



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 10, 2025 – 10:31 PM EST

PDB ID : 6B4V
Title : Antibiotic blasticidin S and E. coli release factor 1 bound to the 70S ribosome
Authors : Svidritskiy, E.; Korostelev, A.A.
Deposited on : 2017-09-27
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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.21
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

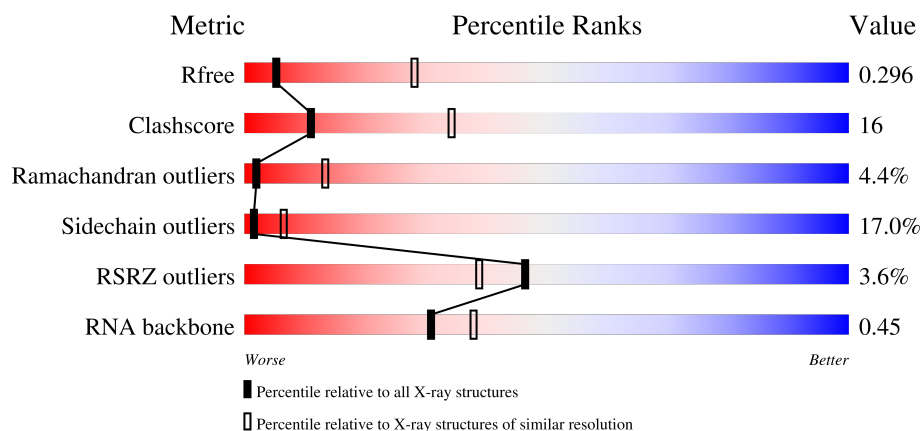
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 3.40 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.



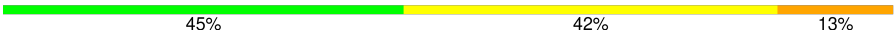

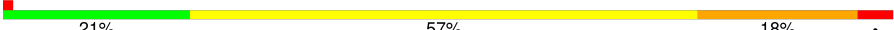
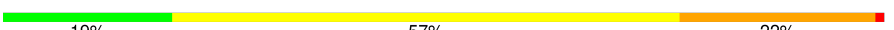

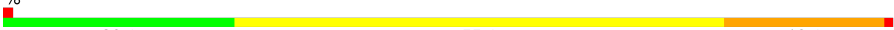




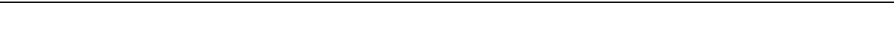

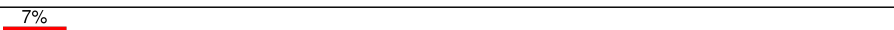
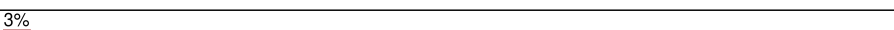











Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)
RNA backbone	3690	1033 (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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1507	
1	EB	1507	
2	B	2880	
2	FB	2880	

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

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

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Mol	Chain	Length	Quality of chain
27	AA	60	
27	EC	60	
28	BA	71	
28	FC	71	
29	CA	60	
29	GC	60	
30	DA	54	
30	HC	54	
31	EA	49	
31	IC	49	
32	FA	65	
32	JC	65	
33	GA	37	
33	KC	37	
34	HA	23	
34	LC	23	
35	JA	368	
35	NC	368	
36	KA	256	
36	OC	256	
37	LA	239	
37	PC	239	
38	MA	209	
38	QC	209	
39	NA	162	

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

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

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 299841 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	EB	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	FB	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
FB	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	GB	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
			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	HB	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			
4	MC	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	IB	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	JB	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	KB	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	LB	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	MB	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	NB	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	OB	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	PB	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	QB	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	RB	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	SB	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	TB	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	UB	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	VB	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	WB	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	XB	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	YB	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	ZB	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	AC	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	BC	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
BC	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	CC	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	DC	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	EC	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	FC	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	GC	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	HC	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	IC	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	JC	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	KC	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	LC	11	Total	C	N	O	P	0	0	0
			220	98	44	67	11			

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

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

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
JA	361	LEU	-	expression tag	UNP A7ZKY5
JA	362	GLU	-	expression tag	UNP A7ZKY5
JA	363	HIS	-	expression tag	UNP A7ZKY5
JA	364	HIS	-	expression tag	UNP A7ZKY5
JA	365	HIS	-	expression tag	UNP A7ZKY5
JA	366	HIS	-	expression tag	UNP A7ZKY5
JA	367	HIS	-	expression tag	UNP A7ZKY5
JA	368	HIS	-	expression tag	UNP A7ZKY5
NC	361	LEU	-	expression tag	UNP A7ZKY5
NC	362	GLU	-	expression tag	UNP A7ZKY5
NC	363	HIS	-	expression tag	UNP A7ZKY5
NC	364	HIS	-	expression tag	UNP A7ZKY5
NC	365	HIS	-	expression tag	UNP A7ZKY5
NC	366	HIS	-	expression tag	UNP A7ZKY5
NC	367	HIS	-	expression tag	UNP A7ZKY5
NC	368	HIS	-	expression tag	UNP A7ZKY5

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	A	214	Total	Mg	0	0
			214	214		
56	B	562	Total	Mg	0	0
			562	562		
56	C	21	Total	Mg	0	0
			21	21		
56	D	5	Total	Mg	0	0
			5	5		
56	E	1	Total	Mg	0	0
			1	1		
56	F	2	Total	Mg	0	0
			2	2		
56	G	2	Total	Mg	0	0
			2	2		
56	H	1	Total	Mg	0	0
			1	1		
56	I	3	Total	Mg	0	0
			3	3		
56	J	2	Total	Mg	0	0
			2	2		
56	K	4	Total	Mg	0	0
			4	4		
56	L	2	Total	Mg	0	0
			2	2		
56	M	5	Total	Mg	0	0
			5	5		
56	O	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	Q	2	Total 2	Mg 2	0	0
56	S	2	Total 2	Mg 2	0	0
56	T	3	Total 3	Mg 3	0	0
56	U	2	Total 2	Mg 2	0	0
56	V	2	Total 2	Mg 2	0	0
56	W	2	Total 2	Mg 2	0	0
56	X	1	Total 1	Mg 1	0	0
56	Y	1	Total 1	Mg 1	0	0
56	Z	4	Total 4	Mg 4	0	0
56	AA	2	Total 2	Mg 2	0	0
56	BA	1	Total 1	Mg 1	0	0
56	CA	1	Total 1	Mg 1	0	0
56	DA	2	Total 2	Mg 2	0	0
56	EA	1	Total 1	Mg 1	0	0
56	HA	3	Total 3	Mg 3	0	0
56	IA	6	Total 6	Mg 6	0	0
56	JA	6	Total 6	Mg 6	0	0
56	KA	1	Total 1	Mg 1	0	0
56	LA	2	Total 2	Mg 2	0	0
56	MA	2	Total 2	Mg 2	0	0
56	NA	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	2	Total 2	Mg 2	0	0
56	SA	3	Total 3	Mg 3	0	0
56	TA	3	Total 3	Mg 3	0	0
56	UA	4	Total 4	Mg 4	0	0
56	XA	6	Total 6	Mg 6	0	0
56	ZA	1	Total 1	Mg 1	0	0
56	AB	2	Total 2	Mg 2	0	0
56	CB	1	Total 1	Mg 1	0	0
56	EB	206	Total 206	Mg 206	0	0
56	FB	475	Total 475	Mg 475	0	0
56	GB	15	Total 15	Mg 15	0	0
56	HB	9	Total 9	Mg 9	0	0
56	IB	4	Total 4	Mg 4	0	0
56	JB	2	Total 2	Mg 2	0	0
56	KB	4	Total 4	Mg 4	0	0
56	MB	2	Total 2	Mg 2	0	0
56	NB	3	Total 3	Mg 3	0	0
56	OB	3	Total 3	Mg 3	0	0
56	PB	1	Total 1	Mg 1	0	0
56	RB	1	Total 1	Mg 1	0	0
56	SB	2	Total 2	Mg 2	0	0

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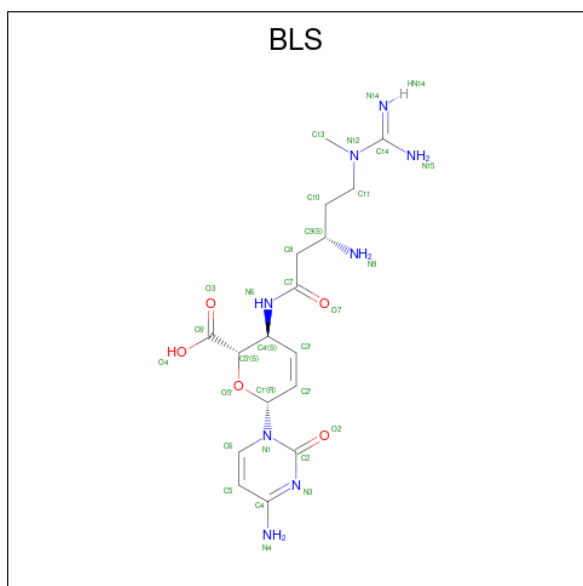
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	TB	1	Total 1	Mg 1	0	0
56	UB	3	Total 3	Mg 3	0	0
56	VB	1	Total 1	Mg 1	0	0
56	WB	1	Total 1	Mg 1	0	0
56	ZB	2	Total 2	Mg 2	0	0
56	BC	1	Total 1	Mg 1	0	0
56	CC	7	Total 7	Mg 7	0	0
56	DC	1	Total 1	Mg 1	0	0
56	EC	1	Total 1	Mg 1	0	0
56	FC	1	Total 1	Mg 1	0	0
56	JC	1	Total 1	Mg 1	0	0
56	LC	1	Total 1	Mg 1	0	0
56	MC	5	Total 5	Mg 5	0	0
56	NC	5	Total 5	Mg 5	0	0
56	OC	5	Total 5	Mg 5	0	0
56	PC	1	Total 1	Mg 1	0	0
56	QC	4	Total 4	Mg 4	0	0
56	RC	3	Total 3	Mg 3	0	0
56	SC	1	Total 1	Mg 1	0	0
56	TC	1	Total 1	Mg 1	0	0
56	UC	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	VC	1	Total	Mg	0	0
			1	1		
56	WC	1	Total	Mg	0	0
			1	1		
56	XC	1	Total	Mg	0	0
			1	1		
56	YC	5	Total	Mg	0	0
			5	5		
56	AD	2	Total	Mg	0	0
			2	2		
56	BD	1	Total	Mg	0	0
			1	1		
56	CD	1	Total	Mg	0	0
			1	1		

- Molecule 57 is BLASTICIDIN S (three-letter code: 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	FB	1	Total	C	N	O	0	0
			30	17	8	5		

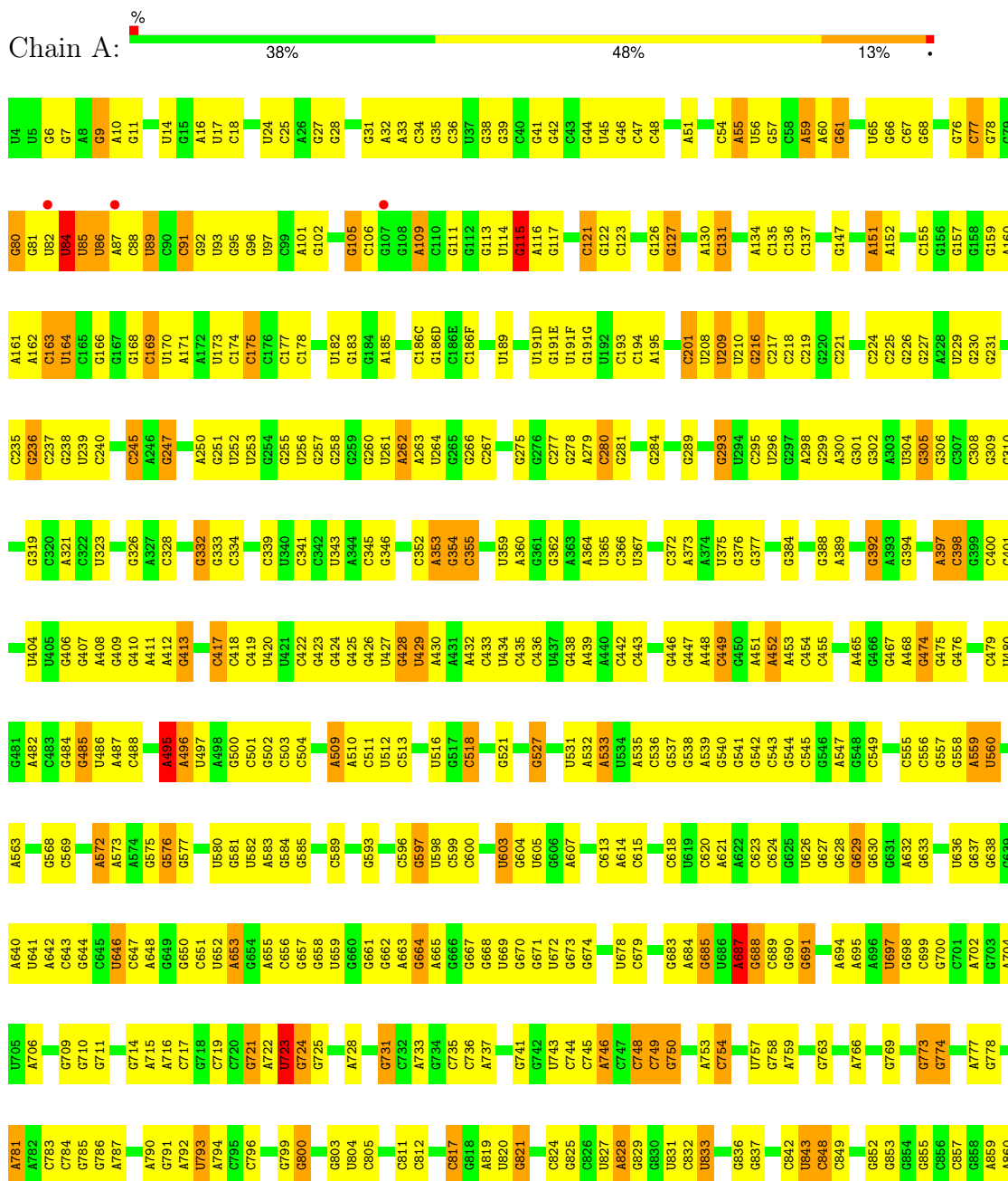
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

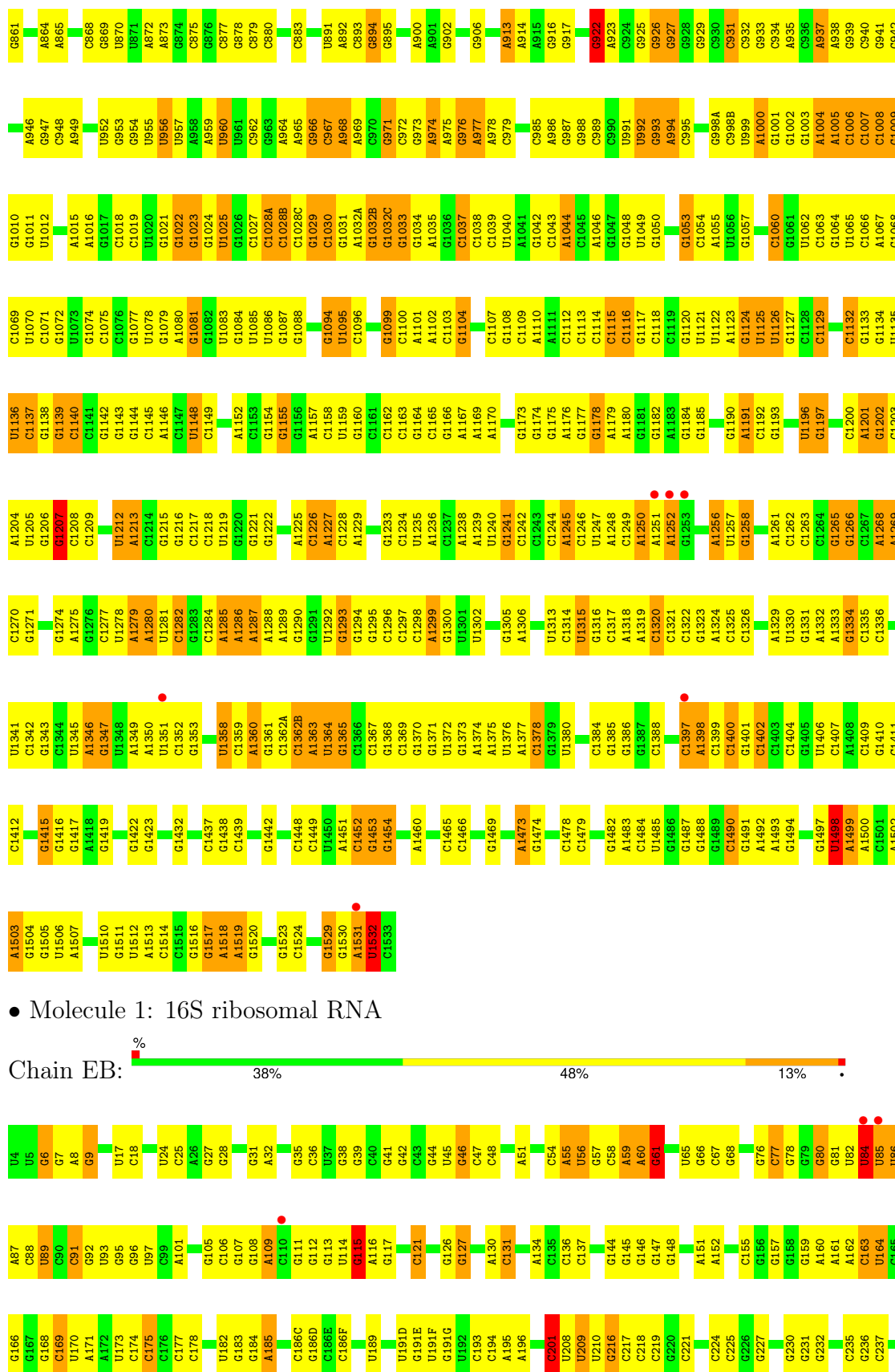
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	V	1	Total 1	Zn 1	0	0
58	BA	1	Total 1	Zn 1	0	0
58	CA	1	Total 1	Zn 1	0	0
58	DA	1	Total 1	Zn 1	0	0
58	GA	1	Total 1	Zn 1	0	0
58	ZB	1	Total 1	Zn 1	0	0
58	FC	1	Total 1	Zn 1	0	0
58	GC	1	Total 1	Zn 1	0	0
58	HC	1	Total 1	Zn 1	0	0
58	KC	1	Total 1	Zn 1	0	0

3 Residue-property plots

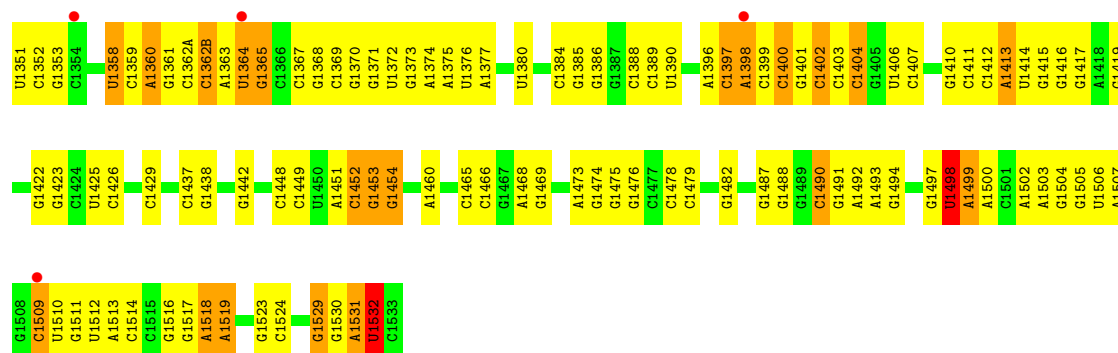
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

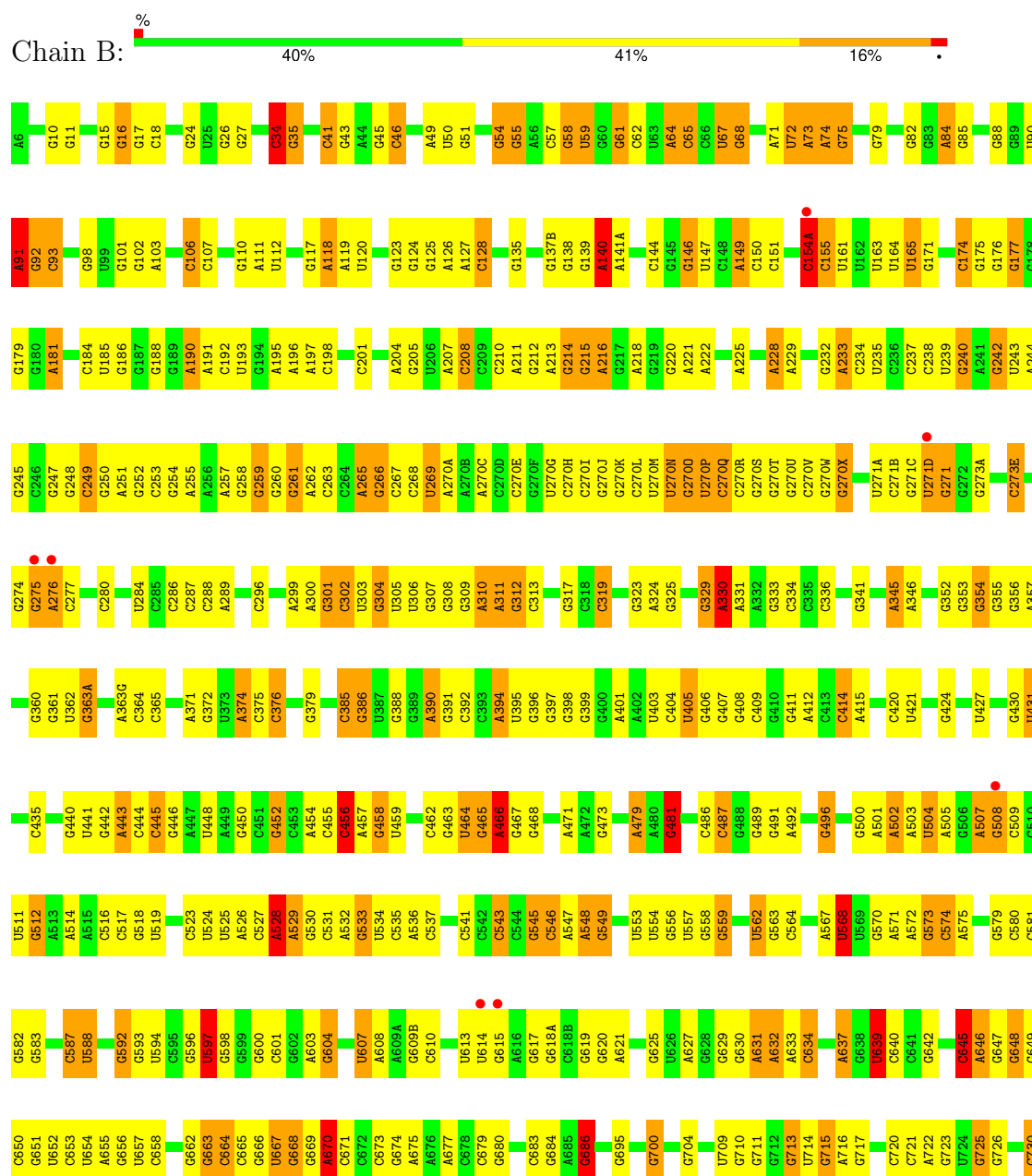




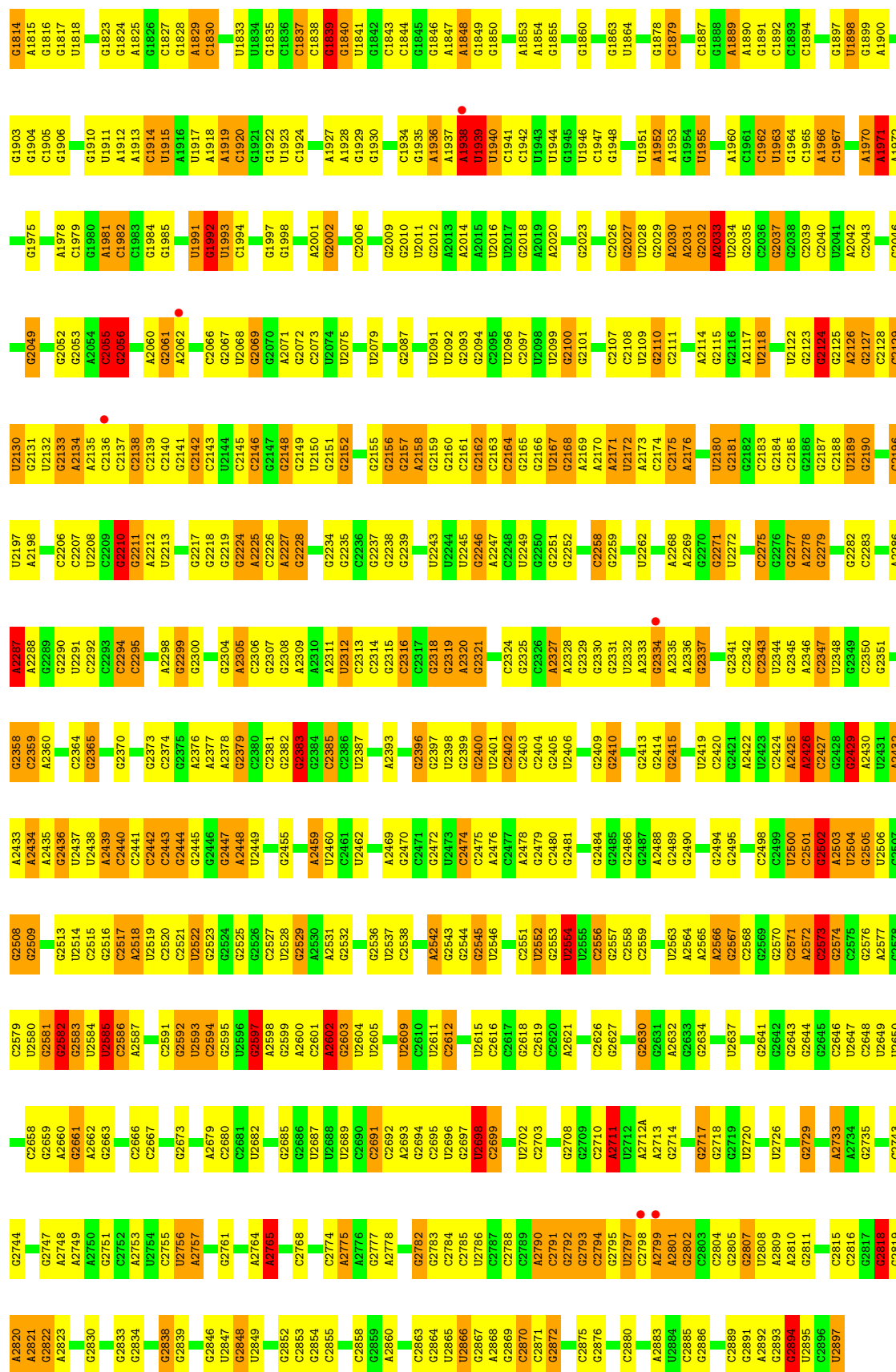
A1285	A1286	A1287	A1288	A1289	G1290	G1291	U1292	G1293	G1294	G1295	G1296	G1297	G1298	A1299	G1300	U1301	U1302	G1305	A1306	U1307	U1308	G1309		U1313	U1314	U1315	U1316	U1317	A1318	A1319	C1320	G1321	C1322	C1323	A1324	C1325	C1326	C1327	C1328	A1329	U1330	G1331	A1332	A1333	G1334	C1335	C1336		U1341	C1342	U1343	C1344	U1345	A1346	U1347	U1348	A1349	A1350																																																																																																																																																																																																																																																																																																																										
C1214	G1215	G1216	C1217	G1218	U1219	G1220	G1221		G1224	A1225	G1226	G1227	G1228	A1229		G1233		A1238	A1239	U1240	G1241	C1242		A1245	G1246	U1247	U1248	G1249	A1250	A1251	A1252	A1256	U1257	G1258		A1261	G1262	C1263	G1264	G1265	G1266	U1267	U1268		A1274	A1275	G1276	U1277	U1278	A1279	A1280	U1281	C1282	A1283	C1284																																																																																																																																																																																																																																																																																																																													
C1147	U1148	C1149		A1152	G1153	G1154	G1155	G1156	A1157	C1158	U1159	G1160	C1161	C1162	G1163	G1164	A1167	A1169	A1170		G1173	G1174	G1175	A1176	G1177	U1178	A1179	A1180	G1181	G1182	A1183	G1184	G1185	G1186	G1187		G1190	A1191	C1192	G1193		U1196	G1197	G1198	U1199	C1200	A1201	G1202	C1203	A1204	U1205	G1206	G1207	A1208	C1209		U1212	G1213	G1214																																																																																																																																																																																																																																																																																																																									
A1080	G1081	U1082	U1083	U1084	U1085	U1086	U1087	U1088		G1094	U1095	C1096		G1099	G1100	A1101	A1102	C1103	G1104		G1107	G1108	C1109	A1110	A1111	C1112	C1113	C1114	C1115	C1116	G1117	C1118	C1119	G1120	U1121	U1122	A1123	G1124	U1125	U1126	U1127	C1128	C1129		C1132	G1133	G1134	G1135	U1136	C1137	G1138	G1139	C1140	G1141	G1142	G1143	G1144	C1145	A1146																																																																																																																																																																																																																																																																																																																									
G1021	G1022	G1023	G1024	U1025	G1026	C1027	C1028A	C1028B	C1028C	G1029	C1030	G1031	A1032A	G1032B	G1032C	C1033	G1034	A1035	G1036	C1037	C1038	C1039	U1040	A1041	G1042	C1043	A1044	C1045	A1046	G1047	G1048	U1049	G1050	G1053	C1054	A1055	U1056	G1057		C1060	G1061	U1062	C1063	G1064	U1065	C1066	A1067	G1068	C1069	U1070	C1071	G1072	U1073	G1074		U1077	G1078	G1079																																																																																																																																																																																																																																																																																																																										
U957	A958	A959	U960	U961	C962	G963	A964	A965	G966	C967	A968	A969	C970	G971	C972	G973	A974	A975	G976	A977	A978	C979		C985	A986	G987	G988	C989	C990	U991	U992	G993	G994		G998A	C998B	U999	A1000	G1001	G1002	A935	C936	A937	A938	G939	C940	G941	C1009	G1010	G1011	U1012	G1013	A1014	A1015	U1016	G1017	C1018	U1019	U1020																																																																																																																																																																																																																																																																																																																									
G869	U870	U871	A872	A873	G874	C875	G876	G877	G878	U879	A880	C881	U882	C883	G884	C885	G886	C887	A888	A889	G890		A893	A894	G895	G896	C897	C898	A899	A900	G901	G902		A913	A914		G917	G918	G919	C920	G921	G922	A923	C924	G925	G926	G927	G928	G929	C930	C931	C932	G933	C934	A935	C936	A937	A938	G939	C940	G941	G942		A946	G947	C948	A949		U952	G953	G954	U955	U956																																																																																																																																																																																																																																																																																																											
C779	A780	A781		G785		A780	G791	A792	U793	A794	C795	C796		G799	G800		G803	U804		C811	C812		C817	G818	A819	U820	G821	C822	C823	C824	G825		A828		G836	G837		C842	U843	C844	C845	C846	C847	C848	C849	U850	G851	G852	G853	G854	G855		A859	A860	A861		U862	G863	A864	A865	C866		A868	G869	G870	C701																																																																																																																																																																																																																																																																																																																		
U560	U561	C562	A563	C564		G568	C569		A572	A573	A574	G575	G576	G577		U580	G581	U582	A583	G584	G585		C589		G593		C596	G597	U598	C599	C600	C601	U602	U603	G604	U605	G606	A607	A608	A609	C610		C613	A614	C615	G616	G617	G618	U619	C620	A621	A622	C623	C624	G625	U626	G627	G628	G629																																																																																																																																																																																																																																																																																																																									
G630	G631	A632	G633		U636	G637	G638	G639	A640	U641	A642	C643	G644	G645	G646	G647	A648	G649	G650	C651	U652	A653		G657	G658	U659	G660	G661	G662	A663	G664	A665	G666	G667	G668		G671	U672	G673	G674		U678	C679		G683	A684	G685	G686	A687	G688	C689	A690	G691		U697	G698	C699	G700																																																																																																																																																																																																																																																																																																																										
A702	G703	A704	U705	A706		G709	G710		G714	A715	A716		G719	G720	G721	A722	U723	G724	G725		G730	G731		C732	A733	G734	C735	C736	A737		G741	G742	U743	C744	G745	A746	C747	C748	C749	G750		A753	C754		U757	G758	A759		G763		A767	A768	G769	C770		G773	G774	A777	G778																																																																																																																																																																																																																																																																																																																									
C779	A780	A781		G785		A780	G791	A792	U793	A794	C795	C796		G799	G800		G803	U804		C811	C812		C817	G818	A819	U820	G821	C822	C823	C824	G825		A828		G836	G837		C842	U843	C844	C845	C846	C847	C848	C849	U850	G851	G852	G853	G854	G855		A859	A860	A861		U862	G863	A864	A865	C866		A868	G869	G870																																																																																																																																																																																																																																																																																																																			
G869	U870	U871	A872	A873	G874	C875	G876	G877	G878	U879	A880	C881	U882	C883	G884	C885	G886	C887	A888	A889	G890		A893	A894	G895	G896	C897	C898	A899	A900	G901	G902		A913	A914		G917	G918	G919	C920	G921	G922	A923	C924	G925	G926	G927	G928	G929	C930	C931	C932	G933	C934	A935	C936	A937	A938	G939	C940	G941	G942		A946	G947	C948	A949		U952	G953	G954	U955	U956																																																																																																																																																																																																																																																																																																											
U957	A958	A959	U960	U961	C962	G963	A964	A965	G966	C967	A968	A969	C970	G971	C972	G973	A974	A975	G976	A977	A978	C979		C985	A986	G987	G988	C989	C990	U991	U992	G993	G994		G998A	C998B	U999	A1000	G1001	G1002	A935	C936	A937	A938	G939	C940	G941	C1009	G1010	G1011	U1012	G1013	A1014	A1015	U1016	G1017	C1018	U1019	U1020																																																																																																																																																																																																																																																																																																																									
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• Molecule 2: 23S ribosomal RNA



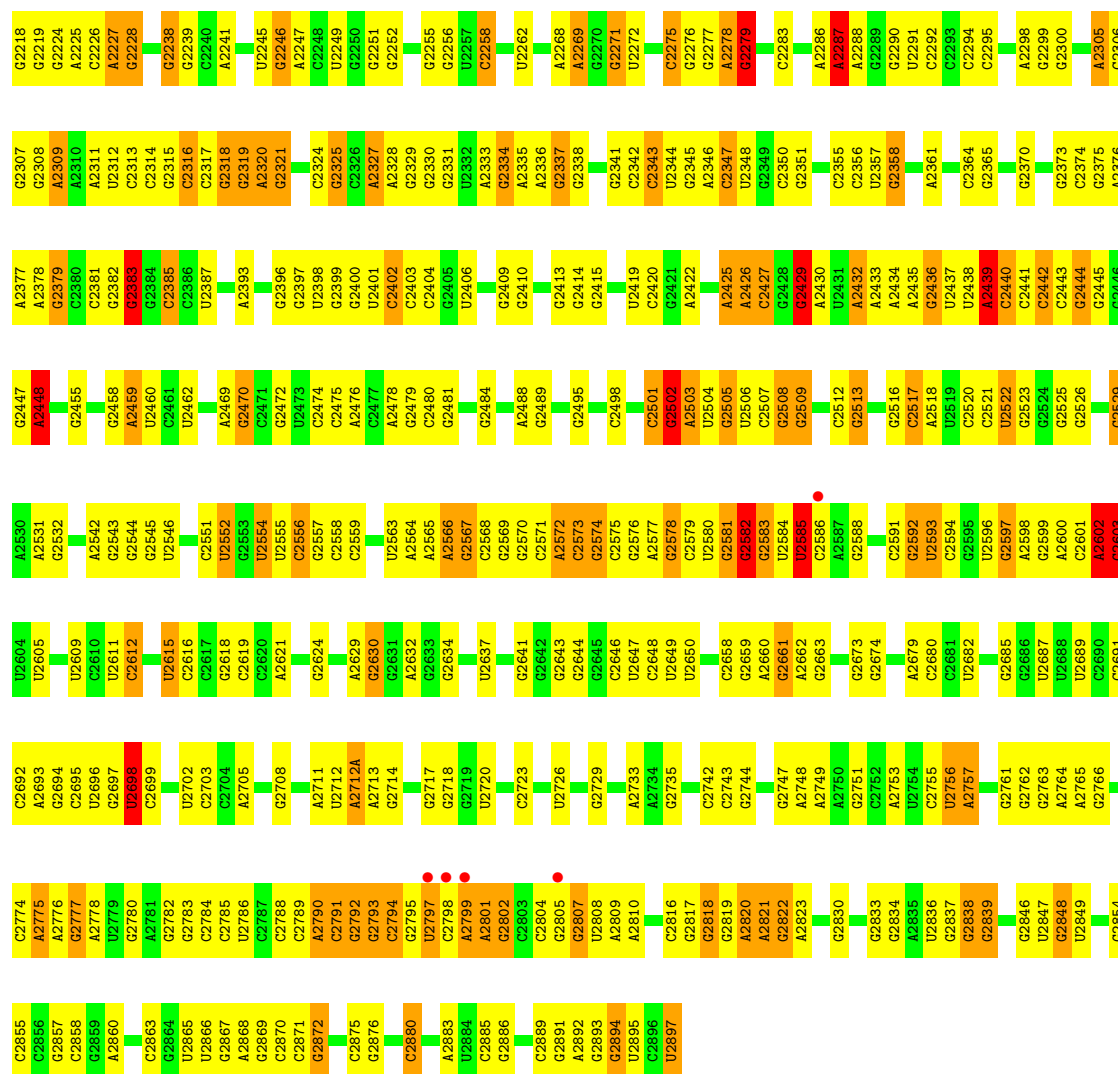
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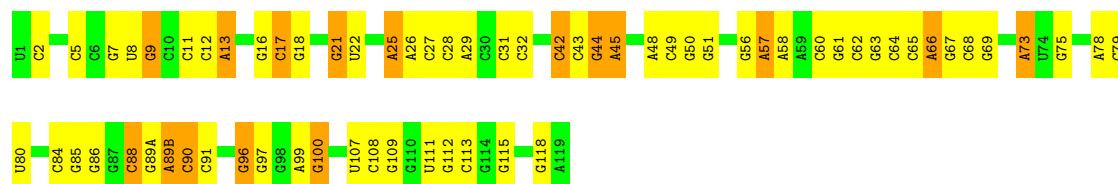
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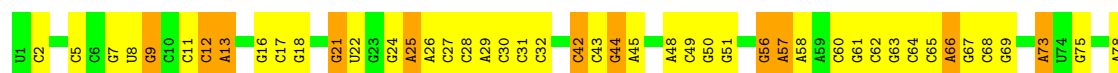
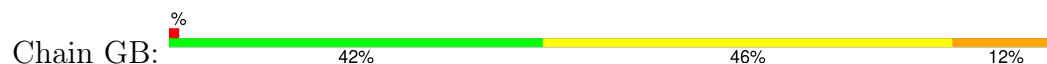
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							C1707	G1463	G1378		
							C1708	G1464	G1379		
							C1709	G1465	G1380		
							C1710	G1466	G1381		
							C1711	G1467	G1382		
							C1712	G1468	G1383		
							C1713	G1469	G1384		
							C1714	G1470	G1385		
							C1715	G1471	G1386		
							C1716	G1472	G1387		
							C1717	G1473	G1388		
							C1718	G1474	G1389		
							C1719	G1475	G1390		
							C1720	G1476	G1391		
							C1721	G1477	G1392		
							C1722	G1478	G1393		
							C1723	G1479	G1394		
							C1724	G1480	G1395		
							C1725	G1481	G1396		
							C1726	G1482	G1397		
							C1727	G1483	G1398		
							C1728	G1484	G1399		
							C1729	G1485	G1400		
							C1730	G1486	G1401		
							C1731	G1487	G1402		
							C1732	G1488	G1403		
							C1733	G1489	G1404		
							C1734	G1490	G1405		
							C1735	G1491	G1406		
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							C173				

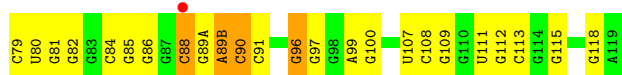


• Molecule 3: 5S ribosomal RNA

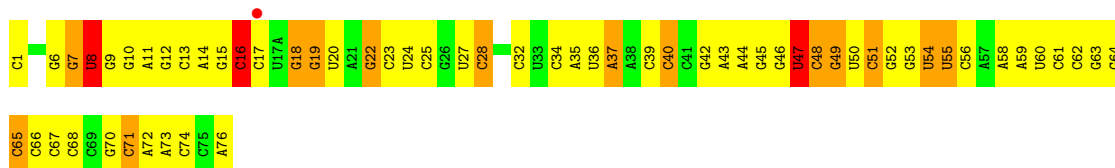


• Molecule 3: 5S ribosomal RNA

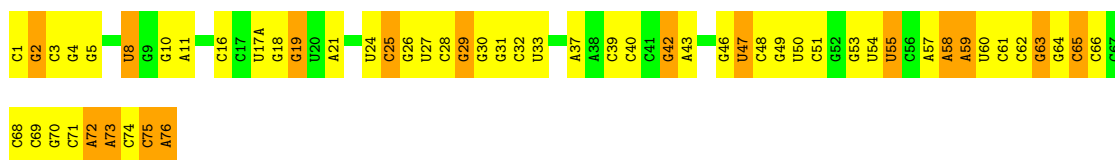
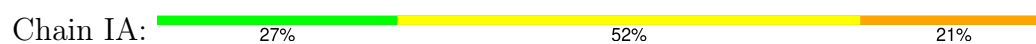




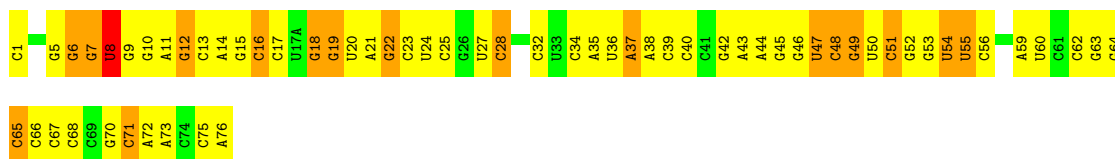
• Molecule 4: tRNA



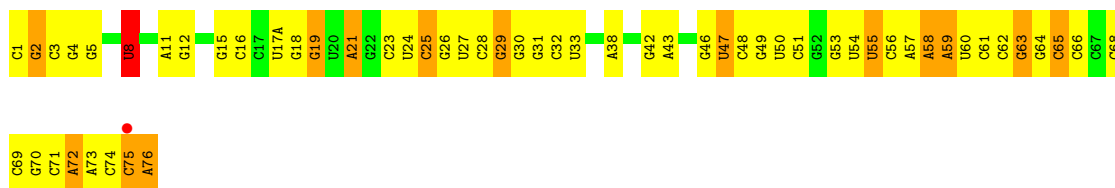
• Molecule 4: tRNA



• Molecule 4: tRNA

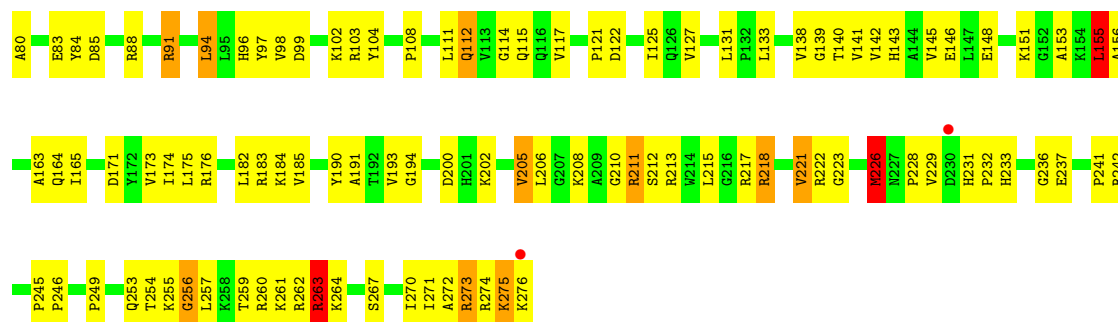


• Molecule 4: tRNA

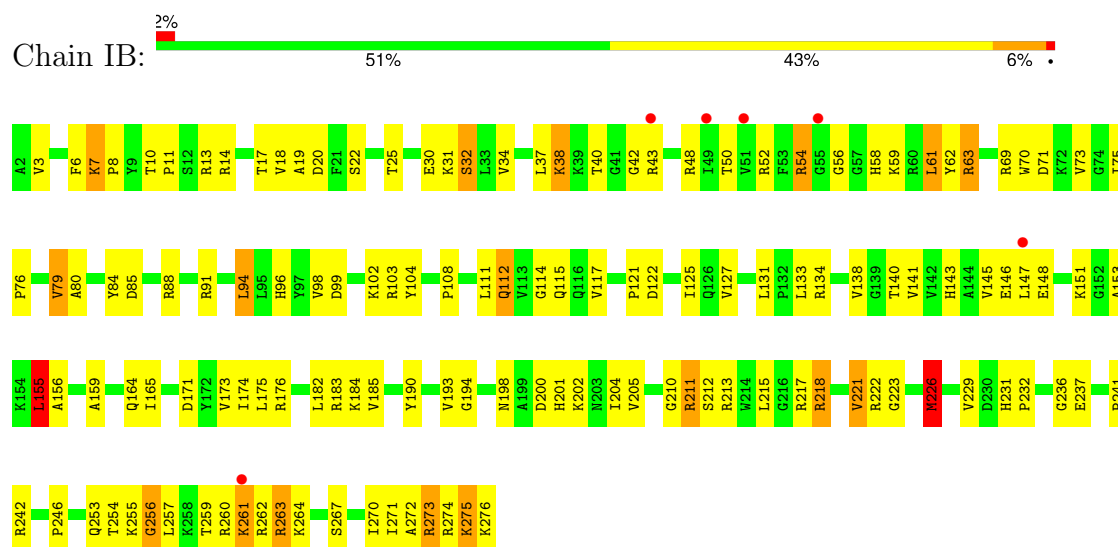


• Molecule 5: 50S ribosomal protein L2

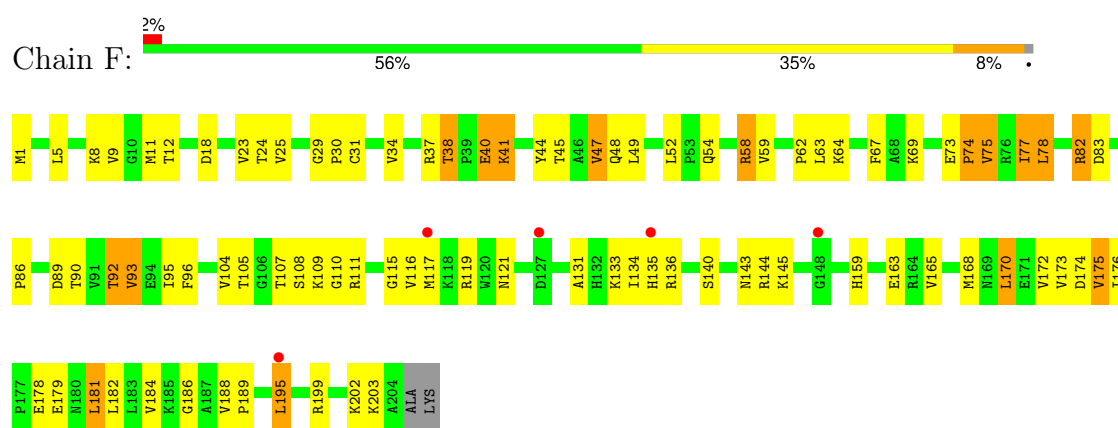




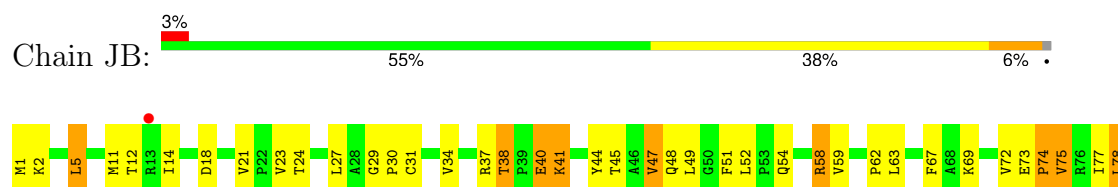
• Molecule 5: 50S ribosomal protein L2

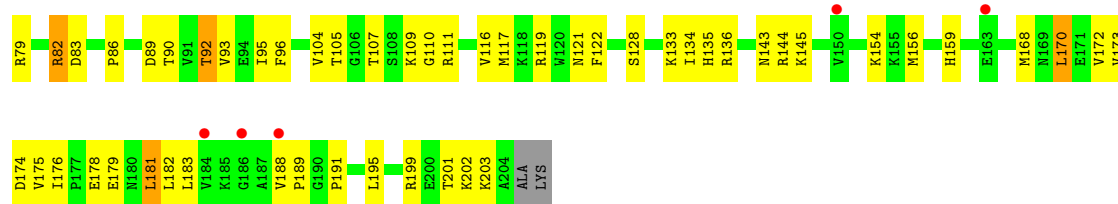


• Molecule 6: 50S ribosomal protein L3



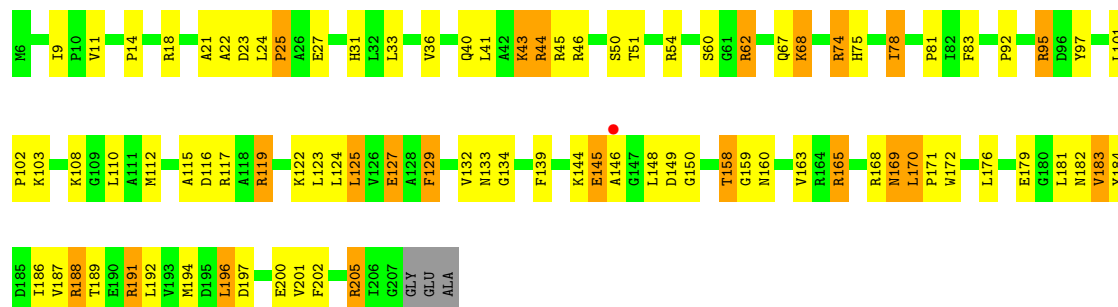
• Molecule 6: 50S ribosomal protein L3





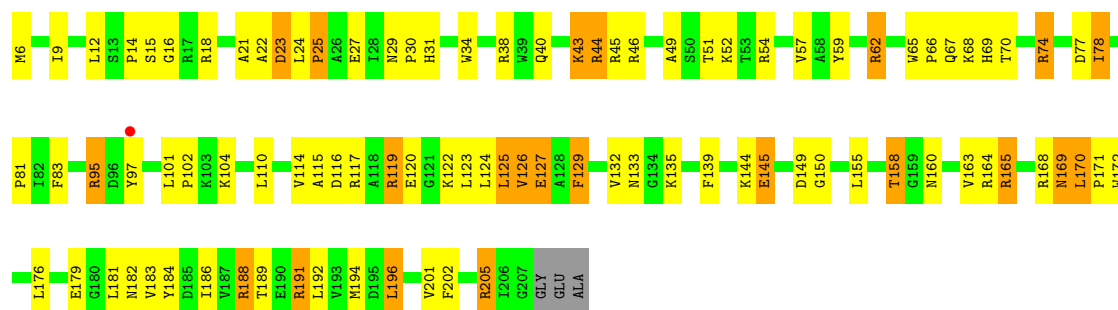
• Molecule 7: 50S ribosomal protein L4

Chain G: 55% 33% 11% .



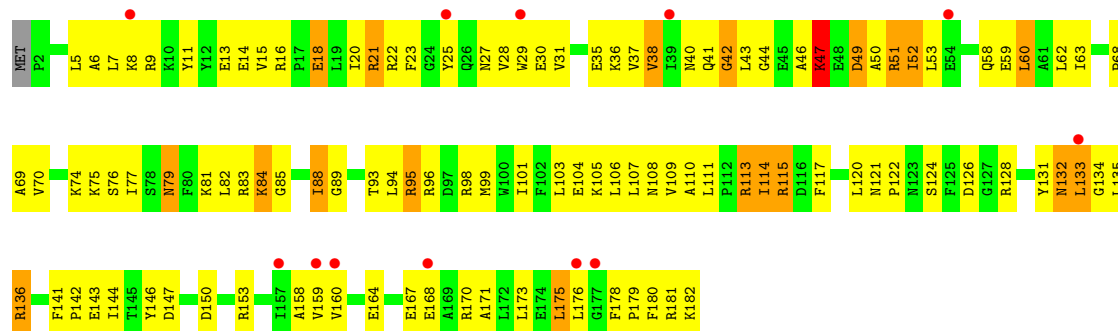
• Molecule 7: 50S ribosomal protein L4

Chain KB: 52% 36% 11% .

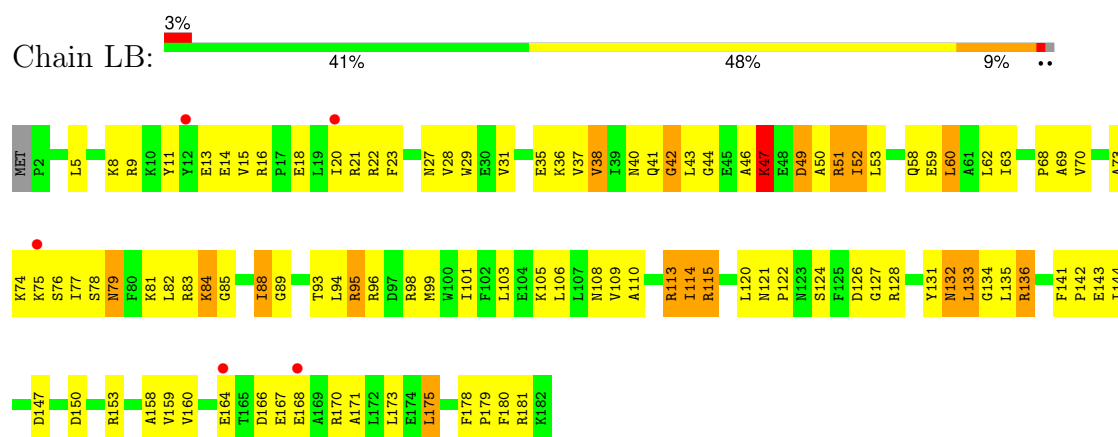


• Molecule 8: 50S ribosomal protein L5

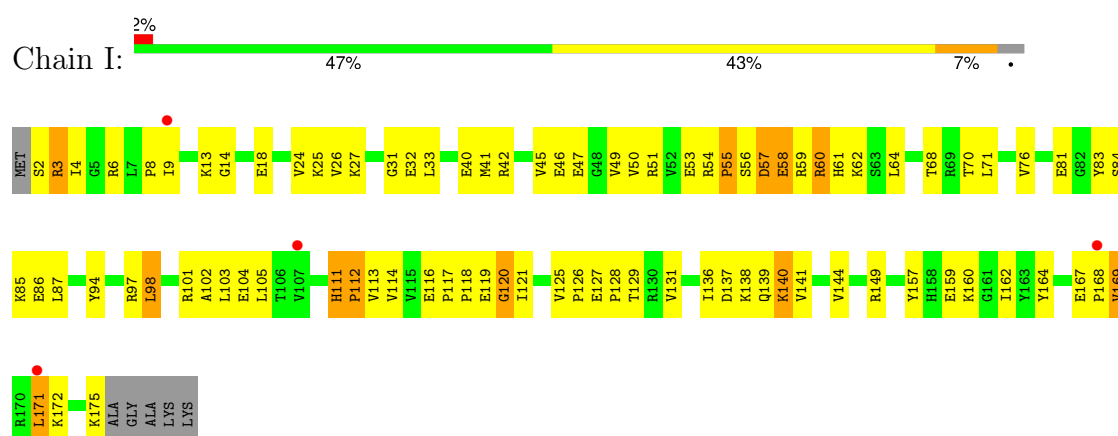
Chain H: 7% 37% 51% 10% ..



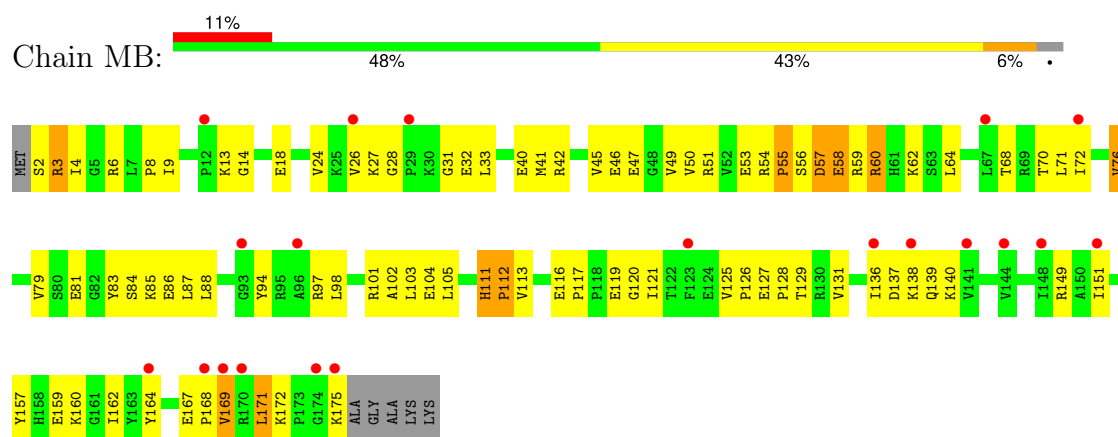
• Molecule 8: 50S ribosomal protein L5



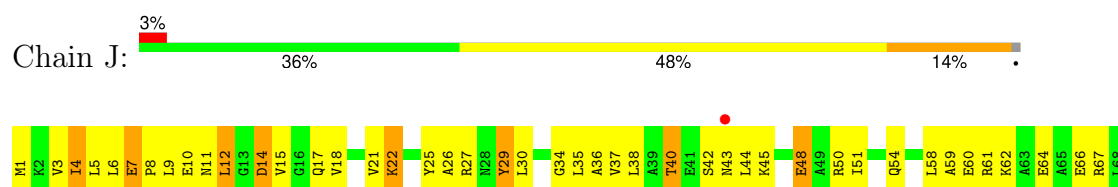
• Molecule 9: 50S ribosomal protein L6

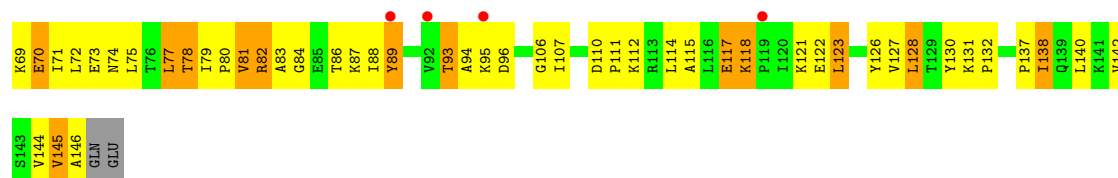


• Molecule 9: 50S ribosomal protein L6

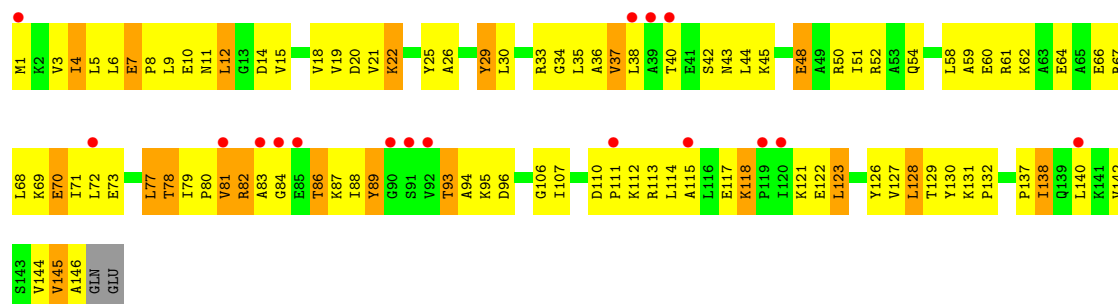


• Molecule 10: 50S ribosomal protein L9

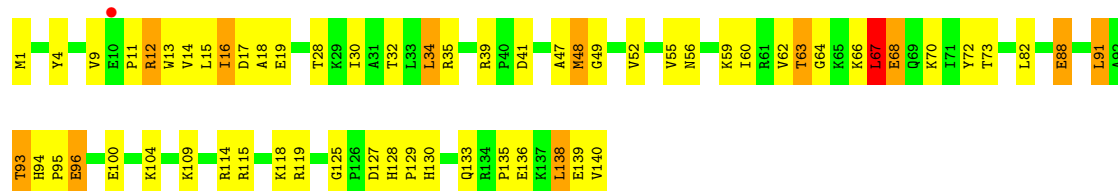




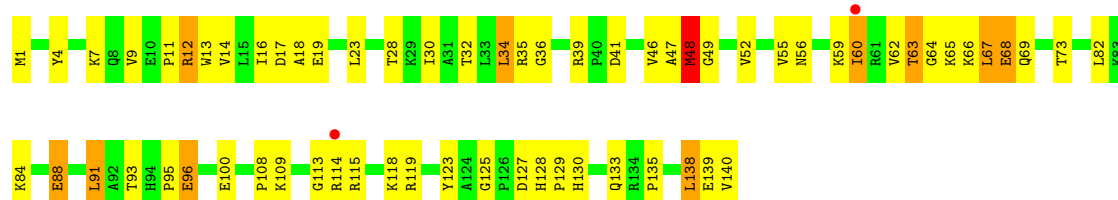
- Molecule 10: 50S ribosomal protein L9



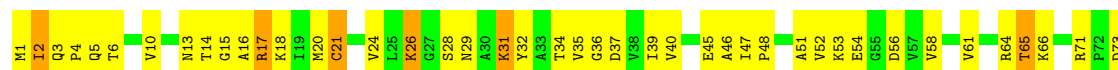
- Molecule 11: 50S ribosomal protein L13



- Molecule 11: 50S ribosomal protein L13

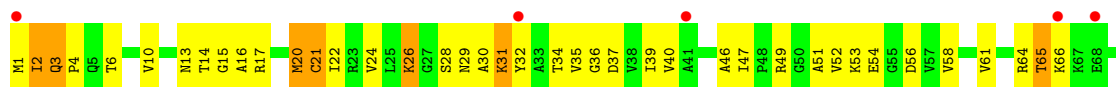


- Molecule 12: 50S ribosomal protein L14

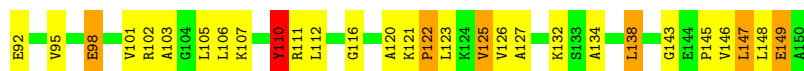
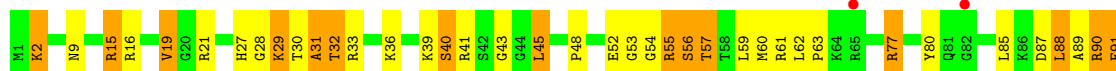




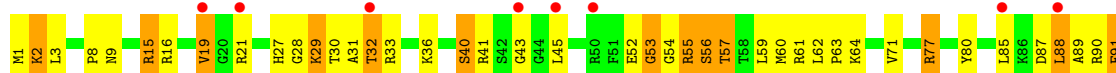
- Molecule 12: 50S ribosomal protein L14



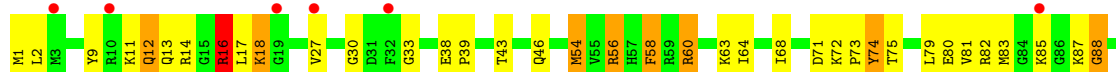
- Molecule 13: 50S ribosomal protein L15



- Molecule 13: 50S ribosomal protein L15

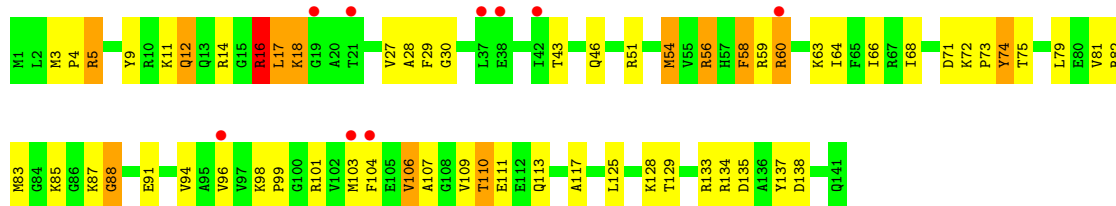


- Molecule 14: 50S ribosomal protein L16

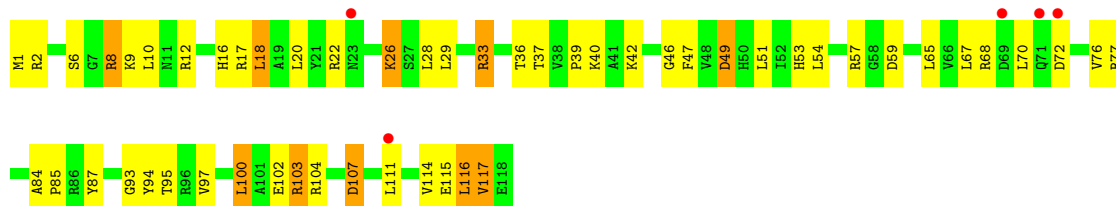


- Molecule 14: 50S ribosomal protein L16

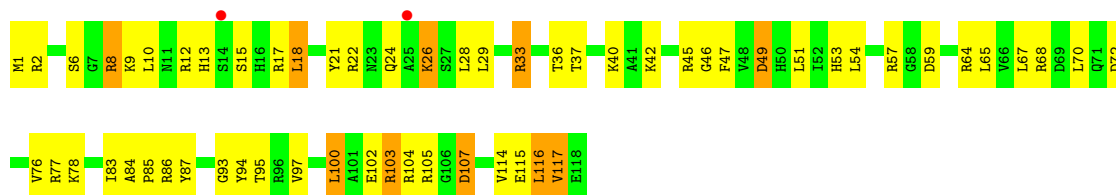




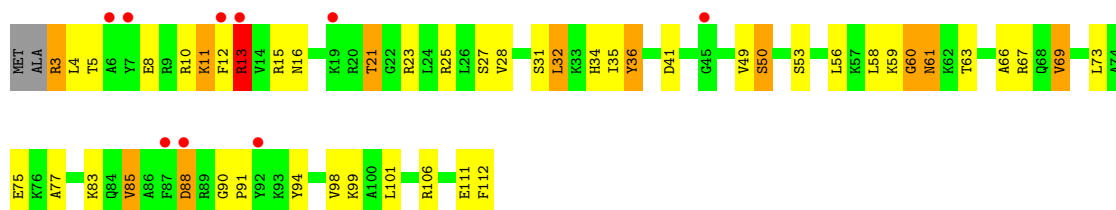
• Molecule 15: 50S ribosomal protein L17



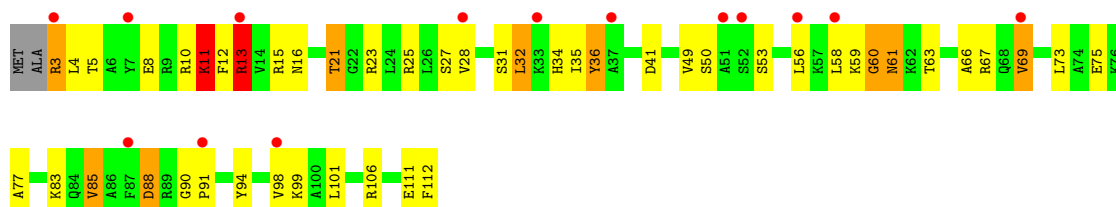
• Molecule 15: 50S ribosomal protein L17



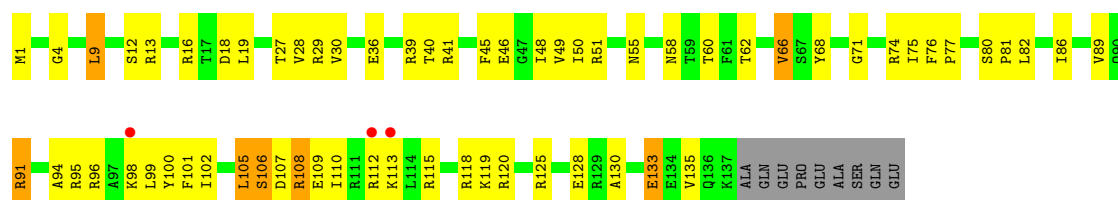
• Molecule 16: 50S ribosomal protein L18



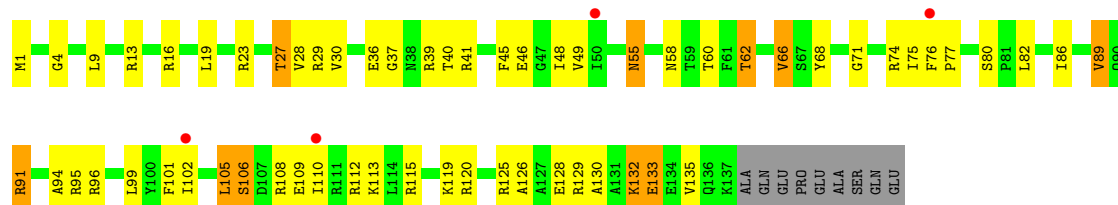
• Molecule 16: 50S ribosomal protein L18



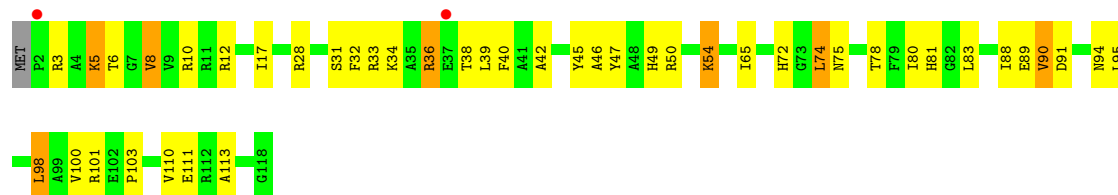
- Molecule 17: 50S ribosomal protein L19



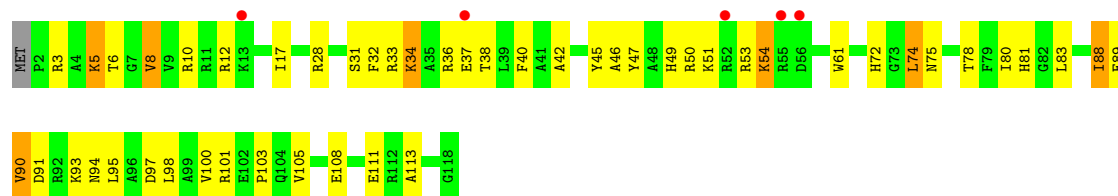
- Molecule 17: 50S ribosomal protein L19



- Molecule 18: 50S ribosomal protein L20

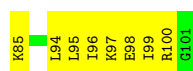


- Molecule 18: 50S ribosomal protein L20

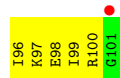


- Molecule 19: 50S ribosomal protein L21

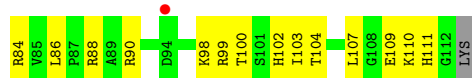
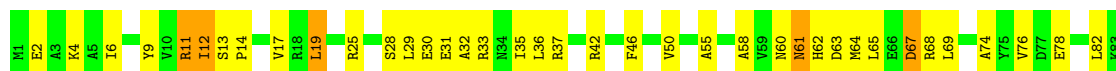




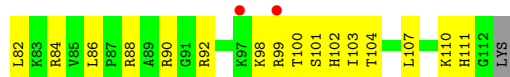
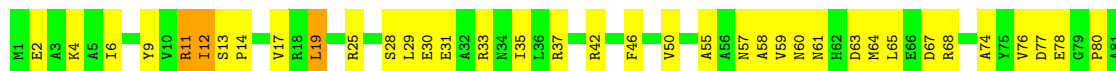
- Molecule 19: 50S ribosomal protein L21



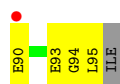
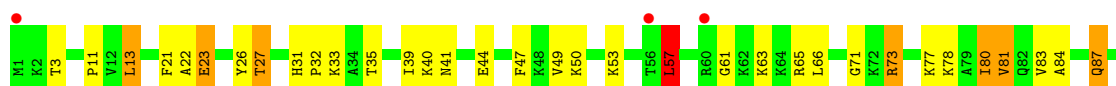
- Molecule 20: 50S ribosomal protein L22



- Molecule 20: 50S ribosomal protein L22

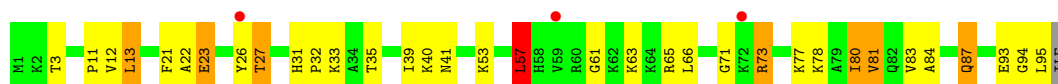


- Molecule 21: 50S ribosomal protein L23

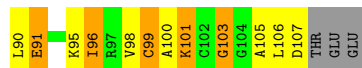


- Molecule 21: 50S ribosomal protein L23

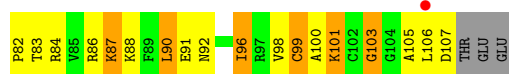
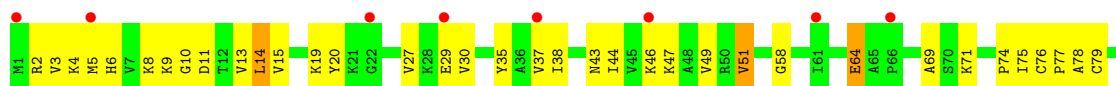




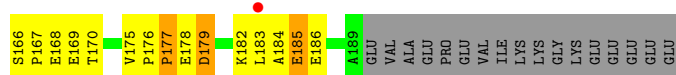
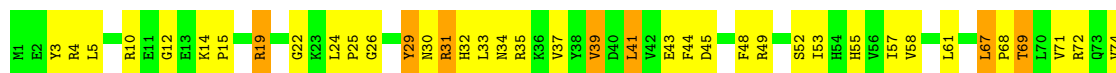
- Molecule 22: 50S ribosomal protein L24



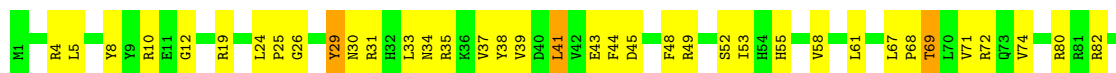
- Molecule 22: 50S ribosomal protein L24

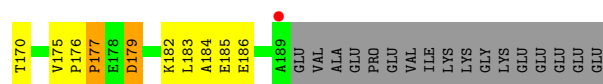


- Molecule 23: 50S ribosomal protein L25

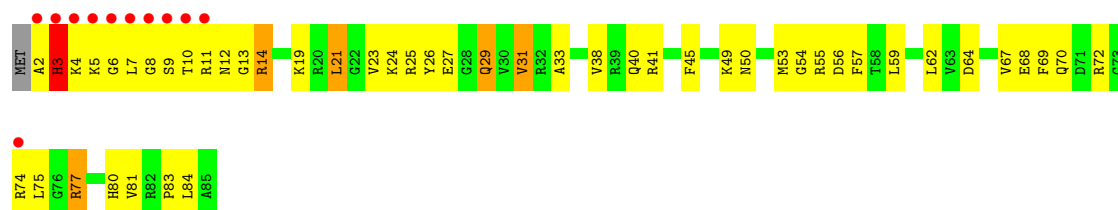


- Molecule 23: 50S ribosomal protein L25





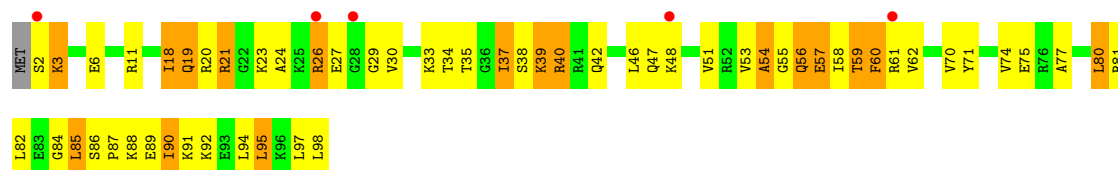
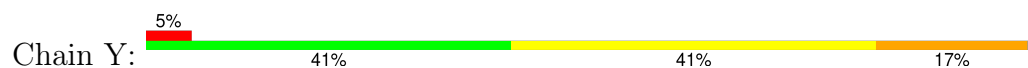
• Molecule 24: 50S ribosomal protein L27



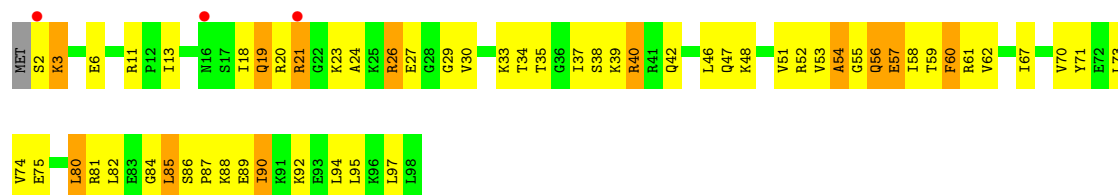
• Molecule 24: 50S ribosomal protein L27



• Molecule 25: 50S ribosomal protein L28

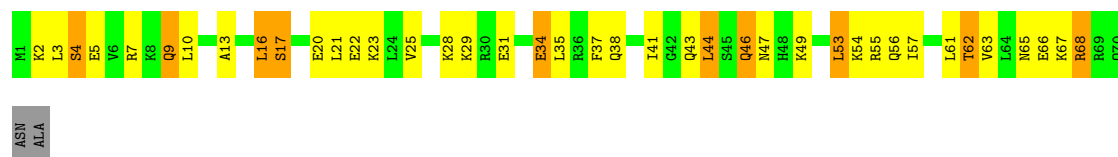


• Molecule 25: 50S ribosomal protein L28

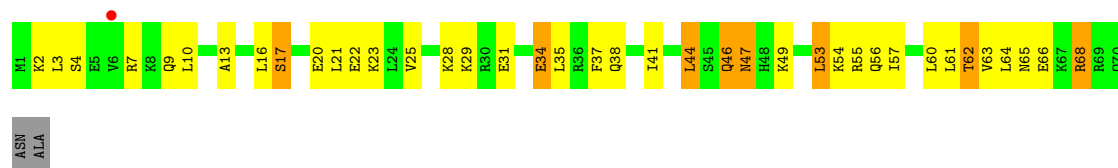
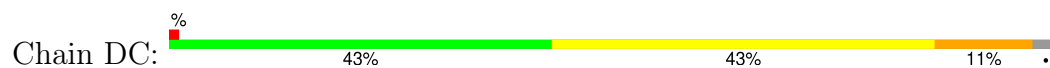


• Molecule 26: 50S ribosomal protein L29





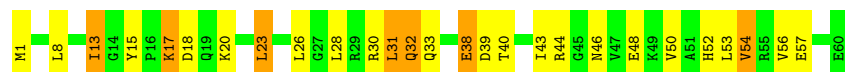
- Molecule 26: 50S ribosomal protein L29



- Molecule 27: 50S ribosomal protein L30



- Molecule 27: 50S ribosomal protein L30



- Molecule 28: 50S ribosomal protein L31

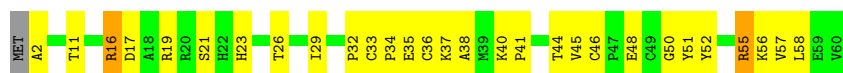


- Molecule 28: 50S ribosomal protein L31



- Molecule 29: 50S ribosomal protein L32

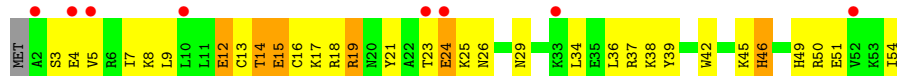




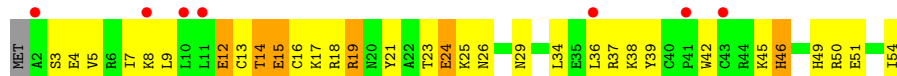
- Molecule 29: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L33



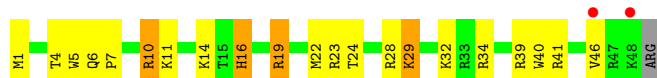
- Molecule 30: 50S ribosomal protein L33



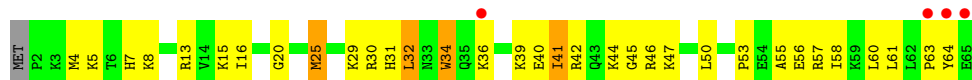
- Molecule 31: 50S ribosomal protein L34



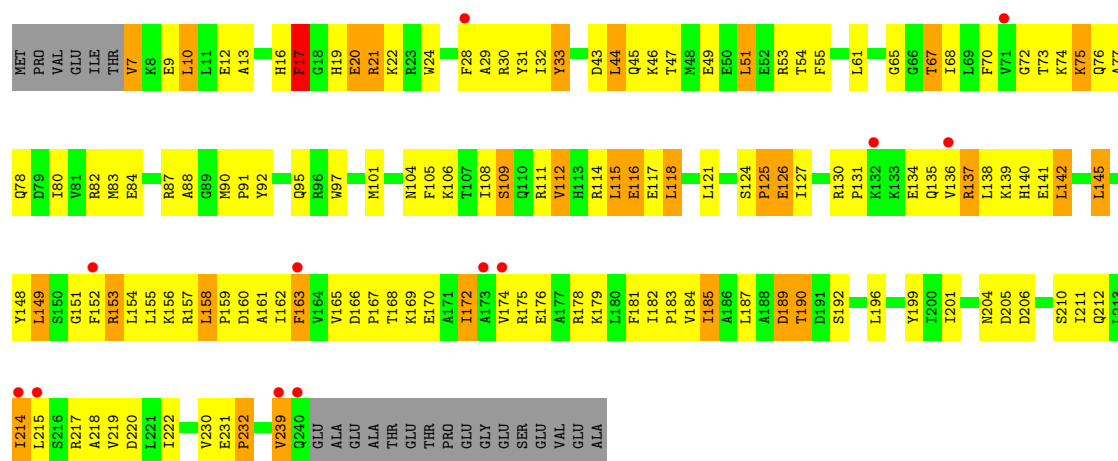
- Molecule 31: 50S ribosomal protein L34



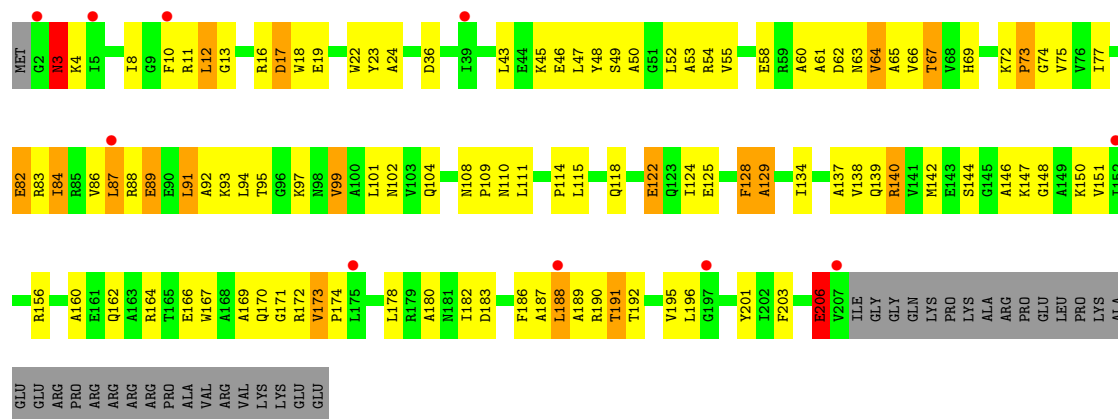
- Molecule 32: 50S ribosomal protein L35



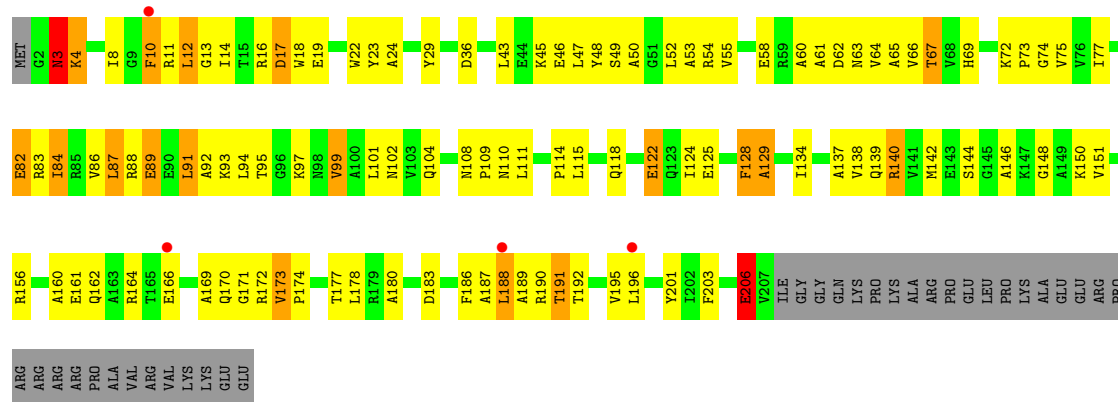
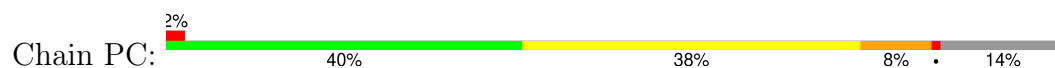
- Molecule 32: 50S ribosomal protein L35



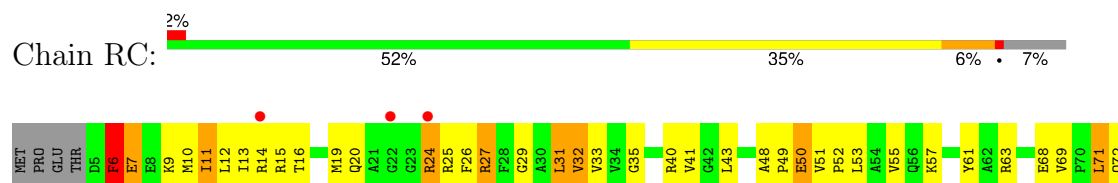
• Molecule 37: 30S ribosomal protein S3



• Molecule 37: 30S ribosomal protein S3



• Molecule 38: 30S ribosomal protein S4

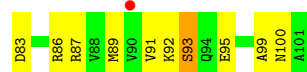
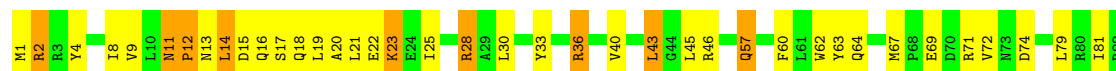




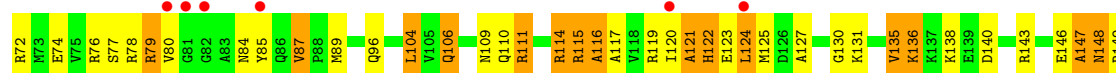
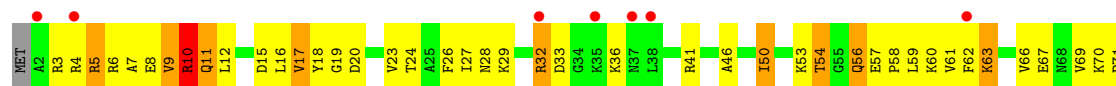
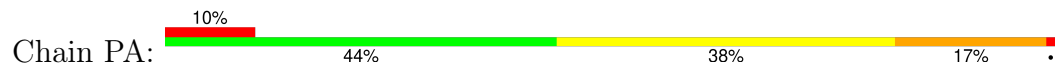
• Molecule 40: 30S ribosomal protein S6



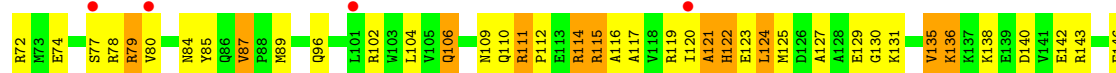
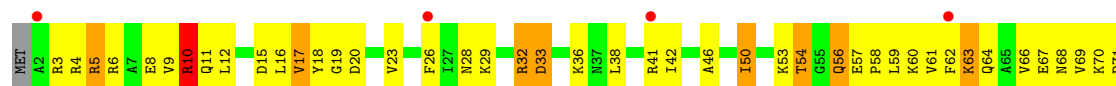
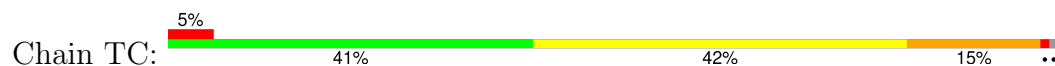
• Molecule 40: 30S ribosomal protein S6



• Molecule 41: 30S ribosomal protein S7

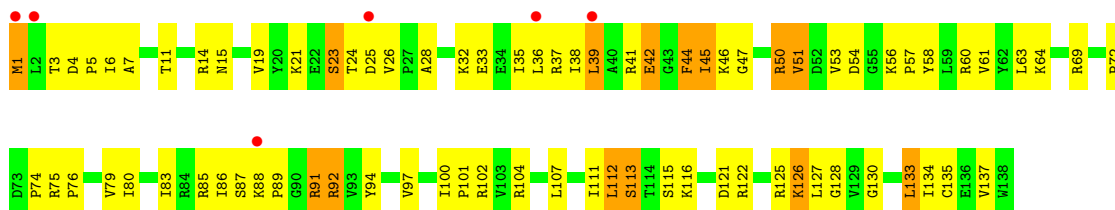


• Molecule 41: 30S ribosomal protein S7

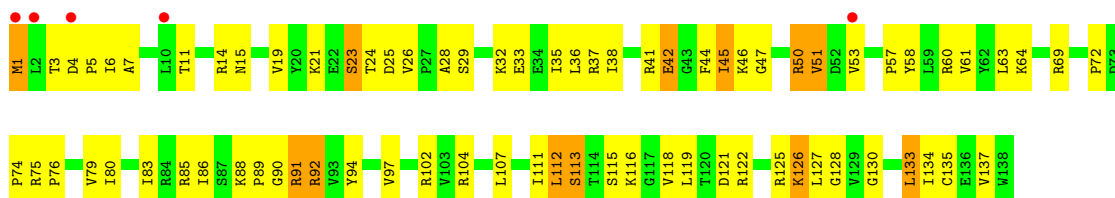




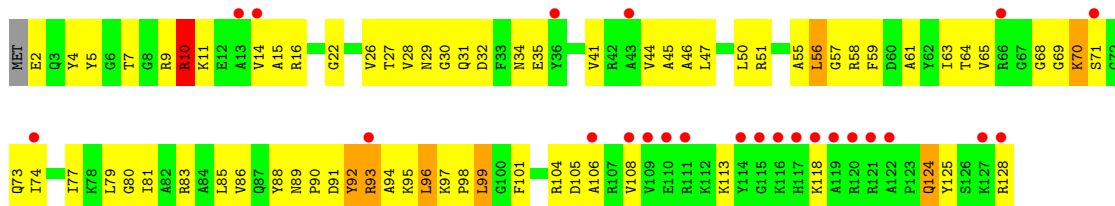
- Molecule 42: 30S ribosomal protein S8



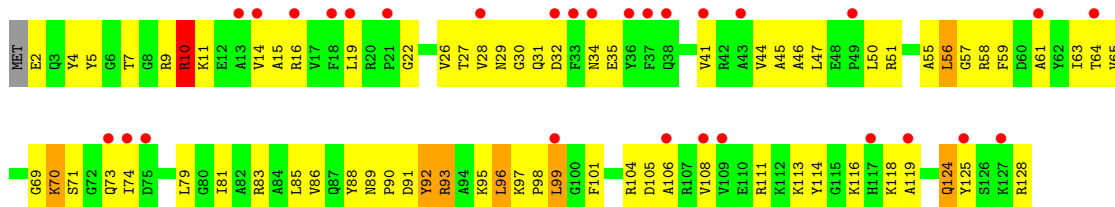
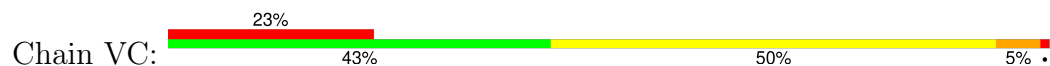
- Molecule 42: 30S ribosomal protein S8



- Molecule 43: 30S ribosomal protein S9

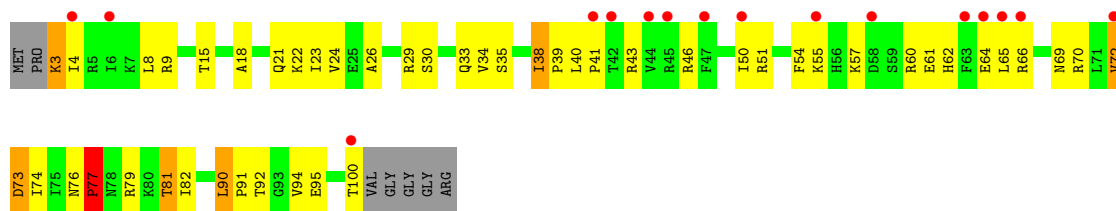


- Molecule 43: 30S ribosomal protein S9

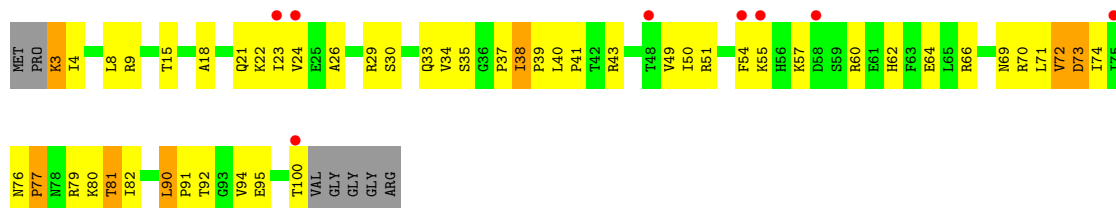


- Molecule 44: 30S ribosomal protein S10

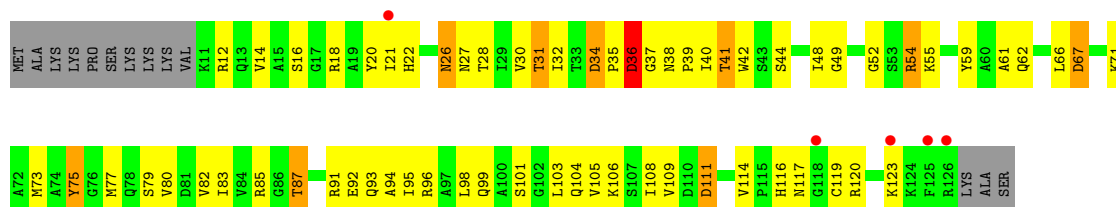




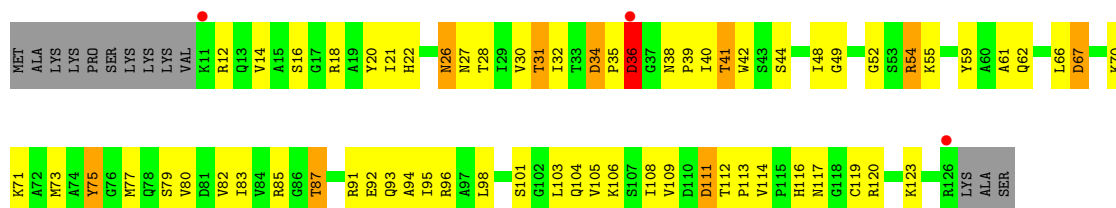
• Molecule 44: 30S ribosomal protein S10



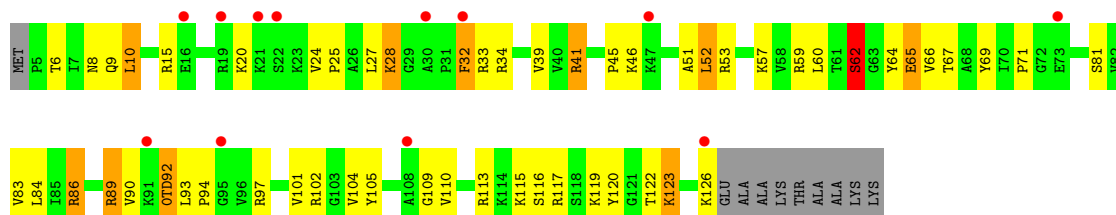
• Molecule 45: 30S ribosomal protein S11



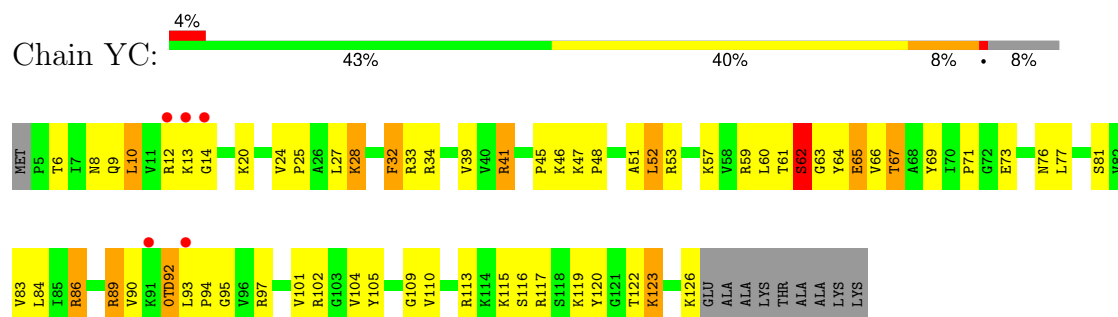
• Molecule 45: 30S ribosomal protein S11



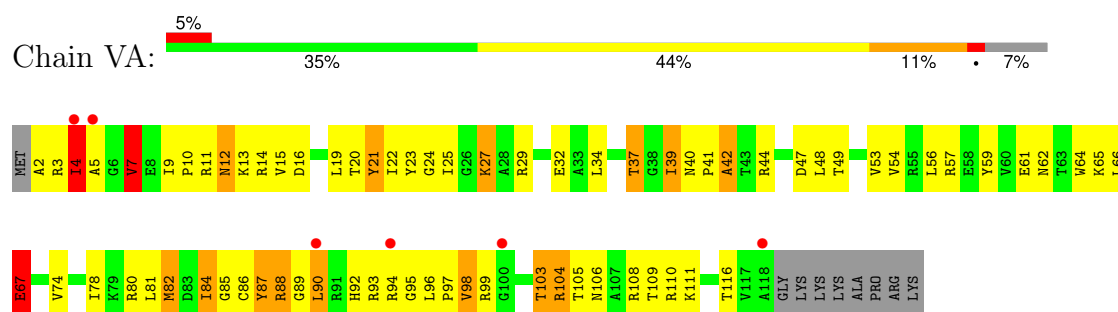
• Molecule 46: 30S ribosomal protein S12



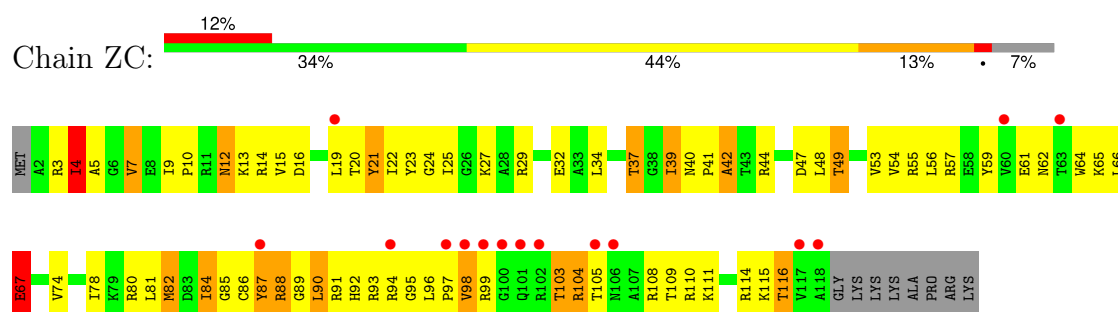
- Molecule 46: 30S ribosomal protein S12



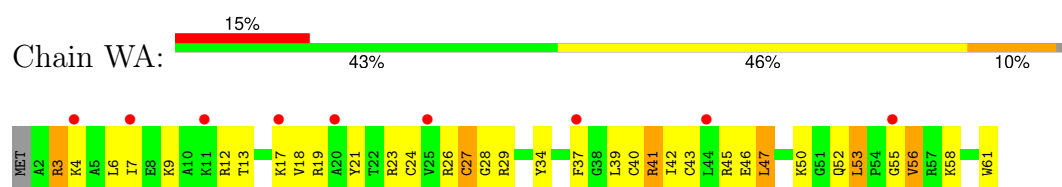
- Molecule 47: 30S ribosomal protein S13



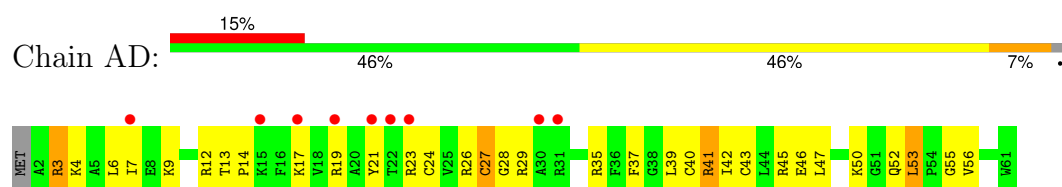
- Molecule 47: 30S ribosomal protein S13



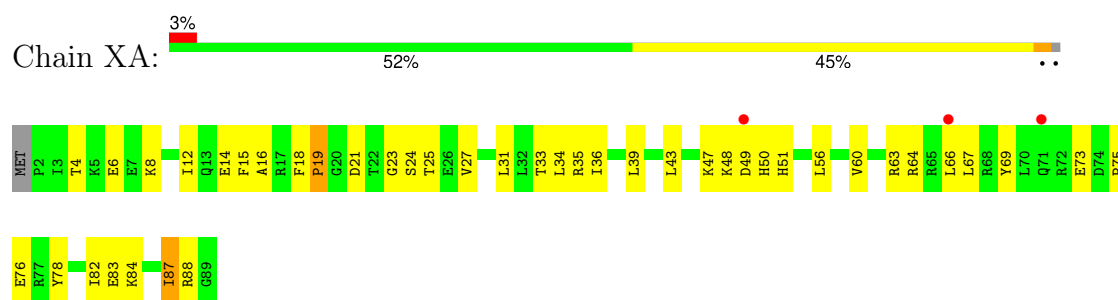
- Molecule 48: 30S ribosomal protein S14 type Z



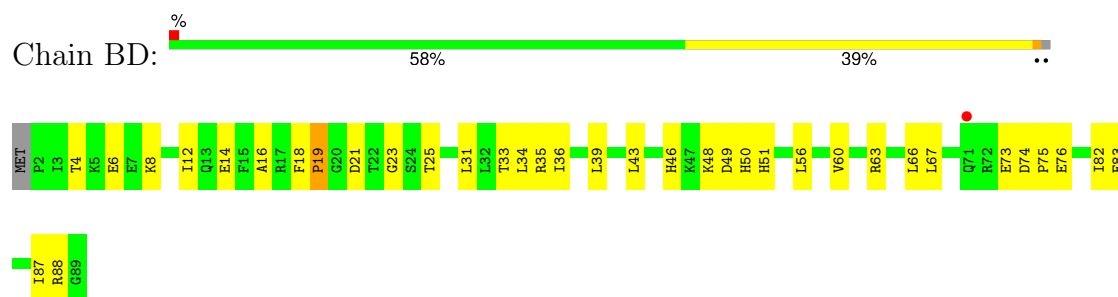
- Molecule 48: 30S ribosomal protein S14 type Z



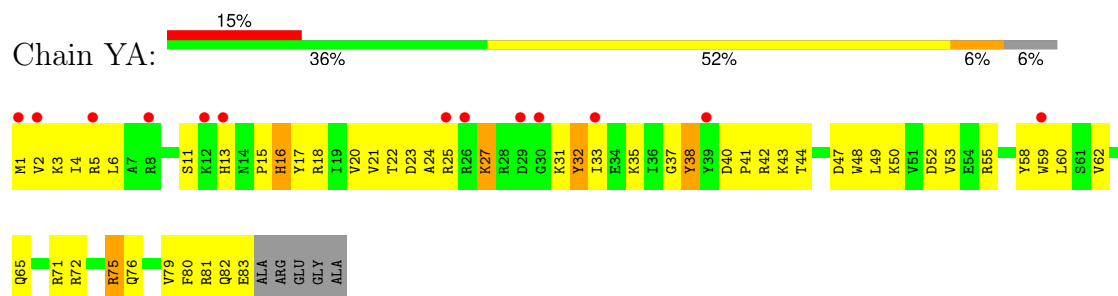
- Molecule 49: 30S ribosomal protein S15



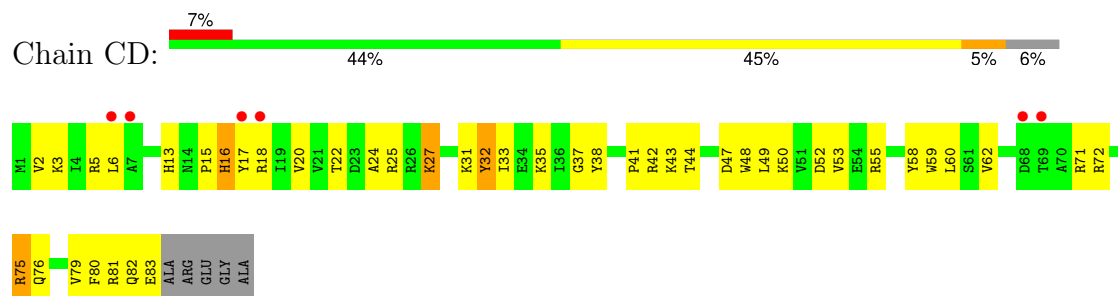
- Molecule 49: 30S ribosomal protein S15



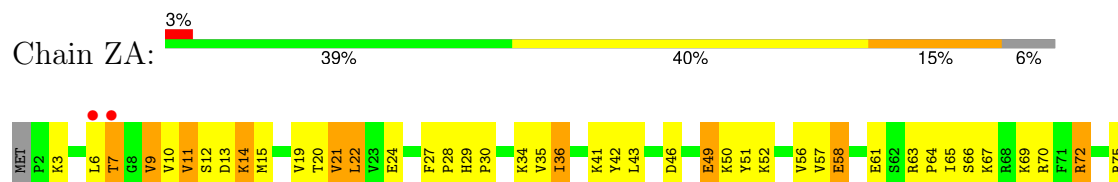
- Molecule 50: 30S ribosomal protein S16



- Molecule 50: 30S ribosomal protein S16

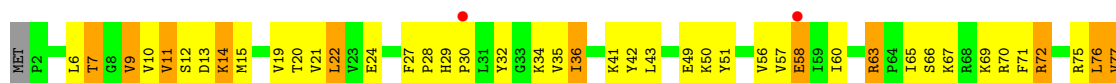
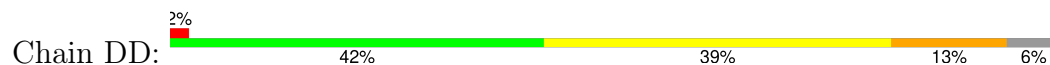


- Molecule 51: 30S ribosomal protein S17

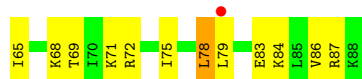
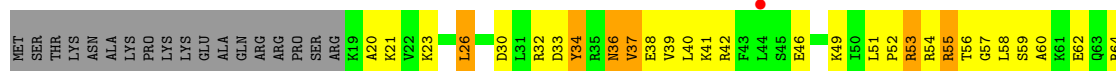




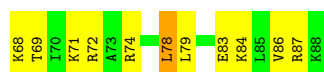
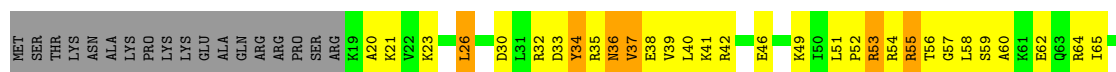
- Molecule 51: 30S ribosomal protein S17



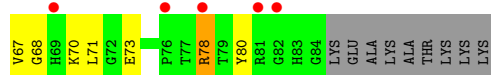
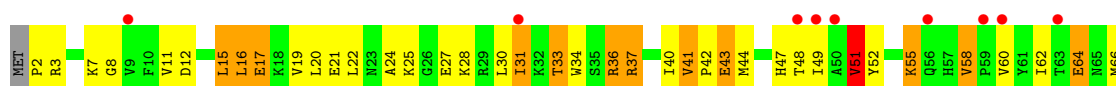
- Molecule 52: 30S ribosomal protein S18



- Molecule 52: 30S ribosomal protein S18

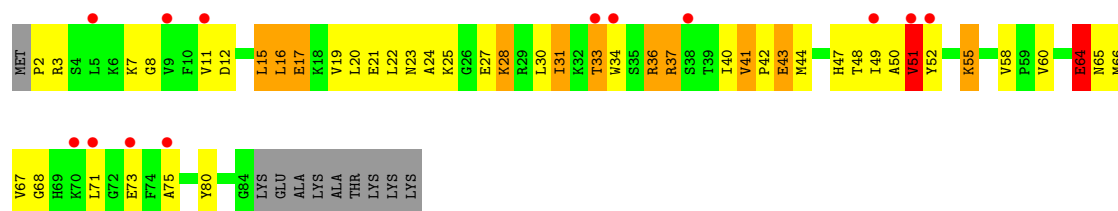


- Molecule 53: 30S ribosomal protein S19

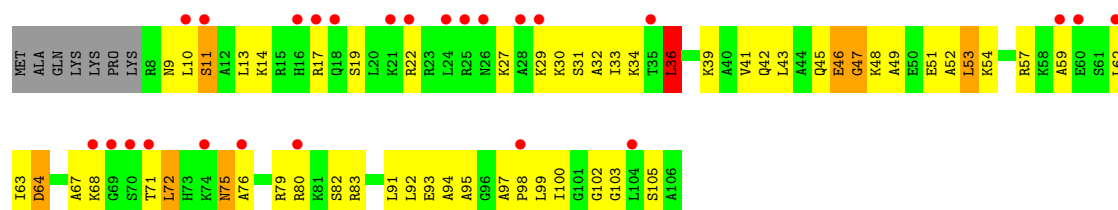


- Molecule 53: 30S ribosomal protein S19

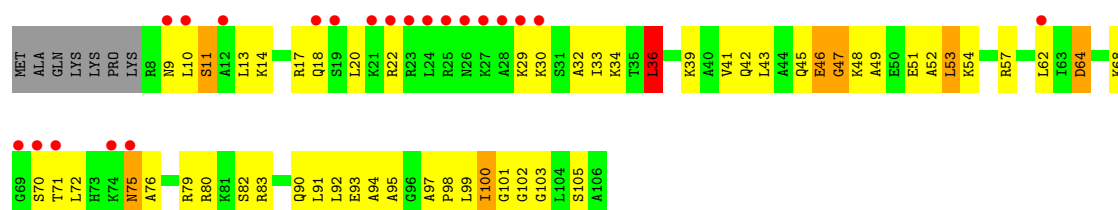
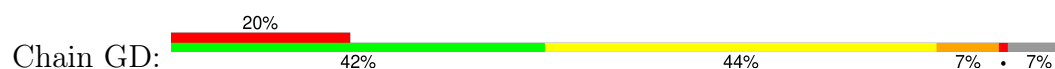




• Molecule 54: 30S ribosomal protein S20



• 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	211.85Å 452.54Å 624.45Å 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) 99.9 (50.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.41Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	(Not available) , (Not available) 0.260 , 0.296	Depositor DCC
R_{free} test set	797375 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	100.4	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	299841	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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: 5MU, 4SU, BLS, 5MC, 7MG, 2MG, UR3, OMG, 0TD, ZN, 2MA, PSU, 4OC, MG, M2G, 2MU, MA6

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.56	0/35961	1.08	64/56125 (0.1%)
1	EB	0.59	0/35961	1.11	67/56125 (0.1%)
2	B	0.90	35/69214 (0.1%)	1.38	667/108048 (0.6%)
2	FB	0.77	20/69214 (0.0%)	1.28	431/108048 (0.4%)
3	C	0.61	0/2881	1.13	3/4494 (0.1%)
3	GB	0.57	0/2881	1.09	1/4494 (0.0%)
4	D	0.43	0/1744	1.04	7/2719 (0.3%)
4	HB	0.43	0/1744	1.04	8/2719 (0.3%)
4	IA	0.53	0/1744	1.04	0/2719
4	MC	0.51	0/1744	1.03	0/2719
5	E	0.71	3/2195 (0.1%)	0.74	2/2955 (0.1%)
5	IB	0.65	2/2195 (0.1%)	0.73	1/2955 (0.0%)
6	F	0.61	1/1596 (0.1%)	0.65	0/2153
6	JB	0.55	2/1596 (0.1%)	0.62	0/2153
7	G	0.63	0/1621	0.66	0/2194
7	KB	0.55	0/1621	0.64	0/2194
8	H	0.36	0/1496	0.58	0/2013
8	LB	0.35	0/1496	0.57	0/2013
9	I	0.49	0/1356	0.58	0/1834
9	MB	0.36	0/1356	0.54	0/1834
10	J	0.44	0/1152	0.62	0/1559
10	NB	0.41	0/1152	0.60	0/1559
11	K	0.54	0/1148	0.64	0/1547
11	OB	0.44	0/1148	0.61	0/1547
12	L	0.65	0/942	0.64	0/1268
12	PB	0.56	0/942	0.64	0/1268
13	M	0.56	0/1162	0.72	0/1544
13	QB	0.51	0/1162	0.69	0/1544
14	N	0.57	0/1142	0.65	0/1525
14	RB	0.51	0/1142	0.63	0/1525
15	O	0.55	0/982	0.68	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	SB	0.51	0/982	0.65	0/1312
16	P	0.38	0/887	0.56	0/1180
16	TB	0.38	0/887	0.56	0/1180
17	Q	0.52	0/1157	0.62	0/1544
17	UB	0.50	0/1157	0.61	0/1544
18	R	0.63	0/982	0.63	0/1306
18	VB	0.51	0/982	0.60	0/1306
19	S	0.61	0/790	0.66	0/1057
19	WB	0.55	0/790	0.65	0/1057
20	T	0.67	0/901	0.67	0/1209
20	XB	0.58	0/901	0.62	0/1209
21	U	0.64	0/764	0.72	1/1025 (0.1%)
21	YB	0.57	0/764	0.69	1/1025 (0.1%)
22	V	0.57	0/827	0.66	0/1103
22	ZB	0.49	0/827	0.63	0/1103
23	AC	0.44	0/1527	0.55	0/2073
23	W	0.50	0/1527	0.57	0/2073
24	BC	0.51	0/671	0.69	0/892
24	X	0.53	0/671	0.70	0/892
25	CC	0.55	0/768	0.64	0/1021
25	Y	0.58	0/768	0.69	0/1021
26	DC	0.51	0/594	0.59	0/785
26	Z	0.63	0/594	0.64	0/785
27	AA	0.56	0/482	0.61	0/646
27	EC	0.52	0/482	0.60	0/646
28	BA	0.33	0/565	0.51	0/761
28	FC	0.34	0/565	0.50	0/761
29	CA	0.58	0/474	0.64	0/640
29	GC	0.47	0/474	0.61	0/640
30	DA	0.35	0/460	0.52	0/613
30	HC	0.33	0/460	0.51	0/613
31	EA	0.67	0/426	0.80	0/561
31	IC	0.60	0/426	0.71	0/561
32	FA	0.56	0/525	0.60	0/691
32	JC	0.54	0/525	0.60	0/691
33	GA	0.50	0/310	0.57	0/407
33	KC	0.46	0/310	0.54	0/407
34	HA	0.72	0/247	1.07	0/382
34	LC	0.74	0/247	1.04	0/382
35	JA	0.44	0/2037	0.61	0/2746
35	NC	0.41	0/2037	0.61	0/2746
36	KA	0.44	2/1935 (0.1%)	0.55	0/2609
36	OC	0.46	2/1935 (0.1%)	0.56	0/2609

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	LA	0.35	0/1636	0.55	0/2205
37	PC	0.38	0/1636	0.56	0/2205
38	MA	0.40	0/1733	0.57	0/2318
38	QC	0.48	0/1733	0.59	0/2318
39	NA	0.43	0/1171	0.59	0/1576
39	RC	0.48	0/1171	0.62	0/1576
40	OA	0.49	0/856	0.59	0/1154
40	SC	0.46	0/856	0.59	0/1154
41	PA	0.35	0/1276	0.51	0/1709
41	TC	0.33	0/1276	0.50	0/1709
42	QA	0.38	0/1136	0.57	0/1527
42	UC	0.42	0/1136	0.60	0/1527
43	RA	0.32	0/1029	0.57	0/1378
43	VC	0.34	0/1029	0.58	0/1378
44	SA	0.33	0/807	0.54	0/1085
44	WC	0.34	0/807	0.55	0/1085
45	TA	0.44	0/879	0.61	0/1187
45	XC	0.43	0/879	0.62	0/1187
46	UA	0.48	0/963	0.62	0/1287
46	YC	0.50	0/963	0.63	0/1287
47	VA	0.32	0/943	0.58	0/1265
47	ZC	0.34	0/943	0.58	0/1265
48	AD	0.38	0/501	0.53	0/664
48	WA	0.38	0/501	0.52	0/664
49	BD	0.47	0/745	0.55	0/992
49	XA	0.46	0/745	0.56	0/992
50	CD	0.42	0/716	0.56	0/963
50	YA	0.38	0/716	0.53	0/963
51	DD	0.51	0/836	0.57	0/1117
51	ZA	0.46	0/836	0.56	0/1117
52	AB	0.43	0/579	0.55	0/768
52	ED	0.44	0/579	0.54	0/768
53	BB	0.34	0/680	0.57	0/915
53	FD	0.33	0/680	0.56	0/915
54	CB	0.36	0/764	0.56	0/1006
54	GD	0.42	0/764	0.59	0/1006
55	DB	0.35	0/212	0.54	0/277
55	HD	0.32	0/212	0.52	0/277
All	All	0.68	67/322254 (0.0%)	1.11	1253/481306 (0.3%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
24	BC	0	1
24	X	0	1
38	MA	0	1
38	QC	0	1
All	All	0	4

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	945	A	N9-C4	12.76	1.45	1.37
2	B	1762	A	N9-C4	11.81	1.45	1.37
2	FB	945	A	N9-C4	11.72	1.44	1.37
2	B	945	A	C5-C6	10.43	1.50	1.41
2	FB	1762	A	N9-C4	10.17	1.44	1.37

The worst 5 of 1253 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	945	A	C2-N3-C4	21.30	121.25	110.60
2	FB	945	A	C2-N3-C4	17.33	119.27	110.60
2	B	945	A	C5-C6-N1	16.78	126.09	117.70
2	B	945	A	N1-C6-N6	-15.09	109.55	118.60
2	FB	945	A	C5-C6-N1	15.07	125.23	117.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	BC	84	LEU	Peptide
38	MA	21	LEU	Peptide
38	QC	21	LEU	Peptide
24	X	84	LEU	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	16368	745	0
1	EB	32394	0	16366	711	0
2	B	62031	0	31274	1148	0
2	FB	62031	0	31274	1141	1
3	C	2576	0	1305	54	0
3	GB	2576	0	1305	60	0
4	D	1642	0	841	45	0
4	HB	1642	0	841	40	0
4	IA	1642	0	841	54	0
4	MC	1642	0	841	49	0
5	E	2145	0	2234	113	0
5	IB	2145	0	2234	105	0
6	F	1563	0	1629	63	0
6	JB	1563	0	1629	63	0
7	G	1586	0	1632	77	0
7	KB	1586	0	1632	79	0
8	H	1471	0	1526	98	0
8	LB	1471	0	1526	87	1
9	I	1330	0	1407	56	0
9	MB	1330	0	1407	58	0
10	J	1137	0	1225	57	0
10	NB	1137	0	1225	59	0
11	K	1121	0	1195	43	0
11	OB	1121	0	1195	46	0
12	L	932	0	994	36	0
12	PB	932	0	994	40	0
13	M	1145	0	1228	58	0
13	QB	1145	0	1228	59	0
14	N	1121	0	1179	53	0
14	RB	1121	0	1179	55	0
15	O	968	0	1033	46	0
15	SB	968	0	1033	45	0
16	P	877	0	938	45	0
16	TB	877	0	938	42	0
17	Q	1143	0	1211	56	0
17	UB	1143	0	1211	53	0
18	R	964	0	1022	34	0
18	VB	964	0	1022	42	0
19	S	779	0	852	26	0
19	WB	779	0	852	31	0
20	T	890	0	951	38	0
20	XB	890	0	951	39	0
21	U	750	0	814	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	YB	750	0	814	24	0
22	V	814	0	906	33	0
22	ZB	814	0	906	36	0
23	AC	1495	0	1521	59	0
23	W	1495	0	1521	74	0
24	BC	662	0	688	39	0
24	X	662	0	688	36	0
25	CC	761	0	837	40	0
25	Y	761	0	837	42	0
26	DC	592	0	654	28	0
26	Z	592	0	654	29	0
27	AA	477	0	529	22	0
27	EC	477	0	529	18	0
28	BA	552	0	537	26	0
28	FC	552	0	537	21	0
29	CA	460	0	480	15	0
29	GC	460	0	480	17	0
30	DA	453	0	476	19	0
30	HC	453	0	476	19	0
31	EA	418	0	467	19	0
31	IC	418	0	467	17	0
32	FA	517	0	582	26	0
32	JC	517	0	582	26	0
33	GA	307	0	335	14	0
33	KC	307	0	335	17	0
34	HA	220	0	108	14	0
34	LC	220	0	108	5	0
35	JA	2005	0	1964	108	0
35	NC	2005	0	1964	95	0
36	KA	1900	0	1951	87	0
36	OC	1900	0	1951	93	0
37	LA	1612	0	1677	74	0
37	PC	1612	0	1677	74	0
38	MA	1703	0	1767	102	0
38	QC	1703	0	1767	105	0
39	NA	1155	0	1213	48	0
39	RC	1155	0	1213	45	0
40	OA	843	0	857	41	0
40	SC	843	0	857	42	0
41	PA	1257	0	1296	84	0
41	TC	1257	0	1296	77	0
42	QA	1116	0	1177	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	UC	1116	0	1177	65	0
43	RA	1011	0	1043	60	0
43	VC	1011	0	1043	61	0
44	SA	794	0	840	44	0
44	WC	794	0	840	43	0
45	TA	864	0	881	51	0
45	XC	864	0	881	50	0
46	UA	958	0	1047	41	0
46	YC	958	0	1047	52	0
47	VA	933	0	992	64	0
47	ZC	933	0	992	63	0
48	AD	492	0	533	32	0
48	WA	492	0	533	37	0
49	BD	734	0	771	26	0
49	XA	734	0	771	30	0
50	CD	700	0	720	40	0
50	YA	700	0	720	48	0
51	DD	823	0	893	46	0
51	ZA	823	0	893	42	0
52	AB	574	0	644	41	0
52	ED	574	0	644	42	0
53	BB	665	0	686	52	0
53	FD	665	0	686	54	0
54	CB	762	0	859	36	0
54	GD	762	0	859	39	0
55	DB	208	0	221	24	0
55	HD	208	0	221	21	0
56	A	214	0	0	0	0
56	AA	2	0	0	0	0
56	AB	2	0	0	0	0
56	AD	2	0	0	0	0
56	B	562	0	0	0	0
56	BA	1	0	0	0	0
56	BC	1	0	0	0	0
56	BD	1	0	0	0	0
56	C	21	0	0	0	0
56	CA	1	0	0	0	0
56	CB	1	0	0	0	0
56	CC	7	0	0	0	0
56	CD	1	0	0	0	0
56	D	5	0	0	0	0
56	DA	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DC	1	0	0	0	0
56	E	1	0	0	0	0
56	EA	1	0	0	0	0
56	EB	206	0	0	0	0
56	EC	1	0	0	0	0
56	F	2	0	0	0	0
56	FB	475	0	0	0	0
56	FC	1	0	0	0	0
56	G	2	0	0	0	0
56	GB	15	0	0	0	0
56	H	1	0	0	0	0
56	HA	3	0	0	0	0
56	HB	9	0	0	0	0
56	I	3	0	0	0	0
56	IA	6	0	0	0	0
56	IB	4	0	0	0	0
56	J	2	0	0	0	0
56	JA	6	0	0	0	0
56	JB	2	0	0	0	0
56	JC	1	0	0	0	0
56	K	4	0	0	0	0
56	KA	1	0	0	0	0
56	KB	4	0	0	0	0
56	L	2	0	0	0	0
56	LA	2	0	0	0	0
56	LC	1	0	0	0	0
56	M	5	0	0	0	0
56	MA	2	0	0	0	0
56	MB	2	0	0	0	0
56	MC	5	0	0	0	0
56	NA	2	0	0	0	0
56	NB	3	0	0	0	0
56	NC	5	0	0	0	0
56	O	2	0	0	0	0
56	OB	3	0	0	0	0
56	OC	5	0	0	0	0
56	PB	1	0	0	0	0
56	PC	1	0	0	0	0
56	Q	2	0	0	0	0
56	QA	2	0	0	0	0
56	QC	4	0	0	0	0
56	RB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	RC	3	0	0	0	0
56	S	2	0	0	0	0
56	SA	3	0	0	0	0
56	SB	2	0	0	0	0
56	SC	1	0	0	0	0
56	T	3	0	0	0	0
56	TA	3	0	0	0	0
56	TB	1	0	0	0	0
56	TC	1	0	0	0	0
56	U	2	0	0	0	0
56	UA	4	0	0	0	0
56	UB	3	0	0	0	0
56	UC	2	0	0	0	0
56	V	2	0	0	0	0
56	VB	1	0	0	0	0
56	VC	1	0	0	0	0
56	W	2	0	0	0	0
56	WB	1	0	0	0	0
56	WC	1	0	0	0	0
56	X	1	0	0	0	0
56	XA	6	0	0	0	0
56	XC	1	0	0	0	0
56	Y	1	0	0	0	0
56	YC	5	0	0	0	0
56	Z	4	0	0	0	0
56	ZA	1	0	0	0	0
56	ZB	2	0	0	0	0
57	B	30	0	24	2	0
57	FB	30	0	24	1	0
58	BA	1	0	0	0	0
58	CA	1	0	0	0	0
58	DA	1	0	0	0	0
58	FC	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	KC	1	0	0	0	0
58	V	1	0	0	0	0
58	ZB	1	0	0	0	0
All	All	299841	0	203748	7838	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 16.

The worst 5 of 7838 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:QC:18:LYS:NZ	38:QC:26:CYS:SG	2.00	1.34
38:MA:9:CYS:SG	38:MA:18:LYS:NZ	2.05	1.30
38:QC:9:CYS:SG	38:QC:18:LYS:NZ	2.03	1.29
2:B:630:G:OP2	32:FA:15:LYS:NZ	1.65	1.29
38:MA:18:LYS:NZ	38:MA:26:CYS:SG	2.04	1.28

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:FB:1412:A:O2'	8:LB:9:ARG:NH1[1_655]	2.16	0.04

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%)	238 (87%)	27 (10%)	8 (3%)	3	19
5	IB	273/275 (99%)	238 (87%)	27 (10%)	8 (3%)	3	19
6	F	202/206 (98%)	171 (85%)	25 (12%)	6 (3%)	3	19
6	JB	202/206 (98%)	171 (85%)	26 (13%)	5 (2%)	4	22
7	G	200/205 (98%)	173 (86%)	22 (11%)	5 (2%)	4	22
7	KB	200/205 (98%)	170 (85%)	26 (13%)	4 (2%)	6	25
8	H	179/182 (98%)	137 (76%)	29 (16%)	13 (7%)	1	5
8	LB	179/182 (98%)	135 (75%)	31 (17%)	13 (7%)	1	5
9	I	172/180 (96%)	138 (80%)	24 (14%)	10 (6%)	1	9
9	MB	172/180 (96%)	138 (80%)	25 (14%)	9 (5%)	1	10
10	J	144/148 (97%)	108 (75%)	27 (19%)	9 (6%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	NB	144/148 (97%)	108 (75%)	27 (19%)	9 (6%)	1	7
11	K	138/140 (99%)	120 (87%)	12 (9%)	6 (4%)	2	14
11	OB	138/140 (99%)	121 (88%)	11 (8%)	6 (4%)	2	14
12	L	120/122 (98%)	105 (88%)	11 (9%)	4 (3%)	3	18
12	PB	120/122 (98%)	105 (88%)	11 (9%)	4 (3%)	3	18
13	M	148/150 (99%)	115 (78%)	24 (16%)	9 (6%)	1	8
13	QB	148/150 (99%)	117 (79%)	24 (16%)	7 (5%)	2	12
14	N	139/141 (99%)	113 (81%)	22 (16%)	4 (3%)	3	19
14	RB	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	3	16
15	O	116/118 (98%)	100 (86%)	14 (12%)	2 (2%)	7	28
15	SB	116/118 (98%)	101 (87%)	12 (10%)	3 (3%)	4	22
16	P	108/112 (96%)	88 (82%)	17 (16%)	3 (3%)	4	20
16	TB	108/112 (96%)	88 (82%)	16 (15%)	4 (4%)	2	16
17	Q	135/146 (92%)	111 (82%)	20 (15%)	4 (3%)	3	19
17	UB	135/146 (92%)	112 (83%)	19 (14%)	4 (3%)	3	19
18	R	115/118 (98%)	104 (90%)	9 (8%)	2 (2%)	7	28
18	VB	115/118 (98%)	104 (90%)	9 (8%)	2 (2%)	7	28
19	S	99/101 (98%)	80 (81%)	14 (14%)	5 (5%)	1	11
19	WB	99/101 (98%)	81 (82%)	14 (14%)	4 (4%)	2	15
20	T	110/113 (97%)	101 (92%)	9 (8%)	0	100	100
20	XB	110/113 (97%)	100 (91%)	9 (8%)	1 (1%)	14	41
21	U	93/96 (97%)	80 (86%)	10 (11%)	3 (3%)	3	18
21	YB	93/96 (97%)	82 (88%)	8 (9%)	3 (3%)	3	18
22	V	105/110 (96%)	83 (79%)	15 (14%)	7 (7%)	1	7
22	ZB	105/110 (96%)	84 (80%)	16 (15%)	5 (5%)	2	12
23	AC	187/206 (91%)	153 (82%)	26 (14%)	8 (4%)	2	14
23	W	187/206 (91%)	150 (80%)	29 (16%)	8 (4%)	2	14
24	BC	82/85 (96%)	67 (82%)	11 (13%)	4 (5%)	2	11
24	X	82/85 (96%)	66 (80%)	10 (12%)	6 (7%)	1	5
25	CC	95/98 (97%)	81 (85%)	10 (10%)	4 (4%)	2	14
25	Y	95/98 (97%)	81 (85%)	10 (10%)	4 (4%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	DC	68/72 (94%)	65 (96%)	2 (3%)	1 (2%)	8	30
26	Z	68/72 (94%)	65 (96%)	2 (3%)	1 (2%)	8	30
27	AA	58/60 (97%)	49 (84%)	8 (14%)	1 (2%)	7	28
27	EC	58/60 (97%)	51 (88%)	6 (10%)	1 (2%)	7	28
28	BA	67/71 (94%)	44 (66%)	14 (21%)	9 (13%)	0	1
28	FC	67/71 (94%)	44 (66%)	16 (24%)	7 (10%)	0	3
29	CA	57/60 (95%)	50 (88%)	7 (12%)	0	100	100
29	GC	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
30	DA	51/54 (94%)	35 (69%)	12 (24%)	4 (8%)	1	5
30	HC	51/54 (94%)	35 (69%)	12 (24%)	4 (8%)	1	5
31	EA	46/49 (94%)	42 (91%)	4 (9%)	0	100	100
31	IC	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
32	FA	62/65 (95%)	56 (90%)	5 (8%)	1 (2%)	8	29
32	JC	62/65 (95%)	57 (92%)	3 (5%)	2 (3%)	3	18
33	GA	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	KC	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
35	JA	256/368 (70%)	197 (77%)	46 (18%)	13 (5%)	1	11
35	NC	256/368 (70%)	197 (77%)	44 (17%)	15 (6%)	1	8
36	KA	232/256 (91%)	180 (78%)	38 (16%)	14 (6%)	1	8
36	OC	232/256 (91%)	180 (78%)	36 (16%)	16 (7%)	1	6
37	LA	204/239 (85%)	158 (78%)	35 (17%)	11 (5%)	1	10
37	PC	204/239 (85%)	158 (78%)	35 (17%)	11 (5%)	1	10
38	MA	206/209 (99%)	159 (77%)	33 (16%)	14 (7%)	1	6
38	QC	206/209 (99%)	159 (77%)	34 (16%)	13 (6%)	1	7
39	NA	149/162 (92%)	121 (81%)	21 (14%)	7 (5%)	2	12
39	RC	149/162 (92%)	120 (80%)	22 (15%)	7 (5%)	2	12
40	OA	99/101 (98%)	81 (82%)	16 (16%)	2 (2%)	6	25
40	SC	99/101 (98%)	83 (84%)	14 (14%)	2 (2%)	6	25
41	PA	153/156 (98%)	115 (75%)	25 (16%)	13 (8%)	0	4
41	TC	153/156 (98%)	114 (74%)	26 (17%)	13 (8%)	0	4
42	QA	136/138 (99%)	120 (88%)	15 (11%)	1 (1%)	19	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	UC	136/138 (99%)	119 (88%)	16 (12%)	1 (1%)	19	47
43	RA	125/128 (98%)	94 (75%)	22 (18%)	9 (7%)	1	6
43	VC	125/128 (98%)	94 (75%)	23 (18%)	8 (6%)	1	7
44	SA	96/105 (91%)	81 (84%)	14 (15%)	1 (1%)	13	39
44	WC	96/105 (91%)	82 (85%)	13 (14%)	1 (1%)	13	39
45	TA	114/129 (88%)	91 (80%)	16 (14%)	7 (6%)	1	8
45	XC	114/129 (88%)	91 (80%)	17 (15%)	6 (5%)	1	10
46	UA	119/132 (90%)	97 (82%)	20 (17%)	2 (2%)	7	28
46	YC	119/132 (90%)	96 (81%)	19 (16%)	4 (3%)	3	17
47	VA	115/126 (91%)	82 (71%)	25 (22%)	8 (7%)	1	6
47	ZC	115/126 (91%)	81 (70%)	25 (22%)	9 (8%)	1	5
48	AD	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	1	10
48	WA	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	17
49	BD	86/89 (97%)	72 (84%)	11 (13%)	3 (4%)	3	17
49	XA	86/89 (97%)	72 (84%)	10 (12%)	4 (5%)	2	12
50	CD	81/88 (92%)	70 (86%)	9 (11%)	2 (2%)	4	22
50	YA	81/88 (92%)	70 (86%)	9 (11%)	2 (2%)	4	22
51	DD	97/105 (92%)	80 (82%)	14 (14%)	3 (3%)	3	18
51	ZA	97/105 (92%)	79 (81%)	15 (16%)	3 (3%)	3	18
52	AB	68/88 (77%)	59 (87%)	7 (10%)	2 (3%)	3	19
52	ED	68/88 (77%)	58 (85%)	8 (12%)	2 (3%)	3	19
53	BB	81/93 (87%)	56 (69%)	19 (24%)	6 (7%)	1	5
53	FD	81/93 (87%)	58 (72%)	17 (21%)	6 (7%)	1	5
54	CB	97/106 (92%)	74 (76%)	14 (14%)	9 (9%)	0	3
54	GD	97/106 (92%)	75 (77%)	14 (14%)	8 (8%)	1	4
55	DB	22/27 (82%)	15 (68%)	5 (23%)	2 (9%)	0	4
55	HD	22/27 (82%)	15 (68%)	5 (23%)	2 (9%)	0	4
All	All	11996/12852 (93%)	9782 (82%)	1686 (14%)	528 (4%)	2	13

5 of 528 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	47	LYS

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Mol	Chain	Res	Type
8	H	51	ARG
8	H	52	ILE
8	H	84	LYS
8	H	126	ASP

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%)	178 (82%)	39 (18%)	1	5
5	IB	217/217 (100%)	176 (81%)	41 (19%)	1	4
6	F	165/166 (99%)	136 (82%)	29 (18%)	1	6
6	JB	165/166 (99%)	137 (83%)	28 (17%)	1	6
7	G	161/162 (99%)	132 (82%)	29 (18%)	1	5
7	KB	161/162 (99%)	132 (82%)	29 (18%)	1	5
8	H	154/156 (99%)	131 (85%)	23 (15%)	2	9
8	LB	154/156 (99%)	131 (85%)	23 (15%)	2	9
9	I	144/148 (97%)	122 (85%)	22 (15%)	2	9
9	MB	144/148 (97%)	122 (85%)	22 (15%)	2	9
10	J	122/124 (98%)	92 (75%)	30 (25%)	0	1
10	NB	122/124 (98%)	91 (75%)	31 (25%)	0	1
11	K	119/119 (100%)	102 (86%)	17 (14%)	2	10
11	OB	119/119 (100%)	102 (86%)	17 (14%)	2	10
12	L	100/100 (100%)	85 (85%)	15 (15%)	2	9
12	PB	100/100 (100%)	85 (85%)	15 (15%)	2	9
13	M	116/116 (100%)	92 (79%)	24 (21%)	1	2
13	QB	116/116 (100%)	93 (80%)	23 (20%)	1	3
14	N	111/111 (100%)	93 (84%)	18 (16%)	2	8
14	RB	111/111 (100%)	93 (84%)	18 (16%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	101/101 (100%)	86 (85%)	15 (15%)	2	9
15	SB	101/101 (100%)	86 (85%)	15 (15%)	2	9
16	P	87/88 (99%)	73 (84%)	14 (16%)	2	8
16	TB	87/88 (99%)	73 (84%)	14 (16%)	2	8
17	Q	121/128 (94%)	108 (89%)	13 (11%)	5	20
17	UB	121/128 (94%)	106 (88%)	15 (12%)	4	14
18	R	93/94 (99%)	81 (87%)	12 (13%)	3	13
18	VB	93/94 (99%)	83 (89%)	10 (11%)	5	20
19	S	82/82 (100%)	66 (80%)	16 (20%)	1	3
19	WB	82/82 (100%)	65 (79%)	17 (21%)	1	2
20	T	91/92 (99%)	77 (85%)	14 (15%)	2	9
20	XB	91/92 (99%)	76 (84%)	15 (16%)	2	7
21	U	77/78 (99%)	65 (84%)	12 (16%)	2	8
21	YB	77/78 (99%)	66 (86%)	11 (14%)	2	10
22	V	87/91 (96%)	71 (82%)	16 (18%)	1	5
22	ZB	87/91 (96%)	71 (82%)	16 (18%)	1	5
23	AC	163/179 (91%)	137 (84%)	26 (16%)	2	8
23	W	163/179 (91%)	137 (84%)	26 (16%)	2	8
24	BC	66/67 (98%)	57 (86%)	9 (14%)	3	12
24	X	66/67 (98%)	57 (86%)	9 (14%)	3	12
25	CC	81/83 (98%)	61 (75%)	20 (25%)	0	1
25	Y	81/83 (98%)	61 (75%)	20 (25%)	0	1
26	DC	66/67 (98%)	52 (79%)	14 (21%)	1	2
26	Z	66/67 (98%)	52 (79%)	14 (21%)	1	2
27	AA	52/52 (100%)	40 (77%)	12 (23%)	0	2
27	EC	52/52 (100%)	40 (77%)	12 (23%)	0	2
28	BA	59/63 (94%)	50 (85%)	9 (15%)	2	9
28	FC	59/63 (94%)	50 (85%)	9 (15%)	2	9
29	CA	51/52 (98%)	39 (76%)	12 (24%)	0	2
29	GC	51/52 (98%)	39 (76%)	12 (24%)	0	2
30	DA	51/52 (98%)	42 (82%)	9 (18%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	HC	51/52 (98%)	42 (82%)	9 (18%)	1	6
31	EA	41/42 (98%)	30 (73%)	11 (27%)	0	1
31	IC	41/42 (98%)	29 (71%)	12 (29%)	0	1
32	FA	54/55 (98%)	46 (85%)	8 (15%)	2	9
32	JC	54/55 (98%)	47 (87%)	7 (13%)	3	13
33	GA	34/34 (100%)	31 (91%)	3 (9%)	8	28
33	KC	34/34 (100%)	31 (91%)	3 (9%)	8	28
35	JA	209/308 (68%)	176 (84%)	33 (16%)	2	8
35	NC	209/308 (68%)	178 (85%)	31 (15%)	2	9
36	KA	202/220 (92%)	164 (81%)	38 (19%)	1	4
36	OC	202/220 (92%)	164 (81%)	38 (19%)	1	4
37	LA	160/188 (85%)	133 (83%)	27 (17%)	1	6
37	PC	160/188 (85%)	133 (83%)	27 (17%)	1	6
38	MA	180/181 (99%)	146 (81%)	34 (19%)	1	4
38	QC	180/181 (99%)	145 (81%)	35 (19%)	1	3
39	NA	116/123 (94%)	102 (88%)	14 (12%)	4	15
39	RC	116/123 (94%)	102 (88%)	14 (12%)	4	15
40	OA	90/90 (100%)	75 (83%)	15 (17%)	2	7
40	SC	90/90 (100%)	75 (83%)	15 (17%)	2	7
41	PA	126/127 (99%)	100 (79%)	26 (21%)	1	3
41	TC	126/127 (99%)	99 (79%)	27 (21%)	1	2
42	QA	119/119 (100%)	100 (84%)	19 (16%)	2	8
42	UC	119/119 (100%)	101 (85%)	18 (15%)	2	9
43	RA	98/99 (99%)	86 (88%)	12 (12%)	4	15
43	VC	98/99 (99%)	86 (88%)	12 (12%)	4	15
44	SA	88/92 (96%)	79 (90%)	9 (10%)	6	22
44	WC	88/92 (96%)	80 (91%)	8 (9%)	7	26
45	TA	88/99 (89%)	71 (81%)	17 (19%)	1	3
45	XC	88/99 (89%)	71 (81%)	17 (19%)	1	3
46	UA	102/108 (94%)	85 (83%)	17 (17%)	2	7
46	YC	102/108 (94%)	85 (83%)	17 (17%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	VA	94/101 (93%)	71 (76%)	23 (24%)	0	1
47	ZC	94/101 (93%)	72 (77%)	22 (23%)	0	2
48	AD	49/50 (98%)	42 (86%)	7 (14%)	2	10
48	WA	49/50 (98%)	42 (86%)	7 (14%)	2	10
49	BD	79/80 (99%)	71 (90%)	8 (10%)	6	22
49	XA	79/80 (99%)	71 (90%)	8 (10%)	6	22
50	CD	72/74 (97%)	62 (86%)	10 (14%)	3	11
50	YA	72/74 (97%)	61 (85%)	11 (15%)	2	9
51	DD	94/97 (97%)	72 (77%)	22 (23%)	0	2
51	ZA	94/97 (97%)	72 (77%)	22 (23%)	0	2
52	AB	61/77 (79%)	50 (82%)	11 (18%)	1	5
52	ED	61/77 (79%)	50 (82%)	11 (18%)	1	5
53	BB	72/80 (90%)	58 (81%)	14 (19%)	1	3
53	FD	72/80 (90%)	59 (82%)	13 (18%)	1	5
54	CB	76/82 (93%)	65 (86%)	11 (14%)	2	10
54	GD	76/82 (93%)	65 (86%)	11 (14%)	2	10
55	DB	19/22 (86%)	15 (79%)	4 (21%)	1	2
55	HD	19/22 (86%)	15 (79%)	4 (21%)	1	2
All	All	10120/10672 (95%)	8397 (83%)	1723 (17%)	1	6

5 of 1723 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	JB	175	VAL
17	UB	89	VAL
46	YC	10	LEU
7	KB	170	LEU
6	JB	173	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
45	XC	26	ASN
47	ZC	62	ASN
53	FD	23	ASN

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Mol	Chain	Res	Type
41	PA	110	GLN
41	PA	109	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1502/1507 (99%)	330 (21%)	13 (0%)
1	EB	1502/1507 (99%)	330 (21%)	13 (0%)
2	B	2876/2880 (99%)	644 (22%)	22 (0%)
2	FB	2876/2880 (99%)	642 (22%)	23 (0%)
3	C	119/120 (99%)	22 (18%)	1 (0%)
3	GB	119/120 (99%)	21 (17%)	1 (0%)
34	HA	9/23 (39%)	5 (55%)	0
34	LC	9/23 (39%)	5 (55%)	0
4	D	76/77 (98%)	25 (32%)	0
4	HB	76/77 (98%)	26 (34%)	0
4	IA	76/77 (98%)	20 (26%)	0
4	MC	76/77 (98%)	20 (26%)	0
All	All	9316/9368 (99%)	2090 (22%)	73 (0%)

5 of 2090 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C

5 of 73 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	FB	974(A)	G
2	FB	2756	U
2	FB	1060	U
2	FB	1939	5MU
2	B	1267	U

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
46	0TD	UA	92	46	8,9,10	3.14	2 (25%)	6,11,13	2.01	3 (50%)
4	4SU	D	8	4	18,21,22	5.94	1 (5%)	25,30,33	0.64	0
1	MA6	A	1518	1	19,26,27	2.14	5 (26%)	18,38,41	1.89	3 (16%)
4	5MU	HB	54	4	19,22,23	2.05	3 (15%)	27,32,35	2.12	8 (29%)
1	5MC	EB	967	1	19,22,23	2.71	4 (21%)	26,32,35	1.10	3 (11%)
1	PSU	EB	516	1	18,21,22	1.73	4 (22%)	21,30,33	1.51	4 (19%)
1	5MC	A	1404	1	19,22,23	2.24	4 (21%)	26,32,35	1.38	3 (11%)
4	5MC	HB	32	4	19,22,23	2.57	5 (26%)	26,32,35	1.01	2 (7%)
4	5MU	IA	54	4	19,22,23	2.09	3 (15%)	27,32,35	2.16	8 (29%)
2	PSU	B	2605	2	18,21,22	1.80	4 (22%)	21,30,33	1.82	4 (19%)
4	5MU	MC	54	4	19,22,23	2.14	3 (15%)	27,32,35	2.00	8 (29%)
1	MA6	A	1519	1	19,26,27	2.14	4 (21%)	18,38,41	1.66	3 (16%)
2	2MA	B	2503	2	17,25,26	1.45	2 (11%)	16,37,40	1.34	3 (18%)
1	UR3	EB	1498	1	19,22,23	1.76	2 (10%)	26,32,35	1.69	5 (19%)
1	5MC	A	1400	1	19,22,23	2.64	5 (26%)	26,32,35	1.11	4 (15%)
2	5MC	B	1942	2	19,22,23	2.74	4 (21%)	26,32,35	1.46	3 (11%)
4	4SU	MC	8	4	18,21,22	5.96	1 (5%)	25,30,33	0.69	0
4	5MC	IA	32	4	19,22,23	2.86	5 (26%)	26,32,35	1.20	3 (11%)
1	M2G	A	966	1	20,27,28	2.35	3 (15%)	19,40,43	1.42	3 (15%)
1	2MG	A	1207	1	18,26,27	2.18	4 (22%)	16,38,41	1.50	2 (12%)
1	5MC	A	1407	1	19,22,23	2.64	4 (21%)	26,32,35	1.35	3 (11%)
2	5MC	B	1962	2	19,22,23	2.77	4 (21%)	26,32,35	1.50	4 (15%)
4	5MC	MC	32	4	19,22,23	2.79	4 (21%)	26,32,35	1.30	3 (11%)
4	PSU	HB	55	4	18,21,22	1.82	2 (11%)	21,30,33	1.67	4 (19%)
1	7MG	A	527	1	23,26,27	3.04	7 (30%)	27,39,42	2.24	7 (25%)
4	5MU	D	54	4	19,22,23	2.10	3 (15%)	27,32,35	2.10	8 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2MU	FB	2552	2	19,22,24	2.50	5 (26%)	25,31,36	2.08	8 (32%)
1	4OC	A	1402	1	20,23,24	0.96	1 (5%)	25,32,35	1.16	2 (8%)
2	PSU	FB	1917	2	18,21,22	1.81	3 (16%)	21,30,33	1.91	6 (28%)
2	4OC	B	1920	2	19,22,24	1.12	1 (5%)	25,31,35	1.15	2 (8%)
1	2MG	EB	1207	1,56	18,26,27	2.21	4 (22%)	16,38,41	1.61	4 (25%)
1	5MC	A	967	1	19,22,23	2.67	4 (21%)	26,32,35	1.11	2 (7%)
1	7MG	EB	527	1	23,26,27	3.16	7 (30%)	27,39,42	2.35	7 (25%)
2	5MU	FB	1915	2	19,22,23	2.13	3 (15%)	27,32,35	2.01	7 (25%)
2	4OC	FB	1920	2	19,22,24	1.10	1 (5%)	25,31,35	1.24	4 (16%)
2	PSU	FB	2605	2	18,21,22	1.63	3 (16%)	21,30,33	1.93	5 (23%)
2	OMG	B	2251	2	19,26,27	1.98	2 (10%)	21,38,41	1.40	4 (19%)
1	5MC	EB	1404	1	19,22,23	2.62	4 (21%)	26,32,35	1.38	4 (15%)
2	5MU	B	1939	2	19,22,23	2.16	4 (21%)	27,32,35	2.49	9 (33%)
4	4SU	HB	8	4	18,21,22	5.94	1 (5%)	25,30,33	0.63	0
2	PSU	FB	1911	2	18,21,22	1.75	3 (16%)	21,30,33	1.89	4 (19%)
2	5MC	FB	1962	2	19,22,23	2.81	5 (26%)	26,32,35	1.20	1 (3%)
1	PSU	A	516	1	18,21,22	1.79	3 (16%)	21,30,33	1.58	5 (23%)
4	PSU	D	55	4	18,21,22	1.78	2 (11%)	21,30,33	1.60	4 (19%)
4	4SU	IA	8	4	18,21,22	5.95	1 (5%)	25,30,33	0.65	0
1	MA6	EB	1518	1	19,26,27	2.26	5 (26%)	18,38,41	2.07	4 (22%)
4	5MC	D	32	4	19,22,23	2.67	5 (26%)	26,32,35	0.98	2 (7%)
1	UR3	A	1498	1	19,22,23	1.81	2 (10%)	26,32,35	1.84	5 (19%)
2	5MC	FB	1942	56,2	19,22,23	2.98	4 (21%)	26,32,35	1.21	1 (3%)
2	5MU	FB	1939	2	19,22,23	2.13	3 (15%)	27,32,35	2.68	9 (33%)
1	5MC	EB	1407	1	19,22,23	2.52	4 (21%)	26,32,35	1.34	2 (7%)
1	MA6	EB	1519	1	19,26,27	1.95	5 (26%)	18,38,41	1.60	3 (16%)
2	OMG	FB	2251	4,2	19,26,27	2.04	4 (21%)	21,38,41	1.36	5 (23%)
2	2MA	FB	2503	56,2	17,25,26	1.46	2 (11%)	16,37,40	1.54	3 (18%)
2	PSU	B	1917	2	18,21,22	1.47	3 (16%)	21,30,33	1.90	6 (28%)
1	5MC	EB	1400	1	19,22,23	2.70	4 (21%)	26,32,35	1.05	2 (7%)
4	PSU	IA	55	4	18,21,22	1.70	2 (11%)	21,30,33	1.66	4 (19%)
46	0TD	YC	92	46	8,9,10	2.11	3 (37%)	6,11,13	2.02	2 (33%)
1	4OC	EB	1402	1	20,23,24	0.96	2 (10%)	25,32,35	1.20	1 (4%)
2	PSU	B	1911	2	18,21,22	1.69	3 (16%)	21,30,33	1.36	3 (14%)
2	5MU	B	1915	56,2	19,22,23	2.06	3 (15%)	27,32,35	2.41	8 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	M2G	EB	966	1	20,27,28	2.36	3 (15%)	19,40,43	1.28	2 (10%)
4	PSU	MC	55	4	18,21,22	1.65	3 (16%)	21,30,33	1.65	4 (19%)
2	2MU	B	2552	2	19,22,24	2.60	5 (26%)	25,31,36	2.36	7 (28%)

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
46	0TD	UA	92	46	-	4/7/12/14	-
4	4SU	D	8	4	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	4/7/29/30	0/3/3/3
4	5MU	HB	54	4	-	0/7/25/26	0/2/2/2
1	5MC	EB	967	1	-	0/7/25/26	0/2/2/2
1	PSU	EB	516	1	-	1/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
4	5MC	HB	32	4	-	0/7/25/26	0/2/2/2
4	5MU	IA	54	4	-	0/7/25/26	0/2/2/2
2	PSU	B	2605	2	-	0/7/25/26	0/2/2/2
4	5MU	MC	54	4	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	5/7/29/30	0/3/3/3
2	2MA	B	2503	2	-	0/3/25/26	0/3/3/3
1	UR3	EB	1498	1	-	2/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	0/7/25/26	0/2/2/2
2	5MC	B	1942	2	-	0/7/25/26	0/2/2/2
4	4SU	MC	8	4	-	0/7/25/26	0/2/2/2
4	5MC	IA	32	4	-	0/7/25/26	0/2/2/2
1	M2G	A	966	1	-	1/7/29/30	0/3/3/3
1	2MG	A	1207	1	-	3/5/27/28	0/3/3/3
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
2	5MC	B	1962	2	-	1/7/25/26	0/2/2/2
4	5MC	MC	32	4	-	0/7/25/26	0/2/2/2
4	PSU	HB	55	4	-	1/7/25/26	0/2/2/2
1	7MG	A	527	1	-	3/7/37/38	0/3/3/3
4	5MU	D	54	4	-	0/7/25/26	0/2/2/2
2	2MU	FB	2552	2	-	1/9/27/28	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
2	PSU	FB	1917	2	-	1/7/25/26	0/2/2/2
2	4OC	B	1920	2	-	2/9/27/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	EB	1207	1,56	-	4/5/27/28	0/3/3/3
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	7MG	EB	527	1	-	3/7/37/38	0/3/3/3
2	5MU	FB	1915	2	-	0/7/25/26	0/2/2/2
2	4OC	FB	1920	2	-	2/9/27/30	0/2/2/2
2	PSU	FB	2605	2	-	0/7/25/26	0/2/2/2
2	OMG	B	2251	2	-	3/5/27/28	0/3/3/3
1	5MC	EB	1404	1	-	0/7/25/26	0/2/2/2
2	5MU	B	1939	2	-	0/7/25/26	0/2/2/2
4	4SU	HB	8	4	-	0/7/25/26	0/2/2/2
2	PSU	FB	1911	2	-	2/7/25/26	0/2/2/2
2	5MC	FB	1962	2	-	1/7/25/26	0/2/2/2
1	PSU	A	516	1	-	1/7/25/26	0/2/2/2
4	PSU	D	55	4	-	1/7/25/26	0/2/2/2
4	4SU	IA	8	4	-	0/7/25/26	0/2/2/2
1	MA6	EB	1518	1	-	4/7/29/30	0/3/3/3
4	5MC	D	32	4	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	2/7/25/26	0/2/2/2
2	5MC	FB	1942	56,2	-	0/7/25/26	0/2/2/2
2	5MU	FB	1939	2	-	0/7/25/26	0/2/2/2
1	5MC	EB	1407	1	-	0/7/25/26	0/2/2/2
1	MA6	EB	1519	1	-	4/7/29/30	0/3/3/3
2	OMG	FB	2251	4,2	-	3/5/27/28	0/3/3/3
2	2MA	FB	2503	56,2	-	0/3/25/26	0/3/3/3
2	PSU	B	1917	2	-	2/7/25/26	0/2/2/2
1	5MC	EB	1400	1	-	0/7/25/26	0/2/2/2
4	PSU	IA	55	4	-	2/7/25/26	0/2/2/2
46	0TD	YC	92	46	-	4/7/12/14	-
1	4OC	EB	1402	1	-	2/9/29/30	0/2/2/2
2	PSU	B	1911	2	-	2/7/25/26	0/2/2/2
2	5MU	B	1915	56,2	-	0/7/25/26	0/2/2/2
1	M2G	EB	966	1	-	1/7/29/30	0/3/3/3
4	PSU	MC	55	4	-	2/7/25/26	0/2/2/2
2	2MU	B	2552	2	-	1/9/27/28	0/2/2/2

The worst 5 of 214 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	MC	8	4SU	C4-S4	-25.21	1.23	1.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	HB	8	4SU	C4-S4	-25.18	1.23	1.68
4	IA	8	4SU	C4-S4	-25.17	1.23	1.68
4	D	8	4SU	C4-S4	-25.16	1.23	1.68
2	FB	1942	5MC	C5-C4	-11.11	1.35	1.44

The worst 5 of 252 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1915	5MU	C5-C4-N3	6.24	120.75	115.32
2	FB	1939	5MU	C4-N3-C2	-6.17	119.25	127.34
2	B	1939	5MU	C4-N3-C2	-6.13	119.30	127.34
2	B	2552	2MU	C4-N3-C2	-6.11	119.03	126.61
2	B	1939	5MU	N3-C2-N1	5.86	122.52	114.89

There are no chirality outliers.

5 of 77 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1207	2MG	O4'-C4'-C5'-O5'
1	A	1207	2MG	N3-C2-N2-CM2
1	A	1518	MA6	O4'-C4'-C5'-O5'
1	A	1518	MA6	C5-C6-N6-C9
1	A	1519	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

38 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	UA	92	0TD	2	0
4	D	8	4SU	2	0
1	A	1518	MA6	2	0
4	HB	54	5MU	3	0
1	EB	967	5MC	2	0
1	EB	516	PSU	1	0
1	A	1519	MA6	4	0
2	B	2503	2MA	1	0
1	EB	1498	UR3	1	0
1	A	1400	5MC	1	0
4	MC	8	4SU	1	0
1	A	1207	2MG	3	0
2	B	1962	5MC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	HB	55	PSU	1	0
4	D	54	5MU	3	0
2	FB	2552	2MU	2	0
1	A	1402	4OC	2	0
2	B	1920	4OC	4	0
1	EB	1207	2MG	1	0
1	A	967	5MC	2	0
2	FB	1915	5MU	1	0
2	FB	1920	4OC	2	0
1	EB	1404	5MC	1	0
2	B	1939	5MU	3	0
4	HB	8	4SU	2	0
2	FB	1962	5MC	1	0
4	D	55	PSU	1	0
1	EB	1518	MA6	1	0
1	A	1498	UR3	1	0
1	EB	1519	MA6	3	0
2	FB	2503	2MA	2	0
1	EB	1400	5MC	1	0
4	IA	55	PSU	1	0
46	YC	92	0TD	3	0
1	EB	1402	4OC	2	0
2	B	1915	5MU	3	0
4	MC	55	PSU	1	0
2	B	2552	2MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1695 ligands modelled in this entry, 1693 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	-	28,31,31	3.07	10 (35%)	26,43,43	2.06	12 (46%)
57	BLS	FB	9001	-	28,31,31	3.10	10 (35%)	26,43,43	2.02	11 (42%)

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	-	-	5/21/38/38	0/2/2/2
57	BLS	FB	9001	-	-	4/21/38/38	0/2/2/2

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	FB	9001	BLS	C14-N12	8.93	1.54	1.35
57	B	9001	BLS	C14-N12	8.56	1.53	1.35
57	FB	9001	BLS	C7-N6	7.29	1.49	1.34
57	B	9001	BLS	C7-N6	7.10	1.49	1.34
57	B	9001	BLS	C3'-C2'	5.00	1.48	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	FB	9001	BLS	C1'-C2'-C3'	-4.87	116.46	122.45
57	B	9001	BLS	C1'-C2'-C3'	-4.31	117.15	122.45
57	FB	9001	BLS	O3-C6'-C5'	-3.69	107.50	120.81
57	B	9001	BLS	O3-C6'-C5'	-3.57	107.91	120.81
57	B	9001	BLS	C13-N12-C11	3.49	122.85	115.90

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

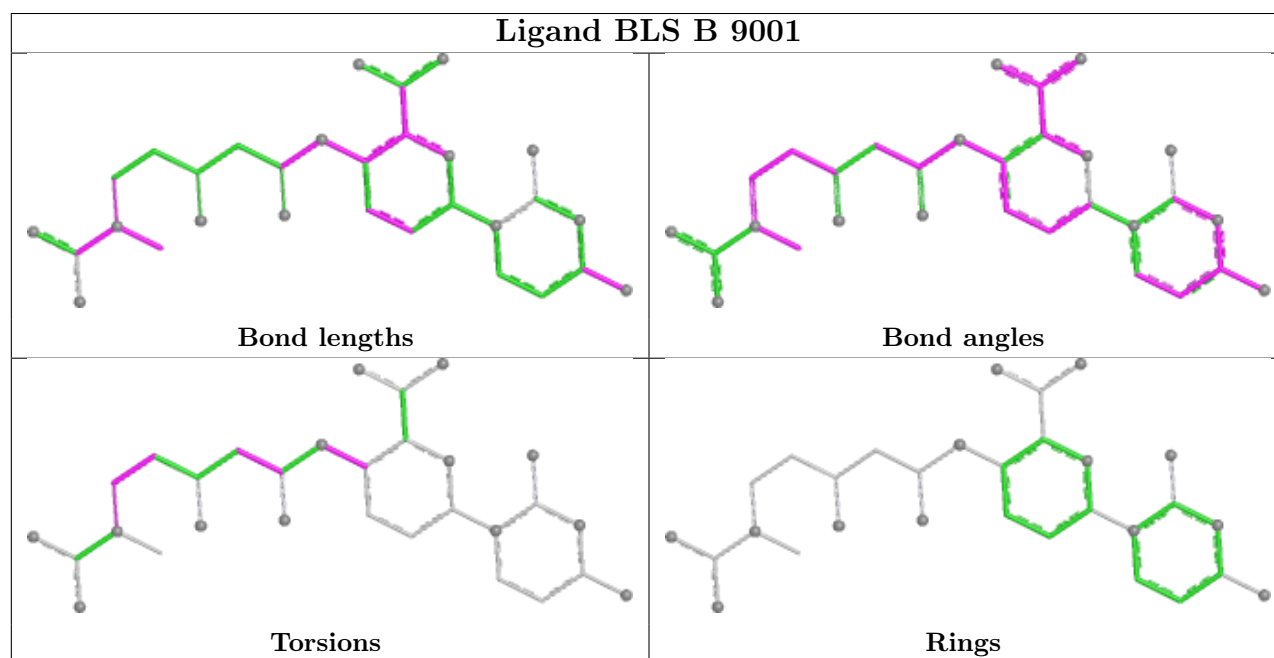
Mol	Chain	Res	Type	Atoms
57	B	9001	BLS	N6-C7-C8-C9
57	B	9001	BLS	O7-C7-C8-C9
57	B	9001	BLS	C9-C10-C11-N12
57	FB	9001	BLS	N6-C7-C8-C9
57	FB	9001	BLS	O7-C7-C8-C9

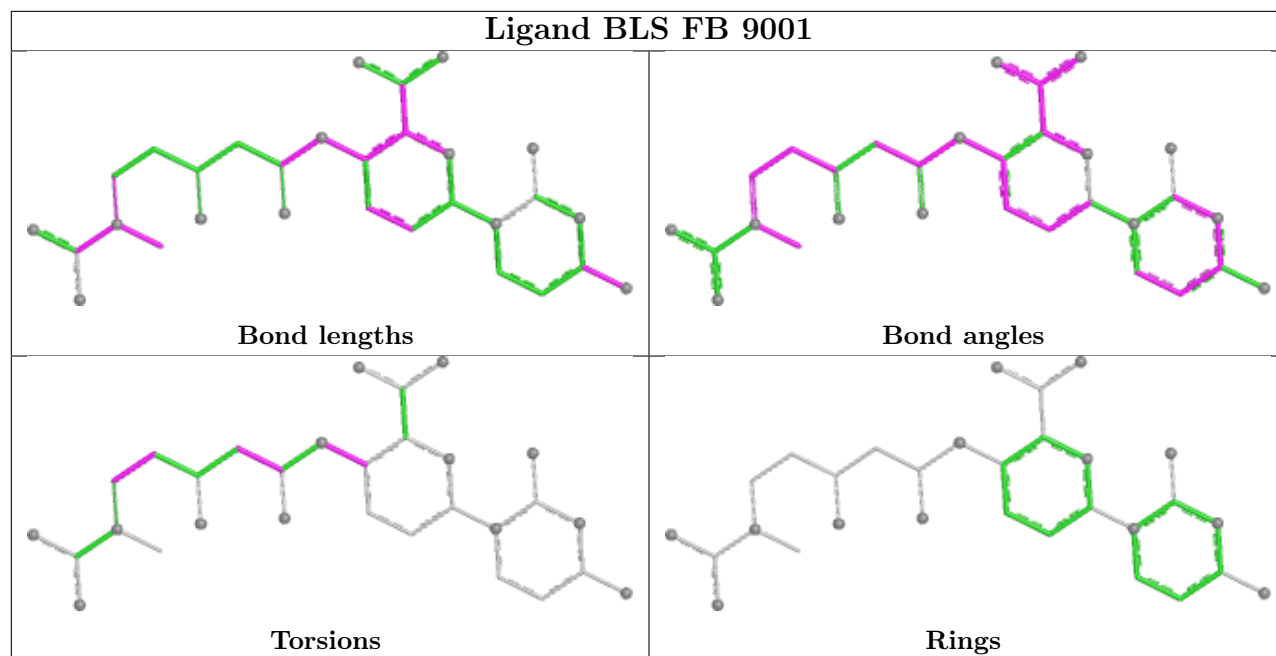
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	B	9001	BLS	2	0
57	FB	9001	BLS	1	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 ⓘ

Warning: The R factor obtained from EDS is 0.2629, which does not match the depositor's R factor of 0.0. Please interpret the results in this section carefully.

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%)	-0.20	9 (0%) 85 80	75, 127, 186, 250	0
1	EB	1495/1507 (99%)	-0.13	13 (0%) 81 73	80, 106, 179, 236	0
2	B	2869/2880 (99%)	-0.34	20 (0%) 84 78	56, 77, 167, 223	0
2	FB	2869/2880 (99%)	-0.14	32 (1%) 77 70	69, 92, 191, 294	0
3	C	120/120 (100%)	-0.30	0 100 100	92, 118, 133, 146	0
3	GB	120/120 (100%)	-0.03	1 (0%) 82 75	102, 127, 142, 153	0
4	D	73/77 (94%)	-0.10	1 (1%) 73 64	98, 185, 199, 203	0
4	HB	73/77 (94%)	-0.08	0 100 100	103, 189, 204, 209	0
4	IA	73/77 (94%)	-0.08	0 100 100	111, 153, 173, 175	0
4	MC	73/77 (94%)	-0.04	1 (1%) 73 64	110, 162, 186, 192	0
5	E	275/275 (100%)	0.06	4 (1%) 71 62	57, 66, 77, 83	0
5	IB	275/275 (100%)	0.21	6 (2%) 62 53	66, 76, 86, 95	0
6	F	204/206 (99%)	-0.07	5 (2%) 58 50	59, 76, 92, 100	0
6	JB	204/206 (99%)	0.31	6 (2%) 54 46	70, 91, 114, 124	0
7	G	202/205 (98%)	-0.12	1 (0%) 87 83	59, 78, 92, 99	0
7	KB	202/205 (98%)	-0.04	1 (0%) 87 83	63, 92, 105, 110	0
8	H	181/182 (99%)	0.53	12 (6%) 26 25	116, 138, 152, 155	0
8	LB	181/182 (99%)	0.28	5 (2%) 55 47	131, 148, 162, 167	0
9	I	174/180 (96%)	0.16	4 (2%) 61 51	90, 96, 102, 117	0
9	MB	174/180 (96%)	0.86	20 (11%) 11 14	130, 166, 175, 183	0
10	J	146/148 (98%)	0.28	5 (3%) 48 41	84, 113, 127, 128	0
10	NB	146/148 (98%)	0.67	17 (11%) 11 14	98, 132, 139, 141	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
11	K	140/140 (100%)	-0.04	1 (0%) 84 78	61, 75, 94, 99	0
11	OB	140/140 (100%)	0.28	2 (1%) 73 64	82, 101, 118, 124	0
12	L	122/122 (100%)	-0.03	0 100 100	63, 74, 82, 85	0
12	PB	122/122 (100%)	0.17	5 (4%) 42 36	76, 86, 93, 95	0
13	M	150/150 (100%)	0.32	2 (1%) 74 66	55, 86, 107, 109	0
13	QB	150/150 (100%)	0.55	10 (6%) 25 25	70, 106, 125, 127	0
14	N	141/141 (100%)	0.44	8 (5%) 30 28	73, 85, 98, 102	0
14	RB	141/141 (100%)	0.54	9 (6%) 27 26	85, 100, 113, 122	0
15	O	118/118 (100%)	0.10	5 (4%) 41 36	61, 72, 85, 92	0
15	SB	118/118 (100%)	0.53	2 (1%) 69 59	75, 89, 97, 102	0
16	P	110/112 (98%)	0.51	9 (8%) 19 20	105, 112, 116, 117	0
16	TB	110/112 (98%)	0.86	14 (12%) 9 11	111, 124, 130, 132	0
17	Q	137/146 (93%)	0.05	3 (2%) 62 53	74, 82, 128, 151	0
17	UB	137/146 (93%)	0.18	4 (2%) 54 46	86, 95, 119, 129	0
18	R	117/118 (99%)	0.01	2 (1%) 69 59	56, 72, 84, 87	0
18	VB	117/118 (99%)	0.42	5 (4%) 40 35	73, 97, 115, 119	0
19	S	101/101 (100%)	-0.05	2 (1%) 64 55	56, 82, 90, 94	0
19	WB	101/101 (100%)	0.35	5 (4%) 35 31	72, 103, 114, 120	0
20	T	112/113 (99%)	-0.15	1 (0%) 81 73	52, 63, 79, 87	0
20	XB	112/113 (99%)	0.16	2 (1%) 67 58	67, 80, 94, 102	0
21	U	95/96 (98%)	0.01	4 (4%) 41 36	62, 70, 80, 86	0
21	YB	95/96 (98%)	0.53	3 (3%) 50 42	85, 93, 101, 103	0
22	V	107/110 (97%)	0.15	0 100 100	77, 83, 91, 96	0
22	ZB	107/110 (97%)	0.69	9 (8%) 18 19	93, 102, 112, 117	0
23	AC	189/206 (91%)	0.14	3 (1%) 70 61	107, 122, 132, 134	0
23	W	189/206 (91%)	0.15	3 (1%) 70 61	92, 106, 119, 124	0
24	BC	84/85 (98%)	1.01	17 (20%) 3 6	94, 98, 126, 134	0
24	X	84/85 (98%)	0.72	11 (13%) 8 11	85, 88, 111, 118	0
25	CC	97/98 (98%)	0.46	3 (3%) 51 44	73, 92, 119, 127	0
25	Y	97/98 (98%)	0.36	5 (5%) 34 30	62, 82, 107, 115	0
26	DC	70/72 (97%)	0.08	1 (1%) 73 64	97, 103, 110, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
26	Z	70/72 (97%)	-0.03	0 100 100	72, 78, 84, 89	0
27	AA	60/60 (100%)	0.19	1 (1%) 69 59	70, 82, 99, 109	0
27	EC	60/60 (100%)	0.32	0 100 100	85, 93, 105, 109	0
28	BA	69/71 (97%)	0.29	1 (1%) 73 64	156, 160, 166, 169	0
28	FC	69/71 (97%)	0.32	0 100 100	165, 174, 188, 191	0
29	CA	59/60 (98%)	-0.16	0 100 100	55, 79, 85, 86	0
29	GC	59/60 (98%)	-0.00	1 (1%) 69 59	69, 93, 102, 106	0
30	DA	53/54 (98%)	1.11	8 (15%) 6 9	158, 159, 159, 159	0
30	HC	53/54 (98%)	0.98	7 (13%) 8 11	164, 168, 172, 173	0
31	EA	48/49 (97%)	0.30	2 (4%) 41 36	56, 60, 64, 65	0
31	IC	48/49 (97%)	0.18	2 (4%) 41 36	67, 71, 80, 84	0
32	FA	64/65 (98%)	0.47	4 (6%) 27 26	63, 75, 95, 103	0
32	JC	64/65 (98%)	0.81	6 (9%) 15 17	75, 85, 102, 110	0
33	GA	37/37 (100%)	1.14	5 (13%) 8 11	96, 97, 98, 98	0
33	KC	37/37 (100%)	1.50	12 (32%) 1 2	111, 119, 128, 132	0
34	HA	11/23 (47%)	0.67	0 100 100	110, 111, 126, 127	0
34	LC	11/23 (47%)	0.55	0 100 100	108, 109, 126, 128	0
35	JA	258/368 (70%)	0.27	17 (6%) 26 25	90, 116, 133, 137	0
35	NC	258/368 (70%)	0.32	14 (5%) 32 29	105, 119, 136, 146	0
36	KA	234/256 (91%)	0.37	11 (4%) 37 33	138, 150, 162, 167	0
36	OC	234/256 (91%)	0.28	12 (5%) 34 30	115, 136, 149, 169	0
37	LA	206/239 (86%)	0.20	10 (4%) 36 31	126, 146, 163, 166	0
37	PC	206/239 (86%)	0.35	4 (1%) 66 57	117, 129, 142, 148	0
38	MA	208/209 (99%)	0.87	23 (11%) 12 14	115, 130, 140, 145	0
38	QC	208/209 (99%)	0.34	9 (4%) 40 35	92, 99, 108, 113	0
39	NA	151/162 (93%)	0.35	8 (5%) 33 29	110, 121, 128, 139	0
39	RC	151/162 (93%)	0.20	4 (2%) 57 49	91, 102, 110, 117	0
40	OA	101/101 (100%)	0.15	2 (1%) 64 55	98, 102, 112, 123	0
40	SC	101/101 (100%)	0.21	1 (0%) 79 71	105, 112, 120, 123	0
41	PA	155/156 (99%)	0.49	16 (10%) 13 15	126, 145, 154, 156	0
41	TC	155/156 (99%)	0.48	8 (5%) 34 30	128, 147, 155, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
42	QA	138/138 (100%)	0.47	6 (4%) 40 35	109, 124, 132, 138	0
42	UC	138/138 (100%)	0.33	5 (3%) 46 39	93, 108, 116, 118	0
43	RA	127/128 (99%)	1.04	24 (18%) 4 6	127, 168, 173, 175	0
43	VC	127/128 (99%)	1.25	29 (22%) 2 5	128, 166, 174, 176	0
44	SA	98/105 (93%)	0.97	16 (16%) 5 8	142, 167, 173, 176	0
44	WC	98/105 (93%)	0.93	8 (8%) 19 20	128, 159, 165, 166	0
45	TA	116/129 (89%)	0.30	5 (4%) 40 35	87, 107, 115, 118	0
45	XC	116/129 (89%)	0.06	3 (2%) 57 49	93, 111, 118, 121	0
46	UA	121/132 (91%)	0.52	12 (9%) 14 16	97, 101, 110, 117	0
46	YC	121/132 (91%)	0.23	5 (4%) 42 36	84, 89, 94, 98	0
47	VA	117/126 (92%)	0.36	6 (5%) 34 30	136, 160, 164, 166	0
47	ZC	117/126 (92%)	0.83	15 (12%) 9 11	140, 168, 172, 172	0
48	AD	60/61 (98%)	1.10	9 (15%) 6 9	128, 138, 154, 154	0
48	WA	60/61 (98%)	1.17	9 (15%) 6 9	141, 149, 154, 155	0
49	BD	88/89 (98%)	0.07	1 (1%) 77 70	91, 101, 109, 111	0
49	XA	88/89 (98%)	0.33	3 (3%) 48 41	94, 106, 116, 117	0
50	CD	83/88 (94%)	0.54	6 (7%) 23 22	92, 100, 115, 126	0
50	YA	83/88 (94%)	1.03	13 (15%) 6 8	122, 134, 146, 157	0
51	DD	99/105 (94%)	0.22	2 (2%) 64 55	87, 92, 96, 97	0
51	ZA	99/105 (94%)	0.42	3 (3%) 52 45	95, 107, 112, 118	0
52	AB	70/88 (79%)	0.06	2 (2%) 54 46	101, 110, 118, 119	0
52	ED	70/88 (79%)	0.08	0 100 100	103, 109, 113, 120	0
53	BB	83/93 (89%)	1.05	14 (16%) 5 7	138, 159, 162, 164	0
53	FD	83/93 (89%)	0.92	13 (15%) 6 8	146, 162, 168, 169	0
54	CB	99/106 (93%)	1.15	25 (25%) 2 4	118, 128, 139, 140	0
54	GD	99/106 (93%)	0.92	21 (21%) 3 5	95, 108, 122, 124	0
55	DB	24/27 (88%)	2.24	12 (50%) 0 0	152, 157, 160, 164	0
55	HD	24/27 (88%)	1.77	7 (29%) 1 3	156, 161, 165, 167	0
All	All	21478/22220 (96%)	0.13	775 (3%) 46 39	52, 102, 169, 294	0

The worst 5 of 775 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	DA	5	VAL	9.3
25	Y	2	SER	8.8
24	X	8	GLY	7.9
24	BC	4	LYS	7.3
54	GD	26	ASN	6.2

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	PSU	HB	55	20/21	0.58	0.13	204,205,205,206	0
4	PSU	D	55	20/21	0.66	0.08	198,199,201,202	0
4	5MU	D	54	21/22	0.66	0.09	196,198,198,199	0
4	5MC	HB	32	21/22	0.67	0.10	149,150,150,150	0
4	4SU	HB	8	20/21	0.69	0.08	194,196,197,198	0
4	5MU	HB	54	21/22	0.69	0.12	201,202,204,204	0
4	4SU	IA	8	20/21	0.72	0.09	149,150,152,152	0
4	PSU	MC	55	20/21	0.73	0.11	178,182,187,188	0
4	PSU	IA	55	20/21	0.74	0.09	170,174,179,180	0
4	4SU	MC	8	20/21	0.76	0.09	160,161,164,164	0
4	5MU	MC	54	21/22	0.76	0.14	180,185,189,190	0
4	4SU	D	8	20/21	0.77	0.08	191,192,192,192	0
4	5MC	MC	32	21/22	0.78	0.14	120,120,120,120	0
46	0TD	UA	92	10/11	0.79	0.26	102,103,103,104	0
4	5MC	D	32	21/22	0.81	0.08	164,164,165,165	0
4	5MU	IA	54	21/22	0.81	0.11	171,176,179,181	0
1	2MG	EB	1207	24/25	0.82	0.12	129,130,132,133	0
2	PSU	FB	1917	20/21	0.84	0.09	97,99,101,102	0
2	PSU	FB	1911	20/21	0.84	0.11	99,102,103,104	0
46	0TD	YC	92	10/11	0.85	0.29	93,94,94,94	0
2	5MU	B	1915	21/22	0.85	0.09	96,98,101,101	0
4	5MC	IA	32	21/22	0.86	0.14	119,119,120,120	0
2	PSU	B	1911	20/21	0.87	0.11	93,96,99,99	0
1	PSU	EB	516	20/21	0.87	0.08	98,99,102,102	0
2	5MU	FB	1915	21/22	0.87	0.09	104,105,108,108	0
1	PSU	A	516	20/21	0.88	0.08	112,114,117,117	0
1	4OC	A	1402	22/23	0.89	0.13	99,100,101,102	0
1	2MG	A	1207	24/25	0.89	0.11	134,135,137,138	0
2	5MC	B	1942	21/22	0.90	0.09	67,69,70,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	UR3	EB	1498	21/22	0.90	0.15	96,96,96,97	0
1	UR3	A	1498	21/22	0.91	0.14	95,95,96,96	0
2	PSU	B	1917	20/21	0.91	0.08	91,92,95,96	0
1	4OC	EB	1402	22/23	0.91	0.12	95,96,97,97	0
1	5MC	EB	967	21/22	0.92	0.09	117,119,122,123	0
2	5MC	FB	1962	21/22	0.93	0.09	78,80,82,82	0
2	PSU	B	2605	20/21	0.93	0.09	59,61,62,62	0
2	5MU	B	1939	21/22	0.93	0.11	63,64,65,66	0
1	5MC	A	967	21/22	0.93	0.10	121,123,125,126	0
1	7MG	EB	527	24/25	0.93	0.16	92,94,95,95	0
1	M2G	EB	966	25/26	0.93	0.12	114,117,120,121	0
2	2MA	B	2503	23/24	0.93	0.12	56,57,57,58	0
2	5MU	FB	1939	21/22	0.93	0.11	73,74,74,75	0
2	5MC	FB	1942	21/22	0.93	0.08	76,78,79,79	0
1	5MC	EB	1400	21/22	0.94	0.10	100,103,105,106	0
1	M2G	A	966	25/26	0.94	0.11	119,121,124,124	0
2	OMG	FB	2251	24/25	0.94	0.11	76,78,80,80	0
1	5MC	EB	1407	21/22	0.94	0.09	89,90,91,91	0
1	5MC	A	1404	21/22	0.94	0.11	91,93,94,94	0
2	5MC	B	1962	21/22	0.94	0.09	70,71,74,75	0
1	5MC	A	1400	21/22	0.94	0.10	105,107,109,111	0
2	2MU	B	2552	21/23	0.94	0.11	64,66,66,66	0
2	4OC	FB	1920	21/23	0.94	0.11	96,98,99,101	0
2	4OC	B	1920	21/23	0.94	0.09	90,93,94,96	0
1	5MC	EB	1404	21/22	0.95	0.13	87,89,89,90	0
2	2MA	FB	2503	23/24	0.95	0.10	70,71,72,72	0
2	PSU	FB	2605	20/21	0.95	0.09	71,72,73,73	0
1	MA6	EB	1519	24/25	0.95	0.15	84,86,87,87	0
1	5MC	A	1407	21/22	0.95	0.10	87,88,90,91	0
1	MA6	A	1518	24/25	0.96	0.10	84,86,88,88	0
2	2MU	FB	2552	21/23	0.96	0.08	74,76,76,77	0
1	7MG	A	527	24/25	0.96	0.09	102,105,106,107	0
1	MA6	EB	1518	24/25	0.96	0.13	84,86,87,88	0
2	OMG	B	2251	24/25	0.96	0.09	64,66,67,67	0
1	MA6	A	1519	24/25	0.97	0.10	85,87,88,89	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	FB	9237	1/1	-0.58	0.26	252,252,252,252	0
56	MG	HB	103	1/1	-0.50	0.22	188,188,188,188	0
56	MG	A	1700	1/1	-0.48	0.29	169,169,169,169	0
56	MG	FB	9157	1/1	-0.47	0.17	181,181,181,181	0
56	MG	HB	101	1/1	-0.44	0.32	204,204,204,204	0
56	MG	A	1781	1/1	-0.33	0.17	232,232,232,232	0
56	MG	FB	9396	1/1	-0.28	0.37	245,245,245,245	0
56	MG	EB	1603	1/1	-0.24	0.42	146,146,146,146	0
56	MG	EB	1669	1/1	-0.23	0.35	148,148,148,148	0
56	MG	EB	1706	1/1	-0.18	0.27	181,181,181,181	0
56	MG	A	1611	1/1	-0.16	0.38	124,124,124,124	0
56	MG	MC	101	1/1	-0.12	0.27	169,169,169,169	0
56	MG	AD	101	1/1	-0.12	0.33	137,137,137,137	0
56	MG	A	1778	1/1	-0.11	0.13	243,243,243,243	0
56	MG	EB	1709	1/1	-0.10	0.23	181,181,181,181	0
56	MG	A	1631	1/1	-0.10	0.24	180,180,180,180	0
56	MG	B	9177	1/1	-0.09	0.34	188,188,188,188	0
56	MG	A	1670	1/1	-0.09	0.19	168,168,168,168	0
56	MG	HB	102	1/1	-0.08	0.23	187,187,187,187	0
56	MG	HB	109	1/1	-0.07	0.23	182,182,182,182	0
56	MG	A	1789	1/1	-0.07	0.19	183,183,183,183	0
56	MG	B	9522	1/1	-0.07	0.28	137,137,137,137	0
56	MG	A	1628	1/1	-0.06	0.45	135,135,135,135	0
56	MG	EB	1611	1/1	-0.05	0.33	172,172,172,172	0
56	MG	A	1746	1/1	-0.04	0.33	156,156,156,156	0
56	MG	EB	1778	1/1	-0.03	0.15	191,191,191,191	0
56	MG	HB	104	1/1	-0.00	0.17	198,198,198,198	0
56	MG	A	1646	1/1	-0.00	0.21	214,214,214,214	0
56	MG	FB	9180	1/1	0.03	0.26	174,174,174,174	0
56	MG	EB	1784	1/1	0.03	0.20	184,184,184,184	0
56	MG	B	9483	1/1	0.04	0.14	202,202,202,202	0
56	MG	B	9219	1/1	0.04	0.20	177,177,177,177	0
56	MG	A	1656	1/1	0.05	0.25	162,162,162,162	0
56	MG	A	1652	1/1	0.07	0.18	151,151,151,151	0
56	MG	EB	1641	1/1	0.07	0.49	136,136,136,136	0
56	MG	EB	1696	1/1	0.08	0.22	167,167,167,167	0
56	MG	B	9414	1/1	0.12	0.23	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	A	1654	1/1	0.14	0.22	169,169,169,169	0
56	MG	FB	9383	1/1	0.15	0.22	184,184,184,184	0
56	MG	A	1658	1/1	0.15	0.28	127,127,127,127	0
56	MG	EB	1675	1/1	0.15	0.21	164,164,164,164	0
56	MG	EB	1760	1/1	0.17	0.22	153,153,153,153	0
56	MG	B	9237	1/1	0.17	0.20	149,149,149,149	0
56	MG	EB	1758	1/1	0.17	0.24	127,127,127,127	0
56	MG	A	1769	1/1	0.19	0.21	162,162,162,162	0
56	MG	EB	1679	1/1	0.20	0.27	137,137,137,137	0
56	MG	EB	1785	1/1	0.20	0.15	185,185,185,185	0
56	MG	A	1685	1/1	0.21	0.38	142,142,142,142	0
56	MG	A	1784	1/1	0.22	0.23	152,152,152,152	0
56	MG	SA	201	1/1	0.23	0.20	170,170,170,170	0
56	MG	A	1675	1/1	0.24	0.32	167,167,167,167	0
56	MG	A	1710	1/1	0.26	0.23	138,138,138,138	0
56	MG	HB	108	1/1	0.26	0.23	146,146,146,146	0
56	MG	A	1727	1/1	0.26	0.22	145,145,145,145	0
56	MG	FB	9308	1/1	0.26	0.24	118,118,118,118	0
56	MG	B	9423	1/1	0.26	0.20	144,144,144,144	0
56	MG	FB	9161	1/1	0.27	0.17	149,149,149,149	0
56	MG	A	1793	1/1	0.27	0.30	123,123,123,123	0
56	MG	C	206	1/1	0.27	0.35	112,112,112,112	0
56	MG	FB	9415	1/1	0.27	0.25	120,120,120,120	0
56	MG	A	1696	1/1	0.28	0.41	141,141,141,141	0
56	MG	B	9298	1/1	0.28	0.24	131,131,131,131	0
56	MG	EB	1616	1/1	0.29	0.39	128,128,128,128	0
56	MG	HB	107	1/1	0.29	0.23	170,170,170,170	0
56	MG	FB	9442	1/1	0.29	0.27	137,137,137,137	0
56	MG	A	1620	1/1	0.29	0.47	118,118,118,118	0
56	MG	A	1692	1/1	0.29	0.15	182,182,182,182	0
56	MG	MC	103	1/1	0.29	0.25	151,151,151,151	0
56	MG	IA	106	1/1	0.29	0.28	144,144,144,144	0
56	MG	A	1648	1/1	0.30	0.31	138,138,138,138	0
56	MG	EB	1720	1/1	0.30	0.26	147,147,147,147	0
56	MG	FB	9407	1/1	0.30	0.20	141,141,141,141	0
56	MG	A	1798	1/1	0.31	0.13	123,123,123,123	0
56	MG	A	1650	1/1	0.34	0.25	126,126,126,126	0
56	MG	F	302	1/1	0.34	0.12	80,80,80,80	0
56	MG	SA	203	1/1	0.34	0.16	147,147,147,147	0
56	MG	VC	201	1/1	0.36	0.26	164,164,164,164	0
56	MG	GB	213	1/1	0.37	0.30	117,117,117,117	0
56	MG	FB	9324	1/1	0.37	0.17	153,153,153,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	FB	9281	1/1	0.37	0.16	151,151,151,151	0
56	MG	EB	1660	1/1	0.37	0.16	171,171,171,171	0
56	MG	B	9300	1/1	0.38	0.26	149,149,149,149	0
56	MG	D	104	1/1	0.38	0.21	185,185,185,185	0
56	MG	EB	1769	1/1	0.38	0.20	149,149,149,149	0
56	MG	EB	1712	1/1	0.39	0.12	182,182,182,182	0
56	MG	B	9226	1/1	0.39	0.23	128,128,128,128	0
56	MG	FB	9099	1/1	0.39	0.22	144,144,144,144	0
56	MG	EB	1791	1/1	0.40	0.43	120,120,120,120	0
56	MG	EB	1663	1/1	0.40	0.13	168,168,168,168	0
56	MG	FB	9377	1/1	0.41	0.18	142,142,142,142	0
56	MG	FB	9040	1/1	0.41	0.20	134,134,134,134	0
56	MG	GB	209	1/1	0.41	0.27	121,121,121,121	0
56	MG	EB	1755	1/1	0.41	0.20	155,155,155,155	0
56	MG	C	204	1/1	0.41	0.22	113,113,113,113	0
56	MG	EB	1749	1/1	0.42	0.37	92,92,92,92	0
56	MG	B	9539	1/1	0.43	0.12	143,143,143,143	0
56	MG	IA	102	1/1	0.43	0.21	158,158,158,158	0
56	MG	FB	9283	1/1	0.43	0.30	116,116,116,116	0
56	MG	EB	1673	1/1	0.43	0.23	139,139,139,139	0
56	MG	FB	9211	1/1	0.44	0.14	144,144,144,144	0
56	MG	B	9356	1/1	0.44	0.21	91,91,91,91	0
56	MG	A	1647	1/1	0.44	0.25	157,157,157,157	0
56	MG	A	1701	1/1	0.44	0.21	120,120,120,120	0
56	MG	FB	9059	1/1	0.44	0.33	102,102,102,102	0
56	MG	EB	1775	1/1	0.45	0.40	125,125,125,125	0
56	MG	EB	1796	1/1	0.45	0.46	109,109,109,109	0
56	MG	GB	201	1/1	0.45	0.51	93,93,93,93	0
56	MG	FB	9355	1/1	0.45	0.19	226,226,226,226	0
56	MG	A	1606	1/1	0.45	0.34	118,118,118,118	0
56	MG	D	105	1/1	0.45	0.18	126,126,126,126	0
56	MG	A	1806	1/1	0.45	0.19	153,153,153,153	0
56	MG	EB	1789	1/1	0.45	0.25	108,108,108,108	0
56	MG	EB	1764	1/1	0.46	0.23	107,107,107,107	0
56	MG	MC	104	1/1	0.46	0.29	115,115,115,115	0
56	MG	OC	302	1/1	0.46	0.25	122,122,122,122	0
56	MG	A	1741	1/1	0.46	0.17	111,111,111,111	0
56	MG	A	1610	1/1	0.46	0.33	128,128,128,128	0
56	MG	A	1678	1/1	0.47	0.15	158,158,158,158	0
56	MG	SA	202	1/1	0.47	0.13	144,144,144,144	0
56	MG	A	1624	1/1	0.47	0.28	131,131,131,131	0
56	MG	A	1751	1/1	0.47	0.38	143,143,143,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	MB	201	1/1	0.47	0.17	148,148,148,148	0
56	MG	MB	202	1/1	0.47	0.17	169,169,169,169	0
56	MG	D	103	1/1	0.48	0.11	158,158,158,158	0
56	MG	MC	102	1/1	0.48	0.19	144,144,144,144	0
56	MG	B	9238	1/1	0.48	0.23	136,136,136,136	0
56	MG	FB	9047	1/1	0.48	0.27	85,85,85,85	0
56	MG	FB	9317	1/1	0.48	0.21	143,143,143,143	0
56	MG	LA	302	1/1	0.48	0.16	113,113,113,113	0
56	MG	EB	1632	1/1	0.48	0.17	136,136,136,136	0
56	MG	FB	9379	1/1	0.49	0.23	117,117,117,117	0
56	MG	A	1683	1/1	0.49	0.23	146,146,146,146	0
56	MG	FB	9021	1/1	0.49	0.18	103,103,103,103	0
56	MG	FB	9321	1/1	0.49	0.18	98,98,98,98	0
56	MG	FB	9153	1/1	0.49	0.24	123,123,123,123	0
56	MG	FB	9432	1/1	0.49	0.14	153,153,153,153	0
56	MG	B	9018	1/1	0.49	0.39	87,87,87,87	0
56	MG	B	9370	1/1	0.49	0.23	73,73,73,73	0
56	MG	GB	203	1/1	0.49	0.35	113,113,113,113	0
56	MG	C	212	1/1	0.50	0.25	109,109,109,109	0
56	MG	MC	105	1/1	0.50	0.21	135,135,135,135	0
56	MG	FB	9177	1/1	0.50	0.30	133,133,133,133	0
56	MG	EB	1691	1/1	0.50	0.17	116,116,116,116	0
56	MG	EB	1670	1/1	0.50	0.34	125,125,125,125	0
56	MG	FB	9361	1/1	0.51	0.21	118,118,118,118	0
56	MG	A	1699	1/1	0.51	0.17	140,140,140,140	0
56	MG	FB	9052	1/1	0.51	0.20	89,89,89,89	0
56	MG	FB	9149	1/1	0.51	0.31	121,121,121,121	0
56	MG	FB	9233	1/1	0.51	0.10	117,117,117,117	0
56	MG	D	101	1/1	0.52	0.17	137,137,137,137	0
56	MG	B	9364	1/1	0.52	0.19	136,136,136,136	0
56	MG	FB	9336	1/1	0.52	0.28	77,77,77,77	0
56	MG	B	9444	1/1	0.52	0.17	110,110,110,110	0
56	MG	A	1718	1/1	0.52	0.15	109,109,109,109	0
56	MG	FB	9307	1/1	0.52	0.26	215,215,215,215	0
56	MG	GB	202	1/1	0.52	0.53	99,99,99,99	0
56	MG	FB	9207	1/1	0.52	0.25	126,126,126,126	0
56	MG	A	1733	1/1	0.52	0.15	161,161,161,161	0
56	MG	FB	9139	1/1	0.53	0.12	146,146,146,146	0
56	MG	EB	1746	1/1	0.53	0.20	126,126,126,126	0
56	MG	A	1651	1/1	0.53	0.33	129,129,129,129	0
56	MG	FB	9425	1/1	0.53	0.17	119,119,119,119	0
56	MG	A	1759	1/1	0.53	0.26	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	EB	1672	1/1	0.53	0.31	122,122,122,122	0
56	MG	A	1662	1/1	0.53	0.27	144,144,144,144	0
56	MG	A	1671	1/1	0.54	0.26	145,145,145,145	0
56	MG	B	9363	1/1	0.54	0.18	111,111,111,111	0
56	MG	EB	1718	1/1	0.54	0.14	125,125,125,125	0
56	MG	BA	102	1/1	0.54	0.15	147,147,147,147	0
56	MG	B	9172	1/1	0.54	0.21	78,78,78,78	0
56	MG	EB	1773	1/1	0.54	0.11	149,149,149,149	0
56	MG	A	1627	1/1	0.54	0.37	103,103,103,103	0
56	MG	CC	106	1/1	0.54	0.24	103,103,103,103	0
56	MG	A	1657	1/1	0.55	0.19	145,145,145,145	0
56	MG	A	1682	1/1	0.55	0.32	127,127,127,127	0
56	MG	FB	9198	1/1	0.55	0.21	128,128,128,128	0
56	MG	FB	9423	1/1	0.55	0.21	137,137,137,137	0
56	MG	OC	304	1/1	0.55	0.29	122,122,122,122	0
56	MG	B	9438	1/1	0.55	0.19	102,102,102,102	0
56	MG	A	1744	1/1	0.55	0.20	150,150,150,150	0
56	MG	A	1779	1/1	0.56	0.26	101,101,101,101	0
56	MG	A	1771	1/1	0.56	0.23	122,122,122,122	0
56	MG	B	9134	1/1	0.56	0.43	53,53,53,53	0
56	MG	A	1688	1/1	0.56	0.16	112,112,112,112	0
56	MG	FB	9403	1/1	0.56	0.25	82,82,82,82	0
56	MG	FB	9393	1/1	0.57	0.13	108,108,108,108	0
56	MG	B	9509	1/1	0.57	0.09	146,146,146,146	0
56	MG	B	9343	1/1	0.57	0.14	121,121,121,121	0
56	MG	EB	1681	1/1	0.57	0.11	107,107,107,107	0
56	MG	A	1736	1/1	0.57	0.24	122,122,122,122	0
56	MG	A	1663	1/1	0.57	0.32	94,94,94,94	0
56	MG	A	1754	1/1	0.57	0.29	123,123,123,123	0
56	MG	EB	1610	1/1	0.57	0.31	96,96,96,96	0
56	MG	A	1693	1/1	0.57	0.22	121,121,121,121	0
56	MG	B	9485	1/1	0.57	0.15	84,84,84,84	0
56	MG	FB	9165	1/1	0.57	0.23	124,124,124,124	0
56	MG	FB	9280	1/1	0.58	0.20	115,115,115,115	0
56	MG	A	1717	1/1	0.58	0.20	119,119,119,119	0
56	MG	HB	106	1/1	0.58	0.16	107,107,107,107	0
56	MG	FB	9349	1/1	0.58	0.17	139,139,139,139	0
56	MG	IA	105	1/1	0.58	0.28	121,121,121,121	0
56	MG	EB	1700	1/1	0.58	0.16	110,110,110,110	0
56	MG	A	1737	1/1	0.58	0.28	97,97,97,97	0
56	MG	A	1619	1/1	0.58	0.25	135,135,135,135	0
56	MG	EB	1633	1/1	0.58	0.30	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	A	1791	1/1	0.59	0.27	110,110,110,110	0
56	MG	CC	102	1/1	0.59	0.19	116,116,116,116	0
56	MG	A	1629	1/1	0.59	0.24	151,151,151,151	0
56	MG	A	1690	1/1	0.59	0.28	133,133,133,133	0
56	MG	FB	9299	1/1	0.59	0.23	89,89,89,89	0
56	MG	EB	1617	1/1	0.59	0.22	134,134,134,134	0
56	MG	FB	9221	1/1	0.59	0.33	96,96,96,96	0
56	MG	FB	9222	1/1	0.59	0.14	97,97,97,97	0
56	MG	FB	9106	1/1	0.59	0.27	83,83,83,83	0
56	MG	FB	9322	1/1	0.59	0.20	132,132,132,132	0
56	MG	JB	302	1/1	0.59	0.21	100,100,100,100	0
56	MG	EB	1788	1/1	0.59	0.13	107,107,107,107	0
56	MG	FB	9053	1/1	0.60	0.31	105,105,105,105	0
56	MG	B	9139	1/1	0.60	0.12	97,97,97,97	0
56	MG	XA	106	1/1	0.60	0.12	109,109,109,109	0
56	MG	FB	9178	1/1	0.60	0.34	94,94,94,94	0
56	MG	EB	1671	1/1	0.60	0.14	156,156,156,156	0
56	MG	FB	9187	1/1	0.60	0.28	116,116,116,116	0
56	MG	A	1801	1/1	0.61	0.22	126,126,126,126	0
56	MG	FB	9357	1/1	0.61	0.13	94,94,94,94	0
56	MG	EB	1800	1/1	0.61	0.48	150,150,150,150	0
56	MG	EB	1693	1/1	0.61	0.16	176,176,176,176	0
56	MG	FB	9124	1/1	0.61	0.23	118,118,118,118	0
56	MG	FB	9471	1/1	0.61	0.15	114,114,114,114	0
56	MG	A	1795	1/1	0.61	0.20	123,123,123,123	0
56	MG	FB	9259	1/1	0.61	0.17	79,79,79,79	0
56	MG	A	1691	1/1	0.61	0.11	240,240,240,240	0
56	MG	B	9174	1/1	0.61	0.17	69,69,69,69	0
56	MG	B	9478	1/1	0.61	0.18	121,121,121,121	0
56	MG	B	9137	1/1	0.62	0.18	103,103,103,103	0
56	MG	HA	102	1/1	0.62	0.37	105,105,105,105	0
56	MG	FB	9472	1/1	0.62	0.27	98,98,98,98	0
56	MG	B	9277	1/1	0.62	0.14	145,145,145,145	0
56	MG	EB	1766	1/1	0.62	0.27	125,125,125,125	0
56	MG	B	9183	1/1	0.62	0.27	125,125,125,125	0
56	MG	A	1721	1/1	0.62	0.41	106,106,106,106	0
56	MG	FB	9402	1/1	0.62	0.25	118,118,118,118	0
56	MG	FB	9272	1/1	0.62	0.19	124,124,124,124	0
56	MG	FB	9278	1/1	0.62	0.33	66,66,66,66	0
56	MG	FB	9410	1/1	0.62	0.09	83,83,83,83	0
56	MG	FB	9344	1/1	0.62	0.21	72,72,72,72	0
56	MG	B	9317	1/1	0.62	0.21	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	9100	1/1	0.62	0.23	88,88,88,88	0
56	MG	YC	205	1/1	0.62	0.26	82,82,82,82	0
56	MG	A	1609	1/1	0.62	0.17	129,129,129,129	0
56	MG	FB	9051	1/1	0.63	0.28	91,91,91,91	0
56	MG	EB	1732	1/1	0.63	0.13	142,142,142,142	0
56	MG	FB	9006	1/1	0.63	0.46	74,74,74,74	0
56	MG	B	9427	1/1	0.63	0.17	96,96,96,96	0
56	MG	FB	9195	1/1	0.63	0.33	113,113,113,113	0
56	MG	FB	9060	1/1	0.63	0.24	97,97,97,97	0
56	MG	EB	1793	1/1	0.63	0.12	140,140,140,140	0
56	MG	B	9286	1/1	0.63	0.20	105,105,105,105	0
56	MG	PC	301	1/1	0.63	0.13	137,137,137,137	0
56	MG	FB	9218	1/1	0.63	0.22	150,150,150,150	0
56	MG	FB	9219	1/1	0.63	0.18	123,123,123,123	0
56	MG	FB	9172	1/1	0.63	0.26	91,91,91,91	0
56	MG	B	9240	1/1	0.64	0.16	156,156,156,156	0
56	MG	FB	9427	1/1	0.64	0.20	105,105,105,105	0
56	MG	B	9503	1/1	0.64	0.29	92,92,92,92	0
56	MG	B	9254	1/1	0.64	0.11	94,94,94,94	0
56	MG	B	9437	1/1	0.64	0.19	117,117,117,117	0
56	MG	SB	201	1/1	0.64	0.41	91,91,91,91	0
56	MG	FB	9366	1/1	0.64	0.26	110,110,110,110	0
56	MG	B	9303	1/1	0.64	0.25	76,76,76,76	0
56	MG	B	9041	1/1	0.64	0.27	71,71,71,71	0
56	MG	FB	9300	1/1	0.64	0.17	94,94,94,94	0
56	MG	FB	9011	1/1	0.64	0.28	66,66,66,66	0
56	MG	EB	1738	1/1	0.64	0.17	99,99,99,99	0
56	MG	FB	9030	1/1	0.64	0.23	83,83,83,83	0
56	MG	FB	9032	1/1	0.64	0.40	90,90,90,90	0
56	MG	EB	1744	1/1	0.64	0.24	117,117,117,117	0
56	MG	B	9186	1/1	0.64	0.31	94,94,94,94	0
56	MG	UC	202	1/1	0.64	0.15	108,108,108,108	0
56	MG	HB	105	1/1	0.64	0.12	151,151,151,151	0
56	MG	B	9482	1/1	0.64	0.19	124,124,124,124	0
56	MG	B	9422	1/1	0.64	0.24	64,64,64,64	0
56	MG	EB	1629	1/1	0.65	0.20	115,115,115,115	0
56	MG	FB	9310	1/1	0.65	0.19	80,80,80,80	0
56	MG	A	1757	1/1	0.65	0.17	135,135,135,135	0
56	MG	EB	1684	1/1	0.65	0.16	96,96,96,96	0
56	MG	B	9563	1/1	0.65	0.16	117,117,117,117	0
56	MG	FB	9120	1/1	0.65	0.22	79,79,79,79	0
56	MG	EB	1638	1/1	0.65	0.30	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	UB	201	1/1	0.65	0.12	86,86,86,86	0
56	MG	H	201	1/1	0.65	0.16	103,103,103,103	0
56	MG	B	9292	1/1	0.65	0.18	88,88,88,88	0
56	MG	FB	9152	1/1	0.65	0.28	99,99,99,99	0
56	MG	EB	1703	1/1	0.65	0.09	98,98,98,98	0
56	MG	FB	9027	1/1	0.65	0.30	97,97,97,97	0
56	MG	B	9244	1/1	0.65	0.19	68,68,68,68	0
56	MG	A	1677	1/1	0.65	0.18	104,104,104,104	0
56	MG	B	9256	1/1	0.65	0.13	92,92,92,92	0
56	MG	EB	1615	1/1	0.65	0.28	90,90,90,90	0
56	MG	FB	9387	1/1	0.65	0.30	77,77,77,77	0
56	MG	A	1687	1/1	0.65	0.25	107,107,107,107	0
56	MG	B	9465	1/1	0.65	0.15	111,111,111,111	0
56	MG	FB	9181	1/1	0.65	0.28	75,75,75,75	0
56	MG	EB	1628	1/1	0.65	0.21	126,126,126,126	0
56	MG	A	1641	1/1	0.66	0.24	123,123,123,123	0
56	MG	FB	9290	1/1	0.66	0.27	91,91,91,91	0
56	MG	B	9102	1/1	0.66	0.30	69,69,69,69	0
56	MG	FB	9169	1/1	0.66	0.18	106,106,106,106	0
56	MG	B	9486	1/1	0.66	0.17	71,71,71,71	0
56	MG	IA	101	1/1	0.66	0.22	131,131,131,131	0
56	MG	A	1680	1/1	0.66	0.22	89,89,89,89	0
56	MG	FB	9127	1/1	0.66	0.37	111,111,111,111	0
56	MG	B	9233	1/1	0.66	0.15	96,96,96,96	0
56	MG	B	9135	1/1	0.66	0.34	100,100,100,100	0
56	MG	FB	9323	1/1	0.66	0.13	177,177,177,177	0
56	MG	B	9328	1/1	0.66	0.30	111,111,111,111	0
56	MG	QA	202	1/1	0.66	0.31	111,111,111,111	0
56	MG	A	1666	1/1	0.66	0.17	142,142,142,142	0
56	MG	EB	1620	1/1	0.67	0.22	90,90,90,90	0
56	MG	EB	1767	1/1	0.67	0.17	128,128,128,128	0
56	MG	A	1660	1/1	0.67	0.23	117,117,117,117	0
56	MG	C	210	1/1	0.67	0.21	102,102,102,102	0
56	MG	B	9250	1/1	0.67	0.31	108,108,108,108	0
56	MG	FB	9236	1/1	0.67	0.14	76,76,76,76	0
56	MG	JA	403	1/1	0.67	0.28	114,114,114,114	0
56	MG	EB	1735	1/1	0.67	0.23	85,85,85,85	0
56	MG	QC	304	1/1	0.67	0.29	102,102,102,102	0
56	MG	FB	9266	1/1	0.67	0.26	86,86,86,86	0
56	MG	EB	1618	1/1	0.67	0.31	74,74,74,74	0
56	MG	FB	9276	1/1	0.67	0.21	76,76,76,76	0
56	MG	FB	9134	1/1	0.67	0.25	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	FB	9416	1/1	0.68	0.26	79,79,79,79	0
56	MG	FB	9418	1/1	0.68	0.18	108,108,108,108	0
56	MG	EB	1605	1/1	0.68	0.31	98,98,98,98	0
56	MG	A	1603	1/1	0.68	0.33	69,69,69,69	0
56	MG	B	9386	1/1	0.68	0.10	115,115,115,115	0
56	MG	FB	9429	1/1	0.68	0.11	107,107,107,107	0
56	MG	FB	9282	1/1	0.68	0.26	92,92,92,92	0
56	MG	EB	1612	1/1	0.68	0.27	101,101,101,101	0
56	MG	EB	1657	1/1	0.68	0.16	99,99,99,99	0
56	MG	FB	9376	1/1	0.68	0.23	94,94,94,94	0
56	MG	EB	1692	1/1	0.68	0.26	129,129,129,129	0
56	MG	NA	201	1/1	0.68	0.12	107,107,107,107	0
56	MG	B	9116	1/1	0.68	0.19	102,102,102,102	0
56	MG	EB	1754	1/1	0.68	0.12	84,84,84,84	0
56	MG	C	219	1/1	0.68	0.24	91,91,91,91	0
56	MG	B	9352	1/1	0.68	0.30	103,103,103,103	0
56	MG	B	9166	1/1	0.68	0.32	96,96,96,96	0
56	MG	A	1765	1/1	0.68	0.21	81,81,81,81	0
56	MG	EB	1801	1/1	0.68	0.12	129,129,129,129	0
56	MG	FB	9118	1/1	0.68	0.22	87,87,87,87	0
56	MG	FB	9412	1/1	0.68	0.21	104,104,104,104	0
56	MG	A	1707	1/1	0.68	0.14	124,124,124,124	0
56	MG	A	1672	1/1	0.69	0.20	102,102,102,102	0
56	MG	FB	9226	1/1	0.69	0.35	100,100,100,100	0
56	MG	FB	9381	1/1	0.69	0.08	117,117,117,117	0
56	MG	EB	1621	1/1	0.69	0.23	119,119,119,119	0
56	MG	FB	9235	1/1	0.69	0.20	124,124,124,124	0
56	MG	A	1782	1/1	0.69	0.21	159,159,159,159	0
56	MG	A	1716	1/1	0.69	0.24	131,131,131,131	0
56	MG	B	9392	1/1	0.69	0.23	125,125,125,125	0
56	MG	IA	103	1/1	0.69	0.25	101,101,101,101	0
56	MG	A	1805	1/1	0.69	0.12	136,136,136,136	0
56	MG	GB	215	1/1	0.69	0.33	120,120,120,120	0
56	MG	EB	1639	1/1	0.69	0.20	102,102,102,102	0
56	MG	B	9249	1/1	0.69	0.25	95,95,95,95	0
56	MG	OC	303	1/1	0.69	0.15	115,115,115,115	0
56	MG	FB	9148	1/1	0.69	0.20	89,89,89,89	0
56	MG	A	1774	1/1	0.69	0.20	111,111,111,111	0
56	MG	B	9017	1/1	0.69	0.29	94,94,94,94	0
56	MG	B	9222	1/1	0.69	0.28	64,64,64,64	0
56	MG	A	1743	1/1	0.69	0.29	108,108,108,108	0
56	MG	A	1753	1/1	0.69	0.17	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	FB	9428	1/1	0.69	0.24	111,111,111,111	0
56	MG	A	1659	1/1	0.70	0.24	85,85,85,85	0
56	MG	FB	9284	1/1	0.70	0.23	95,95,95,95	0
56	MG	XA	102	1/1	0.70	0.22	101,101,101,101	0
56	MG	FB	9158	1/1	0.70	0.31	99,99,99,99	0
56	MG	B	9336	1/1	0.70	0.16	70,70,70,70	0
56	MG	MA	301	1/1	0.70	0.12	130,130,130,130	0
56	MG	FB	9267	1/1	0.70	0.14	89,89,89,89	0
56	MG	A	1601	1/1	0.70	0.30	62,62,62,62	0
56	MG	B	9501	1/1	0.70	0.23	76,76,76,76	0
56	MG	GB	206	1/1	0.70	0.20	114,114,114,114	0
56	MG	A	1617	1/1	0.70	0.17	101,101,101,101	0
56	MG	OB	201	1/1	0.70	0.14	104,104,104,104	0
56	MG	EB	1739	1/1	0.70	0.22	116,116,116,116	0
56	MG	YC	201	1/1	0.70	0.30	82,82,82,82	0
56	MG	FB	9077	1/1	0.70	0.33	95,95,95,95	0
56	MG	D	102	1/1	0.70	0.19	120,120,120,120	0
56	MG	EB	1790	1/1	0.71	0.17	130,130,130,130	0
56	MG	FB	9093	1/1	0.71	0.22	71,71,71,71	0
56	MG	FB	9094	1/1	0.71	0.31	73,73,73,73	0
56	MG	B	9311	1/1	0.71	0.16	99,99,99,99	0
56	MG	EB	1751	1/1	0.71	0.15	130,130,130,130	0
56	MG	FB	9404	1/1	0.71	0.16	101,101,101,101	0
56	MG	FB	9116	1/1	0.71	0.15	92,92,92,92	0
56	MG	FB	9302	1/1	0.71	0.10	109,109,109,109	0
56	MG	A	1702	1/1	0.71	0.20	131,131,131,131	0
56	MG	FB	9210	1/1	0.71	0.27	99,99,99,99	0
56	MG	B	9143	1/1	0.71	0.19	117,117,117,117	0
56	MG	FB	9313	1/1	0.71	0.22	102,102,102,102	0
56	MG	IA	104	1/1	0.71	0.33	118,118,118,118	0
56	MG	B	9291	1/1	0.71	0.15	100,100,100,100	0
56	MG	FB	9009	1/1	0.71	0.20	78,78,78,78	0
56	MG	B	9060	1/1	0.71	0.24	53,53,53,53	0
56	MG	EB	1714	1/1	0.71	0.19	112,112,112,112	0
56	MG	B	9294	1/1	0.71	0.16	118,118,118,118	0
56	MG	LA	301	1/1	0.71	0.18	136,136,136,136	0
56	MG	EB	1770	1/1	0.71	0.15	97,97,97,97	0
56	MG	EB	1728	1/1	0.71	0.16	109,109,109,109	0
56	MG	A	1732	1/1	0.71	0.23	122,122,122,122	0
56	MG	FB	9159	1/1	0.71	0.16	117,117,117,117	0
56	MG	AA	102	1/1	0.71	0.15	75,75,75,75	0
56	MG	FB	9370	1/1	0.71	0.12	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	FB	9163	1/1	0.71	0.27	75,75,75,75	0
56	MG	A	1712	1/1	0.71	0.29	95,95,95,95	0
56	MG	EB	1648	1/1	0.71	0.30	93,93,93,93	0
56	MG	EB	1651	1/1	0.71	0.17	124,124,124,124	0
56	MG	B	9261	1/1	0.71	0.15	69,69,69,69	0
56	MG	B	9369	1/1	0.72	0.32	101,101,101,101	0
56	MG	FB	9070	1/1	0.72	0.27	89,89,89,89	0
56	MG	A	1783	1/1	0.72	0.14	90,90,90,90	0
56	MG	FB	9081	1/1	0.72	0.16	139,139,139,139	0
56	MG	C	201	1/1	0.72	0.40	86,86,86,86	0
56	MG	TB	201	1/1	0.72	0.20	117,117,117,117	0
56	MG	EB	1676	1/1	0.72	0.21	99,99,99,99	0
56	MG	EB	1748	1/1	0.72	0.09	105,105,105,105	0
56	MG	FB	9023	1/1	0.72	0.24	95,95,95,95	0
56	MG	LC	101	1/1	0.72	0.36	86,86,86,86	0
56	MG	B	9476	1/1	0.72	0.10	83,83,83,83	0
56	MG	B	9092	1/1	0.72	0.24	92,92,92,92	0
56	MG	B	9263	1/1	0.72	0.17	60,60,60,60	0
56	MG	GB	210	1/1	0.72	0.17	121,121,121,121	0
56	MG	EB	1668	1/1	0.72	0.15	103,103,103,103	0
56	MG	EB	1721	1/1	0.72	0.18	87,87,87,87	0
56	MG	FB	9128	1/1	0.72	0.37	85,85,85,85	0
56	MG	FB	9411	1/1	0.72	0.15	75,75,75,75	0
56	MG	EB	1722	1/1	0.72	0.38	146,146,146,146	0
56	MG	B	9248	1/1	0.72	0.19	100,100,100,100	0
56	MG	FB	9352	1/1	0.72	0.18	131,131,131,131	0
56	MG	C	214	1/1	0.72	0.25	110,110,110,110	0
56	MG	FB	9209	1/1	0.72	0.17	110,110,110,110	0
56	MG	FB	9057	1/1	0.72	0.33	83,83,83,83	0
56	MG	C	218	1/1	0.72	0.18	115,115,115,115	0
56	MG	BD	101	1/1	0.72	0.16	97,97,97,97	0
56	MG	A	1770	1/1	0.73	0.39	107,107,107,107	0
56	MG	A	1679	1/1	0.73	0.29	103,103,103,103	0
56	MG	A	1785	1/1	0.73	0.13	79,79,79,79	0
56	MG	A	1813	1/1	0.73	0.13	127,127,127,127	0
56	MG	BC	101	1/1	0.73	0.15	93,93,93,93	0
56	MG	B	9209	1/1	0.73	0.30	73,73,73,73	0
56	MG	FB	9125	1/1	0.73	0.19	101,101,101,101	0
56	MG	FC	102	1/1	0.73	0.14	122,122,122,122	0
56	MG	B	9012	1/1	0.73	0.17	52,52,52,52	0
56	MG	FB	9183	1/1	0.73	0.30	89,89,89,89	0
56	MG	GB	212	1/1	0.73	0.35	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	A	1725	1/1	0.73	0.35	109,109,109,109	0
56	MG	TA	203	1/1	0.73	0.12	107,107,107,107	0
56	MG	A	1618	1/1	0.73	0.19	126,126,126,126	0
56	MG	B	9140	1/1	0.73	0.55	69,69,69,69	0
56	MG	AB	102	1/1	0.73	0.11	95,95,95,95	0
56	MG	A	1667	1/1	0.73	0.31	101,101,101,101	0
56	MG	A	1711	1/1	0.73	0.24	88,88,88,88	0
56	MG	FB	9289	1/1	0.73	0.18	124,124,124,124	0
56	MG	EB	1723	1/1	0.73	0.10	99,99,99,99	0
56	MG	A	1720	1/1	0.73	0.15	84,84,84,84	0
56	MG	WC	201	1/1	0.73	0.49	116,116,116,116	0
56	MG	EB	1643	1/1	0.73	0.52	91,91,91,91	0
56	MG	B	9447	1/1	0.73	0.07	78,78,78,78	0
56	MG	FB	9440	1/1	0.73	0.18	93,93,93,93	0
56	MG	FB	9104	1/1	0.73	0.19	96,96,96,96	0
56	MG	EB	1646	1/1	0.74	0.21	98,98,98,98	0
56	MG	B	9339	1/1	0.74	0.07	103,103,103,103	0
56	MG	FB	9389	1/1	0.74	0.22	93,93,93,93	0
56	MG	I	201	1/1	0.74	0.11	89,89,89,89	0
56	MG	FB	9227	1/1	0.74	0.22	74,74,74,74	0
56	MG	FB	9171	1/1	0.74	0.12	117,117,117,117	0
56	MG	EB	1740	1/1	0.74	0.22	112,112,112,112	0
56	MG	FB	9176	1/1	0.74	0.13	81,81,81,81	0
56	MG	J	201	1/1	0.74	0.16	99,99,99,99	0
56	MG	A	1749	1/1	0.74	0.11	119,119,119,119	0
56	MG	B	9217	1/1	0.74	0.17	128,128,128,128	0
56	MG	B	9120	1/1	0.74	0.23	71,71,71,71	0
56	MG	B	9167	1/1	0.74	0.26	92,92,92,92	0
56	MG	A	1623	1/1	0.74	0.25	105,105,105,105	0
56	MG	B	9230	1/1	0.74	0.27	69,69,69,69	0
56	MG	A	1664	1/1	0.74	0.11	121,121,121,121	0
56	MG	FB	9202	1/1	0.74	0.12	94,94,94,94	0
56	MG	B	9556	1/1	0.74	0.17	87,87,87,87	0
56	MG	A	1676	1/1	0.74	0.15	72,72,72,72	0
56	MG	EB	1604	1/1	0.74	0.49	87,87,87,87	0
56	MG	A	1626	1/1	0.74	0.24	91,91,91,91	0
56	MG	FB	9214	1/1	0.74	0.08	150,150,150,150	0
56	MG	EB	1608	1/1	0.74	0.39	72,72,72,72	0
56	MG	B	9106	1/1	0.74	0.18	63,63,63,63	0
58	ZN	FC	101	1/1	0.74	0.18	176,176,176,176	0
56	MG	B	9227	1/1	0.75	0.22	76,76,76,76	0
56	MG	B	9287	1/1	0.75	0.10	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	FB	9332	1/1	0.75	0.13	89,89,89,89	0
56	MG	B	9081	1/1	0.75	0.22	68,68,68,68	0
56	MG	FB	9114	1/1	0.75	0.16	82,82,82,82	0
56	MG	Q	202	1/1	0.75	0.06	78,78,78,78	0
56	MG	EB	1677	1/1	0.75	0.18	83,83,83,83	0
56	MG	EB	1640	1/1	0.75	0.11	110,110,110,110	0
56	MG	B	9210	1/1	0.75	0.15	85,85,85,85	0
56	MG	FB	9434	1/1	0.75	0.11	102,102,102,102	0
56	MG	EB	1734	1/1	0.75	0.14	101,101,101,101	0
56	MG	EB	1774	1/1	0.75	0.10	129,129,129,129	0
56	MG	FB	9046	1/1	0.75	0.40	74,74,74,74	0
56	MG	A	1706	1/1	0.75	0.14	100,100,100,100	0
56	MG	B	9477	1/1	0.75	0.12	101,101,101,101	0
56	MG	A	1705	1/1	0.75	0.26	93,93,93,93	0
56	MG	B	9560	1/1	0.75	0.15	100,100,100,100	0
56	MG	FB	9296	1/1	0.75	0.20	71,71,71,71	0
56	MG	A	1709	1/1	0.75	0.14	97,97,97,97	0
56	MG	UA	201	1/1	0.75	0.38	92,92,92,92	0
56	MG	FB	9391	1/1	0.75	0.18	107,107,107,107	0
56	MG	EB	1619	1/1	0.75	0.47	83,83,83,83	0
56	MG	A	1802	1/1	0.75	0.32	82,82,82,82	0
56	MG	FB	9401	1/1	0.75	0.13	98,98,98,98	0
56	MG	FB	9074	1/1	0.75	0.24	76,76,76,76	0
56	MG	B	9247	1/1	0.75	0.26	75,75,75,75	0
56	MG	FB	9162	1/1	0.75	0.16	93,93,93,93	0
56	MG	C	205	1/1	0.75	0.30	102,102,102,102	0
56	MG	FB	9319	1/1	0.75	0.07	99,99,99,99	0
56	MG	CB	201	1/1	0.75	0.10	128,128,128,128	0
56	MG	EB	1756	1/1	0.75	0.17	90,90,90,90	0
56	MG	B	9550	1/1	0.76	0.14	82,82,82,82	0
56	MG	FB	9031	1/1	0.76	0.35	60,60,60,60	0
56	MG	EB	1704	1/1	0.76	0.14	110,110,110,110	0
56	MG	B	9272	1/1	0.76	0.24	98,98,98,98	0
56	MG	EB	1783	1/1	0.76	0.09	111,111,111,111	0
56	MG	FB	9438	1/1	0.76	0.26	97,97,97,97	0
56	MG	EB	1747	1/1	0.76	0.20	90,90,90,90	0
56	MG	FB	9203	1/1	0.76	0.13	96,96,96,96	0
56	MG	A	1604	1/1	0.76	0.41	99,99,99,99	0
56	MG	A	1661	1/1	0.76	0.35	112,112,112,112	0
56	MG	A	1790	1/1	0.76	0.24	104,104,104,104	0
56	MG	B	9181	1/1	0.76	0.13	74,74,74,74	0
56	MG	B	9145	1/1	0.76	0.16	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	NA	202	1/1	0.76	0.18	122,122,122,122	0
56	MG	FB	9064	1/1	0.76	0.32	98,98,98,98	0
56	MG	A	1812	1/1	0.76	0.26	104,104,104,104	0
56	MG	OC	301	1/1	0.76	0.26	118,118,118,118	0
56	MG	B	9488	1/1	0.76	0.15	115,115,115,115	0
56	MG	B	9188	1/1	0.76	0.37	84,84,84,84	0
56	MG	FB	9078	1/1	0.76	0.18	82,82,82,82	0
56	MG	FB	9003	1/1	0.76	0.30	64,64,64,64	0
56	MG	FB	9086	1/1	0.76	0.26	70,70,70,70	0
56	MG	FB	9004	1/1	0.76	0.27	79,79,79,79	0
56	MG	EB	1765	1/1	0.76	0.23	99,99,99,99	0
56	MG	B	9439	1/1	0.76	0.10	83,83,83,83	0
56	MG	FB	9333	1/1	0.76	0.15	74,74,74,74	0
56	MG	B	9200	1/1	0.76	0.36	67,67,67,67	0
56	MG	B	9520	1/1	0.76	0.11	90,90,90,90	0
56	MG	B	9205	1/1	0.76	0.17	80,80,80,80	0
56	MG	A	1723	1/1	0.76	0.17	99,99,99,99	0
56	MG	FB	9463	1/1	0.77	0.11	83,83,83,83	0
56	MG	B	9452	1/1	0.77	0.07	93,93,93,93	0
56	MG	FB	9067	1/1	0.77	0.18	89,89,89,89	0
56	MG	B	9202	1/1	0.77	0.29	101,101,101,101	0
56	MG	FB	9192	1/1	0.77	0.11	93,93,93,93	0
56	MG	FB	9194	1/1	0.77	0.14	109,109,109,109	0
56	MG	FB	9325	1/1	0.77	0.15	117,117,117,117	0
56	MG	FB	9329	1/1	0.77	0.12	93,93,93,93	0
56	MG	FB	9331	1/1	0.77	0.14	89,89,89,89	0
56	MG	B	9337	1/1	0.77	0.28	111,111,111,111	0
56	MG	A	1799	1/1	0.77	0.15	99,99,99,99	0
56	MG	EB	1715	1/1	0.77	0.17	85,85,85,85	0
56	MG	FB	9339	1/1	0.77	0.13	87,87,87,87	0
56	MG	FB	9080	1/1	0.77	0.25	75,75,75,75	0
56	MG	C	217	1/1	0.77	0.12	85,85,85,85	0
56	MG	B	9043	1/1	0.77	0.27	96,96,96,96	0
56	MG	B	9479	1/1	0.77	0.28	57,57,57,57	0
56	MG	B	9059	1/1	0.77	0.35	85,85,85,85	0
56	MG	A	1704	1/1	0.77	0.25	114,114,114,114	0
56	MG	EB	1724	1/1	0.77	0.20	102,102,102,102	0
56	MG	A	1694	1/1	0.77	0.34	107,107,107,107	0
56	MG	EB	1795	1/1	0.77	0.25	78,78,78,78	0
56	MG	A	1804	1/1	0.77	0.09	138,138,138,138	0
56	MG	EB	1799	1/1	0.77	0.24	82,82,82,82	0
56	MG	B	9487	1/1	0.77	0.10	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	9281	1/1	0.77	0.18	80,80,80,80	0
56	MG	A	1756	1/1	0.77	0.14	94,94,94,94	0
56	MG	A	1735	1/1	0.77	0.11	128,128,128,128	0
56	MG	B	9105	1/1	0.77	0.16	55,55,55,55	0
56	MG	FB	9243	1/1	0.77	0.11	69,69,69,69	0
56	MG	K	204	1/1	0.77	0.06	89,89,89,89	0
56	MG	B	9176	1/1	0.77	0.27	90,90,90,90	0
56	MG	FB	9015	1/1	0.77	0.35	63,63,63,63	0
56	MG	B	9521	1/1	0.77	0.13	125,125,125,125	0
56	MG	A	1758	1/1	0.77	0.08	133,133,133,133	0
56	MG	DA	102	1/1	0.77	0.23	104,104,104,104	0
56	MG	DA	103	1/1	0.77	0.33	95,95,95,95	0
56	MG	B	9109	1/1	0.77	0.28	78,78,78,78	0
56	MG	A	1639	1/1	0.77	0.15	108,108,108,108	0
56	MG	FB	9160	1/1	0.77	0.14	98,98,98,98	0
56	MG	EB	1686	1/1	0.77	0.37	78,78,78,78	0
56	MG	A	1794	1/1	0.77	0.15	73,73,73,73	0
56	MG	A	1645	1/1	0.77	0.18	122,122,122,122	0
56	MG	FB	9049	1/1	0.77	0.19	70,70,70,70	0
56	MG	RC	203	1/1	0.77	0.10	103,103,103,103	0
56	MG	B	9562	1/1	0.77	0.12	75,75,75,75	0
56	MG	A	1740	1/1	0.77	0.21	96,96,96,96	0
56	MG	B	9323	1/1	0.77	0.15	92,92,92,92	0
56	MG	FB	9055	1/1	0.77	0.29	74,74,74,74	0
56	MG	EB	1701	1/1	0.77	0.41	98,98,98,98	0
56	MG	B	9201	1/1	0.77	0.28	73,73,73,73	0
56	MG	AD	102	1/1	0.77	0.15	106,106,106,106	0
56	MG	FB	9179	1/1	0.77	0.12	95,95,95,95	0
56	MG	B	9449	1/1	0.77	0.13	104,104,104,104	0
56	MG	A	1752	1/1	0.78	0.29	101,101,101,101	0
56	MG	UA	203	1/1	0.78	0.26	105,105,105,105	0
56	MG	B	9475	1/1	0.78	0.19	84,84,84,84	0
56	MG	EB	1636	1/1	0.78	0.35	82,82,82,82	0
56	MG	FB	9170	1/1	0.78	0.23	103,103,103,103	0
56	MG	A	1764	1/1	0.78	0.24	99,99,99,99	0
56	MG	B	9415	1/1	0.78	0.09	79,79,79,79	0
56	MG	B	9528	1/1	0.78	0.12	126,126,126,126	0
56	MG	B	9065	1/1	0.78	0.29	71,71,71,71	0
56	MG	FB	9395	1/1	0.78	0.16	66,66,66,66	0
56	MG	B	9546	1/1	0.78	0.10	108,108,108,108	0
56	MG	EB	1806	1/1	0.78	0.21	105,105,105,105	0
56	MG	KB	303	1/1	0.78	0.13	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	FB	9088	1/1	0.78	0.29	69,69,69,69	0
56	MG	EB	1644	1/1	0.78	0.18	93,93,93,93	0
56	MG	B	9077	1/1	0.78	0.15	67,67,67,67	0
56	MG	FB	9301	1/1	0.78	0.19	86,86,86,86	0
56	MG	FB	9408	1/1	0.78	0.17	105,105,105,105	0
56	MG	FB	9098	1/1	0.78	0.32	99,99,99,99	0
56	MG	EB	1647	1/1	0.78	0.23	97,97,97,97	0
56	MG	EB	1757	1/1	0.78	0.13	108,108,108,108	0
56	MG	EB	1607	1/1	0.78	0.42	85,85,85,85	0
56	MG	B	9253	1/1	0.78	0.07	87,87,87,87	0
56	MG	FB	9199	1/1	0.78	0.27	78,78,78,78	0
56	MG	FB	9115	1/1	0.78	0.21	81,81,81,81	0
56	MG	EB	1652	1/1	0.78	0.13	108,108,108,108	0
56	MG	A	1681	1/1	0.78	0.21	121,121,121,121	0
56	MG	EB	1659	1/1	0.78	0.34	87,87,87,87	0
56	MG	A	1792	1/1	0.78	0.15	100,100,100,100	0
56	MG	A	1766	1/1	0.78	0.12	95,95,95,95	0
56	MG	EB	1667	1/1	0.78	0.12	84,84,84,84	0
56	MG	FB	9035	1/1	0.78	0.27	73,73,73,73	0
56	MG	FB	9036	1/1	0.78	0.28	66,66,66,66	0
56	MG	B	9262	1/1	0.78	0.09	97,97,97,97	0
56	MG	QC	301	1/1	0.78	0.26	94,94,94,94	0
56	MG	FB	9462	1/1	0.78	0.19	113,113,113,113	0
56	MG	FB	9140	1/1	0.78	0.27	81,81,81,81	0
56	MG	A	1633	1/1	0.78	0.25	94,94,94,94	0
56	MG	B	9491	1/1	0.78	0.21	86,86,86,86	0
56	MG	EB	1776	1/1	0.78	0.25	98,98,98,98	0
56	MG	A	1788	1/1	0.78	0.10	91,91,91,91	0
56	MG	EB	1782	1/1	0.78	0.10	93,93,93,93	0
56	MG	T	201	1/1	0.78	0.07	65,65,65,65	0
56	MG	V	502	1/1	0.78	0.14	82,82,82,82	0
56	MG	C	209	1/1	0.78	0.21	119,119,119,119	0
56	MG	B	9182	1/1	0.78	0.33	81,81,81,81	0
56	MG	B	9008	1/1	0.79	0.34	67,67,67,67	0
56	MG	EB	1658	1/1	0.79	0.38	90,90,90,90	0
56	MG	EB	1702	1/1	0.79	0.20	94,94,94,94	0
56	MG	A	1726	1/1	0.79	0.24	97,97,97,97	0
56	MG	EB	1622	1/1	0.79	0.32	95,95,95,95	0
56	MG	EB	1662	1/1	0.79	0.36	89,89,89,89	0
56	MG	EB	1623	1/1	0.79	0.30	80,80,80,80	0
56	MG	FB	9312	1/1	0.79	0.33	92,92,92,92	0
56	MG	B	9016	1/1	0.79	0.16	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	FB	9409	1/1	0.79	0.23	74,74,74,74	0
56	MG	A	1703	1/1	0.79	0.12	98,98,98,98	0
56	MG	FB	9216	1/1	0.79	0.18	72,72,72,72	0
56	MG	NB	203	1/1	0.79	0.16	129,129,129,129	0
56	MG	FB	9069	1/1	0.79	0.23	88,88,88,88	0
56	MG	OB	202	1/1	0.79	0.15	99,99,99,99	0
56	MG	FB	9413	1/1	0.79	0.18	87,87,87,87	0
56	MG	B	9359	1/1	0.79	0.17	70,70,70,70	0
56	MG	FB	9072	1/1	0.79	0.28	79,79,79,79	0
56	MG	B	9079	1/1	0.79	0.27	65,65,65,65	0
56	MG	FB	9420	1/1	0.79	0.10	99,99,99,99	0
56	MG	EB	1634	1/1	0.79	0.14	77,77,77,77	0
56	MG	A	1808	1/1	0.79	0.28	108,108,108,108	0
56	MG	FB	9232	1/1	0.79	0.32	75,75,75,75	0
56	MG	I	202	1/1	0.79	0.08	79,79,79,79	0
56	MG	B	9366	1/1	0.79	0.17	60,60,60,60	0
56	MG	FB	9020	1/1	0.79	0.26	60,60,60,60	0
56	MG	B	9313	1/1	0.79	0.10	93,93,93,93	0
56	MG	EB	1726	1/1	0.79	0.20	95,95,95,95	0
56	MG	B	9082	1/1	0.79	0.24	69,69,69,69	0
56	MG	FB	9261	1/1	0.79	0.17	84,84,84,84	0
56	MG	B	9518	1/1	0.79	0.10	132,132,132,132	0
56	MG	B	9030	1/1	0.79	0.22	72,72,72,72	0
56	MG	EB	1645	1/1	0.79	0.24	84,84,84,84	0
56	MG	FB	9364	1/1	0.79	0.11	74,74,74,74	0
56	MG	A	1745	1/1	0.79	0.15	115,115,115,115	0
56	MG	FB	9107	1/1	0.79	0.31	79,79,79,79	0
56	MG	SC	201	1/1	0.79	0.13	104,104,104,104	0
56	MG	FB	9108	1/1	0.79	0.25	68,68,68,68	0
56	MG	B	9329	1/1	0.79	0.12	76,76,76,76	0
56	MG	GB	208	1/1	0.79	0.35	97,97,97,97	0
56	MG	A	1673	1/1	0.79	0.14	104,104,104,104	0
56	MG	B	9050	1/1	0.79	0.29	74,74,74,74	0
56	MG	FB	9188	1/1	0.79	0.18	69,69,69,69	0
56	MG	EB	1745	1/1	0.79	0.17	89,89,89,89	0
56	MG	FB	9048	1/1	0.79	0.26	74,74,74,74	0
56	MG	B	9480	1/1	0.79	0.06	83,83,83,83	0
56	MG	FB	9042	1/1	0.80	0.20	65,65,65,65	0
56	MG	A	1638	1/1	0.80	0.17	96,96,96,96	0
56	MG	JA	402	1/1	0.80	0.30	103,103,103,103	0
56	MG	S	202	1/1	0.80	0.13	89,89,89,89	0
56	MG	JA	404	1/1	0.80	0.10	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	A	1608	1/1	0.80	0.32	99,99,99,99	0
56	MG	B	9395	1/1	0.80	0.29	59,59,59,59	0
56	MG	OB	203	1/1	0.80	0.12	104,104,104,104	0
56	MG	B	9396	1/1	0.80	0.13	116,116,116,116	0
56	MG	A	1674	1/1	0.80	0.10	90,90,90,90	0
56	MG	EB	1771	1/1	0.80	0.11	94,94,94,94	0
56	MG	FB	9303	1/1	0.80	0.28	77,77,77,77	0
56	MG	FB	9447	1/1	0.80	0.37	96,96,96,96	0
56	MG	FB	9173	1/1	0.80	0.13	92,92,92,92	0
56	MG	EB	1666	1/1	0.80	0.24	97,97,97,97	0
56	MG	FB	9468	1/1	0.80	0.17	88,88,88,88	0
56	MG	B	9484	1/1	0.80	0.15	129,129,129,129	0
56	MG	FB	9388	1/1	0.80	0.21	73,73,73,73	0
56	MG	FB	9474	1/1	0.80	0.07	87,87,87,87	0
56	MG	FB	9476	1/1	0.80	0.15	93,93,93,93	0
56	MG	A	1739	1/1	0.80	0.12	101,101,101,101	0
56	MG	FB	9012	1/1	0.80	0.46	78,78,78,78	0
56	MG	FB	9314	1/1	0.80	0.21	64,64,64,64	0
56	MG	FB	9316	1/1	0.80	0.23	87,87,87,87	0
56	MG	HA	101	1/1	0.80	0.36	95,95,95,95	0
56	MG	B	9525	1/1	0.80	0.07	130,130,130,130	0
56	MG	FB	9242	1/1	0.80	0.15	61,61,61,61	0
56	MG	A	1747	1/1	0.80	0.08	99,99,99,99	0
56	MG	FB	9248	1/1	0.80	0.31	83,83,83,83	0
56	MG	B	9535	1/1	0.80	0.21	84,84,84,84	0
56	MG	TC	201	1/1	0.80	0.12	117,117,117,117	0
56	MG	B	9048	1/1	0.80	0.15	71,71,71,71	0
56	MG	A	1622	1/1	0.80	0.38	101,101,101,101	0
56	MG	FB	9330	1/1	0.80	0.14	72,72,72,72	0
56	MG	EB	1786	1/1	0.80	0.13	103,103,103,103	0
56	MG	UA	204	1/1	0.80	0.07	100,100,100,100	0
56	MG	A	1637	1/1	0.80	0.16	106,106,106,106	0
56	MG	FB	9155	1/1	0.80	0.15	87,87,87,87	0
56	MG	EB	1650	1/1	0.80	0.24	84,84,84,84	0
58	ZN	BA	101	1/1	0.80	0.17	162,162,162,162	0
56	MG	EB	1680	1/1	0.80	0.17	90,90,90,90	0
56	MG	A	1803	1/1	0.81	0.18	108,108,108,108	0
56	MG	B	9431	1/1	0.81	0.14	57,57,57,57	0
56	MG	FB	9338	1/1	0.81	0.22	104,104,104,104	0
56	MG	EB	1768	1/1	0.81	0.16	90,90,90,90	0
56	MG	FB	9131	1/1	0.81	0.21	66,66,66,66	0
56	MG	FB	9347	1/1	0.81	0.31	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	FB	9348	1/1	0.81	0.11	107,107,107,107	0
56	MG	B	9502	1/1	0.81	0.23	74,74,74,74	0
56	MG	B	9378	1/1	0.81	0.22	107,107,107,107	0
56	MG	RB	201	1/1	0.81	0.26	92,92,92,92	0
56	MG	B	9349	1/1	0.81	0.16	93,93,93,93	0
56	MG	FB	9143	1/1	0.81	0.16	103,103,103,103	0
56	MG	FB	9359	1/1	0.81	0.31	91,91,91,91	0
56	MG	ZB	702	1/1	0.81	0.13	94,94,94,94	0
56	MG	B	9515	1/1	0.81	0.20	81,81,81,81	0
56	MG	FB	9204	1/1	0.81	0.24	88,88,88,88	0
56	MG	B	9293	1/1	0.81	0.17	78,78,78,78	0
56	MG	DC	101	1/1	0.81	0.08	93,93,93,93	0
56	MG	FB	9449	1/1	0.81	0.11	107,107,107,107	0
56	MG	FB	9453	1/1	0.81	0.13	85,85,85,85	0
56	MG	XA	105	1/1	0.81	0.15	97,97,97,97	0
56	MG	A	1636	1/1	0.81	0.21	84,84,84,84	0
56	MG	EB	1661	1/1	0.81	0.39	90,90,90,90	0
56	MG	FB	9028	1/1	0.81	0.40	67,67,67,67	0
56	MG	FB	9380	1/1	0.81	0.20	87,87,87,87	0
56	MG	NC	401	1/1	0.81	0.13	114,114,114,114	0
56	MG	NC	403	1/1	0.81	0.17	93,93,93,93	0
56	MG	B	9083	1/1	0.81	0.20	79,79,79,79	0
56	MG	C	207	1/1	0.81	0.13	99,99,99,99	0
56	MG	FB	9090	1/1	0.81	0.27	95,95,95,95	0
56	MG	EB	1665	1/1	0.81	0.29	95,95,95,95	0
56	MG	OC	305	1/1	0.81	0.15	120,120,120,120	0
56	MG	B	9114	1/1	0.81	0.19	78,78,78,78	0
56	MG	FB	9097	1/1	0.81	0.23	65,65,65,65	0
56	MG	M	203	1/1	0.81	0.20	87,87,87,87	0
56	MG	FB	9315	1/1	0.81	0.25	84,84,84,84	0
56	MG	JA	405	1/1	0.81	0.13	111,111,111,111	0
56	MG	EB	1707	1/1	0.81	0.17	103,103,103,103	0
56	MG	B	9221	1/1	0.81	0.24	88,88,88,88	0
56	MG	B	9453	1/1	0.81	0.12	68,68,68,68	0
56	MG	B	9306	1/1	0.81	0.12	61,61,61,61	0
56	MG	C	215	1/1	0.81	0.21	123,123,123,123	0
56	MG	B	9208	1/1	0.81	0.25	82,82,82,82	0
56	MG	EB	1759	1/1	0.81	0.14	81,81,81,81	0
56	MG	EB	1674	1/1	0.81	0.27	84,84,84,84	0
56	MG	B	9543	1/1	0.81	0.08	63,63,63,63	0
56	MG	FB	9123	1/1	0.81	0.20	80,80,80,80	0
56	MG	B	9489	1/1	0.81	0.18	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	A	1787	1/1	0.82	0.11	116,116,116,116	0
56	MG	B	9312	1/1	0.82	0.28	103,103,103,103	0
56	MG	XA	104	1/1	0.82	0.21	101,101,101,101	0
56	MG	B	9007	1/1	0.82	0.37	61,61,61,61	0
56	MG	A	1761	1/1	0.82	0.17	85,85,85,85	0
56	MG	EB	1743	1/1	0.82	0.11	86,86,86,86	0
56	MG	ZA	201	1/1	0.82	0.10	94,94,94,94	0
56	MG	A	1669	1/1	0.82	0.20	95,95,95,95	0
56	MG	B	9441	1/1	0.82	0.14	67,67,67,67	0
56	MG	B	9251	1/1	0.82	0.16	72,72,72,72	0
56	MG	E	301	1/1	0.82	0.05	78,78,78,78	0
56	MG	FB	9320	1/1	0.82	0.12	67,67,67,67	0
56	MG	B	9445	1/1	0.82	0.11	101,101,101,101	0
56	MG	FB	9154	1/1	0.82	0.19	71,71,71,71	0
56	MG	B	9561	1/1	0.82	0.19	91,91,91,91	0
56	MG	PB	201	1/1	0.82	0.17	85,85,85,85	0
56	MG	EB	1752	1/1	0.82	0.15	78,78,78,78	0
56	MG	B	9171	1/1	0.82	0.10	52,52,52,52	0
56	MG	SB	202	1/1	0.82	0.13	81,81,81,81	0
56	MG	B	9494	1/1	0.82	0.14	76,76,76,76	0
56	MG	FB	9421	1/1	0.82	0.16	118,118,118,118	0
56	MG	FB	9234	1/1	0.82	0.20	108,108,108,108	0
56	MG	I	203	1/1	0.82	0.09	92,92,92,92	0
56	MG	B	9498	1/1	0.82	0.28	89,89,89,89	0
56	MG	EB	1655	1/1	0.82	0.17	100,100,100,100	0
56	MG	EB	1613	1/1	0.82	0.32	71,71,71,71	0
56	MG	EB	1614	1/1	0.82	0.23	88,88,88,88	0
56	MG	FB	9244	1/1	0.82	0.24	86,86,86,86	0
56	MG	FB	9342	1/1	0.82	0.14	92,92,92,92	0
56	MG	FB	9343	1/1	0.82	0.15	72,72,72,72	0
56	MG	FB	9441	1/1	0.82	0.22	133,133,133,133	0
56	MG	FB	9246	1/1	0.82	0.29	73,73,73,73	0
56	MG	B	9125	1/1	0.82	0.17	63,63,63,63	0
56	MG	FB	9092	1/1	0.82	0.22	84,84,84,84	0
56	MG	MA	302	1/1	0.82	0.10	111,111,111,111	0
56	MG	FB	9264	1/1	0.82	0.08	61,61,61,61	0
56	MG	B	9051	1/1	0.82	0.24	67,67,67,67	0
56	MG	FB	9022	1/1	0.82	0.35	72,72,72,72	0
56	MG	FB	9470	1/1	0.82	0.12	86,86,86,86	0
56	MG	B	9338	1/1	0.82	0.13	75,75,75,75	0
56	MG	A	1797	1/1	0.82	0.14	83,83,83,83	0
56	MG	A	1728	1/1	0.82	0.15	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	FB	9029	1/1	0.82	0.33	78,78,78,78	0
56	MG	B	9403	1/1	0.82	0.28	77,77,77,77	0
56	MG	B	9344	1/1	0.82	0.23	74,74,74,74	0
56	MG	FB	9111	1/1	0.82	0.20	77,77,77,77	0
56	MG	A	1695	1/1	0.82	0.30	111,111,111,111	0
56	MG	GB	207	1/1	0.82	0.27	109,109,109,109	0
56	MG	EB	1625	1/1	0.82	0.17	98,98,98,98	0
56	MG	FB	9191	1/1	0.82	0.31	90,90,90,90	0
56	MG	A	1665	1/1	0.82	0.14	98,98,98,98	0
56	MG	FB	9384	1/1	0.82	0.14	120,120,120,120	0
56	MG	UA	202	1/1	0.82	0.17	88,88,88,88	0
56	MG	EB	1630	1/1	0.82	0.27	81,81,81,81	0
56	MG	EB	1779	1/1	0.82	0.11	102,102,102,102	0
56	MG	B	9354	1/1	0.82	0.12	71,71,71,71	0
56	MG	FB	9073	1/1	0.83	0.36	74,74,74,74	0
56	MG	A	1686	1/1	0.83	0.32	101,101,101,101	0
56	MG	B	9397	1/1	0.83	0.13	104,104,104,104	0
56	MG	A	1742	1/1	0.83	0.19	110,110,110,110	0
56	MG	B	9409	1/1	0.83	0.09	66,66,66,66	0
56	MG	FB	9417	1/1	0.83	0.16	99,99,99,99	0
56	MG	EB	1763	1/1	0.83	0.09	85,85,85,85	0
56	MG	FB	9014	1/1	0.83	0.27	64,64,64,64	0
56	MG	B	9214	1/1	0.83	0.13	57,57,57,57	0
56	MG	B	9014	1/1	0.83	0.21	79,79,79,79	0
56	MG	B	9345	1/1	0.83	0.14	56,56,56,56	0
56	MG	B	9180	1/1	0.83	0.13	57,57,57,57	0
56	MG	B	9136	1/1	0.83	0.27	64,64,64,64	0
56	MG	FB	9095	1/1	0.83	0.32	65,65,65,65	0
56	MG	K	202	1/1	0.83	0.23	73,73,73,73	0
56	MG	WB	201	1/1	0.83	0.14	106,106,106,106	0
56	MG	B	9428	1/1	0.83	0.07	70,70,70,70	0
56	MG	B	9095	1/1	0.83	0.14	64,64,64,64	0
56	MG	M	204	1/1	0.83	0.16	89,89,89,89	0
56	MG	CC	103	1/1	0.83	0.18	72,72,72,72	0
56	MG	C	202	1/1	0.83	0.18	80,80,80,80	0
56	MG	FB	9275	1/1	0.83	0.30	71,71,71,71	0
56	MG	S	201	1/1	0.83	0.13	80,80,80,80	0
56	MG	C	203	1/1	0.83	0.14	80,80,80,80	0
56	MG	A	1649	1/1	0.83	0.28	103,103,103,103	0
56	MG	FB	9113	1/1	0.83	0.34	80,80,80,80	0
56	MG	A	1605	1/1	0.83	0.26	68,68,68,68	0
56	MG	A	1708	1/1	0.83	0.15	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	9231	1/1	0.83	0.31	89,89,89,89	0
56	MG	B	9314	1/1	0.83	0.10	76,76,76,76	0
56	MG	B	9070	1/1	0.83	0.23	57,57,57,57	0
56	MG	FB	9295	1/1	0.83	0.12	58,58,58,58	0
56	MG	B	9075	1/1	0.83	0.17	54,54,54,54	0
56	MG	B	9376	1/1	0.83	0.21	68,68,68,68	0
56	MG	B	9279	1/1	0.83	0.20	87,87,87,87	0
56	MG	FB	9126	1/1	0.83	0.15	84,84,84,84	0
56	MG	EB	1683	1/1	0.83	0.28	84,84,84,84	0
56	MG	A	1762	1/1	0.83	0.18	103,103,103,103	0
56	MG	B	9454	1/1	0.83	0.28	70,70,70,70	0
56	MG	EB	1690	1/1	0.83	0.13	97,97,97,97	0
56	MG	B	9457	1/1	0.83	0.37	102,102,102,102	0
56	MG	FB	9311	1/1	0.83	0.22	89,89,89,89	0
56	MG	B	9390	1/1	0.83	0.23	61,61,61,61	0
56	MG	FB	9400	1/1	0.83	0.10	88,88,88,88	0
56	MG	FB	9212	1/1	0.83	0.12	103,103,103,103	0
56	MG	A	1814	1/1	0.83	0.12	171,171,171,171	0
56	MG	FB	9144	1/1	0.83	0.26	65,65,65,65	0
56	MG	EB	1649	1/1	0.83	0.55	81,81,81,81	0
56	MG	JA	401	1/1	0.83	0.15	108,108,108,108	0
56	MG	FB	9150	1/1	0.83	0.19	84,84,84,84	0
56	MG	FB	9071	1/1	0.83	0.30	73,73,73,73	0
56	MG	A	1621	1/1	0.83	0.34	93,93,93,93	0
56	MG	EB	1626	1/1	0.84	0.23	90,90,90,90	0
56	MG	FB	9287	1/1	0.84	0.26	72,72,72,72	0
56	MG	B	9153	1/1	0.84	0.21	85,85,85,85	0
56	MG	GB	214	1/1	0.84	0.16	82,82,82,82	0
56	MG	T	202	1/1	0.84	0.08	69,69,69,69	0
56	MG	B	9516	1/1	0.84	0.18	102,102,102,102	0
56	MG	EB	1631	1/1	0.84	0.22	83,83,83,83	0
56	MG	B	9353	1/1	0.84	0.14	67,67,67,67	0
56	MG	FB	9054	1/1	0.84	0.30	76,76,76,76	0
56	MG	C	213	1/1	0.84	0.11	103,103,103,103	0
56	MG	XA	101	1/1	0.84	0.29	99,99,99,99	0
56	MG	FB	9208	1/1	0.84	0.29	78,78,78,78	0
56	MG	A	1632	1/1	0.84	0.17	100,100,100,100	0
56	MG	A	1730	1/1	0.84	0.16	73,73,73,73	0
56	MG	A	1807	1/1	0.84	0.17	92,92,92,92	0
56	MG	KB	301	1/1	0.84	0.10	80,80,80,80	0
56	MG	FB	9065	1/1	0.84	0.32	75,75,75,75	0
56	MG	A	1653	1/1	0.84	0.21	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	FB	9068	1/1	0.84	0.15	64,64,64,64	0
56	MG	B	9527	1/1	0.84	0.10	82,82,82,82	0
56	MG	B	9009	1/1	0.84	0.47	55,55,55,55	0
56	MG	B	9531	1/1	0.84	0.13	58,58,58,58	0
56	MG	B	9365	1/1	0.84	0.16	104,104,104,104	0
56	MG	B	9034	1/1	0.84	0.31	84,84,84,84	0
56	MG	EB	1695	1/1	0.84	0.12	77,77,77,77	0
56	MG	FB	9228	1/1	0.84	0.09	115,115,115,115	0
56	MG	B	9011	1/1	0.84	0.35	58,58,58,58	0
56	MG	EB	1606	1/1	0.84	0.27	77,77,77,77	0
56	MG	B	9434	1/1	0.84	0.14	68,68,68,68	0
56	MG	B	9144	1/1	0.84	0.20	79,79,79,79	0
56	MG	FB	9326	1/1	0.84	0.38	94,94,94,94	0
56	MG	ZB	703	1/1	0.84	0.24	91,91,91,91	0
56	MG	B	9373	1/1	0.84	0.08	60,60,60,60	0
56	MG	FB	9424	1/1	0.84	0.10	97,97,97,97	0
56	MG	FB	9019	1/1	0.84	0.21	59,59,59,59	0
56	MG	FB	9240	1/1	0.84	0.15	99,99,99,99	0
56	MG	B	9375	1/1	0.84	0.10	51,51,51,51	0
56	MG	A	1772	1/1	0.84	0.16	101,101,101,101	0
56	MG	JC	101	1/1	0.84	0.33	89,89,89,89	0
56	MG	FB	9431	1/1	0.84	0.23	86,86,86,86	0
56	MG	FB	9334	1/1	0.84	0.23	65,65,65,65	0
56	MG	FB	9433	1/1	0.84	0.47	90,90,90,90	0
56	MG	B	9211	1/1	0.84	0.10	72,72,72,72	0
56	MG	B	9301	1/1	0.84	0.17	75,75,75,75	0
56	MG	FB	9247	1/1	0.84	0.14	79,79,79,79	0
56	MG	K	201	1/1	0.84	0.32	76,76,76,76	0
56	MG	FB	9253	1/1	0.84	0.25	67,67,67,67	0
56	MG	FB	9254	1/1	0.84	0.19	78,78,78,78	0
56	MG	FB	9255	1/1	0.84	0.35	89,89,89,89	0
56	MG	B	9446	1/1	0.84	0.15	55,55,55,55	0
56	MG	FB	9454	1/1	0.84	0.11	81,81,81,81	0
56	MG	B	9497	1/1	0.84	0.12	69,69,69,69	0
56	MG	B	9149	1/1	0.84	0.13	60,60,60,60	0
56	MG	FB	9103	1/1	0.84	0.29	78,78,78,78	0
56	MG	FB	9356	1/1	0.84	0.17	89,89,89,89	0
56	MG	QA	201	1/1	0.84	0.21	111,111,111,111	0
56	MG	B	9265	1/1	0.84	0.06	74,74,74,74	0
56	MG	FB	9473	1/1	0.84	0.10	107,107,107,107	0
56	MG	FB	9360	1/1	0.84	0.17	83,83,83,83	0
56	MG	B	9393	1/1	0.84	0.15	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	9346	1/1	0.84	0.34	68,68,68,68	0
56	MG	XC	201	1/1	0.84	0.11	97,97,97,97	0
56	MG	B	9243	1/1	0.84	0.12	73,73,73,73	0
56	MG	FB	9112	1/1	0.84	0.33	91,91,91,91	0
56	MG	GB	205	1/1	0.84	0.23	103,103,103,103	0
56	MG	FB	9375	1/1	0.84	0.14	80,80,80,80	0
56	MG	EB	1624	1/1	0.84	0.11	96,96,96,96	0
56	MG	FB	9043	1/1	0.84	0.26	81,81,81,81	0
56	MG	TA	202	1/1	0.84	0.16	90,90,90,90	0
56	MG	B	9223	1/1	0.85	0.27	93,93,93,93	0
56	MG	FB	9269	1/1	0.85	0.07	97,97,97,97	0
56	MG	FB	9196	1/1	0.85	0.27	84,84,84,84	0
56	MG	FB	9197	1/1	0.85	0.41	74,74,74,74	0
56	MG	FB	9345	1/1	0.85	0.10	92,92,92,92	0
56	MG	A	1614	1/1	0.85	0.12	82,82,82,82	0
56	MG	FB	9277	1/1	0.85	0.44	65,65,65,65	0
56	MG	B	9290	1/1	0.85	0.17	63,63,63,63	0
56	MG	A	1729	1/1	0.85	0.13	71,71,71,71	0
56	MG	FB	9136	1/1	0.85	0.16	84,84,84,84	0
56	MG	FB	9013	1/1	0.85	0.30	56,56,56,56	0
56	MG	FB	9206	1/1	0.85	0.14	91,91,91,91	0
56	MG	FB	9437	1/1	0.85	0.09	99,99,99,99	0
56	MG	FB	9358	1/1	0.85	0.11	75,75,75,75	0
56	MG	B	9023	1/1	0.85	0.28	48,48,48,48	0
56	MG	EB	1682	1/1	0.85	0.26	90,90,90,90	0
56	MG	FB	9017	1/1	0.85	0.16	85,85,85,85	0
56	MG	FB	9075	1/1	0.85	0.21	62,62,62,62	0
56	MG	B	9544	1/1	0.85	0.13	68,68,68,68	0
56	MG	EB	1730	1/1	0.85	0.09	97,97,97,97	0
56	MG	Q	201	1/1	0.85	0.16	121,121,121,121	0
56	MG	CC	104	1/1	0.85	0.18	79,79,79,79	0
56	MG	FB	9457	1/1	0.85	0.09	77,77,77,77	0
56	MG	EB	1733	1/1	0.85	0.17	109,109,109,109	0
56	MG	EB	1685	1/1	0.85	0.23	71,71,71,71	0
56	MG	FB	9024	1/1	0.85	0.34	60,60,60,60	0
56	MG	B	9320	1/1	0.85	0.35	85,85,85,85	0
56	MG	EB	1736	1/1	0.85	0.10	85,85,85,85	0
56	MG	EB	1737	1/1	0.85	0.10	113,113,113,113	0
56	MG	KA	301	1/1	0.85	0.14	119,119,119,119	0
56	MG	EB	1780	1/1	0.85	0.20	101,101,101,101	0
56	MG	B	9027	1/1	0.85	0.21	73,73,73,73	0
56	MG	B	9554	1/1	0.85	0.12	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	9391	1/1	0.85	0.16	81,81,81,81	0
56	MG	NC	404	1/1	0.85	0.12	119,119,119,119	0
56	MG	B	9559	1/1	0.85	0.13	71,71,71,71	0
56	MG	GB	204	1/1	0.85	0.14	118,118,118,118	0
56	MG	FB	9394	1/1	0.85	0.18	72,72,72,72	0
56	MG	A	1775	1/1	0.85	0.09	70,70,70,70	0
56	MG	W	301	1/1	0.85	0.12	104,104,104,104	0
56	MG	B	9297	1/1	0.85	0.17	57,57,57,57	0
56	MG	EB	1635	1/1	0.85	0.30	87,87,87,87	0
56	MG	A	1634	1/1	0.85	0.22	79,79,79,79	0
56	MG	EB	1637	1/1	0.85	0.21	107,107,107,107	0
56	MG	A	1750	1/1	0.85	0.11	79,79,79,79	0
56	MG	B	9519	1/1	0.85	0.12	75,75,75,75	0
56	MG	EB	1798	1/1	0.85	0.17	97,97,97,97	0
56	MG	B	9280	1/1	0.85	0.30	84,84,84,84	0
56	MG	EB	1711	1/1	0.85	0.21	85,85,85,85	0
56	MG	B	9091	1/1	0.85	0.10	71,71,71,71	0
56	MG	FB	9258	1/1	0.85	0.09	126,126,126,126	0
56	MG	B	9408	1/1	0.85	0.15	73,73,73,73	0
56	MG	FB	9002	1/1	0.85	0.37	62,62,62,62	0
56	MG	FB	9262	1/1	0.85	0.09	61,61,61,61	0
56	MG	B	9368	1/1	0.85	0.19	78,78,78,78	0
56	MG	B	9284	1/1	0.85	0.20	65,65,65,65	0
56	MG	IB	302	1/1	0.85	0.20	64,64,64,64	0
56	MG	EB	1653	1/1	0.86	0.20	77,77,77,77	0
56	MG	A	1731	1/1	0.86	0.13	72,72,72,72	0
56	MG	FB	9101	1/1	0.86	0.19	76,76,76,76	0
56	MG	FB	9382	1/1	0.86	0.21	80,80,80,80	0
56	MG	EB	1656	1/1	0.86	0.19	78,78,78,78	0
56	MG	FB	9189	1/1	0.86	0.13	93,93,93,93	0
56	MG	FB	9190	1/1	0.86	0.32	79,79,79,79	0
56	MG	B	9196	1/1	0.86	0.19	70,70,70,70	0
56	MG	B	9537	1/1	0.86	0.13	59,59,59,59	0
56	MG	B	9538	1/1	0.86	0.18	74,74,74,74	0
56	MG	EB	1713	1/1	0.86	0.14	96,96,96,96	0
56	MG	B	9413	1/1	0.86	0.23	62,62,62,62	0
56	MG	FB	9297	1/1	0.86	0.36	75,75,75,75	0
56	MG	B	9268	1/1	0.86	0.21	49,49,49,49	0
56	MG	FB	9033	1/1	0.86	0.45	76,76,76,76	0
56	MG	EB	1717	1/1	0.86	0.17	90,90,90,90	0
56	MG	A	1689	1/1	0.86	0.34	78,78,78,78	0
56	MG	B	9273	1/1	0.86	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	9154	1/1	0.86	0.18	68,68,68,68	0
56	MG	FB	9405	1/1	0.86	0.18	73,73,73,73	0
56	MG	FB	9406	1/1	0.86	0.15	100,100,100,100	0
56	MG	B	9553	1/1	0.86	0.12	63,63,63,63	0
56	MG	FB	9122	1/1	0.86	0.10	64,64,64,64	0
56	MG	FB	9045	1/1	0.86	0.54	79,79,79,79	0
56	MG	B	9165	1/1	0.86	0.15	53,53,53,53	0
56	MG	EB	1781	1/1	0.86	0.19	95,95,95,95	0
56	MG	B	9315	1/1	0.86	0.24	112,112,112,112	0
56	MG	B	9047	1/1	0.86	0.23	68,68,68,68	0
56	MG	FB	9050	1/1	0.86	0.15	87,87,87,87	0
56	MG	FB	9129	1/1	0.86	0.22	87,87,87,87	0
56	MG	EB	1727	1/1	0.86	0.15	99,99,99,99	0
56	MG	UB	203	1/1	0.86	0.25	91,91,91,91	0
56	MG	B	9121	1/1	0.86	0.18	54,54,54,54	0
56	MG	FB	9135	1/1	0.86	0.09	93,93,93,93	0
56	MG	B	9322	1/1	0.86	0.12	55,55,55,55	0
56	MG	FB	9224	1/1	0.86	0.24	73,73,73,73	0
56	MG	B	9169	1/1	0.86	0.20	69,69,69,69	0
56	MG	B	9324	1/1	0.86	0.08	78,78,78,78	0
56	MG	B	9325	1/1	0.86	0.11	53,53,53,53	0
56	MG	FB	9229	1/1	0.86	0.37	69,69,69,69	0
56	MG	B	9499	1/1	0.86	0.10	51,51,51,51	0
56	MG	EB	1792	1/1	0.86	0.25	76,76,76,76	0
56	MG	B	9500	1/1	0.86	0.09	88,88,88,88	0
56	MG	B	9326	1/1	0.86	0.20	69,69,69,69	0
56	MG	FB	9066	1/1	0.86	0.35	69,69,69,69	0
56	MG	A	1724	1/1	0.86	0.13	80,80,80,80	0
56	MG	A	1780	1/1	0.86	0.14	79,79,79,79	0
56	MG	B	9330	1/1	0.86	0.08	81,81,81,81	0
56	MG	FB	9340	1/1	0.86	0.09	76,76,76,76	0
56	MG	FB	9341	1/1	0.86	0.22	75,75,75,75	0
56	MG	NC	402	1/1	0.86	0.11	125,125,125,125	0
56	MG	FB	9445	1/1	0.86	0.21	72,72,72,72	0
56	MG	A	1616	1/1	0.86	0.15	69,69,69,69	0
56	MG	NC	405	1/1	0.86	0.20	82,82,82,82	0
56	MG	B	9052	1/1	0.86	0.26	60,60,60,60	0
56	MG	FB	9451	1/1	0.86	0.15	73,73,73,73	0
56	MG	C	211	1/1	0.86	0.11	111,111,111,111	0
56	MG	B	9025	1/1	0.86	0.20	49,49,49,49	0
56	MG	A	1773	1/1	0.86	0.13	98,98,98,98	0
56	MG	EB	1601	1/1	0.86	0.45	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	9061	1/1	0.86	0.14	64,64,64,64	0
56	MG	QC	303	1/1	0.86	0.20	101,101,101,101	0
56	MG	FB	9350	1/1	0.86	0.13	91,91,91,91	0
56	MG	FB	9164	1/1	0.86	0.15	67,67,67,67	0
56	MG	FB	9007	1/1	0.86	0.36	69,69,69,69	0
56	MG	FB	9168	1/1	0.86	0.18	85,85,85,85	0
56	MG	B	9462	1/1	0.86	0.09	69,69,69,69	0
56	MG	A	1625	1/1	0.86	0.14	96,96,96,96	0
56	MG	FB	9263	1/1	0.86	0.18	78,78,78,78	0
56	MG	EB	1694	1/1	0.86	0.34	90,90,90,90	0
56	MG	B	9523	1/1	0.86	0.16	65,65,65,65	0
56	MG	YC	202	1/1	0.86	0.19	76,76,76,76	0
56	MG	A	1800	1/1	0.86	0.10	116,116,116,116	0
56	MG	EB	1698	1/1	0.86	0.16	82,82,82,82	0
56	MG	C	220	1/1	0.86	0.14	99,99,99,99	0
56	MG	EB	1609	1/1	0.86	0.28	86,86,86,86	0
56	MG	B	9402	1/1	0.86	0.11	60,60,60,60	0
56	MG	B	9036	1/1	0.86	0.17	68,68,68,68	0
56	MG	IB	304	1/1	0.87	0.25	62,62,62,62	0
56	MG	FB	9044	1/1	0.87	0.41	73,73,73,73	0
56	MG	A	1722	1/1	0.87	0.17	126,126,126,126	0
56	MG	FB	9213	1/1	0.87	0.23	61,61,61,61	0
56	MG	FB	9354	1/1	0.87	0.14	69,69,69,69	0
56	MG	A	1697	1/1	0.87	0.11	101,101,101,101	0
56	MG	EB	1761	1/1	0.87	0.24	82,82,82,82	0
56	MG	EB	1804	1/1	0.87	0.16	79,79,79,79	0
56	MG	FB	9294	1/1	0.87	0.10	118,118,118,118	0
56	MG	B	9168	1/1	0.87	0.11	64,64,64,64	0
56	MG	B	9122	1/1	0.87	0.21	79,79,79,79	0
56	MG	B	9511	1/1	0.87	0.07	77,77,77,77	0
56	MG	FB	9362	1/1	0.87	0.06	84,84,84,84	0
56	MG	A	1612	1/1	0.87	0.29	83,83,83,83	0
56	MG	B	9128	1/1	0.87	0.17	72,72,72,72	0
56	MG	EB	1688	1/1	0.87	0.25	99,99,99,99	0
56	MG	FB	9443	1/1	0.87	0.19	96,96,96,96	0
56	MG	FB	9373	1/1	0.87	0.10	76,76,76,76	0
56	MG	B	9252	1/1	0.87	0.14	69,69,69,69	0
56	MG	A	1635	1/1	0.87	0.31	103,103,103,103	0
56	MG	FB	9058	1/1	0.87	0.26	68,68,68,68	0
56	MG	CC	101	1/1	0.87	0.17	82,82,82,82	0
56	MG	B	9296	1/1	0.87	0.14	72,72,72,72	0
56	MG	B	9084	1/1	0.87	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	FB	9455	1/1	0.87	0.13	83,83,83,83	0
56	MG	FB	9117	1/1	0.87	0.14	96,96,96,96	0
56	MG	FB	9458	1/1	0.87	0.13	85,85,85,85	0
56	MG	FB	9459	1/1	0.87	0.08	92,92,92,92	0
56	MG	B	9085	1/1	0.87	0.22	67,67,67,67	0
56	MG	B	9033	1/1	0.87	0.26	75,75,75,75	0
56	MG	FB	9465	1/1	0.87	0.11	94,94,94,94	0
56	MG	FB	9466	1/1	0.87	0.14	74,74,74,74	0
56	MG	FB	9239	1/1	0.87	0.08	111,111,111,111	0
56	MG	B	9057	1/1	0.87	0.20	62,62,62,62	0
56	MG	FB	9018	1/1	0.87	0.26	77,77,77,77	0
56	MG	EB	1697	1/1	0.87	0.09	98,98,98,98	0
56	MG	A	1719	1/1	0.87	0.09	105,105,105,105	0
56	MG	EB	1664	1/1	0.87	0.36	83,83,83,83	0
56	MG	EB	1742	1/1	0.87	0.17	82,82,82,82	0
56	MG	A	1713	1/1	0.87	0.17	99,99,99,99	0
56	MG	FB	9250	1/1	0.87	0.25	75,75,75,75	0
56	MG	FB	9397	1/1	0.87	0.14	85,85,85,85	0
56	MG	B	9530	1/1	0.87	0.19	71,71,71,71	0
56	MG	FB	9130	1/1	0.87	0.36	76,76,76,76	0
56	MG	B	9037	1/1	0.87	0.23	65,65,65,65	0
56	MG	B	9064	1/1	0.87	0.27	73,73,73,73	0
56	MG	B	9193	1/1	0.87	0.20	59,59,59,59	0
56	MG	B	9448	1/1	0.87	0.13	78,78,78,78	0
56	MG	FB	9138	1/1	0.87	0.48	66,66,66,66	0
56	MG	GB	211	1/1	0.87	0.19	104,104,104,104	0
56	MG	B	9038	1/1	0.87	0.13	53,53,53,53	0
56	MG	B	9040	1/1	0.87	0.24	57,57,57,57	0
56	MG	FB	9141	1/1	0.87	0.28	82,82,82,82	0
56	MG	A	1715	1/1	0.87	0.26	113,113,113,113	0
56	MG	U	102	1/1	0.87	0.13	69,69,69,69	0
56	MG	FB	9145	1/1	0.87	0.16	66,66,66,66	0
56	MG	FB	9274	1/1	0.87	0.15	78,78,78,78	0
56	MG	FB	9205	1/1	0.87	0.22	84,84,84,84	0
56	MG	FB	9089	1/1	0.87	0.12	76,76,76,76	0
56	MG	A	1796	1/1	0.87	0.08	81,81,81,81	0
56	MG	V	503	1/1	0.87	0.14	66,66,66,66	0
56	MG	B	9547	1/1	0.87	0.19	127,127,127,127	0
56	MG	Y	101	1/1	0.87	0.11	66,66,66,66	0
56	MG	FB	9422	1/1	0.87	0.13	104,104,104,104	0
56	MG	B	9270	1/1	0.88	0.27	57,57,57,57	0
56	MG	FB	9337	1/1	0.88	0.18	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	FB	9256	1/1	0.88	0.31	87,87,87,87	0
56	MG	FB	9257	1/1	0.88	0.25	76,76,76,76	0
56	MG	JB	301	1/1	0.88	0.19	69,69,69,69	0
56	MG	B	9129	1/1	0.88	0.10	65,65,65,65	0
56	MG	B	9101	1/1	0.88	0.21	61,61,61,61	0
56	MG	B	9361	1/1	0.88	0.08	56,56,56,56	0
56	MG	B	9239	1/1	0.88	0.14	94,94,94,94	0
56	MG	B	9316	1/1	0.88	0.20	58,58,58,58	0
56	MG	B	9435	1/1	0.88	0.10	63,63,63,63	0
56	MG	FB	9119	1/1	0.88	0.10	84,84,84,84	0
56	MG	EB	1687	1/1	0.88	0.26	95,95,95,95	0
56	MG	B	9056	1/1	0.88	0.23	63,63,63,63	0
56	MG	B	9207	1/1	0.88	0.15	57,57,57,57	0
56	MG	B	9321	1/1	0.88	0.15	77,77,77,77	0
56	MG	A	1734	1/1	0.88	0.07	89,89,89,89	0
56	MG	Z	103	1/1	0.88	0.18	82,82,82,82	0
56	MG	FB	9439	1/1	0.88	0.13	91,91,91,91	0
56	MG	B	9245	1/1	0.88	0.18	77,77,77,77	0
56	MG	EB	1802	1/1	0.88	0.06	108,108,108,108	0
56	MG	VB	201	1/1	0.88	0.31	69,69,69,69	0
56	MG	FB	9279	1/1	0.88	0.19	70,70,70,70	0
56	MG	EB	1803	1/1	0.88	0.29	88,88,88,88	0
56	MG	A	1748	1/1	0.88	0.17	82,82,82,82	0
56	MG	FB	9446	1/1	0.88	0.07	83,83,83,83	0
56	MG	C	208	1/1	0.88	0.18	99,99,99,99	0
56	MG	B	9510	1/1	0.88	0.06	120,120,120,120	0
56	MG	B	9108	1/1	0.88	0.18	71,71,71,71	0
56	MG	B	9512	1/1	0.88	0.13	59,59,59,59	0
56	MG	FB	9288	1/1	0.88	0.08	73,73,73,73	0
56	MG	FB	9371	1/1	0.88	0.09	79,79,79,79	0
56	MG	FB	9372	1/1	0.88	0.18	81,81,81,81	0
56	MG	FB	9005	1/1	0.88	0.35	53,53,53,53	0
56	MG	A	1607	1/1	0.88	0.41	84,84,84,84	0
56	MG	B	9110	1/1	0.88	0.24	58,58,58,58	0
56	MG	FB	9008	1/1	0.88	0.34	63,63,63,63	0
56	MG	B	9179	1/1	0.88	0.19	58,58,58,58	0
56	MG	B	9388	1/1	0.88	0.07	71,71,71,71	0
56	MG	B	9015	1/1	0.88	0.35	77,77,77,77	0
56	MG	FB	9469	1/1	0.88	0.19	74,74,74,74	0
56	MG	B	9335	1/1	0.88	0.11	77,77,77,77	0
56	MG	A	1643	1/1	0.88	0.18	73,73,73,73	0
56	MG	FB	9076	1/1	0.88	0.31	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	9460	1/1	0.88	0.08	76,76,76,76	0
56	MG	FB	9016	1/1	0.88	0.41	75,75,75,75	0
56	MG	B	9148	1/1	0.88	0.28	65,65,65,65	0
56	MG	FB	9225	1/1	0.88	0.18	71,71,71,71	0
56	MG	B	9463	1/1	0.88	0.09	72,72,72,72	0
56	MG	FB	9156	1/1	0.88	0.31	89,89,89,89	0
56	MG	A	1776	1/1	0.88	0.12	93,93,93,93	0
56	MG	B	9468	1/1	0.88	0.17	62,62,62,62	0
56	MG	B	9473	1/1	0.88	0.07	70,70,70,70	0
56	MG	B	9035	1/1	0.88	0.24	49,49,49,49	0
56	MG	B	9536	1/1	0.88	0.15	71,71,71,71	0
56	MG	A	1811	1/1	0.88	0.15	100,100,100,100	0
56	MG	FB	9026	1/1	0.88	0.31	81,81,81,81	0
56	MG	B	9164	1/1	0.88	0.32	65,65,65,65	0
56	MG	B	9099	1/1	0.88	0.07	60,60,60,60	0
56	MG	B	9405	1/1	0.88	0.05	73,73,73,73	0
56	MG	B	9407	1/1	0.88	0.09	75,75,75,75	0
56	MG	B	9266	1/1	0.88	0.07	74,74,74,74	0
56	MG	B	9307	1/1	0.88	0.19	72,72,72,72	0
56	MG	B	9351	1/1	0.88	0.15	82,82,82,82	0
56	MG	EB	1731	1/1	0.88	0.16	79,79,79,79	0
56	MG	FB	9175	1/1	0.88	0.36	87,87,87,87	0
56	MG	B	9309	1/1	0.88	0.19	73,73,73,73	0
56	MG	FB	9038	1/1	0.88	0.20	70,70,70,70	0
56	MG	B	9019	1/1	0.88	0.19	44,44,44,44	0
56	MG	FB	9450	1/1	0.89	0.11	71,71,71,71	0
56	MG	B	9111	1/1	0.89	0.27	64,64,64,64	0
56	MG	B	9401	1/1	0.89	0.15	66,66,66,66	0
56	MG	HA	103	1/1	0.89	0.24	104,104,104,104	0
56	MG	B	9026	1/1	0.89	0.14	53,53,53,53	0
56	MG	B	9155	1/1	0.89	0.22	76,76,76,76	0
56	MG	B	9203	1/1	0.89	0.36	57,57,57,57	0
56	MG	FB	9102	1/1	0.89	0.18	79,79,79,79	0
56	MG	B	9178	1/1	0.89	0.14	65,65,65,65	0
56	MG	B	9278	1/1	0.89	0.20	67,67,67,67	0
56	MG	EB	1699	1/1	0.89	0.07	81,81,81,81	0
56	MG	B	9371	1/1	0.89	0.09	75,75,75,75	0
56	MG	FB	9467	1/1	0.89	0.10	82,82,82,82	0
56	MG	M	201	1/1	0.89	0.27	78,78,78,78	0
56	MG	M	202	1/1	0.89	0.17	83,83,83,83	0
56	MG	B	9156	1/1	0.89	0.21	79,79,79,79	0
56	MG	B	9042	1/1	0.89	0.27	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	FB	9061	1/1	0.89	0.24	66,66,66,66	0
56	MG	B	9058	1/1	0.89	0.23	59,59,59,59	0
56	MG	B	9039	1/1	0.89	0.28	56,56,56,56	0
56	MG	EC	101	1/1	0.89	0.17	78,78,78,78	0
56	MG	FB	9475	1/1	0.89	0.17	77,77,77,77	0
56	MG	B	9464	1/1	0.89	0.13	78,78,78,78	0
56	MG	B	9382	1/1	0.89	0.24	66,66,66,66	0
56	MG	B	9545	1/1	0.89	0.13	99,99,99,99	0
56	MG	B	9385	1/1	0.89	0.22	63,63,63,63	0
56	MG	B	9327	1/1	0.89	0.30	90,90,90,90	0
56	MG	EB	1753	1/1	0.89	0.12	93,93,93,93	0
56	MG	B	9088	1/1	0.89	0.32	59,59,59,59	0
56	MG	EB	1794	1/1	0.89	0.10	88,88,88,88	0
56	MG	B	9389	1/1	0.89	0.16	57,57,57,57	0
56	MG	A	1642	1/1	0.89	0.23	69,69,69,69	0
56	MG	FB	9291	1/1	0.89	0.13	65,65,65,65	0
56	MG	FB	9292	1/1	0.89	0.22	85,85,85,85	0
56	MG	B	9357	1/1	0.89	0.20	62,62,62,62	0
56	MG	Z	101	1/1	0.89	0.17	82,82,82,82	0
56	MG	FB	9034	1/1	0.89	0.23	69,69,69,69	0
56	MG	FB	9182	1/1	0.89	0.23	60,60,60,60	0
56	MG	FB	9079	1/1	0.89	0.24	73,73,73,73	0
56	MG	FB	9185	1/1	0.89	0.13	104,104,104,104	0
56	MG	B	9358	1/1	0.89	0.12	64,64,64,64	0
56	MG	FB	9241	1/1	0.89	0.30	84,84,84,84	0
56	MG	AA	101	1/1	0.89	0.17	80,80,80,80	0
56	MG	FB	9306	1/1	0.89	0.17	71,71,71,71	0
56	MG	FB	9083	1/1	0.89	0.34	82,82,82,82	0
56	MG	B	9053	1/1	0.89	0.19	48,48,48,48	0
56	MG	FB	9309	1/1	0.89	0.09	70,70,70,70	0
56	MG	EB	1725	1/1	0.89	0.10	111,111,111,111	0
56	MG	FB	9374	1/1	0.89	0.14	84,84,84,84	0
56	MG	B	9481	1/1	0.89	0.09	58,58,58,58	0
56	MG	FB	9193	1/1	0.89	0.18	80,80,80,80	0
56	MG	FB	9249	1/1	0.89	0.14	88,88,88,88	0
56	MG	YC	204	1/1	0.89	0.17	74,74,74,74	0
56	MG	KB	302	1/1	0.89	0.10	84,84,84,84	0
56	MG	FB	9378	1/1	0.89	0.09	85,85,85,85	0
56	MG	B	9093	1/1	0.89	0.22	60,60,60,60	0
56	MG	FB	9251	1/1	0.89	0.26	77,77,77,77	0
56	MG	B	9062	1/1	0.89	0.23	70,70,70,70	0
56	MG	EB	1729	1/1	0.89	0.19	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	9147	1/1	0.90	0.12	52,52,52,52	0
56	MG	B	9191	1/1	0.90	0.24	67,67,67,67	0
56	MG	B	9049	1/1	0.90	0.16	65,65,65,65	0
56	MG	B	9514	1/1	0.90	0.13	59,59,59,59	0
56	MG	EB	1772	1/1	0.90	0.24	102,102,102,102	0
56	MG	B	9258	1/1	0.90	0.10	88,88,88,88	0
56	MG	B	9170	1/1	0.90	0.18	75,75,75,75	0
56	MG	EB	1678	1/1	0.90	0.20	74,74,74,74	0
56	MG	FB	9390	1/1	0.90	0.14	67,67,67,67	0
56	MG	A	1668	1/1	0.90	0.12	80,80,80,80	0
56	MG	FB	9460	1/1	0.90	0.13	73,73,73,73	0
56	MG	FB	9461	1/1	0.90	0.14	71,71,71,71	0
56	MG	FB	9392	1/1	0.90	0.10	77,77,77,77	0
56	MG	FB	9137	1/1	0.90	0.48	71,71,71,71	0
56	MG	B	9472	1/1	0.90	0.12	80,80,80,80	0
56	MG	B	9097	1/1	0.90	0.12	67,67,67,67	0
56	MG	B	9138	1/1	0.90	0.12	69,69,69,69	0
56	MG	B	9175	1/1	0.90	0.17	64,64,64,64	0
56	MG	B	9302	1/1	0.90	0.22	58,58,58,58	0
56	MG	Z	102	1/1	0.90	0.14	64,64,64,64	0
56	MG	B	9204	1/1	0.90	0.09	76,76,76,76	0
56	MG	B	9113	1/1	0.90	0.12	64,64,64,64	0
56	MG	FB	9273	1/1	0.90	0.08	76,76,76,76	0
56	MG	B	9429	1/1	0.90	0.10	56,56,56,56	0
56	MG	C	216	1/1	0.90	0.08	117,117,117,117	0
56	MG	B	9271	1/1	0.90	0.09	89,89,89,89	0
56	MG	B	9340	1/1	0.90	0.36	64,64,64,64	0
56	MG	B	9308	1/1	0.90	0.24	70,70,70,70	0
56	MG	B	9383	1/1	0.90	0.13	74,74,74,74	0
56	MG	A	1760	1/1	0.90	0.10	74,74,74,74	0
56	MG	FB	9215	1/1	0.90	0.18	70,70,70,70	0
56	MG	FB	9041	1/1	0.90	0.24	61,61,61,61	0
56	MG	FB	9414	1/1	0.90	0.17	76,76,76,76	0
56	MG	B	9241	1/1	0.90	0.08	54,54,54,54	0
56	MG	B	9158	1/1	0.90	0.26	77,77,77,77	0
56	MG	FB	9100	1/1	0.90	0.23	83,83,83,83	0
56	MG	B	9542	1/1	0.90	0.12	54,54,54,54	0
56	MG	B	9443	1/1	0.90	0.09	57,57,57,57	0
56	MG	B	9347	1/1	0.90	0.10	90,90,90,90	0
56	MG	F	301	1/1	0.90	0.16	60,60,60,60	0
56	MG	B	9490	1/1	0.90	0.23	65,65,65,65	0
56	MG	G	302	1/1	0.90	0.09	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	9162	1/1	0.90	0.16	71,71,71,71	0
56	MG	B	9493	1/1	0.90	0.09	71,71,71,71	0
56	MG	B	9549	1/1	0.90	0.11	59,59,59,59	0
56	MG	B	9163	1/1	0.90	0.16	54,54,54,54	0
56	MG	EB	1710	1/1	0.90	0.15	96,96,96,96	0
56	MG	B	9141	1/1	0.90	0.18	56,56,56,56	0
56	MG	FB	9056	1/1	0.90	0.37	72,72,72,72	0
56	MG	B	9213	1/1	0.90	0.11	53,53,53,53	0
56	MG	FB	9305	1/1	0.90	0.14	72,72,72,72	0
56	MG	IB	303	1/1	0.90	0.18	59,59,59,59	0
56	MG	B	9080	1/1	0.90	0.19	59,59,59,59	0
56	MG	EB	1762	1/1	0.90	0.15	84,84,84,84	0
56	MG	B	9355	1/1	0.90	0.05	74,74,74,74	0
56	MG	FB	9121	1/1	0.90	0.15	53,53,53,53	0
56	MG	B	9130	1/1	0.90	0.29	53,53,53,53	0
56	MG	B	9118	1/1	0.90	0.15	64,64,64,64	0
56	MG	B	9456	1/1	0.90	0.14	53,53,53,53	0
56	MG	B	9187	1/1	0.90	0.13	56,56,56,56	0
56	MG	NB	201	1/1	0.90	0.19	124,124,124,124	0
56	MG	FB	9186	1/1	0.91	0.14	75,75,75,75	0
56	MG	FB	9260	1/1	0.91	0.20	70,70,70,70	0
56	MG	B	9173	1/1	0.91	0.06	69,69,69,69	0
56	MG	B	9010	1/1	0.91	0.44	67,67,67,67	0
56	MG	EB	1797	1/1	0.91	0.05	97,97,97,97	0
56	MG	EB	1741	1/1	0.91	0.16	87,87,87,87	0
56	MG	B	9069	1/1	0.91	0.13	63,63,63,63	0
56	MG	EB	1689	1/1	0.91	0.12	81,81,81,81	0
56	MG	FB	9268	1/1	0.91	0.12	70,70,70,70	0
56	MG	KB	304	1/1	0.91	0.10	93,93,93,93	0
56	MG	B	9380	1/1	0.91	0.11	51,51,51,51	0
56	MG	W	302	1/1	0.91	0.16	87,87,87,87	0
56	MG	EB	1642	1/1	0.91	0.15	92,92,92,92	0
56	MG	NB	202	1/1	0.91	0.14	113,113,113,113	0
56	MG	X	101	1/1	0.91	0.18	77,77,77,77	0
56	MG	FB	9435	1/1	0.91	0.39	72,72,72,72	0
56	MG	EB	1805	1/1	0.91	0.18	84,84,84,84	0
56	MG	B	9029	1/1	0.91	0.21	46,46,46,46	0
56	MG	B	9142	1/1	0.91	0.28	65,65,65,65	0
56	MG	FB	9200	1/1	0.91	0.18	93,93,93,93	0
56	MG	FB	9062	1/1	0.91	0.21	87,87,87,87	0
56	MG	FB	9063	1/1	0.91	0.20	63,63,63,63	0
56	MG	B	9229	1/1	0.91	0.10	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AB	101	1/1	0.91	0.13	92,92,92,92	0
56	MG	B	9255	1/1	0.91	0.16	66,66,66,66	0
56	MG	B	9533	1/1	0.91	0.10	53,53,53,53	0
56	MG	FB	9286	1/1	0.91	0.15	72,72,72,72	0
56	MG	FB	9367	1/1	0.91	0.09	70,70,70,70	0
56	MG	B	9534	1/1	0.91	0.08	81,81,81,81	0
56	MG	FB	9452	1/1	0.91	0.14	67,67,67,67	0
56	MG	EB	1602	1/1	0.91	0.41	72,72,72,72	0
56	MG	B	9350	1/1	0.91	0.14	60,60,60,60	0
56	MG	A	1615	1/1	0.91	0.13	63,63,63,63	0
56	MG	B	9257	1/1	0.91	0.15	61,61,61,61	0
56	MG	B	9032	1/1	0.91	0.20	78,78,78,78	0
56	MG	CC	107	1/1	0.91	0.10	68,68,68,68	0
56	MG	B	9260	1/1	0.91	0.08	60,60,60,60	0
56	MG	EB	1708	1/1	0.91	0.09	115,115,115,115	0
56	MG	B	9540	1/1	0.91	0.09	65,65,65,65	0
56	MG	A	1738	1/1	0.91	0.16	103,103,103,103	0
56	MG	B	9394	1/1	0.91	0.09	96,96,96,96	0
56	MG	FB	9220	1/1	0.91	0.28	66,66,66,66	0
56	MG	B	9492	1/1	0.91	0.12	59,59,59,59	0
56	MG	B	9021	1/1	0.91	0.26	54,54,54,54	0
56	MG	B	9022	1/1	0.91	0.18	47,47,47,47	0
56	MG	FB	9385	1/1	0.91	0.17	77,77,77,77	0
56	MG	B	9495	1/1	0.91	0.12	69,69,69,69	0
56	MG	FB	9084	1/1	0.91	0.11	76,76,76,76	0
56	MG	FB	9085	1/1	0.91	0.18	71,71,71,71	0
56	MG	EB	1716	1/1	0.91	0.07	84,84,84,84	0
56	MG	A	1809	1/1	0.91	0.14	93,93,93,93	0
56	MG	B	9184	1/1	0.91	0.27	76,76,76,76	0
56	MG	EB	1719	1/1	0.91	0.18	121,121,121,121	0
56	MG	B	9551	1/1	0.91	0.22	90,90,90,90	0
56	MG	B	9360	1/1	0.91	0.16	63,63,63,63	0
56	MG	B	9185	1/1	0.91	0.16	78,78,78,78	0
56	MG	J	202	1/1	0.91	0.06	104,104,104,104	0
56	MG	FB	9167	1/1	0.91	0.13	65,65,65,65	0
56	MG	B	9150	1/1	0.91	0.17	61,61,61,61	0
56	MG	B	9406	1/1	0.91	0.10	60,60,60,60	0
56	MG	B	9151	1/1	0.91	0.28	66,66,66,66	0
56	MG	B	9331	1/1	0.91	0.10	63,63,63,63	0
56	MG	B	9332	1/1	0.91	0.08	52,52,52,52	0
56	MG	B	9304	1/1	0.91	0.16	72,72,72,72	0
56	MG	FB	9174	1/1	0.91	0.26	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	FB	9039	1/1	0.91	0.31	78,78,78,78	0
56	MG	B	9305	1/1	0.91	0.09	76,76,76,76	0
56	MG	FB	9327	1/1	0.91	0.26	69,69,69,69	0
56	MG	M	205	1/1	0.91	0.16	75,75,75,75	0
56	MG	B	9469	1/1	0.91	0.10	59,59,59,59	0
56	MG	B	9471	1/1	0.91	0.18	74,74,74,74	0
56	MG	B	9216	1/1	0.91	0.10	61,61,61,61	0
56	MG	TA	201	1/1	0.91	0.11	96,96,96,96	0
56	MG	A	1644	1/1	0.91	0.25	83,83,83,83	0
56	MG	A	1640	1/1	0.91	0.07	84,84,84,84	0
56	MG	B	9424	1/1	0.91	0.10	82,82,82,82	0
56	MG	FB	9270	1/1	0.92	0.08	78,78,78,78	0
56	MG	Z	104	1/1	0.92	0.06	76,76,76,76	0
56	MG	B	9218	1/1	0.92	0.25	58,58,58,58	0
56	MG	EB	1787	1/1	0.92	0.07	113,113,113,113	0
56	MG	B	9412	1/1	0.92	0.18	50,50,50,50	0
56	MG	B	9206	1/1	0.92	0.21	65,65,65,65	0
56	MG	FB	9184	1/1	0.92	0.17	61,61,61,61	0
56	MG	CA	602	1/1	0.92	0.10	62,62,62,62	0
56	MG	FB	9231	1/1	0.92	0.12	81,81,81,81	0
56	MG	FB	9436	1/1	0.92	0.06	69,69,69,69	0
56	MG	FB	9142	1/1	0.92	0.24	71,71,71,71	0
56	MG	B	9220	1/1	0.92	0.11	64,64,64,64	0
56	MG	B	9504	1/1	0.92	0.08	59,59,59,59	0
56	MG	B	9508	1/1	0.92	0.09	70,70,70,70	0
56	MG	FB	9147	1/1	0.92	0.13	74,74,74,74	0
56	MG	B	9295	1/1	0.92	0.08	61,61,61,61	0
56	MG	FB	9335	1/1	0.92	0.25	69,69,69,69	0
56	MG	FB	9105	1/1	0.92	0.17	67,67,67,67	0
56	MG	L	202	1/1	0.92	0.07	81,81,81,81	0
56	MG	B	9086	1/1	0.92	0.16	66,66,66,66	0
56	MG	XA	103	1/1	0.92	0.40	96,96,96,96	0
56	MG	FB	9110	1/1	0.92	0.38	62,62,62,62	0
56	MG	B	9450	1/1	0.92	0.12	58,58,58,58	0
56	MG	FB	9293	1/1	0.92	0.16	68,68,68,68	0
56	MG	EB	1627	1/1	0.92	0.16	73,73,73,73	0
56	MG	B	9131	1/1	0.92	0.23	62,62,62,62	0
56	MG	B	9242	1/1	0.92	0.15	67,67,67,67	0
56	MG	A	1777	1/1	0.92	0.10	86,86,86,86	0
56	MG	FB	9298	1/1	0.92	0.08	61,61,61,61	0
56	MG	B	9225	1/1	0.92	0.08	52,52,52,52	0
56	MG	B	9517	1/1	0.92	0.09	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	QC	302	1/1	0.92	0.07	95,95,95,95	0
56	MG	B	9318	1/1	0.92	0.06	79,79,79,79	0
56	MG	B	9430	1/1	0.92	0.06	68,68,68,68	0
56	MG	B	9400	1/1	0.92	0.08	119,119,119,119	0
56	MG	FB	9304	1/1	0.92	0.14	66,66,66,66	0
56	MG	B	9433	1/1	0.92	0.06	69,69,69,69	0
56	MG	A	1698	1/1	0.92	0.15	75,75,75,75	0
56	MG	EB	1705	1/1	0.92	0.12	82,82,82,82	0
56	MG	B	9557	1/1	0.92	0.11	58,58,58,58	0
56	MG	A	1810	1/1	0.92	0.06	110,110,110,110	0
56	MG	EB	1777	1/1	0.92	0.06	116,116,116,116	0
56	MG	B	9436	1/1	0.92	0.08	70,70,70,70	0
56	MG	B	9381	1/1	0.92	0.06	71,71,71,71	0
56	MG	B	9067	1/1	0.92	0.15	66,66,66,66	0
56	MG	B	9529	1/1	0.92	0.09	62,62,62,62	0
56	MG	UB	202	1/1	0.92	0.05	83,83,83,83	0
56	MG	A	1768	1/1	0.92	0.12	78,78,78,78	0
56	MG	B	9157	1/1	0.92	0.07	69,69,69,69	0
56	MG	B	9096	1/1	0.92	0.10	55,55,55,55	0
58	ZN	HC	101	1/1	0.92	0.15	135,135,135,135	0
56	MG	B	9466	1/1	0.93	0.05	69,69,69,69	0
56	MG	A	1763	1/1	0.93	0.15	95,95,95,95	0
56	MG	EB	1654	1/1	0.93	0.13	71,71,71,71	0
56	MG	B	9192	1/1	0.93	0.23	54,54,54,54	0
56	MG	B	9342	1/1	0.93	0.20	56,56,56,56	0
56	MG	B	9087	1/1	0.93	0.15	60,60,60,60	0
56	MG	FB	9230	1/1	0.93	0.07	70,70,70,70	0
56	MG	B	9195	1/1	0.93	0.16	62,62,62,62	0
56	MG	B	9103	1/1	0.93	0.21	53,53,53,53	0
56	MG	B	9197	1/1	0.93	0.18	65,65,65,65	0
56	MG	B	9198	1/1	0.93	0.09	56,56,56,56	0
56	MG	B	9348	1/1	0.93	0.08	59,59,59,59	0
56	MG	FB	9037	1/1	0.93	0.09	130,130,130,130	0
56	MG	B	9013	1/1	0.93	0.34	66,66,66,66	0
56	MG	CC	105	1/1	0.93	0.23	67,67,67,67	0
56	MG	FB	9238	1/1	0.93	0.09	68,68,68,68	0
56	MG	O	202	1/1	0.93	0.45	76,76,76,76	0
56	MG	B	9224	1/1	0.93	0.13	47,47,47,47	0
56	MG	B	9288	1/1	0.93	0.10	58,58,58,58	0
56	MG	B	9319	1/1	0.93	0.18	75,75,75,75	0
56	MG	B	9526	1/1	0.93	0.12	65,65,65,65	0
56	MG	FB	9091	1/1	0.93	0.40	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	9161	1/1	0.93	0.19	67,67,67,67	0
56	MG	B	9078	1/1	0.93	0.32	56,56,56,56	0
56	MG	B	9440	1/1	0.93	0.07	55,55,55,55	0
56	MG	B	9020	1/1	0.93	0.22	45,45,45,45	0
56	MG	FB	9363	1/1	0.93	0.08	63,63,63,63	0
56	MG	B	9228	1/1	0.93	0.14	62,62,62,62	0
56	MG	FB	9365	1/1	0.93	0.06	72,72,72,72	0
56	MG	A	1655	1/1	0.93	0.15	74,74,74,74	0
56	MG	FB	9252	1/1	0.93	0.08	79,79,79,79	0
56	MG	FB	9369	1/1	0.93	0.19	63,63,63,63	0
56	MG	B	9066	1/1	0.93	0.17	57,57,57,57	0
56	MG	B	9003	1/1	0.93	0.32	54,54,54,54	0
56	MG	FB	9151	1/1	0.93	0.09	127,127,127,127	0
56	MG	B	9232	1/1	0.93	0.08	79,79,79,79	0
56	MG	B	9112	1/1	0.93	0.17	66,66,66,66	0
56	MG	B	9235	1/1	0.93	0.10	80,80,80,80	0
56	MG	B	9264	1/1	0.93	0.28	74,74,74,74	0
56	MG	C	221	1/1	0.93	0.09	100,100,100,100	0
56	MG	B	9004	1/1	0.93	0.28	40,40,40,40	0
56	MG	B	9005	1/1	0.93	0.30	47,47,47,47	0
56	MG	FB	9318	1/1	0.93	0.14	68,68,68,68	0
56	MG	B	9334	1/1	0.93	0.19	64,64,64,64	0
56	MG	FB	9109	1/1	0.93	0.18	61,61,61,61	0
56	MG	FB	9265	1/1	0.93	0.14	69,69,69,69	0
56	MG	FB	9448	1/1	0.93	0.17	79,79,79,79	0
56	MG	B	9152	1/1	0.93	0.13	50,50,50,50	0
56	MG	B	9411	1/1	0.93	0.07	73,73,73,73	0
56	MG	B	9458	1/1	0.93	0.05	58,58,58,58	0
56	MG	B	9115	1/1	0.93	0.20	48,48,48,48	0
56	MG	B	9548	1/1	0.93	0.12	84,84,84,84	0
56	MG	G	301	1/1	0.93	0.04	85,85,85,85	0
56	MG	B	9071	1/1	0.93	0.20	49,49,49,49	0
56	MG	B	9189	1/1	0.93	0.07	52,52,52,52	0
56	MG	B	9505	1/1	0.93	0.14	60,60,60,60	0
56	MG	B	9374	1/1	0.93	0.09	62,62,62,62	0
56	MG	B	9420	1/1	0.93	0.07	103,103,103,103	0
56	MG	FB	9223	1/1	0.93	0.07	68,68,68,68	0
56	MG	B	9461	1/1	0.94	0.28	67,67,67,67	0
56	MG	B	9425	1/1	0.94	0.15	86,86,86,86	0
56	MG	B	9159	1/1	0.94	0.24	65,65,65,65	0
56	MG	B	9072	1/1	0.94	0.21	55,55,55,55	0
56	MG	U	101	1/1	0.94	0.09	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	9146	1/1	0.94	0.07	53,53,53,53	0
56	MG	B	9341	1/1	0.94	0.15	69,69,69,69	0
56	MG	FB	9146	1/1	0.94	0.15	61,61,61,61	0
56	MG	B	9467	1/1	0.94	0.19	71,71,71,71	0
56	MG	B	9073	1/1	0.94	0.15	48,48,48,48	0
56	MG	FB	9285	1/1	0.94	0.16	73,73,73,73	0
56	MG	B	9432	1/1	0.94	0.08	67,67,67,67	0
56	MG	B	9470	1/1	0.94	0.12	97,97,97,97	0
56	MG	B	9269	1/1	0.94	0.08	53,53,53,53	0
56	MG	B	9212	1/1	0.94	0.12	77,77,77,77	0
56	MG	B	9074	1/1	0.94	0.29	54,54,54,54	0
56	MG	B	9552	1/1	0.94	0.07	56,56,56,56	0
56	MG	A	1755	1/1	0.94	0.08	110,110,110,110	0
56	MG	B	9215	1/1	0.94	0.06	71,71,71,71	0
56	MG	B	9274	1/1	0.94	0.15	68,68,68,68	0
56	MG	B	9404	1/1	0.94	0.09	65,65,65,65	0
56	MG	B	9076	1/1	0.94	0.22	53,53,53,53	0
56	MG	B	9031	1/1	0.94	0.13	60,60,60,60	0
56	MG	B	9377	1/1	0.94	0.07	61,61,61,61	0
56	MG	B	9236	1/1	0.94	0.26	63,63,63,63	0
56	MG	FB	9398	1/1	0.94	0.10	72,72,72,72	0
56	MG	FB	9399	1/1	0.94	0.21	71,71,71,71	0
56	MG	B	9089	1/1	0.94	0.17	59,59,59,59	0
56	MG	B	9024	1/1	0.94	0.24	57,57,57,57	0
56	MG	B	9282	1/1	0.94	0.21	53,53,53,53	0
56	MG	FB	9456	1/1	0.94	0.09	76,76,76,76	0
56	MG	FB	9166	1/1	0.94	0.13	80,80,80,80	0
56	MG	FB	9353	1/1	0.94	0.09	76,76,76,76	0
56	MG	B	9283	1/1	0.94	0.16	67,67,67,67	0
56	MG	RC	201	1/1	0.94	0.05	85,85,85,85	0
56	MG	K	203	1/1	0.94	0.10	71,71,71,71	0
56	MG	B	9384	1/1	0.94	0.12	52,52,52,52	0
56	MG	FB	9082	1/1	0.94	0.07	62,62,62,62	0
56	MG	UC	201	1/1	0.94	0.25	98,98,98,98	0
56	MG	L	201	1/1	0.94	0.15	57,57,57,57	0
56	MG	A	1602	1/1	0.94	0.33	60,60,60,60	0
56	MG	B	9417	1/1	0.94	0.19	67,67,67,67	0
56	MG	B	9419	1/1	0.94	0.06	58,58,58,58	0
56	MG	A	1714	1/1	0.94	0.11	98,98,98,98	0
56	MG	B	9421	1/1	0.94	0.21	57,57,57,57	0
56	MG	YC	203	1/1	0.94	0.14	80,80,80,80	0
56	MG	FB	9133	1/1	0.94	0.14	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	9127	1/1	0.94	0.13	52,52,52,52	0
56	MG	JA	406	1/1	0.94	0.13	74,74,74,74	0
56	MG	FB	9271	1/1	0.94	0.22	64,64,64,64	0
56	MG	FB	9419	1/1	0.94	0.12	72,72,72,72	0
56	MG	A	1684	1/1	0.94	0.20	74,74,74,74	0
56	MG	B	9459	1/1	0.94	0.05	71,71,71,71	0
56	MG	A	1767	1/1	0.94	0.05	94,94,94,94	0
56	MG	FB	9368	1/1	0.95	0.16	74,74,74,74	0
56	MG	B	9160	1/1	0.95	0.16	60,60,60,60	0
56	MG	B	9426	1/1	0.95	0.12	48,48,48,48	0
56	MG	B	9046	1/1	0.95	0.14	51,51,51,51	0
56	MG	FB	9201	1/1	0.95	0.07	67,67,67,67	0
56	MG	B	9246	1/1	0.95	0.32	61,61,61,61	0
56	MG	FB	9010	1/1	0.95	0.55	60,60,60,60	0
56	MG	B	9132	1/1	0.95	0.11	46,46,46,46	0
56	MG	B	9068	1/1	0.95	0.16	52,52,52,52	0
56	MG	B	9379	1/1	0.95	0.16	54,54,54,54	0
56	MG	EA	101	1/1	0.95	0.17	57,57,57,57	0
56	MG	B	9094	1/1	0.95	0.26	53,53,53,53	0
56	MG	B	9107	1/1	0.95	0.29	58,58,58,58	0
56	MG	B	9028	1/1	0.95	0.17	54,54,54,54	0
56	MG	B	9199	1/1	0.95	0.14	54,54,54,54	0
56	MG	B	9234	1/1	0.95	0.18	59,59,59,59	0
56	MG	B	9410	1/1	0.95	0.05	69,69,69,69	0
56	MG	RC	202	1/1	0.95	0.09	92,92,92,92	0
56	MG	B	9275	1/1	0.95	0.11	59,59,59,59	0
56	MG	B	9362	1/1	0.95	0.27	76,76,76,76	0
56	MG	B	9387	1/1	0.95	0.06	56,56,56,56	0
56	MG	A	1630	1/1	0.95	0.07	66,66,66,66	0
56	MG	FB	9025	1/1	0.95	0.24	53,53,53,53	0
56	MG	B	9442	1/1	0.95	0.15	65,65,65,65	0
56	MG	FB	9426	1/1	0.95	0.12	71,71,71,71	0
56	MG	B	9124	1/1	0.95	0.14	55,55,55,55	0
56	MG	IB	301	1/1	0.95	0.14	65,65,65,65	0
56	MG	B	9063	1/1	0.95	0.16	56,56,56,56	0
56	MG	B	9126	1/1	0.95	0.21	54,54,54,54	0
56	MG	B	9474	1/1	0.95	0.05	75,75,75,75	0
56	MG	A	1613	1/1	0.95	0.13	76,76,76,76	0
56	MG	B	9002	1/1	0.95	0.50	45,45,45,45	0
56	MG	FB	9096	1/1	0.95	0.16	73,73,73,73	0
56	MG	B	9090	1/1	0.95	0.10	49,49,49,49	0
57	BLS	B	9001	30/30	0.95	0.12	80,80,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	BLS	FB	9001	30/30	0.95	0.12	83,84,84,84	0
56	MG	B	9044	1/1	0.95	0.26	48,48,48,48	0
56	MG	B	9190	1/1	0.95	0.27	52,52,52,52	0
56	MG	B	9451	1/1	0.95	0.11	55,55,55,55	0
56	MG	B	9399	1/1	0.96	0.06	67,67,67,67	0
56	MG	B	9524	1/1	0.96	0.13	62,62,62,62	0
56	MG	FB	9087	1/1	0.96	0.23	65,65,65,65	0
56	MG	B	9123	1/1	0.96	0.07	46,46,46,46	0
56	MG	FB	9430	1/1	0.96	0.06	75,75,75,75	0
56	MG	B	9117	1/1	0.96	0.42	69,69,69,69	0
56	MG	B	9006	1/1	0.96	0.22	51,51,51,51	0
56	MG	B	9416	1/1	0.96	0.12	59,59,59,59	0
56	MG	B	9133	1/1	0.96	0.10	61,61,61,61	0
56	MG	FB	9386	1/1	0.96	0.08	72,72,72,72	0
56	MG	EB	1750	1/1	0.96	0.12	85,85,85,85	0
56	MG	B	9418	1/1	0.96	0.18	72,72,72,72	0
56	MG	FB	9464	1/1	0.96	0.14	76,76,76,76	0
56	MG	B	9513	1/1	0.96	0.21	61,61,61,61	0
56	MG	B	9119	1/1	0.96	0.10	49,49,49,49	0
56	MG	B	9496	1/1	0.96	0.06	55,55,55,55	0
56	MG	B	9285	1/1	0.96	0.10	61,61,61,61	0
56	MG	B	9367	1/1	0.96	0.09	57,57,57,57	0
56	MG	B	9054	1/1	0.96	0.32	50,50,50,50	0
56	MG	FB	9444	1/1	0.96	0.05	84,84,84,84	0
56	MG	B	9558	1/1	0.96	0.07	62,62,62,62	0
56	MG	B	9276	1/1	0.96	0.09	57,57,57,57	0
56	MG	CD	101	1/1	0.96	0.21	94,94,94,94	0
56	MG	B	9098	1/1	0.96	0.17	53,53,53,53	0
56	MG	FB	9351	1/1	0.96	0.10	68,68,68,68	0
56	MG	A	1786	1/1	0.96	0.05	119,119,119,119	0
56	MG	B	9541	1/1	0.96	0.08	55,55,55,55	0
56	MG	B	9259	1/1	0.96	0.18	61,61,61,61	0
56	MG	FB	9217	1/1	0.97	0.08	138,138,138,138	0
56	MG	B	9398	1/1	0.97	0.10	54,54,54,54	0
56	MG	B	9532	1/1	0.97	0.24	62,62,62,62	0
56	MG	B	9055	1/1	0.97	0.23	57,57,57,57	0
56	MG	B	9045	1/1	0.97	0.20	49,49,49,49	0
56	MG	O	201	1/1	0.97	0.12	63,63,63,63	0
56	MG	FB	9132	1/1	0.97	0.22	67,67,67,67	0
56	MG	B	9333	1/1	0.97	0.32	64,64,64,64	0
56	MG	B	9299	1/1	0.97	0.18	49,49,49,49	0
56	MG	B	9310	1/1	0.97	0.24	54,54,54,54	0

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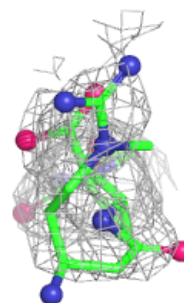
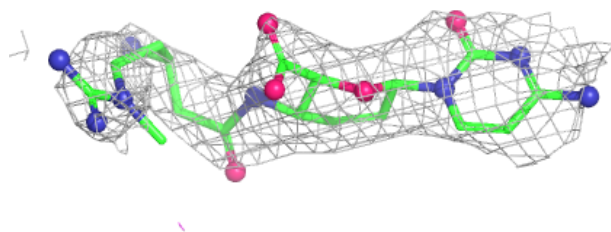
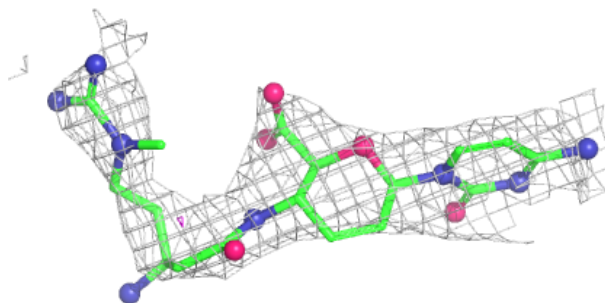
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	FB	9346	1/1	0.97	0.20	83,83,83,83	0
56	MG	B	9194	1/1	0.97	0.20	56,56,56,56	0
56	MG	B	9372	1/1	0.97	0.18	55,55,55,55	0
56	MG	FB	9245	1/1	0.97	0.14	63,63,63,63	0
56	MG	B	9506	1/1	0.97	0.08	61,61,61,61	0
56	MG	B	9507	1/1	0.97	0.11	64,64,64,64	0
58	ZN	ZB	701	1/1	0.97	0.04	106,106,106,106	0
56	MG	B	9267	1/1	0.97	0.23	56,56,56,56	0
56	MG	B	9555	1/1	0.97	0.10	79,79,79,79	0
56	MG	T	203	1/1	0.98	0.03	72,72,72,72	0
58	ZN	V	501	1/1	0.98	0.06	100,100,100,100	0
56	MG	B	9455	1/1	0.98	0.12	67,67,67,67	0
58	ZN	DA	101	1/1	0.98	0.11	133,133,133,133	0
56	MG	B	9289	1/1	0.98	0.09	62,62,62,62	0
56	MG	B	9104	1/1	0.98	0.04	78,78,78,78	0
56	MG	FB	9328	1/1	0.98	0.03	70,70,70,70	0
58	ZN	GA	101	1/1	0.99	0.02	94,94,94,94	0
58	ZN	GC	101	1/1	0.99	0.03	104,104,104,104	0
58	ZN	CA	601	1/1	0.99	0.03	82,82,82,82	0
58	ZN	KC	101	1/1	0.99	0.03	121,121,121,121	0

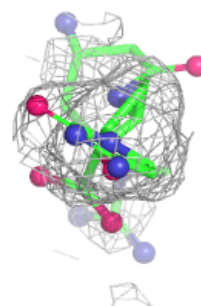
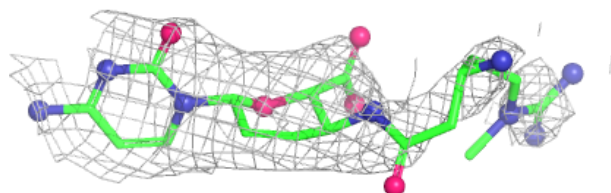
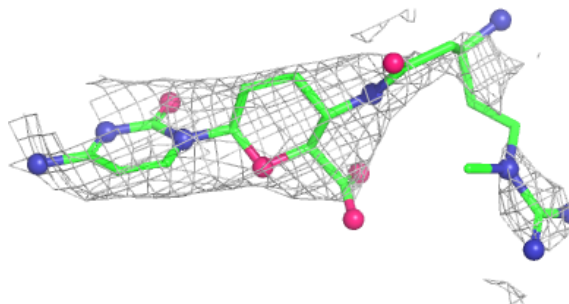
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BLS B 9001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around BLS FB 9001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.