



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 10, 2025 – 10:27 PM EST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

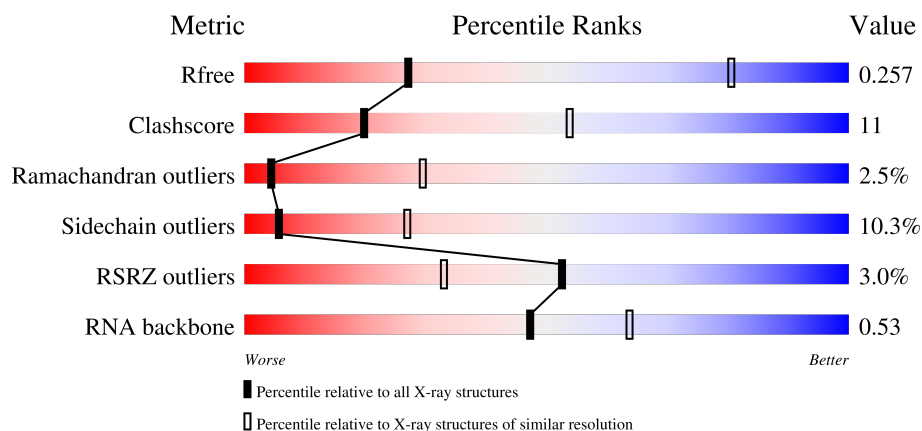
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 Å.

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





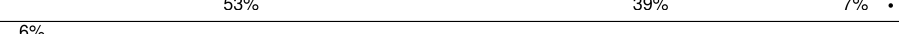
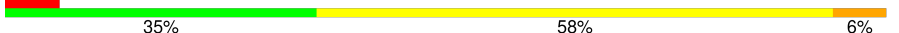
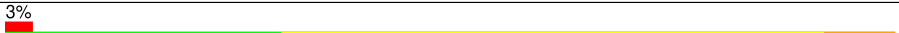
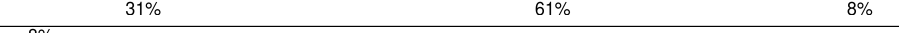

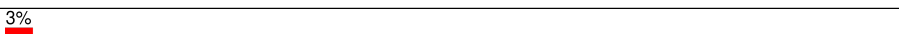


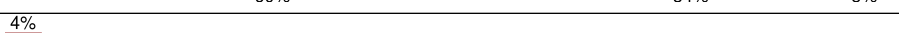


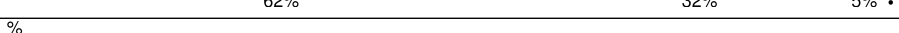


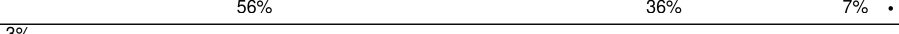








Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1261 (3.62-3.50)
Clashscore	180529	1351 (3.62-3.50)
Ramachandran outliers	177936	1336 (3.62-3.50)
Sidechain outliers	177891	1337 (3.62-3.50)
RSRZ outliers	164620	1260 (3.62-3.50)
RNA backbone	3690	1097 (4.10-3.00)

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	 2% 49% 41% 9% .
1	DB	1507	 2% 49% 41% 9% .
2	B	2880	 % 43% 41% 14% .
2	EB	2880	 2% 47% 39% 12% .











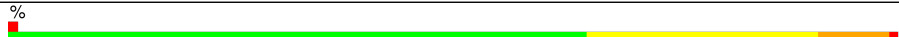


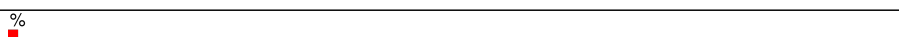
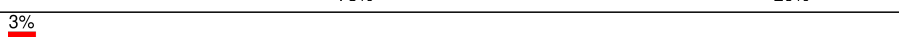
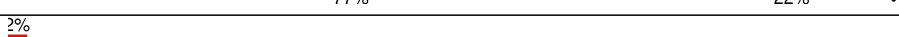



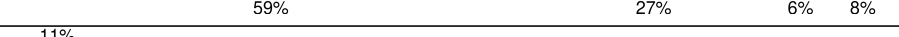





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Mol	Chain	Length	Quality of chain
3	C	120	
3	FB	120	
4	D	77	
4	GB	77	
4	IA	77	
4	LC	77	
5	E	275	
5	HB	275	
6	F	206	
6	IB	206	
7	G	205	
7	JB	205	
8	H	182	
8	KB	182	
9	I	180	
9	LB	180	
10	J	148	
10	MB	148	
11	K	140	
11	NB	140	
12	L	122	
12	OB	122	
13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


















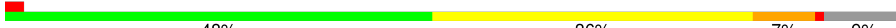







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Mol	Chain	Length	Quality of chain
14	QB	141	
15	O	118	
15	RB	118	
16	P	112	
16	SB	112	
17	Q	146	
17	TB	146	
18	R	118	
18	UB	118	
19	S	101	
19	VB	101	
20	T	113	
20	WB	113	
21	U	96	
21	XB	96	
22	V	110	
22	YB	110	
23	W	206	
23	ZB	206	
24	AC	85	
24	X	85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

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

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

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Mol	Chain	Length	Quality of chain
52	AB	93	<div><div></div><div>52%</div><div>33%</div><div>•</div><div>11%</div></div>
52	DD	93	<div><div>2%</div><div></div><div>48%</div><div>38%</div><div>•</div><div>11%</div></div>
53	BB	106	<div><div>10%</div><div></div><div>56%</div><div>33%</div><div>5%</div><div>7%</div></div>
53	ED	106	<div><div>7%</div><div></div><div>52%</div><div>38%</div><div>•</div><div>7%</div></div>
54	CB	27	<div><div>15%</div><div></div><div>63%</div><div>26%</div><div></div><div>11%</div></div>
54	FD	27	<div><div>26%</div><div></div><div>48%</div><div>37%</div><div>•</div><div>11%</div></div>
55	GD	365	<div><div>2%</div><div></div><div>42%</div><div>23%</div><div>•</div><div>30%</div></div>
55	HD	365	<div><div>2%</div><div></div><div>43%</div><div>22%</div><div>5%</div><div>30%</div></div>

2 Entry composition [i](#)

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 34 is a RNA chain called mRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 22 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

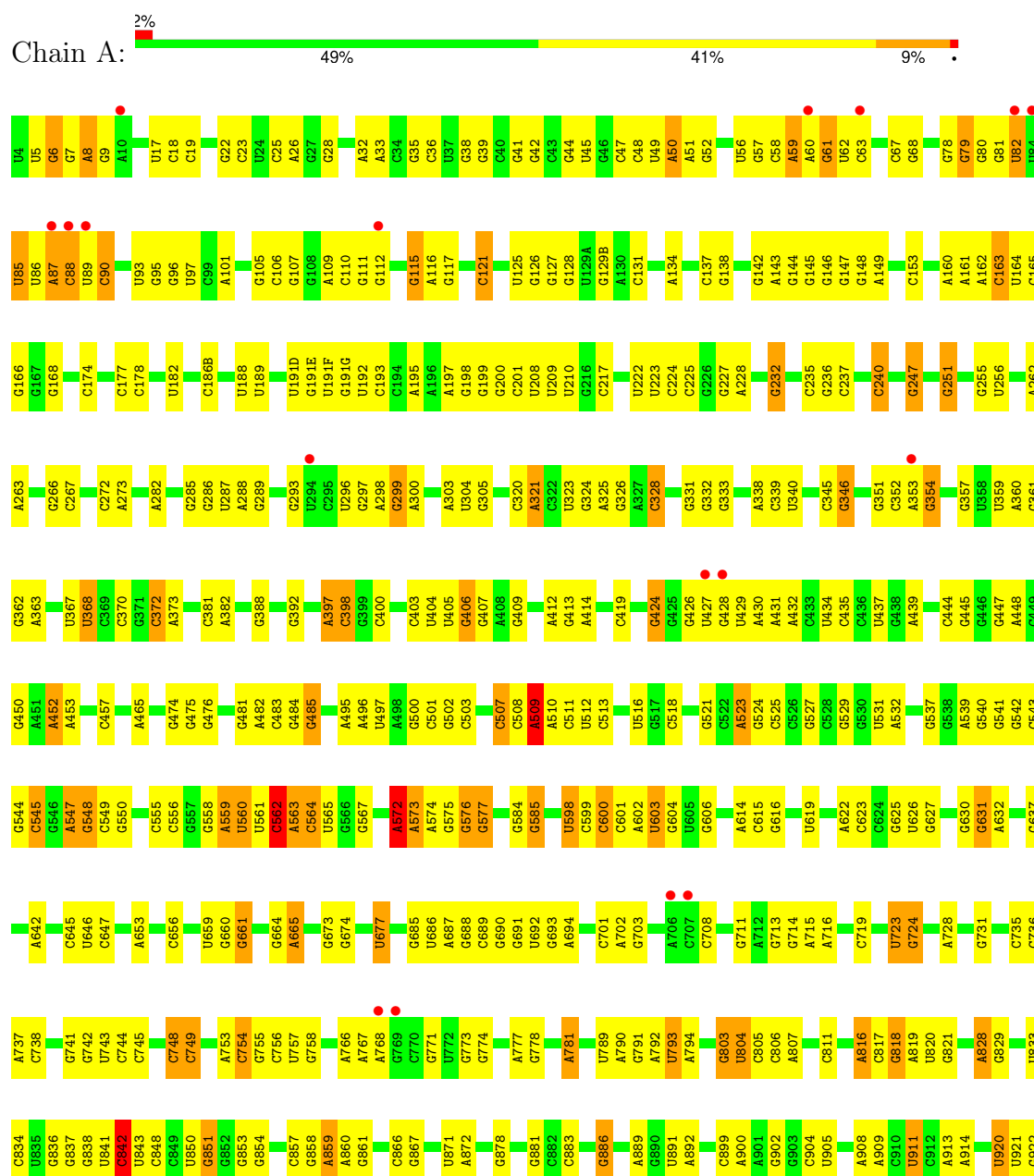
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

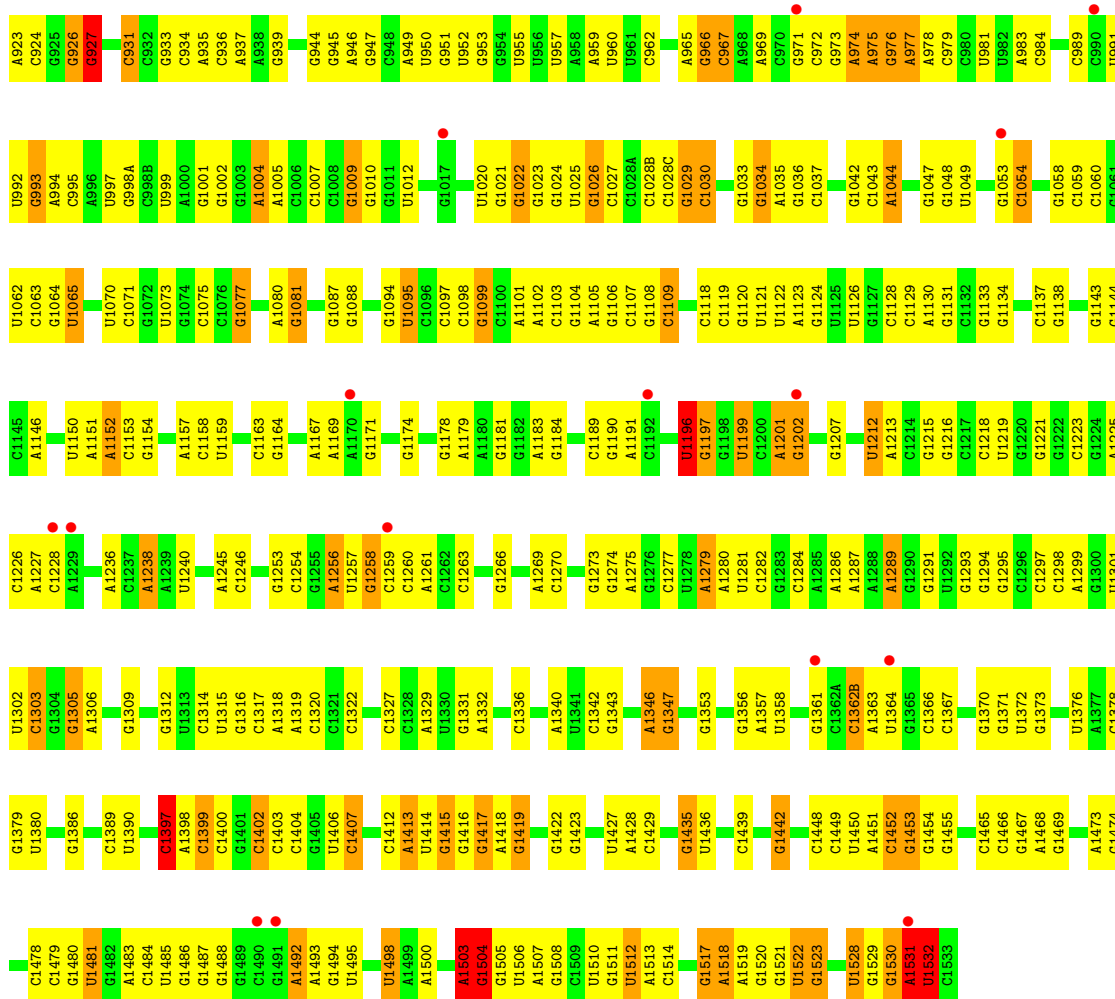
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	V	1	Total	Zn	0	0
			1	1		
57	BA	1	Total	Zn	0	0
			1	1		
57	CA	1	Total	Zn	0	0
			1	1		
57	DA	1	Total	Zn	0	0
			1	1		
57	GA	1	Total	Zn	0	0
			1	1		
57	YB	1	Total	Zn	0	0
			1	1		
57	EC	1	Total	Zn	0	0
			1	1		
57	FC	1	Total	Zn	0	0
			1	1		
57	GC	1	Total	Zn	0	0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

3 Residue-property plots

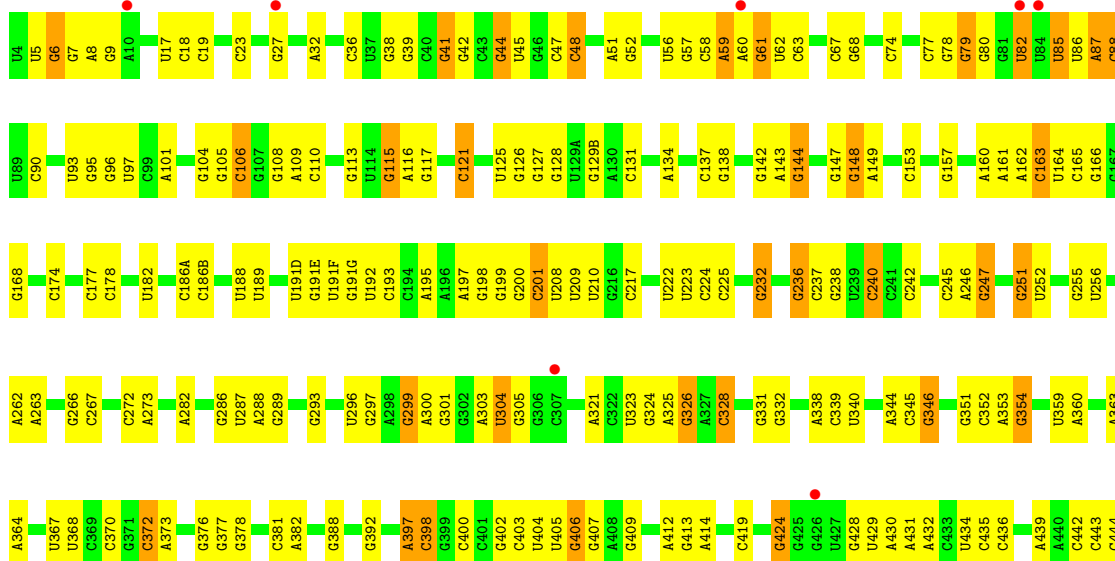
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

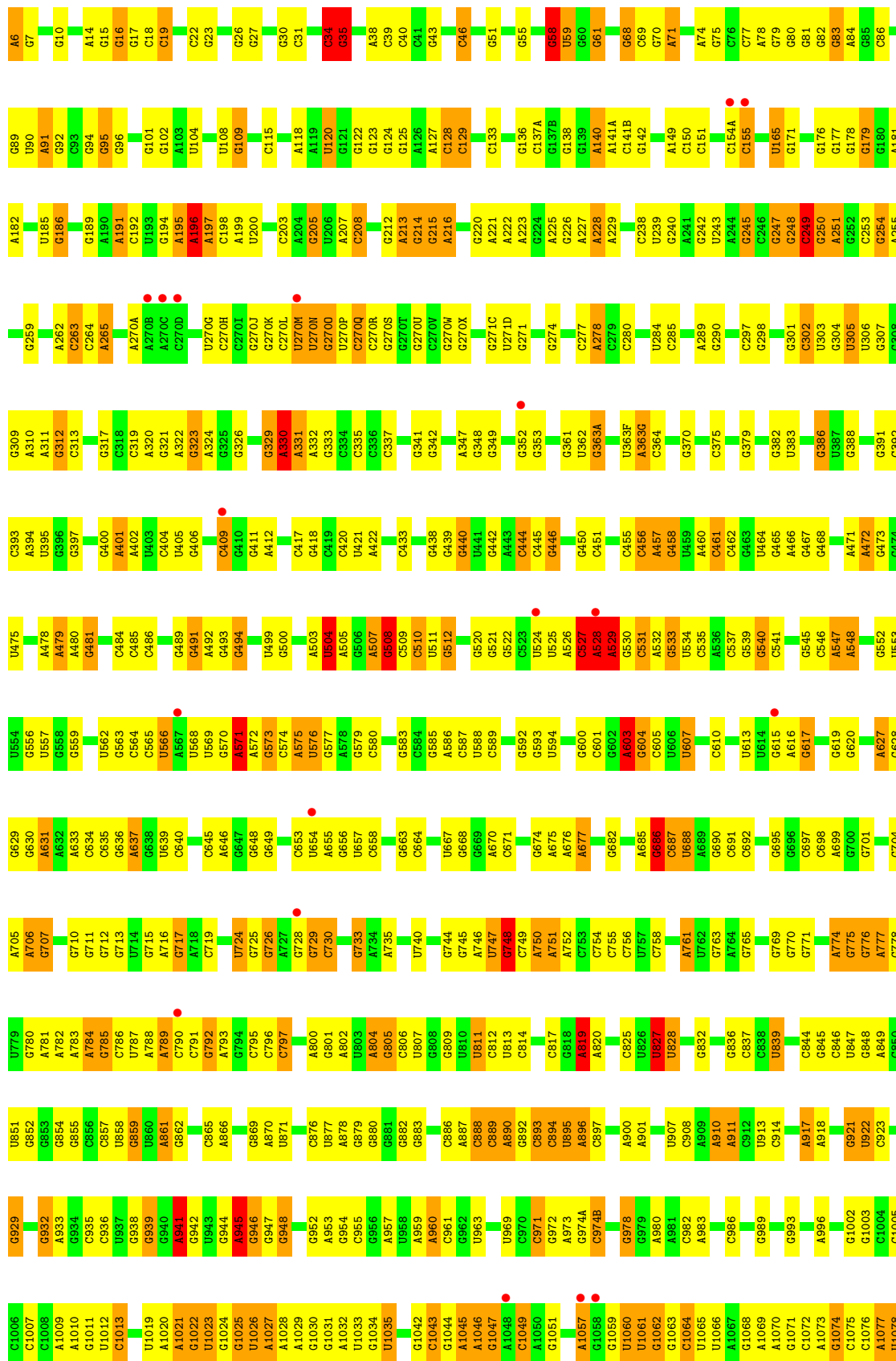




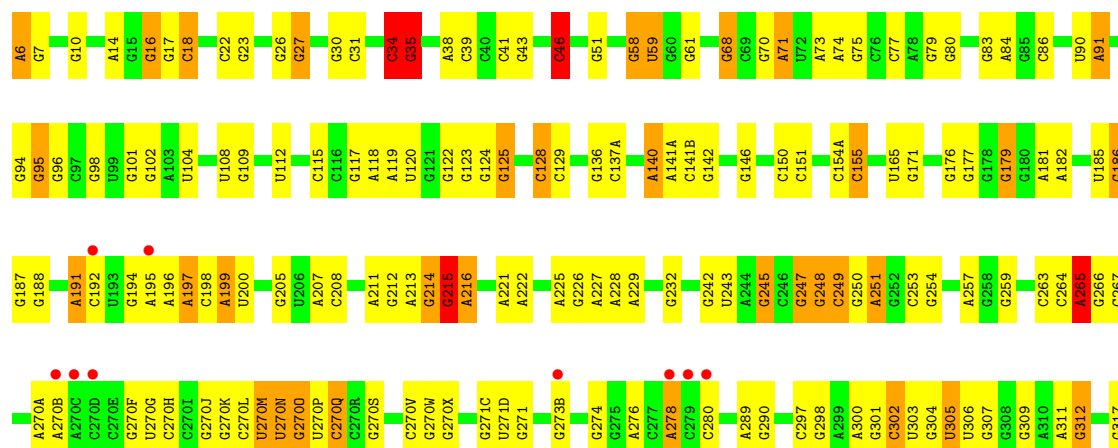
• Molecule 1: 16S ribosomal RNA





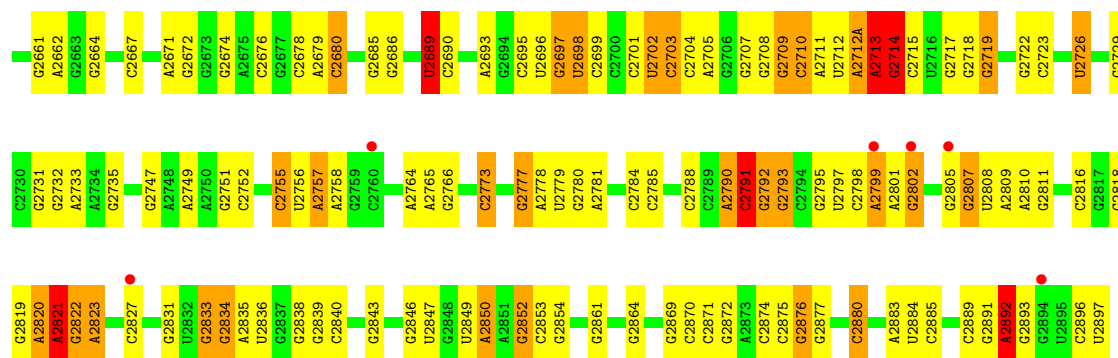


A2117	G2038	C1985	G1897	C1800	G1717	A1837	C1565	G1483	U1394	A1322	G1244	C1161	G1079
U2118	C2039	A1966	U1898	G1801	U1727	C1640	A1566	G1484	A1396	U1323	G1245	C1161	G1080
A2119	G2040	C1967	G1899	A1802	G1728	U1641	A1567	G1488	U1396	G1325	A1246	G1164	U1081
G2123	U2041	G1968	A1900	U1805	U1729	G1642	G1568	U1489	U1397	G1326	U1251	U1165	U1082
G2124	A2042	A1969	A1901	U1806	U1730	G1643	A1569	C1402	C1402	C1327	G1252	G1173	U1083
G2125	C2043	A1970	G1902	A1810	G1731	G1644	G1573	C1403	U1405	G1328	A1253	A1174	A1085
A2126	G2049	A1972	G1903	G1811	A1732	C1645	U1578	A1494	U1406	A1331	A1254	U1175	A1086
G2127	G1973	G1973	A1812	G1813	C1742	C1648	U1578	U1497	C1407	G1332	A1255	G1176	G1087
C2128	G2052	C1974	G1907	G1813	C1743	C1648	U1578	U1497	C1408	G1333	G1256	A1177	A1088
G2129	G2053	G1975	C1908	G1814	G1743	C1648	U1578	U1497	C1409	G1334	G1259	C1178	G1089
U2130	A2054	U1976	U1911	G1815	G1750	G1651	G1581	C1501	G1410	G1335	G1260	C1179	C1092
G2131	C2055	G1989	A1912	G1816	C1751	G1652	G1582	A1508	G1416	A1336	C1261	C1180	G1093
U2132	G2056	G1992	A1913	G1817	C1752	G1653	A1583	A1509	G1417	G1339	G1264	C1185	U1094
G2133	A2057	U1993	A1914	G1818	G1753	G1654	C1586	A1510	C1418	U1340	A1265	A1095	A1095
A2134	C2058	G1980	A1915	G1819	C1754	C1657	A1587	A1511	G1419	U1341	A1266	G1187	A1096
A2135	A2059	A1981	U1915	G1820	A1755	C1658	C1588	G1512	U1420	G1342	U1267	U1188	U1097
G2136	C2060	C1983	A1916	G1821	G1756	U1659	C1589	C1513	U1421	G1343	A1268	A1189	A1098
C2137	G2061	G1984	U1917	G1822	U1757	G1660	U1590	U1516	G1422	G1344	A1269	G1190	G1099
G2138	A2062	U1989	A1918	G1823	U1758	G1661	G1591	G1517	G1425	G1345	G1271	G1193	U1101
C2139	C2063	G1992	A1919	G1824	A1759	G1662	G1592	C1518	G1426	U1272	A1273	G1104	U1105
G2140	C2064	G1992	C1920	G1825	A1760	A1664	G1593	G1519	G1427	U1273	U1274	G1106	U1106
G2141	C2065	U1993	G1921	G1826	G1761	G1667	G1594	U1520	A1427	A1274	A1275	G1107	G1107
C2142	C2066	G1997	U1922	G1827	A1762	G1668	C1588	G1521	C1428	A1349	G1276	C1203	G1110
G2143	G2067	G1997	G1923	G1828	G1763	U1669	C1599	U1522	G1429	U1352	A1277	G1202	G1111
U2144	U2068	G1998	C1924	A1829	G1764	G1670	C1599	G1523	U1434	A1353	G1278	A1204	G1112
C2145	G2069	G1998	U1925	A1830	G1765	C1671	U1602	G1524	A1435	A1354	A1279	U1205	G1113
G2146	G2070	A2001	U1926	C1838	U1766	C1672	A1603	G1525	G1436	G1355	U1282	G1206	G1113
G2147	A2071	G2002	A1927	G1839	U1767	U1673	C1604	G1526	U1437	G1356	U1282	G1209	G1125
G2148	G2072	G2003	A1928	G1840	U1768	U1674	C1605	G1527	U1438	U1357	A1286	A1211	A1126
G2149	C2073	G2004	G1930	G1842	U1771	C1675	C1605	G1530	G1441	G1358	A1287	G1212	A1127
U2150	G2080	A2005	U1931	G1845	G1772	A1676	A1608	C1531	A1444B	A1360	U1288	G1215	A1128
G2151	C2081	C2006	A1932	G1846	U1773	G1681	A1610	C1532	A1449B	G1364	C1291	G1216	A1129
G2152	G2083	C2007	G1933	A1847	C1774	G1681	A1611	G1533	G1449	A1365	U1292	G1217	U1130
G2153	C2084	C2008	C1934	G1848	U1775	U1688	C1612	G1534	C1450	A1366	C1293	C1218	G1131
C2154	G2085	G2009	G1935	G1857	U1776	A1689	G1613	U1535	U1454	G1367	C1297	G1219	C1135
G2155	U2086	G2010	A1936	G1858	U1777	A1689	G1614	G1536	G1455	A1449	C1298	A1220	G1136
G2156	G2087	U2011	A1937	G1859	U1778	U1692	A1614	G1537	G1455	A1367	C1299	G1221	G1137
G2157	U2091	A2013	U1939	G1863	U1779	U1693	C1617	G1538	U1454	G1371	U1300	C1221A	G1138
G2158	U2092	A2014	U1940	U1864	C1781	G1694	A1618	G1539	G1455	U1372	A1301	C1224	G1139
G2159	G2093	C1941	C1942	U1865	C1782	G1695	G1622	G1540	G1461	G1373	G1303	G1225	A1142B
C2161	G2094	A2020	U1943	G1869	A1783	G1696	G1623	G1541	G1465	A1378	A1304	A1226	A1143
G2162	C2095	U2022	A1946	G1871	A1784	G1697	G1624	G1542	G1466	A1379	A1307	G1227	G1144
C2163	G2096	G2023	C1947	A1872	A1785	A1698	G1625	A1543	G1467	G1380	G1310	G1231	G1149
G2164	C2097	C2023	U1947	G1878	A1786	G1699	C1626	A1553	G1468	G1381	G1310	U1234	C1152
G2165	G2100	C2026	U1951	C1879	A1787	A1700	G1627	A1554	A1469	G1382	G1314	G1235	G1153
G2166	C2107	G2027	A1952	G1882	C1788	A1701	G1628	C1544	G1470	G1383	C1315	G1236	G1154
U2167	C2108	U2028	A1953	G1883	A1789	G1702	G1629	C1550	A1471	G1384	C1319	U1240	A1155
A2168	C2109	G2029	A1954	G1889	C1790	G1703	G1630	C1551	G1477	G1385	C1320	U1243	C1158
A2169	U2109	A2030	G1954	A1890	C1791	G1704	G1630B	G1552	G1478	G1386	A1392	G1243	
A2170	G2110	A2031	U1955	A1891	G1792	G1705	A1554	A1554	G1479	G1387	A1392	G1243	
A2171	G2111	A2032	U1956	G1891	G1793	U1706	A1631	C1557	G1479	G1388	A1392	G1243	
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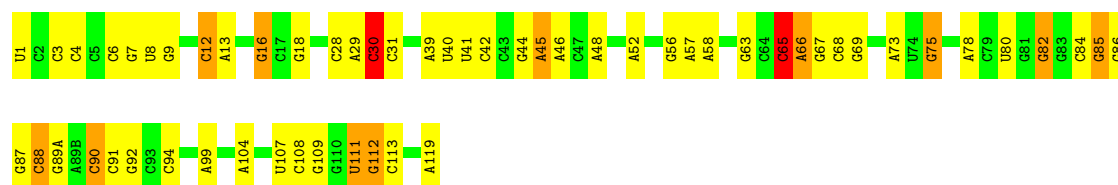


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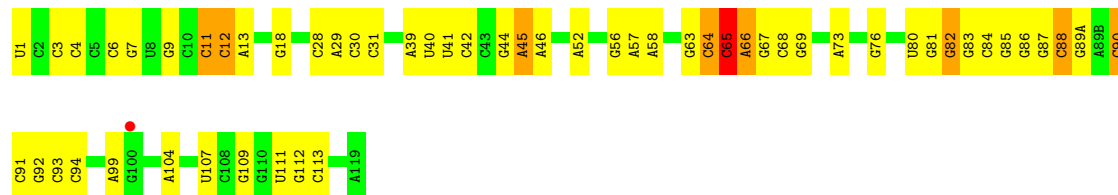
- Molecule 3: 5S ribosomal RNA

Chain C: 52% 37% 9% .



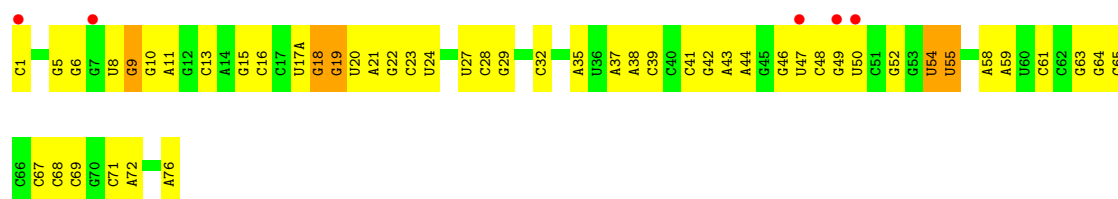
- Molecule 3: 5S ribosomal RNA

Chain FB: 53% 39% 7% .



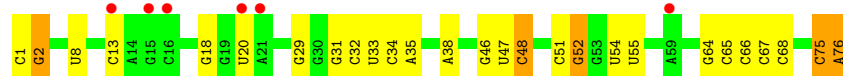
- Molecule 4: 16S ribosomal RNA

Chain D: 6% 35% 58% 6%

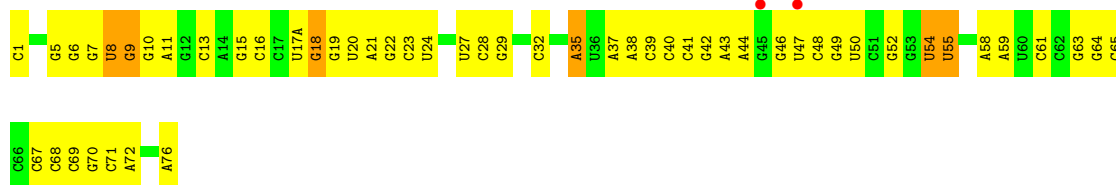


- Molecule 4: 16S ribosomal RNA

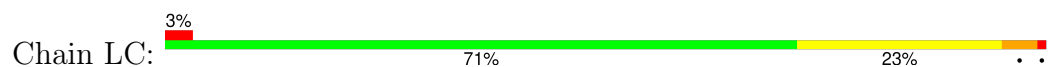
Chain IA: 8% 65% 29% 6%



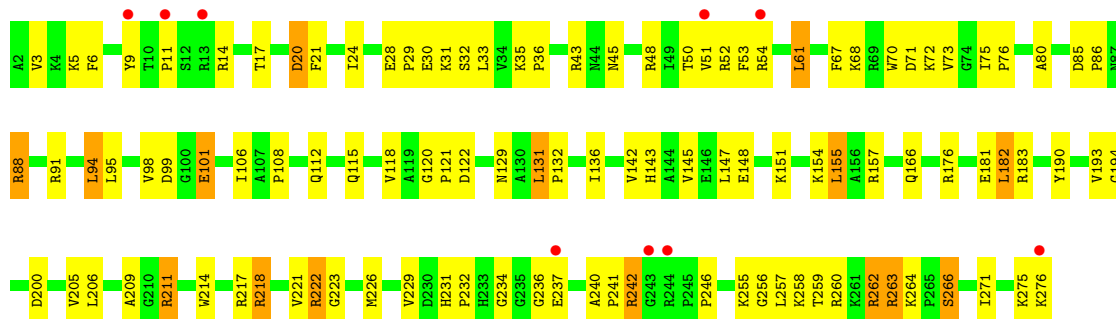
- Molecule 4: 16S ribosomal RNA



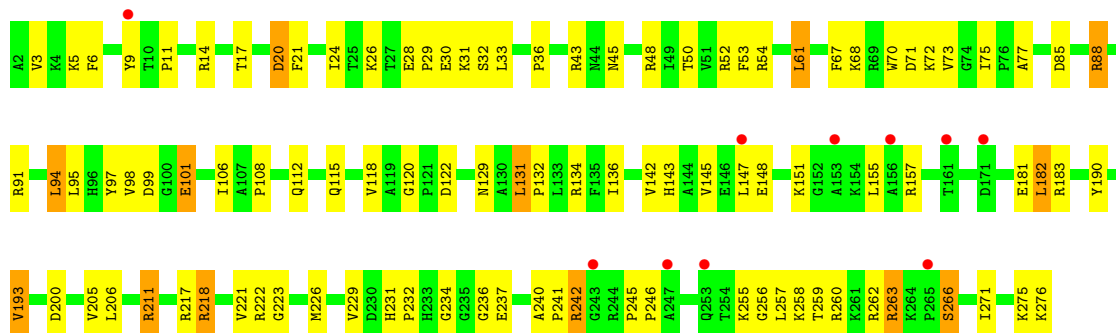
• Molecule 4: 16S ribosomal RNA



• Molecule 5: 50S ribosomal protein L2



• Molecule 5: 50S ribosomal protein L2

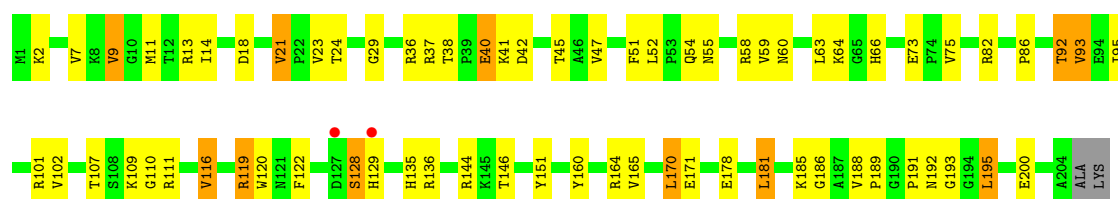


• Molecule 6: 50S ribosomal protein L3

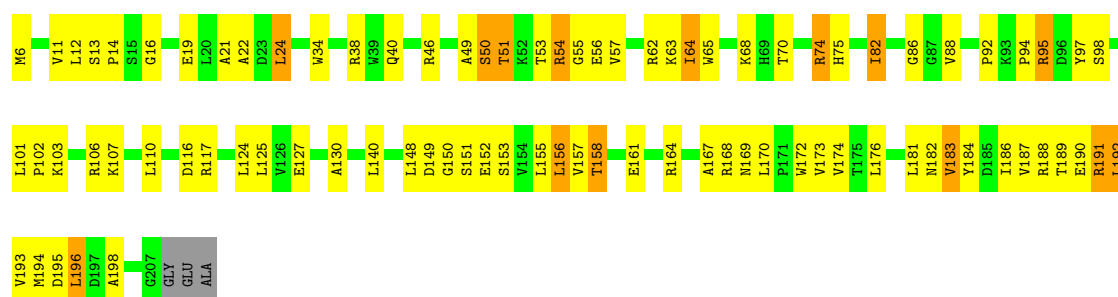




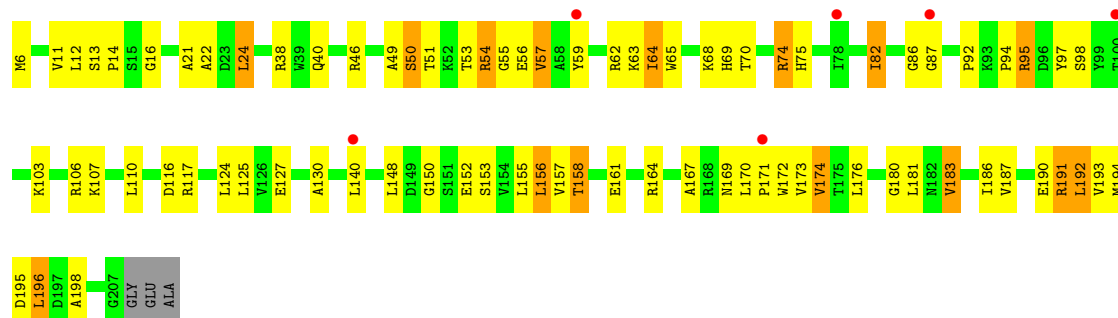
- Molecule 6: 50S ribosomal protein L3



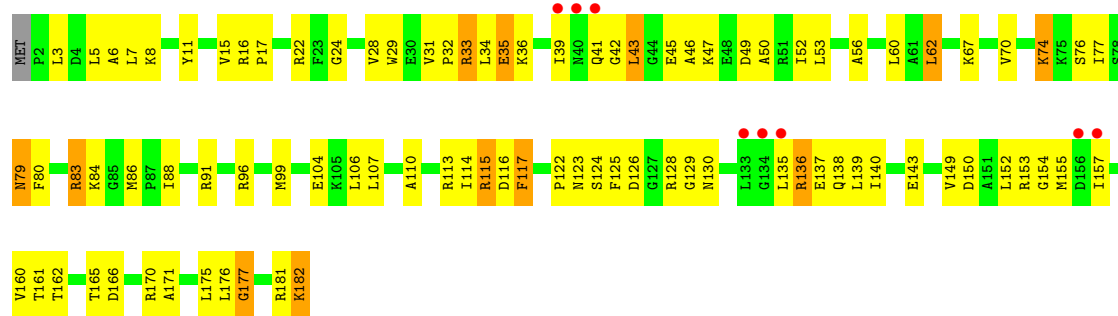
- Molecule 7: 50S ribosomal protein L4



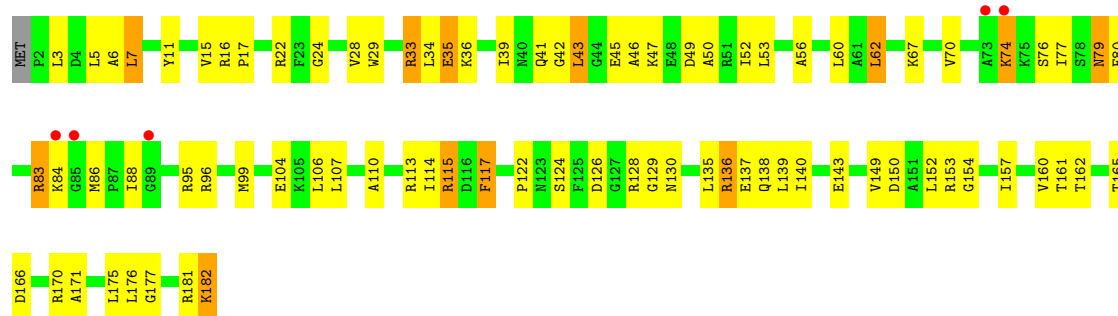
- Molecule 7: 50S ribosomal protein L4



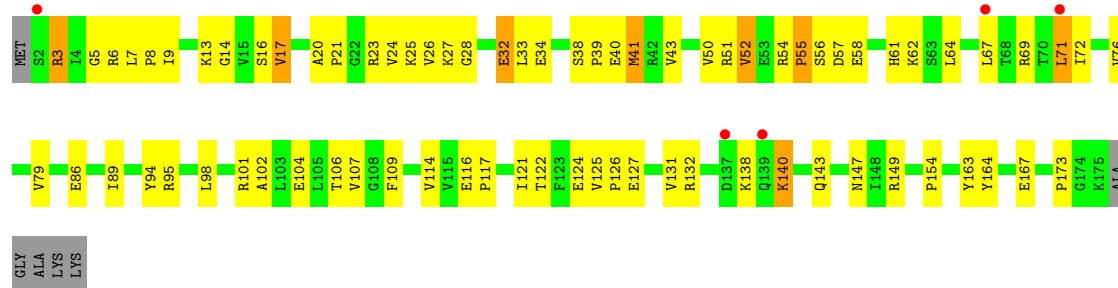
- Molecule 8: 50S ribosomal protein L5



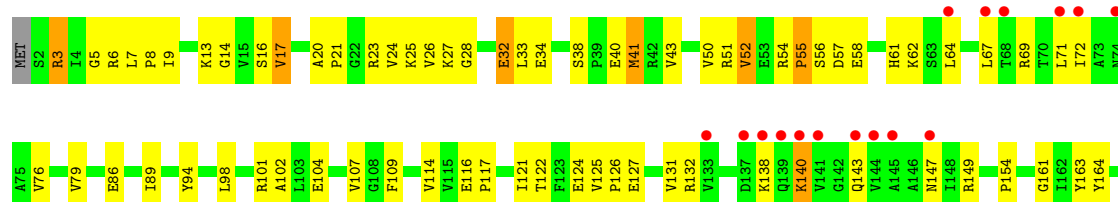
• Molecule 8: 50S ribosomal protein L5

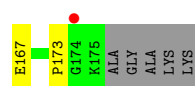


• Molecule 9: 50S ribosomal protein L6

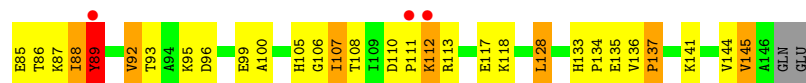
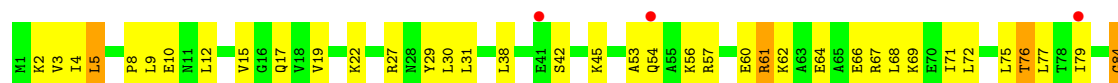


• Molecule 9: 50S ribosomal protein L6

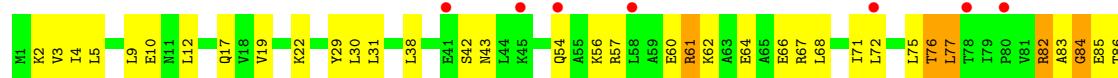




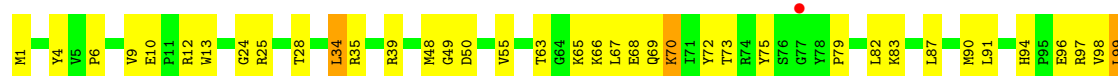
- Molecule 10: 50S ribosomal protein L9



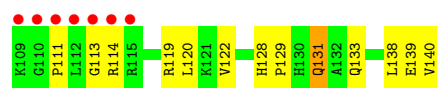
- Molecule 10: 50S ribosomal protein L9



- Molecule 11: 50S ribosomal protein L13

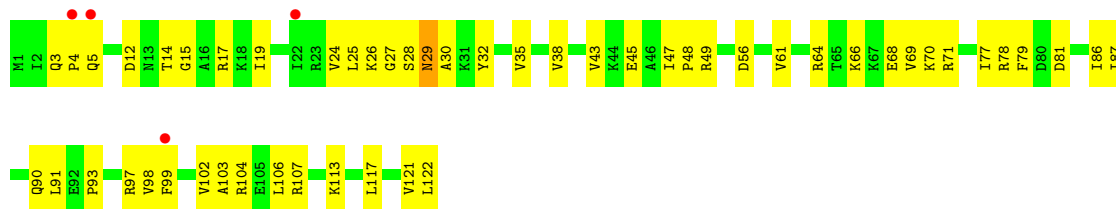


- Molecule 11: 50S ribosomal protein L13

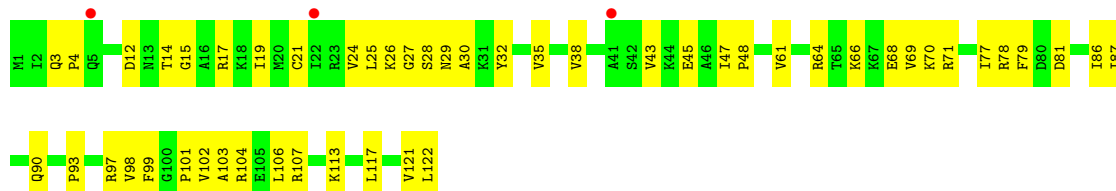


- Molecule 12: 50S ribosomal protein L14

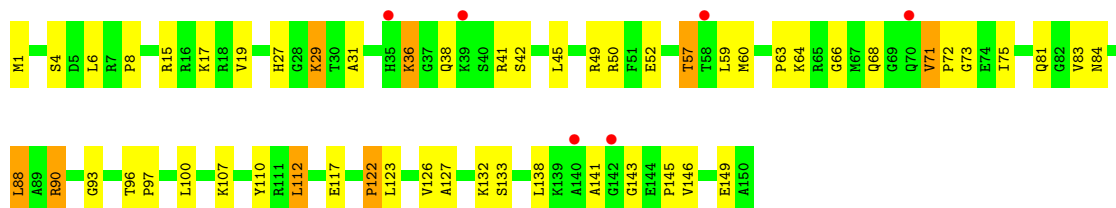




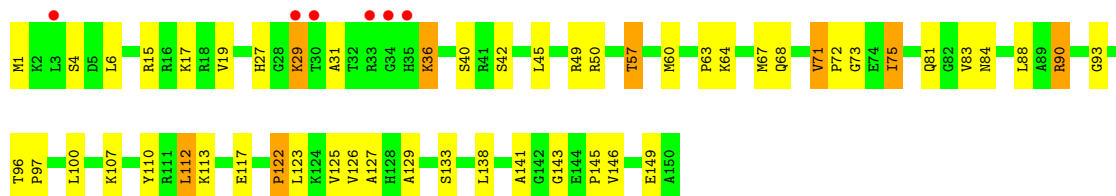
• Molecule 12: 50S ribosomal protein L14



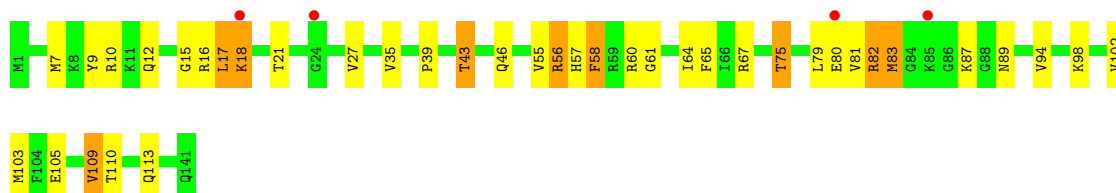
• Molecule 13: 50S ribosomal protein L15



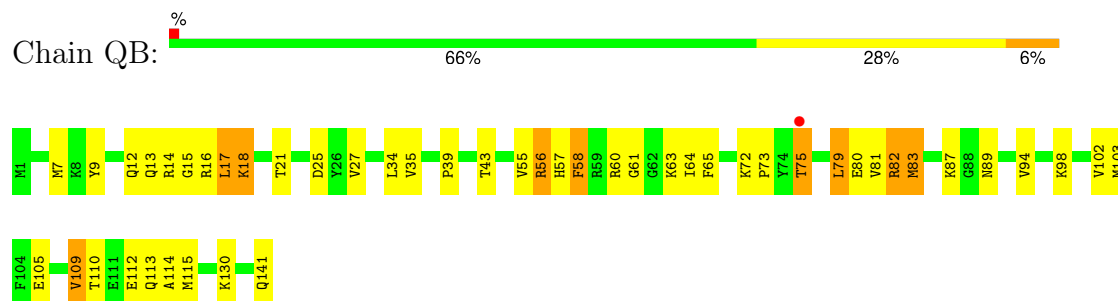
• Molecule 13: 50S ribosomal protein L15



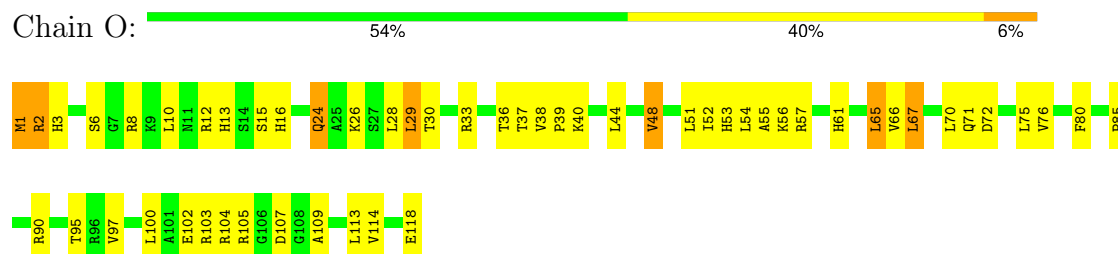
• Molecule 14: 50S ribosomal protein L16



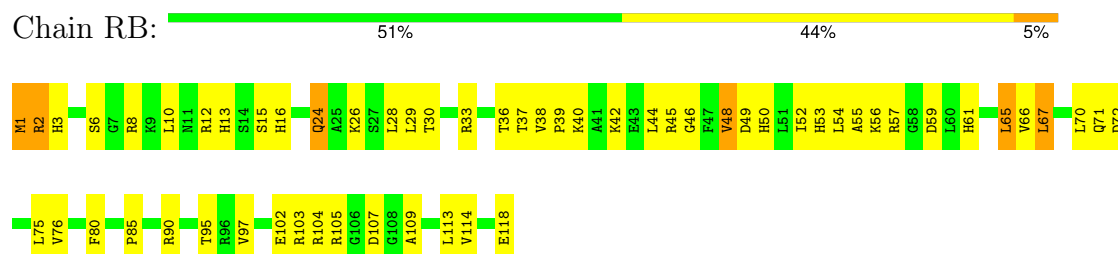
- Molecule 14: 50S ribosomal protein L16



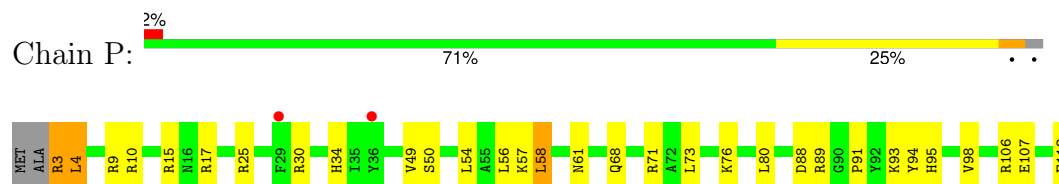
- Molecule 15: 50S ribosomal protein L17



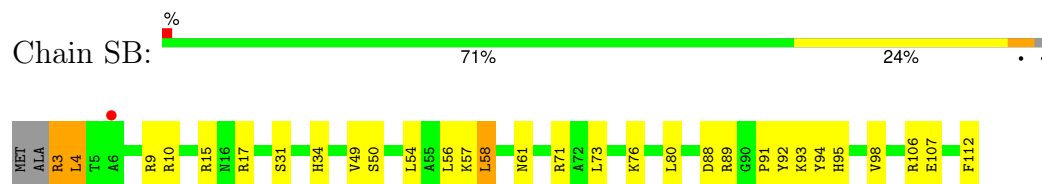
- Molecule 15: 50S ribosomal protein L17



- Molecule 16: 50S ribosomal protein L18

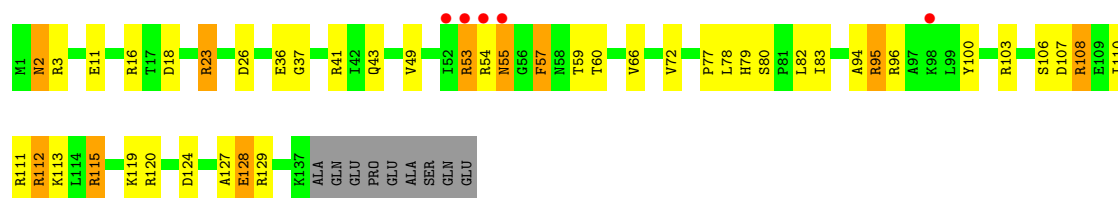


- Molecule 16: 50S ribosomal protein L18

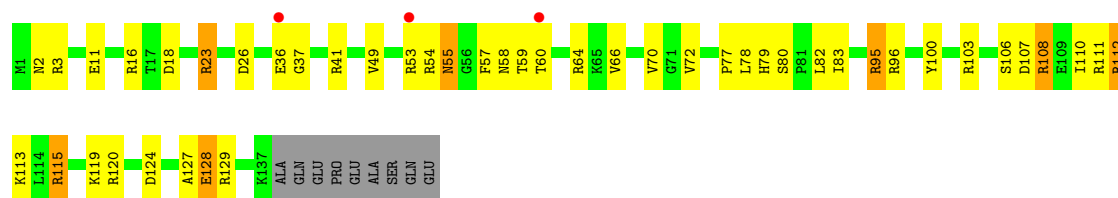


- Molecule 17: 50S ribosomal protein L19

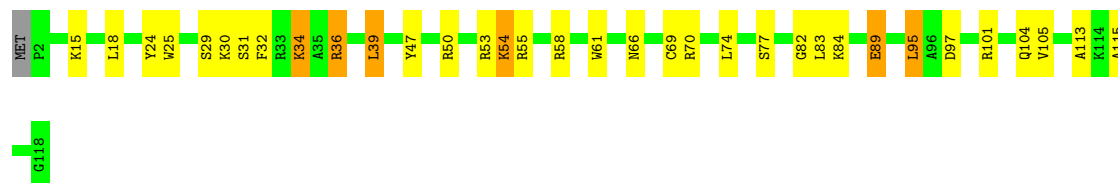




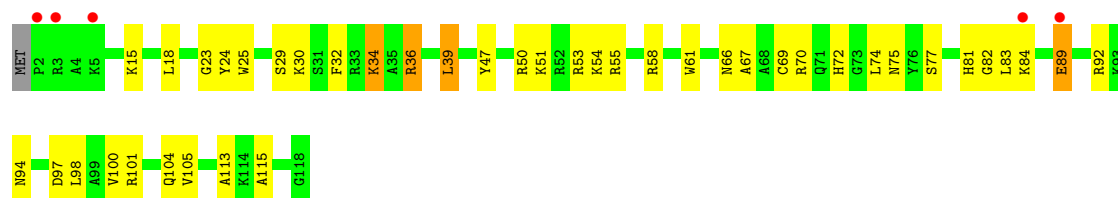
• Molecule 17: 50S ribosomal protein L19



• Molecule 18: 50S ribosomal protein L20



• Molecule 18: 50S ribosomal protein L20

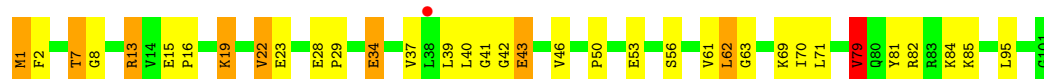


• Molecule 19: 50S ribosomal protein L21

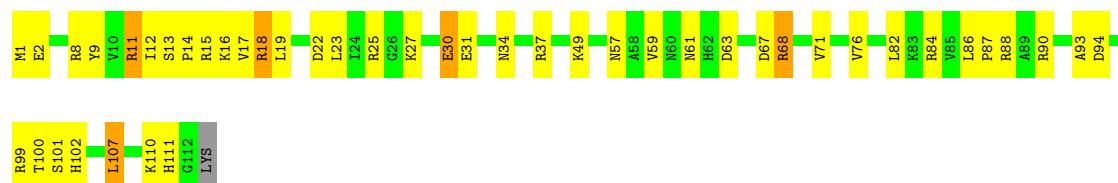


• Molecule 19: 50S ribosomal protein L21





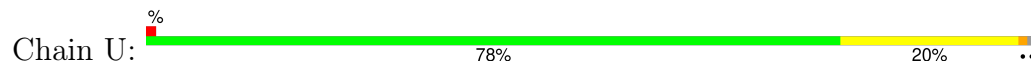
- Molecule 20: 50S ribosomal protein L22



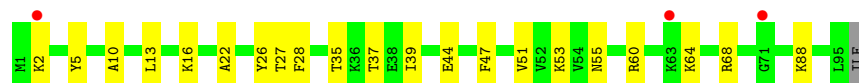
- Molecule 20: 50S ribosomal protein L22



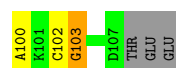
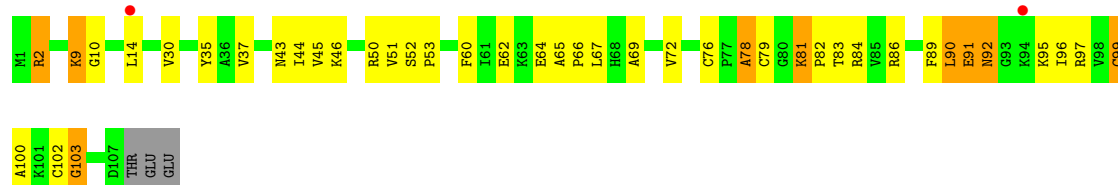
- Molecule 21: 50S ribosomal protein L23



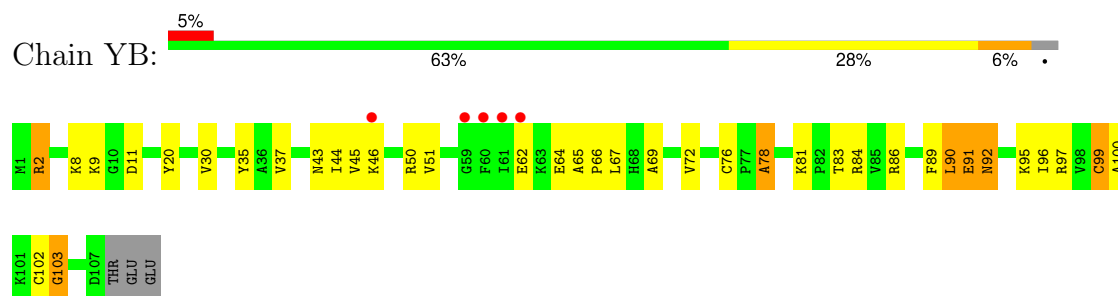
- Molecule 21: 50S ribosomal protein L23



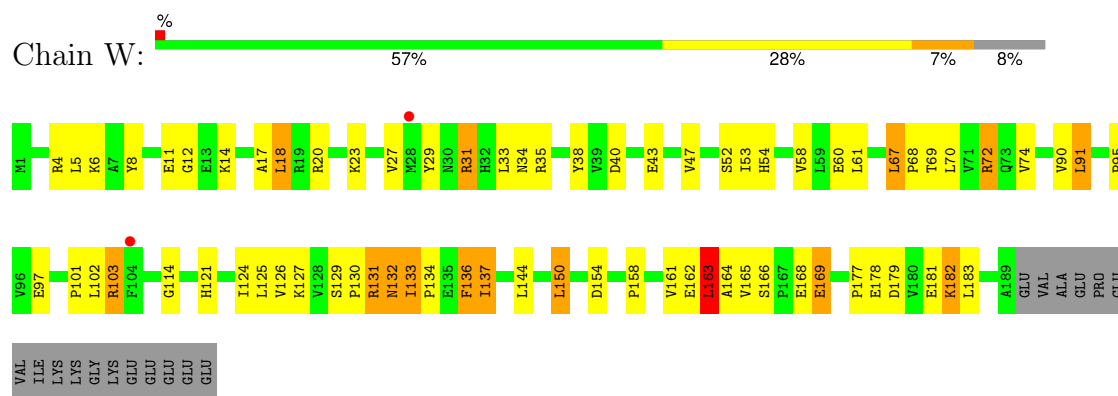
- Molecule 22: 50S ribosomal protein L24



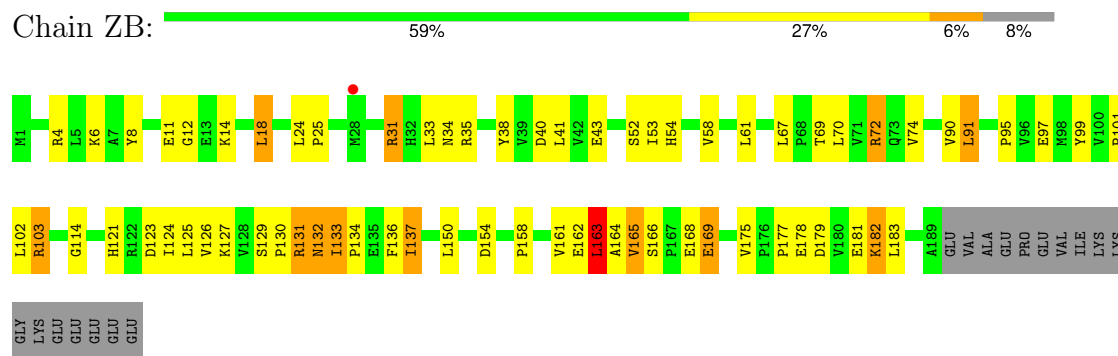
- Molecule 22: 50S ribosomal protein L24



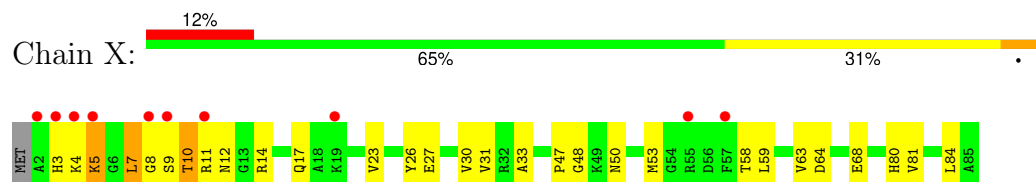
- Molecule 23: 50S ribosomal protein L25



- Molecule 23: 50S ribosomal protein L25



- Molecule 24: 50S ribosomal protein L27

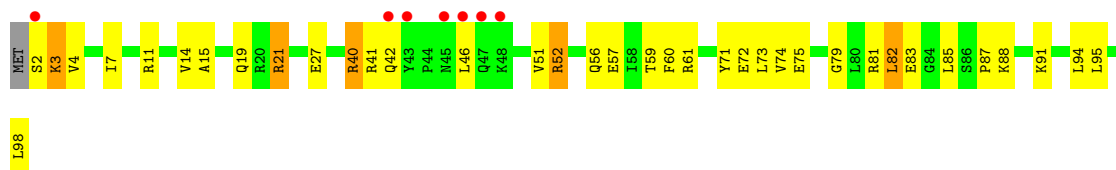


- Molecule 24: 50S ribosomal protein L27

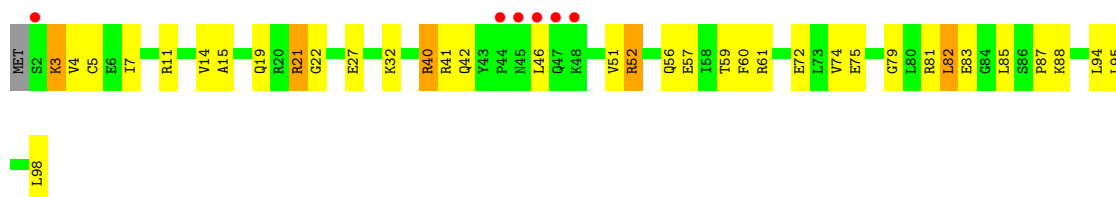




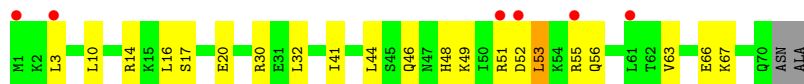
- Molecule 25: 50S ribosomal protein L28



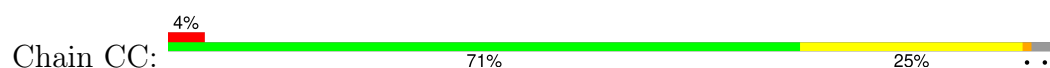
- Molecule 25: 50S ribosomal protein L28



- 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



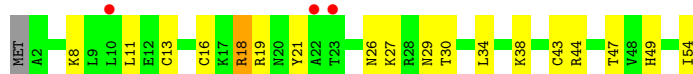
- Molecule 29: 50S ribosomal protein L32



- Molecule 29: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L33



- Molecule 30: 50S ribosomal protein L33

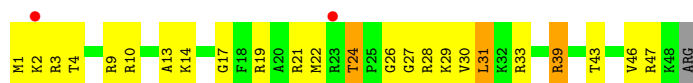


- Molecule 31: 50S ribosomal protein L34





- Molecule 31: 50S ribosomal protein L34



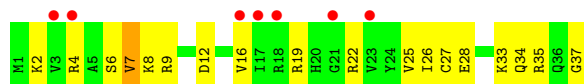
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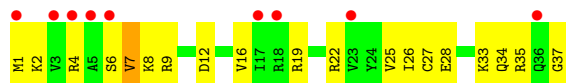
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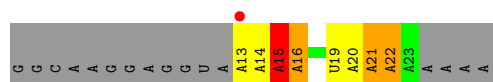
- Molecule 33: 50S ribosomal protein L36



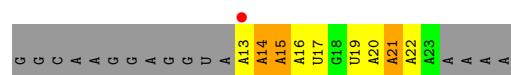
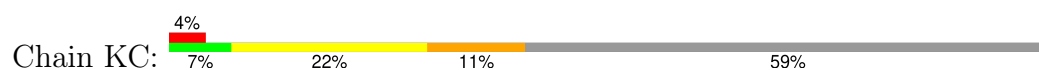
- Molecule 33: 50S ribosomal protein L36



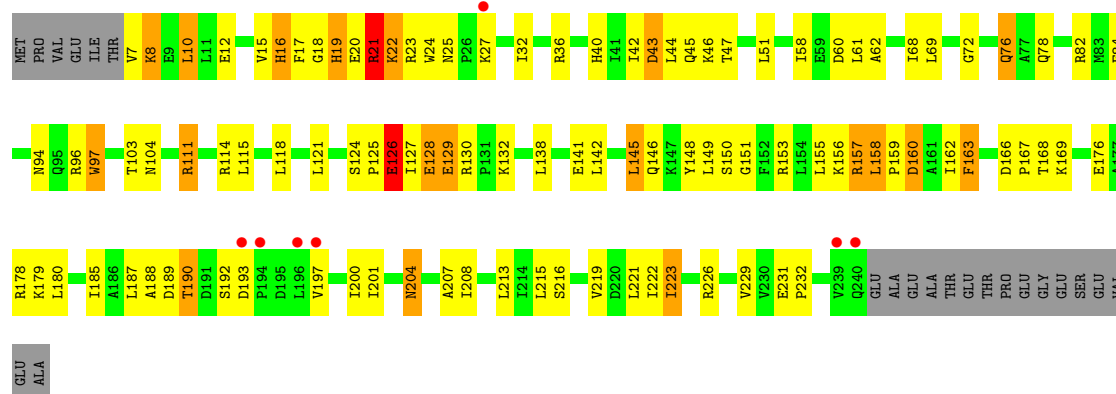
- Molecule 34: mRNA



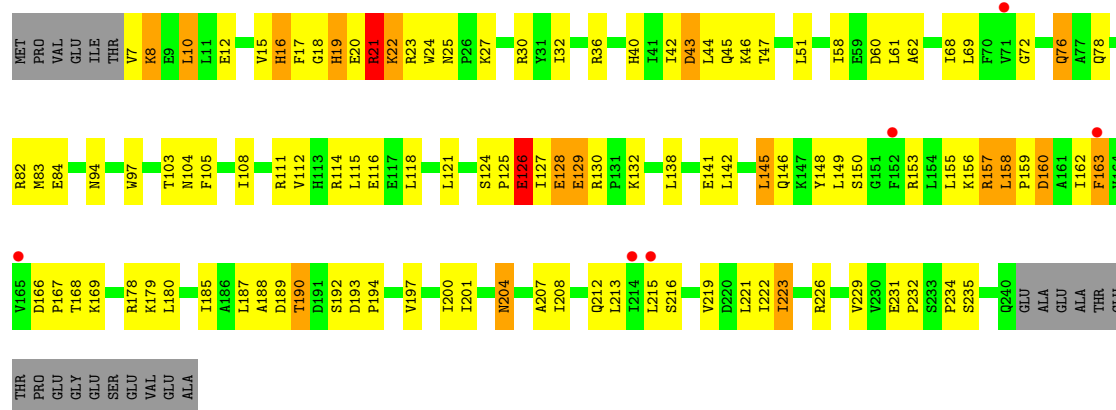
- Molecule 34: mRNA



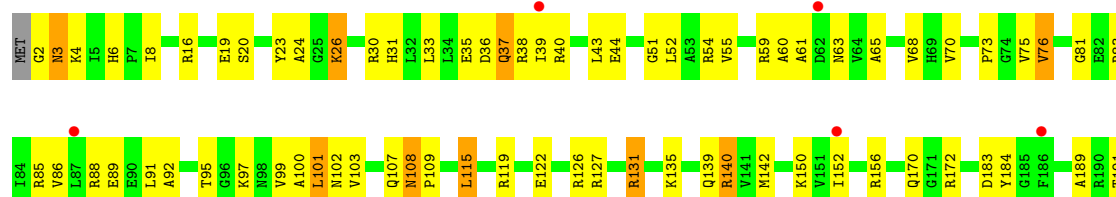
• Molecule 35: 30S ribosomal protein S2

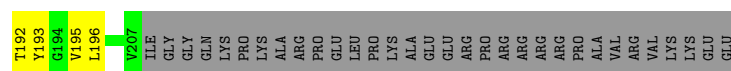


• Molecule 35: 30S ribosomal protein S2

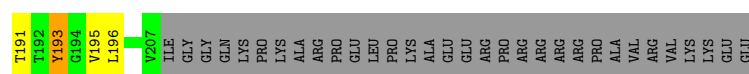


• Molecule 36: 30S ribosomal protein S3

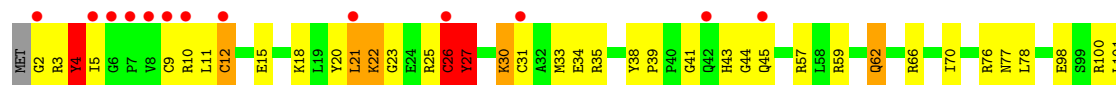




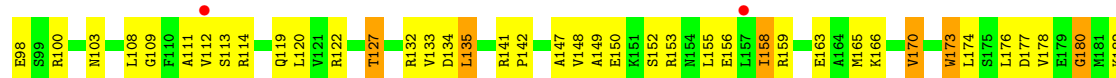
- Molecule 36: 30S ribosomal protein S3



- Molecule 37: 30S ribosomal protein S4

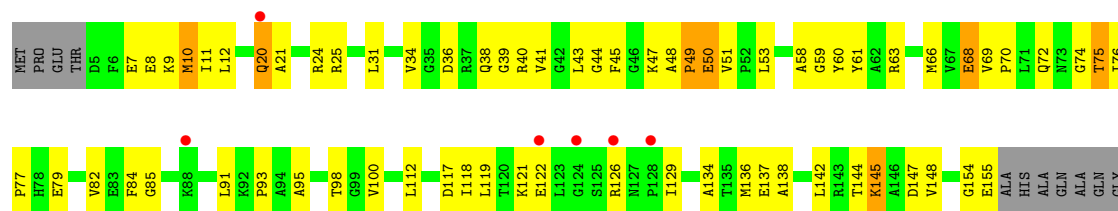


- Molecule 37: 30S ribosomal protein S4

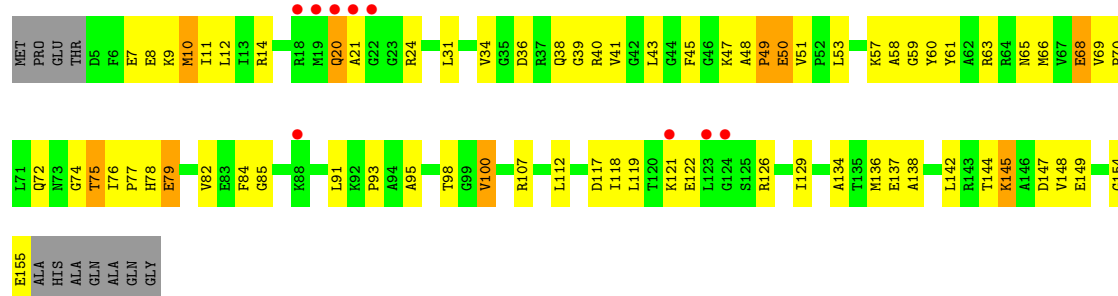


- Molecule 38: 30S ribosomal protein S5

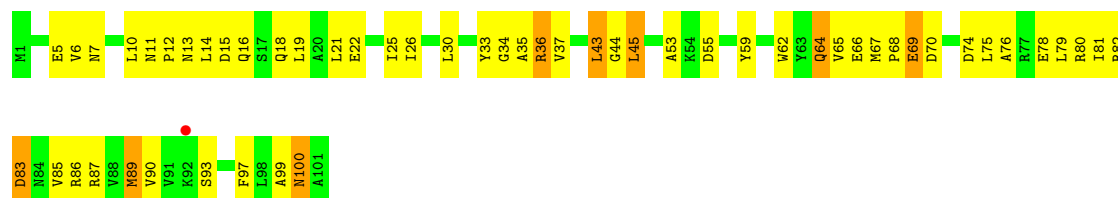




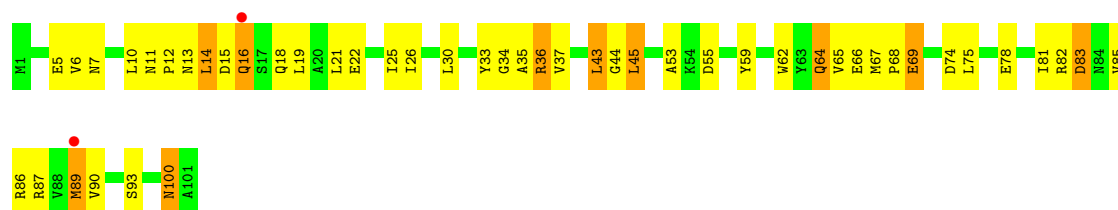
• Molecule 38: 30S ribosomal protein S5



• Molecule 39: 30S ribosomal protein S6



• Molecule 39: 30S ribosomal protein S6

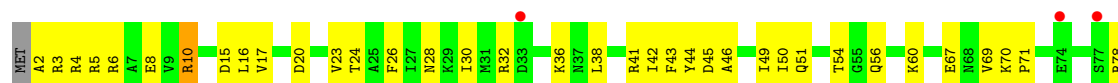


• Molecule 40: 30S ribosomal protein S7





- Molecule 40: 30S ribosomal protein S7



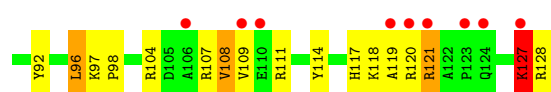
- Molecule 41: 30S ribosomal protein S8



- Molecule 41: 30S ribosomal protein S8

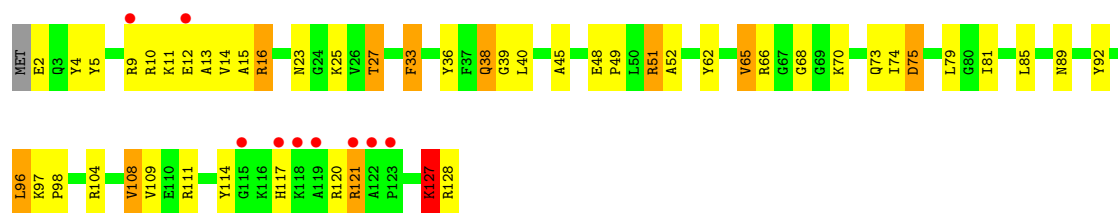


- Molecule 42: 30S ribosomal protein S9

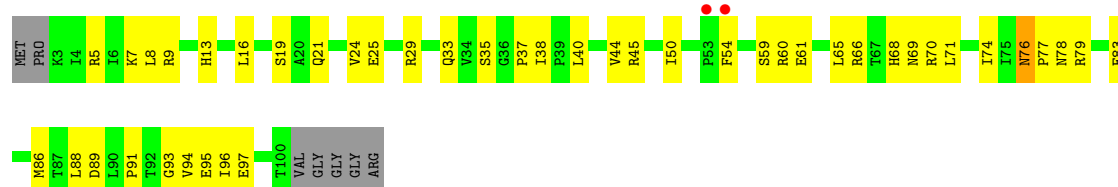


- Molecule 42: 30S ribosomal protein S9

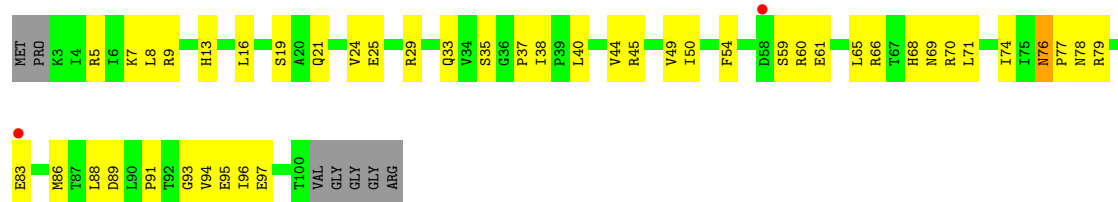




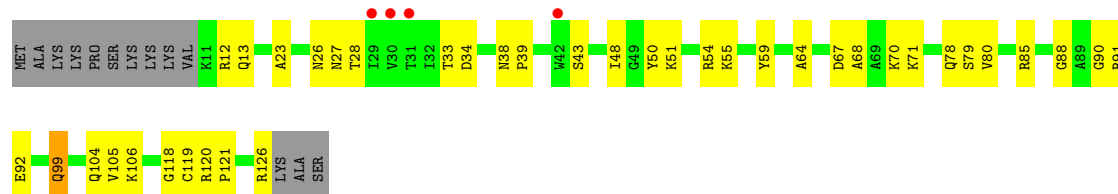
• Molecule 43: 30S ribosomal protein S10



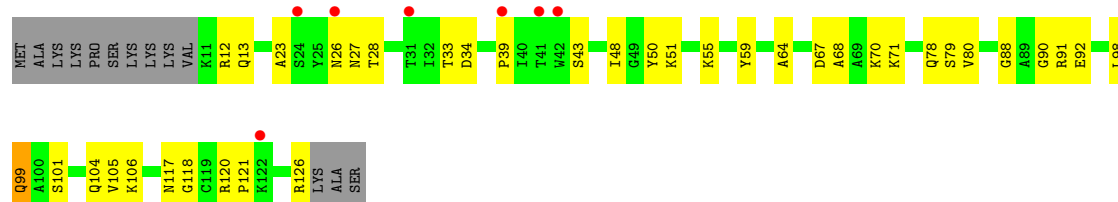
• Molecule 43: 30S ribosomal protein S10



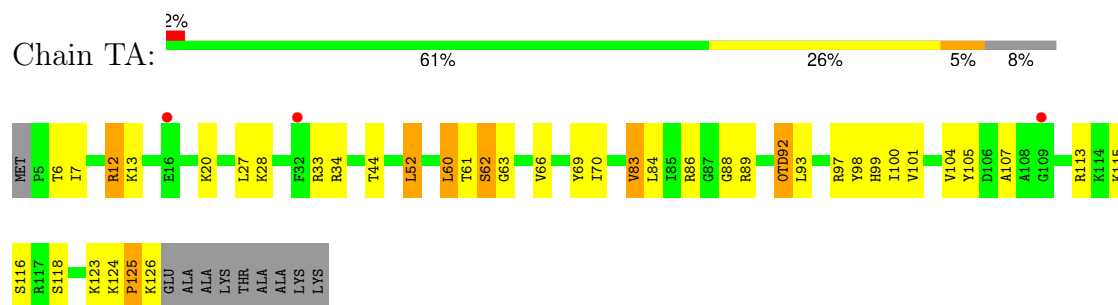
• Molecule 44: 30S ribosomal protein S11



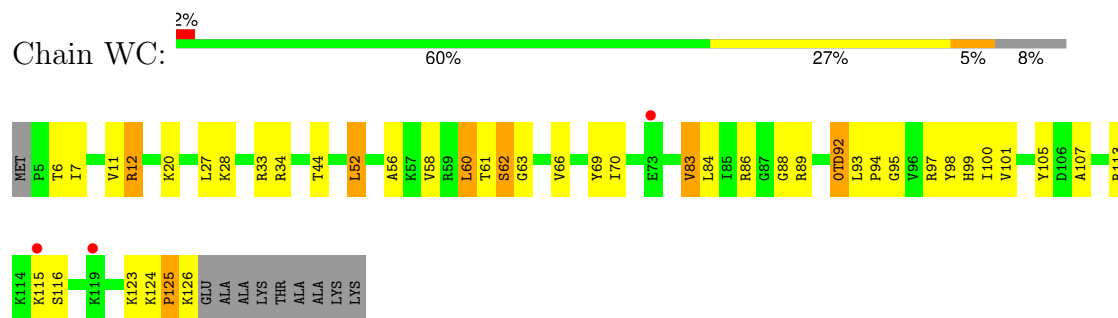
• Molecule 44: 30S ribosomal protein S11



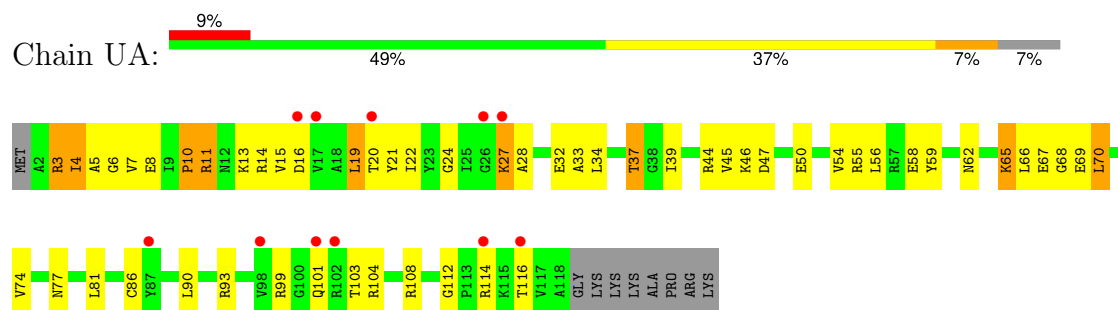
- Molecule 45: 30S ribosomal protein S12



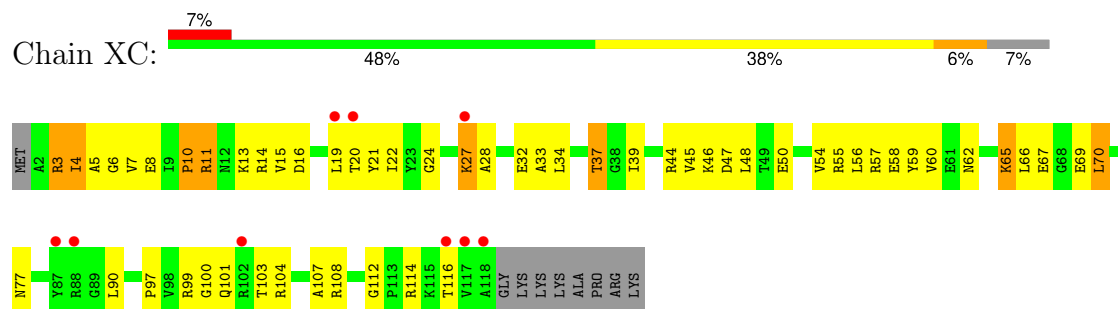
- Molecule 45: 30S ribosomal protein S12



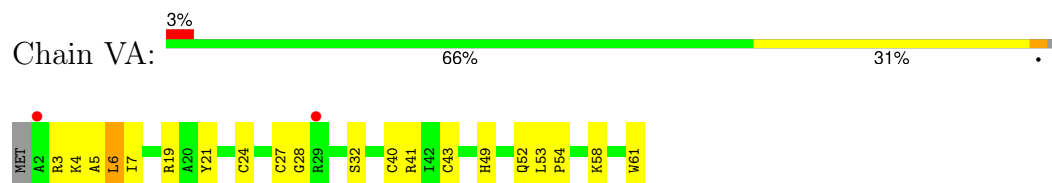
- Molecule 46: 30S ribosomal protein S13



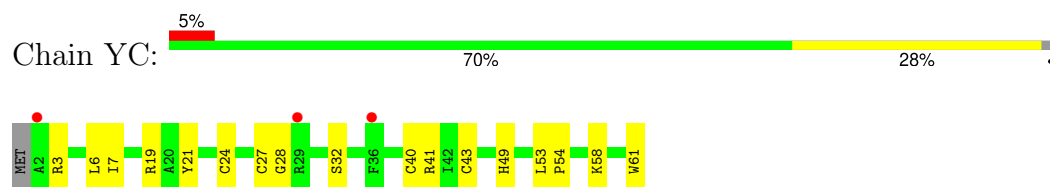
- Molecule 46: 30S ribosomal protein S13



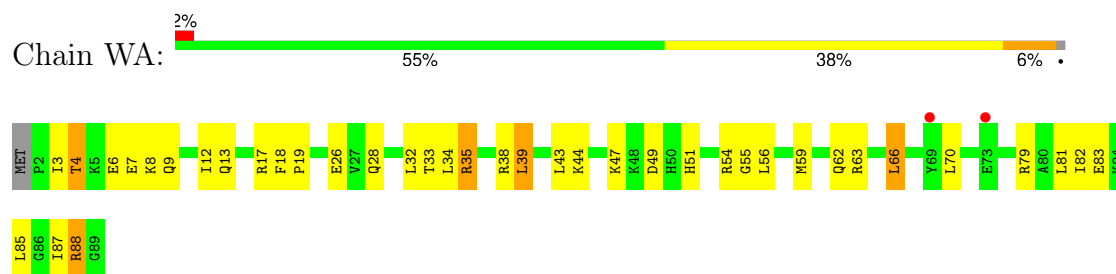
- Molecule 47: 30S ribosomal protein S14 type Z



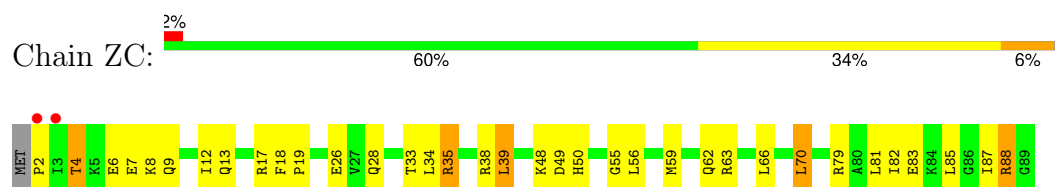
- Molecule 47: 30S ribosomal protein S14 type Z



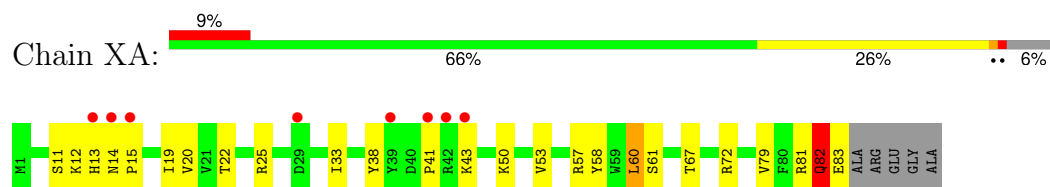
- Molecule 48: 30S ribosomal protein S15



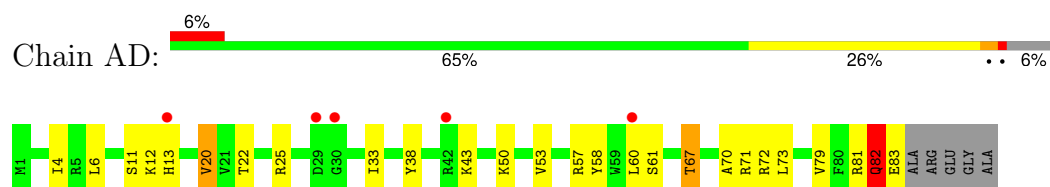
- Molecule 48: 30S ribosomal protein S15



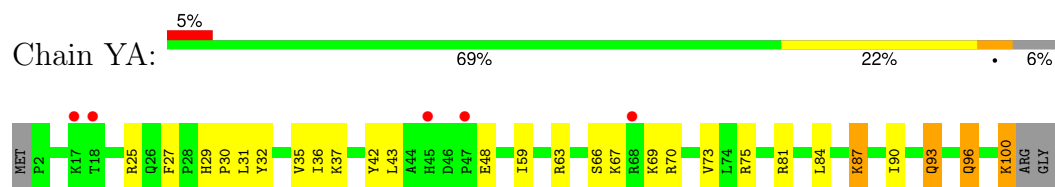
- Molecule 49: 30S ribosomal protein S16



- Molecule 49: 30S ribosomal protein S16

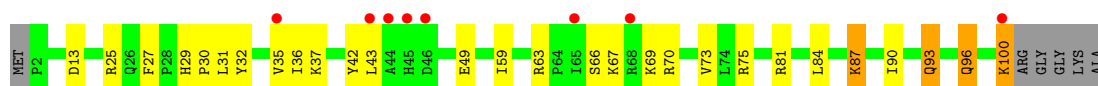


- Molecule 50: 30S ribosomal protein S17

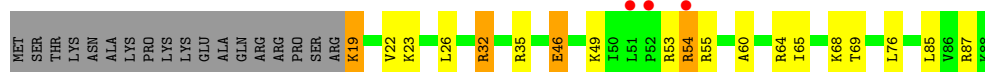


- Molecule 50: 30S ribosomal protein S17

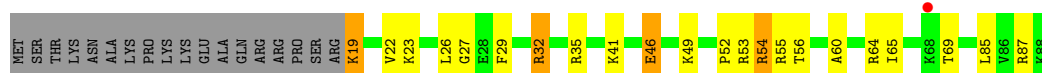




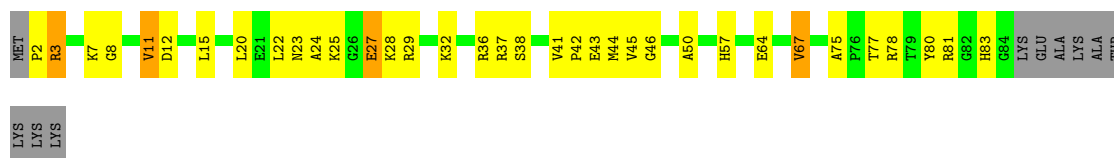
- Molecule 51: 30S ribosomal protein S18



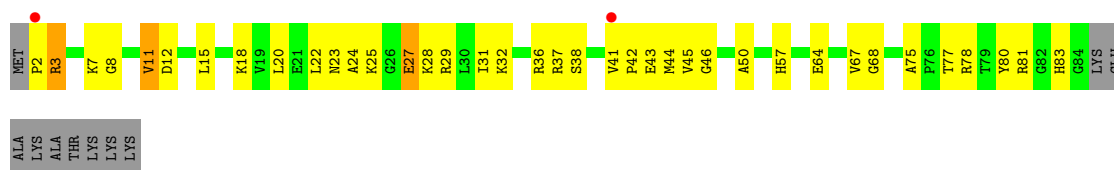
- Molecule 51: 30S ribosomal protein S18



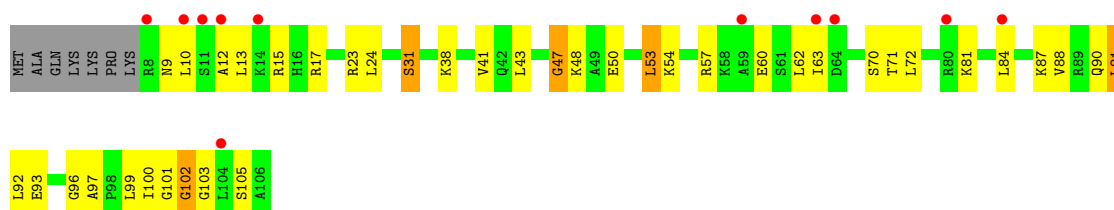
- Molecule 52: 30S ribosomal protein S19



- Molecule 52: 30S ribosomal protein S19

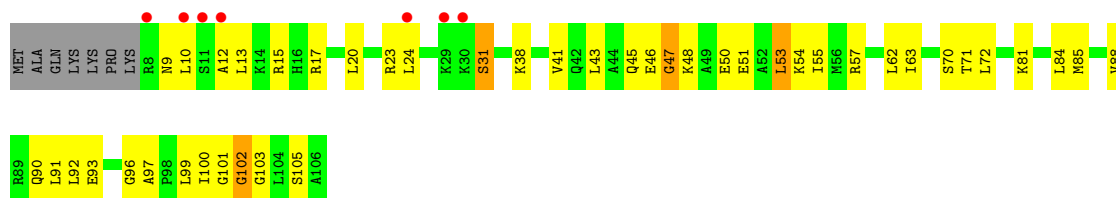


- Molecule 53: 30S ribosomal protein S20



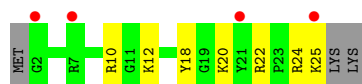
- Molecule 53: 30S ribosomal protein S20

Chain ED:  7% 52% 38% 7%



- Molecule 54: 30S ribosomal protein Thx

Chain CB: 



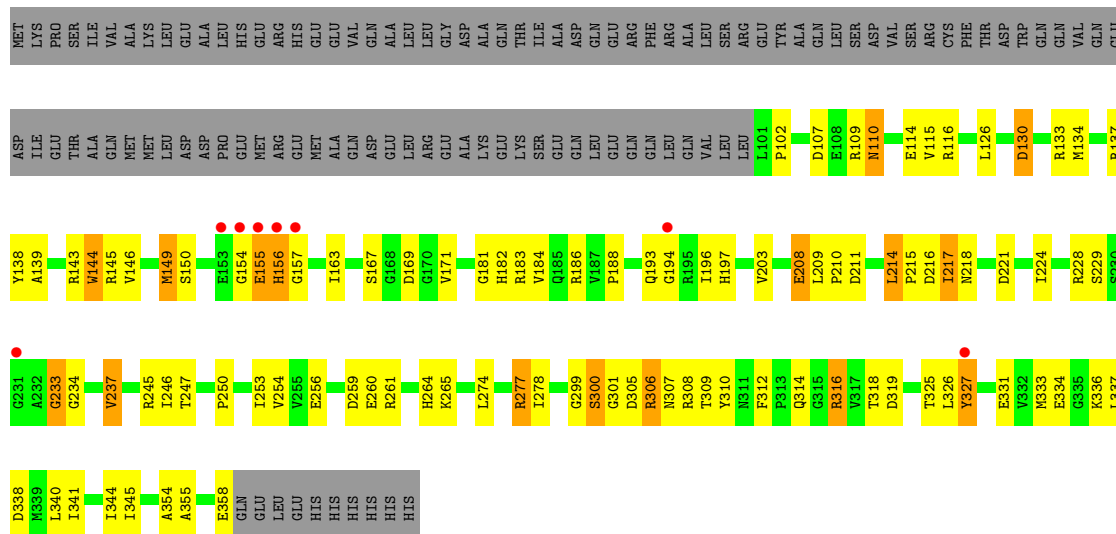
- Molecule 54: 30S ribosomal protein Thx

Chain FD: 

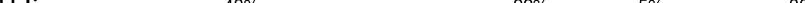


- Molecule 55: Peptide chain release factor 1

Chain GD: 



- Molecule 55: Peptide chain release factor 1

Chain HD: 



D130	D216	E334	ASP
M134	I217	G335	ILE
R137	N218	K336	GLU
Y138		L337	THR
A139	D221	D338	ALA
	I224	K339	GLN
		L340	MET
		I341	MET
			LEU
R143	R228	I345	ASP
W144	S229		ASP
R145	S230	A354	PRO
V146	G231	A355	GLU
	A232		MET
M149	G233	E358	ARG
S150	G234	GLN	GLU
		LEU	GLU
E153	V237	LEU	MET
G154		GLU	ALA
E155	R245	GLU	GLN
H156	I246	HIS	ASP
G157		HIS	GLU
	I253	HIS	LEU
K160	E256	HIS	ARG
		HIS	GLU
	K265		ALA
I163			LYS
A164	L274		GLU
K165			LYS
I166	L277		SER
S167	I278		GLU
G168			GLN
D169	Q287		LEU
G170			GLU
V171			GLN
E178	G299		GLN
	S300		LEU
	G301		GLN
	D305		VAL
G181	R306		LEU
H182	N307		LEU
R183	R308		LEU
V184	T309		P101
Q185	Y310		P102
R196	N311		
V187	F312		D107
P188	P313		E108
	Q193		R109
	G194		N110
Q195	Q314		A111
R196	G315		F112
I196	R316		L113
H197	V317		E114
	T318		V115
	D319		R116
V203	T325		T119
E208	L326		
L209	Y327		E123
P210			
D211	E331		L126
	V332		
L214	M333		
P215			

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.82Å 450.45Å 615.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.55 50.00 – 3.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-3.55) 99.8 (50.00-3.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.58Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	(Not available) , (Not available) 0.221 , 0.257	Depositor DCC
R_{free} test set	684222 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	124.9	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 83.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	299566	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.66	8/35961 (0.0%)	1.15	147/56125 (0.3%)
1	DB	0.69	5/35961 (0.0%)	1.18	176/56125 (0.3%)
2	B	1.01	76/69214 (0.1%)	1.49	1088/108048 (1.0%)
2	EB	0.88	60/69214 (0.1%)	1.38	770/108048 (0.7%)
3	C	0.69	0/2881	1.20	18/4494 (0.4%)
3	FB	0.61	0/2881	1.09	11/4494 (0.2%)
4	D	0.47	0/1744	0.88	0/2719
4	GB	0.48	0/1744	0.88	0/2719
4	IA	0.74	0/1744	1.17	7/2719 (0.3%)
4	LC	0.70	1/1744 (0.1%)	1.12	5/2719 (0.2%)
5	E	0.78	4/2195 (0.2%)	0.74	0/2955
5	HB	0.70	3/2195 (0.1%)	0.72	0/2955
6	F	0.63	0/1596	0.67	0/2153
6	IB	0.57	0/1596	0.65	0/2153
7	G	0.70	0/1621	0.69	0/2194
7	JB	0.61	0/1621	0.65	0/2194
8	H	0.44	0/1496	0.57	0/2013
8	KB	0.40	0/1496	0.56	0/2013
9	I	0.52	0/1356	0.56	0/1834
9	LB	0.38	0/1356	0.52	0/1834
10	J	0.51	0/1152	0.58	0/1559
10	MB	0.47	0/1152	0.58	0/1559
11	K	0.62	0/1148	0.66	0/1547
11	NB	0.51	0/1148	0.63	0/1547
12	L	0.67	0/942	0.68	0/1268
12	OB	0.67	0/942	0.67	0/1268
13	M	0.64	0/1162	0.69	0/1544
13	PB	0.56	0/1162	0.67	0/1544
14	N	0.67	0/1142	0.63	0/1525
14	QB	0.60	0/1142	0.63	0/1525
15	O	0.60	0/982	0.72	0/1312
15	RB	0.57	0/982	0.68	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	P	0.45	0/887	0.58	0/1180
16	SB	0.40	0/887	0.53	0/1180
17	Q	0.61	0/1157	0.65	0/1544
17	TB	0.58	0/1157	0.65	0/1544
18	R	0.67	0/982	0.68	0/1306
18	UB	0.57	0/982	0.65	0/1306
19	S	0.65	0/790	0.67	0/1057
19	VB	0.56	0/790	0.65	0/1057
20	T	0.74	0/901	0.73	0/1209
20	WB	0.65	0/901	0.69	0/1209
21	U	0.76	0/764	0.69	0/1025
21	XB	0.63	0/764	0.65	0/1025
22	V	0.64	0/827	0.66	0/1103
22	YB	0.60	0/827	0.65	0/1103
23	W	0.49	0/1527	0.58	0/2073
23	ZB	0.43	0/1527	0.55	0/2073
24	AC	0.61	0/671	0.71	0/892
24	X	0.71	0/671	0.73	0/892
25	BC	0.65	0/768	0.71	0/1021
25	Y	0.70	0/768	0.72	0/1021
26	CC	0.57	0/594	0.60	0/785
26	Z	0.68	0/594	0.64	0/785
27	AA	0.60	0/482	0.62	0/646
27	DC	0.57	0/482	0.63	0/646
28	BA	0.42	0/565	0.46	0/761
28	EC	0.39	0/565	0.46	0/761
29	CA	0.60	0/474	0.63	0/640
29	FC	0.55	0/474	0.64	0/640
30	DA	0.41	0/460	0.50	0/613
30	GC	0.40	0/460	0.48	0/613
31	EA	0.79	0/426	0.89	3/561 (0.5%)
31	HC	0.69	0/426	0.78	1/561 (0.2%)
32	FA	0.74	1/525 (0.2%)	0.68	0/691
32	IC	0.61	0/525	0.66	0/691
33	GA	0.45	0/310	0.53	0/407
33	JC	0.46	0/310	0.53	0/407
34	HA	1.01	0/247	1.24	3/382 (0.8%)
34	KC	1.01	0/247	1.14	0/382
35	JA	0.41	0/1935	0.55	0/2609
35	MC	0.41	0/1935	0.54	0/2609
36	KA	0.41	0/1636	0.53	0/2205
36	NC	0.40	0/1636	0.53	0/2205
37	LA	0.51	1/1733 (0.1%)	0.60	1/2318 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	OC	0.58	1/1733 (0.1%)	0.62	1/2318 (0.0%)
38	MA	0.48	0/1171	0.61	0/1576
38	PC	0.51	0/1171	0.63	0/1576
39	NA	0.53	0/856	0.59	0/1154
39	QC	0.50	0/856	0.59	0/1154
40	OA	0.42	0/1276	0.51	0/1709
40	RC	0.44	0/1276	0.52	0/1709
41	PA	0.45	0/1136	0.59	0/1527
41	SC	0.46	0/1136	0.60	0/1527
42	QA	0.36	0/1029	0.49	0/1378
42	TC	0.36	0/1029	0.49	0/1378
43	RA	0.38	0/807	0.49	0/1085
43	UC	0.38	0/807	0.49	0/1085
44	SA	0.52	0/879	0.61	0/1187
44	VC	0.50	0/879	0.61	0/1187
45	TA	0.55	0/963	0.63	0/1287
45	WC	0.56	0/963	0.63	0/1287
46	UA	0.38	0/943	0.53	0/1265
46	XC	0.38	0/943	0.52	0/1265
47	VA	0.42	0/501	0.54	0/664
47	YC	0.39	0/501	0.53	0/664
48	WA	0.50	0/745	0.56	0/992
48	ZC	0.51	0/745	0.56	0/992
49	AD	0.49	0/716	0.58	0/963
49	XA	0.40	0/716	0.55	0/963
50	BD	0.53	0/836	0.58	0/1117
50	YA	0.52	0/836	0.59	0/1117
51	CD	0.50	0/579	0.55	0/768
51	ZA	0.52	0/579	0.57	0/768
52	AB	0.36	0/680	0.51	0/915
52	DD	0.35	0/680	0.51	0/915
53	BB	0.40	0/764	0.52	0/1006
53	ED	0.44	0/764	0.55	0/1006
54	CB	0.35	0/212	0.46	0/277
54	FD	0.36	0/212	0.46	0/277
55	GD	0.54	0/2012	0.62	0/2713
55	HD	0.48	0/2012	0.60	0/2713
All	All	0.77	160/322204 (0.0%)	1.18	2231/481240 (0.5%)

The worst 5 of 160 bond length outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1762	A	N9-C4	14.42	1.46	1.37
2	EB	1762	A	N9-C4	13.35	1.45	1.37
2	B	1142(B)	A	N9-C4	-10.33	1.31	1.37
1	A	1503	A	N9-C4	9.28	1.43	1.37
1	A	1531	A	N9-C4	9.11	1.43	1.37

The worst 5 of 2231 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EB	2053	G	N1-C6-O6	19.40	131.54	119.90
2	EB	2053	G	C5-C6-O6	-15.62	119.23	128.60
2	B	2053	G	N1-C6-O6	15.42	129.15	119.90
2	B	2593	U	N3-C4-C5	-14.85	105.69	114.60
2	B	1602	U	N3-C4-C5	-14.74	105.75	114.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32394	0	16367	505	0
1	DB	32394	0	16367	492	0
2	B	62031	0	31275	829	0
2	EB	62031	0	31275	802	0
3	C	2576	0	1305	35	0
3	FB	2576	0	1305	35	0
4	D	1642	0	841	26	0
4	GB	1642	0	841	29	0
4	IA	1642	0	841	12	0
4	LC	1642	0	841	10	0
5	E	2145	0	2234	91	0
5	HB	2145	0	2234	78	0
6	F	1563	0	1629	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	IB	1563	0	1629	55	0
7	G	1586	0	1632	65	0
7	JB	1586	0	1632	61	0
8	H	1471	0	1526	67	0
8	KB	1471	0	1526	62	0
9	I	1330	0	1407	57	0
9	LB	1330	0	1407	51	0
10	J	1137	0	1225	50	0
10	MB	1137	0	1225	40	0
11	K	1121	0	1195	34	0
11	NB	1121	0	1195	31	0
12	L	932	0	994	32	0
12	OB	932	0	994	27	0
13	M	1145	0	1228	40	0
13	PB	1145	0	1228	35	0
14	N	1121	0	1179	36	0
14	QB	1121	0	1179	42	0
15	O	968	0	1033	39	0
15	RB	968	0	1033	43	0
16	P	877	0	938	28	0
16	SB	877	0	938	29	0
17	Q	1143	0	1211	37	0
17	TB	1143	0	1211	33	0
18	R	964	0	1022	25	0
18	UB	964	0	1022	30	0
19	S	779	0	852	28	0
19	VB	779	0	852	29	0
20	T	890	0	951	34	0
20	WB	890	0	951	26	0
21	U	750	0	814	14	0
21	XB	750	0	814	14	0
22	V	814	0	907	28	0
22	YB	814	0	907	25	0
23	W	1495	0	1521	51	0
23	ZB	1495	0	1521	50	0
24	AC	662	0	688	23	0
24	X	662	0	688	23	0
25	BC	761	0	837	28	0
25	Y	761	0	837	30	0
26	CC	592	0	654	16	0
26	Z	592	0	654	16	0
27	AA	477	0	529	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	DC	477	0	529	16	0
28	BA	552	0	537	23	0
28	EC	552	0	537	22	0
29	CA	460	0	484	17	0
29	FC	460	0	484	19	0
30	DA	453	0	477	11	0
30	GC	453	0	477	11	0
31	EA	418	0	467	17	0
31	HC	418	0	467	17	0
32	FA	517	0	582	17	0
32	IC	517	0	582	19	0
33	GA	307	0	338	15	0
33	JC	307	0	337	16	0
34	HA	220	0	108	7	0
34	KC	220	0	108	9	0
35	JA	1900	0	1951	69	0
35	MC	1900	0	1951	69	0
36	KA	1612	0	1677	49	0
36	NC	1612	0	1677	48	0
37	LA	1703	0	1765	74	0
37	OC	1703	0	1765	68	0
38	MA	1155	0	1213	45	0
38	PC	1155	0	1213	51	0
39	NA	843	0	857	44	0
39	QC	843	0	857	40	0
40	OA	1257	0	1296	38	0
40	RC	1257	0	1296	42	0
41	PA	1116	0	1177	49	0
41	SC	1116	0	1177	48	0
42	QA	1011	0	1043	43	0
42	TC	1011	0	1043	43	0
43	RA	794	0	840	25	0
43	UC	794	0	840	27	0
44	SA	864	0	881	25	0
44	VC	864	0	881	21	0
45	TA	958	0	1047	31	0
45	WC	958	0	1047	31	0
46	UA	933	0	992	50	0
46	XC	933	0	992	47	0
47	VA	492	0	533	20	0
47	YC	492	0	533	17	0
48	WA	734	0	771	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	ZC	734	0	771	27	0
49	AD	700	0	720	20	0
49	XA	700	0	720	20	0
50	BD	823	0	893	24	0
50	YA	823	0	893	21	0
51	CD	574	0	644	17	0
51	ZA	574	0	644	19	0
52	AB	665	0	686	28	0
52	DD	665	0	686	29	0
53	BB	762	0	859	27	0
53	ED	762	0	859	27	0
54	CB	208	0	221	4	0
54	FD	208	0	221	12	0
55	GD	1980	0	1942	69	0
55	HD	1980	0	1942	63	0
56	A	160	0	0	0	0
56	AB	1	0	0	0	0
56	AC	2	0	0	0	0
56	AD	1	0	0	0	0
56	B	514	0	0	0	0
56	BB	1	0	0	0	0
56	BC	1	0	0	0	0
56	BD	2	0	0	0	0
56	C	23	0	0	0	0
56	CA	1	0	0	0	0
56	CD	2	0	0	0	0
56	D	6	0	0	0	0
56	DB	177	0	0	0	0
56	DC	1	0	0	0	0
56	E	4	0	0	0	0
56	EA	1	0	0	0	0
56	EB	395	0	0	0	0
56	ED	1	0	0	0	0
56	F	1	0	0	0	0
56	FA	1	0	0	0	0
56	FB	17	0	0	0	0
56	FC	1	0	0	0	0
56	G	4	0	0	0	0
56	GB	5	0	0	0	0
56	GD	5	0	0	0	0
56	H	1	0	0	0	0
56	HA	1	0	0	0	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	SB	1	0	0	0	0
56	SC	1	0	0	0	0
56	T	2	0	0	0	0
56	TA	3	0	0	0	0
56	TB	5	0	0	0	0
56	TC	2	0	0	0	0
56	U	2	0	0	0	0
56	UC	1	0	0	0	0
56	V	5	0	0	0	0
56	VA	2	0	0	0	0
56	VB	1	0	0	0	0
56	W	12	0	0	0	0
56	WA	3	0	0	0	0
56	WB	3	0	0	0	0
56	WC	2	0	0	0	0
56	XB	2	0	0	0	0
56	XC	2	0	0	0	0
56	Y	4	0	0	0	0
56	YA	2	0	0	0	0
56	YB	3	0	0	0	0
56	YC	1	0	0	0	0
56	Z	3	0	0	0	0
56	ZA	1	0	0	0	0
56	ZB	2	0	0	0	0
56	ZC	1	0	0	0	0
57	BA	1	0	0	0	0
57	CA	1	0	0	0	0
57	DA	1	0	0	0	0
57	EC	1	0	0	0	0
57	FC	1	0	0	0	0
57	GA	1	0	0	0	0
57	GC	1	0	0	0	0
57	JC	1	0	0	0	0
57	V	1	0	0	0	0
57	YB	1	0	0	0	0
All	All	299566	0	203671	5481	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 5481 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	273/275 (99%)	243 (89%)	25 (9%)	5 (2%)	7	36
5	HB	273/275 (99%)	243 (89%)	25 (9%)	5 (2%)	7	36
6	F	202/206 (98%)	180 (89%)	20 (10%)	2 (1%)	13	47
6	IB	202/206 (98%)	181 (90%)	19 (9%)	2 (1%)	13	47
7	G	200/205 (98%)	187 (94%)	9 (4%)	4 (2%)	6	34
7	JB	200/205 (98%)	186 (93%)	10 (5%)	4 (2%)	6	34
8	H	179/182 (98%)	152 (85%)	20 (11%)	7 (4%)	2	21
8	KB	179/182 (98%)	151 (84%)	22 (12%)	6 (3%)	3	25
9	I	172/180 (96%)	155 (90%)	14 (8%)	3 (2%)	7	37
9	LB	172/180 (96%)	154 (90%)	15 (9%)	3 (2%)	7	37
10	J	144/148 (97%)	118 (82%)	17 (12%)	9 (6%)	1	13
10	MB	144/148 (97%)	118 (82%)	16 (11%)	10 (7%)	1	11
11	K	138/140 (99%)	125 (91%)	12 (9%)	1 (1%)	19	53
11	NB	138/140 (99%)	126 (91%)	11 (8%)	1 (1%)	19	53
12	L	120/122 (98%)	106 (88%)	12 (10%)	2 (2%)	7	37
12	OB	120/122 (98%)	106 (88%)	12 (10%)	2 (2%)	7	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	148/150 (99%)	132 (89%)	11 (7%)	5 (3%)	3	25
13	PB	148/150 (99%)	131 (88%)	12 (8%)	5 (3%)	3	25
14	N	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	9	40
14	QB	139/141 (99%)	125 (90%)	12 (9%)	2 (1%)	9	40
15	O	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	7	37
15	RB	116/118 (98%)	107 (92%)	7 (6%)	2 (2%)	7	37
16	P	108/112 (96%)	99 (92%)	7 (6%)	2 (2%)	6	35
16	SB	108/112 (96%)	100 (93%)	6 (6%)	2 (2%)	6	35
17	Q	135/146 (92%)	118 (87%)	12 (9%)	5 (4%)	2	22
17	TB	135/146 (92%)	118 (87%)	13 (10%)	4 (3%)	3	26
18	R	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	14	49
18	UB	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	49
19	S	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	6	34
19	VB	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	6	34
20	T	110/113 (97%)	104 (94%)	4 (4%)	2 (2%)	7	36
20	WB	110/113 (97%)	103 (94%)	5 (4%)	2 (2%)	7	36
21	U	93/96 (97%)	84 (90%)	8 (9%)	1 (1%)	12	45
21	XB	93/96 (97%)	84 (90%)	8 (9%)	1 (1%)	12	45
22	V	105/110 (96%)	89 (85%)	11 (10%)	5 (5%)	2	17
22	YB	105/110 (96%)	91 (87%)	9 (9%)	5 (5%)	2	17
23	W	187/206 (91%)	165 (88%)	21 (11%)	1 (0%)	25	59
23	ZB	187/206 (91%)	165 (88%)	21 (11%)	1 (0%)	25	59
24	AC	82/85 (96%)	70 (85%)	10 (12%)	2 (2%)	5	30
24	X	82/85 (96%)	69 (84%)	11 (13%)	2 (2%)	5	30
25	BC	95/98 (97%)	84 (88%)	10 (10%)	1 (1%)	12	45
25	Y	95/98 (97%)	86 (90%)	8 (8%)	1 (1%)	12	45
26	CC	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
26	Z	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
27	AA	58/60 (97%)	53 (91%)	4 (7%)	1 (2%)	7	37
27	DC	58/60 (97%)	53 (91%)	4 (7%)	1 (2%)	7	37
28	BA	67/71 (94%)	47 (70%)	19 (28%)	1 (2%)	8	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	EC	67/71 (94%)	47 (70%)	20 (30%)	0	100	100
29	CA	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	7	36
29	FC	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	7	36
30	DA	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
30	GC	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
31	EA	46/49 (94%)	46 (100%)	0	0	100	100
31	HC	46/49 (94%)	46 (100%)	0	0	100	100
32	FA	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
32	IC	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
33	GA	35/37 (95%)	27 (77%)	8 (23%)	0	100	100
33	JC	35/37 (95%)	27 (77%)	8 (23%)	0	100	100
35	JA	232/256 (91%)	189 (82%)	29 (12%)	14 (6%)	1	13
35	MC	232/256 (91%)	188 (81%)	30 (13%)	14 (6%)	1	13
36	KA	204/239 (85%)	172 (84%)	24 (12%)	8 (4%)	2	21
36	NC	204/239 (85%)	172 (84%)	24 (12%)	8 (4%)	2	21
37	LA	206/209 (99%)	179 (87%)	20 (10%)	7 (3%)	3	25
37	OC	206/209 (99%)	182 (88%)	16 (8%)	8 (4%)	2	21
38	MA	149/162 (92%)	132 (89%)	11 (7%)	6 (4%)	2	21
38	PC	149/162 (92%)	132 (89%)	10 (7%)	7 (5%)	2	18
39	NA	99/101 (98%)	88 (89%)	9 (9%)	2 (2%)	6	34
39	QC	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	6	34
40	OA	153/156 (98%)	133 (87%)	13 (8%)	7 (5%)	2	18
40	RC	153/156 (98%)	133 (87%)	13 (8%)	7 (5%)	2	18
41	PA	136/138 (99%)	125 (92%)	9 (7%)	2 (2%)	8	39
41	SC	136/138 (99%)	126 (93%)	9 (7%)	1 (1%)	19	53
42	QA	125/128 (98%)	105 (84%)	17 (14%)	3 (2%)	5	30
42	TC	125/128 (98%)	105 (84%)	16 (13%)	4 (3%)	3	25
43	RA	96/105 (91%)	81 (84%)	12 (12%)	3 (3%)	3	26
43	UC	96/105 (91%)	81 (84%)	12 (12%)	3 (3%)	3	26
44	SA	114/129 (88%)	101 (89%)	10 (9%)	3 (3%)	4	28
44	VC	114/129 (88%)	101 (89%)	9 (8%)	4 (4%)	3	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	TA	119/132 (90%)	104 (87%)	11 (9%)	4 (3%)	3	25
45	WC	119/132 (90%)	104 (87%)	11 (9%)	4 (3%)	3	25
46	UA	115/126 (91%)	102 (89%)	12 (10%)	1 (1%)	14	49
46	XC	115/126 (91%)	102 (89%)	11 (10%)	2 (2%)	7	37
47	VA	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
47	YC	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
48	WA	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	5	31
48	ZC	86/89 (97%)	81 (94%)	3 (4%)	2 (2%)	5	31
49	AD	81/88 (92%)	73 (90%)	7 (9%)	1 (1%)	11	43
49	XA	81/88 (92%)	73 (90%)	7 (9%)	1 (1%)	11	43
50	BD	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
50	YA	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
51	CD	68/88 (77%)	62 (91%)	5 (7%)	1 (2%)	8	39
51	ZA	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	8	39
52	AB	81/93 (87%)	63 (78%)	14 (17%)	4 (5%)	2	17
52	DD	81/93 (87%)	63 (78%)	14 (17%)	4 (5%)	2	17
53	BB	97/106 (92%)	90 (93%)	3 (3%)	4 (4%)	2	20
53	ED	97/106 (92%)	90 (93%)	3 (3%)	4 (4%)	2	20
54	CB	22/27 (82%)	18 (82%)	4 (18%)	0	100	100
54	FD	22/27 (82%)	18 (82%)	4 (18%)	0	100	100
55	GD	253/365 (69%)	207 (82%)	35 (14%)	11 (4%)	2	19
55	HD	253/365 (69%)	206 (81%)	37 (15%)	10 (4%)	2	21
All	All	11990/12846 (93%)	10568 (88%)	1121 (9%)	301 (2%)	4	29

5 of 301 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	31	LYS
6	F	192	ASN
7	G	21	ALA
7	G	130	ALA
8	H	74	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	217/217 (100%)	197 (91%)	20 (9%)	7	31
5	HB	217/217 (100%)	197 (91%)	20 (9%)	7	31
6	F	165/166 (99%)	145 (88%)	20 (12%)	4	21
6	IB	165/166 (99%)	145 (88%)	20 (12%)	4	21
7	G	161/162 (99%)	142 (88%)	19 (12%)	4	22
7	JB	161/162 (99%)	142 (88%)	19 (12%)	4	22
8	H	154/156 (99%)	134 (87%)	20 (13%)	3	19
8	KB	154/156 (99%)	136 (88%)	18 (12%)	4	22
9	I	144/148 (97%)	130 (90%)	14 (10%)	6	28
9	LB	144/148 (97%)	130 (90%)	14 (10%)	6	28
10	J	122/124 (98%)	105 (86%)	17 (14%)	3	17
10	MB	122/124 (98%)	106 (87%)	16 (13%)	3	18
11	K	119/119 (100%)	107 (90%)	12 (10%)	6	27
11	NB	119/119 (100%)	108 (91%)	11 (9%)	7	31
12	L	100/100 (100%)	91 (91%)	9 (9%)	8	31
12	OB	100/100 (100%)	90 (90%)	10 (10%)	6	28
13	M	116/116 (100%)	103 (89%)	13 (11%)	5	24
13	PB	116/116 (100%)	101 (87%)	15 (13%)	3	19
14	N	111/111 (100%)	99 (89%)	12 (11%)	5	25
14	QB	111/111 (100%)	98 (88%)	13 (12%)	4	22
15	O	101/101 (100%)	89 (88%)	12 (12%)	4	22
15	RB	101/101 (100%)	89 (88%)	12 (12%)	4	22
16	P	87/88 (99%)	83 (95%)	4 (5%)	23	52
16	SB	87/88 (99%)	83 (95%)	4 (5%)	23	52
17	Q	121/128 (94%)	112 (93%)	9 (7%)	11	37
17	TB	121/128 (94%)	113 (93%)	8 (7%)	14	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	R	93/94 (99%)	83 (89%)	10 (11%)	5	25
18	UB	93/94 (99%)	84 (90%)	9 (10%)	6	28
19	S	82/82 (100%)	70 (85%)	12 (15%)	2	15
19	VB	82/82 (100%)	72 (88%)	10 (12%)	4	20
20	T	91/92 (99%)	81 (89%)	10 (11%)	5	25
20	WB	91/92 (99%)	81 (89%)	10 (11%)	5	25
21	U	77/78 (99%)	73 (95%)	4 (5%)	19	49
21	XB	77/78 (99%)	73 (95%)	4 (5%)	19	49
22	V	87/91 (96%)	81 (93%)	6 (7%)	13	40
22	YB	87/91 (96%)	81 (93%)	6 (7%)	13	40
23	W	163/179 (91%)	142 (87%)	21 (13%)	3	19
23	ZB	163/179 (91%)	143 (88%)	20 (12%)	4	20
24	AC	66/67 (98%)	57 (86%)	9 (14%)	3	17
24	X	66/67 (98%)	57 (86%)	9 (14%)	3	17
25	BC	81/83 (98%)	70 (86%)	11 (14%)	3	17
25	Y	81/83 (98%)	70 (86%)	11 (14%)	3	17
26	CC	66/67 (98%)	62 (94%)	4 (6%)	15	44
26	Z	66/67 (98%)	62 (94%)	4 (6%)	15	44
27	AA	52/52 (100%)	48 (92%)	4 (8%)	10	36
27	DC	52/52 (100%)	49 (94%)	3 (6%)	17	45
28	BA	59/63 (94%)	51 (86%)	8 (14%)	3	17
28	EC	59/63 (94%)	51 (86%)	8 (14%)	3	17
29	CA	51/52 (98%)	46 (90%)	5 (10%)	6	28
29	FC	51/52 (98%)	46 (90%)	5 (10%)	6	28
30	DA	51/52 (98%)	47 (92%)	4 (8%)	10	35
30	GC	51/52 (98%)	46 (90%)	5 (10%)	6	28
31	EA	41/42 (98%)	35 (85%)	6 (15%)	2	15
31	HC	41/42 (98%)	35 (85%)	6 (15%)	2	15
32	FA	54/55 (98%)	47 (87%)	7 (13%)	3	19
32	IC	54/55 (98%)	48 (89%)	6 (11%)	5	24
33	GA	34/34 (100%)	30 (88%)	4 (12%)	4	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	JC	34/34 (100%)	30 (88%)	4 (12%)	4	22
35	JA	202/220 (92%)	177 (88%)	25 (12%)	4	20
35	MC	202/220 (92%)	177 (88%)	25 (12%)	4	20
36	KA	160/188 (85%)	146 (91%)	14 (9%)	8	32
36	NC	160/188 (85%)	145 (91%)	15 (9%)	7	30
37	LA	180/181 (99%)	159 (88%)	21 (12%)	4	22
37	OC	180/181 (99%)	157 (87%)	23 (13%)	3	19
38	MA	116/123 (94%)	100 (86%)	16 (14%)	3	17
38	PC	116/123 (94%)	99 (85%)	17 (15%)	2	15
39	NA	90/90 (100%)	80 (89%)	10 (11%)	5	24
39	QC	90/90 (100%)	79 (88%)	11 (12%)	4	20
40	OA	126/127 (99%)	120 (95%)	6 (5%)	21	51
40	RC	126/127 (99%)	120 (95%)	6 (5%)	21	51
41	PA	119/119 (100%)	107 (90%)	12 (10%)	6	27
41	SC	119/119 (100%)	108 (91%)	11 (9%)	7	31
42	QA	98/99 (99%)	86 (88%)	12 (12%)	4	20
42	TC	98/99 (99%)	86 (88%)	12 (12%)	4	20
43	RA	88/92 (96%)	81 (92%)	7 (8%)	10	35
43	UC	88/92 (96%)	81 (92%)	7 (8%)	10	35
44	SA	88/99 (89%)	85 (97%)	3 (3%)	32	60
44	VC	88/99 (89%)	85 (97%)	3 (3%)	32	60
45	TA	102/108 (94%)	95 (93%)	7 (7%)	13	40
45	WC	102/108 (94%)	95 (93%)	7 (7%)	13	40
46	UA	94/101 (93%)	82 (87%)	12 (13%)	3	19
46	XC	94/101 (93%)	83 (88%)	11 (12%)	4	22
47	VA	49/50 (98%)	47 (96%)	2 (4%)	26	55
47	YC	49/50 (98%)	47 (96%)	2 (4%)	26	55
48	WA	79/80 (99%)	72 (91%)	7 (9%)	8	32
48	ZC	79/80 (99%)	72 (91%)	7 (9%)	8	32
49	AD	72/74 (97%)	66 (92%)	6 (8%)	9	33
49	XA	72/74 (97%)	66 (92%)	6 (8%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	BD	94/97 (97%)	86 (92%)	8 (8%)	8	33
50	YA	94/97 (97%)	86 (92%)	8 (8%)	8	33
51	CD	61/77 (79%)	56 (92%)	5 (8%)	9	34
51	ZA	61/77 (79%)	56 (92%)	5 (8%)	9	34
52	AB	72/80 (90%)	65 (90%)	7 (10%)	6	28
52	DD	72/80 (90%)	65 (90%)	7 (10%)	6	28
53	BB	76/82 (93%)	70 (92%)	6 (8%)	10	35
53	ED	76/82 (93%)	70 (92%)	6 (8%)	10	35
54	CB	19/22 (86%)	18 (95%)	1 (5%)	19	48
54	FD	19/22 (86%)	18 (95%)	1 (5%)	19	48
55	GD	206/305 (68%)	179 (87%)	27 (13%)	3	18
55	HD	206/305 (68%)	179 (87%)	27 (13%)	3	18
All	All	10114/10666 (95%)	9077 (90%)	1037 (10%)	6	27

5 of 1037 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	WC	52	LEU
49	AD	67	THR
45	WC	44	THR
39	NA	69	GLU
38	MA	136	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
10	MB	54	GLN
55	HD	236	HIS
23	ZB	75	ASN
55	HD	197	HIS
50	BD	26	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1502/1507 (99%)	228 (15%)	10 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	DB	1502/1507 (99%)	223 (14%)	10 (0%)
2	B	2876/2880 (99%)	498 (17%)	15 (0%)
2	EB	2876/2880 (99%)	496 (17%)	15 (0%)
3	C	119/120 (99%)	18 (15%)	0
3	FB	119/120 (99%)	17 (14%)	0
34	HA	9/27 (33%)	4 (44%)	1 (11%)
34	KC	9/27 (33%)	4 (44%)	1 (11%)
4	D	76/77 (98%)	13 (17%)	0
4	GB	76/77 (98%)	13 (17%)	0
4	IA	76/77 (98%)	7 (9%)	0
4	LC	76/77 (98%)	7 (9%)	0
All	All	9316/9376 (99%)	1528 (16%)	52 (0%)

5 of 1528 RNA backbone outliers are listed below:

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

5 of 52 RNA pucker outliers are listed below:

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	DB	516	1	18,21,22	1.82	3 (16%)	21,30,33	1.34	3 (14%)
2	OMG	EB	2251	4,2	19,26,27	2.04	5 (26%)	21,38,41	1.39	4 (19%)
1	5MC	A	1400	1	19,22,23	2.34	4 (21%)	26,32,35	1.21	4 (15%)
2	PSU	B	1911	2	18,21,22	1.52	2 (11%)	21,30,33	1.71	5 (23%)
4	5MU	IA	54	4,56	19,22,23	2.14	3 (15%)	27,32,35	2.22	10 (37%)
2	5MU	EB	1939	2	19,22,23	2.22	5 (26%)	27,32,35	2.60	8 (29%)
1	5MC	DB	1407	1	19,22,23	3.12	4 (21%)	26,32,35	1.17	2 (7%)
1	MA6	A	1518	1	19,26,27	1.98	5 (26%)	18,38,41	1.78	3 (16%)
4	5MC	IA	32	4	19,22,23	2.61	4 (21%)	26,32,35	1.30	3 (11%)
4	4SU	D	8	4	18,21,22	4.82	7 (38%)	25,30,33	5.36	10 (40%)
1	5MC	A	967	1	19,22,23	2.52	5 (26%)	26,32,35	1.31	3 (11%)
2	5MC	B	1962	2	19,22,23	2.65	4 (21%)	26,32,35	1.29	2 (7%)
1	M2G	DB	966	1	20,27,28	2.28	5 (25%)	19,40,43	1.31	3 (15%)
1	4OC	DB	1402	1	20,23,24	1.07	2 (10%)	25,32,35	1.59	7 (28%)
1	2MG	A	1207	1	18,26,27	2.17	3 (16%)	16,38,41	1.68	4 (25%)
4	5MU	GB	54	4	19,22,23	2.07	3 (15%)	27,32,35	2.12	8 (29%)
1	2MG	DB	1207	1	18,26,27	2.19	3 (16%)	16,38,41	1.72	4 (25%)
2	PSU	EB	2605	2	18,21,22	1.48	2 (11%)	21,30,33	1.66	5 (23%)
4	4SU	IA	8	4	18,21,22	4.77	7 (38%)	25,30,33	5.16	11 (44%)
4	5MC	GB	32	4	19,22,23	2.65	4 (21%)	26,32,35	1.13	3 (11%)
2	PSU	EB	1917	2	18,21,22	1.71	2 (11%)	21,30,33	1.82	6 (28%)
1	MA6	DB	1519	1	19,26,27	2.02	5 (26%)	18,38,41	1.76	3 (16%)
45	0TD	WC	92	45	8,9,10	3.17	2 (25%)	6,11,13	3.11	3 (50%)
2	4OC	B	1920	2	19,22,24	1.14	1 (5%)	25,31,35	0.85	1 (4%)
1	MA6	A	1519	1	19,26,27	2.04	5 (26%)	18,38,41	1.82	3 (16%)
1	UR3	DB	1498	1	19,22,23	1.92	1 (5%)	26,32,35	1.42	3 (11%)
2	2MU	B	2552	2	19,22,24	2.72	5 (26%)	25,31,36	2.18	6 (24%)
2	PSU	B	1917	2	18,21,22	1.77	3 (16%)	21,30,33	1.84	5 (23%)
1	5MC	DB	967	1	19,22,23	2.39	5 (26%)	26,32,35	1.32	3 (11%)
2	PSU	EB	1911	2	18,21,22	1.58	2 (11%)	21,30,33	2.09	6 (28%)
4	PSU	LC	55	4	18,21,22	1.90	3 (16%)	21,30,33	1.71	5 (23%)
1	PSU	A	516	1	18,21,22	1.93	3 (16%)	21,30,33	1.47	5 (23%)
2	5MC	B	1942	2	19,22,23	2.99	4 (21%)	26,32,35	1.38	4 (15%)
2	2MA	B	2503	2	17,25,26	1.46	2 (11%)	16,37,40	1.53	3 (18%)
4	5MU	D	54	4	19,22,23	2.10	3 (15%)	27,32,35	1.99	8 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	GB	55	4	18,21,22	1.65	3 (16%)	21,30,33	1.58	3 (14%)
4	PSU	IA	55	4	18,21,22	1.91	2 (11%)	21,30,33	1.87	6 (28%)
1	M2G	A	966	1	20,27,28	2.33	4 (20%)	19,40,43	1.37	3 (15%)
1	UR3	A	1498	1	19,22,23	1.79	2 (10%)	26,32,35	1.55	4 (15%)
2	PSU	B	2605	2	18,21,22	1.59	3 (16%)	21,30,33	1.69	4 (19%)
4	4SU	GB	8	4	18,21,22	4.63	7 (38%)	25,30,33	6.22	9 (36%)
4	5MC	D	32	4	19,22,23	2.65	4 (21%)	26,32,35	0.97	2 (7%)
2	5MU	B	1915	2	19,22,23	1.95	3 (15%)	27,32,35	2.45	6 (22%)
45	0TD	TA	92	45	8,9,10	2.60	2 (25%)	6,11,13	3.29	3 (50%)
1	5MC	DB	1400	1	19,22,23	2.45	4 (21%)	26,32,35	1.26	4 (15%)
1	7MG	DB	527	1	23,26,27	2.94	7 (30%)	27,39,42	2.28	9 (33%)
2	2MU	EB	2552	56,2	19,22,24	2.56	3 (15%)	25,31,36	2.26	5 (20%)
4	PSU	D	55	4	18,21,22	1.76	2 (11%)	21,30,33	1.48	2 (9%)
4	4SU	LC	8	4	18,21,22	4.70	7 (38%)	25,30,33	6.03	11 (44%)
2	5MC	EB	1942	2	19,22,23	2.95	4 (21%)	26,32,35	1.44	4 (15%)
2	4OC	EB	1920	2	19,22,24	1.03	1 (5%)	25,31,35	0.84	0
2	5MC	EB	1962	56,2	19,22,23	2.61	5 (26%)	26,32,35	1.24	2 (7%)
2	2MA	EB	2503	2	17,25,26	1.45	2 (11%)	16,37,40	1.73	3 (18%)
2	OMG	B	2251	4,2	19,26,27	2.05	3 (15%)	21,38,41	1.22	4 (19%)
1	5MC	A	1407	1	19,22,23	2.87	4 (21%)	26,32,35	1.24	1 (3%)
1	5MC	DB	1404	1	19,22,23	2.61	4 (21%)	26,32,35	1.28	3 (11%)
1	MA6	DB	1518	1	19,26,27	2.01	5 (26%)	18,38,41	2.03	3 (16%)
4	5MC	LC	32	4	19,22,23	2.33	4 (21%)	26,32,35	1.32	3 (11%)
1	4OC	A	1402	1	20,23,24	1.11	2 (10%)	25,32,35	1.30	5 (20%)
1	5MC	A	1404	1	19,22,23	2.78	4 (21%)	26,32,35	1.21	1 (3%)
2	5MU	B	1939	2	19,22,23	2.28	3 (15%)	27,32,35	2.47	8 (29%)
4	5MU	LC	54	4	19,22,23	2.22	3 (15%)	27,32,35	1.83	7 (25%)
2	5MU	EB	1915	2	19,22,23	2.02	3 (15%)	27,32,35	2.31	5 (18%)
1	7MG	A	527	1	23,26,27	2.98	7 (30%)	27,39,42	2.09	8 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	DB	516	1	-	0/7/25/26	0/2/2/2
2	OMG	EB	2251	4,2	-	1/5/27/28	0/3/3/3
1	5MC	A	1400	1	-	1/7/25/26	0/2/2/2
2	PSU	B	1911	2	-	0/7/25/26	0/2/2/2
4	5MU	IA	54	4,56	-	0/7/25/26	0/2/2/2
2	5MU	EB	1939	2	-	0/7/25/26	0/2/2/2
1	5MC	DB	1407	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	1/7/29/30	0/3/3/3
4	5MC	IA	32	4	-	0/7/25/26	0/2/2/2
4	4SU	D	8	4	-	2/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
2	5MC	B	1962	2	-	0/7/25/26	0/2/2/2
1	M2G	DB	966	1	-	0/7/29/30	0/3/3/3
1	4OC	DB	1402	1	-	2/9/29/30	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
4	5MU	GB	54	4	-	0/7/25/26	0/2/2/2
1	2MG	DB	1207	1	-	0/5/27/28	0/3/3/3
2	PSU	EB	2605	2	-	0/7/25/26	0/2/2/2
4	4SU	IA	8	4	-	0/7/25/26	0/2/2/2
4	5MC	GB	32	4	-	0/7/25/26	0/2/2/2
2	PSU	EB	1917	2	-	0/7/25/26	0/2/2/2
1	MA6	DB	1519	1	-	3/7/29/30	0/3/3/3
45	0TD	WC	92	45	-	5/7/12/14	-
2	4OC	B	1920	2	-	4/9/27/30	0/2/2/2
1	MA6	A	1519	1	-	3/7/29/30	0/3/3/3
1	UR3	DB	1498	1	-	0/7/25/26	0/2/2/2
2	2MU	B	2552	2	-	0/9/27/28	0/2/2/2
2	PSU	B	1917	2	-	0/7/25/26	0/2/2/2
1	5MC	DB	967	1	-	0/7/25/26	0/2/2/2
2	PSU	EB	1911	2	-	0/7/25/26	0/2/2/2
4	PSU	LC	55	4	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
2	5MC	B	1942	2	-	0/7/25/26	0/2/2/2
2	2MA	B	2503	2	-	1/3/25/26	0/3/3/3
4	5MU	D	54	4	-	0/7/25/26	0/2/2/2
4	PSU	GB	55	4	-	0/7/25/26	0/2/2/2
4	PSU	IA	55	4	-	0/7/25/26	0/2/2/2
1	M2G	A	966	1	-	0/7/29/30	0/3/3/3
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
2	PSU	B	2605	2	-	0/7/25/26	0/2/2/2
4	4SU	GB	8	4	-	2/7/25/26	0/2/2/2
4	5MC	D	32	4	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5MU	B	1915	2	-	0/7/25/26	0/2/2/2
45	0TD	TA	92	45	-	4/7/12/14	-
1	5MC	DB	1400	1	-	2/7/25/26	0/2/2/2
1	7MG	DB	527	1	-	2/7/37/38	0/3/3/3
2	2MU	EB	2552	56,2	-	0/9/27/28	0/2/2/2
4	PSU	D	55	4	-	0/7/25/26	0/2/2/2
4	4SU	LC	8	4	-	0/7/25/26	0/2/2/2
2	5MC	EB	1942	2	-	0/7/25/26	0/2/2/2
2	4OC	EB	1920	2	-	3/9/27/30	0/2/2/2
2	5MC	EB	1962	56,2	-	0/7/25/26	0/2/2/2
2	2MA	EB	2503	2	-	1/3/25/26	0/3/3/3
2	OMG	B	2251	4,2	-	1/5/27/28	0/3/3/3
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	5MC	DB	1404	1	-	0/7/25/26	0/2/2/2
1	MA6	DB	1518	1	-	1/7/29/30	0/3/3/3
4	5MC	LC	32	4	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
2	5MU	B	1939	2	-	0/7/25/26	0/2/2/2
4	5MU	LC	54	4	-	0/7/25/26	0/2/2/2
2	5MU	EB	1915	2	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3

The worst 5 of 233 bond length outliers are listed below:

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

The worst 5 of 294 bond angle outliers are listed below:

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

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1519	MA6	O4'-C4'-C5'-O5'
2	B	1920	4OC	C1'-C2'-O2'-CM2
2	B	2251	OMG	C1'-C2'-O2'-CM2
45	TA	92	0TD	CA-CB-SB-CSB
45	TA	92	0TD	SB-CB-CG-OD2

There are no ring outliers.

31 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	EB	1939	5MU	1	0
1	DB	1407	5MC	1	0
1	A	1518	MA6	1	0
1	A	967	5MC	1	0
1	DB	966	M2G	1	0
1	DB	1402	4OC	1	0
4	GB	54	5MU	1	0
2	EB	1917	PSU	1	0
1	DB	1519	MA6	1	0
45	WC	92	0TD	3	0
2	B	1920	4OC	1	0
1	DB	1498	UR3	1	0
2	B	2552	2MU	2	0
1	DB	967	5MC	1	0
2	B	2503	2MA	3	0
4	D	54	5MU	1	0
4	GB	55	PSU	1	0
1	A	966	M2G	1	0
1	A	1498	UR3	1	0
4	GB	8	4SU	1	0
2	B	1915	5MU	1	0
45	TA	92	0TD	3	0
2	EB	2552	2MU	2	0
4	D	55	PSU	1	0
2	EB	1942	5MC	1	0
2	EB	2503	2MA	4	0
1	A	1407	5MC	1	0
1	DB	1518	MA6	1	0
1	A	1402	4OC	2	0
2	B	1939	5MU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	EB	1915	5MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Warning: The R factor obtained from EDS is 0.2204, 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%)	-0.07	32 (2%) 63 41	94, 141, 205, 274	0
1	DB	1495/1507 (99%)	0.03	28 (1%) 66 44	100, 130, 190, 262	0
2	B	2869/2880 (99%)	-0.17	40 (1%) 73 51	77, 97, 192, 252	0
2	EB	2869/2880 (99%)	-0.02	52 (1%) 67 45	88, 112, 211, 267	0
3	C	120/120 (100%)	-0.24	0 100 100	108, 129, 142, 160	0
3	FB	120/120 (100%)	0.11	1 (0%) 82 64	119, 157, 177, 190	0
4	D	73/77 (94%)	0.17	5 (6%) 25 17	112, 214, 233, 236	0
4	GB	73/77 (94%)	0.19	2 (2%) 56 35	131, 210, 227, 231	0
4	IA	73/77 (94%)	0.16	6 (8%) 19 13	90, 125, 134, 141	0
4	LC	73/77 (94%)	-0.07	2 (2%) 56 35	108, 132, 144, 148	0
5	E	275/275 (100%)	-0.06	9 (3%) 49 30	79, 88, 98, 107	0
5	HB	275/275 (100%)	-0.05	10 (3%) 46 29	86, 102, 112, 122	0
6	F	204/206 (99%)	-0.09	1 (0%) 87 72	78, 102, 123, 133	0
6	IB	204/206 (99%)	-0.14	2 (0%) 79 59	90, 116, 136, 147	0
7	G	202/205 (98%)	-0.31	0 100 100	71, 100, 121, 131	0
7	JB	202/205 (98%)	-0.12	6 (2%) 52 33	84, 115, 132, 137	0
8	H	181/182 (99%)	-0.01	8 (4%) 39 25	132, 140, 158, 161	0
8	KB	181/182 (99%)	0.08	5 (2%) 55 34	146, 166, 178, 180	0
9	I	174/180 (96%)	-0.14	5 (2%) 54 34	112, 121, 128, 139	0
9	LB	174/180 (96%)	0.55	17 (9%) 14 10	158, 192, 207, 212	0
10	J	146/148 (98%)	0.10	6 (4%) 42 26	102, 140, 148, 150	0
10	MB	146/148 (98%)	0.40	11 (7%) 22 15	123, 153, 164, 166	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
11	K	140/140 (100%)	-0.18	1 (0%) 84 66	84, 100, 119, 128	0
11	NB	140/140 (100%)	0.08	9 (6%) 27 18	100, 122, 137, 142	0
12	L	122/122 (100%)	-0.13	4 (3%) 49 30	87, 100, 110, 114	0
12	OB	122/122 (100%)	-0.11	3 (2%) 58 37	97, 107, 115, 118	0
13	M	150/150 (100%)	0.03	6 (4%) 43 26	76, 106, 131, 135	0
13	PB	150/150 (100%)	0.09	6 (4%) 43 26	93, 118, 148, 150	0
14	N	141/141 (100%)	-0.09	4 (2%) 55 34	94, 105, 118, 126	0
14	QB	141/141 (100%)	-0.02	1 (0%) 84 66	106, 126, 140, 148	0
15	O	118/118 (100%)	-0.25	0 100 100	87, 101, 114, 120	0
15	RB	118/118 (100%)	-0.20	0 100 100	97, 111, 121, 125	0
16	P	110/112 (98%)	-0.19	2 (1%) 67 45	116, 127, 132, 134	0
16	SB	110/112 (98%)	0.07	1 (0%) 81 61	139, 155, 162, 165	0
17	Q	137/146 (93%)	-0.11	5 (3%) 46 29	99, 111, 155, 184	0
17	TB	137/146 (93%)	-0.02	3 (2%) 62 40	108, 117, 147, 158	0
18	R	117/118 (99%)	-0.28	0 100 100	78, 95, 108, 111	0
18	UB	117/118 (99%)	0.10	5 (4%) 40 25	92, 116, 131, 137	0
19	S	101/101 (100%)	-0.42	0 100 100	80, 105, 116, 121	0
19	VB	101/101 (100%)	-0.18	1 (0%) 79 59	96, 127, 136, 141	0
20	T	112/113 (99%)	-0.42	0 100 100	77, 90, 113, 123	0
20	WB	112/113 (99%)	-0.26	1 (0%) 81 61	89, 102, 121, 133	0
21	U	95/96 (98%)	-0.24	1 (1%) 77 56	87, 93, 104, 111	0
21	XB	95/96 (98%)	0.07	3 (3%) 50 31	107, 121, 129, 131	0
22	V	107/110 (97%)	-0.05	2 (1%) 66 44	97, 106, 122, 125	0
22	YB	107/110 (97%)	0.32	5 (4%) 37 24	114, 124, 143, 146	0
23	W	189/206 (91%)	-0.18	2 (1%) 77 56	111, 129, 139, 142	0
23	ZB	189/206 (91%)	-0.13	1 (0%) 87 72	132, 151, 162, 167	0
24	AC	84/85 (98%)	0.48	9 (10%) 12 9	116, 122, 137, 141	0
24	X	84/85 (98%)	0.35	10 (11%) 10 8	100, 105, 124, 130	0
25	BC	97/98 (98%)	0.34	6 (6%) 28 18	92, 116, 142, 154	0
25	Y	97/98 (98%)	0.26	7 (7%) 23 16	82, 99, 125, 135	0
26	CC	70/72 (97%)	0.23	3 (4%) 40 25	126, 133, 136, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
26	Z	70/72 (97%)	-0.04	6 (8%)	18 12	95, 101, 106, 112	0
27	AA	60/60 (100%)	-0.41	0	100 100	92, 104, 123, 130	0
27	DC	60/60 (100%)	-0.17	0	100 100	108, 120, 133, 138	0
28	BA	69/71 (97%)	-0.10	0	100 100	162, 179, 201, 205	0
28	EC	69/71 (97%)	-0.04	0	100 100	189, 197, 207, 209	0
29	CA	59/60 (98%)	-0.05	1 (1%)	69 47	79, 106, 122, 126	0
29	FC	59/60 (98%)	-0.11	1 (1%)	69 47	88, 116, 131, 133	0
30	DA	53/54 (98%)	0.38	3 (5%)	30 19	161, 165, 168, 169	0
30	GC	53/54 (98%)	0.66	6 (11%)	11 8	188, 192, 195, 195	0
31	EA	48/49 (97%)	0.32	5 (10%)	13 9	72, 77, 87, 89	0
31	HC	48/49 (97%)	0.54	2 (4%)	41 25	89, 92, 102, 107	0
32	FA	64/65 (98%)	0.07	2 (3%)	51 32	83, 94, 110, 118	0
32	IC	64/65 (98%)	0.02	3 (4%)	37 24	98, 109, 127, 132	0
33	GA	37/37 (100%)	0.87	7 (18%)	4 4	154, 154, 155, 155	0
33	JC	37/37 (100%)	1.14	9 (24%)	2 2	167, 167, 167, 167	0
34	HA	11/27 (40%)	0.61	1 (9%)	16 11	120, 128, 144, 147	0
34	KC	11/27 (40%)	0.33	1 (9%)	16 11	124, 129, 145, 145	0
35	JA	234/256 (91%)	-0.02	7 (2%)	52 33	148, 164, 183, 190	0
35	MC	234/256 (91%)	-0.01	6 (2%)	57 36	139, 159, 176, 188	0
36	KA	206/239 (86%)	-0.14	5 (2%)	59 38	143, 156, 173, 176	0
36	NC	206/239 (86%)	-0.09	2 (0%)	79 59	142, 155, 172, 176	0
37	LA	208/209 (99%)	0.58	18 (8%)	17 12	132, 148, 157, 161	0
37	OC	208/209 (99%)	0.35	18 (8%)	17 12	117, 128, 135, 139	0
38	MA	151/162 (93%)	0.08	6 (3%)	43 26	125, 138, 145, 157	0
38	PC	151/162 (93%)	-0.05	9 (5%)	29 19	114, 125, 133, 144	0
39	NA	101/101 (100%)	-0.24	1 (0%)	79 59	119, 129, 134, 144	0
39	QC	101/101 (100%)	-0.28	2 (1%)	64 43	125, 134, 141, 147	0
40	OA	155/156 (99%)	0.13	8 (5%)	34 21	141, 155, 164, 165	0
40	RC	155/156 (99%)	0.12	9 (5%)	30 19	142, 153, 160, 163	0
41	PA	138/138 (100%)	0.03	7 (5%)	34 22	124, 141, 147, 152	0
41	SC	138/138 (100%)	-0.21	1 (0%)	84 66	116, 129, 137, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
42	QA	127/128 (99%)	0.21	11 (8%) 17 12	134, 179, 187, 189	0
42	TC	127/128 (99%)	0.22	9 (7%) 23 16	145, 173, 181, 183	0
43	RA	98/105 (93%)	0.22	2 (2%) 64 43	144, 182, 195, 196	0
43	UC	98/105 (93%)	0.17	2 (2%) 64 43	148, 176, 181, 183	0
44	SA	116/129 (89%)	0.02	4 (3%) 48 30	108, 126, 133, 142	0
44	VC	116/129 (89%)	0.03	7 (6%) 29 19	109, 130, 137, 143	0
45	TA	121/132 (91%)	0.06	3 (2%) 58 37	115, 121, 128, 132	0
45	WC	121/132 (91%)	-0.18	3 (2%) 58 37	108, 114, 123, 128	0
46	UA	117/126 (92%)	0.28	11 (9%) 15 11	132, 167, 173, 174	0
46	XC	117/126 (92%)	0.25	9 (7%) 21 14	147, 178, 186, 187	0
47	VA	60/61 (98%)	0.25	2 (3%) 49 30	151, 158, 167, 168	0
47	YC	60/61 (98%)	0.32	3 (5%) 35 22	152, 160, 176, 177	0
48	WA	88/89 (98%)	-0.16	2 (2%) 61 39	108, 126, 138, 140	0
48	ZC	88/89 (98%)	-0.34	2 (2%) 61 39	110, 127, 133, 135	0
49	AD	83/88 (94%)	0.07	5 (6%) 29 19	118, 123, 137, 154	0
49	XA	83/88 (94%)	0.54	8 (9%) 15 11	137, 156, 170, 187	0
50	BD	99/105 (94%)	0.13	8 (8%) 19 13	111, 120, 124, 126	0
50	YA	99/105 (94%)	0.18	5 (5%) 34 22	109, 128, 135, 138	0
51	CD	70/88 (79%)	-0.11	1 (1%) 73 51	125, 134, 141, 144	0
51	ZA	70/88 (79%)	-0.12	3 (4%) 40 25	120, 130, 138, 141	0
52	AB	83/93 (89%)	0.01	0 100 100	143, 170, 175, 177	0
52	DD	83/93 (89%)	0.13	2 (2%) 59 38	158, 183, 188, 189	0
53	BB	99/106 (93%)	0.40	11 (11%) 12 9	141, 154, 170, 172	0
53	ED	99/106 (93%)	0.15	7 (7%) 23 16	119, 140, 155, 156	0
54	CB	24/27 (88%)	1.15	4 (16%) 5 5	155, 165, 170, 174	0
54	FD	24/27 (88%)	1.35	7 (29%) 1 2	160, 168, 173, 175	0
55	GD	255/365 (69%)	-0.09	8 (3%) 51 32	94, 137, 163, 184	0
55	HD	255/365 (69%)	-0.06	8 (3%) 51 32	117, 143, 169, 180	0
All	All	21472/22222 (96%)	-0.01	642 (2%) 52 33	71, 124, 185, 274	0

The worst 5 of 642 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	BC	2	SER	11.3
25	Y	2	SER	9.9
24	AC	3	HIS	8.4
24	X	3	HIS	8.0
9	LB	71	LEU	6.9

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

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

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	5MC	IA	32	21/22	0.92	0.11	126,126,126,127	0
1	7MG	DB	527	24/25	0.92	0.11	117,118,119,120	0
2	5MU	B	1939	21/22	0.92	0.13	84,85,86,86	0
1	PSU	A	516	20/21	0.93	0.07	132,134,137,137	0
2	5MC	EB	1942	21/22	0.93	0.08	101,103,104,104	0
2	5MC	EB	1962	21/22	0.93	0.11	98,99,101,102	0
1	5MC	DB	1400	21/22	0.93	0.11	119,121,123,124	0
2	5MC	B	1942	21/22	0.93	0.09	90,92,93,94	0
1	UR3	DB	1498	21/22	0.93	0.14	111,111,112,112	0
2	4OC	B	1920	21/23	0.93	0.10	102,104,106,107	0
4	4SU	LC	8	20/21	0.93	0.13	130,133,134,134	0
1	M2G	DB	966	25/26	0.93	0.10	130,132,134,134	0
1	5MC	DB	967	21/22	0.93	0.08	131,133,135,136	0
2	2MA	EB	2503	23/24	0.94	0.10	88,89,90,90	0
1	4OC	A	1402	22/23	0.94	0.11	115,116,117,117	0
2	PSU	B	1917	20/21	0.94	0.07	107,108,111,112	0
1	5MC	A	1407	21/22	0.94	0.08	104,105,107,108	0
1	MA6	DB	1518	24/25	0.94	0.17	102,104,105,106	0
1	7MG	A	527	24/25	0.94	0.11	122,124,125,126	0
2	2MU	EB	2552	21/23	0.95	0.14	96,97,98,98	0
1	M2G	A	966	25/26	0.95	0.10	129,130,132,132	0
2	5MC	B	1962	21/22	0.95	0.07	92,93,95,97	0
2	PSU	EB	1911	20/21	0.95	0.07	113,116,117,118	0
1	5MC	A	1404	21/22	0.95	0.09	106,107,108,109	0
2	PSU	B	2605	20/21	0.95	0.10	79,81,81,81	0
1	MA6	A	1518	24/25	0.96	0.11	99,102,104,104	0
1	MA6	DB	1519	24/25	0.96	0.13	103,105,106,106	0
2	2MA	B	2503	23/24	0.96	0.08	78,78,79,79	0
1	5MC	DB	1407	21/22	0.96	0.09	107,109,110,110	0
2	OMG	EB	2251	24/25	0.96	0.11	95,96,98,98	0
1	UR3	A	1498	21/22	0.96	0.11	107,108,109,109	0
2	2MU	B	2552	21/23	0.97	0.13	84,86,86,86	0
1	MA6	A	1519	24/25	0.97	0.10	100,102,104,104	0
2	PSU	EB	2605	20/21	0.97	0.08	89,90,91,91	0
1	5MC	DB	1404	21/22	0.97	0.09	107,108,109,109	0

6.3 Carbohydrates

There are no 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	EB	3285	1/1	-0.40	0.20	220,220,220,220	0
56	MG	EB	3189	1/1	-0.39	0.12	241,241,241,241	0
56	MG	B	3188	1/1	-0.38	0.35	217,217,217,217	0
56	MG	B	3142	1/1	-0.33	0.19	214,214,214,214	0
56	MG	D	105	1/1	-0.29	0.20	208,208,208,208	0
56	MG	EB	3170	1/1	-0.29	0.15	187,187,187,187	0
56	MG	LB	204	1/1	-0.28	0.23	197,197,197,197	0
56	MG	A	1746	1/1	-0.22	0.35	173,173,173,173	0
56	MG	A	1688	1/1	-0.22	0.20	167,167,167,167	0
56	MG	DB	1736	1/1	-0.16	0.25	212,212,212,212	0
56	MG	RC	201	1/1	-0.10	0.39	142,142,142,142	0
56	MG	B	3391	1/1	-0.08	0.15	240,240,240,240	0
56	MG	DB	1729	1/1	-0.08	0.18	159,159,159,159	0
56	MG	EB	3026	1/1	-0.07	0.14	175,175,175,175	0
56	MG	EB	3016	1/1	-0.05	0.35	243,243,243,243	0
56	MG	EB	3195	1/1	-0.01	0.22	152,152,152,152	0
56	MG	A	1711	1/1	-0.01	0.37	130,130,130,130	0
56	MG	A	1728	1/1	0.00	0.20	160,160,160,160	0
56	MG	GB	103	1/1	-0.00	0.23	211,211,211,211	0
56	MG	A	1680	1/1	0.00	0.37	176,176,176,176	0
56	MG	B	3352	1/1	0.00	0.20	183,183,183,183	0
56	MG	DB	1681	1/1	0.01	0.33	149,149,149,149	0
56	MG	B	3288	1/1	0.03	0.22	208,208,208,208	0
56	MG	VA	101	1/1	0.03	0.44	140,140,140,140	0
56	MG	A	1640	1/1	0.05	0.39	134,134,134,134	0
56	MG	DB	1690	1/1	0.06	0.31	139,139,139,139	0
56	MG	RA	201	1/1	0.08	0.18	165,165,165,165	0
56	MG	B	3392	1/1	0.08	0.18	192,192,192,192	0
56	MG	A	1755	1/1	0.08	0.19	176,176,176,176	0
56	MG	EB	2945	1/1	0.09	0.52	139,139,139,139	0
56	MG	B	3025	1/1	0.10	0.35	234,234,234,234	0
56	MG	EB	3014	1/1	0.11	0.21	136,136,136,136	0
56	MG	A	1729	1/1	0.11	0.40	152,152,152,152	0
56	MG	B	3304	1/1	0.12	0.28	237,237,237,237	0
56	MG	KB	201	1/1	0.12	0.19	173,173,173,173	0
56	MG	KA	301	1/1	0.13	0.34	157,157,157,157	0
56	MG	B	3175	1/1	0.13	0.45	154,154,154,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	W	302	1/1	0.13	0.38	129,129,129,129	0
56	MG	GB	102	1/1	0.13	0.13	204,204,204,204	0
56	MG	W	310	1/1	0.14	0.13	134,134,134,134	0
56	MG	B	2960	1/1	0.16	0.57	223,223,223,223	0
56	MG	GD	404	1/1	0.17	0.27	135,135,135,135	0
56	MG	B	3315	1/1	0.20	0.13	203,203,203,203	0
56	MG	A	1707	1/1	0.20	0.20	163,163,163,163	0
56	MG	EB	3177	1/1	0.20	0.21	122,122,122,122	0
56	MG	B	3384	1/1	0.20	0.25	161,161,161,161	0
56	MG	EB	3251	1/1	0.22	0.09	158,158,158,158	0
56	MG	DB	1742	1/1	0.22	0.26	142,142,142,142	0
56	MG	B	2966	1/1	0.22	0.43	106,106,106,106	0
56	MG	A	1742	1/1	0.22	0.23	179,179,179,179	0
56	MG	Q	202	1/1	0.23	0.22	148,148,148,148	0
56	MG	EB	2936	1/1	0.23	0.48	128,128,128,128	0
56	MG	FB	216	1/1	0.23	0.36	141,141,141,141	0
56	MG	DB	1761	1/1	0.25	0.19	152,152,152,152	0
56	MG	GB	101	1/1	0.25	0.21	202,202,202,202	0
56	MG	A	1627	1/1	0.25	0.26	127,127,127,127	0
56	MG	EB	2944	1/1	0.25	0.26	102,102,102,102	0
56	MG	A	1745	1/1	0.25	0.19	219,219,219,219	0
56	MG	EB	2982	1/1	0.25	0.40	133,133,133,133	0
56	MG	DB	1617	1/1	0.25	0.44	136,136,136,136	0
56	MG	TC	201	1/1	0.25	0.27	177,177,177,177	0
56	MG	B	3274	1/1	0.25	0.32	118,118,118,118	0
56	MG	EB	3132	1/1	0.26	0.33	140,140,140,140	0
56	MG	XC	201	1/1	0.26	0.14	171,171,171,171	0
56	MG	EB	3050	1/1	0.26	0.36	160,160,160,160	0
56	MG	EB	3067	1/1	0.27	0.17	131,131,131,131	0
56	MG	GB	105	1/1	0.27	0.24	172,172,172,172	0
56	MG	LB	202	1/1	0.28	0.32	181,181,181,181	0
56	MG	EB	3102	1/1	0.28	0.21	126,126,126,126	0
56	MG	D	102	1/1	0.28	0.15	210,210,210,210	0
56	MG	DB	1601	1/1	0.29	0.40	122,122,122,122	0
56	MG	B	3124	1/1	0.29	0.22	155,155,155,155	0
56	MG	EB	3120	1/1	0.29	0.39	143,143,143,143	0
56	MG	JC	102	1/1	0.29	0.17	146,146,146,146	0
56	MG	EB	3019	1/1	0.30	0.30	113,113,113,113	0
56	MG	DB	1685	1/1	0.30	0.19	177,177,177,177	0
56	MG	A	1618	1/1	0.31	0.34	126,126,126,126	0
56	MG	A	1634	1/1	0.31	0.50	134,134,134,134	0
56	MG	EB	3103	1/1	0.31	0.41	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	EB	2971	1/1	0.31	0.40	112,112,112,112	0
56	MG	DB	1602	1/1	0.32	0.54	97,97,97,97	0
56	MG	DB	1703	1/1	0.32	0.44	163,163,163,163	0
56	MG	DB	1714	1/1	0.32	0.38	99,99,99,99	0
56	MG	B	3262	1/1	0.32	0.45	143,143,143,143	0
56	MG	LB	205	1/1	0.32	0.10	197,197,197,197	0
56	MG	B	2908	1/1	0.33	0.33	95,95,95,95	0
56	MG	A	1675	1/1	0.33	0.30	118,118,118,118	0
56	MG	FB	208	1/1	0.34	0.15	171,171,171,171	0
56	MG	DB	1623	1/1	0.34	0.28	121,121,121,121	0
56	MG	DB	1686	1/1	0.34	0.35	124,124,124,124	0
56	MG	VA	102	1/1	0.35	0.11	159,159,159,159	0
56	MG	EB	3259	1/1	0.35	0.24	141,141,141,141	0
56	MG	B	3176	1/1	0.35	0.22	144,144,144,144	0
56	MG	DB	1648	1/1	0.36	0.17	143,143,143,143	0
56	MG	A	1659	1/1	0.36	0.16	153,153,153,153	0
56	MG	B	3134	1/1	0.36	0.36	129,129,129,129	0
56	MG	FB	212	1/1	0.36	0.33	160,160,160,160	0
56	MG	A	1635	1/1	0.36	0.25	138,138,138,138	0
56	MG	B	3287	1/1	0.36	0.25	151,151,151,151	0
56	MG	B	3022	1/1	0.36	0.28	118,118,118,118	0
56	MG	DB	1712	1/1	0.36	0.17	199,199,199,199	0
56	MG	A	1705	1/1	0.36	0.38	143,143,143,143	0
56	MG	JA	303	1/1	0.37	0.11	161,161,161,161	0
56	MG	A	1752	1/1	0.37	0.33	160,160,160,160	0
56	MG	IB	302	1/1	0.37	0.34	95,95,95,95	0
56	MG	EB	2966	1/1	0.38	0.40	99,99,99,99	0
56	MG	A	1662	1/1	0.38	0.26	154,154,154,154	0
56	MG	LA	301	1/1	0.38	0.19	139,139,139,139	0
56	MG	GD	402	1/1	0.38	0.20	124,124,124,124	0
56	MG	MC	301	1/1	0.38	0.23	149,149,149,149	0
56	MG	FB	205	1/1	0.39	0.41	143,143,143,143	0
56	MG	EB	3201	1/1	0.39	0.24	133,133,133,133	0
56	MG	JA	301	1/1	0.39	0.22	143,143,143,143	0
56	MG	DB	1615	1/1	0.39	0.68	122,122,122,122	0
56	MG	A	1656	1/1	0.39	0.18	229,229,229,229	0
56	MG	A	1622	1/1	0.40	0.37	147,147,147,147	0
56	MG	LC	102	1/1	0.40	0.24	124,124,124,124	0
56	MG	A	1633	1/1	0.40	0.20	140,140,140,140	0
56	MG	DB	1654	1/1	0.40	0.21	165,165,165,165	0
56	MG	TB	203	1/1	0.41	0.19	152,152,152,152	0
56	MG	A	1726	1/1	0.41	0.22	167,167,167,167	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DB	1645	1/1	0.41	0.28	139,139,139,139	0
56	MG	DB	1733	1/1	0.42	0.38	127,127,127,127	0
56	MG	A	1657	1/1	0.42	0.34	164,164,164,164	0
56	MG	A	1699	1/1	0.43	0.28	143,143,143,143	0
56	MG	B	3282	1/1	0.43	0.23	147,147,147,147	0
56	MG	FB	203	1/1	0.43	0.37	125,125,125,125	0
56	MG	B	3119	1/1	0.43	0.46	100,100,100,100	0
56	MG	A	1649	1/1	0.43	0.47	125,125,125,125	0
56	MG	SB	201	1/1	0.44	0.09	149,149,149,149	0
56	MG	EB	2969	1/1	0.44	0.29	127,127,127,127	0
56	MG	D	103	1/1	0.44	0.09	175,175,175,175	0
56	MG	EB	2925	1/1	0.44	0.55	88,88,88,88	0
56	MG	EB	2995	1/1	0.44	0.30	152,152,152,152	0
56	MG	GD	405	1/1	0.44	0.28	117,117,117,117	0
56	MG	LC	105	1/1	0.45	0.15	136,136,136,136	0
56	MG	EB	2989	1/1	0.45	0.30	179,179,179,179	0
56	MG	A	1647	1/1	0.45	0.40	149,149,149,149	0
56	MG	DB	1725	1/1	0.45	0.34	166,166,166,166	0
56	MG	A	1623	1/1	0.45	0.54	132,132,132,132	0
56	MG	FB	206	1/1	0.45	0.38	124,124,124,124	0
56	MG	B	3086	1/1	0.45	0.14	151,151,151,151	0
56	MG	P	201	1/1	0.45	0.13	129,129,129,129	0
56	MG	DB	1610	1/1	0.46	0.85	109,109,109,109	0
56	MG	A	1661	1/1	0.46	0.37	145,145,145,145	0
56	MG	EB	3191	1/1	0.46	0.19	151,151,151,151	0
56	MG	A	1758	1/1	0.46	0.19	188,188,188,188	0
56	MG	DB	1758	1/1	0.46	0.28	207,207,207,207	0
56	MG	A	1615	1/1	0.46	0.30	118,118,118,118	0
56	MG	EB	3066	1/1	0.46	0.19	172,172,172,172	0
56	MG	C	206	1/1	0.47	0.30	130,130,130,130	0
56	MG	EB	3266	1/1	0.47	0.23	138,138,138,138	0
56	MG	B	3154	1/1	0.47	0.28	136,136,136,136	0
56	MG	FB	201	1/1	0.47	0.42	117,117,117,117	0
56	MG	LC	106	1/1	0.47	0.12	124,124,124,124	0
56	MG	C	202	1/1	0.47	0.20	106,106,106,106	0
56	MG	B	3180	1/1	0.48	0.22	179,179,179,179	0
56	MG	DB	1756	1/1	0.48	0.33	119,119,119,119	0
56	MG	C	213	1/1	0.48	0.20	139,139,139,139	0
56	MG	EB	3181	1/1	0.48	0.38	155,155,155,155	0
56	MG	LC	108	1/1	0.48	0.11	125,125,125,125	0
56	MG	A	1636	1/1	0.48	0.25	140,140,140,140	0
56	MG	DB	1640	1/1	0.49	0.31	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	2936	1/1	0.49	0.62	94,94,94,94	0
56	MG	DB	1627	1/1	0.49	0.31	104,104,104,104	0
56	MG	AC	102	1/1	0.49	0.48	98,98,98,98	0
56	MG	UC	201	1/1	0.49	0.34	164,164,164,164	0
56	MG	DB	1722	1/1	0.49	0.17	117,117,117,117	0
56	MG	ZC	101	1/1	0.49	0.10	126,126,126,126	0
56	MG	DB	1628	1/1	0.49	0.23	115,115,115,115	0
56	MG	FB	217	1/1	0.49	0.18	139,139,139,139	0
56	MG	EB	3250	1/1	0.49	0.23	134,134,134,134	0
56	MG	DB	1684	1/1	0.50	0.27	133,133,133,133	0
56	MG	EB	3022	1/1	0.50	0.39	114,114,114,114	0
56	MG	B	3123	1/1	0.50	0.33	103,103,103,103	0
56	MG	A	1611	1/1	0.50	0.26	149,149,149,149	0
56	MG	K	202	1/1	0.50	0.33	105,105,105,105	0
56	MG	B	3010	1/1	0.50	0.30	116,116,116,116	0
56	MG	WA	102	1/1	0.50	0.14	124,124,124,124	0
56	MG	A	1691	1/1	0.50	0.20	113,113,113,113	0
56	MG	EB	2951	1/1	0.51	0.26	95,95,95,95	0
56	MG	EB	3142	1/1	0.51	0.38	136,136,136,136	0
56	MG	EB	2992	1/1	0.51	0.39	91,91,91,91	0
56	MG	DB	1709	1/1	0.51	0.13	107,107,107,107	0
56	MG	A	1717	1/1	0.51	0.74	144,144,144,144	0
56	MG	YA	201	1/1	0.51	0.28	106,106,106,106	0
56	MG	EB	2979	1/1	0.51	0.49	111,111,111,111	0
56	MG	DB	1668	1/1	0.51	0.26	99,99,99,99	0
56	MG	EB	2978	1/1	0.52	0.32	103,103,103,103	0
56	MG	B	2944	1/1	0.52	0.31	115,115,115,115	0
56	MG	A	1735	1/1	0.52	0.15	131,131,131,131	0
56	MG	DB	1621	1/1	0.52	0.32	110,110,110,110	0
56	MG	JB	302	1/1	0.52	0.12	116,116,116,116	0
56	MG	EB	2939	1/1	0.52	0.41	99,99,99,99	0
56	MG	B	3026	1/1	0.52	0.18	116,116,116,116	0
56	MG	LB	203	1/1	0.52	0.21	168,168,168,168	0
56	MG	EB	3059	1/1	0.52	0.22	122,122,122,122	0
56	MG	B	3246	1/1	0.53	0.14	125,125,125,125	0
56	MG	EB	2984	1/1	0.53	0.30	127,127,127,127	0
56	MG	EB	3186	1/1	0.53	0.22	124,124,124,124	0
56	MG	DB	1660	1/1	0.53	0.20	131,131,131,131	0
56	MG	B	3218	1/1	0.53	0.11	109,109,109,109	0
56	MG	DB	1718	1/1	0.53	0.28	145,145,145,145	0
56	MG	DB	1717	1/1	0.54	0.21	124,124,124,124	0
56	MG	A	1701	1/1	0.54	0.45	141,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	EB	2942	1/1	0.54	0.23	138,138,138,138	0
56	MG	IA	102	1/1	0.54	0.28	124,124,124,124	0
56	MG	B	3131	1/1	0.54	0.23	112,112,112,112	0
56	MG	A	1703	1/1	0.54	0.16	136,136,136,136	0
56	MG	B	2903	1/1	0.54	0.44	107,107,107,107	0
56	MG	CD	102	1/1	0.54	0.12	122,122,122,122	0
56	MG	EB	3128	1/1	0.54	0.30	161,161,161,161	0
56	MG	EB	3049	1/1	0.54	0.27	106,106,106,106	0
56	MG	EB	3134	1/1	0.54	0.26	154,154,154,154	0
56	MG	EB	3260	1/1	0.55	0.28	220,220,220,220	0
56	MG	EB	3149	1/1	0.55	0.27	113,113,113,113	0
56	MG	HB	304	1/1	0.55	0.29	100,100,100,100	0
56	MG	DB	1657	1/1	0.55	0.17	102,102,102,102	0
56	MG	A	1704	1/1	0.55	0.30	137,137,137,137	0
56	MG	EA	101	1/1	0.55	0.17	91,91,91,91	0
56	MG	A	1613	1/1	0.55	0.47	116,116,116,116	0
56	MG	EB	2950	1/1	0.55	0.41	124,124,124,124	0
56	MG	DB	1614	1/1	0.55	0.42	94,94,94,94	0
56	MG	B	3404	1/1	0.55	0.23	121,121,121,121	0
56	MG	DB	1721	1/1	0.55	0.41	134,134,134,134	0
56	MG	EB	2911	1/1	0.55	0.55	111,111,111,111	0
56	MG	J	202	1/1	0.55	0.26	138,138,138,138	0
56	MG	W	304	1/1	0.55	0.26	119,119,119,119	0
56	MG	A	1696	1/1	0.56	0.32	152,152,152,152	0
56	MG	B	3145	1/1	0.56	0.38	123,123,123,123	0
56	MG	YB	202	1/1	0.56	0.23	116,116,116,116	0
56	MG	ZB	302	1/1	0.56	0.14	154,154,154,154	0
56	MG	DB	1697	1/1	0.56	0.31	105,105,105,105	0
56	MG	A	1738	1/1	0.56	0.40	144,144,144,144	0
56	MG	EB	3203	1/1	0.56	0.19	130,130,130,130	0
56	MG	EB	3205	1/1	0.56	0.21	138,138,138,138	0
56	MG	A	1678	1/1	0.56	0.29	145,145,145,145	0
56	MG	A	1644	1/1	0.56	0.41	114,114,114,114	0
56	MG	A	1718	1/1	0.57	0.15	171,171,171,171	0
56	MG	C	212	1/1	0.57	0.23	128,128,128,128	0
56	MG	DB	1641	1/1	0.57	0.29	146,146,146,146	0
56	MG	DB	1603	1/1	0.57	0.44	108,108,108,108	0
56	MG	A	1630	1/1	0.57	0.49	116,116,116,116	0
56	MG	B	3046	1/1	0.57	0.25	126,126,126,126	0
56	MG	EB	3138	1/1	0.57	0.09	116,116,116,116	0
56	MG	B	3251	1/1	0.57	0.15	154,154,154,154	0
56	MG	B	3261	1/1	0.57	0.10	187,187,187,187	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	LB	201	1/1	0.57	0.23	159,159,159,159	0
56	MG	EB	3047	1/1	0.57	0.47	98,98,98,98	0
56	MG	EB	2974	1/1	0.57	0.21	114,114,114,114	0
56	MG	W	311	1/1	0.57	0.11	134,134,134,134	0
56	MG	DB	1680	1/1	0.57	0.34	137,137,137,137	0
56	MG	D	106	1/1	0.57	0.18	227,227,227,227	0
56	MG	B	3063	1/1	0.57	0.30	100,100,100,100	0
56	MG	EB	3087	1/1	0.57	0.17	156,156,156,156	0
56	MG	HD	402	1/1	0.57	0.20	128,128,128,128	0
56	MG	DB	1775	1/1	0.58	0.19	143,143,143,143	0
56	MG	B	2916	1/1	0.58	0.36	93,93,93,93	0
56	MG	BB	201	1/1	0.58	0.25	131,131,131,131	0
56	MG	C	223	1/1	0.58	0.22	132,132,132,132	0
56	MG	B	2933	1/1	0.58	0.40	89,89,89,89	0
56	MG	B	3137	1/1	0.58	0.26	132,132,132,132	0
56	MG	EB	3153	1/1	0.58	0.27	103,103,103,103	0
56	MG	W	303	1/1	0.58	0.20	125,125,125,125	0
56	MG	PA	202	1/1	0.58	0.19	142,142,142,142	0
56	MG	A	1651	1/1	0.58	0.38	107,107,107,107	0
56	MG	A	1601	1/1	0.58	0.37	94,94,94,94	0
56	MG	J	201	1/1	0.58	0.28	134,134,134,134	0
56	MG	B	3150	1/1	0.58	0.23	113,113,113,113	0
56	MG	DB	1612	1/1	0.59	0.21	112,112,112,112	0
56	MG	V	502	1/1	0.59	0.28	100,100,100,100	0
56	MG	A	1721	1/1	0.59	0.21	95,95,95,95	0
56	MG	NA	202	1/1	0.59	0.11	126,126,126,126	0
56	MG	EB	2988	1/1	0.59	0.41	104,104,104,104	0
56	MG	DB	1620	1/1	0.59	0.38	126,126,126,126	0
56	MG	DB	1704	1/1	0.59	0.20	127,127,127,127	0
56	MG	DB	1707	1/1	0.59	0.17	108,108,108,108	0
56	MG	EB	3002	1/1	0.59	0.35	116,116,116,116	0
56	MG	OA	202	1/1	0.59	0.10	135,135,135,135	0
56	MG	A	1709	1/1	0.59	0.35	164,164,164,164	0
56	MG	FB	213	1/1	0.59	0.29	137,137,137,137	0
56	MG	B	2947	1/1	0.59	0.49	108,108,108,108	0
56	MG	TA	202	1/1	0.59	0.32	114,114,114,114	0
56	MG	EB	3237	1/1	0.59	0.29	123,123,123,123	0
56	MG	B	3308	1/1	0.59	0.28	109,109,109,109	0
56	MG	A	1628	1/1	0.60	0.65	116,116,116,116	0
56	MG	OA	201	1/1	0.60	0.23	142,142,142,142	0
56	MG	EB	3232	1/1	0.60	0.22	145,145,145,145	0
56	MG	DB	1606	1/1	0.60	0.23	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	DB	1607	1/1	0.60	0.74	110,110,110,110	0
56	MG	A	1681	1/1	0.60	0.25	169,169,169,169	0
56	MG	DB	1705	1/1	0.60	0.27	130,130,130,130	0
56	MG	DB	1611	1/1	0.60	0.38	101,101,101,101	0
56	MG	XC	202	1/1	0.60	0.24	157,157,157,157	0
56	MG	YC	101	1/1	0.60	0.20	158,158,158,158	0
56	MG	A	1679	1/1	0.60	0.58	116,116,116,116	0
56	MG	B	2967	1/1	0.60	0.41	125,125,125,125	0
56	MG	AC	101	1/1	0.60	0.21	115,115,115,115	0
56	MG	DB	1751	1/1	0.60	0.32	130,130,130,130	0
56	MG	EB	3200	1/1	0.60	0.31	111,111,111,111	0
56	MG	MA	202	1/1	0.60	0.13	129,129,129,129	0
56	MG	EB	3284	1/1	0.61	0.23	103,103,103,103	0
56	MG	B	2942	1/1	0.61	0.43	116,116,116,116	0
56	MG	B	3159	1/1	0.61	0.26	90,90,90,90	0
56	MG	CD	101	1/1	0.61	0.12	124,124,124,124	0
56	MG	B	3347	1/1	0.61	0.12	124,124,124,124	0
56	MG	A	1692	1/1	0.61	0.77	145,145,145,145	0
56	MG	B	3037	1/1	0.61	0.38	102,102,102,102	0
56	MG	TA	201	1/1	0.61	0.16	118,118,118,118	0
56	MG	EB	3275	1/1	0.61	0.40	135,135,135,135	0
56	MG	B	3089	1/1	0.62	0.39	86,86,86,86	0
56	MG	B	3006	1/1	0.62	0.45	97,97,97,97	0
56	MG	B	3302	1/1	0.62	0.20	105,105,105,105	0
56	MG	HB	302	1/1	0.62	0.14	120,120,120,120	0
56	MG	DB	1770	1/1	0.62	0.27	137,137,137,137	0
56	MG	DB	1773	1/1	0.62	0.35	109,109,109,109	0
56	MG	EB	3283	1/1	0.62	0.12	166,166,166,166	0
56	MG	A	1602	1/1	0.62	0.44	98,98,98,98	0
56	MG	DB	1699	1/1	0.62	0.59	106,106,106,106	0
56	MG	EB	2913	1/1	0.62	0.36	89,89,89,89	0
56	MG	B	3075	1/1	0.62	0.38	76,76,76,76	0
56	MG	DB	1667	1/1	0.62	0.20	115,115,115,115	0
56	MG	WA	101	1/1	0.62	0.12	126,126,126,126	0
56	MG	B	3126	1/1	0.62	0.17	99,99,99,99	0
56	MG	DB	1740	1/1	0.62	0.11	130,130,130,130	0
56	MG	DB	1741	1/1	0.62	0.31	135,135,135,135	0
56	MG	IA	104	1/1	0.62	0.25	123,123,123,123	0
56	MG	B	2968	1/1	0.62	0.33	97,97,97,97	0
56	MG	EB	3139	1/1	0.62	0.35	103,103,103,103	0
56	MG	B	2940	1/1	0.63	0.27	88,88,88,88	0
56	MG	B	3213	1/1	0.63	0.13	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	A	1645	1/1	0.63	0.35	137,137,137,137	0
56	MG	B	3219	1/1	0.63	0.34	131,131,131,131	0
56	MG	EB	3135	1/1	0.63	0.13	111,111,111,111	0
56	MG	B	2963	1/1	0.63	0.35	86,86,86,86	0
56	MG	DB	1677	1/1	0.63	0.28	158,158,158,158	0
56	MG	A	1694	1/1	0.63	0.12	168,168,168,168	0
56	MG	EB	3084	1/1	0.63	0.32	87,87,87,87	0
56	MG	C	216	1/1	0.63	0.24	123,123,123,123	0
56	MG	DC	101	1/1	0.63	0.20	112,112,112,112	0
56	MG	JB	301	1/1	0.63	0.50	89,89,89,89	0
56	MG	DB	1760	1/1	0.63	0.30	102,102,102,102	0
56	MG	B	3257	1/1	0.63	0.19	96,96,96,96	0
56	MG	EB	3180	1/1	0.63	0.16	114,114,114,114	0
56	MG	EB	3107	1/1	0.64	0.33	108,108,108,108	0
56	MG	W	307	1/1	0.64	0.14	125,125,125,125	0
56	MG	DB	1670	1/1	0.64	0.35	167,167,167,167	0
56	MG	B	3291	1/1	0.64	0.17	142,142,142,142	0
56	MG	EB	2909	1/1	0.64	0.60	88,88,88,88	0
56	MG	LC	101	1/1	0.64	0.15	132,132,132,132	0
56	MG	DB	1678	1/1	0.64	0.23	106,106,106,106	0
56	MG	EB	3246	1/1	0.64	0.46	105,105,105,105	0
56	MG	B	3003	1/1	0.64	0.23	84,84,84,84	0
56	MG	B	3362	1/1	0.64	0.11	118,118,118,118	0
56	MG	A	1612	1/1	0.64	0.26	118,118,118,118	0
56	MG	A	1663	1/1	0.64	0.46	113,113,113,113	0
56	MG	EB	3060	1/1	0.64	0.21	95,95,95,95	0
56	MG	EB	3271	1/1	0.64	0.09	127,127,127,127	0
56	MG	EB	3163	1/1	0.64	0.16	144,144,144,144	0
56	MG	B	3170	1/1	0.64	0.14	117,117,117,117	0
56	MG	DB	1663	1/1	0.64	0.26	96,96,96,96	0
56	MG	EB	3082	1/1	0.64	0.38	112,112,112,112	0
56	MG	DB	1691	1/1	0.64	0.19	109,109,109,109	0
56	MG	EB	3086	1/1	0.64	0.24	104,104,104,104	0
56	MG	EB	2946	1/1	0.64	0.20	124,124,124,124	0
56	MG	C	220	1/1	0.64	0.23	122,122,122,122	0
56	MG	WB	202	1/1	0.64	0.18	96,96,96,96	0
56	MG	EB	3011	1/1	0.64	0.14	163,163,163,163	0
56	MG	EB	3244	1/1	0.65	0.20	96,96,96,96	0
56	MG	B	3065	1/1	0.65	0.34	98,98,98,98	0
56	MG	B	3343	1/1	0.65	0.09	106,106,106,106	0
56	MG	C	208	1/1	0.65	0.32	99,99,99,99	0
56	MG	B	3249	1/1	0.65	0.28	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AB	3301	1/1	0.65	0.12	136,136,136,136	0
56	MG	PC	201	1/1	0.65	0.40	106,106,106,106	0
56	MG	EB	3216	1/1	0.65	0.36	129,129,129,129	0
56	MG	H	201	1/1	0.65	0.11	129,129,129,129	0
56	MG	W	308	1/1	0.65	0.14	132,132,132,132	0
56	MG	B	3195	1/1	0.66	0.26	115,115,115,115	0
56	MG	B	2951	1/1	0.66	0.34	111,111,111,111	0
56	MG	DB	1682	1/1	0.66	0.12	128,128,128,128	0
56	MG	EB	3176	1/1	0.66	0.09	106,106,106,106	0
56	MG	EB	3018	1/1	0.66	0.15	110,110,110,110	0
56	MG	EB	3179	1/1	0.66	0.39	121,121,121,121	0
56	MG	B	2953	1/1	0.66	0.42	107,107,107,107	0
56	MG	B	2984	1/1	0.66	0.36	96,96,96,96	0
56	MG	DB	1604	1/1	0.66	0.42	103,103,103,103	0
56	MG	EB	3110	1/1	0.66	0.26	120,120,120,120	0
56	MG	EB	3112	1/1	0.66	0.21	124,124,124,124	0
56	MG	EB	3035	1/1	0.66	0.60	116,116,116,116	0
56	MG	EB	3122	1/1	0.66	0.16	174,174,174,174	0
56	MG	B	3031	1/1	0.66	0.30	87,87,87,87	0
56	MG	A	1629	1/1	0.66	0.32	123,123,123,123	0
56	MG	A	1610	1/1	0.66	0.32	108,108,108,108	0
56	MG	DB	1636	1/1	0.66	0.25	137,137,137,137	0
56	MG	GD	401	1/1	0.66	0.41	95,95,95,95	0
56	MG	A	1631	1/1	0.66	0.29	131,131,131,131	0
56	MG	IA	108	1/1	0.66	0.20	130,130,130,130	0
56	MG	EB	2960	1/1	0.66	0.50	95,95,95,95	0
56	MG	EB	3076	1/1	0.66	0.34	116,116,116,116	0
56	MG	EB	2904	1/1	0.67	0.65	79,79,79,79	0
56	MG	SA	201	1/1	0.67	0.16	106,106,106,106	0
56	MG	FA	101	1/1	0.67	0.52	111,111,111,111	0
56	MG	QB	203	1/1	0.67	0.10	103,103,103,103	0
56	MG	EB	3262	1/1	0.67	0.10	112,112,112,112	0
56	MG	HA	101	1/1	0.67	0.13	123,123,123,123	0
56	MG	VB	201	1/1	0.67	0.16	114,114,114,114	0
56	MG	A	1607	1/1	0.67	0.53	92,92,92,92	0
56	MG	A	1617	1/1	0.67	0.17	100,100,100,100	0
56	MG	Q	203	1/1	0.67	0.15	106,106,106,106	0
56	MG	EB	3029	1/1	0.67	0.13	90,90,90,90	0
56	MG	EB	2941	1/1	0.67	0.37	103,103,103,103	0
56	MG	EB	3290	1/1	0.67	0.08	131,131,131,131	0
56	MG	DB	1720	1/1	0.67	0.19	143,143,143,143	0
56	MG	DB	1674	1/1	0.67	0.12	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3056	1/1	0.67	0.33	117,117,117,117	0
56	MG	B	2924	1/1	0.67	0.42	87,87,87,87	0
56	MG	DB	1726	1/1	0.67	0.21	135,135,135,135	0
56	MG	ZA	101	1/1	0.67	0.22	124,124,124,124	0
56	MG	DB	1626	1/1	0.67	0.22	111,111,111,111	0
56	MG	FB	214	1/1	0.67	0.34	128,128,128,128	0
56	MG	A	1734	1/1	0.67	0.30	110,110,110,110	0
56	MG	EB	3190	1/1	0.67	0.09	111,111,111,111	0
56	MG	C	211	1/1	0.67	0.23	119,119,119,119	0
56	MG	W	305	1/1	0.67	0.27	129,129,129,129	0
56	MG	DB	1638	1/1	0.67	0.21	103,103,103,103	0
56	MG	B	3380	1/1	0.67	0.21	97,97,97,97	0
56	MG	B	3074	1/1	0.67	0.32	94,94,94,94	0
56	MG	DB	1644	1/1	0.67	0.25	105,105,105,105	0
56	MG	DB	1698	1/1	0.67	0.34	112,112,112,112	0
56	MG	B	3225	1/1	0.67	0.21	116,116,116,116	0
56	MG	DB	1764	1/1	0.67	0.29	110,110,110,110	0
56	MG	DB	1646	1/1	0.67	0.24	101,101,101,101	0
56	MG	J	204	1/1	0.67	0.11	138,138,138,138	0
56	MG	C	217	1/1	0.67	0.16	113,113,113,113	0
56	MG	EB	2986	1/1	0.68	0.24	95,95,95,95	0
56	MG	B	2956	1/1	0.68	0.35	99,99,99,99	0
56	MG	EB	3123	1/1	0.68	0.42	103,103,103,103	0
56	MG	EB	3057	1/1	0.68	0.56	95,95,95,95	0
56	MG	B	3181	1/1	0.68	0.24	106,106,106,106	0
56	MG	DB	1766	1/1	0.68	0.31	122,122,122,122	0
56	MG	EB	3199	1/1	0.68	0.28	117,117,117,117	0
56	MG	A	1706	1/1	0.68	0.21	135,135,135,135	0
56	MG	A	1670	1/1	0.68	0.14	139,139,139,139	0
56	MG	B	3018	1/1	0.68	0.44	88,88,88,88	0
56	MG	EB	2902	1/1	0.68	0.45	89,89,89,89	0
56	MG	FB	204	1/1	0.68	0.22	130,130,130,130	0
56	MG	DB	1622	1/1	0.68	0.47	103,103,103,103	0
56	MG	QB	201	1/1	0.68	0.16	99,99,99,99	0
56	MG	B	2921	1/1	0.68	0.35	88,88,88,88	0
56	MG	EB	3235	1/1	0.68	0.14	122,122,122,122	0
56	MG	MA	201	1/1	0.68	0.38	114,114,114,114	0
56	MG	A	1604	1/1	0.68	0.54	105,105,105,105	0
56	MG	EB	3245	1/1	0.68	0.12	128,128,128,128	0
56	MG	A	1605	1/1	0.68	0.29	103,103,103,103	0
56	MG	DB	1664	1/1	0.68	0.13	137,137,137,137	0
56	MG	A	1660	1/1	0.68	0.35	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	HD	401	1/1	0.68	0.49	97,97,97,97	0
56	MG	B	3370	1/1	0.68	0.63	214,214,214,214	0
56	MG	B	3186	1/1	0.69	0.12	109,109,109,109	0
56	MG	EB	2993	1/1	0.69	0.19	88,88,88,88	0
56	MG	DB	1750	1/1	0.69	0.28	116,116,116,116	0
56	MG	DB	1671	1/1	0.69	0.39	112,112,112,112	0
56	MG	IA	103	1/1	0.69	0.31	124,124,124,124	0
56	MG	LC	103	1/1	0.69	0.48	126,126,126,126	0
56	MG	DB	1639	1/1	0.69	0.68	140,140,140,140	0
56	MG	B	3152	1/1	0.69	0.21	107,107,107,107	0
56	MG	EB	2947	1/1	0.69	0.44	106,106,106,106	0
56	MG	B	3309	1/1	0.69	0.19	111,111,111,111	0
56	MG	B	3133	1/1	0.69	0.12	169,169,169,169	0
56	MG	QC	201	1/1	0.69	0.36	120,120,120,120	0
56	MG	C	205	1/1	0.69	0.21	114,114,114,114	0
56	MG	A	1616	1/1	0.69	0.33	99,99,99,99	0
56	MG	B	2915	1/1	0.69	0.37	85,85,85,85	0
56	MG	I	201	1/1	0.69	0.15	130,130,130,130	0
56	MG	MB	201	1/1	0.69	0.16	153,153,153,153	0
56	MG	B	3051	1/1	0.69	0.34	106,106,106,106	0
56	MG	A	1730	1/1	0.69	0.29	119,119,119,119	0
56	MG	DB	1693	1/1	0.69	0.21	111,111,111,111	0
56	MG	B	3236	1/1	0.69	0.09	122,122,122,122	0
56	MG	TB	205	1/1	0.69	0.05	121,121,121,121	0
56	MG	J	205	1/1	0.69	0.14	134,134,134,134	0
56	MG	A	1698	1/1	0.69	0.20	160,160,160,160	0
56	MG	EB	2935	1/1	0.69	0.46	98,98,98,98	0
56	MG	EB	3072	1/1	0.69	0.37	98,98,98,98	0
56	MG	B	3151	1/1	0.69	0.22	105,105,105,105	0
56	MG	DB	1700	1/1	0.70	0.20	145,145,145,145	0
56	MG	DB	1616	1/1	0.70	0.28	100,100,100,100	0
56	MG	A	1710	1/1	0.70	0.27	126,126,126,126	0
56	MG	A	1732	1/1	0.70	0.33	149,149,149,149	0
56	MG	B	3085	1/1	0.70	0.20	106,106,106,106	0
56	MG	EB	2976	1/1	0.70	0.27	113,113,113,113	0
56	MG	EB	3119	1/1	0.70	0.20	134,134,134,134	0
56	MG	B	2928	1/1	0.70	0.24	107,107,107,107	0
56	MG	EB	3038	1/1	0.70	0.20	97,97,97,97	0
56	MG	EB	2927	1/1	0.70	0.32	90,90,90,90	0
56	MG	B	3127	1/1	0.70	0.28	96,96,96,96	0
56	MG	A	1632	1/1	0.70	0.20	124,124,124,124	0
56	MG	B	3103	1/1	0.70	0.23	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	DB	1609	1/1	0.70	0.28	116,116,116,116	0
56	MG	EB	3230	1/1	0.70	0.10	100,100,100,100	0
56	MG	TB	201	1/1	0.70	0.19	112,112,112,112	0
56	MG	B	3110	1/1	0.70	0.38	94,94,94,94	0
56	MG	B	3205	1/1	0.70	0.33	82,82,82,82	0
56	MG	DB	1694	1/1	0.70	0.28	125,125,125,125	0
56	MG	B	3314	1/1	0.70	0.15	99,99,99,99	0
56	MG	EB	3000	1/1	0.70	0.26	114,114,114,114	0
56	MG	EB	3079	1/1	0.70	0.29	139,139,139,139	0
56	MG	B	3160	1/1	0.70	0.19	92,92,92,92	0
56	MG	DB	1774	1/1	0.70	0.24	128,128,128,128	0
56	MG	B	3316	1/1	0.70	0.13	151,151,151,151	0
56	MG	A	1713	1/1	0.71	0.15	116,116,116,116	0
56	MG	B	3178	1/1	0.71	0.13	140,140,140,140	0
56	MG	DB	1752	1/1	0.71	0.08	156,156,156,156	0
56	MG	B	2904	1/1	0.71	0.45	74,74,74,74	0
56	MG	EB	3053	1/1	0.71	0.22	113,113,113,113	0
56	MG	B	3093	1/1	0.71	0.23	120,120,120,120	0
56	MG	B	3356	1/1	0.71	0.13	92,92,92,92	0
56	MG	A	1684	1/1	0.71	0.36	113,113,113,113	0
56	MG	DB	1633	1/1	0.71	0.51	106,106,106,106	0
56	MG	DB	1635	1/1	0.71	0.25	120,120,120,120	0
56	MG	B	3367	1/1	0.71	0.22	102,102,102,102	0
56	MG	EB	3141	1/1	0.71	0.31	96,96,96,96	0
56	MG	FB	209	1/1	0.71	0.26	132,132,132,132	0
56	MG	MA	203	1/1	0.71	0.13	143,143,143,143	0
56	MG	B	3053	1/1	0.71	0.37	101,101,101,101	0
56	MG	S	203	1/1	0.71	0.07	112,112,112,112	0
56	MG	F	301	1/1	0.71	0.27	106,106,106,106	0
56	MG	DB	1738	1/1	0.71	0.43	108,108,108,108	0
56	MG	DB	1643	1/1	0.71	0.38	109,109,109,109	0
56	MG	EB	2910	1/1	0.71	0.38	87,87,87,87	0
56	MG	B	3244	1/1	0.71	0.12	82,82,82,82	0
56	MG	EB	3106	1/1	0.71	0.14	120,120,120,120	0
56	MG	B	2911	1/1	0.71	0.18	61,61,61,61	0
56	MG	EB	2924	1/1	0.71	0.34	89,89,89,89	0
56	MG	EB	3257	1/1	0.72	0.18	103,103,103,103	0
56	MG	OB	202	1/1	0.72	0.14	100,100,100,100	0
56	MG	B	2989	1/1	0.72	0.32	109,109,109,109	0
56	MG	EB	2948	1/1	0.72	0.49	123,123,123,123	0
56	MG	B	3390	1/1	0.72	0.20	124,124,124,124	0
56	MG	B	3216	1/1	0.72	0.15	157,157,157,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	A	1683	1/1	0.72	0.51	106,106,106,106	0
56	MG	B	3036	1/1	0.72	0.37	110,110,110,110	0
56	MG	EB	3001	1/1	0.72	0.25	112,112,112,112	0
56	MG	EB	2933	1/1	0.72	0.29	95,95,95,95	0
56	MG	EB	3225	1/1	0.72	0.17	115,115,115,115	0
56	MG	B	3122	1/1	0.72	0.19	90,90,90,90	0
56	MG	C	204	1/1	0.72	0.19	114,114,114,114	0
56	MG	A	1654	1/1	0.72	0.18	154,154,154,154	0
56	MG	A	1723	1/1	0.72	0.29	180,180,180,180	0
56	MG	A	1643	1/1	0.72	0.39	117,117,117,117	0
56	MG	EB	3182	1/1	0.72	0.21	107,107,107,107	0
56	MG	A	1727	1/1	0.72	0.23	106,106,106,106	0
56	MG	A	1682	1/1	0.72	0.15	191,191,191,191	0
56	MG	B	3099	1/1	0.72	0.27	87,87,87,87	0
56	MG	EB	3278	1/1	0.73	0.22	106,106,106,106	0
56	MG	DB	1618	1/1	0.73	0.57	101,101,101,101	0
56	MG	B	3125	1/1	0.73	0.42	107,107,107,107	0
56	MG	EB	3207	1/1	0.73	0.10	121,121,121,121	0
56	MG	EB	3101	1/1	0.73	0.20	96,96,96,96	0
56	MG	B	3247	1/1	0.73	0.07	146,146,146,146	0
56	MG	B	2959	1/1	0.73	0.18	78,78,78,78	0
56	MG	EB	2996	1/1	0.73	0.46	86,86,86,86	0
56	MG	DB	1673	1/1	0.73	0.26	105,105,105,105	0
56	MG	EB	3109	1/1	0.73	0.13	112,112,112,112	0
56	MG	MB	202	1/1	0.73	0.16	148,148,148,148	0
56	MG	EB	3054	1/1	0.73	0.28	102,102,102,102	0
56	MG	K	201	1/1	0.73	0.14	111,111,111,111	0
56	MG	FB	210	1/1	0.73	0.26	143,143,143,143	0
56	MG	DB	1624	1/1	0.73	0.35	111,111,111,111	0
56	MG	B	3276	1/1	0.73	0.14	83,83,83,83	0
56	MG	OA	203	1/1	0.73	0.14	142,142,142,142	0
56	MG	B	3054	1/1	0.73	0.38	89,89,89,89	0
56	MG	EB	3068	1/1	0.73	0.29	92,92,92,92	0
56	MG	B	3401	1/1	0.73	0.14	111,111,111,111	0
56	MG	B	3283	1/1	0.73	0.42	226,226,226,226	0
56	MG	EB	3263	1/1	0.73	0.11	133,133,133,133	0
56	MG	B	3285	1/1	0.73	0.59	132,132,132,132	0
56	MG	B	2923	1/1	0.73	0.40	78,78,78,78	0
56	MG	DB	1665	1/1	0.73	0.24	129,129,129,129	0
56	MG	EB	3121	1/1	0.74	0.22	116,116,116,116	0
56	MG	A	1753	1/1	0.74	0.21	125,125,125,125	0
56	MG	WB	201	1/1	0.74	0.24	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	A	1743	1/1	0.74	0.12	174,174,174,174	0
56	MG	B	2914	1/1	0.74	0.41	93,93,93,93	0
56	MG	B	2929	1/1	0.74	0.34	90,90,90,90	0
56	MG	EB	3133	1/1	0.74	0.23	91,91,91,91	0
56	MG	A	1603	1/1	0.74	0.35	88,88,88,88	0
56	MG	BC	101	1/1	0.74	0.20	116,116,116,116	0
56	MG	I	202	1/1	0.74	0.09	122,122,122,122	0
56	MG	DB	1649	1/1	0.74	0.33	106,106,106,106	0
56	MG	C	210	1/1	0.74	0.13	123,123,123,123	0
56	MG	A	1671	1/1	0.74	0.18	131,131,131,131	0
56	MG	EB	3074	1/1	0.74	0.21	91,91,91,91	0
56	MG	DB	1772	1/1	0.74	0.09	109,109,109,109	0
56	MG	B	3132	1/1	0.74	0.41	104,104,104,104	0
56	MG	Y	103	1/1	0.74	0.20	115,115,115,115	0
56	MG	EB	3166	1/1	0.74	0.36	113,113,113,113	0
56	MG	MC	302	1/1	0.74	0.12	138,138,138,138	0
56	MG	EB	3012	1/1	0.74	0.33	90,90,90,90	0
56	MG	EB	3085	1/1	0.74	0.26	117,117,117,117	0
56	MG	B	2918	1/1	0.74	0.30	76,76,76,76	0
56	MG	DB	1732	1/1	0.74	0.17	147,147,147,147	0
56	MG	EB	2961	1/1	0.74	0.30	94,94,94,94	0
56	MG	B	3116	1/1	0.74	0.31	122,122,122,122	0
56	MG	B	3266	1/1	0.74	0.10	149,149,149,149	0
56	MG	EB	3105	1/1	0.74	0.20	97,97,97,97	0
56	MG	B	3273	1/1	0.74	0.12	104,104,104,104	0
56	MG	EB	2973	1/1	0.74	0.39	91,91,91,91	0
56	MG	EB	3286	1/1	0.74	0.26	123,123,123,123	0
56	MG	A	1712	1/1	0.74	0.15	125,125,125,125	0
56	MG	B	3077	1/1	0.74	0.42	99,99,99,99	0
56	MG	TA	203	1/1	0.74	0.07	113,113,113,113	0
56	MG	DB	1746	1/1	0.74	0.32	104,104,104,104	0
56	MG	B	3340	1/1	0.74	0.12	89,89,89,89	0
56	MG	TB	204	1/1	0.74	0.15	112,112,112,112	0
56	MG	HD	403	1/1	0.74	0.14	129,129,129,129	0
56	MG	B	3098	1/1	0.75	0.30	86,86,86,86	0
56	MG	EB	2962	1/1	0.75	0.55	114,114,114,114	0
56	MG	N	202	1/1	0.75	0.20	96,96,96,96	0
56	MG	B	3268	1/1	0.75	0.08	94,94,94,94	0
56	MG	DB	1749	1/1	0.75	0.17	113,113,113,113	0
56	MG	EB	2914	1/1	0.75	0.35	94,94,94,94	0
56	MG	EB	3094	1/1	0.75	0.19	110,110,110,110	0
56	MG	D	104	1/1	0.75	0.14	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3190	1/1	0.75	0.28	88,88,88,88	0
56	MG	PC	202	1/1	0.75	0.21	123,123,123,123	0
56	MG	B	3369	1/1	0.75	0.09	89,89,89,89	0
56	MG	RB	204	1/1	0.75	0.16	100,100,100,100	0
56	MG	B	2906	1/1	0.75	0.38	78,78,78,78	0
56	MG	TC	202	1/1	0.75	0.09	156,156,156,156	0
56	MG	IA	105	1/1	0.75	0.43	116,116,116,116	0
56	MG	B	3082	1/1	0.75	0.27	90,90,90,90	0
56	MG	DB	1661	1/1	0.75	0.28	97,97,97,97	0
56	MG	DB	1762	1/1	0.75	0.26	122,122,122,122	0
56	MG	A	1668	1/1	0.75	0.28	126,126,126,126	0
56	MG	BD	202	1/1	0.75	0.08	108,108,108,108	0
56	MG	EB	2991	1/1	0.75	0.28	90,90,90,90	0
56	MG	A	1676	1/1	0.75	0.37	127,127,127,127	0
56	MG	B	2905	1/1	0.75	0.59	80,80,80,80	0
56	MG	DB	1666	1/1	0.75	0.27	108,108,108,108	0
56	MG	B	3258	1/1	0.75	0.22	107,107,107,107	0
56	MG	B	2986	1/1	0.75	0.40	81,81,81,81	0
56	MG	DB	1669	1/1	0.75	0.30	154,154,154,154	0
56	MG	B	3096	1/1	0.75	0.27	111,111,111,111	0
56	MG	C	201	1/1	0.75	0.41	94,94,94,94	0
56	MG	B	3228	1/1	0.76	0.14	119,119,119,119	0
56	MG	A	1697	1/1	0.76	0.38	104,104,104,104	0
56	MG	DB	1631	1/1	0.76	0.26	106,106,106,106	0
56	MG	EB	2972	1/1	0.76	0.18	104,104,104,104	0
56	MG	L	207	1/1	0.76	0.17	101,101,101,101	0
56	MG	EB	3289	1/1	0.76	0.26	109,109,109,109	0
56	MG	E	301	1/1	0.76	0.29	71,71,71,71	0
56	MG	E	302	1/1	0.76	0.16	93,93,93,93	0
56	MG	NA	201	1/1	0.76	0.16	129,129,129,129	0
56	MG	EB	3231	1/1	0.76	0.35	119,119,119,119	0
56	MG	NB	201	1/1	0.76	0.18	115,115,115,115	0
56	MG	A	1748	1/1	0.76	0.09	97,97,97,97	0
56	MG	B	3163	1/1	0.76	0.18	89,89,89,89	0
56	MG	B	3184	1/1	0.76	0.29	116,116,116,116	0
56	MG	RB	203	1/1	0.76	0.38	114,114,114,114	0
56	MG	EB	3240	1/1	0.76	0.08	155,155,155,155	0
56	MG	DB	1767	1/1	0.76	0.11	106,106,106,106	0
56	MG	FB	211	1/1	0.76	0.16	146,146,146,146	0
56	MG	DB	1731	1/1	0.76	0.22	133,133,133,133	0
56	MG	B	3317	1/1	0.76	0.25	120,120,120,120	0
56	MG	B	3331	1/1	0.76	0.42	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	B	3078	1/1	0.76	0.28	89,89,89,89	0
56	MG	J	203	1/1	0.76	0.20	104,104,104,104	0
56	MG	B	3100	1/1	0.76	0.34	97,97,97,97	0
56	MG	A	1759	1/1	0.76	0.18	176,176,176,176	0
56	MG	EB	2954	1/1	0.76	0.67	103,103,103,103	0
56	MG	DB	1650	1/1	0.76	0.34	103,103,103,103	0
56	MG	DB	1708	1/1	0.76	0.21	106,106,106,106	0
56	MG	EB	3073	1/1	0.76	0.20	105,105,105,105	0
56	MG	DB	1652	1/1	0.76	0.35	122,122,122,122	0
56	MG	EB	2915	1/1	0.77	0.57	96,96,96,96	0
56	MG	EB	2922	1/1	0.77	0.38	79,79,79,79	0
56	MG	FB	207	1/1	0.77	0.15	138,138,138,138	0
56	MG	EB	3030	1/1	0.77	0.22	110,110,110,110	0
56	MG	XB	102	1/1	0.77	0.15	124,124,124,124	0
56	MG	A	1614	1/1	0.77	0.21	108,108,108,108	0
56	MG	YB	204	1/1	0.77	0.09	118,118,118,118	0
56	MG	B	2964	1/1	0.77	0.57	88,88,88,88	0
56	MG	EB	3043	1/1	0.77	0.17	119,119,119,119	0
56	MG	EB	3044	1/1	0.77	0.14	118,118,118,118	0
56	MG	B	3114	1/1	0.77	0.21	86,86,86,86	0
56	MG	EB	2929	1/1	0.77	0.29	98,98,98,98	0
56	MG	EB	2930	1/1	0.77	0.39	84,84,84,84	0
56	MG	Y	104	1/1	0.77	0.08	101,101,101,101	0
56	MG	Z	103	1/1	0.77	0.05	92,92,92,92	0
56	MG	B	2912	1/1	0.77	0.18	86,86,86,86	0
56	MG	G	302	1/1	0.77	0.42	73,73,73,73	0
56	MG	DB	1692	1/1	0.77	0.11	137,137,137,137	0
56	MG	B	3040	1/1	0.77	0.14	79,79,79,79	0
56	MG	EB	2943	1/1	0.77	0.38	93,93,93,93	0
56	MG	B	3394	1/1	0.77	0.33	107,107,107,107	0
56	MG	B	3024	1/1	0.77	0.30	85,85,85,85	0
56	MG	A	1725	1/1	0.77	0.09	119,119,119,119	0
56	MG	EB	3160	1/1	0.77	0.25	108,108,108,108	0
56	MG	QC	202	1/1	0.77	0.19	124,124,124,124	0
56	MG	EB	2999	1/1	0.77	0.22	101,101,101,101	0
56	MG	B	3238	1/1	0.77	0.40	93,93,93,93	0
56	MG	EB	3077	1/1	0.77	0.20	133,133,133,133	0
56	MG	DB	1613	1/1	0.77	0.35	97,97,97,97	0
56	MG	B	3165	1/1	0.77	0.17	75,75,75,75	0
56	MG	EB	3004	1/1	0.77	0.45	102,102,102,102	0
56	MG	EB	3281	1/1	0.77	0.17	95,95,95,95	0
56	MG	EB	2903	1/1	0.77	0.46	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	AD	101	1/1	0.77	0.34	108,108,108,108	0
56	MG	B	2952	1/1	0.77	0.29	78,78,78,78	0
56	MG	OB	203	1/1	0.77	0.07	95,95,95,95	0
56	MG	JA	302	1/1	0.77	0.20	146,146,146,146	0
56	MG	W	306	1/1	0.77	0.18	122,122,122,122	0
56	MG	EB	3287	1/1	0.77	0.33	110,110,110,110	0
56	MG	B	3275	1/1	0.77	0.13	116,116,116,116	0
56	MG	B	3029	1/1	0.77	0.45	85,85,85,85	0
56	MG	EB	3021	1/1	0.77	0.18	111,111,111,111	0
56	MG	W	309	1/1	0.77	0.19	121,121,121,121	0
56	MG	EB	3025	1/1	0.77	0.89	103,103,103,103	0
56	MG	B	3138	1/1	0.78	0.35	106,106,106,106	0
56	MG	B	3193	1/1	0.78	0.25	81,81,81,81	0
56	MG	B	2976	1/1	0.78	0.44	96,96,96,96	0
56	MG	DB	1765	1/1	0.78	0.14	122,122,122,122	0
56	MG	EB	3223	1/1	0.78	0.11	97,97,97,97	0
56	MG	ZB	301	1/1	0.78	0.21	137,137,137,137	0
56	MG	A	1693	1/1	0.78	0.23	107,107,107,107	0
56	MG	B	3248	1/1	0.78	0.33	103,103,103,103	0
56	MG	B	3207	1/1	0.78	0.48	98,98,98,98	0
56	MG	B	3208	1/1	0.78	0.11	118,118,118,118	0
56	MG	A	1646	1/1	0.78	0.22	117,117,117,117	0
56	MG	EB	2998	1/1	0.78	0.23	86,86,86,86	0
56	MG	IA	107	1/1	0.78	0.41	108,108,108,108	0
56	MG	EB	3070	1/1	0.78	0.17	104,104,104,104	0
56	MG	EB	3071	1/1	0.78	0.35	100,100,100,100	0
56	MG	HB	301	1/1	0.78	0.24	103,103,103,103	0
56	MG	B	3305	1/1	0.78	0.08	120,120,120,120	0
56	MG	LC	107	1/1	0.78	0.10	110,110,110,110	0
56	MG	A	1669	1/1	0.78	0.27	93,93,93,93	0
56	MG	HB	307	1/1	0.78	0.14	102,102,102,102	0
56	MG	B	3002	1/1	0.78	0.52	85,85,85,85	0
56	MG	EB	3159	1/1	0.78	0.10	104,104,104,104	0
56	MG	A	1652	1/1	0.78	0.34	123,123,123,123	0
56	MG	EB	3009	1/1	0.78	0.18	93,93,93,93	0
56	MG	EB	3164	1/1	0.78	0.08	114,114,114,114	0
56	MG	A	1667	1/1	0.78	0.23	105,105,105,105	0
56	MG	EB	3168	1/1	0.78	0.33	88,88,88,88	0
56	MG	EB	2957	1/1	0.78	0.42	91,91,91,91	0
56	MG	EB	3174	1/1	0.78	0.33	98,98,98,98	0
56	MG	WC	201	1/1	0.78	0.11	96,96,96,96	0
56	MG	WC	202	1/1	0.78	0.15	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3267	1/1	0.78	0.13	112,112,112,112	0
56	MG	EB	3279	1/1	0.78	0.42	95,95,95,95	0
56	MG	DB	1629	1/1	0.78	0.24	100,100,100,100	0
56	MG	DB	1743	1/1	0.78	0.14	104,104,104,104	0
56	MG	A	1722	1/1	0.78	0.12	96,96,96,96	0
56	MG	EB	2968	1/1	0.78	0.22	112,112,112,112	0
56	MG	B	3231	1/1	0.78	0.28	91,91,91,91	0
56	MG	B	3335	1/1	0.78	0.10	128,128,128,128	0
56	MG	EB	2923	1/1	0.78	0.38	97,97,97,97	0
56	MG	B	3232	1/1	0.78	0.20	83,83,83,83	0
56	MG	C	207	1/1	0.78	0.37	127,127,127,127	0
56	MG	B	3233	1/1	0.78	0.34	95,95,95,95	0
56	MG	EB	2928	1/1	0.78	0.33	95,95,95,95	0
56	MG	B	2971	1/1	0.78	0.16	82,82,82,82	0
56	MG	B	3277	1/1	0.78	0.18	106,106,106,106	0
56	MG	B	3346	1/1	0.79	0.11	85,85,85,85	0
56	MG	A	1666	1/1	0.79	0.29	105,105,105,105	0
56	MG	EB	3156	1/1	0.79	0.61	109,109,109,109	0
56	MG	EB	3078	1/1	0.79	0.24	110,110,110,110	0
56	MG	DB	1724	1/1	0.79	0.34	107,107,107,107	0
56	MG	B	3139	1/1	0.79	0.19	97,97,97,97	0
56	MG	KC	101	1/1	0.79	0.20	113,113,113,113	0
56	MG	EB	3256	1/1	0.79	0.08	106,106,106,106	0
56	MG	B	3076	1/1	0.79	0.17	88,88,88,88	0
56	MG	DB	1769	1/1	0.79	0.14	92,92,92,92	0
56	MG	B	3357	1/1	0.79	0.14	88,88,88,88	0
56	MG	IB	303	1/1	0.79	0.10	112,112,112,112	0
56	MG	EB	2983	1/1	0.79	0.32	88,88,88,88	0
56	MG	EB	3088	1/1	0.79	0.36	97,97,97,97	0
56	MG	B	3027	1/1	0.79	0.22	95,95,95,95	0
56	MG	EB	2985	1/1	0.79	0.23	91,91,91,91	0
56	MG	EB	3036	1/1	0.79	0.31	102,102,102,102	0
56	MG	EB	3037	1/1	0.79	0.22	95,95,95,95	0
56	MG	A	1625	1/1	0.79	0.13	137,137,137,137	0
56	MG	A	1624	1/1	0.79	0.30	111,111,111,111	0
56	MG	EB	3183	1/1	0.79	0.34	119,119,119,119	0
56	MG	RC	202	1/1	0.79	0.22	152,152,152,152	0
56	MG	B	3032	1/1	0.79	0.24	87,87,87,87	0
56	MG	EB	3187	1/1	0.79	0.18	134,134,134,134	0
56	MG	B	3111	1/1	0.79	0.20	84,84,84,84	0
56	MG	B	2945	1/1	0.79	0.34	82,82,82,82	0
56	MG	DB	1605	1/1	0.79	0.25	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	EB	3113	1/1	0.79	0.43	114,114,114,114	0
56	MG	EB	3052	1/1	0.79	0.38	106,106,106,106	0
56	MG	EB	2907	1/1	0.79	0.38	97,97,97,97	0
56	MG	A	1747	1/1	0.79	0.92	150,150,150,150	0
56	MG	B	3326	1/1	0.79	0.07	94,94,94,94	0
56	MG	B	3330	1/1	0.79	0.10	88,88,88,88	0
56	MG	B	3284	1/1	0.79	0.26	79,79,79,79	0
56	MG	B	3118	1/1	0.79	0.23	96,96,96,96	0
56	MG	RA	202	1/1	0.79	0.18	152,152,152,152	0
56	MG	B	2950	1/1	0.79	0.41	92,92,92,92	0
56	MG	B	3407	1/1	0.79	0.08	78,78,78,78	0
56	MG	EB	3010	1/1	0.79	0.20	84,84,84,84	0
56	MG	B	3408	1/1	0.79	0.19	119,119,119,119	0
56	MG	U	102	1/1	0.79	0.05	102,102,102,102	0
56	MG	B	3263	1/1	0.79	0.17	99,99,99,99	0
56	MG	IC	102	1/1	0.80	0.12	105,105,105,105	0
56	MG	A	1731	1/1	0.80	0.26	102,102,102,102	0
56	MG	DB	1715	1/1	0.80	0.43	107,107,107,107	0
56	MG	B	3239	1/1	0.80	0.13	78,78,78,78	0
56	MG	B	2930	1/1	0.80	0.33	78,78,78,78	0
56	MG	B	3001	1/1	0.80	0.29	88,88,88,88	0
56	MG	A	1642	1/1	0.80	0.19	106,106,106,106	0
56	MG	A	1689	1/1	0.80	0.30	105,105,105,105	0
56	MG	EB	2975	1/1	0.80	0.36	105,105,105,105	0
56	MG	DB	1689	1/1	0.80	0.22	111,111,111,111	0
56	MG	B	3318	1/1	0.80	0.15	95,95,95,95	0
56	MG	B	3280	1/1	0.80	0.22	94,94,94,94	0
56	MG	DB	1728	1/1	0.80	0.10	99,99,99,99	0
56	MG	B	3083	1/1	0.80	0.34	100,100,100,100	0
56	MG	B	3250	1/1	0.80	0.10	96,96,96,96	0
56	MG	B	2910	1/1	0.80	0.43	83,83,83,83	0
56	MG	EB	3083	1/1	0.80	0.28	106,106,106,106	0
56	MG	EB	3219	1/1	0.80	0.32	105,105,105,105	0
56	MG	SC	201	1/1	0.80	0.18	124,124,124,124	0
56	MG	EB	3221	1/1	0.80	0.39	103,103,103,103	0
56	MG	D	101	1/1	0.80	0.10	123,123,123,123	0
56	MG	L	201	1/1	0.80	0.21	99,99,99,99	0
56	MG	B	3220	1/1	0.80	0.08	88,88,88,88	0
56	MG	DB	1739	1/1	0.80	0.25	113,113,113,113	0
56	MG	B	3155	1/1	0.80	0.19	101,101,101,101	0
56	MG	EB	3092	1/1	0.80	0.25	108,108,108,108	0
56	MG	EB	3236	1/1	0.80	0.15	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3187	1/1	0.80	0.18	84,84,84,84	0
56	MG	EB	3239	1/1	0.80	0.20	123,123,123,123	0
56	MG	EB	3098	1/1	0.80	0.38	102,102,102,102	0
56	MG	B	3061	1/1	0.80	0.33	109,109,109,109	0
56	MG	A	1650	1/1	0.80	0.39	108,108,108,108	0
56	MG	EB	3169	1/1	0.80	0.32	87,87,87,87	0
56	MG	R	202	1/1	0.80	0.21	101,101,101,101	0
56	MG	EB	3104	1/1	0.80	0.30	103,103,103,103	0
56	MG	A	1702	1/1	0.80	0.22	115,115,115,115	0
56	MG	T	201	1/1	0.80	0.16	94,94,94,94	0
56	MG	A	1665	1/1	0.80	0.18	115,115,115,115	0
56	MG	EB	2917	1/1	0.80	0.34	89,89,89,89	0
56	MG	WA	103	1/1	0.81	0.17	126,126,126,126	0
56	MG	B	3128	1/1	0.81	0.28	94,94,94,94	0
56	MG	EB	3254	1/1	0.81	0.16	123,123,123,123	0
56	MG	IC	101	1/1	0.81	0.22	108,108,108,108	0
56	MG	EB	3108	1/1	0.81	0.34	127,127,127,127	0
56	MG	B	3224	1/1	0.81	0.08	93,93,93,93	0
56	MG	HB	306	1/1	0.81	0.15	108,108,108,108	0
56	MG	B	3325	1/1	0.81	0.25	113,113,113,113	0
56	MG	HB	308	1/1	0.81	0.14	108,108,108,108	0
56	MG	B	3147	1/1	0.81	0.21	94,94,94,94	0
56	MG	B	3226	1/1	0.81	0.17	90,90,90,90	0
56	MG	EB	3116	1/1	0.81	0.31	93,93,93,93	0
56	MG	B	3171	1/1	0.81	0.42	81,81,81,81	0
56	MG	EB	3188	1/1	0.81	0.17	89,89,89,89	0
56	MG	EB	2931	1/1	0.81	0.23	80,80,80,80	0
56	MG	A	1672	1/1	0.81	0.22	137,137,137,137	0
56	MG	B	3197	1/1	0.81	0.07	116,116,116,116	0
56	MG	B	2962	1/1	0.81	0.26	83,83,83,83	0
56	MG	EB	3197	1/1	0.81	0.38	94,94,94,94	0
56	MG	EB	2981	1/1	0.81	0.21	97,97,97,97	0
56	MG	B	3015	1/1	0.81	0.29	71,71,71,71	0
56	MG	B	2993	1/1	0.81	0.24	86,86,86,86	0
56	MG	DB	1701	1/1	0.81	0.10	119,119,119,119	0
56	MG	DB	1608	1/1	0.81	0.41	94,94,94,94	0
56	MG	PB	202	1/1	0.81	0.44	103,103,103,103	0
56	MG	A	1626	1/1	0.81	0.27	122,122,122,122	0
56	MG	EB	3213	1/1	0.81	0.31	103,103,103,103	0
56	MG	B	3269	1/1	0.81	0.41	110,110,110,110	0
56	MG	B	3272	1/1	0.81	0.30	104,104,104,104	0
56	MG	EB	2990	1/1	0.81	0.26	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	EB	2908	1/1	0.81	0.27	88,88,88,88	0
56	MG	EB	3089	1/1	0.81	0.25	109,109,109,109	0
56	MG	EB	3090	1/1	0.81	0.23	86,86,86,86	0
56	MG	B	3214	1/1	0.81	0.13	79,79,79,79	0
56	MG	B	3363	1/1	0.81	0.54	229,229,229,229	0
56	MG	EB	3097	1/1	0.81	0.14	87,87,87,87	0
56	MG	DB	1710	1/1	0.81	0.21	136,136,136,136	0
56	MG	W	301	1/1	0.81	0.10	107,107,107,107	0
56	MG	A	1658	1/1	0.81	0.39	109,109,109,109	0
56	MG	A	1749	1/1	0.81	0.15	95,95,95,95	0
56	MG	B	3097	1/1	0.81	0.46	99,99,99,99	0
56	MG	EB	3173	1/1	0.81	0.19	103,103,103,103	0
56	MG	B	3373	1/1	0.81	0.08	109,109,109,109	0
57	ZN	BA	101	1/1	0.81	0.17	180,180,180,180	0
56	MG	A	1695	1/1	0.82	0.17	105,105,105,105	0
56	MG	B	2917	1/1	0.82	0.42	79,79,79,79	0
56	MG	B	3320	1/1	0.82	0.14	85,85,85,85	0
56	MG	IA	101	1/1	0.82	0.17	119,119,119,119	0
56	MG	EB	3081	1/1	0.82	0.25	81,81,81,81	0
56	MG	B	3177	1/1	0.82	0.12	92,92,92,92	0
56	MG	EB	3023	1/1	0.82	0.26	101,101,101,101	0
56	MG	A	1608	1/1	0.82	0.25	82,82,82,82	0
56	MG	A	1736	1/1	0.82	0.14	148,148,148,148	0
56	MG	B	3130	1/1	0.82	0.23	82,82,82,82	0
56	MG	EB	2934	1/1	0.82	0.64	86,86,86,86	0
56	MG	EB	3143	1/1	0.82	0.34	89,89,89,89	0
56	MG	EB	3146	1/1	0.82	0.18	99,99,99,99	0
56	MG	DB	1656	1/1	0.82	0.21	105,105,105,105	0
56	MG	T	202	1/1	0.82	0.26	98,98,98,98	0
56	MG	DB	1771	1/1	0.82	0.10	106,106,106,106	0
56	MG	EB	3226	1/1	0.82	0.38	102,102,102,102	0
56	MG	EB	3091	1/1	0.82	0.11	97,97,97,97	0
56	MG	B	3055	1/1	0.82	0.28	82,82,82,82	0
56	MG	B	2978	1/1	0.82	0.38	78,78,78,78	0
56	MG	B	2948	1/1	0.82	0.35	93,93,93,93	0
56	MG	DB	1734	1/1	0.82	0.13	121,121,121,121	0
56	MG	EB	2901	1/1	0.82	0.37	79,79,79,79	0
56	MG	B	3062	1/1	0.82	0.26	86,86,86,86	0
56	MG	DB	1737	1/1	0.82	0.32	110,110,110,110	0
56	MG	B	2934	1/1	0.82	0.34	82,82,82,82	0
56	MG	B	3227	1/1	0.82	0.36	83,83,83,83	0
56	MG	B	3192	1/1	0.82	0.20	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	A	1685	1/1	0.82	0.36	149,149,149,149	0
56	MG	B	3038	1/1	0.82	0.19	80,80,80,80	0
56	MG	B	2902	1/1	0.82	0.55	61,61,61,61	0
56	MG	B	3234	1/1	0.82	0.14	87,87,87,87	0
56	MG	B	3313	1/1	0.82	0.18	133,133,133,133	0
56	MG	EB	2965	1/1	0.82	0.30	84,84,84,84	0
56	MG	B	3271	1/1	0.82	0.10	100,100,100,100	0
56	MG	B	3199	1/1	0.82	0.40	98,98,98,98	0
56	MG	HC	101	1/1	0.82	0.14	102,102,102,102	0
56	MG	B	3378	1/1	0.82	0.27	101,101,101,101	0
56	MG	B	3172	1/1	0.82	0.39	97,97,97,97	0
57	ZN	EC	101	1/1	0.82	0.11	199,199,199,199	0
56	MG	EB	3148	1/1	0.83	0.15	134,134,134,134	0
56	MG	B	3395	1/1	0.83	0.20	99,99,99,99	0
56	MG	EB	3152	1/1	0.83	0.25	106,106,106,106	0
56	MG	B	3286	1/1	0.83	0.11	95,95,95,95	0
56	MG	B	2922	1/1	0.83	0.32	74,74,74,74	0
56	MG	DB	1757	1/1	0.83	0.34	106,106,106,106	0
56	MG	EB	3032	1/1	0.83	0.25	95,95,95,95	0
56	MG	B	3017	1/1	0.83	0.53	84,84,84,84	0
56	MG	DB	1630	1/1	0.83	0.21	105,105,105,105	0
56	MG	B	3167	1/1	0.83	0.29	100,100,100,100	0
56	MG	B	3298	1/1	0.83	0.16	96,96,96,96	0
56	MG	GB	104	1/1	0.83	0.14	152,152,152,152	0
56	MG	A	1641	1/1	0.83	0.36	107,107,107,107	0
56	MG	B	3019	1/1	0.83	0.19	83,83,83,83	0
56	MG	EB	3249	1/1	0.83	0.33	137,137,137,137	0
56	MG	B	3200	1/1	0.83	0.14	111,111,111,111	0
56	MG	DB	1679	1/1	0.83	0.20	134,134,134,134	0
56	MG	EB	3253	1/1	0.83	0.30	120,120,120,120	0
56	MG	B	3058	1/1	0.83	0.61	89,89,89,89	0
56	MG	IB	301	1/1	0.83	0.18	88,88,88,88	0
56	MG	I	203	1/1	0.83	0.08	111,111,111,111	0
56	MG	B	3140	1/1	0.83	0.18	84,84,84,84	0
56	MG	DB	1683	1/1	0.83	0.31	109,109,109,109	0
56	MG	B	3033	1/1	0.83	0.23	101,101,101,101	0
56	MG	B	3243	1/1	0.83	0.15	97,97,97,97	0
56	MG	DB	1730	1/1	0.83	0.08	108,108,108,108	0
56	MG	B	3020	1/1	0.83	0.45	91,91,91,91	0
56	MG	EB	3114	1/1	0.83	0.11	135,135,135,135	0
56	MG	EB	3273	1/1	0.83	0.13	88,88,88,88	0
56	MG	B	3094	1/1	0.83	0.18	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3021	1/1	0.83	0.47	93,93,93,93	0
56	MG	C	214	1/1	0.83	0.17	97,97,97,97	0
56	MG	EB	3280	1/1	0.83	0.12	105,105,105,105	0
56	MG	A	1653	1/1	0.83	0.26	114,114,114,114	0
56	MG	EB	2958	1/1	0.83	0.31	78,78,78,78	0
56	MG	EB	3008	1/1	0.83	0.18	92,92,92,92	0
56	MG	EB	2959	1/1	0.83	0.25	99,99,99,99	0
56	MG	QB	202	1/1	0.83	0.11	103,103,103,103	0
56	MG	B	3383	1/1	0.83	0.20	114,114,114,114	0
56	MG	BD	201	1/1	0.83	0.07	122,122,122,122	0
56	MG	M	201	1/1	0.83	0.19	77,77,77,77	0
56	MG	B	3069	1/1	0.83	0.14	79,79,79,79	0
56	MG	DB	1619	1/1	0.83	0.36	86,86,86,86	0
56	MG	EB	3291	1/1	0.83	0.23	90,90,90,90	0
56	MG	TB	202	1/1	0.83	0.07	111,111,111,111	0
56	MG	O	201	1/1	0.83	0.30	93,93,93,93	0
56	MG	EB	3209	1/1	0.83	0.32	97,97,97,97	0
56	MG	B	3005	1/1	0.83	0.14	72,72,72,72	0
56	MG	DB	1662	1/1	0.83	0.36	108,108,108,108	0
56	MG	B	3043	1/1	0.83	0.42	85,85,85,85	0
56	MG	B	2920	1/1	0.83	0.19	82,82,82,82	0
56	MG	A	1637	1/1	0.83	0.39	92,92,92,92	0
56	MG	B	3106	1/1	0.84	0.19	103,103,103,103	0
56	MG	B	3303	1/1	0.84	0.26	91,91,91,91	0
56	MG	DB	1748	1/1	0.84	0.17	121,121,121,121	0
56	MG	B	3364	1/1	0.84	0.21	95,95,95,95	0
56	MG	B	3156	1/1	0.84	0.17	92,92,92,92	0
56	MG	P	202	1/1	0.84	0.14	126,126,126,126	0
56	MG	EB	3125	1/1	0.84	0.20	96,96,96,96	0
56	MG	EB	2932	1/1	0.84	0.46	80,80,80,80	0
56	MG	B	3107	1/1	0.84	0.24	96,96,96,96	0
56	MG	EB	3222	1/1	0.84	0.27	92,92,92,92	0
56	MG	C	218	1/1	0.84	0.21	123,123,123,123	0
56	MG	C	219	1/1	0.84	0.23	131,131,131,131	0
56	MG	B	3229	1/1	0.84	0.17	112,112,112,112	0
56	MG	EB	2994	1/1	0.84	0.37	87,87,87,87	0
56	MG	B	3191	1/1	0.84	0.14	81,81,81,81	0
56	MG	A	1715	1/1	0.84	0.14	137,137,137,137	0
56	MG	B	3008	1/1	0.84	0.38	96,96,96,96	0
56	MG	B	3113	1/1	0.84	0.26	96,96,96,96	0
56	MG	B	3166	1/1	0.84	0.14	105,105,105,105	0
56	MG	B	3386	1/1	0.84	0.13	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	B	2949	1/1	0.84	0.40	82,82,82,82	0
56	MG	PA	201	1/1	0.84	0.10	129,129,129,129	0
56	MG	EB	3005	1/1	0.84	0.28	99,99,99,99	0
56	MG	EB	3006	1/1	0.84	0.56	103,103,103,103	0
56	MG	EB	3247	1/1	0.84	0.26	156,156,156,156	0
56	MG	EB	3158	1/1	0.84	0.14	105,105,105,105	0
56	MG	A	1751	1/1	0.84	0.07	116,116,116,116	0
56	MG	B	3242	1/1	0.84	0.38	89,89,89,89	0
56	MG	B	3049	1/1	0.84	0.15	73,73,73,73	0
56	MG	DB	1672	1/1	0.84	0.29	104,104,104,104	0
56	MG	B	3071	1/1	0.84	0.19	90,90,90,90	0
56	MG	B	3327	1/1	0.84	0.22	92,92,92,92	0
56	MG	B	2926	1/1	0.84	0.34	74,74,74,74	0
56	MG	A	1638	1/1	0.84	0.25	102,102,102,102	0
56	MG	EB	3172	1/1	0.84	0.49	120,120,120,120	0
56	MG	B	3334	1/1	0.84	0.32	87,87,87,87	0
56	MG	A	1655	1/1	0.84	0.36	96,96,96,96	0
56	MG	B	3338	1/1	0.84	0.23	119,119,119,119	0
56	MG	B	3148	1/1	0.84	0.40	103,103,103,103	0
56	MG	CA	102	1/1	0.84	0.23	81,81,81,81	0
56	MG	EB	3099	1/1	0.84	0.32	103,103,103,103	0
56	MG	B	3179	1/1	0.84	0.10	106,106,106,106	0
56	MG	DB	1735	1/1	0.84	0.18	101,101,101,101	0
56	MG	YA	202	1/1	0.84	0.15	128,128,128,128	0
56	MG	A	1720	1/1	0.84	0.20	110,110,110,110	0
56	MG	ED	201	1/1	0.84	0.31	122,122,122,122	0
56	MG	EB	3034	1/1	0.84	0.35	106,106,106,106	0
56	MG	B	2957	1/1	0.84	0.22	81,81,81,81	0
56	MG	A	1621	1/1	0.84	0.20	115,115,115,115	0
56	MG	EB	2921	1/1	0.84	0.29	77,77,77,77	0
56	MG	EB	2977	1/1	0.84	0.20	120,120,120,120	0
56	MG	EB	3042	1/1	0.84	0.27	113,113,113,113	0
56	MG	B	3297	1/1	0.84	0.15	100,100,100,100	0
56	MG	L	203	1/1	0.84	0.21	104,104,104,104	0
56	MG	B	3105	1/1	0.84	0.20	83,83,83,83	0
56	MG	B	3115	1/1	0.85	0.27	114,114,114,114	0
56	MG	EB	2940	1/1	0.85	0.31	108,108,108,108	0
56	MG	B	3348	1/1	0.85	0.13	98,98,98,98	0
56	MG	G	301	1/1	0.85	0.32	89,89,89,89	0
56	MG	B	2938	1/1	0.85	0.17	86,86,86,86	0
56	MG	EB	3238	1/1	0.85	0.31	100,100,100,100	0
56	MG	FC	102	1/1	0.85	0.12	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DB	1776	1/1	0.85	0.12	94,94,94,94	0
56	MG	B	3217	1/1	0.85	0.23	93,93,93,93	0
56	MG	EB	3241	1/1	0.85	0.21	102,102,102,102	0
56	MG	B	3004	1/1	0.85	0.38	80,80,80,80	0
56	MG	B	3361	1/1	0.85	0.15	95,95,95,95	0
56	MG	A	1724	1/1	0.85	0.18	122,122,122,122	0
56	MG	EB	3051	1/1	0.85	0.26	95,95,95,95	0
56	MG	B	3311	1/1	0.85	0.17	87,87,87,87	0
56	MG	A	1639	1/1	0.85	0.27	95,95,95,95	0
56	MG	DB	1745	1/1	0.85	0.25	102,102,102,102	0
56	MG	B	3007	1/1	0.85	0.29	88,88,88,88	0
56	MG	B	3101	1/1	0.85	0.33	95,95,95,95	0
56	MG	B	2988	1/1	0.85	0.33	87,87,87,87	0
56	MG	EB	3065	1/1	0.85	0.12	92,92,92,92	0
56	MG	A	1760	1/1	0.85	0.34	101,101,101,101	0
56	MG	B	3045	1/1	0.85	0.28	84,84,84,84	0
56	MG	EB	3115	1/1	0.85	0.24	106,106,106,106	0
56	MG	Y	102	1/1	0.85	0.09	79,79,79,79	0
56	MG	EB	3117	1/1	0.85	0.24	92,92,92,92	0
56	MG	EB	2963	1/1	0.85	0.18	85,85,85,85	0
56	MG	EB	2918	1/1	0.85	0.35	92,92,92,92	0
56	MG	B	2927	1/1	0.85	0.36	87,87,87,87	0
56	MG	B	3230	1/1	0.85	0.10	93,93,93,93	0
56	MG	B	3068	1/1	0.85	0.22	82,82,82,82	0
56	MG	EB	3196	1/1	0.85	0.17	100,100,100,100	0
56	MG	EB	3075	1/1	0.85	0.17	95,95,95,95	0
56	MG	B	3091	1/1	0.85	0.25	86,86,86,86	0
56	MG	EB	3130	1/1	0.85	0.29	97,97,97,97	0
56	MG	B	3289	1/1	0.85	0.18	93,93,93,93	0
56	MG	A	1677	1/1	0.85	0.17	115,115,115,115	0
56	MG	DB	1763	1/1	0.85	0.05	120,120,120,120	0
56	MG	EB	3080	1/1	0.85	0.29	92,92,92,92	0
56	MG	B	3292	1/1	0.85	0.10	107,107,107,107	0
56	MG	B	3295	1/1	0.85	0.10	90,90,90,90	0
56	MG	EB	3295	1/1	0.85	0.10	109,109,109,109	0
56	MG	EB	3215	1/1	0.85	0.98	119,119,119,119	0
56	MG	FB	202	1/1	0.85	0.15	135,135,135,135	0
56	MG	B	3296	1/1	0.85	0.16	101,101,101,101	0
56	MG	B	2977	1/1	0.85	0.27	83,83,83,83	0
56	MG	DB	1768	1/1	0.85	0.24	104,104,104,104	0
56	MG	B	3209	1/1	0.85	0.26	97,97,97,97	0
56	MG	B	3158	1/1	0.85	0.13	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DB	1696	1/1	0.85	0.27	105,105,105,105	0
56	MG	EB	3151	1/1	0.85	0.09	119,119,119,119	0
57	ZN	YB	201	1/1	0.85	0.25	147,147,147,147	0
56	MG	EB	2937	1/1	0.85	0.44	95,95,95,95	0
56	MG	Z	102	1/1	0.86	0.05	95,95,95,95	0
56	MG	B	3332	1/1	0.86	0.12	102,102,102,102	0
56	MG	C	209	1/1	0.86	0.14	96,96,96,96	0
56	MG	EB	3136	1/1	0.86	0.10	96,96,96,96	0
56	MG	A	1687	1/1	0.86	0.06	167,167,167,167	0
56	MG	G	304	1/1	0.86	0.13	80,80,80,80	0
56	MG	EB	3198	1/1	0.86	0.38	92,92,92,92	0
56	MG	B	2958	1/1	0.86	0.32	80,80,80,80	0
56	MG	EB	3093	1/1	0.86	0.13	115,115,115,115	0
56	MG	EB	2970	1/1	0.86	0.21	90,90,90,90	0
56	MG	EB	3144	1/1	0.86	0.15	106,106,106,106	0
56	MG	A	1733	1/1	0.86	0.17	91,91,91,91	0
56	MG	A	1744	1/1	0.86	0.14	118,118,118,118	0
56	MG	A	1620	1/1	0.86	0.33	98,98,98,98	0
56	MG	EB	3100	1/1	0.86	0.28	92,92,92,92	0
56	MG	A	1664	1/1	0.86	0.43	105,105,105,105	0
56	MG	V	503	1/1	0.86	0.07	99,99,99,99	0
56	MG	EB	3217	1/1	0.86	0.18	93,93,93,93	0
56	MG	EB	3062	1/1	0.86	0.12	89,89,89,89	0
56	MG	EB	3064	1/1	0.86	0.24	91,91,91,91	0
56	MG	A	1690	1/1	0.86	0.06	111,111,111,111	0
56	MG	B	3034	1/1	0.86	0.29	109,109,109,109	0
56	MG	EB	3015	1/1	0.86	0.14	94,94,94,94	0
56	MG	A	1606	1/1	0.86	0.48	99,99,99,99	0
56	MG	EB	3227	1/1	0.86	0.34	109,109,109,109	0
56	MG	EB	3229	1/1	0.86	0.11	111,111,111,111	0
56	MG	EB	3165	1/1	0.86	0.15	88,88,88,88	0
56	MG	DB	1754	1/1	0.86	0.25	129,129,129,129	0
56	MG	B	2994	1/1	0.86	0.28	75,75,75,75	0
56	MG	EB	3234	1/1	0.86	0.12	168,168,168,168	0
56	MG	EB	3020	1/1	0.86	0.20	90,90,90,90	0
56	MG	B	3153	1/1	0.86	0.07	165,165,165,165	0
56	MG	B	3108	1/1	0.86	0.13	124,124,124,124	0
56	MG	A	1739	1/1	0.86	0.06	151,151,151,151	0
56	MG	A	1740	1/1	0.86	0.36	129,129,129,129	0
56	MG	EB	2916	1/1	0.86	0.42	78,78,78,78	0
56	MG	EB	2949	1/1	0.86	0.36	93,93,93,93	0
56	MG	EB	3242	1/1	0.86	0.32	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	2943	1/1	0.86	0.20	77,77,77,77	0
56	MG	B	2972	1/1	0.86	0.25	72,72,72,72	0
56	MG	EB	2919	1/1	0.86	0.55	80,80,80,80	0
56	MG	B	3136	1/1	0.86	0.10	91,91,91,91	0
56	MG	W	312	1/1	0.86	0.07	126,126,126,126	0
56	MG	N	203	1/1	0.86	0.12	113,113,113,113	0
56	MG	B	3095	1/1	0.86	0.32	99,99,99,99	0
56	MG	B	3300	1/1	0.86	0.12	117,117,117,117	0
56	MG	B	3161	1/1	0.87	0.20	81,81,81,81	0
56	MG	EB	3243	1/1	0.87	0.12	106,106,106,106	0
56	MG	B	2995	1/1	0.87	0.43	84,84,84,84	0
56	MG	EB	3124	1/1	0.87	0.34	115,115,115,115	0
56	MG	B	2979	1/1	0.87	0.47	86,86,86,86	0
56	MG	R	201	1/1	0.87	0.27	100,100,100,100	0
56	MG	EB	2905	1/1	0.87	0.35	78,78,78,78	0
56	MG	B	3255	1/1	0.87	0.09	89,89,89,89	0
56	MG	B	3374	1/1	0.87	0.40	102,102,102,102	0
56	MG	B	3376	1/1	0.87	0.56	92,92,92,92	0
56	MG	DB	1676	1/1	0.87	0.18	120,120,120,120	0
56	MG	DB	1642	1/1	0.87	0.22	92,92,92,92	0
56	MG	EB	3039	1/1	0.87	0.36	102,102,102,102	0
56	MG	DB	1713	1/1	0.87	0.28	143,143,143,143	0
56	MG	EB	3140	1/1	0.87	0.20	124,124,124,124	0
56	MG	EB	3261	1/1	0.87	0.05	115,115,115,115	0
56	MG	B	2981	1/1	0.87	0.28	82,82,82,82	0
56	MG	B	2969	1/1	0.87	0.23	83,83,83,83	0
56	MG	EB	2956	1/1	0.87	0.39	92,92,92,92	0
56	MG	EB	3269	1/1	0.87	0.12	103,103,103,103	0
56	MG	MC	303	1/1	0.87	0.07	140,140,140,140	0
56	MG	B	2985	1/1	0.87	0.25	89,89,89,89	0
56	MG	EB	3272	1/1	0.87	0.35	128,128,128,128	0
56	MG	EB	3145	1/1	0.87	0.10	95,95,95,95	0
56	MG	B	3057	1/1	0.87	0.44	76,76,76,76	0
56	MG	DB	1719	1/1	0.87	0.09	113,113,113,113	0
56	MG	EB	3214	1/1	0.87	0.07	128,128,128,128	0
56	MG	DB	1647	1/1	0.87	0.15	123,123,123,123	0
56	MG	B	2925	1/1	0.87	0.28	73,73,73,73	0
56	MG	B	3264	1/1	0.87	0.19	97,97,97,97	0
56	MG	OB	201	1/1	0.87	0.19	96,96,96,96	0
56	MG	EB	3218	1/1	0.87	0.23	92,92,92,92	0
56	MG	DB	1723	1/1	0.87	0.13	102,102,102,102	0
56	MG	B	3265	1/1	0.87	0.16	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3023	1/1	0.87	0.25	79,79,79,79	0
56	MG	EB	3061	1/1	0.87	0.28	86,86,86,86	0
56	MG	EB	2926	1/1	0.87	0.52	101,101,101,101	0
56	MG	B	2907	1/1	0.87	0.15	79,79,79,79	0
56	MG	EB	3293	1/1	0.87	0.15	85,85,85,85	0
56	MG	B	3354	1/1	0.87	0.13	103,103,103,103	0
56	MG	A	1609	1/1	0.87	0.20	74,74,74,74	0
56	MG	EB	3013	1/1	0.87	0.28	81,81,81,81	0
56	MG	B	2992	1/1	0.87	0.43	80,80,80,80	0
56	MG	EB	3069	1/1	0.87	0.21	86,86,86,86	0
56	MG	B	3406	1/1	0.87	0.29	86,86,86,86	0
56	MG	A	1756	1/1	0.87	0.07	170,170,170,170	0
56	MG	DB	1695	1/1	0.87	0.15	109,109,109,109	0
56	MG	B	3322	1/1	0.87	0.12	90,90,90,90	0
56	MG	B	3410	1/1	0.87	0.14	127,127,127,127	0
56	MG	B	3203	1/1	0.87	0.19	82,82,82,82	0
56	MG	YB	203	1/1	0.87	0.17	130,130,130,130	0
56	MG	B	2935	1/1	0.87	0.40	79,79,79,79	0
56	MG	DB	1632	1/1	0.87	0.72	110,110,110,110	0
56	MG	EB	3157	1/1	0.88	0.34	88,88,88,88	0
56	MG	B	3306	1/1	0.88	0.14	82,82,82,82	0
56	MG	EB	3048	1/1	0.88	0.15	88,88,88,88	0
56	MG	L	202	1/1	0.88	0.41	91,91,91,91	0
56	MG	EB	3162	1/1	0.88	0.10	87,87,87,87	0
56	MG	EB	2997	1/1	0.88	0.29	85,85,85,85	0
56	MG	EB	2952	1/1	0.88	0.21	94,94,94,94	0
56	MG	B	2987	1/1	0.88	0.46	82,82,82,82	0
56	MG	B	3341	1/1	0.88	0.08	94,94,94,94	0
56	MG	Z	101	1/1	0.88	0.23	97,97,97,97	0
56	MG	B	3121	1/1	0.88	0.18	95,95,95,95	0
56	MG	EB	3003	1/1	0.88	0.40	86,86,86,86	0
56	MG	B	2946	1/1	0.88	0.27	84,84,84,84	0
56	MG	B	3312	1/1	0.88	0.18	80,80,80,80	0
56	MG	B	3135	1/1	0.88	0.12	66,66,66,66	0
56	MG	EB	3063	1/1	0.88	0.23	109,109,109,109	0
56	MG	B	3398	1/1	0.88	0.19	89,89,89,89	0
56	MG	B	3052	1/1	0.88	0.25	78,78,78,78	0
56	MG	B	2939	1/1	0.88	0.16	76,76,76,76	0
56	MG	B	2999	1/1	0.88	0.29	68,68,68,68	0
56	MG	HB	303	1/1	0.88	0.37	94,94,94,94	0
56	MG	DB	1675	1/1	0.88	0.20	110,110,110,110	0
56	MG	B	3042	1/1	0.88	0.44	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3358	1/1	0.88	0.26	83,83,83,83	0
56	MG	DB	1637	1/1	0.88	0.41	106,106,106,106	0
56	MG	R	203	1/1	0.88	0.47	84,84,84,84	0
56	MG	B	2991	1/1	0.88	0.30	84,84,84,84	0
56	MG	E	303	1/1	0.88	0.09	104,104,104,104	0
56	MG	B	3411	1/1	0.88	0.11	83,83,83,83	0
56	MG	B	3412	1/1	0.88	0.16	91,91,91,91	0
56	MG	B	3294	1/1	0.88	0.12	92,92,92,92	0
56	MG	B	3072	1/1	0.88	0.30	88,88,88,88	0
56	MG	V	505	1/1	0.88	0.15	113,113,113,113	0
56	MG	B	3323	1/1	0.88	0.14	83,83,83,83	0
56	MG	EB	3270	1/1	0.88	0.24	89,89,89,89	0
56	MG	EB	2938	1/1	0.88	0.34	90,90,90,90	0
56	MG	B	3366	1/1	0.88	0.19	108,108,108,108	0
56	MG	EB	3031	1/1	0.88	0.20	95,95,95,95	0
56	MG	B	3144	1/1	0.88	0.12	100,100,100,100	0
56	MG	EB	3206	1/1	0.88	0.17	93,93,93,93	0
56	MG	B	3182	1/1	0.88	0.28	98,98,98,98	0
56	MG	EB	3208	1/1	0.88	0.45	99,99,99,99	0
56	MG	B	3129	1/1	0.88	0.09	106,106,106,106	0
56	MG	B	3328	1/1	0.88	0.16	93,93,93,93	0
56	MG	DB	1653	1/1	0.88	0.17	95,95,95,95	0
56	MG	A	1648	1/1	0.88	0.13	139,139,139,139	0
56	MG	RB	202	1/1	0.88	0.11	98,98,98,98	0
56	MG	B	3256	1/1	0.88	0.47	94,94,94,94	0
56	MG	EB	3041	1/1	0.88	0.19	90,90,90,90	0
56	MG	B	3212	1/1	0.88	0.18	95,95,95,95	0
56	MG	B	3035	1/1	0.88	0.19	78,78,78,78	0
56	MG	B	3259	1/1	0.88	0.28	85,85,85,85	0
56	MG	EB	3292	1/1	0.88	0.10	91,91,91,91	0
56	MG	EB	3095	1/1	0.88	0.29	110,110,110,110	0
56	MG	EB	3096	1/1	0.88	0.26	96,96,96,96	0
56	MG	EB	3224	1/1	0.88	0.22	93,93,93,93	0
56	MG	EB	3154	1/1	0.88	0.07	114,114,114,114	0
56	MG	EB	3046	1/1	0.88	0.30	104,104,104,104	0
56	MG	A	1750	1/1	0.89	0.18	130,130,130,130	0
56	MG	B	3349	1/1	0.89	0.30	81,81,81,81	0
56	MG	EB	3233	1/1	0.89	0.21	83,83,83,83	0
56	MG	EB	3184	1/1	0.89	0.10	120,120,120,120	0
56	MG	EB	3288	1/1	0.89	0.12	111,111,111,111	0
56	MG	B	3092	1/1	0.89	0.22	86,86,86,86	0
56	MG	B	3073	1/1	0.89	0.17	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3194	1/1	0.89	0.06	110,110,110,110	0
56	MG	B	3385	1/1	0.89	0.11	83,83,83,83	0
56	MG	B	3210	1/1	0.89	0.20	87,87,87,87	0
56	MG	EB	3033	1/1	0.89	0.39	103,103,103,103	0
56	MG	EB	3193	1/1	0.89	0.19	106,106,106,106	0
56	MG	B	3389	1/1	0.89	0.10	98,98,98,98	0
56	MG	PB	201	1/1	0.89	0.22	99,99,99,99	0
56	MG	L	204	1/1	0.89	0.12	104,104,104,104	0
56	MG	B	3237	1/1	0.89	0.27	73,73,73,73	0
56	MG	IA	106	1/1	0.89	0.06	112,112,112,112	0
56	MG	B	3011	1/1	0.89	0.09	91,91,91,91	0
56	MG	EB	3111	1/1	0.89	0.16	127,127,127,127	0
56	MG	M	204	1/1	0.89	0.32	88,88,88,88	0
56	MG	N	201	1/1	0.89	0.08	111,111,111,111	0
56	MG	DB	1651	1/1	0.89	0.23	107,107,107,107	0
56	MG	B	3299	1/1	0.89	0.13	103,103,103,103	0
56	MG	B	3336	1/1	0.89	0.15	86,86,86,86	0
56	MG	EB	3255	1/1	0.89	0.19	108,108,108,108	0
56	MG	EB	3161	1/1	0.89	0.10	78,78,78,78	0
56	MG	EB	3045	1/1	0.89	0.31	84,84,84,84	0
56	MG	EB	3210	1/1	0.89	0.36	103,103,103,103	0
56	MG	DB	1625	1/1	0.89	0.18	87,87,87,87	0
56	MG	B	3013	1/1	0.89	0.24	84,84,84,84	0
56	MG	DB	1688	1/1	0.89	0.12	113,113,113,113	0
56	MG	B	3365	1/1	0.89	0.17	82,82,82,82	0
56	MG	B	3339	1/1	0.89	0.24	98,98,98,98	0
56	MG	B	3240	1/1	0.89	0.16	100,100,100,100	0
56	MG	DB	1759	1/1	0.89	0.12	102,102,102,102	0
56	MG	Y	101	1/1	0.89	0.34	88,88,88,88	0
56	MG	B	2996	1/1	0.89	0.35	75,75,75,75	0
56	MG	EB	3017	1/1	0.89	0.18	93,93,93,93	0
56	MG	EB	3175	1/1	0.89	0.07	106,106,106,106	0
56	MG	B	2998	1/1	0.89	0.18	66,66,66,66	0
56	MG	B	3090	1/1	0.89	0.20	85,85,85,85	0
56	MG	B	3290	1/1	0.89	0.09	90,90,90,90	0
56	MG	R	204	1/1	0.89	0.34	86,86,86,86	0
56	MG	EB	2953	1/1	0.89	0.31	94,94,94,94	0
56	MG	B	3009	1/1	0.90	0.13	81,81,81,81	0
56	MG	EB	3126	1/1	0.90	0.10	82,82,82,82	0
56	MG	Q	201	1/1	0.90	0.13	115,115,115,115	0
56	MG	B	3206	1/1	0.90	0.07	105,105,105,105	0
56	MG	A	1741	1/1	0.90	0.12	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	EB	3167	1/1	0.90	0.23	103,103,103,103	0
56	MG	B	3396	1/1	0.90	0.15	101,101,101,101	0
56	MG	B	3254	1/1	0.90	0.24	102,102,102,102	0
56	MG	B	2990	1/1	0.90	0.29	72,72,72,72	0
56	MG	EB	2964	1/1	0.90	0.12	98,98,98,98	0
56	MG	B	3012	1/1	0.90	0.33	98,98,98,98	0
56	MG	B	3164	1/1	0.90	0.38	91,91,91,91	0
56	MG	E	304	1/1	0.90	0.08	92,92,92,92	0
56	MG	B	3319	1/1	0.90	0.10	80,80,80,80	0
56	MG	EB	3294	1/1	0.90	0.17	117,117,117,117	0
56	MG	B	2954	1/1	0.90	0.25	67,67,67,67	0
56	MG	B	3059	1/1	0.90	0.11	74,74,74,74	0
56	MG	M	202	1/1	0.90	0.17	87,87,87,87	0
56	MG	EB	3024	1/1	0.90	0.23	100,100,100,100	0
56	MG	B	3120	1/1	0.90	0.26	80,80,80,80	0
56	MG	B	3387	1/1	0.90	0.28	87,87,87,87	0
56	MG	EB	3058	1/1	0.90	0.32	102,102,102,102	0
56	MG	EB	3028	1/1	0.90	0.32	95,95,95,95	0
56	MG	B	3414	1/1	0.90	0.17	93,93,93,93	0
56	MG	B	3109	1/1	0.90	0.41	86,86,86,86	0
56	MG	EB	3118	1/1	0.90	0.09	102,102,102,102	0
56	MG	EB	3155	1/1	0.90	0.17	108,108,108,108	0
56	MG	B	3060	1/1	0.90	0.37	95,95,95,95	0
56	MG	DB	1687	1/1	0.90	0.14	96,96,96,96	0
56	MG	DB	1711	1/1	0.90	0.26	115,115,115,115	0
56	MG	EB	2955	1/1	0.90	0.27	85,85,85,85	0
56	MG	EB	3007	1/1	0.90	0.30	89,89,89,89	0
56	MG	EB	3277	1/1	0.90	0.17	91,91,91,91	0
56	MG	B	3079	1/1	0.90	0.17	86,86,86,86	0
56	MG	B	3388	1/1	0.91	0.15	93,93,93,93	0
56	MG	B	3067	1/1	0.91	0.16	71,71,71,71	0
56	MG	B	3310	1/1	0.91	0.17	93,93,93,93	0
56	MG	B	3201	1/1	0.91	0.11	87,87,87,87	0
56	MG	DB	1753	1/1	0.91	0.24	119,119,119,119	0
56	MG	RB	205	1/1	0.91	0.21	95,95,95,95	0
56	MG	EB	2906	1/1	0.91	0.50	79,79,79,79	0
56	MG	B	3202	1/1	0.91	0.26	74,74,74,74	0
56	MG	B	3252	1/1	0.91	0.27	90,90,90,90	0
56	MG	DB	1727	1/1	0.91	0.23	108,108,108,108	0
56	MG	B	3235	1/1	0.91	0.34	82,82,82,82	0
56	MG	A	1757	1/1	0.91	0.07	99,99,99,99	0
56	MG	EB	3127	1/1	0.91	0.14	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	2955	1/1	0.91	0.39	76,76,76,76	0
56	MG	EB	3129	1/1	0.91	0.20	80,80,80,80	0
56	MG	B	3399	1/1	0.91	0.36	89,89,89,89	0
56	MG	C	215	1/1	0.91	0.06	123,123,123,123	0
56	MG	B	3221	1/1	0.91	0.18	89,89,89,89	0
56	MG	B	3047	1/1	0.91	0.38	88,88,88,88	0
56	MG	B	2980	1/1	0.91	0.24	75,75,75,75	0
56	MG	EB	3171	1/1	0.91	0.25	93,93,93,93	0
56	MG	B	2970	1/1	0.91	0.49	72,72,72,72	0
56	MG	EB	2920	1/1	0.91	0.64	87,87,87,87	0
56	MG	EB	2980	1/1	0.91	0.35	82,82,82,82	0
56	MG	B	3087	1/1	0.91	0.17	83,83,83,83	0
56	MG	A	1719	1/1	0.91	0.19	126,126,126,126	0
56	MG	S	202	1/1	0.91	0.08	105,105,105,105	0
56	MG	B	3245	1/1	0.91	0.16	85,85,85,85	0
56	MG	EB	3220	1/1	0.91	0.09	107,107,107,107	0
56	MG	GD	403	1/1	0.91	0.07	95,95,95,95	0
56	MG	B	2941	1/1	0.91	0.31	79,79,79,79	0
56	MG	B	3353	1/1	0.91	0.07	93,93,93,93	0
56	MG	B	2901	1/1	0.91	0.40	60,60,60,60	0
56	MG	B	2919	1/1	0.91	0.18	74,74,74,74	0
56	MG	B	3329	1/1	0.91	0.13	105,105,105,105	0
57	ZN	V	501	1/1	0.91	0.15	130,130,130,130	0
56	MG	LC	104	1/1	0.91	0.14	101,101,101,101	0
56	MG	EB	3185	1/1	0.91	0.20	101,101,101,101	0
56	MG	L	206	1/1	0.91	0.09	97,97,97,97	0
56	MG	B	3368	1/1	0.92	0.17	90,90,90,90	0
56	MG	EB	3056	1/1	0.92	0.25	87,87,87,87	0
56	MG	EB	3211	1/1	0.92	0.21	100,100,100,100	0
56	MG	EB	3212	1/1	0.92	0.15	100,100,100,100	0
56	MG	B	3403	1/1	0.92	0.20	101,101,101,101	0
56	MG	B	3215	1/1	0.92	0.07	156,156,156,156	0
56	MG	V	504	1/1	0.92	0.18	101,101,101,101	0
56	MG	DB	1655	1/1	0.92	0.24	116,116,116,116	0
56	MG	B	3405	1/1	0.92	0.17	120,120,120,120	0
56	MG	B	3198	1/1	0.92	0.07	107,107,107,107	0
56	MG	DB	1658	1/1	0.92	0.19	109,109,109,109	0
56	MG	B	3371	1/1	0.92	0.65	80,80,80,80	0
56	MG	FB	215	1/1	0.92	0.09	135,135,135,135	0
56	MG	EB	3265	1/1	0.92	0.10	98,98,98,98	0
56	MG	B	3102	1/1	0.92	0.42	84,84,84,84	0
56	MG	B	3409	1/1	0.92	0.08	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3041	1/1	0.92	0.38	81,81,81,81	0
56	MG	A	1754	1/1	0.92	0.17	112,112,112,112	0
56	MG	B	3278	1/1	0.92	0.15	83,83,83,83	0
56	MG	B	3413	1/1	0.92	0.09	98,98,98,98	0
56	MG	DB	1634	1/1	0.92	0.20	99,99,99,99	0
56	MG	B	3185	1/1	0.92	0.13	82,82,82,82	0
56	MG	B	3050	1/1	0.92	0.15	87,87,87,87	0
56	MG	B	3222	1/1	0.92	0.12	96,96,96,96	0
56	MG	EB	3150	1/1	0.92	0.23	88,88,88,88	0
56	MG	B	3223	1/1	0.92	0.19	82,82,82,82	0
56	MG	B	3355	1/1	0.92	0.12	81,81,81,81	0
56	MG	EB	3040	1/1	0.92	0.49	115,115,115,115	0
56	MG	B	3066	1/1	0.92	0.30	77,77,77,77	0
56	MG	B	3307	1/1	0.92	0.12	86,86,86,86	0
56	MG	A	1700	1/1	0.92	0.21	96,96,96,96	0
56	MG	B	3359	1/1	0.92	0.10	79,79,79,79	0
56	MG	DB	1744	1/1	0.92	0.11	126,126,126,126	0
56	MG	B	3141	1/1	0.92	0.34	89,89,89,89	0
56	MG	B	3044	1/1	0.92	0.16	69,69,69,69	0
56	MG	B	3143	1/1	0.92	0.27	83,83,83,83	0
56	MG	A	1674	1/1	0.92	0.06	98,98,98,98	0
56	MG	A	1708	1/1	0.92	0.14	89,89,89,89	0
56	MG	DB	1716	1/1	0.92	0.08	119,119,119,119	0
56	MG	B	3146	1/1	0.92	0.43	81,81,81,81	0
56	MG	B	3080	1/1	0.92	0.25	99,99,99,99	0
56	MG	B	3279	1/1	0.93	0.14	79,79,79,79	0
56	MG	B	2973	1/1	0.93	0.48	80,80,80,80	0
56	MG	B	3301	1/1	0.93	0.20	101,101,101,101	0
56	MG	B	3281	1/1	0.93	0.10	88,88,88,88	0
56	MG	WB	203	1/1	0.93	0.20	82,82,82,82	0
56	MG	B	3324	1/1	0.93	0.07	94,94,94,94	0
56	MG	B	2983	1/1	0.93	0.24	71,71,71,71	0
56	MG	DB	1659	1/1	0.93	0.13	106,106,106,106	0
56	MG	EB	3267	1/1	0.93	0.15	82,82,82,82	0
56	MG	B	2974	1/1	0.93	0.53	68,68,68,68	0
56	MG	B	3088	1/1	0.93	0.48	88,88,88,88	0
56	MG	B	3048	1/1	0.93	0.22	80,80,80,80	0
56	MG	A	1737	1/1	0.93	0.07	97,97,97,97	0
56	MG	EB	3178	1/1	0.93	0.49	90,90,90,90	0
56	MG	B	2931	1/1	0.93	0.34	74,74,74,74	0
56	MG	EB	3276	1/1	0.93	0.20	121,121,121,121	0
56	MG	B	2965	1/1	0.93	0.39	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3270	1/1	0.93	0.07	81,81,81,81	0
56	MG	L	205	1/1	0.93	0.06	110,110,110,110	0
56	MG	B	3253	1/1	0.93	0.46	98,98,98,98	0
56	MG	B	3081	1/1	0.93	0.19	76,76,76,76	0
56	MG	B	2913	1/1	0.93	0.51	66,66,66,66	0
56	MG	B	3196	1/1	0.93	0.06	158,158,158,158	0
56	MG	RB	201	1/1	0.93	0.16	105,105,105,105	0
56	MG	M	203	1/1	0.93	0.20	84,84,84,84	0
56	MG	B	3241	1/1	0.93	0.35	92,92,92,92	0
56	MG	B	2937	1/1	0.93	0.41	81,81,81,81	0
56	MG	B	3183	1/1	0.93	0.15	85,85,85,85	0
56	MG	B	3168	1/1	0.93	0.21	79,79,79,79	0
56	MG	B	3400	1/1	0.93	0.42	83,83,83,83	0
56	MG	B	3345	1/1	0.93	0.10	82,82,82,82	0
56	MG	B	3402	1/1	0.93	0.20	109,109,109,109	0
56	MG	EB	3258	1/1	0.93	0.14	90,90,90,90	0
56	MG	B	3039	1/1	0.94	0.12	83,83,83,83	0
56	MG	DB	1747	1/1	0.94	0.12	106,106,106,106	0
56	MG	B	3397	1/1	0.94	0.15	85,85,85,85	0
56	MG	A	1686	1/1	0.94	0.09	116,116,116,116	0
56	MG	B	3377	1/1	0.94	0.13	93,93,93,93	0
56	MG	EB	3027	1/1	0.94	0.13	95,95,95,95	0
56	MG	B	3016	1/1	0.94	0.47	81,81,81,81	0
56	MG	B	3379	1/1	0.94	0.12	104,104,104,104	0
56	MG	EB	3248	1/1	0.94	0.12	100,100,100,100	0
56	MG	EB	3282	1/1	0.94	0.11	95,95,95,95	0
56	MG	DB	1706	1/1	0.94	0.12	111,111,111,111	0
56	MG	B	3070	1/1	0.94	0.10	72,72,72,72	0
56	MG	B	3382	1/1	0.94	0.05	92,92,92,92	0
56	MG	B	3173	1/1	0.94	0.08	74,74,74,74	0
56	MG	B	3174	1/1	0.94	0.20	96,96,96,96	0
56	MG	A	1619	1/1	0.94	0.26	100,100,100,100	0
56	MG	B	3189	1/1	0.94	0.12	96,96,96,96	0
56	MG	B	3204	1/1	0.94	0.14	76,76,76,76	0
56	MG	EB	3228	1/1	0.94	0.11	111,111,111,111	0
56	MG	B	2982	1/1	0.94	0.29	96,96,96,96	0
56	MG	B	2961	1/1	0.94	0.24	77,77,77,77	0
56	MG	EB	3202	1/1	0.94	0.08	89,89,89,89	0
56	MG	EB	2912	1/1	0.94	0.30	76,76,76,76	0
56	MG	V	506	1/1	0.94	0.09	119,119,119,119	0
56	MG	B	3351	1/1	0.94	0.06	99,99,99,99	0
56	MG	B	3117	1/1	0.94	0.17	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3000	1/1	0.94	0.17	76,76,76,76	0
56	MG	C	222	1/1	0.94	0.07	119,119,119,119	0
56	MG	B	3028	1/1	0.94	0.12	72,72,72,72	0
56	MG	A	1673	1/1	0.94	0.12	153,153,153,153	0
56	MG	B	3162	1/1	0.95	0.28	88,88,88,88	0
56	MG	B	3030	1/1	0.95	0.20	76,76,76,76	0
56	MG	A	1716	1/1	0.95	0.14	95,95,95,95	0
56	MG	EB	3131	1/1	0.95	0.12	97,97,97,97	0
56	MG	C	221	1/1	0.95	0.11	121,121,121,121	0
56	MG	S	201	1/1	0.95	0.20	98,98,98,98	0
56	MG	EB	3204	1/1	0.95	0.13	92,92,92,92	0
56	MG	B	3344	1/1	0.95	0.13	93,93,93,93	0
56	MG	EB	3252	1/1	0.95	0.13	99,99,99,99	0
56	MG	B	2932	1/1	0.95	0.23	73,73,73,73	0
56	MG	EB	2987	1/1	0.95	0.22	82,82,82,82	0
56	MG	B	3372	1/1	0.95	0.11	76,76,76,76	0
56	MG	DB	1702	1/1	0.95	0.10	111,111,111,111	0
56	MG	B	3084	1/1	0.95	0.04	89,89,89,89	0
56	MG	U	101	1/1	0.95	0.13	85,85,85,85	0
56	MG	B	3360	1/1	0.95	0.06	78,78,78,78	0
56	MG	XB	101	1/1	0.95	0.12	119,119,119,119	0
56	MG	B	3375	1/1	0.95	0.11	79,79,79,79	0
56	MG	B	2975	1/1	0.95	0.26	72,72,72,72	0
56	MG	B	3393	1/1	0.95	0.09	99,99,99,99	0
56	MG	B	3064	1/1	0.95	0.23	89,89,89,89	0
56	MG	EB	3264	1/1	0.95	0.09	93,93,93,93	0
56	MG	B	3112	1/1	0.95	0.18	84,84,84,84	0
56	MG	B	3211	1/1	0.95	0.11	81,81,81,81	0
56	MG	B	2997	1/1	0.95	0.27	75,75,75,75	0
56	MG	B	3014	1/1	0.95	0.27	78,78,78,78	0
57	ZN	FC	101	1/1	0.95	0.06	142,142,142,142	0
56	MG	EB	3268	1/1	0.96	0.10	94,94,94,94	0
56	MG	B	3350	1/1	0.96	0.11	79,79,79,79	0
56	MG	B	3293	1/1	0.96	0.06	87,87,87,87	0
56	MG	EB	3137	1/1	0.96	0.39	91,91,91,91	0
56	MG	B	3104	1/1	0.96	0.10	76,76,76,76	0
56	MG	B	3342	1/1	0.96	0.19	80,80,80,80	0
56	MG	B	3333	1/1	0.96	0.13	91,91,91,91	0
56	MG	A	1714	1/1	0.96	0.56	115,115,115,115	0
56	MG	HB	305	1/1	0.96	0.13	96,96,96,96	0
56	MG	B	3260	1/1	0.96	0.11	98,98,98,98	0
56	MG	EB	3192	1/1	0.96	0.12	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B	3321	1/1	0.96	0.19	88,88,88,88	0
56	MG	EB	3194	1/1	0.96	0.16	89,89,89,89	0
56	MG	B	3337	1/1	0.96	0.17	101,101,101,101	0
56	MG	B	2909	1/1	0.96	0.25	74,74,74,74	0
56	MG	B	3169	1/1	0.96	0.29	82,82,82,82	0
57	ZN	GC	101	1/1	0.96	0.09	156,156,156,156	0
56	MG	DB	1755	1/1	0.97	0.05	142,142,142,142	0
56	MG	EB	3274	1/1	0.97	0.20	100,100,100,100	0
56	MG	B	3381	1/1	0.97	0.11	80,80,80,80	0
57	ZN	CA	101	1/1	0.97	0.03	134,134,134,134	0
56	MG	DB	1777	1/1	0.97	0.10	110,110,110,110	0
56	MG	B	3157	1/1	0.97	0.21	77,77,77,77	0
56	MG	C	203	1/1	0.97	0.06	125,125,125,125	0
56	MG	G	303	1/1	0.97	0.08	75,75,75,75	0
56	MG	B	3149	1/1	0.98	0.08	92,92,92,92	0
56	MG	EB	3055	1/1	0.98	0.14	80,80,80,80	0
56	MG	EB	2967	1/1	0.98	0.33	86,86,86,86	0
57	ZN	DA	101	1/1	0.98	0.05	141,141,141,141	0
57	ZN	JC	101	1/1	0.98	0.05	159,159,159,159	0
57	ZN	GA	101	1/1	0.99	0.02	132,132,132,132	0
56	MG	EB	3147	1/1	0.99	0.03	165,165,165,165	0

6.5 Other polymers

There are no such residues in this entry.