56	MG	B	9128	1/1	0.92	0.18	106,106,106,106	0
56	MG	GB	9266	1/1	0.92	0.08	118,118,118,118	0
56	MG	VA	202	1/1	0.92	0.13	127,127,127,127	0
56	MG	GB	9003	1/1	0.92	0.30	67,67,67,67	0
56	MG	RB	203	1/1	0.92	0.09	103,103,103,103	0
56	MG	FB	1711	1/1	0.92	0.10	118,118,118,118	0
56	MG	GB	9305	1/1	0.92	0.06	80,80,80,80	0
56	MG	B	9137	1/1	0.92	0.12	83,83,83,83	0
56	MG	A	1629	1/1	0.92	0.25	85,85,85,85	0
56	MG	B	9299	1/1	0.92	0.10	101,101,101,101	0
56	MG	B	9390	1/1	0.92	0.09	89,89,89,89	0
56	MG	B	9065	1/1	0.92	0.14	69,69,69,69	0
56	MG	BB	101	1/1	0.92	0.13	118,118,118,118	0
56	MG	B	9412	1/1	0.92	0.07	82,82,82,82	0
56	MG	FB	1747	1/1	0.92	0.07	116,116,116,116	0
56	MG	GB	9315	1/1	0.92	0.04	151,151,151,151	0
56	MG	B	9170	1/1	0.92	0.11	78,78,78,78	0
56	MG	B	9123	1/1	0.92	0.15	88,88,88,88	0
56	MG	B	9354	1/1	0.92	0.11	103,103,103,103	0
56	MG	GB	9186	1/1	0.92	0.15	80,80,80,80	0
56	MG	B	9172	1/1	0.92	0.14	87,87,87,87	0
56	MG	B	9275	1/1	0.92	0.12	76,76,76,76	0
56	MG	M	201	1/1	0.92	0.07	104,104,104,104	0
56	MG	A	1703	1/1	0.92	0.15	101,101,101,101	0
56	MG	E	301	1/1	0.92	0.22	68,68,68,68	0
56	MG	B	9051	1/1	0.92	0.11	93,93,93,93	0
56	MG	B	9047	1/1	0.92	0.26	89,89,89,89	0
56	MG	FB	1758	1/1	0.92	0.06	104,104,104,104	0
56	MG	B	9360	1/1	0.92	0.03	106,106,106,106	0
56	MG	GB	9260	1/1	0.92	0.13	109,109,109,109	0
56	MG	C	212	1/1	0.92	0.13	138,138,138,138	0
58	ZN	IC	101	1/1	0.92	0.13	158,158,158,158	0
56	MG	FB	1769	1/1	0.93	0.11	109,109,109,109	0
56	MG	GB	9221	1/1	0.93	0.12	80,80,80,80	0
56	MG	B	9097	1/1	0.93	0.12	73,73,73,73	0
56	MG	B	9160	1/1	0.93	0.19	103,103,103,103	0
56	MG	OC	401	1/1	0.93	0.15	171,171,171,171	0
56	MG	A	1753	1/1	0.93	0.07	132,132,132,132	0
56	MG	B	9332	1/1	0.93	0.09	96,96,96,96	0
56	MG	B	9377	1/1	0.93	0.06	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9147	1/1	0.93	0.08	103,103,103,103	0
56	MG	PA	202	1/1	0.93	0.07	125,125,125,125	0
56	MG	GB	9009	1/1	0.93	0.29	78,78,78,78	0
56	MG	B	9163	1/1	0.93	0.11	85,85,85,85	0
56	MG	JB	301	1/1	0.93	0.13	75,75,75,75	0
56	MG	GB	9365	1/1	0.93	0.11	87,87,87,87	0
56	MG	ZB	101	1/1	0.93	0.10	103,103,103,103	0
56	MG	B	9034	1/1	0.93	0.15	69,69,69,69	0
56	MG	B	9035	1/1	0.93	0.28	69,69,69,69	0
56	MG	GB	9340	1/1	0.93	0.11	111,111,111,111	0
56	MG	E	304	1/1	0.93	0.08	85,85,85,85	0
56	MG	GB	9037	1/1	0.93	0.22	82,82,82,82	0
56	MG	B	9415	1/1	0.93	0.11	97,97,97,97	0
56	MG	GB	9344	1/1	0.93	0.13	100,100,100,100	0
56	MG	B	9366	1/1	0.93	0.09	76,76,76,76	0
56	MG	KC	101	1/1	0.93	0.18	117,117,117,117	0
56	MG	B	9214	1/1	0.93	0.07	93,93,93,93	0
56	MG	FB	1743	1/1	0.93	0.06	98,98,98,98	0
56	MG	FB	1786	1/1	0.93	0.08	96,96,96,96	0
56	MG	GB	9379	1/1	0.93	0.22	89,89,89,89	0
56	MG	A	1724	1/1	0.93	0.06	100,100,100,100	0
56	MG	B	9205	1/1	0.93	0.12	120,120,120,120	0
56	MG	A	1769	1/1	0.93	0.13	117,117,117,117	0
56	MG	G	302	1/1	0.93	0.14	90,90,90,90	0
58	ZN	BA	101	1/1	0.93	0.04	194,194,194,194	0
56	MG	FB	1768	1/1	0.93	0.15	105,105,105,105	0
56	MG	FB	1719	1/1	0.94	0.05	150,150,150,150	0
56	MG	B	9325	1/1	0.94	0.18	92,92,92,92	0
56	MG	GB	9307	1/1	0.94	0.06	109,109,109,109	0
56	MG	GB	9193	1/1	0.94	0.13	95,95,95,95	0
56	MG	GB	9376	1/1	0.94	0.06	143,143,143,143	0
56	MG	FB	1789	1/1	0.94	0.19	107,107,107,107	0
56	MG	FB	1775	1/1	0.94	0.06	119,119,119,119	0
56	MG	B	9353	1/1	0.94	0.13	92,92,92,92	0
56	MG	B	9386	1/1	0.94	0.08	114,114,114,114	0
56	MG	GB	9198	1/1	0.94	0.07	89,89,89,89	0
56	MG	B	9427	1/1	0.94	0.17	84,84,84,84	0
56	MG	B	9216	1/1	0.94	0.13	85,85,85,85	0
56	MG	B	9242	1/1	0.94	0.18	93,93,93,93	0
56	MG	B	9312	1/1	0.94	0.04	122,122,122,122	0
56	MG	B	9247	1/1	0.94	0.10	93,93,93,93	0
56	MG	GB	9277	1/1	0.94	0.08	82,82,82,82	0

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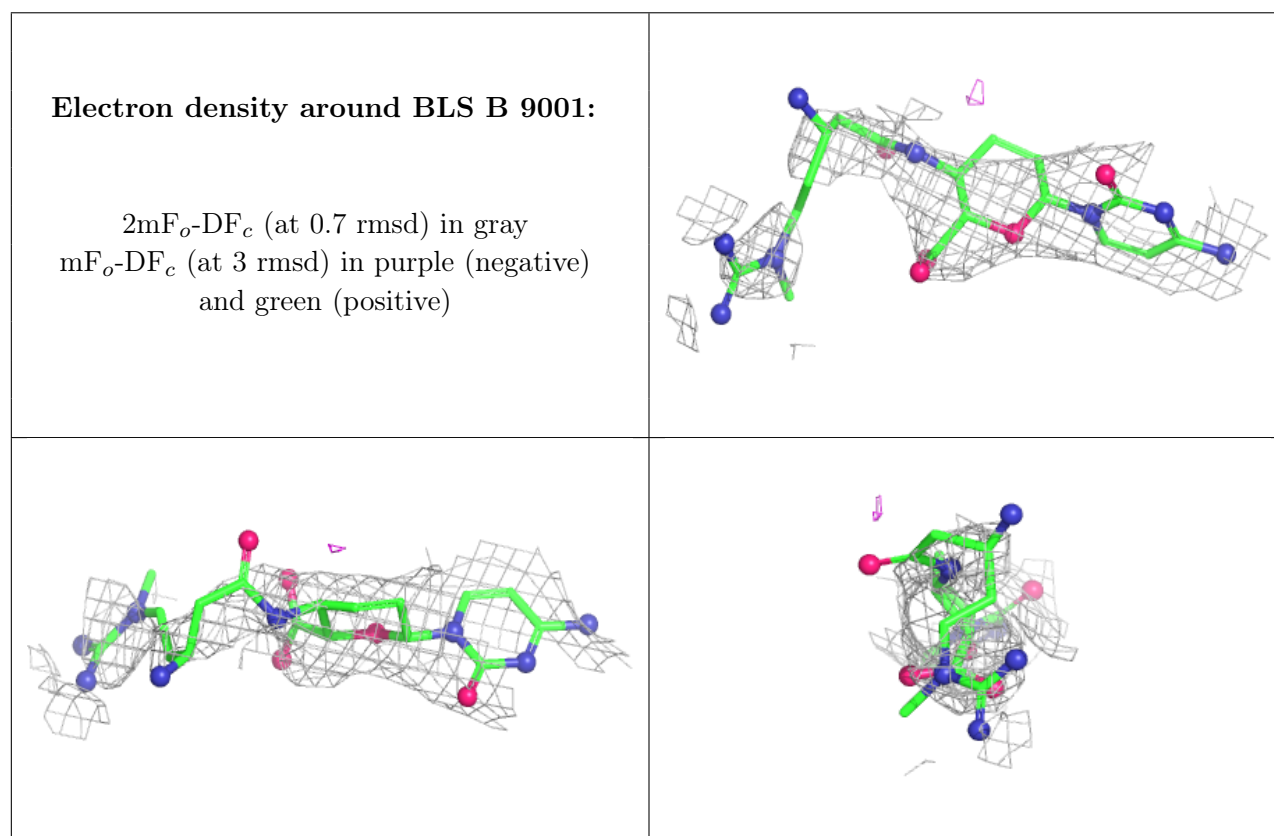
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9019	1/1	0.94	0.37	79,79,79,79	0
56	MG	GB	9299	1/1	0.94	0.06	162,162,162,162	0
56	MG	GB	9223	1/1	0.94	0.05	85,85,85,85	0
56	MG	B	9420	1/1	0.94	0.20	94,94,94,94	0
56	MG	GB	9302	1/1	0.94	0.05	112,112,112,112	0
56	MG	FB	1656	1/1	0.94	0.08	120,120,120,120	0
58	ZN	GC	101	1/1	0.94	0.05	206,206,206,206	0
56	MG	B	9410	1/1	0.94	0.07	84,84,84,84	0
56	MG	GB	9236	1/1	0.95	0.06	87,87,87,87	0
56	MG	B	9085	1/1	0.95	0.09	77,77,77,77	0
56	MG	A	1681	1/1	0.95	0.05	132,132,132,132	0
56	MG	B	9041	1/1	0.95	0.21	71,71,71,71	0
56	MG	GB	9396	1/1	0.95	0.09	78,78,78,78	0
56	MG	FB	1676	1/1	0.95	0.14	94,94,94,94	0
56	MG	B	9173	1/1	0.95	0.28	86,86,86,86	0
56	MG	B	9421	1/1	0.95	0.10	85,85,85,85	0
56	MG	E	305	1/1	0.95	0.04	85,85,85,85	0
56	MG	B	9278	1/1	0.95	0.10	101,101,101,101	0
56	MG	B	9279	1/1	0.95	0.16	93,93,93,93	0
56	MG	B	9374	1/1	0.95	0.07	94,94,94,94	0
56	MG	B	9425	1/1	0.95	0.07	83,83,83,83	0
56	MG	B	9003	1/1	0.95	0.38	64,64,64,64	0
56	MG	B	9340	1/1	0.95	0.05	85,85,85,85	0
56	MG	B	9371	1/1	0.96	0.07	81,81,81,81	0
56	MG	B	9202	1/1	0.96	0.05	80,80,80,80	0
56	MG	GB	9204	1/1	0.96	0.09	130,130,130,130	0
56	MG	B	9416	1/1	0.96	0.04	82,82,82,82	0
56	MG	FB	1746	1/1	0.96	0.07	96,96,96,96	0
56	MG	B	9379	1/1	0.96	0.06	100,100,100,100	0
56	MG	B	9409	1/1	0.96	0.16	83,83,83,83	0
56	MG	A	1741	1/1	0.96	0.04	109,109,109,109	0
56	MG	A	1651	1/1	0.96	0.04	175,175,175,175	0
56	MG	B	9306	1/1	0.96	0.06	83,83,83,83	0
56	MG	M	202	1/1	0.96	0.05	81,81,81,81	0
57	BLS	B	9001	30/30	0.96	0.11	105,105,106,106	0
57	BLS	GB	9001	30/30	0.96	0.09	104,104,105,105	0
58	ZN	V	501	1/1	0.96	0.06	123,123,123,123	0
56	MG	B	9261	1/1	0.96	0.15	66,66,66,66	0
58	ZN	DA	101	1/1	0.96	0.05	160,160,160,160	0
56	MG	GB	9161	1/1	0.96	0.07	101,101,101,101	0
56	MG	GB	9005	1/1	0.96	0.45	68,68,68,68	0
56	MG	B	9027	1/1	0.97	0.32	68,68,68,68	0

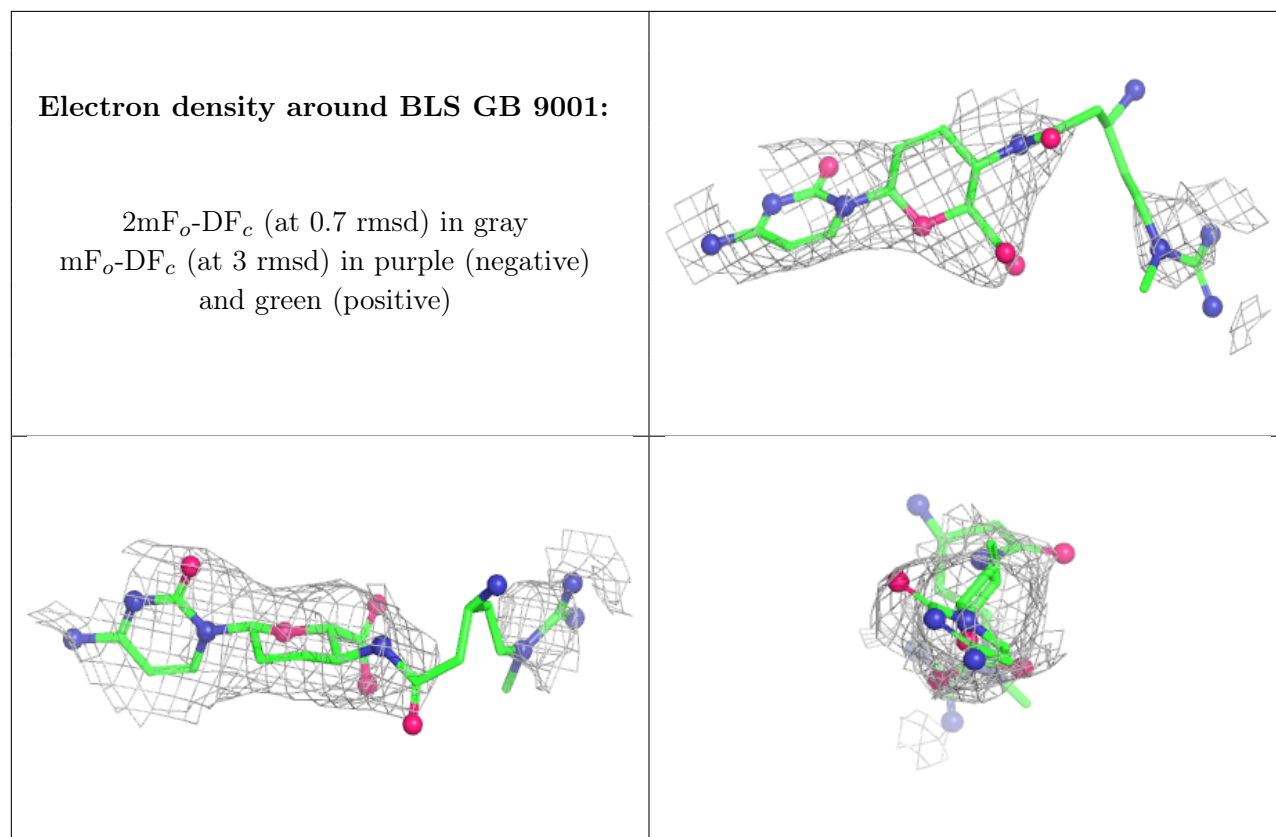
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9039	1/1	0.97	0.05	68,68,68,68	0
56	MG	FB	1742	1/1	0.97	0.04	121,121,121,121	0
56	MG	B	9096	1/1	0.97	0.08	78,78,78,78	0
56	MG	B	9339	1/1	0.97	0.11	88,88,88,88	0
56	MG	B	9365	1/1	0.97	0.09	84,84,84,84	0
56	MG	B	9394	1/1	0.97	0.06	71,71,71,71	0
58	ZN	GA	101	1/1	0.97	0.06	153,153,153,153	0
58	ZN	AC	201	1/1	0.97	0.05	147,147,147,147	0
56	MG	B	9226	1/1	0.97	0.33	70,70,70,70	0
56	MG	B	9300	1/1	0.97	0.09	89,89,89,89	0
56	MG	GB	9370	1/1	0.98	0.03	127,127,127,127	0
56	MG	B	9246	1/1	0.98	0.05	84,84,84,84	0
56	MG	GB	9284	1/1	0.98	0.07	91,91,91,91	0
56	MG	B	9344	1/1	0.98	0.12	93,93,93,93	0
58	ZN	LC	101	1/1	0.98	0.07	171,171,171,171	0
58	ZN	CA	101	1/1	0.99	0.02	125,125,125,125	0
58	ZN	HC	101	1/1	1.00	0.01	126,126,126,126	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.