



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 11:38 AM UTC

PDB ID : 4YZV / pdb_00004yzv
Title : Precleavage 70S structure of the *P. vulgaris* HigB deltaH92 toxin bound to the ACA codon
Authors : Schureck, M.A.; Dunkle, J.A.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2015-03-25
Resolution : 3.10 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

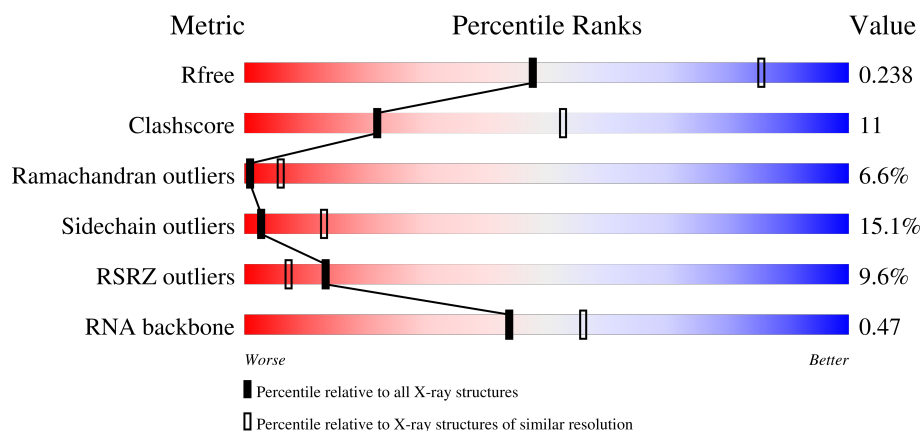
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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

Mol	Chain	Length	Quality of chain
1	QA	1522	5% 57% 31% 11% .
1	XA	1522	3% 58% 33% 8% .
2	QB	256	17% 52% 31% 9% 8%
2	XB	256	19% 49% 35% 8% 8%

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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	

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Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	25	
21	XU	25	
22	QV	77	
22	XV	77	
23	QX	24	
23	XX	24	
24	QY	117	
24	XY	117	
25	RA	2916	
25	YA	2916	
26	RB	124	
26	YB	124	
27	RD	276	
27	YD	276	

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Mol	Chain	Length	Quality of chain
28	RE	206	
28	YE	206	
29	RF	210	
29	YF	210	
30	RG	182	
30	YG	182	
31	RH	180	
31	YH	180	
32	RI	148	
32	YI	148	
33	RN	140	
33	YN	140	
34	RO	122	
34	YO	122	
35	RP	150	
35	YP	150	
36	RQ	141	
36	YQ	141	
37	RR	118	
37	YR	118	
38	RS	112	
38	YS	112	
39	RT	146	
39	YT	146	
40	RU	118	

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Mol	Chain	Length	Quality of chain
40	YU	118	
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	71	
51	R5	60	
51	Y5	60	
52	R6	54	
52	Y6	54	

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Mol	Chain	Length	Quality of chain
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	
56	Z6	3	
56	Z7	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	QA	1639	-	-	-	X
57	MG	QA	1735	-	-	-	X
57	MG	RA	3261	-	-	-	X
57	MG	RA	3323	-	-	-	X
57	MG	YA	3348	-	-	-	X
57	MG	YA	3448	-	-	-	X

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 294445 atoms, of which 18 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1511	Total	C	N	O	P	0	0	0
			32472	14453	6011	10497	1511			
1	XA	1508	Total	C	N	O	P	0	0	0
			32409	14425	6001	10475	1508			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	236	Total	C	N	O	S	0	0	0
			1915	1223	343	344	5			
2	XB	236	Total	C	N	O	S	0	0	0
			1915	1223	343	344	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	QD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	XD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	QE	154	Total	C	N	O	S	0	0	0
			1178	743	221	210	4			
5	XE	154	Total	C	N	O	S	0	0	0
			1178	743	221	210	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	QF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	XF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	QG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	XG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	XH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	QI	128	Total	C	N	O	S	0	0	0
			1018	644	198	175	1			
9	XI	128	Total	C	N	O	S	0	0	0
			1018	644	198	175	1			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	QJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	XJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	121	Total	C	N	O	S	0	0	0
			901	560	171	167	3			
11	XK	121	Total	C	N	O	S	0	0	0
			901	560	171	167	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	QL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	XL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			
13	XM	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	QN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	XN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	QO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	XO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	QP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	XP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	QQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	XQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	71	Total	C	N	O	0	0	0
			585	373	116	96			
18	XR	71	Total	C	N	O	0	0	0
			585	373	116	96			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	82	Total	C	N	O	S	0	0	0
			656	419	121	114	2			
19	XS	82	Total	C	N	O	S	0	0	0
			656	419	121	114	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	XT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	QU	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	XU	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	XV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	QX	20	Total	C	H	N	O	P	0	0	0
			444	198	9	87	131	19			
23	XX	20	Total	C	H	N	O	P	0	0	0
			444	198	9	87	131	19			

- Molecule 24 is a protein called Killer protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	QY	91	Total	C	N	O	0	0	0
			746	478	131	137			
24	XY	91	Total	C	N	O	0	0	0
			746	478	131	137			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QY	0	MET	-	initiating methionine	UNP Q7A225
QY	1	GLY	-	expression tag	UNP Q7A225
QY	92	LYS	-	expression tag	UNP Q7A225
QY	93	LEU	-	expression tag	UNP Q7A225
QY	94	GLY	-	expression tag	UNP Q7A225
QY	95	PRO	-	expression tag	UNP Q7A225
QY	96	GLU	-	expression tag	UNP Q7A225
QY	97	GLN	-	expression tag	UNP Q7A225
QY	98	LYS	-	expression tag	UNP Q7A225
QY	99	LEU	-	expression tag	UNP Q7A225
QY	100	ILE	-	expression tag	UNP Q7A225

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Chain	Residue	Modelled	Actual	Comment	Reference
QY	101	SER	-	expression tag	UNP Q7A225
QY	102	GLU	-	expression tag	UNP Q7A225
QY	103	GLU	-	expression tag	UNP Q7A225
QY	104	ASP	-	expression tag	UNP Q7A225
QY	105	LEU	-	expression tag	UNP Q7A225
QY	106	ASN	-	expression tag	UNP Q7A225
QY	107	SER	-	expression tag	UNP Q7A225
QY	108	ALA	-	expression tag	UNP Q7A225
QY	109	VAL	-	expression tag	UNP Q7A225
QY	110	ASP	-	expression tag	UNP Q7A225
QY	111	HIS	-	expression tag	UNP Q7A225
QY	112	HIS	-	expression tag	UNP Q7A225
QY	113	HIS	-	expression tag	UNP Q7A225
QY	114	HIS	-	expression tag	UNP Q7A225
QY	115	HIS	-	expression tag	UNP Q7A225
QY	116	HIS	-	expression tag	UNP Q7A225
XY	0	MET	-	initiating methionine	UNP Q7A225
XY	1	GLY	-	expression tag	UNP Q7A225
XY	92	LYS	-	expression tag	UNP Q7A225
XY	93	LEU	-	expression tag	UNP Q7A225
XY	94	GLY	-	expression tag	UNP Q7A225
XY	95	PRO	-	expression tag	UNP Q7A225
XY	96	GLU	-	expression tag	UNP Q7A225
XY	97	GLN	-	expression tag	UNP Q7A225
XY	98	LYS	-	expression tag	UNP Q7A225
XY	99	LEU	-	expression tag	UNP Q7A225
XY	100	ILE	-	expression tag	UNP Q7A225
XY	101	SER	-	expression tag	UNP Q7A225
XY	102	GLU	-	expression tag	UNP Q7A225
XY	103	GLU	-	expression tag	UNP Q7A225
XY	104	ASP	-	expression tag	UNP Q7A225
XY	105	LEU	-	expression tag	UNP Q7A225
XY	106	ASN	-	expression tag	UNP Q7A225
XY	107	SER	-	expression tag	UNP Q7A225
XY	108	ALA	-	expression tag	UNP Q7A225
XY	109	VAL	-	expression tag	UNP Q7A225
XY	110	ASP	-	expression tag	UNP Q7A225
XY	111	HIS	-	expression tag	UNP Q7A225
XY	112	HIS	-	expression tag	UNP Q7A225
XY	113	HIS	-	expression tag	UNP Q7A225
XY	114	HIS	-	expression tag	UNP Q7A225
XY	115	HIS	-	expression tag	UNP Q7A225

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Chain	Residue	Modelled	Actual	Comment	Reference
XY	116	HIS	-	expression tag	UNP Q7A225

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	RA	2891	Total	C	N	O	P	0	0	0
			62269	27713	11649	20016	2891			
25	YA	2875	Total	C	N	O	P	0	0	0
			61924	27560	11583	19906	2875			

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	RB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
26	YB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	RD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
27	YD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
28	YE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	RF	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			
29	YF	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	RG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
30	YG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	RH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			
31	YH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	RI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
32	YI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	RN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
33	YN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	RO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
34	YO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
35	YP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RQ	140	Total	C	N	O	S	0	0	0
			1112	710	210	185	7			
36	YQ	139	Total	C	N	O	S	0	0	0
			1107	707	209	184	7			

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	RR	117	Total	C	N	O	0	0	0
			960	599	202	159			
37	YR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	RS	111	Total	C	N	O	0	0	0
			882	556	176	150			
38	YS	111	Total	C	N	O	0	0	0
			882	556	176	150			

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
39	YT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	YU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
41	YV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
42	YW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	RX	92	Total	C	N	O	0	0	0
			725	471	131	123			
43	YX	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	RY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
44	YY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RZ	176	Total	C	N	O	S	0	0	0
			1404	897	252	252	3			
45	YZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R0	83	Total	C	N	O	S	0	0	0
			657	407	139	110	1			
46	Y0	83	Total	C	N	O	S	0	0	0
			657	407	139	110	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
47	Y1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
48	Y2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	R3	59	Total	C	N	O	0	0	0
			469	298	90	81			
49	Y3	59	Total	C	N	O	0	0	0
			469	298	90	81			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	R4	70	Total	C	N	O	S	0	0	0
			573	359	107	103	4			
50	Y4	70	Total	C	N	O	S	0	0	0
			573	359	107	103	4			

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
51	Y5	57	Total	C	N	O	S	0	0	0
			442	278	88	71	5			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	R6	48	Total	C	N	O	S	0	0	0
			417	259	86	68	4			
52	Y6	48	Total	C	N	O	S	0	0	0
			417	259	86	68	4			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	R7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
53	Y7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	R8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
54	Y8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	R9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
55	Y9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 56 is a RNA chain called CC-puromycin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	Z6	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	Z7	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	151	Total	Mg	0	0
			151	151		
57	QD	2	Total	Mg	0	0
			2	2		
57	QE	1	Total	Mg	0	0
			1	1		
57	QL	1	Total	Mg	0	0
			1	1		
57	QN	1	Total	Mg	0	0
			1	1		
57	QV	5	Total	Mg	0	0
			5	5		
57	RA	451	Total	Mg	0	0
			451	451		
57	RB	5	Total	Mg	0	0
			5	5		
57	RD	2	Total	Mg	0	0
			2	2		
57	RE	3	Total	Mg	0	0
			3	3		
57	RF	1	Total	Mg	0	0
			1	1		
57	RP	2	Total	Mg	0	0
			2	2		
57	RQ	2	Total	Mg	0	0
			2	2		
57	RR	1	Total	Mg	0	0
			1	1		
57	RV	1	Total	Mg	0	0
			1	1		
57	RY	2	Total	Mg	0	0
			2	2		
57	R0	2	Total	Mg	0	0
			2	2		
57	R2	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	R5	3	Total 3	Mg 3	0	0
57	XA	164	Total 164	Mg 164	0	0
57	XD	1	Total 1	Mg 1	0	0
57	XE	1	Total 1	Mg 1	0	0
57	XF	1	Total 1	Mg 1	0	0
57	XK	1	Total 1	Mg 1	0	0
57	XL	1	Total 1	Mg 1	0	0
57	XN	1	Total 1	Mg 1	0	0
57	XS	1	Total 1	Mg 1	0	0
57	XV	4	Total 4	Mg 4	0	0
57	YA	504	Total 504	Mg 504	0	0
57	YB	6	Total 6	Mg 6	0	0
57	YD	1	Total 1	Mg 1	0	0
57	YE	2	Total 2	Mg 2	0	0
57	YF	2	Total 2	Mg 2	0	0
57	YG	1	Total 1	Mg 1	0	0
57	YH	2	Total 2	Mg 2	0	0
57	YN	1	Total 1	Mg 1	0	0
57	YO	1	Total 1	Mg 1	0	0
57	YP	2	Total 2	Mg 2	0	0
57	YQ	2	Total 2	Mg 2	0	0

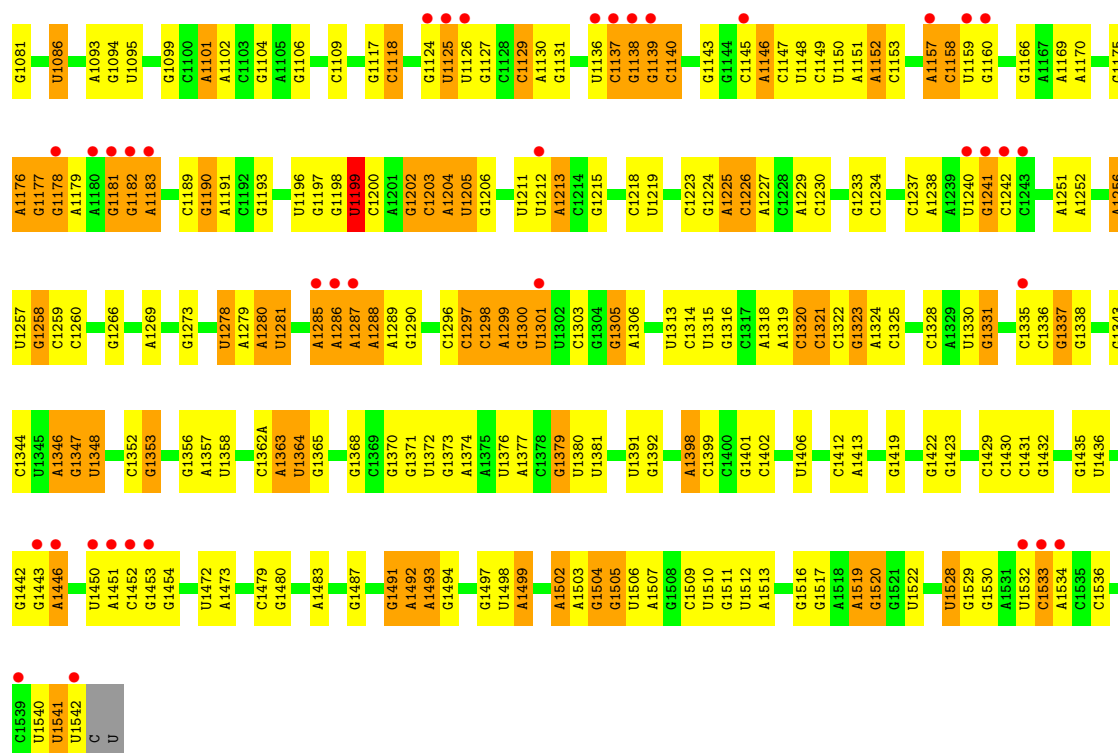
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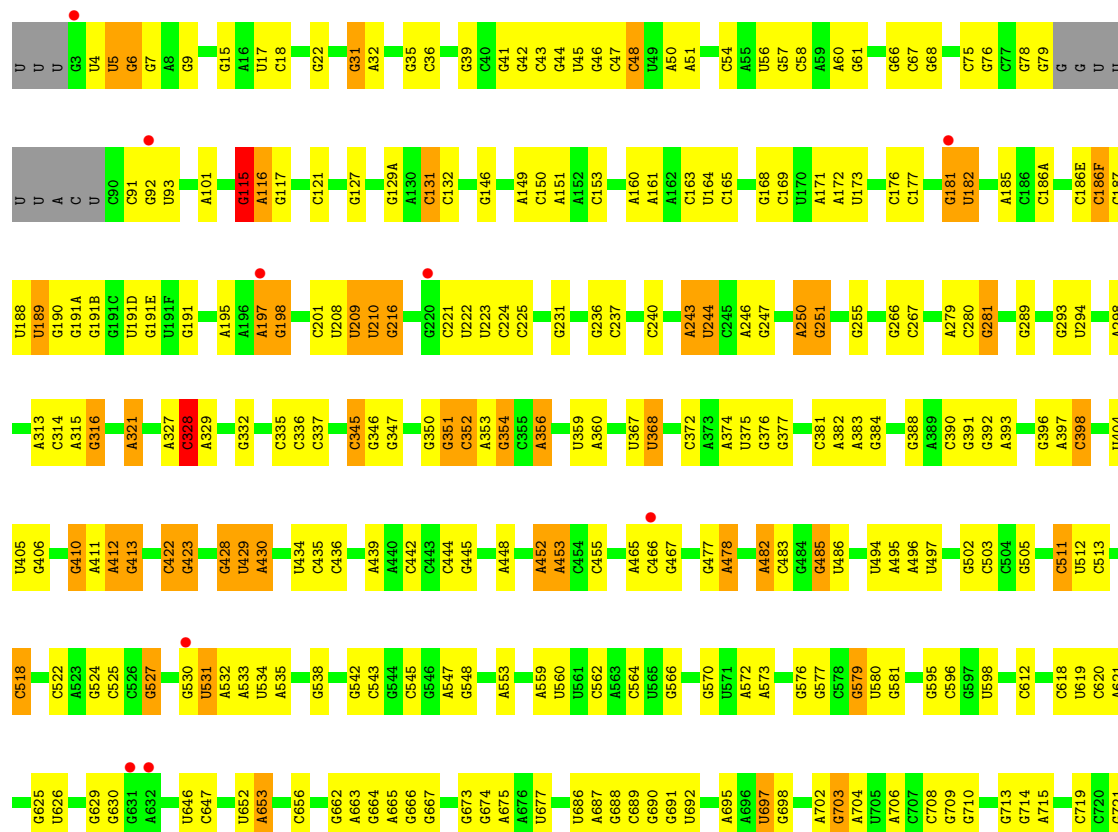
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YR	1	Total	Mg	0	0
			1	1		
57	YU	1	Total	Mg	0	0
			1	1		
57	YV	1	Total	Mg	0	0
			1	1		
57	YW	1	Total	Mg	0	0
			1	1		
57	Y0	1	Total	Mg	0	0
			1	1		
57	Y5	3	Total	Mg	0	0
			3	3		
57	Y7	1	Total	Mg	0	0
			1	1		
57	Z7	1	Total	Mg	0	0
			1	1		

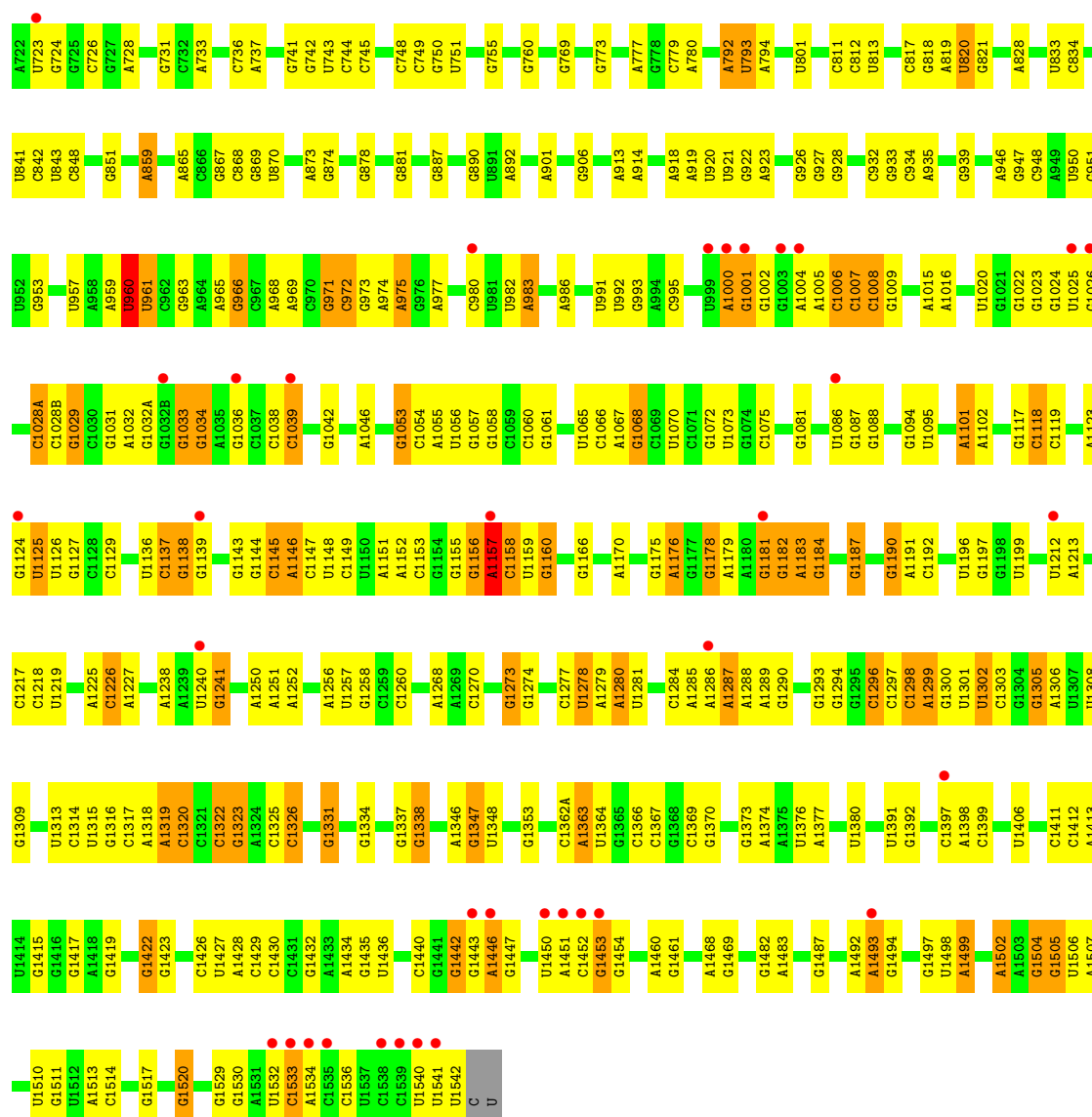
- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	QD	1	Total	Zn	0	0
			1	1		
58	QN	1	Total	Zn	0	0
			1	1		
58	XD	1	Total	Zn	0	0
			1	1		
58	XN	1	Total	Zn	0	0
			1	1		

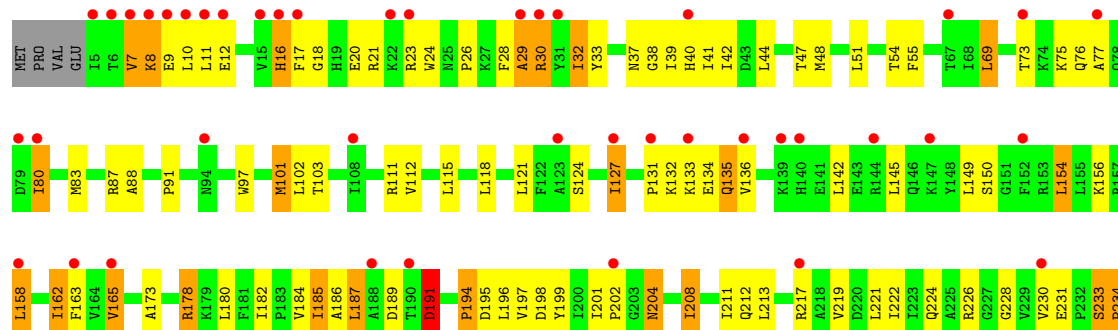


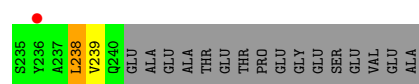
• Molecule 1: 16S rRNA



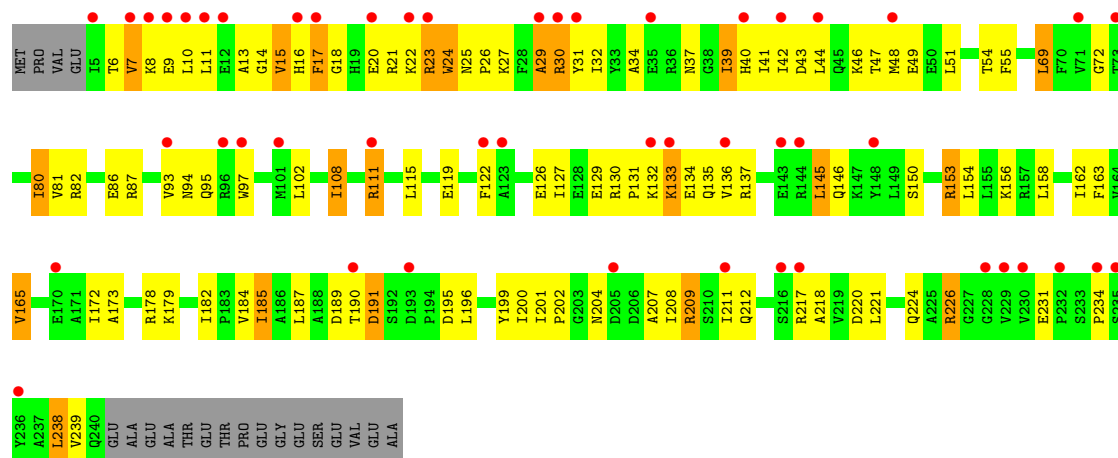


• Molecule 2: 30S ribosomal protein S2

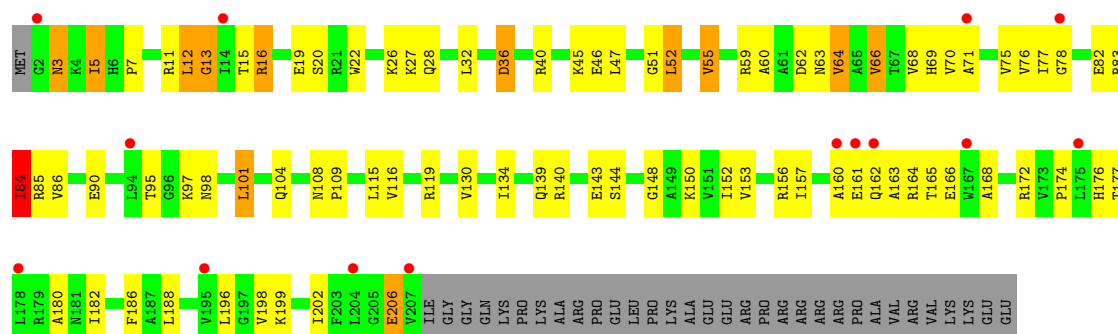




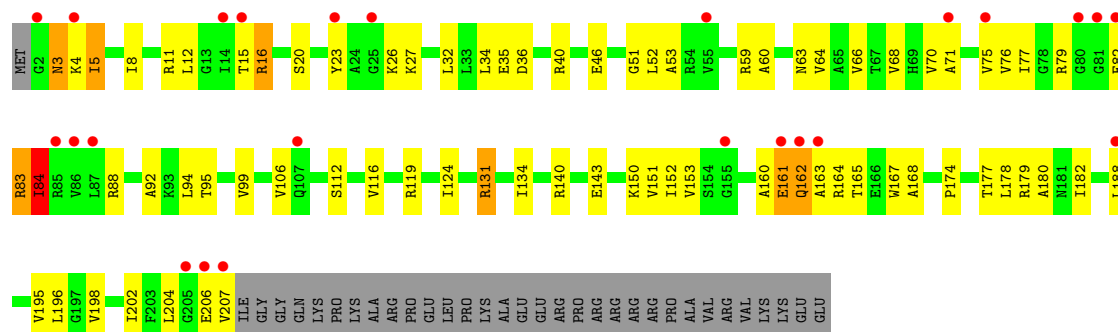
• Molecule 2: 30S ribosomal protein S2



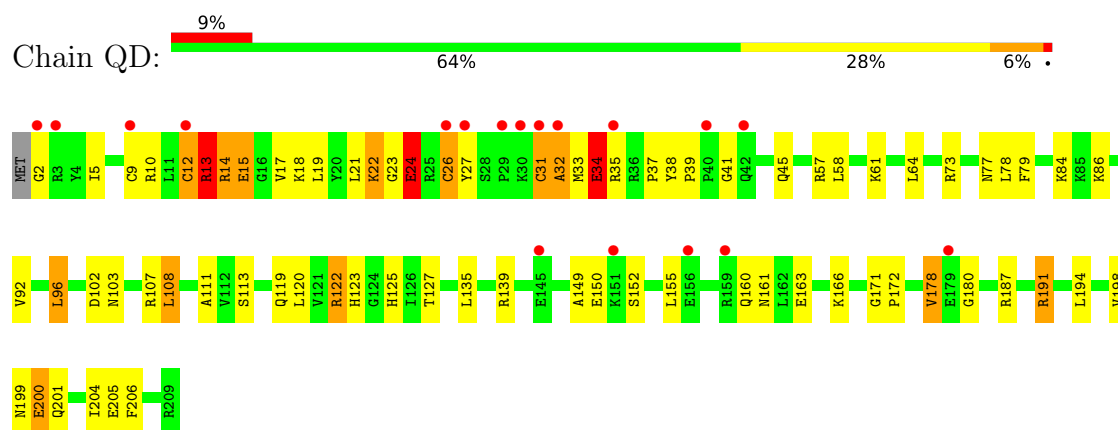
• Molecule 3: 30S ribosomal protein S3



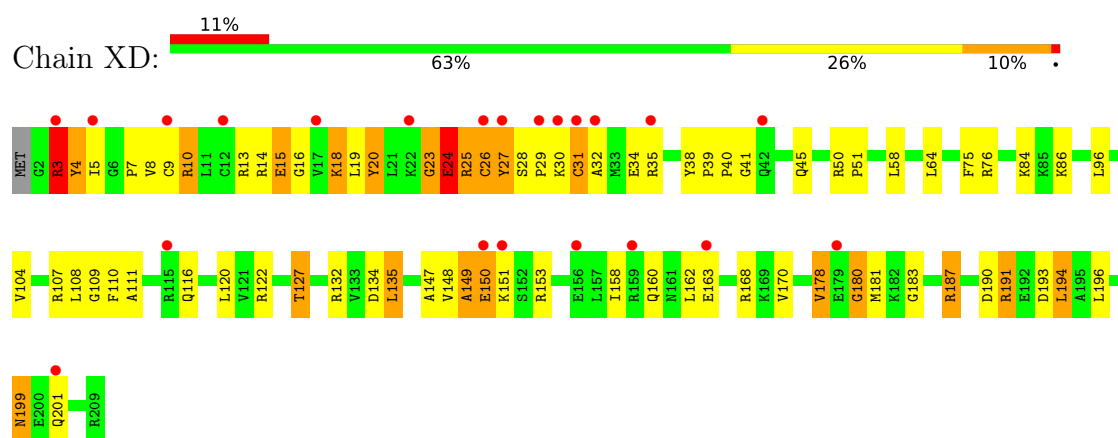
• Molecule 3: 30S ribosomal protein S3



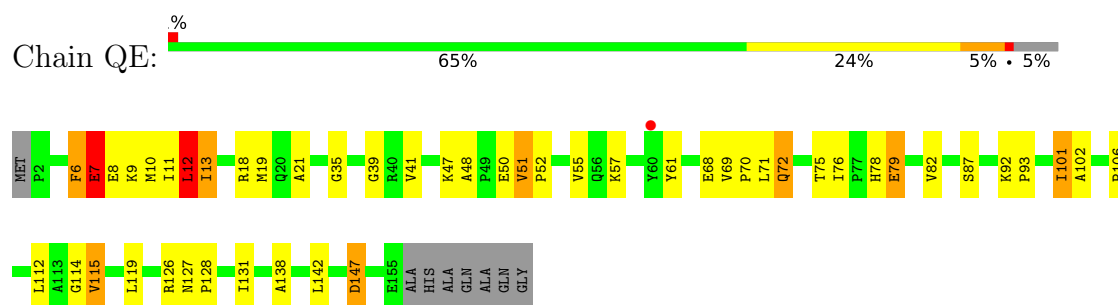
- Molecule 4: 30S ribosomal protein S4



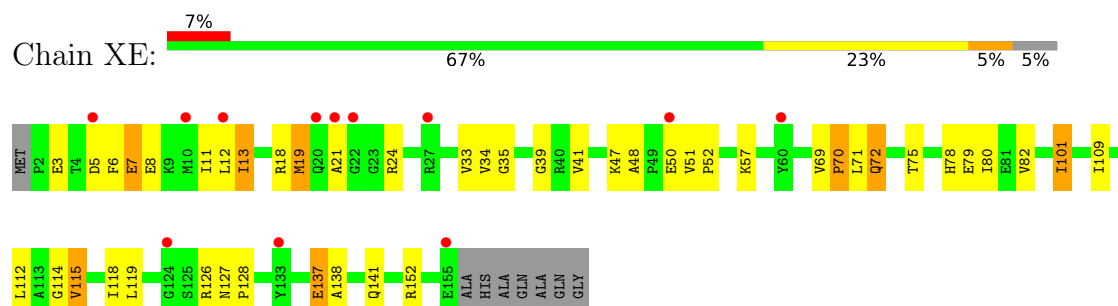
- Molecule 4: 30S ribosomal protein S4



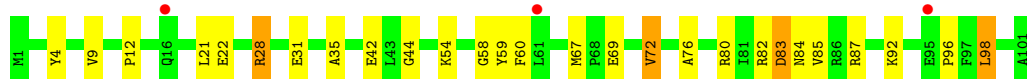
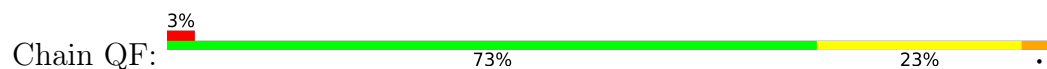
- Molecule 5: 30S ribosomal protein S5



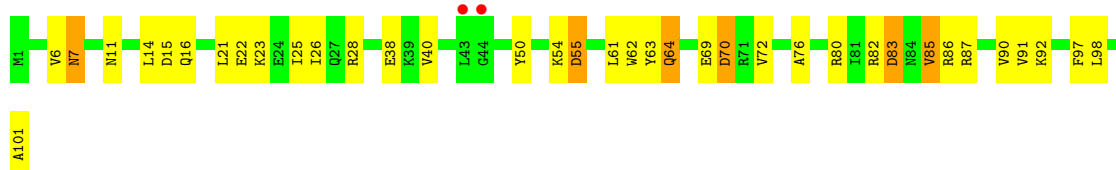
- Molecule 5: 30S ribosomal protein S5



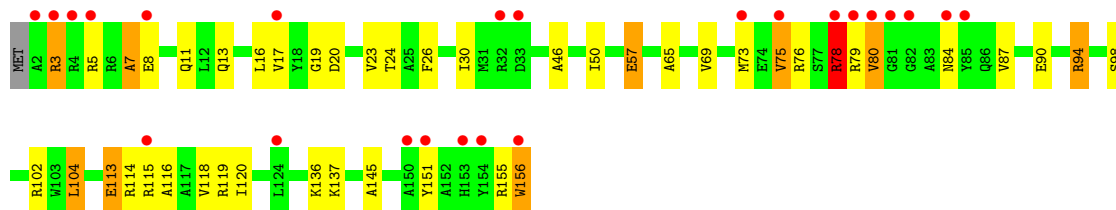
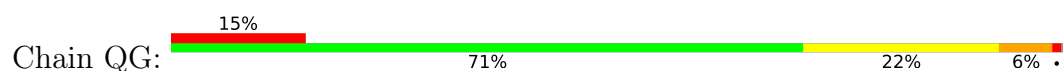
- Molecule 6: 30S ribosomal protein S6



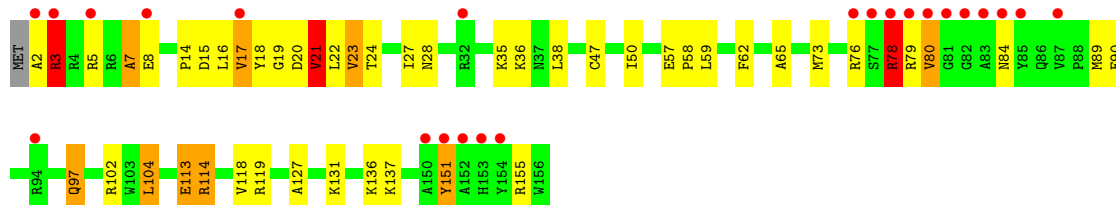
- Molecule 6: 30S ribosomal protein S6



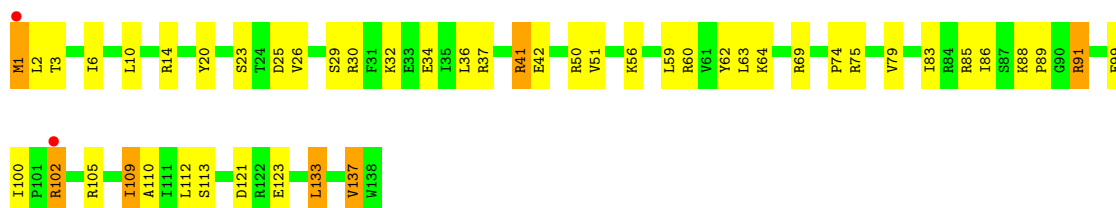
- Molecule 7: 30S ribosomal protein S7



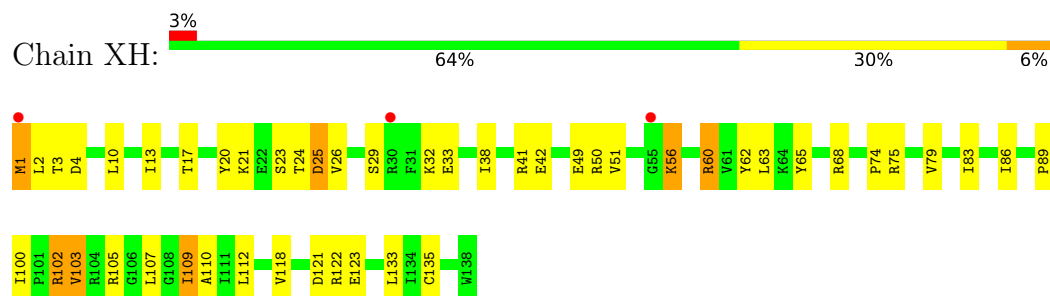
- Molecule 7: 30S ribosomal protein S7



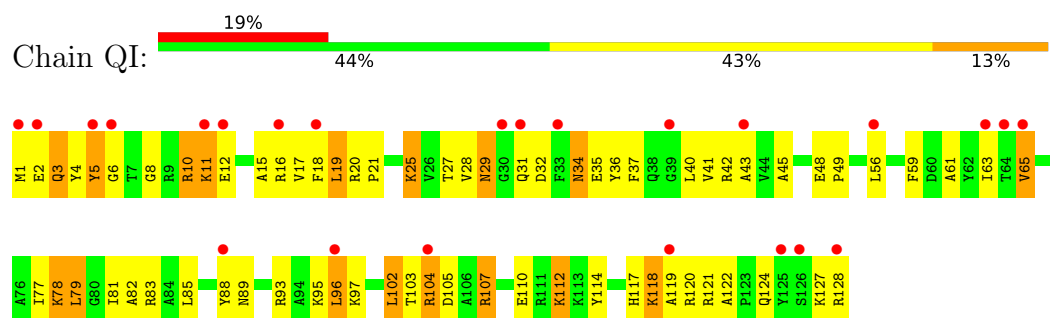
- Molecule 8: 30S ribosomal protein S8



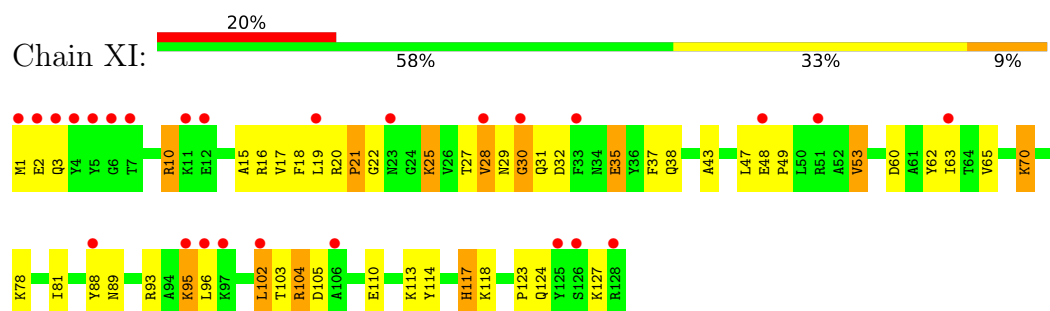
- Molecule 8: 30S ribosomal protein S8



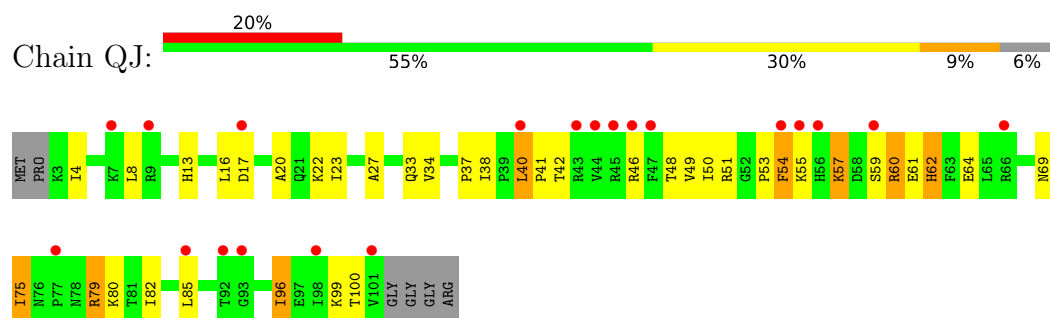
- Molecule 9: 30S ribosomal protein S9



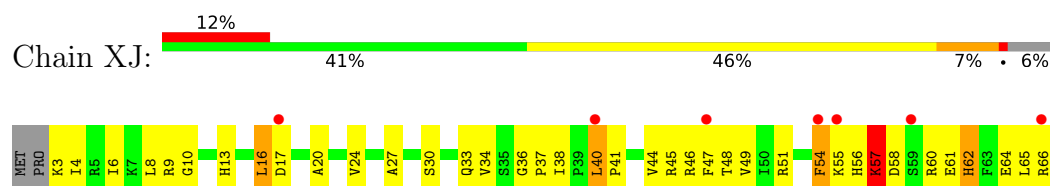
- Molecule 9: 30S ribosomal protein S9

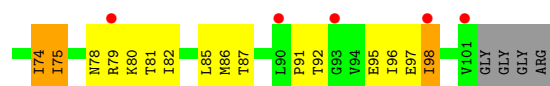


- Molecule 10: 30S ribosomal protein S10

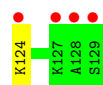
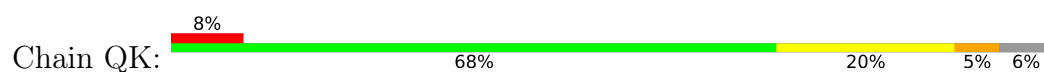


- Molecule 10: 30S ribosomal protein S10

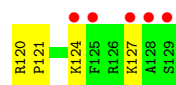




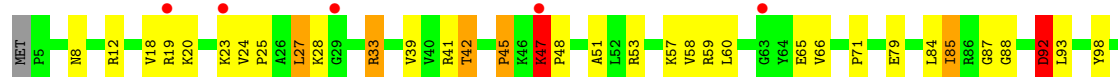
- Molecule 11: 30S ribosomal protein S11



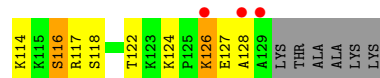
- Molecule 11: 30S ribosomal protein S11



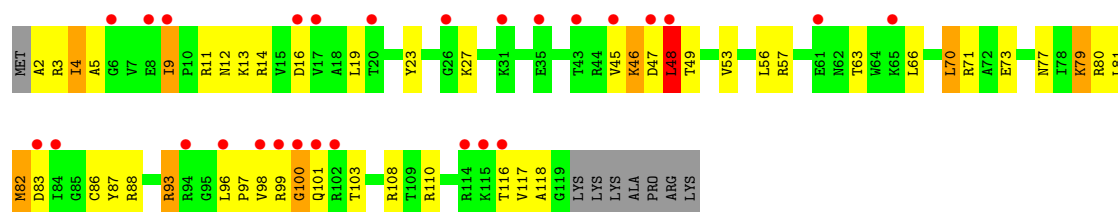
- Molecule 12: 30S ribosomal protein S12



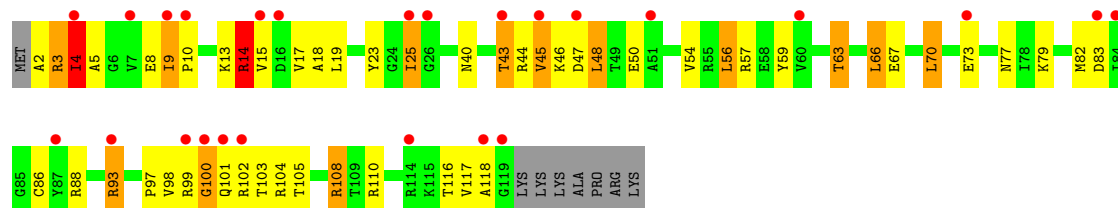
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



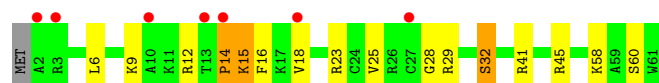
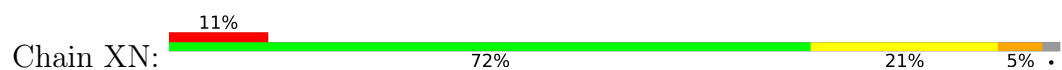
- Molecule 13: 30S ribosomal protein S13



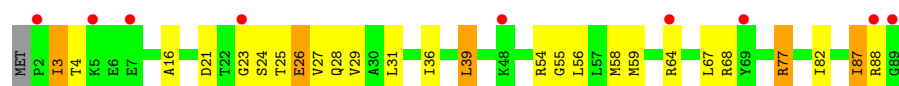
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S14 type Z



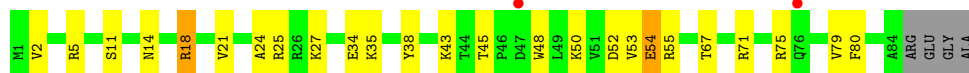
- Molecule 15: 30S ribosomal protein S15



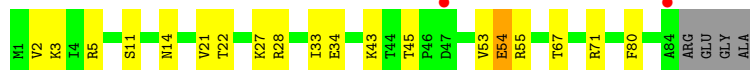
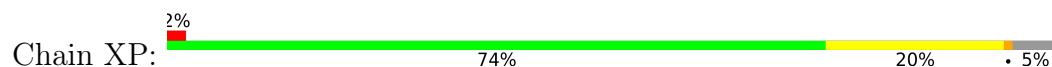
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



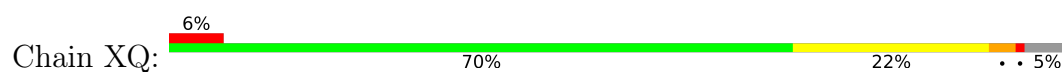
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



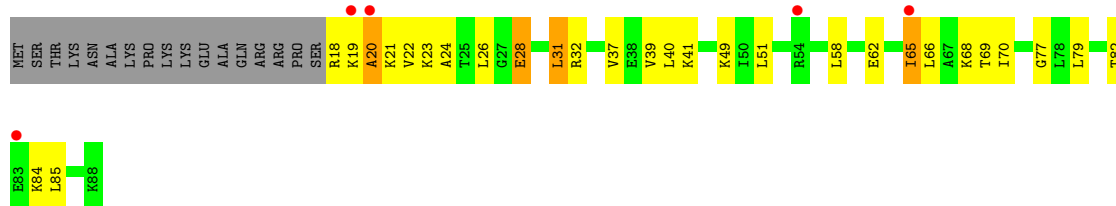
- Molecule 17: 30S ribosomal protein S17



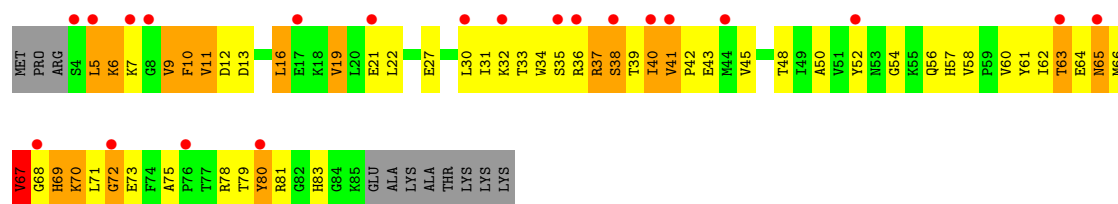
- Molecule 18: 30S ribosomal protein S18



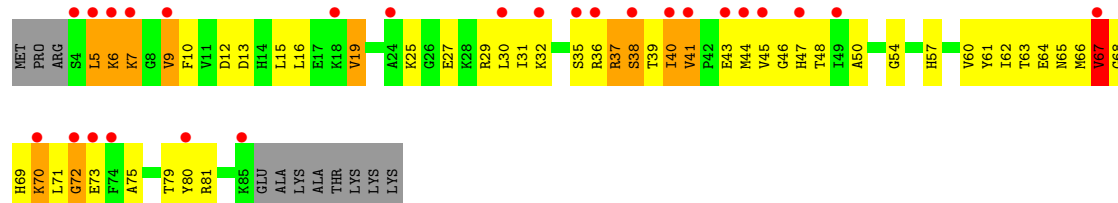
- Molecule 18: 30S ribosomal protein S18



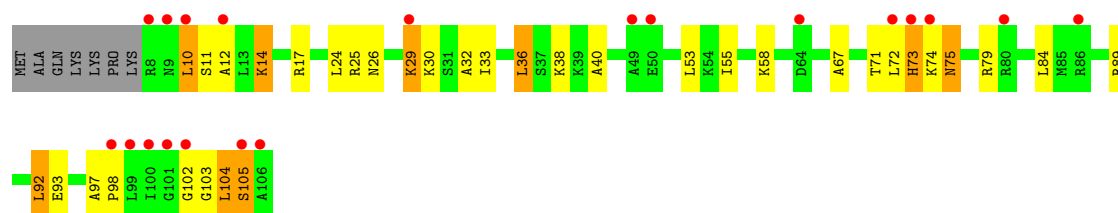
- Molecule 19: 30S ribosomal protein S19



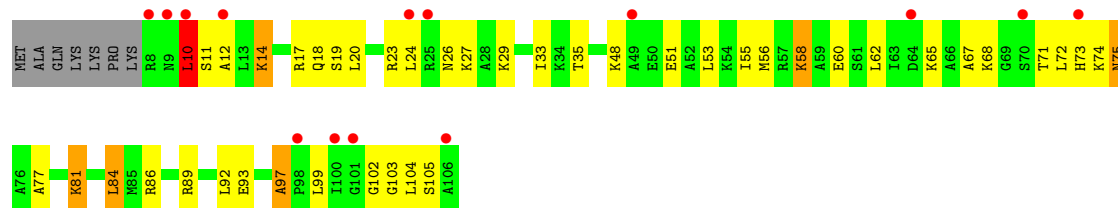
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

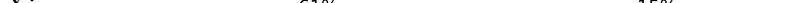


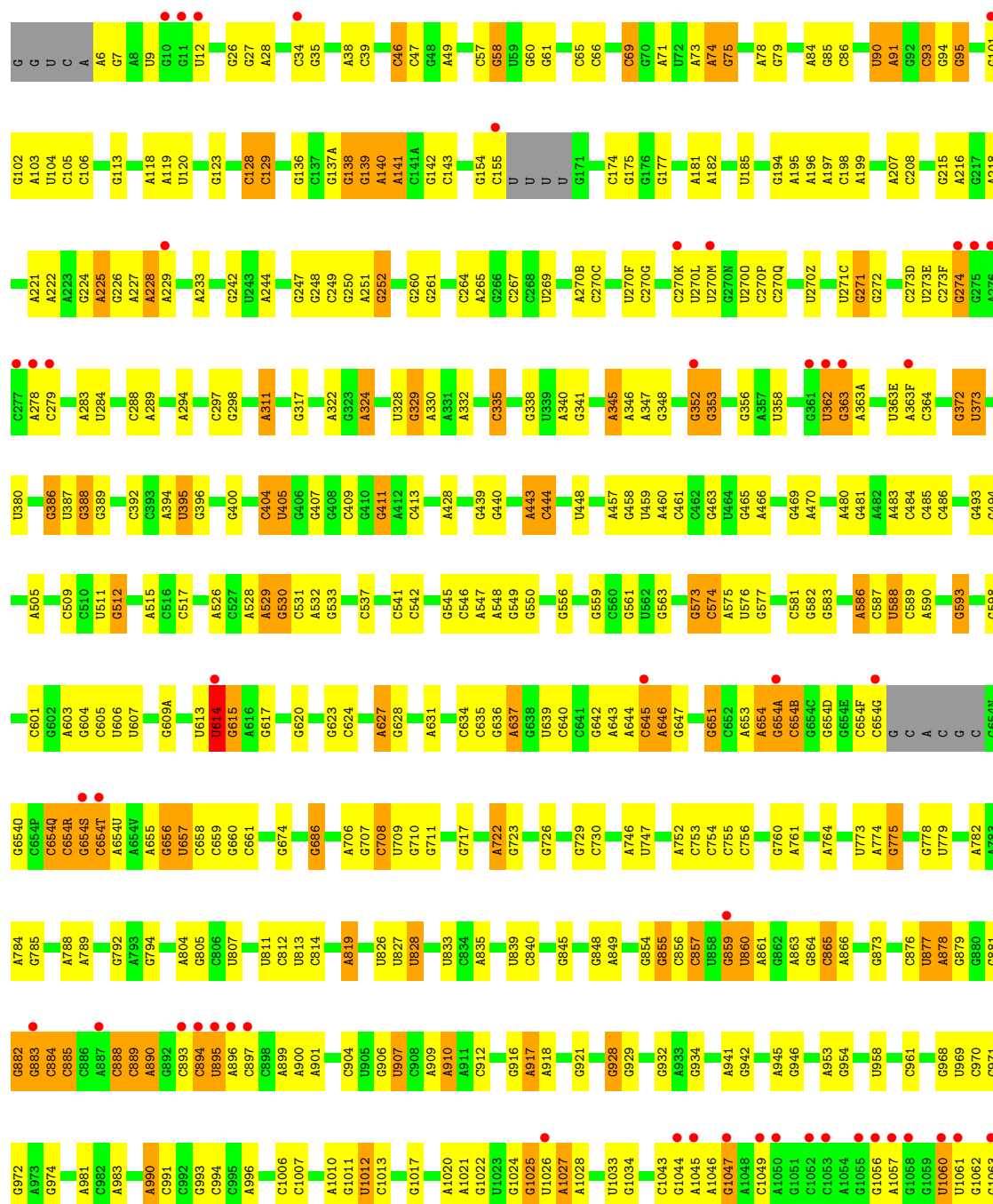
- Molecule 20: 30S ribosomal protein S20



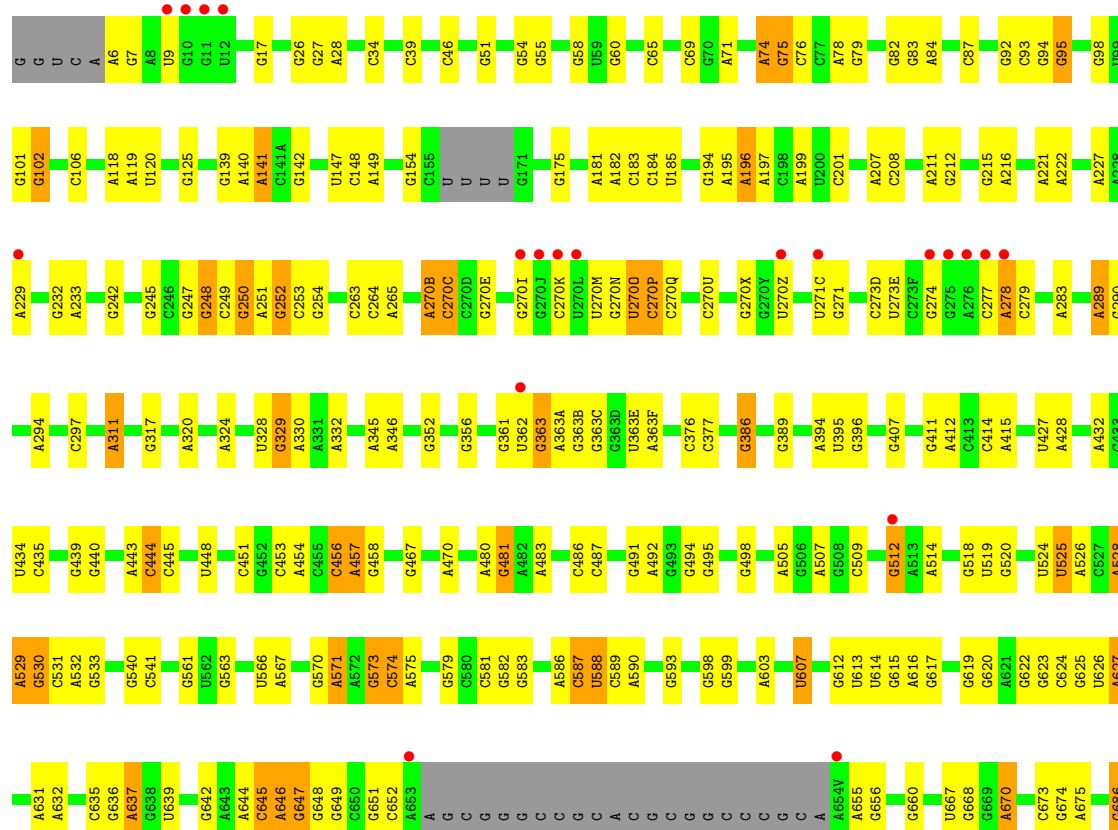
- Molecule 21: 30S ribosomal protein Thx



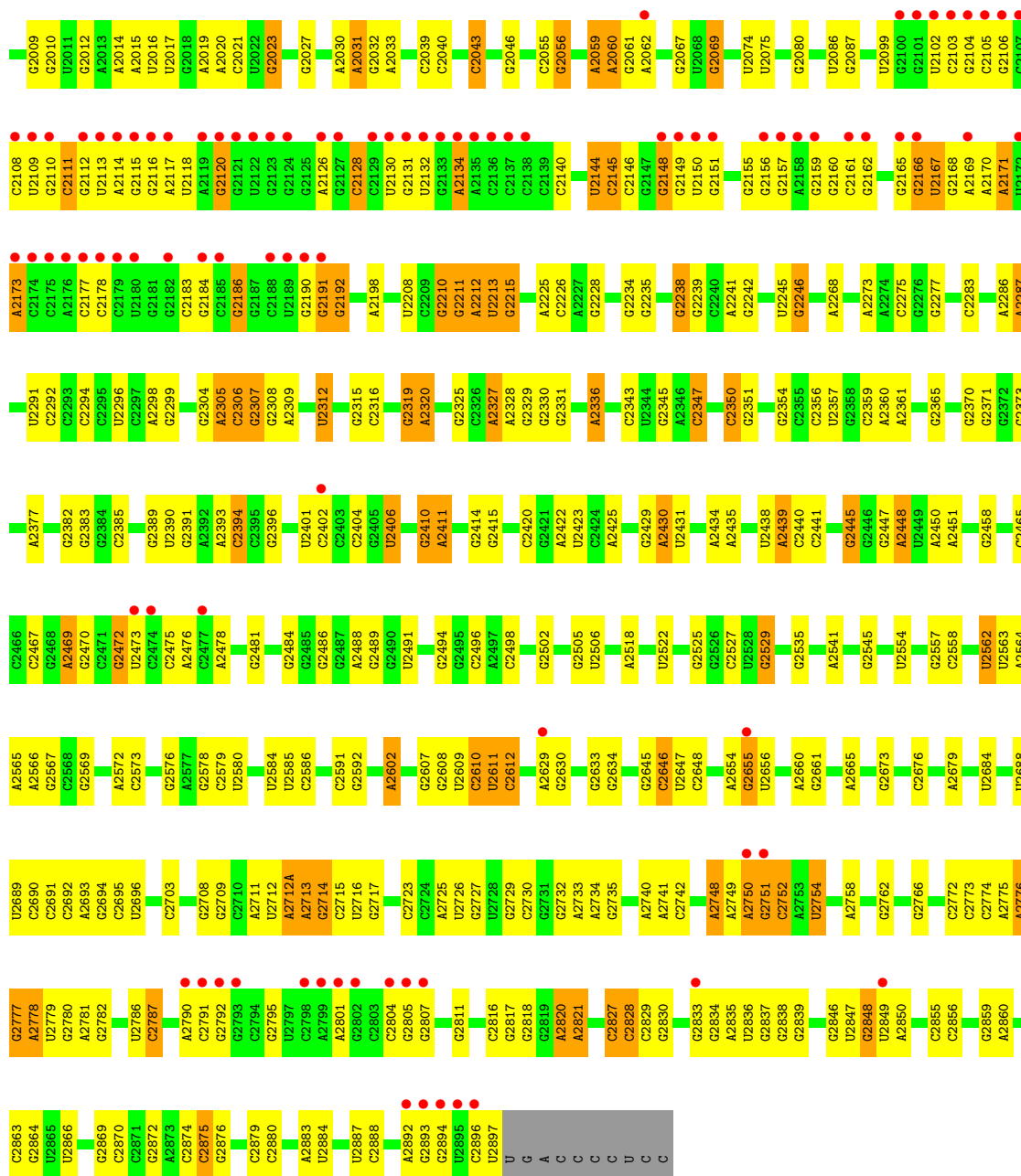
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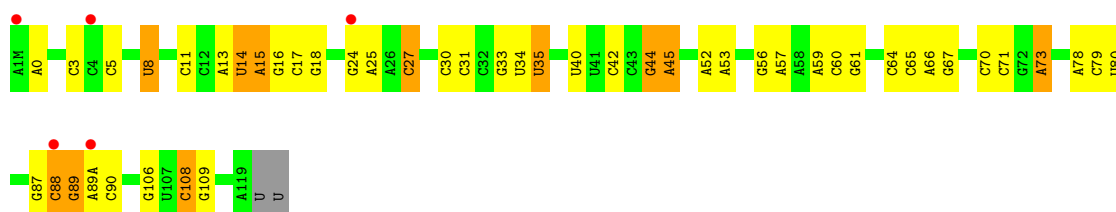


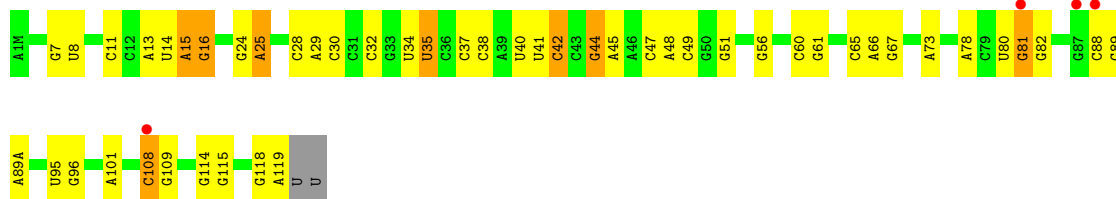


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G1904	G1905	A1784	A1654	A1545	G1459	A1379	G1252	A1143	U1066	G987	C894	A706
G1906	G1903	A1785	C1657	C1547	C1548	G1385	A1253	G1149	A1067	A988	U895	G707
G1906	G1903	A1786	C1658	C1549	C1548	C1386	A1254	C1150	G1068	G989	A896	C708
A1912	A1913	A1787	A1665	C1549	C1467	C1387	U1255	A1155	A1069	C991	C897	U709
A1913	A1912	A1788	A1666	C1549	C1467	C1388	G1256	A1155	U1070	C992	A900	C316
A1914	A1915	A1789	G1666	A1554	A1471	G1389	A1262	G1182	C1071	G993	A901	C717
A1916	A1913	A1790	G1667	A1554	A1471	G1388	U1263	U1165	A1073	C995	G906	A722
G1922	U1923	C1800	C1675	G1559	A1477	G1389	A1265	C1166	G1074	A996	U907	G723
U1923	U1805	G1806	C1694	G1572	C1488	U1394	G1266	A1185	C1075	G997	C906	U724
G1929	G1816	G1816	G1695	C1573	A1489	A1395	A1269	G1170	A1084	C998	A909	U826
U1931	G1930	G1930	G1696	C1574	A1490	U1406	A1278	C1179	C1076	U999	A910	U827
A1932	A1933	A1819	A1701	U1578	C1493	C1407	G1281	C1180	G1093	A1000	A911	U828
G1934	G1934	U1820	G1702	A1579	A1494	C1408	U1282	G1183	U1094	A1001	C912	
G1935	G1826	G1826	G1703	A1495	A1495	G1416	C1289	G1186	A1096	A1007	C912	
A1938	A1829	A1829	U1709	G1581	C1498	C1417	U1497	U1175	G1088	C1007	A917	U740
U1946	U1833	C1710	C1710	C1585	C1489	A1419	U1294	G1190	U1098	A1010	A918	G741
C1947	U1834	C1711	C1711	A1586	G1500	U1420	U1300	G1195	C1100	C934	A919	
G1948	G1835	C1712	C1712	A1587	C1501	G1421	A1301	A1195	A1029	C835	A941	U747
G1949	G1733	G1725	G1725	C1588	C1502	G1424	G1309	U1198	G1031	C836	C957	G748
A1952	C1838	C1728	A1505	C1592	C1505	G1425	G1309	U1199	A1032	U858	A945	A764
U1955	G1845	A1729	G1593	G1593	A1508	G1426	U1313	C1280	U1105	U860	C947	
G1963	A1846	U1730	G1594	G1594	C1509	A1427	C1314	C1201	G1106	A961	A953	G768
G1964	G1731	G1731	G1595	G1595	A1510	G1429	G1203	G1202	A1048	C962		
G1964	A1848	A1732	C1598	C1598	A1514	C1430	G1319	A1204	C1109	G1036		
G1967	A1854	G1734	A1603	A1603	C1515	U1431	U1341	C1222	G1122	G1042	G956	G771
C1967	G1858	C1735	A1608	A1608	U1516	C1437	U1329	C1217	G1112	C1043	A957	A774
G1968	C1741	C1741	A1608	A1608	G1517	C1437	C1330	C1218	U1113	G1044	U958	A774
A1969	A1859	C1742	A1609	A1609	C1518	G1441	A1336	G1219	G1114	A1045	A959	G775
A1970	G1860	G1743	A1610	A1610	A1519	G1442	A1336	A1220	G1115	G1047	C961	G776
A1971	G1861				G1519	G1442	U1341	C1222	A1048	U877	C964	U872
A1972		G1750	A1614	A1614	G1522	A1444A	U1341	C1222	G1122	C1049	C964	A782
C1979	G1869		C1615	C1615	G1526	C1445	U1362	C1223	G1125	A1050	U969	A783
G1979	A1870	C1754	C1617	C1617	G1527	G1446	U1362	C1225	A1128	G1051	C970	A784
A1981	A1872	G1756	A1618	A1618	A1528	G1447	U1357	C1225	G1135	C1052	C981	G785
C1982	G1878				A1528	G1448	A1359	G1228	C1135	G1054	G974	A788
		C1761	U1639	U1639	G1534	G1449A	A1360	C1230	G1136	G1055	C974A	G792
C1990	C1881	A1762	C1640	C1640	U1535	C1450	A1360	G1230	U1057	G1056	C975	
U1991	G1763	C1882	A1871	A1871	A1536	G1451	A1365	G1231	G1137	A1057	C886	C796
G1992	G1883	G1764	C1648	C1648	C1537	U1453	A1365	G1236	U1058	G1058	A987	C797
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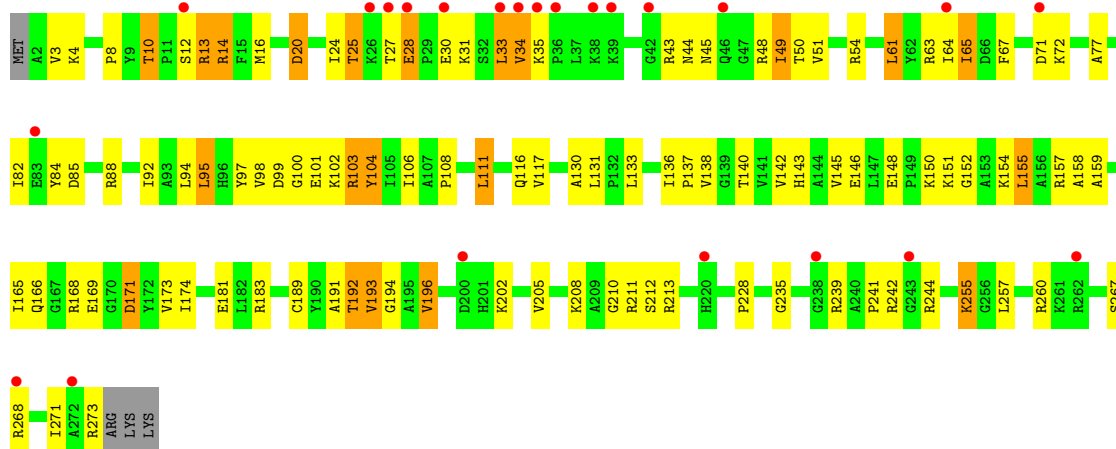


• Molecule 26: 5S rRNA

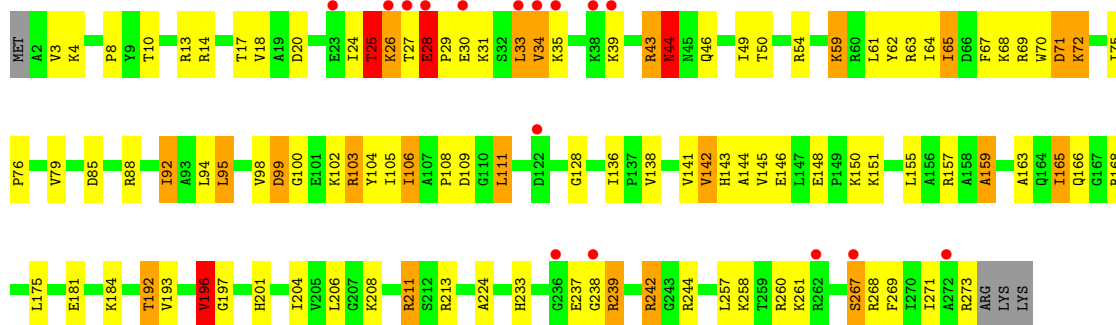




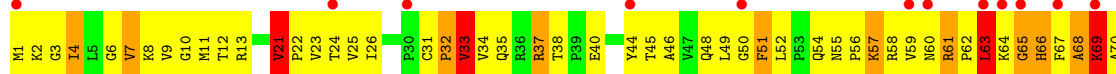
• Molecule 27: 50S ribosomal protein L2

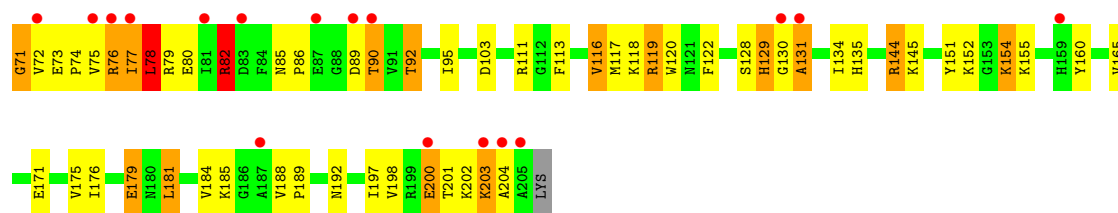


• Molecule 27: 50S ribosomal protein L2

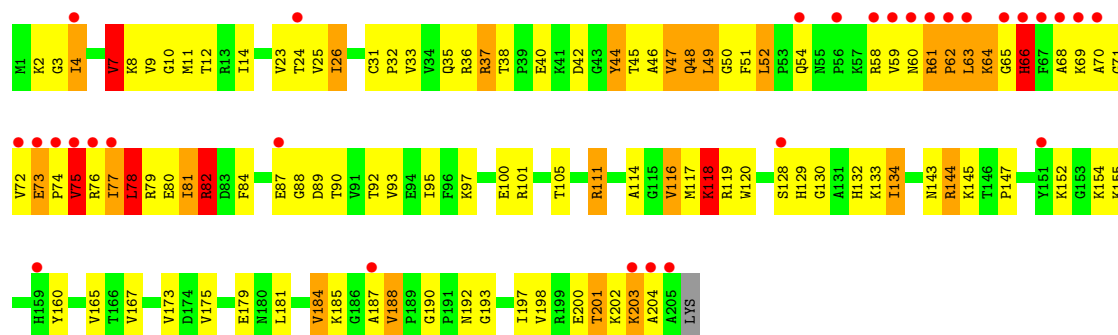


• Molecule 28: 50S ribosomal protein L3

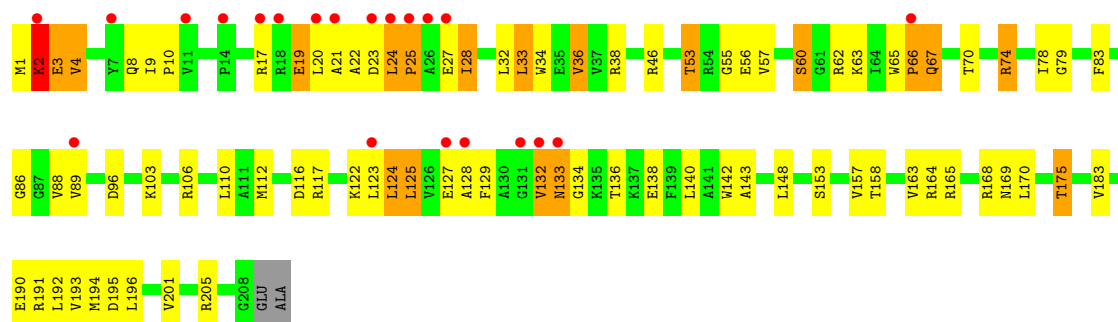




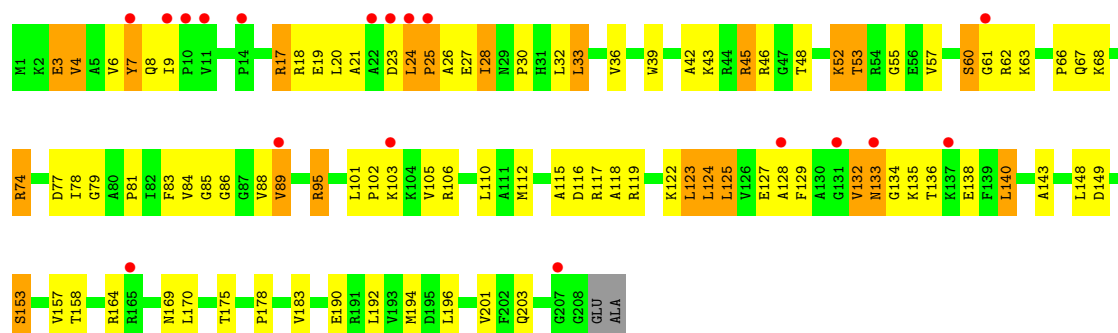
• Molecule 28: 50S ribosomal protein L3



• Molecule 29: 50S ribosomal protein L4

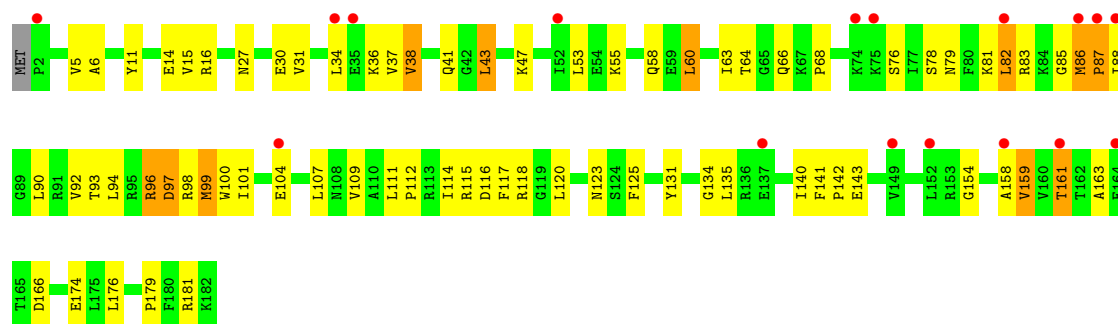


• Molecule 29: 50S ribosomal protein L4



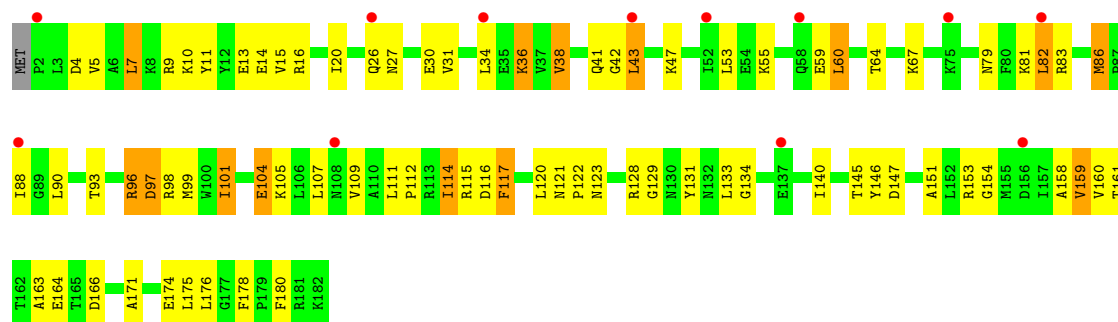
- Molecule 30: 50S ribosomal protein L5

Chain RG: 



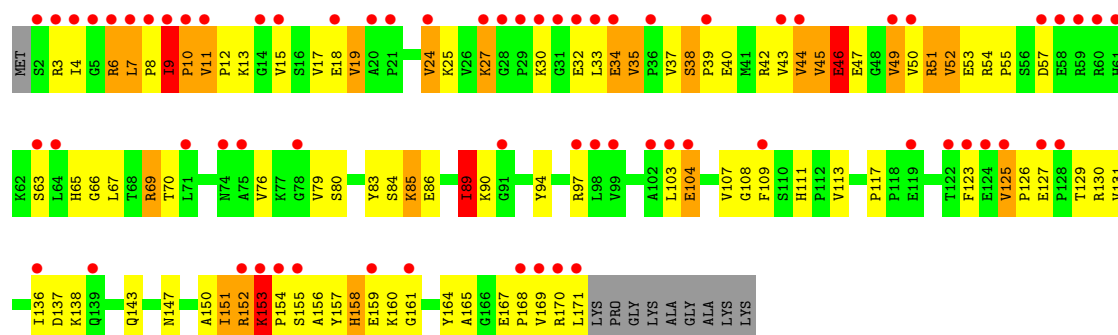
- Molecule 30: 50S ribosomal protein L5

Chain YG: 



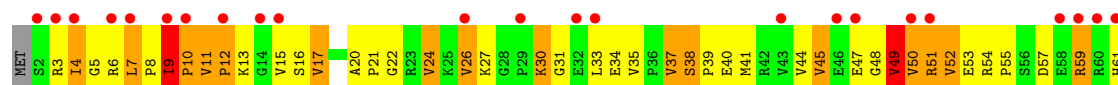
- Molecule 31: 50S ribosomal protein L6

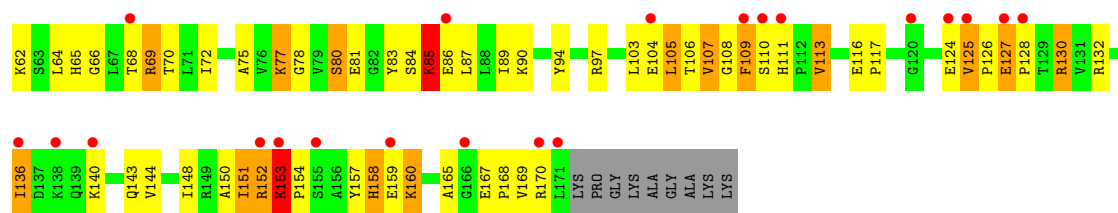
Chain RH: 



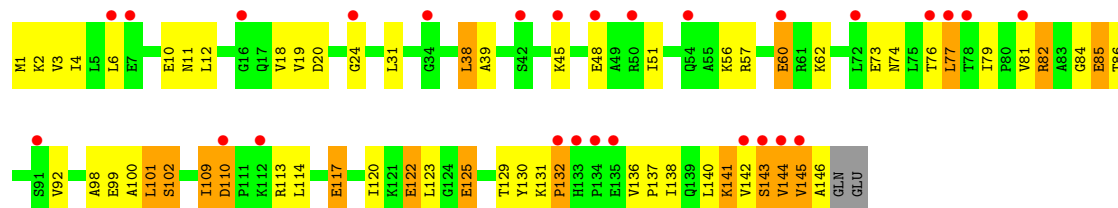
- Molecule 31: 50S ribosomal protein L6

Chain YH: 

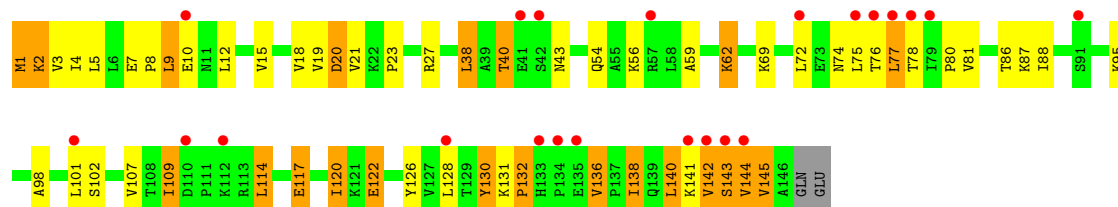




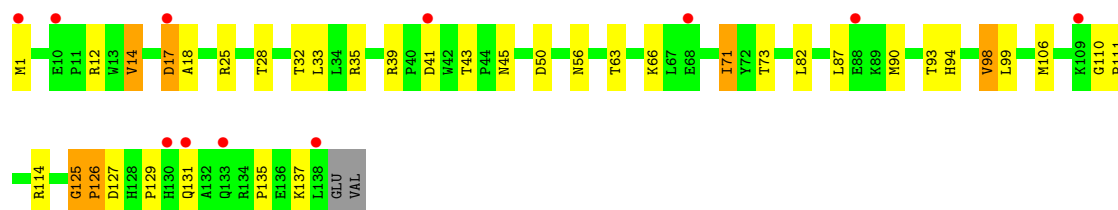
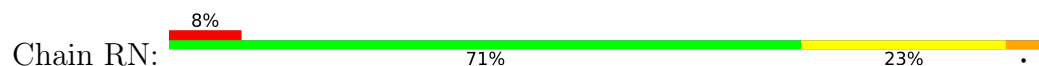
• Molecule 32: 50S ribosomal protein L9



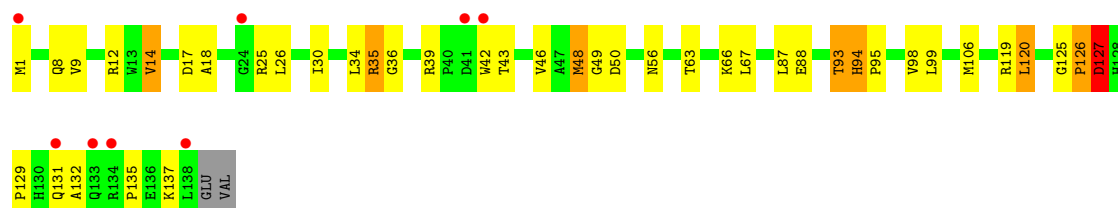
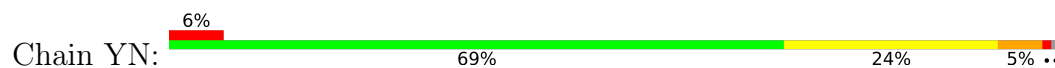
• Molecule 32: 50S ribosomal protein L9



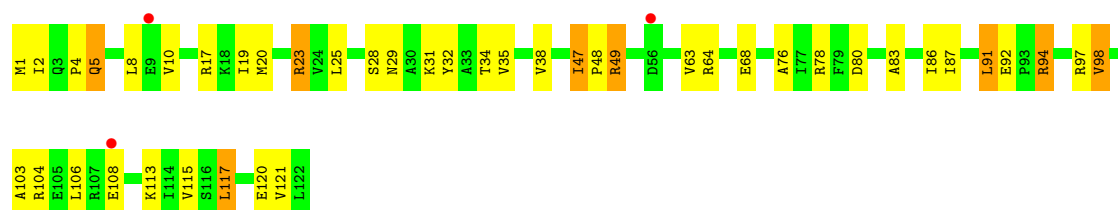
• Molecule 33: 50S ribosomal protein L13



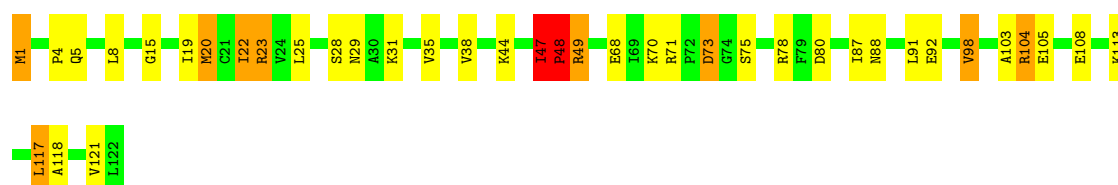
• Molecule 33: 50S ribosomal protein L13



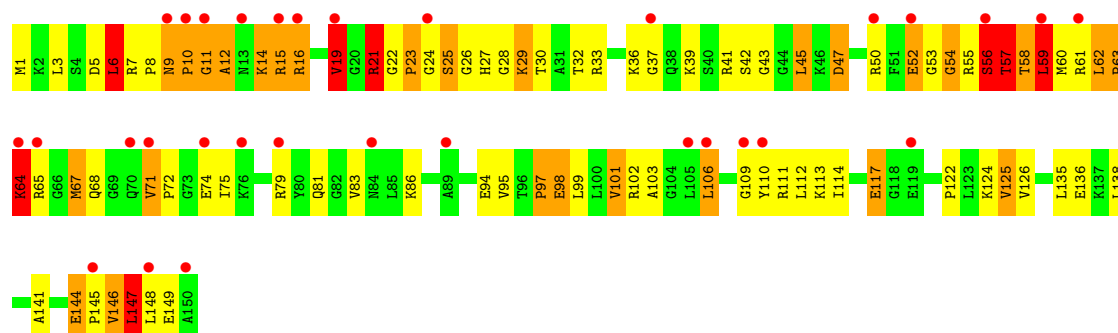
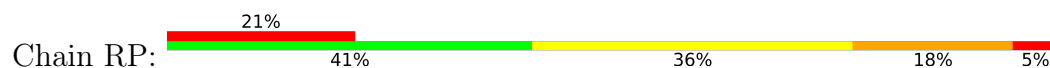
- Molecule 34: 50S ribosomal protein L14



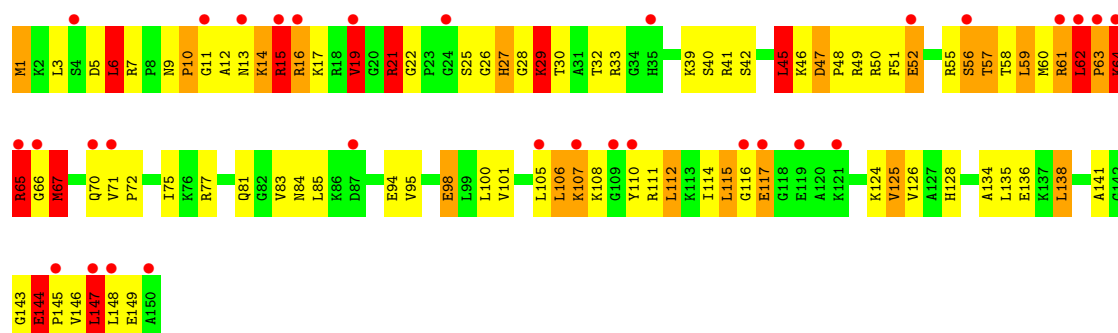
- Molecule 34: 50S ribosomal protein L14



- Molecule 35: 50S ribosomal protein L15

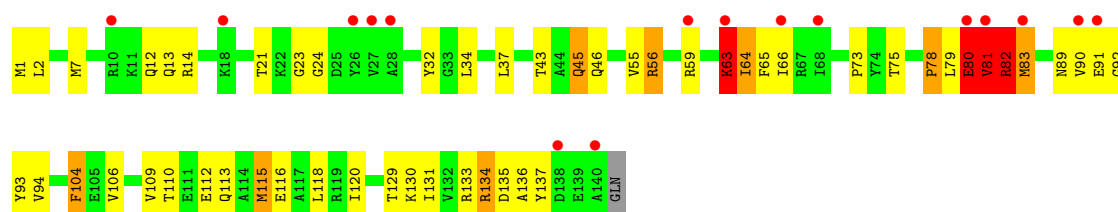


- Molecule 35: 50S ribosomal protein L15



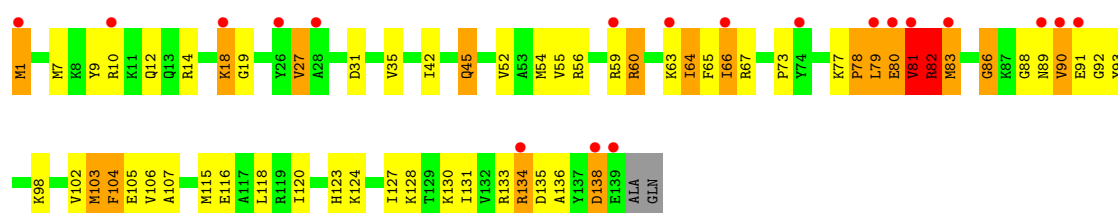
- Molecule 36: 50S ribosomal protein L16

Chain RQ: 



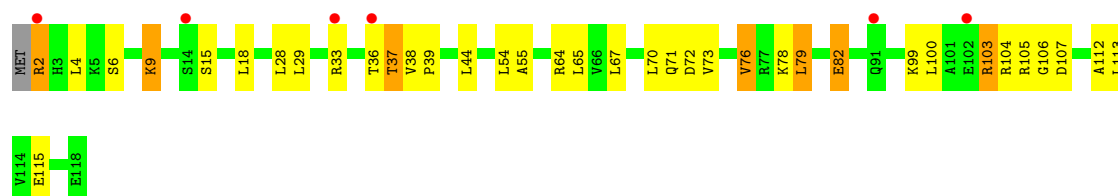
- Molecule 36: 50S ribosomal protein L16

Chain YQ: 



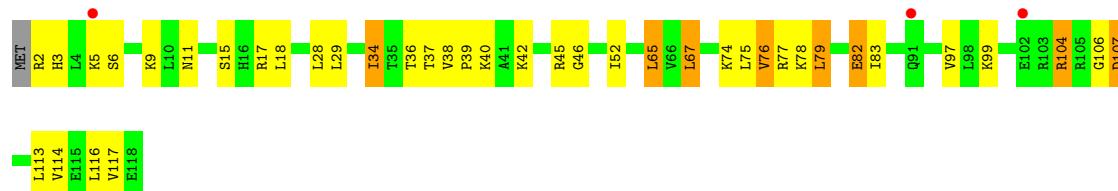
- Molecule 37: 50S ribosomal protein L17

Chain RR: 



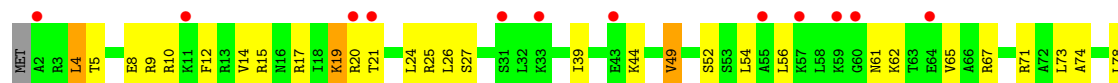
- Molecule 37: 50S ribosomal protein L17

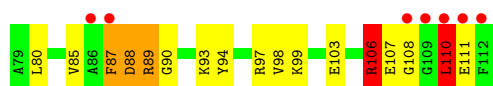
Chain YR: 



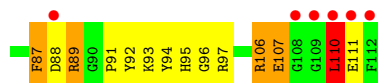
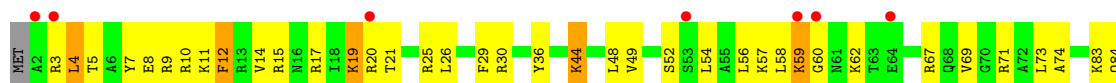
- Molecule 38: 50S ribosomal protein L18

Chain RS: 

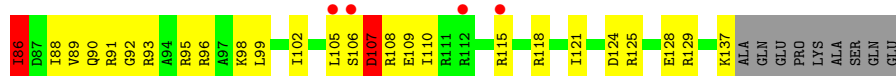




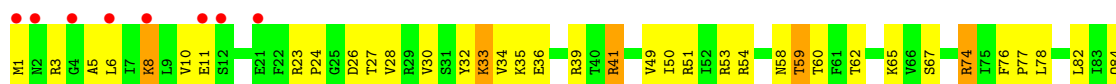
• Molecule 38: 50S ribosomal protein L18



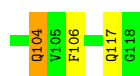
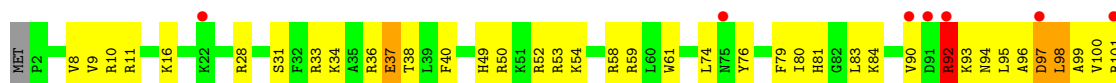
• Molecule 39: 50S ribosomal protein L19



• Molecule 39: 50S ribosomal protein L19

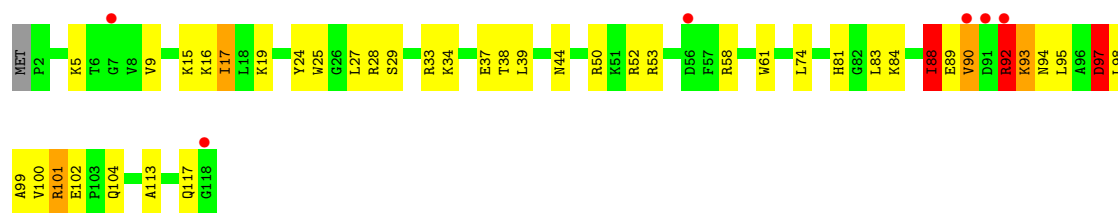


• Molecule 40: 50S ribosomal protein L20

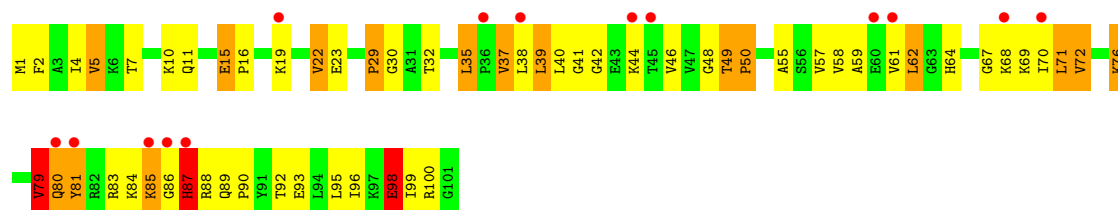
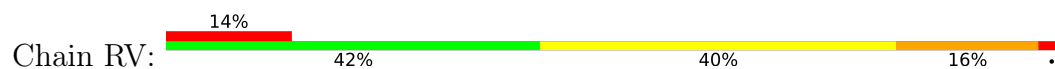


• Molecule 40: 50S ribosomal protein L20

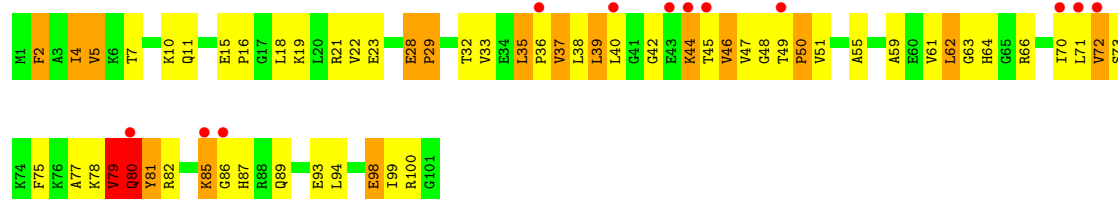
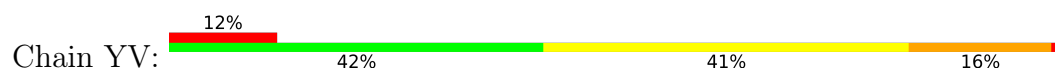




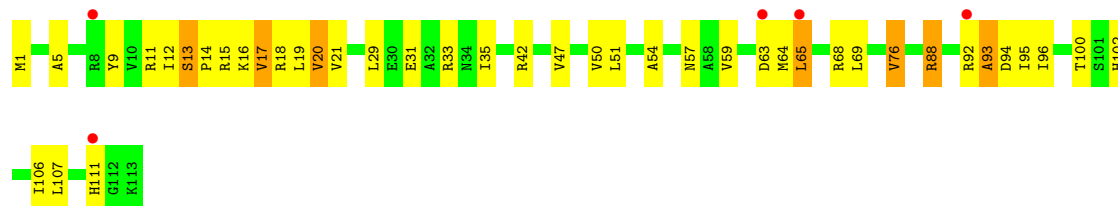
• Molecule 41: 50S ribosomal protein L21



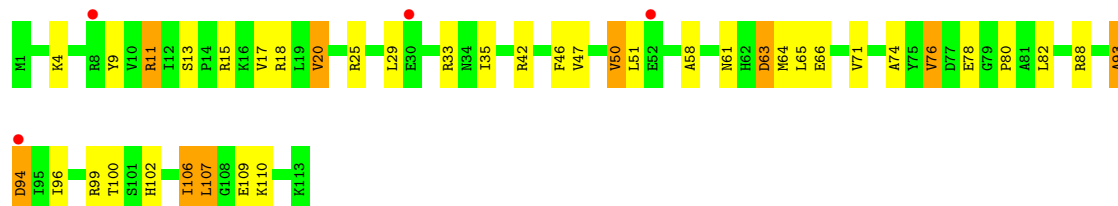
• Molecule 41: 50S ribosomal protein L21



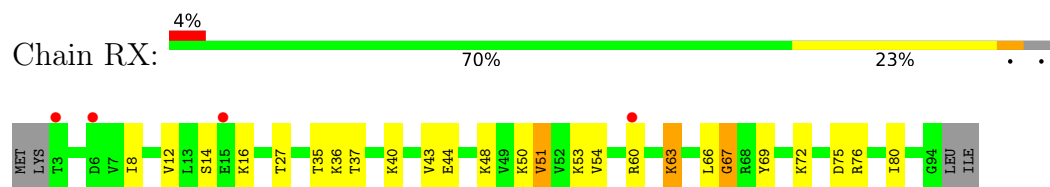
• Molecule 42: 50S ribosomal protein L22



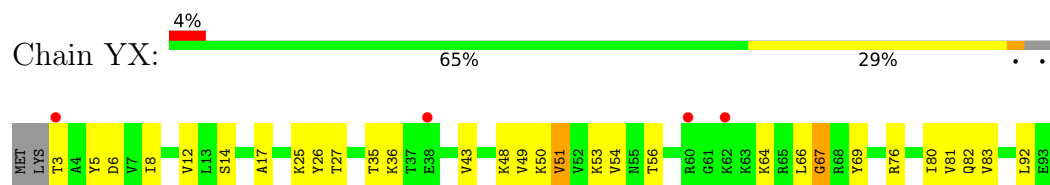
• Molecule 42: 50S ribosomal protein L22



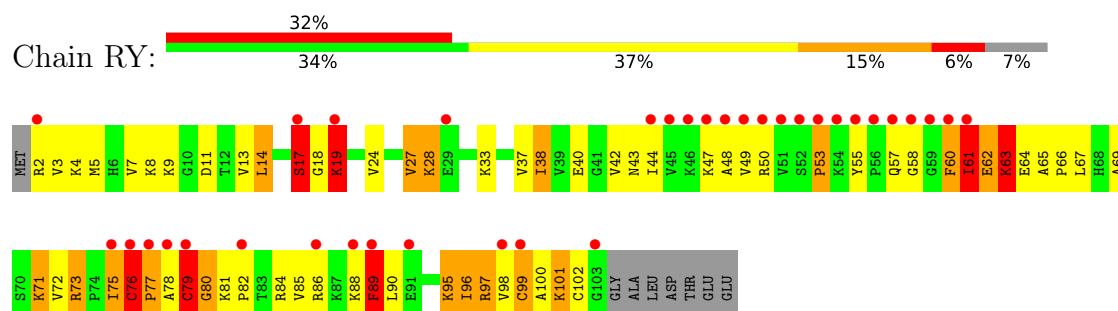
- Molecule 43: 50S ribosomal protein L23



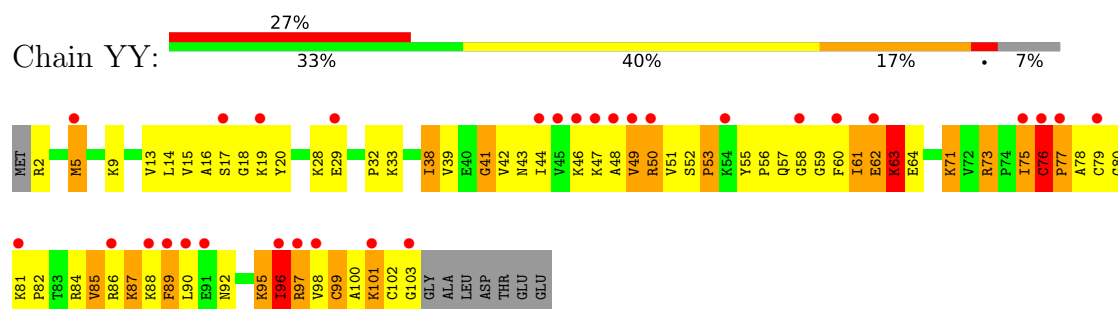
- Molecule 43: 50S ribosomal protein L23



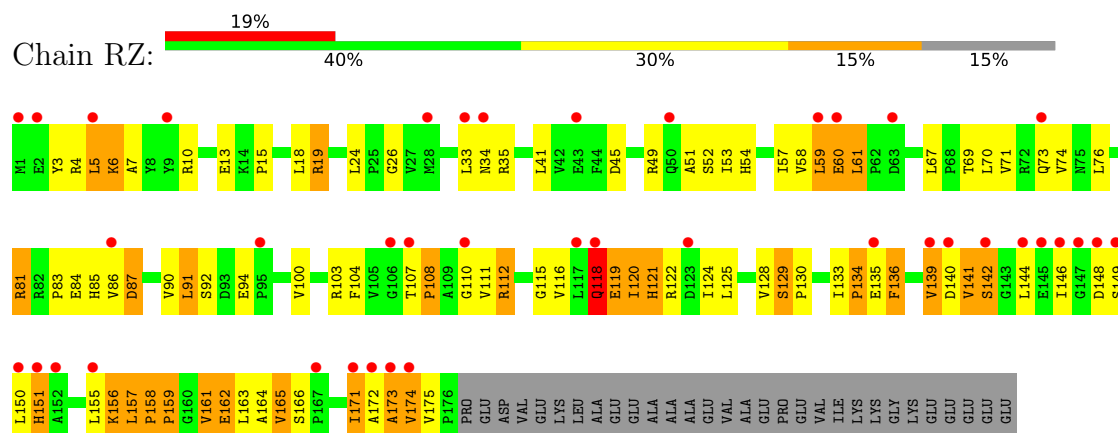
- Molecule 44: 50S ribosomal protein L24



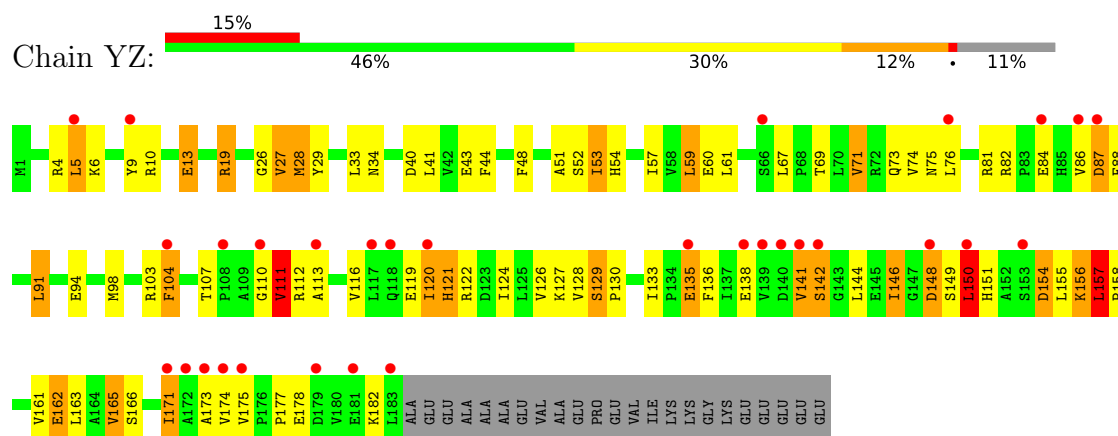
- Molecule 44: 50S ribosomal protein L24



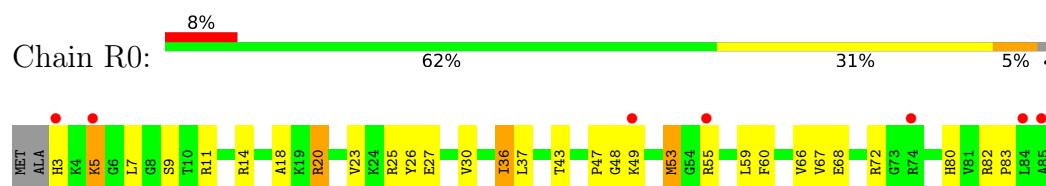
- Molecule 45: 50S ribosomal protein L25



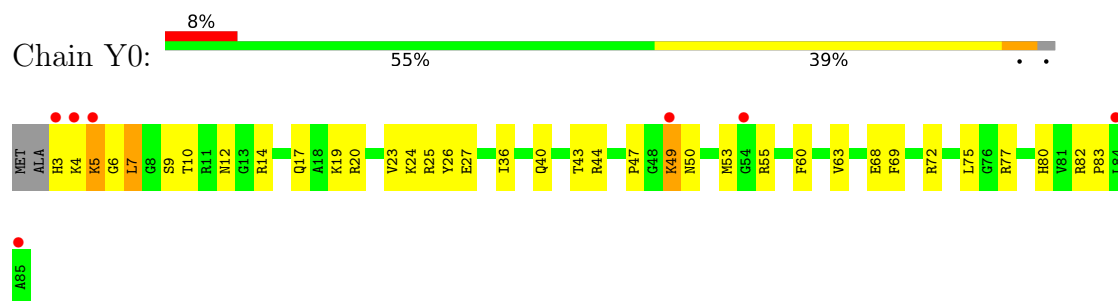
• Molecule 45: 50S ribosomal protein L25



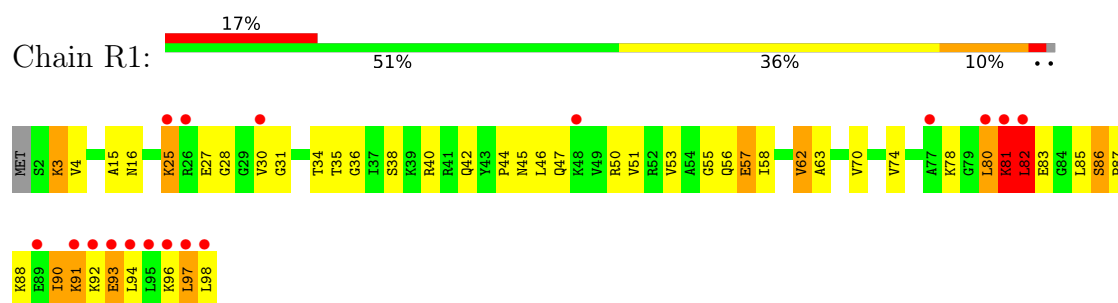
• Molecule 46: 50S ribosomal protein L27



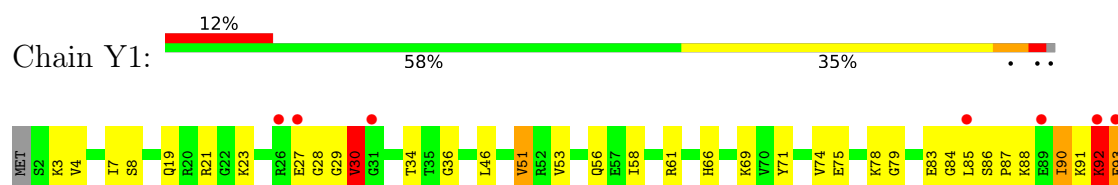
• Molecule 46: 50S ribosomal protein L27

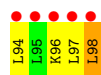


• Molecule 47: 50S ribosomal protein L28

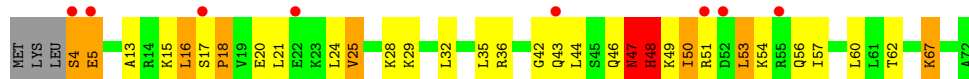


• Molecule 47: 50S ribosomal protein L28

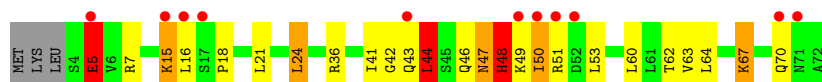




- Molecule 48: 50S ribosomal protein L29



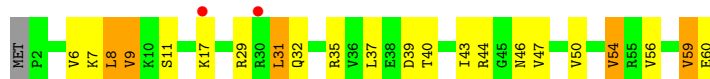
- Molecule 48: 50S ribosomal protein L29



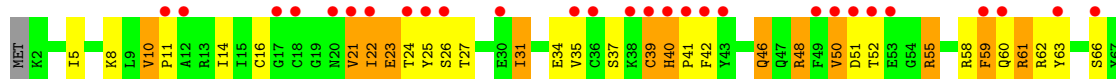
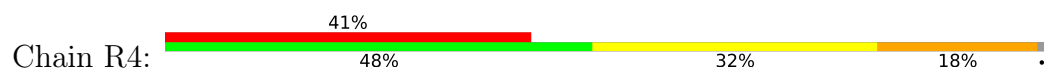
- Molecule 49: 50S ribosomal protein L30



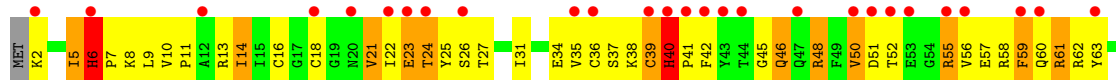
- Molecule 49: 50S ribosomal protein L30



- Molecule 50: 50S ribosomal protein L31

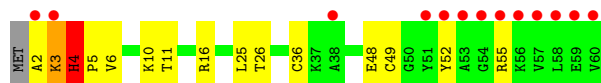
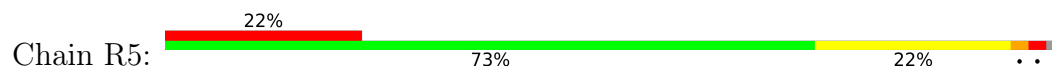


- Molecule 50: 50S ribosomal protein L31

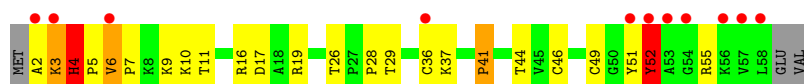




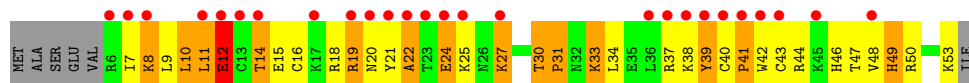
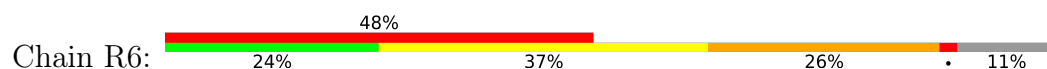
- Molecule 51: 50S ribosomal protein L32



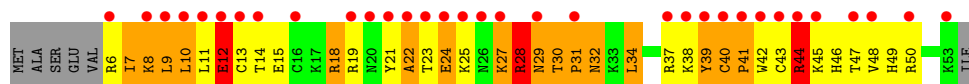
- Molecule 51: 50S ribosomal protein L32



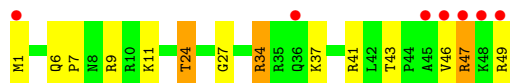
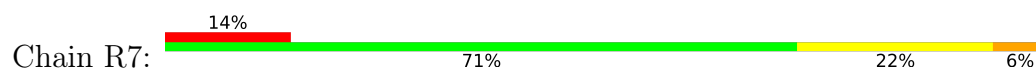
- Molecule 52: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L33



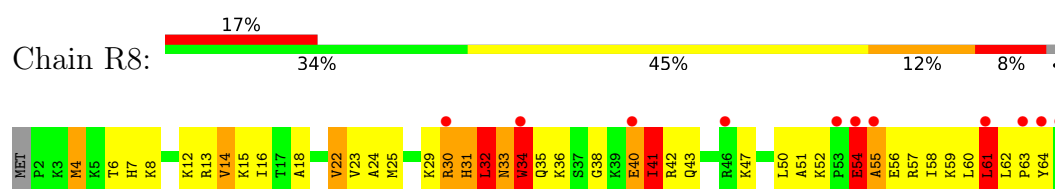
- Molecule 53: 50S ribosomal protein L34



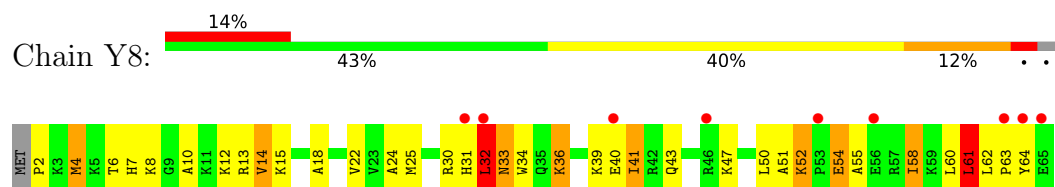
- Molecule 53: 50S ribosomal protein L34



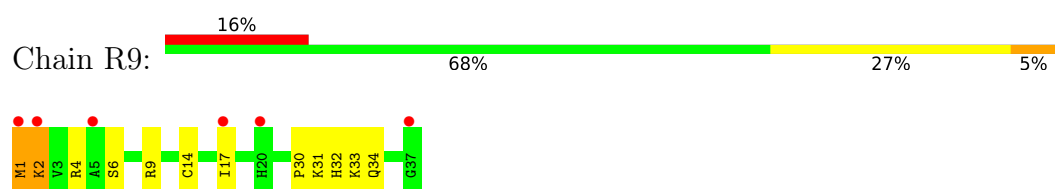
- Molecule 54: 50S ribosomal protein L35



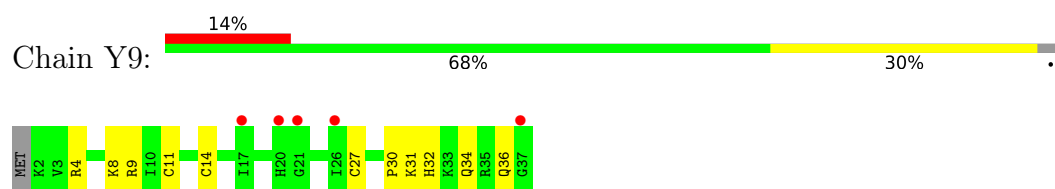
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: CC-puromycin



- Molecule 56: CC-puromycin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	214.20Å 453.27Å 609.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.93 – 3.10 34.93 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (34.93-3.10) 99.3 (34.93-3.10)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.13Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.203 , 0.237 0.205 , 0.238	Depositor DCC
R_{free} test set	49438 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 74.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	294445	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% 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: OMC, ZN, A2M, PPU, MG

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	QA	0.18	0/36346	0.38	3/56724 (0.0%)
1	XA	0.20	0/36276	0.40	7/56615 (0.0%)
2	QB	0.33	0/1950	0.81	2/2630 (0.1%)
2	XB	0.33	0/1950	0.82	2/2630 (0.1%)
3	QC	0.33	0/1636	0.77	0/2205
3	XC	0.36	0/1636	0.79	0/2205
4	QD	0.36	0/1733	0.85	2/2318 (0.1%)
4	XD	0.36	0/1733	0.83	3/2318 (0.1%)
5	QE	0.37	0/1195	0.86	0/1609
5	XE	0.41	0/1195	0.80	0/1609
6	QF	0.31	0/856	0.74	0/1154
6	XF	0.33	0/856	0.75	0/1154
7	QG	0.33	0/1276	0.80	2/1709 (0.1%)
7	XG	0.36	0/1276	0.85	2/1709 (0.1%)
8	QH	0.33	0/1136	0.82	0/1527
8	XH	0.36	0/1136	0.81	2/1527 (0.1%)
9	QI	0.34	0/1037	0.83	1/1389 (0.1%)
9	XI	0.35	0/1037	0.83	2/1389 (0.1%)
10	QJ	0.31	0/814	0.77	0/1095
10	XJ	0.31	0/814	0.78	0/1095
11	QK	0.33	0/916	0.82	1/1234 (0.1%)
11	XK	0.38	0/916	0.86	1/1234 (0.1%)
12	QL	0.39	0/991	0.88	2/1327 (0.2%)
12	XL	0.43	1/991 (0.1%)	0.92	8/1327 (0.6%)
13	QM	0.36	0/947	0.84	0/1270
13	XM	0.35	0/947	0.85	0/1270
14	QN	0.32	0/501	0.80	0/664
14	XN	0.35	0/501	0.79	0/664
15	QO	0.31	0/745	0.70	0/992
15	XO	0.35	0/745	0.75	0/992
16	QP	0.33	0/721	0.75	0/970
16	XP	0.34	0/721	0.75	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.31	0/847	0.79	0/1131
17	XQ	0.34	0/847	0.74	0/1131
18	QR	0.33	0/590	0.78	0/782
18	XR	0.33	0/590	0.77	0/782
19	QS	0.37	0/670	0.86	1/901 (0.1%)
19	XS	0.41	0/670	0.88	0/901
20	QT	0.35	0/765	0.80	1/1007 (0.1%)
20	XT	0.34	0/765	0.80	1/1007 (0.1%)
21	QU	0.28	0/221	0.78	0/288
21	XU	0.28	0/221	0.74	0/288
22	QV	0.19	0/1832	0.34	0/2855
22	XV	0.21	0/1832	0.34	0/2855
23	QX	0.34	1/414 (0.2%)	0.34	0/645
23	XX	0.34	1/414 (0.2%)	0.42	0/645
24	QY	0.43	0/762	0.74	1/1028 (0.1%)
24	XY	0.31	0/762	0.72	0/1028
25	RA	0.24	0/69742	0.42	5/108874 (0.0%)
25	YA	0.25	0/69356	0.42	3/108271 (0.0%)
26	RB	0.18	0/2928	0.38	0/4568
26	YB	0.18	0/2928	0.38	0/4568
27	RD	0.43	0/2165	0.89	4/2919 (0.1%)
27	YD	0.47	0/2165	0.93	5/2919 (0.2%)
28	RE	0.41	0/1601	0.89	5/2160 (0.2%)
28	YE	0.47	0/1601	0.95	6/2160 (0.3%)
29	RF	0.45	0/1662	0.92	4/2249 (0.2%)
29	YF	0.41	0/1662	0.91	2/2249 (0.1%)
30	RG	0.34	0/1499	0.78	2/2016 (0.1%)
30	YG	0.35	0/1499	0.78	0/2016
31	RH	0.38	0/1332	1.03	10/1802 (0.6%)
31	YH	0.39	0/1332	0.97	6/1802 (0.3%)
32	RI	0.34	0/1151	0.84	1/1558 (0.1%)
32	YI	0.40	0/1151	0.93	5/1558 (0.3%)
33	RN	0.35	0/1131	0.85	3/1525 (0.2%)
33	YN	0.38	0/1131	0.87	2/1525 (0.1%)
34	RO	0.39	0/943	0.86	2/1269 (0.2%)
34	YO	0.42	0/943	0.87	2/1269 (0.2%)
35	RP	0.45	0/1162	0.97	5/1544 (0.3%)
35	YP	0.47	0/1162	0.97	3/1544 (0.2%)
36	RQ	0.45	0/1133	0.88	1/1515 (0.1%)
36	YQ	0.46	0/1128	0.91	2/1508 (0.1%)
37	RR	0.39	0/974	0.80	0/1302
37	YR	0.42	0/974	0.80	1/1302 (0.1%)
38	RS	0.32	0/892	0.77	1/1187 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YS	0.36	0/892	0.83	1/1187 (0.1%)
39	RT	0.35	0/1155	0.78	2/1542 (0.1%)
39	YT	0.39	0/1155	0.81	0/1542
40	RU	0.42	0/982	0.86	3/1306 (0.2%)
40	YU	0.41	0/982	0.91	4/1306 (0.3%)
41	RV	0.52	0/790	1.01	4/1057 (0.4%)
41	YV	0.48	0/790	1.02	5/1057 (0.5%)
42	RW	0.42	0/911	0.84	3/1220 (0.2%)
42	YW	0.42	0/911	0.82	2/1220 (0.2%)
43	RX	0.40	0/739	0.85	0/993
43	YX	0.45	0/739	0.89	1/993 (0.1%)
44	RY	0.46	0/798	0.95	0/1064
44	YY	0.46	0/798	0.99	2/1064 (0.2%)
45	RZ	0.40	0/1435	0.91	2/1947 (0.1%)
45	YZ	0.43	0/1493	0.96	6/2026 (0.3%)
46	R0	0.40	0/666	0.85	0/885
46	Y0	0.39	0/666	0.87	1/885 (0.1%)
47	R1	0.42	0/770	0.84	0/1022
47	Y1	0.49	0/770	0.84	0/1022
48	R2	0.33	0/583	0.92	1/771 (0.1%)
48	Y2	0.41	0/583	0.90	1/771 (0.1%)
49	R3	0.37	0/474	0.77	0/635
49	Y3	0.37	0/474	0.80	0/635
50	R4	0.34	0/586	0.77	0/785
50	Y4	0.44	0/586	0.82	1/785 (0.1%)
51	R5	0.44	0/473	1.07	2/639 (0.3%)
51	Y5	0.67	3/456 (0.7%)	1.15	9/617 (1.5%)
52	R6	0.41	0/424	0.98	2/565 (0.4%)
52	Y6	0.53	0/424	1.07	1/565 (0.2%)
53	R7	0.42	0/438	0.80	0/575
53	Y7	0.44	0/438	0.83	2/575 (0.3%)
54	R8	0.56	0/525	1.13	5/691 (0.7%)
54	Y8	0.54	0/525	1.13	3/691 (0.4%)
55	R9	0.33	0/310	0.72	0/407
55	Y9	0.31	0/302	0.71	0/397
56	Z6	0.50	0/40	0.86	0/60
56	Z7	0.42	0/40	0.89	0/60
All	All	0.29	6/318202 (0.0%)	0.57	187/475540 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	Y5	4	HIS	C-N	6.42	1.41	1.33
51	Y5	6	VAL	C-N	5.53	1.41	1.33
51	Y5	7	PRO	N-CD	5.33	1.55	1.47
23	QX	21	A2M	O3'-P	5.29	1.61	1.56
23	XX	21	A2M	O3'-P	5.27	1.61	1.56

The worst 5 of 187 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	Y8	41	ILE	N-CA-C	-12.65	101.69	113.71
54	R8	41	ILE	N-CA-C	-11.87	102.44	113.71
36	YQ	82	ARG	N-CA-C	11.18	124.86	109.54
25	RA	614	U	C2'-C3'-O3'	-9.94	98.79	113.70
1	QA	1528	U	C4'-C3'-O3'	9.92	124.28	109.40

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	QA	32472	0	16393	412	0
1	XA	32409	0	16361	380	0
2	QB	1915	0	1969	59	0
2	XB	1915	0	1969	63	0
3	QC	1612	0	1677	51	0
3	XC	1612	0	1677	35	0
4	QD	1703	0	1765	41	0
4	XD	1703	0	1766	39	0
5	QE	1178	0	1233	30	0
5	XE	1178	0	1234	26	0
6	QF	843	0	857	16	0
6	XF	843	0	857	19	0
7	QG	1257	0	1296	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	32	0
8	QH	1116	0	1177	34	0
8	XH	1116	0	1177	27	0
9	QI	1018	0	1049	55	0
9	XI	1018	0	1049	40	0
10	QJ	801	0	849	34	0
10	XJ	801	0	849	46	0
11	QK	901	0	926	20	0
11	XK	901	0	926	20	0
12	QL	975	0	1062	26	0
12	XL	975	0	1062	22	0
13	QM	937	0	994	32	0
13	XM	937	0	994	60	0
14	QN	492	0	529	17	0
14	XN	492	0	529	11	0
15	QO	734	0	771	16	0
15	XO	734	0	771	18	0
16	QP	705	0	725	13	0
16	XP	705	0	725	10	0
17	QQ	834	0	904	15	0
17	XQ	834	0	904	16	0
18	QR	585	0	657	9	0
18	XR	585	0	657	19	0
19	QS	656	0	678	48	0
19	XS	656	0	678	44	0
20	QT	763	0	861	21	0
20	XT	763	0	861	26	0
21	QU	217	0	234	9	0
21	XU	217	0	234	14	0
22	QV	1640	0	837	11	0
22	XV	1640	0	837	11	0
23	QX	435	9	225	18	0
23	XX	435	9	225	16	0
24	QY	746	0	742	15	0
24	XY	746	0	742	14	0
25	RA	62269	0	31392	695	0
25	YA	61924	0	31214	650	0
26	RB	2617	0	1328	27	0
26	YB	2617	0	1328	25	0
27	RD	2115	0	2195	68	0
27	YD	2115	0	2195	72	0
28	RE	1568	0	1634	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	YE	1568	0	1634	78	0
29	RF	1627	0	1680	57	0
29	YF	1627	0	1680	58	0
30	RG	1474	0	1535	46	0
30	YG	1474	0	1535	47	0
31	RH	1307	0	1382	94	0
31	YH	1307	0	1381	86	0
32	RI	1136	0	1223	53	0
32	YI	1136	0	1223	69	0
33	RN	1104	0	1180	15	0
33	YN	1104	0	1180	21	0
34	RO	933	0	996	28	0
34	YO	933	0	996	30	0
35	RP	1145	0	1228	119	0
35	YP	1145	0	1228	142	0
36	RQ	1112	0	1170	40	0
36	YQ	1107	0	1165	40	0
37	RR	960	0	1021	16	0
37	YR	960	0	1021	25	0
38	RS	882	0	943	31	0
38	YS	882	0	943	35	0
39	RT	1141	0	1202	44	0
39	YT	1141	0	1202	41	0
40	RU	964	0	1022	37	0
40	YU	964	0	1022	37	0
41	RV	779	0	852	58	0
41	YV	779	0	852	57	0
42	RW	900	0	964	23	0
42	YW	900	0	964	21	0
43	RX	725	0	778	18	0
43	YX	725	0	778	16	0
44	RY	785	0	877	67	0
44	YY	785	0	878	47	0
45	RZ	1404	0	1437	92	0
45	YZ	1461	0	1493	51	0
46	R0	657	0	683	21	0
46	Y0	657	0	683	24	0
47	R1	763	0	848	28	0
47	Y1	763	0	848	23	0
48	R2	581	0	629	18	0
48	Y2	581	0	629	16	0
49	R3	469	0	518	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Y3	469	0	518	9	0
50	R4	573	0	565	23	0
50	Y4	573	0	565	37	0
51	R5	459	0	480	10	0
51	Y5	442	0	465	23	0
52	R6	417	0	441	26	0
52	Y6	417	0	441	54	0
53	R7	430	0	480	8	0
53	Y7	430	0	480	13	0
54	R8	517	0	582	48	0
54	Y8	517	0	582	68	0
55	R9	307	0	338	8	0
55	Y9	299	0	326	7	0
56	Z6	74	0	51	9	0
56	Z7	74	0	51	10	0
57	QA	151	0	0	0	0
57	QD	2	0	0	0	0
57	QE	1	0	0	0	0
57	QL	1	0	0	0	0
57	QN	1	0	0	0	0
57	QV	5	0	0	0	0
57	R0	2	0	0	0	0
57	R2	1	0	0	0	0
57	R5	3	0	0	0	0
57	RA	451	0	0	0	0
57	RB	5	0	0	0	0
57	RD	2	0	0	0	0
57	RE	3	0	0	0	0
57	RF	1	0	0	0	0
57	RP	2	0	0	0	0
57	RQ	2	0	0	0	0
57	RR	1	0	0	0	0
57	RV	1	0	0	0	0
57	RY	2	0	0	0	0
57	XA	164	0	0	0	0
57	XD	1	0	0	0	0
57	XE	1	0	0	0	0
57	XF	1	0	0	0	0
57	XK	1	0	0	0	0
57	XL	1	0	0	0	0
57	XN	1	0	0	0	0
57	XS	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	XV	4	0	0	0	0
57	Y0	1	0	0	0	0
57	Y5	3	0	0	0	0
57	Y7	1	0	0	0	0
57	YA	504	0	0	0	0
57	YB	6	0	0	0	0
57	YD	1	0	0	0	0
57	YE	2	0	0	0	0
57	YF	2	0	0	0	0
57	YG	1	0	0	0	0
57	YH	2	0	0	0	0
57	YN	1	0	0	0	0
57	YO	1	0	0	0	0
57	YP	2	0	0	0	0
57	YQ	2	0	0	0	0
57	YR	1	0	0	0	0
57	YU	1	0	0	0	0
57	YV	1	0	0	0	0
57	YW	1	0	0	0	0
57	Z7	1	0	0	0	0
58	QD	1	0	0	0	0
58	QN	1	0	0	0	0
58	XD	1	0	0	0	0
58	XN	1	0	0	0	0
All	All	294427	18	199944	5106	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 5106 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)
41:YV:49:THR:CG2	41:YV:50:PRO:HD3	1.35	1.52
31:RH:9:ILE:CG2	31:RH:10:PRO:HA	1.36	1.51
50:Y4:6:HIS:HB2	50:Y4:7:PRO:CD	1.43	1.47
31:YH:9:ILE:CG2	31:YH:10:PRO:HA	1.39	1.47
41:RV:49:THR:CG2	41:RV:50:PRO:HD3	1.48	1.42

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	234/256 (91%)	186 (80%)	29 (12%)	19 (8%)	1	4
2	XB	234/256 (91%)	189 (81%)	27 (12%)	18 (8%)	1	4
3	QC	204/239 (85%)	161 (79%)	27 (13%)	16 (8%)	1	4
3	XC	204/239 (85%)	160 (78%)	31 (15%)	13 (6%)	1	6
4	QD	206/209 (99%)	169 (82%)	26 (13%)	11 (5%)	1	10
4	XD	206/209 (99%)	168 (82%)	22 (11%)	16 (8%)	1	4
5	QE	152/162 (94%)	135 (89%)	12 (8%)	5 (3%)	3	17
5	XE	152/162 (94%)	137 (90%)	9 (6%)	6 (4%)	2	14
6	QF	99/101 (98%)	89 (90%)	10 (10%)	0	100	100
6	XF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
7	QG	153/156 (98%)	136 (89%)	13 (8%)	4 (3%)	4	21
7	XG	153/156 (98%)	133 (87%)	15 (10%)	5 (3%)	3	17
8	QH	136/138 (99%)	126 (93%)	7 (5%)	3 (2%)	5	24
8	XH	136/138 (99%)	123 (90%)	10 (7%)	3 (2%)	5	24
9	QI	126/128 (98%)	94 (75%)	24 (19%)	8 (6%)	1	6
9	XI	126/128 (98%)	97 (77%)	22 (18%)	7 (6%)	1	8
10	QJ	97/105 (92%)	80 (82%)	13 (13%)	4 (4%)	2	13
10	XJ	97/105 (92%)	81 (84%)	11 (11%)	5 (5%)	1	10
11	QK	119/129 (92%)	102 (86%)	13 (11%)	4 (3%)	3	16
11	XK	119/129 (92%)	105 (88%)	10 (8%)	4 (3%)	3	16
12	QL	123/132 (93%)	99 (80%)	16 (13%)	8 (6%)	1	6
12	XL	123/132 (93%)	97 (79%)	18 (15%)	8 (6%)	1	6
13	QM	116/126 (92%)	88 (76%)	17 (15%)	11 (10%)	0	3
13	XM	116/126 (92%)	88 (76%)	17 (15%)	11 (10%)	0	3
14	QN	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	XN	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	1	10
15	QO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
15	XO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
16	QP	82/88 (93%)	72 (88%)	10 (12%)	0	100	100
16	XP	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
17	QQ	98/105 (93%)	90 (92%)	7 (7%)	1 (1%)	12	41
17	XQ	98/105 (93%)	89 (91%)	7 (7%)	2 (2%)	6	25
18	QR	69/88 (78%)	61 (88%)	8 (12%)	0	100	100
18	XR	69/88 (78%)	62 (90%)	6 (9%)	1 (1%)	9	34
19	QS	80/93 (86%)	52 (65%)	18 (22%)	10 (12%)	0	1
19	XS	80/93 (86%)	52 (65%)	18 (22%)	10 (12%)	0	1
20	QT	97/106 (92%)	79 (81%)	15 (16%)	3 (3%)	3	18
20	XT	97/106 (92%)	80 (82%)	14 (14%)	3 (3%)	3	18
21	QU	23/25 (92%)	16 (70%)	6 (26%)	1 (4%)	2	12
21	XU	23/25 (92%)	18 (78%)	3 (13%)	2 (9%)	0	4
24	QY	89/117 (76%)	80 (90%)	9 (10%)	0	100	100
24	XY	89/117 (76%)	83 (93%)	6 (7%)	0	100	100
27	RD	270/276 (98%)	224 (83%)	38 (14%)	8 (3%)	3	19
27	YD	270/276 (98%)	228 (84%)	32 (12%)	10 (4%)	2	15
28	RE	203/206 (98%)	137 (68%)	38 (19%)	28 (14%)	0	1
28	YE	203/206 (98%)	134 (66%)	39 (19%)	30 (15%)	0	0
29	RF	206/210 (98%)	167 (81%)	26 (13%)	13 (6%)	1	6
29	YF	206/210 (98%)	168 (82%)	22 (11%)	16 (8%)	1	4
30	RG	179/182 (98%)	141 (79%)	26 (14%)	12 (7%)	1	6
30	YG	179/182 (98%)	147 (82%)	21 (12%)	11 (6%)	1	7
31	RH	168/180 (93%)	104 (62%)	37 (22%)	27 (16%)	0	0
31	YH	168/180 (93%)	98 (58%)	42 (25%)	28 (17%)	0	0
32	RI	144/148 (97%)	109 (76%)	28 (19%)	7 (5%)	1	11
32	YI	144/148 (97%)	116 (81%)	24 (17%)	4 (3%)	4	20
33	RN	136/140 (97%)	116 (85%)	13 (10%)	7 (5%)	1	10
33	YN	136/140 (97%)	110 (81%)	19 (14%)	7 (5%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	RO	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	16	47
34	YO	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	16	47
35	RP	148/150 (99%)	97 (66%)	23 (16%)	28 (19%)	0	0
35	YP	148/150 (99%)	102 (69%)	22 (15%)	24 (16%)	0	0
36	RQ	138/141 (98%)	110 (80%)	17 (12%)	11 (8%)	1	4
36	YQ	137/141 (97%)	111 (81%)	15 (11%)	11 (8%)	1	4
37	RR	115/118 (98%)	107 (93%)	4 (4%)	4 (4%)	3	16
37	YR	115/118 (98%)	109 (95%)	3 (3%)	3 (3%)	4	21
38	RS	109/112 (97%)	84 (77%)	17 (16%)	8 (7%)	1	5
38	YS	109/112 (97%)	85 (78%)	13 (12%)	11 (10%)	0	3
39	RT	135/146 (92%)	109 (81%)	24 (18%)	2 (2%)	8	32
39	YT	135/146 (92%)	113 (84%)	17 (13%)	5 (4%)	2	15
40	RU	115/118 (98%)	107 (93%)	6 (5%)	2 (2%)	7	30
40	YU	115/118 (98%)	103 (90%)	9 (8%)	3 (3%)	4	21
41	RV	99/101 (98%)	72 (73%)	12 (12%)	15 (15%)	0	0
41	YV	99/101 (98%)	71 (72%)	15 (15%)	13 (13%)	0	1
42	RW	111/113 (98%)	107 (96%)	1 (1%)	3 (3%)	4	20
42	YW	111/113 (98%)	104 (94%)	3 (3%)	4 (4%)	2	16
43	RX	90/96 (94%)	76 (84%)	12 (13%)	2 (2%)	5	24
43	YX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	5	24
44	RY	100/110 (91%)	56 (56%)	28 (28%)	16 (16%)	0	0
44	YY	100/110 (91%)	57 (57%)	27 (27%)	16 (16%)	0	0
45	RZ	174/206 (84%)	117 (67%)	33 (19%)	24 (14%)	0	1
45	YZ	181/206 (88%)	122 (67%)	42 (23%)	17 (9%)	0	3
46	R0	81/85 (95%)	73 (90%)	5 (6%)	3 (4%)	2	15
46	Y0	81/85 (95%)	67 (83%)	11 (14%)	3 (4%)	2	15
47	R1	95/98 (97%)	71 (75%)	12 (13%)	12 (13%)	0	1
47	Y1	95/98 (97%)	76 (80%)	13 (14%)	6 (6%)	1	6
48	R2	67/72 (93%)	54 (81%)	8 (12%)	5 (8%)	1	4
48	Y2	67/72 (93%)	56 (84%)	5 (8%)	6 (9%)	0	3
49	R3	57/60 (95%)	51 (90%)	6 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	Y3	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
50	R4	68/71 (96%)	43 (63%)	12 (18%)	13 (19%)	0	0
50	Y4	68/71 (96%)	38 (56%)	15 (22%)	15 (22%)	0	0
51	R5	57/60 (95%)	46 (81%)	9 (16%)	2 (4%)	3	16
51	Y5	55/60 (92%)	48 (87%)	4 (7%)	3 (6%)	1	9
52	R6	46/54 (85%)	22 (48%)	15 (33%)	9 (20%)	0	0
52	Y6	46/54 (85%)	16 (35%)	17 (37%)	13 (28%)	0	0
53	R7	47/49 (96%)	47 (100%)	0	0	100	100
53	Y7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
54	R8	62/65 (95%)	48 (77%)	7 (11%)	7 (11%)	0	2
54	Y8	62/65 (95%)	49 (79%)	6 (10%)	7 (11%)	0	2
55	R9	35/37 (95%)	34 (97%)	0	1 (3%)	3	19
55	Y9	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
All	All	11647/12358 (94%)	9391 (81%)	1489 (13%)	767 (7%)	1	6

5 of 767 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	29	ALA
2	QB	165	VAL
2	QB	195	ASP
2	QB	238	LEU
3	QC	64	VAL

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	
2	QB	204/220 (93%)	176 (86%)	28 (14%)	3	15
2	XB	204/220 (93%)	175 (86%)	29 (14%)	3	14
3	QC	160/188 (85%)	143 (89%)	17 (11%)	6	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	XC	160/188 (85%)	139 (87%)	21 (13%)	4	17
4	QD	180/181 (99%)	157 (87%)	23 (13%)	4	18
4	XD	180/181 (99%)	151 (84%)	29 (16%)	2	11
5	QE	119/123 (97%)	104 (87%)	15 (13%)	4	19
5	XE	119/123 (97%)	106 (89%)	13 (11%)	6	24
6	QF	90/90 (100%)	84 (93%)	6 (7%)	15	43
6	XF	90/90 (100%)	75 (83%)	15 (17%)	2	10
7	QG	126/127 (99%)	112 (89%)	14 (11%)	6	24
7	XG	126/127 (99%)	107 (85%)	19 (15%)	3	13
8	QH	119/119 (100%)	108 (91%)	11 (9%)	8	31
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	24
9	QI	99/99 (100%)	78 (79%)	21 (21%)	1	5
9	XI	99/99 (100%)	83 (84%)	16 (16%)	2	11
10	QJ	89/92 (97%)	78 (88%)	11 (12%)	4	19
10	XJ	89/92 (97%)	76 (85%)	13 (15%)	3	14
11	QK	92/99 (93%)	84 (91%)	8 (9%)	9	34
11	XK	92/99 (93%)	84 (91%)	8 (9%)	9	34
12	QL	104/109 (95%)	89 (86%)	15 (14%)	3	14
12	XL	104/109 (95%)	82 (79%)	22 (21%)	1	5
13	QM	94/101 (93%)	79 (84%)	15 (16%)	2	12
13	XM	94/101 (93%)	83 (88%)	11 (12%)	5	22
14	QN	49/50 (98%)	46 (94%)	3 (6%)	17	46
14	XN	49/50 (98%)	45 (92%)	4 (8%)	10	36
15	QO	79/80 (99%)	71 (90%)	8 (10%)	7	28
15	XO	79/80 (99%)	72 (91%)	7 (9%)	9	33
16	QP	72/74 (97%)	65 (90%)	7 (10%)	8	30
16	XP	72/74 (97%)	65 (90%)	7 (10%)	8	30
17	QQ	95/97 (98%)	90 (95%)	5 (5%)	20	51
17	XQ	95/97 (98%)	88 (93%)	7 (7%)	13	40
18	QR	62/77 (80%)	57 (92%)	5 (8%)	11	36
18	XR	62/77 (80%)	55 (89%)	7 (11%)	5	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	QS	71/80 (89%)	52 (73%)	19 (27%)	0	2
19	XS	71/80 (89%)	56 (79%)	15 (21%)	1	5
20	QT	76/82 (93%)	61 (80%)	15 (20%)	1	6
20	XT	76/82 (93%)	63 (83%)	13 (17%)	2	10
21	QU	20/20 (100%)	19 (95%)	1 (5%)	22	53
21	XU	20/20 (100%)	18 (90%)	2 (10%)	7	29
24	QY	78/102 (76%)	76 (97%)	2 (3%)	40	68
24	XY	78/102 (76%)	74 (95%)	4 (5%)	21	52
27	RD	214/218 (98%)	175 (82%)	39 (18%)	2	8
27	YD	214/218 (98%)	172 (80%)	42 (20%)	1	6
28	RE	165/166 (99%)	134 (81%)	31 (19%)	1	7
28	YE	165/166 (99%)	130 (79%)	35 (21%)	1	5
29	RF	165/166 (99%)	139 (84%)	26 (16%)	2	12
29	YF	165/166 (99%)	141 (86%)	24 (14%)	3	14
30	RG	155/156 (99%)	143 (92%)	12 (8%)	12	38
30	YG	155/156 (99%)	138 (89%)	17 (11%)	6	24
31	RH	142/148 (96%)	120 (84%)	22 (16%)	2	12
31	YH	142/148 (96%)	113 (80%)	29 (20%)	1	5
32	RI	122/124 (98%)	99 (81%)	23 (19%)	1	7
32	YI	122/124 (98%)	100 (82%)	22 (18%)	2	8
33	RN	117/119 (98%)	104 (89%)	13 (11%)	6	24
33	YN	117/119 (98%)	105 (90%)	12 (10%)	7	27
34	RO	100/100 (100%)	88 (88%)	12 (12%)	5	21
34	YO	100/100 (100%)	86 (86%)	14 (14%)	3	15
35	RP	116/116 (100%)	82 (71%)	34 (29%)	0	1
35	YP	116/116 (100%)	80 (69%)	36 (31%)	0	0
36	RQ	110/111 (99%)	94 (86%)	16 (14%)	3	14
36	YQ	110/111 (99%)	91 (83%)	19 (17%)	2	9
37	RR	100/101 (99%)	81 (81%)	19 (19%)	1	7
37	YR	100/101 (99%)	84 (84%)	16 (16%)	2	12
38	RS	87/88 (99%)	77 (88%)	10 (12%)	5	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	YS	87/88 (99%)	74 (85%)	13 (15%)	3	13
39	RT	120/127 (94%)	99 (82%)	21 (18%)	2	9
39	YT	120/127 (94%)	99 (82%)	21 (18%)	2	9
40	RU	93/94 (99%)	85 (91%)	8 (9%)	10	34
40	YU	93/94 (99%)	84 (90%)	9 (10%)	8	30
41	RV	82/82 (100%)	68 (83%)	14 (17%)	2	10
41	YV	82/82 (100%)	63 (77%)	19 (23%)	1	4
42	RW	92/92 (100%)	78 (85%)	14 (15%)	3	13
42	YW	92/92 (100%)	79 (86%)	13 (14%)	3	15
43	RX	74/78 (95%)	64 (86%)	10 (14%)	4	16
43	YX	74/78 (95%)	66 (89%)	8 (11%)	6	25
44	RY	85/91 (93%)	61 (72%)	24 (28%)	0	1
44	YY	85/91 (93%)	62 (73%)	23 (27%)	0	2
45	RZ	155/179 (87%)	125 (81%)	30 (19%)	1	7
45	YZ	162/179 (90%)	132 (82%)	30 (18%)	1	8
46	R0	66/67 (98%)	60 (91%)	6 (9%)	9	32
46	Y0	66/67 (98%)	59 (89%)	7 (11%)	6	26
47	R1	82/83 (99%)	68 (83%)	14 (17%)	2	10
47	Y1	82/83 (99%)	71 (87%)	11 (13%)	4	17
48	R2	64/67 (96%)	52 (81%)	12 (19%)	1	7
48	Y2	64/67 (96%)	55 (86%)	9 (14%)	3	15
49	R3	51/52 (98%)	43 (84%)	8 (16%)	2	12
49	Y3	51/52 (98%)	41 (80%)	10 (20%)	1	6
50	R4	62/63 (98%)	49 (79%)	13 (21%)	1	5
50	Y4	62/63 (98%)	45 (73%)	17 (27%)	0	1
51	R5	51/52 (98%)	43 (84%)	8 (16%)	2	12
51	Y5	49/52 (94%)	43 (88%)	6 (12%)	5	20
52	R6	47/52 (90%)	34 (72%)	13 (28%)	0	1
52	Y6	47/52 (90%)	29 (62%)	18 (38%)	0	0
53	R7	42/42 (100%)	35 (83%)	7 (17%)	2	10
53	Y7	42/42 (100%)	36 (86%)	6 (14%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	R8	54/55 (98%)	43 (80%)	11 (20%)	1	5
54	Y8	54/55 (98%)	44 (82%)	10 (18%)	1	8
55	R9	34/34 (100%)	32 (94%)	2 (6%)	18	48
55	Y9	33/34 (97%)	33 (100%)	0	100	100
All	All	9854/10266 (96%)	8362 (85%)	1492 (15%)	3	13

5 of 1492 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	XM	70	LEU
32	YI	9	LEU
17	XQ	74	LEU
13	XM	66	LEU
28	YE	12	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
2	XB	94	ASN
51	Y5	23	HIS
11	XK	13	GLN
51	Y5	4	HIS
45	YZ	132	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1509/1522 (99%)	311 (20%)	50 (3%)
1	XA	1506/1522 (98%)	308 (20%)	41 (2%)
22	QV	76/77 (98%)	16 (21%)	0
22	XV	76/77 (98%)	13 (17%)	1 (1%)
23	QX	19/24 (79%)	9 (47%)	2 (10%)
23	XX	19/24 (79%)	8 (42%)	0
25	RA	2888/2916 (99%)	602 (20%)	54 (1%)
25	YA	2872/2916 (98%)	585 (20%)	41 (1%)
26	RB	121/124 (97%)	23 (19%)	1 (0%)
26	YB	121/124 (97%)	24 (19%)	1 (0%)
56	Z6	1/3 (33%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
56	Z7	1/3 (33%)	0	0
All	All	9209/9332 (98%)	1899 (20%)	191 (2%)

5 of 1899 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	4	U
1	QA	5	U
1	QA	6	G
1	QA	9	G
1	QA	22	G

5 of 191 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	243	A
1	XA	1181	G
1	XA	328	C
1	XA	812	C
25	YA	101	G

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

8 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
56	PPU	Z6	76	25,56	37,40,41	1.24	4 (10%)	47,57,60	2.24	15 (31%)
23	OMC	QX	20	23	19,22,23	0.83	0	25,31,34	0.97	1 (4%)
23	A2M	QX	21	23,1	22,25,26	1.57	3 (13%)	30,36,39	2.10	11 (36%)
23	A2M	XX	19	23,22	22,25,26	1.38	3 (13%)	30,36,39	2.32	11 (36%)
23	OMC	XX	20	23	19,22,23	0.80	0	25,31,34	0.96	1 (4%)
23	A2M	QX	19	23,22	22,25,26	1.53	4 (18%)	30,36,39	2.08	11 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PPU	Z7	76	25,56	37,40,41	1.28	4 (10%)	47,57,60	2.03	13 (27%)
23	A2M	XX	21	23,1	22,25,26	1.53	4 (18%)	30,36,39	2.01	9 (30%)

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
56	PPU	Z6	76	25,56	-	2/25/43/44	0/4/4/4
23	OMC	QX	20	23	-	3/9/27/28	0/2/2/2
23	A2M	QX	21	23,1	-	4/9/27/28	0/3/3/3
23	A2M	XX	19	23,22	-	1/9/27/28	0/3/3/3
23	OMC	XX	20	23	-	2/9/27/28	0/2/2/2
23	A2M	QX	19	23,22	-	0/9/27/28	0/3/3/3
56	PPU	Z7	76	25,56	-	3/25/43/44	0/4/4/4
23	A2M	XX	21	23,1	-	3/9/27/28	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	QX	21	A2M	C5-C4	5.01	1.48	1.39
23	XX	21	A2M	C5-C4	4.95	1.47	1.39
23	QX	19	A2M	C5-C4	4.83	1.47	1.39
56	Z7	76	PPU	C5-C4	4.16	1.46	1.39
56	Z6	76	PPU	C5-C4	4.05	1.46	1.39

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z7	76	PPU	C5-C4-N3	-5.79	118.75	126.72
56	Z6	76	PPU	C5-C4-N3	-5.75	118.81	126.72
56	Z6	76	PPU	N1-C6-N6	5.64	123.72	116.86
23	XX	19	A2M	C5-C4-N3	-5.58	119.03	126.72
23	QX	21	A2M	C5-C4-N3	-5.44	119.23	126.72

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	QX	21	A2M	C3'-C2'-O2'-CM'
23	XX	21	A2M	C3'-C2'-O2'-CM'
56	Z7	76	PPU	C5-C6-N6-C10
23	QX	20	OMC	O4'-C4'-C5'-O5'
23	XX	21	A2M	C3'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z6	76	PPU	8	0
23	QX	20	OMC	1	0
23	QX	21	A2M	1	0
23	XX	19	A2M	1	0
23	XX	20	OMC	1	0
23	QX	19	A2M	1	0
56	Z7	76	PPU	9	0
23	XX	21	A2M	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1350 ligands modelled in this entry, 1350 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1511/1522 (99%)	0.22	71 (4%) 36 19	34, 73, 167, 323	0
1	XA	1508/1522 (99%)	0.03	45 (2%) 52 31	27, 64, 152, 309	0
2	QB	236/256 (92%)	1.12	43 (18%) 3 1	56, 114, 192, 239	0
2	XB	236/256 (92%)	1.06	49 (20%) 2 1	51, 99, 182, 208	0
3	QC	206/239 (86%)	0.68	14 (6%) 23 12	42, 97, 183, 230	0
3	XC	206/239 (86%)	0.77	24 (11%) 9 5	48, 84, 156, 235	0
4	QD	208/209 (99%)	0.42	18 (8%) 16 9	37, 65, 105, 184	0
4	XD	208/209 (99%)	0.55	22 (10%) 11 6	39, 67, 113, 170	0
5	QE	154/162 (95%)	0.32	1 (0%) 85 70	38, 64, 127, 212	0
5	XE	154/162 (95%)	0.37	12 (7%) 19 10	33, 60, 127, 229	0
6	QF	101/101 (100%)	0.65	3 (2%) 52 31	51, 87, 129, 142	0
6	XF	101/101 (100%)	0.20	2 (1%) 65 44	34, 64, 107, 165	0
7	QG	155/156 (99%)	1.09	24 (15%) 5 2	71, 109, 182, 224	0
7	XG	155/156 (99%)	0.89	23 (14%) 5 3	49, 89, 156, 201	0
8	QH	138/138 (100%)	0.33	2 (1%) 73 53	48, 72, 106, 156	0
8	XH	138/138 (100%)	0.18	4 (2%) 53 32	41, 64, 110, 142	0
9	QI	128/128 (100%)	1.31	24 (18%) 3 1	69, 127, 198, 231	0
9	XI	128/128 (100%)	1.17	26 (20%) 3 1	46, 97, 172, 248	0
10	QJ	99/105 (94%)	1.39	21 (21%) 2 1	67, 123, 200, 249	0
10	XJ	99/105 (94%)	1.23	13 (13%) 7 4	45, 109, 178, 237	0
11	QK	121/129 (93%)	0.73	10 (8%) 17 9	42, 85, 170, 226	0
11	XK	121/129 (93%)	0.53	11 (9%) 15 8	33, 65, 157, 195	0
12	QL	125/132 (94%)	0.35	7 (5%) 30 16	34, 58, 110, 215	0
12	XL	125/132 (94%)	0.34	7 (5%) 30 16	28, 55, 96, 205	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	118/126 (93%)	1.41	27 (22%) 2 1	66, 113, 181, 242	0
13	XM	118/126 (93%)	1.19	25 (21%) 2 1	52, 97, 150, 259	0
14	QN	60/61 (98%)	1.23	10 (16%) 4 2	63, 95, 133, 188	0
14	XN	60/61 (98%)	0.96	7 (11%) 9 5	50, 77, 123, 190	0
15	QO	88/89 (98%)	0.59	9 (10%) 12 6	42, 75, 119, 154	0
15	XO	88/89 (98%)	0.36	4 (4%) 38 20	30, 63, 104, 120	0
16	QP	84/88 (95%)	0.27	2 (2%) 59 38	46, 66, 101, 182	0
16	XP	84/88 (95%)	0.32	2 (2%) 59 38	50, 70, 104, 198	0
17	QQ	100/105 (95%)	0.51	6 (6%) 27 15	44, 74, 105, 120	0
17	XQ	100/105 (95%)	0.47	6 (6%) 27 15	41, 67, 103, 183	0
18	QR	71/88 (80%)	0.82	4 (5%) 30 16	59, 91, 157, 210	0
18	XR	71/88 (80%)	0.45	5 (7%) 22 12	36, 63, 144, 203	0
19	QS	82/93 (88%)	1.45	21 (25%) 1 1	64, 120, 198, 256	0
19	XS	82/93 (88%)	1.50	26 (31%) 1 1	52, 100, 182, 224	0
20	QT	99/106 (93%)	1.23	20 (20%) 3 1	47, 80, 163, 206	0
20	XT	99/106 (93%)	0.99	14 (14%) 6 3	47, 80, 163, 198	0
21	QU	25/25 (100%)	2.10	7 (28%) 1 1	68, 98, 172, 193	0
21	XU	25/25 (100%)	1.78	12 (48%) 0 0	65, 95, 117, 174	0
22	QV	77/77 (100%)	0.36	3 (3%) 43 24	29, 71, 129, 189	0
22	XV	77/77 (100%)	0.20	2 (2%) 57 36	29, 68, 106, 175	0
23	QX	17/24 (70%)	2.23	9 (52%) 0 0	51, 206, 281, 292	0
23	XX	17/24 (70%)	1.68	7 (41%) 0 0	37, 216, 350, 357	0
24	QY	91/117 (77%)	0.55	7 (7%) 19 10	53, 81, 111, 140	0
24	XY	91/117 (77%)	0.54	7 (7%) 19 10	50, 78, 103, 123	0
25	RA	2891/2916 (99%)	0.02	172 (5%) 28 15	21, 50, 223, 352	0
25	YA	2875/2916 (98%)	-0.04	172 (5%) 27 15	19, 45, 231, 375	0
26	RB	122/124 (98%)	0.37	5 (4%) 41 23	40, 82, 126, 193	0
26	YB	122/124 (98%)	0.35	4 (3%) 49 29	41, 72, 121, 208	0
27	RD	272/276 (98%)	0.29	23 (8%) 16 9	16, 46, 89, 168	0
27	YD	272/276 (98%)	0.18	16 (5%) 28 15	10, 36, 80, 191	0
28	RE	205/206 (99%)	0.76	29 (14%) 6 3	26, 63, 143, 241	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YE	205/206 (99%)	0.81	30 (14%) 6 3	23, 58, 148, 254	0
29	RF	208/210 (99%)	0.42	21 (10%) 12 6	18, 44, 142, 240	0
29	YF	208/210 (99%)	0.48	18 (8%) 16 9	21, 51, 167, 229	0
30	RG	181/182 (99%)	0.83	17 (9%) 14 8	56, 92, 150, 174	0
30	YG	181/182 (99%)	0.65	12 (6%) 24 13	45, 81, 134, 169	0
31	RH	170/180 (94%)	1.95	68 (40%) 1 0	53, 125, 218, 256	0
31	YH	170/180 (94%)	1.57	44 (25%) 1 1	54, 104, 201, 250	0
32	RI	146/148 (98%)	1.07	27 (18%) 3 1	46, 96, 156, 246	0
32	YI	146/148 (98%)	0.91	22 (15%) 5 3	30, 84, 153, 224	0
33	RN	138/140 (98%)	0.51	11 (7%) 18 10	30, 65, 114, 163	0
33	YN	138/140 (98%)	0.42	8 (5%) 29 16	30, 61, 121, 149	0
34	RO	122/122 (100%)	0.17	3 (2%) 58 37	32, 55, 86, 131	0
34	YO	122/122 (100%)	-0.01	0 100 100	25, 46, 77, 97	0
35	RP	150/150 (100%)	1.10	31 (20%) 2 1	17, 63, 133, 211	0
35	YP	150/150 (100%)	1.19	31 (20%) 2 1	19, 54, 139, 202	0
36	RQ	140/141 (99%)	0.65	16 (11%) 10 5	28, 59, 104, 202	0
36	YQ	139/141 (98%)	0.60	19 (13%) 6 4	31, 55, 114, 204	0
37	RR	117/118 (99%)	0.29	6 (5%) 33 18	24, 56, 91, 123	0
37	YR	117/118 (99%)	0.16	3 (2%) 57 36	25, 51, 87, 124	0
38	RS	111/112 (99%)	1.10	19 (17%) 4 2	50, 83, 148, 217	0
38	YS	111/112 (99%)	0.69	13 (11%) 9 5	38, 67, 122, 171	0
39	RT	137/146 (93%)	0.61	12 (8%) 15 9	34, 67, 146, 241	0
39	YT	137/146 (93%)	0.57	19 (13%) 6 4	29, 59, 155, 214	0
40	RU	117/118 (99%)	0.31	7 (5%) 27 15	24, 48, 105, 151	0
40	YU	117/118 (99%)	0.53	6 (5%) 33 18	29, 54, 101, 169	0
41	RV	101/101 (100%)	0.58	14 (13%) 6 4	20, 65, 123, 222	0
41	YV	101/101 (100%)	0.89	12 (11%) 9 5	28, 75, 133, 247	0
42	RW	113/113 (100%)	0.12	5 (4%) 39 21	24, 49, 94, 175	0
42	YW	113/113 (100%)	0.15	4 (3%) 47 27	25, 46, 99, 194	0
43	RX	92/96 (95%)	0.44	4 (4%) 40 22	39, 62, 87, 135	0
43	YX	92/96 (95%)	0.27	4 (4%) 40 22	16, 47, 89, 103	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RY	102/110 (92%)	1.67	35 (34%) 1 0	40, 75, 179, 238	0
44	YY	102/110 (92%)	1.67	30 (29%) 1 1	33, 79, 184, 214	0
45	RZ	176/206 (85%)	1.30	40 (22%) 2 1	49, 93, 187, 286	0
45	YZ	183/206 (88%)	1.13	31 (16%) 4 2	41, 92, 163, 211	0
46	R0	83/85 (97%)	0.20	7 (8%) 17 9	27, 50, 94, 200	0
46	Y0	83/85 (97%)	0.37	7 (8%) 17 9	24, 50, 81, 189	0
47	R1	97/98 (98%)	0.87	17 (17%) 4 2	29, 58, 172, 241	0
47	Y1	97/98 (98%)	0.67	12 (12%) 8 5	22, 46, 176, 235	0
48	R2	69/72 (95%)	0.92	8 (11%) 9 5	39, 79, 141, 190	0
48	Y2	69/72 (95%)	0.73	11 (15%) 5 2	29, 60, 106, 196	0
49	R3	59/60 (98%)	0.19	2 (3%) 48 28	33, 53, 103, 126	0
49	Y3	59/60 (98%)	0.30	2 (3%) 48 28	35, 61, 112, 167	0
50	R4	70/71 (98%)	2.06	29 (41%) 0 0	79, 165, 243, 284	0
50	Y4	70/71 (98%)	1.94	28 (40%) 1 0	79, 143, 226, 269	0
51	R5	59/60 (98%)	0.86	13 (22%) 2 1	23, 53, 179, 237	0
51	Y5	57/60 (95%)	0.96	11 (19%) 3 1	21, 53, 161, 284	0
52	R6	48/54 (88%)	3.00	26 (54%) 0 0	73, 134, 213, 253	0
52	Y6	48/54 (88%)	3.30	33 (68%) 0 0	73, 129, 207, 245	0
53	R7	49/49 (100%)	0.45	7 (14%) 6 3	21, 33, 127, 192	0
53	Y7	49/49 (100%)	0.30	5 (10%) 12 6	18, 29, 82, 193	0
54	R8	64/65 (98%)	0.99	11 (17%) 4 2	19, 47, 122, 180	0
54	Y8	64/65 (98%)	0.90	9 (14%) 6 3	16, 44, 72, 174	0
55	R9	37/37 (100%)	1.21	6 (16%) 4 2	52, 78, 134, 165	0
55	Y9	36/37 (97%)	0.94	5 (13%) 6 4	36, 76, 110, 130	0
56	Z6	2/3 (66%)	-0.39	0 100 100	29, 29, 29, 38	0
56	Z7	2/3 (66%)	0.22	0 100 100	30, 30, 30, 43	0
All	All	21068/21690 (97%)	0.46	2030 (9%) 13 7	10, 65, 171, 375	0

The worst 5 of 2030 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
52	R6	23	THR	12.7
36	RQ	140	ALA	11.3

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Mol	Chain	Res	Type	RSRZ
52	Y6	41	PRO	11.0
44	YY	48	ALA	10.4
35	YP	13	ASN	10.2

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
23	A2M	QX	21	23/24	0.77	0.19	44,130,130,130	0
23	A2M	XX	21	23/24	0.85	0.19	44,118,118,118	0
23	OMC	XX	20	21/22	0.91	0.10	44,74,74,74	0
23	A2M	XX	19	23/24	0.92	0.11	62,62,104,137	0
23	OMC	QX	20	21/22	0.93	0.09	44,77,77,77	0
23	A2M	QX	19	23/24	0.94	0.08	39,73,73,73	0
56	PPU	Z6	76	37/38	0.95	0.12	26,33,40,43	0
56	PPU	Z7	76	37/38	0.95	0.11	27,32,49,62	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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
57	MG	RA	3036	1/1	0.25	0.34	51,51,51,51	0
57	MG	QA	1630	1/1	0.30	0.26	63,63,63,63	0
57	MG	XA	1690	1/1	0.34	0.25	52,52,52,52	0
57	MG	YA	3228	1/1	0.34	0.31	69,69,69,69	0
57	MG	YA	3082	1/1	0.35	0.23	24,24,24,24	0
57	MG	RA	3083	1/1	0.36	0.27	30,30,30,30	0
57	MG	YA	3255	1/1	0.37	0.28	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3448	1/1	0.43	0.42	82,82,82,82	0
57	MG	RA	3414	1/1	0.48	0.12	42,42,42,42	0
57	MG	YA	3294	1/1	0.48	0.26	45,45,45,45	0
57	MG	RA	3261	1/1	0.48	0.43	79,79,79,79	0
57	MG	YA	3149	1/1	0.50	0.26	34,34,34,34	0
57	MG	RA	3345	1/1	0.51	0.20	73,73,73,73	0
57	MG	XA	1656	1/1	0.54	0.31	65,65,65,65	0
57	MG	RA	3102	1/1	0.54	0.31	28,28,28,28	0
57	MG	YA	3457	1/1	0.54	0.18	24,24,24,24	0
57	MG	RA	3210	1/1	0.55	0.27	64,64,64,64	0
57	MG	YA	3186	1/1	0.56	0.22	48,48,48,48	0
57	MG	YA	3502	1/1	0.56	0.26	32,32,32,32	0
57	MG	YA	3287	1/1	0.57	0.23	58,58,58,58	0
57	MG	YA	3104	1/1	0.59	0.38	76,76,76,76	0
57	MG	RA	3198	1/1	0.59	0.30	50,50,50,50	0
57	MG	YA	3268	1/1	0.60	0.31	55,55,55,55	0
57	MG	XA	1629	1/1	0.61	0.29	54,54,54,54	0
57	MG	RA	3322	1/1	0.61	0.10	84,84,84,84	0
57	MG	YA	3428	1/1	0.61	0.21	32,32,32,32	0
57	MG	RY	202	1/1	0.62	0.13	50,50,50,50	0
57	MG	XA	1628	1/1	0.62	0.19	52,52,52,52	0
57	MG	XA	1732	1/1	0.63	0.17	56,56,56,56	0
57	MG	RA	3343	1/1	0.63	0.12	56,56,56,56	0
57	MG	YA	3201	1/1	0.63	0.25	35,35,35,35	0
57	MG	XA	1625	1/1	0.63	0.14	37,37,37,37	0
57	MG	QA	1678	1/1	0.64	0.24	70,70,70,70	0
57	MG	YA	3493	1/1	0.64	0.22	63,63,63,63	0
57	MG	QA	1631	1/1	0.64	0.28	55,55,55,55	0
57	MG	RA	3214	1/1	0.65	0.25	57,57,57,57	0
57	MG	YA	3376	1/1	0.66	0.25	63,63,63,63	0
57	MG	QA	1720	1/1	0.66	0.16	67,67,67,67	0
57	MG	YA	3501	1/1	0.67	0.26	31,31,31,31	0
57	MG	YA	3352	1/1	0.67	0.39	84,84,84,84	0
57	MG	QA	1722	1/1	0.68	0.20	57,57,57,57	0
57	MG	RA	3095	1/1	0.68	0.30	38,38,38,38	0
57	MG	QA	1694	1/1	0.68	0.23	55,55,55,55	0
57	MG	RA	3211	1/1	0.69	0.12	31,31,31,31	0
57	MG	YA	3371	1/1	0.69	0.17	64,64,64,64	0
57	MG	RA	3092	1/1	0.69	0.23	56,56,56,56	0
57	MG	YA	3283	1/1	0.70	0.26	52,52,52,52	0
57	MG	QA	1642	1/1	0.70	0.21	50,50,50,50	0
57	MG	RA	3358	1/1	0.70	0.20	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3100	1/1	0.70	0.27	20,20,20,20	0
57	MG	QA	1703	1/1	0.70	0.22	86,86,86,86	0
57	MG	XA	1698	1/1	0.70	0.36	75,75,75,75	0
57	MG	RA	3118	1/1	0.71	0.30	55,55,55,55	0
57	MG	QA	1669	1/1	0.71	0.14	53,53,53,53	0
57	MG	RA	3446	1/1	0.71	0.23	33,33,33,33	0
57	MG	RA	3106	1/1	0.71	0.23	41,41,41,41	0
57	MG	RA	3361	1/1	0.72	0.17	65,65,65,65	0
57	MG	RA	3392	1/1	0.72	0.35	42,42,42,42	0
57	MG	RA	3217	1/1	0.72	0.20	50,50,50,50	0
57	MG	YA	3472	1/1	0.72	0.28	66,66,66,66	0
57	MG	QA	1672	1/1	0.72	0.27	71,71,71,71	0
57	MG	RA	3075	1/1	0.72	0.23	42,42,42,42	0
57	MG	YA	3143	1/1	0.72	0.34	48,48,48,48	0
57	MG	YA	3013	1/1	0.73	0.34	27,27,27,27	0
57	MG	YA	3281	1/1	0.73	0.31	52,52,52,52	0
57	MG	RA	3264	1/1	0.73	0.23	41,41,41,41	0
57	MG	XA	1630	1/1	0.73	0.35	75,75,75,75	0
57	MG	XA	1728	1/1	0.73	0.28	59,59,59,59	0
57	MG	QN	102	1/1	0.73	0.21	61,61,61,61	0
57	MG	YA	3362	1/1	0.73	0.32	61,61,61,61	0
57	MG	YA	3265	1/1	0.73	0.23	45,45,45,45	0
57	MG	XA	1704	1/1	0.74	0.36	62,62,62,62	0
57	MG	RA	3366	1/1	0.74	0.29	71,71,71,71	0
57	MG	RA	3002	1/1	0.74	0.18	55,55,55,55	0
57	MG	YA	3301	1/1	0.74	0.15	55,55,55,55	0
57	MG	RA	3179	1/1	0.74	0.22	47,47,47,47	0
57	MG	YA	3333	1/1	0.75	0.24	53,53,53,53	0
57	MG	QA	1637	1/1	0.75	0.37	74,74,74,74	0
57	MG	RA	3234	1/1	0.75	0.18	49,49,49,49	0
57	MG	XA	1763	1/1	0.75	0.14	59,59,59,59	0
57	MG	RA	3277	1/1	0.75	0.16	57,57,57,57	0
57	MG	RA	3372	1/1	0.75	0.22	74,74,74,74	0
57	MG	QA	1735	1/1	0.76	0.48	73,73,73,73	0
57	MG	RQ	201	1/1	0.76	0.16	34,34,34,34	0
57	MG	YA	3451	1/1	0.76	0.31	66,66,66,66	0
57	MG	YA	3410	1/1	0.76	0.28	62,62,62,62	0
57	MG	XA	1670	1/1	0.77	0.15	16,16,16,16	0
57	MG	XA	1680	1/1	0.77	0.25	50,50,50,50	0
57	MG	QA	1639	1/1	0.77	0.49	76,76,76,76	0
57	MG	RA	3376	1/1	0.77	0.23	66,66,66,66	0
57	MG	RA	3274	1/1	0.77	0.33	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3401	1/1	0.77	0.24	58,58,58,58	0
57	MG	QA	1737	1/1	0.77	0.25	56,56,56,56	0
57	MG	XA	1757	1/1	0.77	0.25	68,68,68,68	0
57	MG	QA	1609	1/1	0.77	0.37	61,61,61,61	0
57	MG	RA	3323	1/1	0.77	0.66	87,87,87,87	0
57	MG	RA	3093	1/1	0.77	0.23	38,38,38,38	0
57	MG	YA	3090	1/1	0.77	0.14	46,46,46,46	0
57	MG	YA	3099	1/1	0.77	0.25	53,53,53,53	0
57	MG	YA	3394	1/1	0.77	0.25	56,56,56,56	0
57	MG	R2	101	1/1	0.77	0.24	68,68,68,68	0
57	MG	YA	3421	1/1	0.77	0.15	38,38,38,38	0
57	MG	QA	1675	1/1	0.77	0.24	48,48,48,48	0
57	MG	QA	1652	1/1	0.77	0.19	34,34,34,34	0
57	MG	RA	3041	1/1	0.77	0.23	23,23,23,23	0
57	MG	YA	3169	1/1	0.77	0.33	46,46,46,46	0
57	MG	RA	3362	1/1	0.77	0.21	56,56,56,56	0
57	MG	XA	1655	1/1	0.77	0.26	53,53,53,53	0
57	MG	YA	3500	1/1	0.77	0.25	71,71,71,71	0
57	MG	RA	3069	1/1	0.77	0.19	18,18,18,18	0
57	MG	YA	3236	1/1	0.77	0.21	40,40,40,40	0
57	MG	YU	201	1/1	0.77	0.24	45,45,45,45	0
57	MG	YA	3192	1/1	0.78	0.23	34,34,34,34	0
57	MG	RA	3281	1/1	0.78	0.07	53,53,53,53	0
57	MG	QA	1745	1/1	0.78	0.20	52,52,52,52	0
57	MG	RA	3014	1/1	0.78	0.30	17,17,17,17	0
57	MG	YB	204	1/1	0.78	0.09	69,69,69,69	0
57	MG	YO	201	1/1	0.78	0.12	66,66,66,66	0
57	MG	RA	3328	1/1	0.78	0.29	61,61,61,61	0
57	MG	RA	3445	1/1	0.79	0.24	18,18,18,18	0
57	MG	YA	3176	1/1	0.79	0.16	57,57,57,57	0
57	MG	RA	3309	1/1	0.79	0.23	60,60,60,60	0
57	MG	YA	3475	1/1	0.79	0.14	40,40,40,40	0
57	MG	QA	1665	1/1	0.79	0.24	54,54,54,54	0
57	MG	YA	3387	1/1	0.79	0.13	71,71,71,71	0
57	MG	RA	3357	1/1	0.79	0.28	61,61,61,61	0
57	MG	QA	1633	1/1	0.79	0.30	57,57,57,57	0
57	MG	RA	3294	1/1	0.79	0.23	63,63,63,63	0
57	MG	RA	3332	1/1	0.79	0.30	67,67,67,67	0
57	MG	YA	3348	1/1	0.79	0.42	77,77,77,77	0
57	MG	YA	3191	1/1	0.80	0.26	30,30,30,30	0
57	MG	RA	3355	1/1	0.80	0.32	81,81,81,81	0
57	MG	YA	3386	1/1	0.80	0.14	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3182	1/1	0.80	0.33	78,78,78,78	0
57	MG	XD	302	1/1	0.80	0.10	51,51,51,51	0
57	MG	YA	3229	1/1	0.80	0.20	29,29,29,29	0
57	MG	XA	1638	1/1	0.80	0.31	59,59,59,59	0
57	MG	RA	3438	1/1	0.80	0.30	58,58,58,58	0
57	MG	YA	3440	1/1	0.80	0.22	49,49,49,49	0
57	MG	QA	1704	1/1	0.80	0.33	59,59,59,59	0
57	MG	QV	105	1/1	0.80	0.26	31,31,31,31	0
57	MG	RD	301	1/1	0.80	0.14	28,28,28,28	0
57	MG	QA	1677	1/1	0.80	0.10	50,50,50,50	0
57	MG	YA	3128	1/1	0.80	0.08	38,38,38,38	0
57	MG	RA	3168	1/1	0.80	0.22	48,48,48,48	0
57	MG	XA	1699	1/1	0.80	0.23	52,52,52,52	0
57	MG	YA	3313	1/1	0.80	0.24	37,37,37,37	0
57	MG	RA	3333	1/1	0.80	0.20	55,55,55,55	0
57	MG	QA	1673	1/1	0.80	0.27	60,60,60,60	0
57	MG	YA	3182	1/1	0.80	0.24	52,52,52,52	0
57	MG	RA	3218	1/1	0.80	0.28	35,35,35,35	0
57	MG	YA	3183	1/1	0.81	0.16	45,45,45,45	0
57	MG	YA	3349	1/1	0.81	0.38	62,62,62,62	0
57	MG	XA	1693	1/1	0.81	0.26	89,89,89,89	0
57	MG	RA	3449	1/1	0.81	0.23	32,32,32,32	0
57	MG	QA	1734	1/1	0.81	0.28	55,55,55,55	0
57	MG	XA	1657	1/1	0.81	0.24	37,37,37,37	0
57	MG	YA	3377	1/1	0.81	0.14	43,43,43,43	0
57	MG	YA	3288	1/1	0.81	0.20	51,51,51,51	0
57	MG	RA	3157	1/1	0.81	0.14	40,40,40,40	0
57	MG	YA	3173	1/1	0.81	0.13	28,28,28,28	0
57	MG	YA	3309	1/1	0.81	0.32	73,73,73,73	0
57	MG	YH	202	1/1	0.81	0.13	47,47,47,47	0
57	MG	QA	1688	1/1	0.81	0.19	56,56,56,56	0
57	MG	QA	1686	1/1	0.81	0.17	43,43,43,43	0
57	MG	RA	3111	1/1	0.82	0.11	45,45,45,45	0
57	MG	XA	1624	1/1	0.82	0.26	39,39,39,39	0
57	MG	YA	3404	1/1	0.82	0.20	63,63,63,63	0
57	MG	YA	3134	1/1	0.82	0.25	47,47,47,47	0
57	MG	RA	3043	1/1	0.82	0.25	36,36,36,36	0
57	MG	YA	3425	1/1	0.82	0.10	33,33,33,33	0
57	MG	RA	3415	1/1	0.82	0.28	23,23,23,23	0
57	MG	RA	3138	1/1	0.82	0.28	40,40,40,40	0
57	MG	RA	3225	1/1	0.82	0.27	67,67,67,67	0
57	MG	XA	1634	1/1	0.82	0.13	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1740	1/1	0.82	0.28	56,56,56,56	0
57	MG	YA	3458	1/1	0.82	0.22	28,28,28,28	0
57	MG	XA	1636	1/1	0.82	0.13	46,46,46,46	0
57	MG	YA	3473	1/1	0.82	0.09	39,39,39,39	0
57	MG	RA	3368	1/1	0.82	0.30	55,55,55,55	0
57	MG	YA	3478	1/1	0.82	0.41	81,81,81,81	0
57	MG	YA	3492	1/1	0.82	0.29	55,55,55,55	0
57	MG	RA	3205	1/1	0.82	0.17	30,30,30,30	0
57	MG	QA	1742	1/1	0.82	0.11	44,44,44,44	0
57	MG	YA	3198	1/1	0.82	0.34	54,54,54,54	0
57	MG	RA	3385	1/1	0.82	0.24	57,57,57,57	0
57	MG	RQ	202	1/1	0.82	0.27	58,58,58,58	0
57	MG	YE	301	1/1	0.82	0.13	40,40,40,40	0
57	MG	YA	3091	1/1	0.82	0.20	40,40,40,40	0
57	MG	XA	1672	1/1	0.82	0.21	52,52,52,52	0
57	MG	QA	1751	1/1	0.82	0.19	84,84,84,84	0
57	MG	YA	3047	1/1	0.83	0.22	18,18,18,18	0
57	MG	YA	3392	1/1	0.83	0.29	51,51,51,51	0
57	MG	YA	3226	1/1	0.83	0.28	48,48,48,48	0
57	MG	YA	3068	1/1	0.83	0.14	32,32,32,32	0
57	MG	RA	3387	1/1	0.83	0.31	56,56,56,56	0
57	MG	QA	1716	1/1	0.83	0.28	76,76,76,76	0
57	MG	QA	1655	1/1	0.83	0.25	46,46,46,46	0
57	MG	RA	3192	1/1	0.83	0.22	36,36,36,36	0
57	MG	XA	1697	1/1	0.83	0.15	62,62,62,62	0
57	MG	RA	3134	1/1	0.83	0.25	46,46,46,46	0
57	MG	YA	3118	1/1	0.83	0.20	40,40,40,40	0
57	MG	RA	3433	1/1	0.83	0.14	49,49,49,49	0
57	MG	YA	3133	1/1	0.83	0.18	38,38,38,38	0
57	MG	XA	1703	1/1	0.83	0.26	55,55,55,55	0
57	MG	RA	3072	1/1	0.83	0.21	32,32,32,32	0
57	MG	RA	3147	1/1	0.83	0.21	48,48,48,48	0
57	MG	QA	1699	1/1	0.83	0.22	58,58,58,58	0
57	MG	YA	3479	1/1	0.83	0.11	42,42,42,42	0
57	MG	RA	3371	1/1	0.83	0.19	70,70,70,70	0
57	MG	XA	1747	1/1	0.83	0.28	64,64,64,64	0
57	MG	YA	3498	1/1	0.83	0.26	57,57,57,57	0
57	MG	YA	3499	1/1	0.83	0.14	67,67,67,67	0
57	MG	RA	3334	1/1	0.83	0.42	71,71,71,71	0
57	MG	RE	303	1/1	0.83	0.11	51,51,51,51	0
57	MG	YA	3360	1/1	0.83	0.32	61,61,61,61	0
57	MG	YA	3503	1/1	0.83	0.21	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1727	1/1	0.83	0.24	57,57,57,57	0
57	MG	YA	3001	1/1	0.83	0.47	68,68,68,68	0
57	MG	RA	3216	1/1	0.83	0.20	32,32,32,32	0
57	MG	YA	3040	1/1	0.83	0.19	26,26,26,26	0
57	MG	YQ	202	1/1	0.83	0.10	39,39,39,39	0
57	MG	YA	3199	1/1	0.83	0.20	54,54,54,54	0
57	MG	YA	3029	1/1	0.84	0.10	33,33,33,33	0
57	MG	YA	3120	1/1	0.84	0.30	41,41,41,41	0
57	MG	YA	3035	1/1	0.84	0.21	39,39,39,39	0
57	MG	QA	1728	1/1	0.84	0.23	45,45,45,45	0
57	MG	RA	3276	1/1	0.84	0.27	50,50,50,50	0
57	MG	YA	3399	1/1	0.84	0.13	47,47,47,47	0
57	MG	YA	3402	1/1	0.84	0.12	56,56,56,56	0
57	MG	RA	3206	1/1	0.84	0.11	18,18,18,18	0
57	MG	YA	3147	1/1	0.84	0.07	25,25,25,25	0
57	MG	YA	3419	1/1	0.84	0.14	37,37,37,37	0
57	MG	RA	3394	1/1	0.84	0.13	31,31,31,31	0
57	MG	XA	1646	1/1	0.84	0.63	87,87,87,87	0
57	MG	YA	3232	1/1	0.84	0.14	35,35,35,35	0
57	MG	YA	3437	1/1	0.84	0.12	37,37,37,37	0
57	MG	RA	3448	1/1	0.84	0.26	27,27,27,27	0
57	MG	RA	3249	1/1	0.84	0.18	48,48,48,48	0
57	MG	YA	3179	1/1	0.84	0.19	63,63,63,63	0
57	MG	QA	1736	1/1	0.84	0.21	47,47,47,47	0
57	MG	QA	1670	1/1	0.84	0.31	54,54,54,54	0
57	MG	RA	3325	1/1	0.85	0.21	41,41,41,41	0
57	MG	XA	1639	1/1	0.85	0.41	74,74,74,74	0
57	MG	QA	1743	1/1	0.85	0.19	52,52,52,52	0
57	MG	RA	3246	1/1	0.85	0.24	39,39,39,39	0
57	MG	RA	3413	1/1	0.85	0.12	41,41,41,41	0
57	MG	RA	3364	1/1	0.85	0.27	64,64,64,64	0
57	MG	YA	3335	1/1	0.85	0.20	52,52,52,52	0
57	MG	YA	3345	1/1	0.85	0.29	70,70,70,70	0
57	MG	XA	1663	1/1	0.85	0.21	42,42,42,42	0
57	MG	QA	1661	1/1	0.85	0.17	52,52,52,52	0
57	MG	YA	3130	1/1	0.85	0.23	34,34,34,34	0
57	MG	YA	3477	1/1	0.85	0.16	44,44,44,44	0
57	MG	YA	3215	1/1	0.85	0.28	33,33,33,33	0
57	MG	YA	3219	1/1	0.85	0.30	46,46,46,46	0
57	MG	YA	3490	1/1	0.85	0.24	63,63,63,63	0
57	MG	YA	3367	1/1	0.85	0.41	70,70,70,70	0
57	MG	XA	1604	1/1	0.85	0.27	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3495	1/1	0.85	0.35	63,63,63,63	0
57	MG	RA	3420	1/1	0.85	0.24	49,49,49,49	0
57	MG	YA	3139	1/1	0.85	0.27	29,29,29,29	0
57	MG	RA	3287	1/1	0.85	0.13	30,30,30,30	0
57	MG	QA	1659	1/1	0.85	0.34	43,43,43,43	0
57	MG	YA	3245	1/1	0.85	0.23	40,40,40,40	0
57	MG	YA	3148	1/1	0.85	0.09	59,59,59,59	0
57	MG	QA	1671	1/1	0.85	0.24	49,49,49,49	0
57	MG	YA	3160	1/1	0.85	0.17	37,37,37,37	0
57	MG	YH	201	1/1	0.85	0.13	58,58,58,58	0
57	MG	RA	3346	1/1	0.85	0.14	38,38,38,38	0
57	MG	RA	3269	1/1	0.85	0.29	50,50,50,50	0
57	MG	YA	3285	1/1	0.85	0.11	52,52,52,52	0
57	MG	RA	3156	1/1	0.85	0.13	42,42,42,42	0
57	MG	RA	3231	1/1	0.86	0.19	41,41,41,41	0
57	MG	YA	3011	1/1	0.86	0.31	22,22,22,22	0
57	MG	RA	3232	1/1	0.86	0.23	53,53,53,53	0
57	MG	RA	3173	1/1	0.86	0.11	28,28,28,28	0
57	MG	YA	3397	1/1	0.86	0.27	62,62,62,62	0
57	MG	RA	3235	1/1	0.86	0.30	48,48,48,48	0
57	MG	RA	3242	1/1	0.86	0.19	40,40,40,40	0
57	MG	RA	3339	1/1	0.86	0.17	52,52,52,52	0
57	MG	RA	3342	1/1	0.86	0.24	52,52,52,52	0
57	MG	RA	3245	1/1	0.86	0.12	34,34,34,34	0
57	MG	QA	1632	1/1	0.86	0.34	58,58,58,58	0
57	MG	YA	3423	1/1	0.86	0.16	57,57,57,57	0
57	MG	RA	3434	1/1	0.86	0.15	46,46,46,46	0
57	MG	QA	1657	1/1	0.86	0.30	42,42,42,42	0
57	MG	RA	3347	1/1	0.86	0.23	65,65,65,65	0
57	MG	YA	3102	1/1	0.86	0.32	40,40,40,40	0
57	MG	RA	3353	1/1	0.86	0.19	46,46,46,46	0
57	MG	XA	1681	1/1	0.86	0.21	38,38,38,38	0
57	MG	XA	1687	1/1	0.86	0.19	55,55,55,55	0
57	MG	QA	1711	1/1	0.86	0.22	55,55,55,55	0
57	MG	QA	1605	1/1	0.86	0.24	36,36,36,36	0
57	MG	QA	1643	1/1	0.86	0.17	40,40,40,40	0
57	MG	YA	3474	1/1	0.86	0.17	37,37,37,37	0
57	MG	RA	3070	1/1	0.86	0.21	28,28,28,28	0
57	MG	YA	3291	1/1	0.86	0.17	54,54,54,54	0
57	MG	YA	3137	1/1	0.86	0.23	34,34,34,34	0
57	MG	YA	3300	1/1	0.86	0.37	51,51,51,51	0
57	MG	RA	3208	1/1	0.86	0.31	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1721	1/1	0.86	0.29	52,52,52,52	0
57	MG	QA	1693	1/1	0.86	0.34	63,63,63,63	0
57	MG	XA	1719	1/1	0.86	0.09	43,43,43,43	0
57	MG	RA	3152	1/1	0.86	0.28	43,43,43,43	0
57	MG	XA	1601	1/1	0.86	0.31	36,36,36,36	0
57	MG	YA	3164	1/1	0.86	0.15	50,50,50,50	0
57	MG	QA	1603	1/1	0.86	0.09	53,53,53,53	0
57	MG	QA	1667	1/1	0.86	0.18	43,43,43,43	0
57	MG	YA	3354	1/1	0.86	0.19	41,41,41,41	0
57	MG	XA	1752	1/1	0.86	0.13	56,56,56,56	0
57	MG	YA	3177	1/1	0.86	0.30	59,59,59,59	0
57	MG	RA	3163	1/1	0.86	0.30	55,55,55,55	0
57	MG	XA	1761	1/1	0.86	0.23	53,53,53,53	0
57	MG	YN	201	1/1	0.86	0.15	38,38,38,38	0
57	MG	RA	3378	1/1	0.86	0.16	49,49,49,49	0
57	MG	QA	1700	1/1	0.86	0.11	51,51,51,51	0
57	MG	YA	3380	1/1	0.86	0.35	54,54,54,54	0
57	MG	YA	3158	1/1	0.87	0.06	30,30,30,30	0
57	MG	RA	3124	1/1	0.87	0.16	40,40,40,40	0
57	MG	QA	1647	1/1	0.87	0.34	60,60,60,60	0
57	MG	XA	1615	1/1	0.87	0.21	38,38,38,38	0
57	MG	XA	1684	1/1	0.87	0.25	55,55,55,55	0
57	MG	RA	3431	1/1	0.87	0.28	53,53,53,53	0
57	MG	RA	3338	1/1	0.87	0.42	70,70,70,70	0
57	MG	YA	3447	1/1	0.87	0.21	44,44,44,44	0
57	MG	XA	1627	1/1	0.87	0.21	71,71,71,71	0
57	MG	QA	1708	1/1	0.87	0.33	60,60,60,60	0
57	MG	RA	3176	1/1	0.87	0.35	57,57,57,57	0
57	MG	QA	1651	1/1	0.87	0.22	39,39,39,39	0
57	MG	YA	3470	1/1	0.87	0.27	50,50,50,50	0
57	MG	QA	1638	1/1	0.87	0.20	48,48,48,48	0
57	MG	XA	1635	1/1	0.87	0.26	43,43,43,43	0
57	MG	XA	1709	1/1	0.87	0.35	54,54,54,54	0
57	MG	XA	1710	1/1	0.87	0.26	58,58,58,58	0
57	MG	XA	1712	1/1	0.87	0.26	61,61,61,61	0
57	MG	YA	3109	1/1	0.87	0.33	40,40,40,40	0
57	MG	YA	3361	1/1	0.87	0.16	48,48,48,48	0
57	MG	RA	3317	1/1	0.87	0.18	36,36,36,36	0
57	MG	RA	3318	1/1	0.87	0.22	51,51,51,51	0
57	MG	YA	3368	1/1	0.87	0.16	49,49,49,49	0
57	MG	XA	1730	1/1	0.87	0.25	49,49,49,49	0
57	MG	RA	3348	1/1	0.87	0.29	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3183	1/1	0.87	0.28	65,65,65,65	0
57	MG	XA	1648	1/1	0.87	0.21	55,55,55,55	0
57	MG	YA	3383	1/1	0.87	0.27	51,51,51,51	0
57	MG	YA	3237	1/1	0.87	0.28	54,54,54,54	0
57	MG	XA	1748	1/1	0.87	0.37	62,62,62,62	0
57	MG	YA	3391	1/1	0.87	0.26	49,49,49,49	0
57	MG	YB	206	1/1	0.87	0.10	49,49,49,49	0
57	MG	RA	3185	1/1	0.87	0.17	32,32,32,32	0
57	MG	RA	3091	1/1	0.87	0.09	24,24,24,24	0
57	MG	QA	1640	1/1	0.87	0.21	60,60,60,60	0
57	MG	YA	3274	1/1	0.87	0.30	48,48,48,48	0
57	MG	RA	3203	1/1	0.87	0.14	18,18,18,18	0
57	MG	YA	3282	1/1	0.87	0.17	31,31,31,31	0
57	MG	R5	103	1/1	0.87	0.09	40,40,40,40	0
57	MG	YA	3418	1/1	0.88	0.24	24,24,24,24	0
57	MG	RA	3254	1/1	0.88	0.13	47,47,47,47	0
57	MG	YA	3036	1/1	0.88	0.28	21,21,21,21	0
57	MG	RA	3256	1/1	0.88	0.44	67,67,67,67	0
57	MG	RA	3451	1/1	0.88	0.27	23,23,23,23	0
57	MG	XA	1637	1/1	0.88	0.22	57,57,57,57	0
57	MG	YA	3307	1/1	0.88	0.23	68,68,68,68	0
57	MG	XA	1705	1/1	0.88	0.35	47,47,47,47	0
57	MG	QA	1713	1/1	0.88	0.23	58,58,58,58	0
57	MG	YA	3324	1/1	0.88	0.25	53,53,53,53	0
57	MG	RA	3003	1/1	0.88	0.21	22,22,22,22	0
57	MG	YA	3452	1/1	0.88	0.20	49,49,49,49	0
57	MG	YA	3097	1/1	0.88	0.08	20,20,20,20	0
57	MG	XA	1642	1/1	0.88	0.20	61,61,61,61	0
57	MG	RA	3397	1/1	0.88	0.35	52,52,52,52	0
57	MG	QA	1714	1/1	0.88	0.30	46,46,46,46	0
57	MG	QA	1610	1/1	0.88	0.20	76,76,76,76	0
57	MG	R0	102	1/1	0.88	0.46	57,57,57,57	0
57	MG	XA	1736	1/1	0.88	0.19	56,56,56,56	0
57	MG	YA	3476	1/1	0.88	0.13	53,53,53,53	0
57	MG	QA	1668	1/1	0.88	0.17	44,44,44,44	0
57	MG	QA	1738	1/1	0.88	0.09	43,43,43,43	0
57	MG	RA	3417	1/1	0.88	0.24	53,53,53,53	0
57	MG	RA	3146	1/1	0.88	0.19	37,37,37,37	0
57	MG	RA	3285	1/1	0.88	0.15	35,35,35,35	0
57	MG	YA	3372	1/1	0.88	0.22	55,55,55,55	0
57	MG	YA	3135	1/1	0.88	0.19	31,31,31,31	0
57	MG	XA	1759	1/1	0.88	0.39	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3246	1/1	0.88	0.21	38,38,38,38	0
57	MG	YA	3248	1/1	0.88	0.34	61,61,61,61	0
57	MG	XA	1760	1/1	0.88	0.17	77,77,77,77	0
57	MG	YA	3263	1/1	0.88	0.27	44,44,44,44	0
57	MG	RA	3046	1/1	0.88	0.21	16,16,16,16	0
57	MG	RA	3048	1/1	0.88	0.23	13,13,13,13	0
57	MG	XA	1686	1/1	0.88	0.17	39,39,39,39	0
57	MG	RA	3437	1/1	0.88	0.14	52,52,52,52	0
57	MG	YA	3157	1/1	0.88	0.18	34,34,34,34	0
57	MG	RA	3302	1/1	0.88	0.32	59,59,59,59	0
57	MG	RA	3307	1/1	0.88	0.38	64,64,64,64	0
57	MG	YA	3406	1/1	0.88	0.20	49,49,49,49	0
57	MG	QA	1741	1/1	0.88	0.19	46,46,46,46	0
57	MG	YA	3411	1/1	0.88	0.20	67,67,67,67	0
57	MG	Y5	102	1/1	0.88	0.20	50,50,50,50	0
57	MG	RA	3312	1/1	0.89	0.34	47,47,47,47	0
57	MG	RA	3314	1/1	0.89	0.42	62,62,62,62	0
57	MG	YA	3336	1/1	0.89	0.15	52,52,52,52	0
57	MG	YA	3340	1/1	0.89	0.33	54,54,54,54	0
57	MG	QA	1729	1/1	0.89	0.14	30,30,30,30	0
57	MG	QA	1732	1/1	0.89	0.24	44,44,44,44	0
57	MG	RA	3384	1/1	0.89	0.12	28,28,28,28	0
57	MG	XA	1608	1/1	0.89	0.36	47,47,47,47	0
57	MG	XA	1721	1/1	0.89	0.10	32,32,32,32	0
57	MG	YA	3356	1/1	0.89	0.30	54,54,54,54	0
57	MG	XA	1722	1/1	0.89	0.14	42,42,42,42	0
57	MG	XA	1726	1/1	0.89	0.27	54,54,54,54	0
57	MG	YA	3155	1/1	0.89	0.25	44,44,44,44	0
57	MG	YA	3366	1/1	0.89	0.30	57,57,57,57	0
57	MG	YA	3156	1/1	0.89	0.17	29,29,29,29	0
57	MG	RA	3321	1/1	0.89	0.12	53,53,53,53	0
57	MG	RA	3128	1/1	0.89	0.07	35,35,35,35	0
57	MG	RA	3133	1/1	0.89	0.34	59,59,59,59	0
57	MG	RA	3084	1/1	0.89	0.25	33,33,33,33	0
57	MG	YA	3168	1/1	0.89	0.19	31,31,31,31	0
57	MG	RA	3187	1/1	0.89	0.30	55,55,55,55	0
57	MG	YA	3382	1/1	0.89	0.20	55,55,55,55	0
57	MG	XA	1743	1/1	0.89	0.18	56,56,56,56	0
57	MG	RA	3398	1/1	0.89	0.08	24,24,24,24	0
57	MG	QA	1719	1/1	0.89	0.25	60,60,60,60	0
57	MG	XA	1751	1/1	0.89	0.15	46,46,46,46	0
57	MG	RA	3408	1/1	0.89	0.14	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3141	1/1	0.89	0.09	34,34,34,34	0
57	MG	QA	1710	1/1	0.89	0.27	50,50,50,50	0
57	MG	QA	1666	1/1	0.89	0.26	42,42,42,42	0
57	MG	QV	101	1/1	0.89	0.12	15,15,15,15	0
57	MG	RA	3153	1/1	0.89	0.11	23,23,23,23	0
57	MG	XA	1641	1/1	0.89	0.14	51,51,51,51	0
57	MG	XK	201	1/1	0.89	0.21	37,37,37,37	0
57	MG	YA	3207	1/1	0.89	0.14	20,20,20,20	0
57	MG	YA	3414	1/1	0.89	0.34	60,60,60,60	0
57	MG	YA	3212	1/1	0.89	0.15	28,28,28,28	0
57	MG	XN	102	1/1	0.89	0.13	52,52,52,52	0
57	MG	YA	3216	1/1	0.89	0.21	30,30,30,30	0
57	MG	RA	3426	1/1	0.89	0.27	56,56,56,56	0
57	MG	YA	3220	1/1	0.89	0.29	39,39,39,39	0
57	MG	XA	1644	1/1	0.89	0.28	40,40,40,40	0
57	MG	YA	3227	1/1	0.89	0.18	51,51,51,51	0
57	MG	YA	3439	1/1	0.89	0.19	42,42,42,42	0
57	MG	RA	3155	1/1	0.89	0.17	30,30,30,30	0
57	MG	YA	3022	1/1	0.89	0.30	72,72,72,72	0
57	MG	YA	3025	1/1	0.89	0.32	34,34,34,34	0
57	MG	RA	3096	1/1	0.89	0.16	45,45,45,45	0
57	MG	QA	1622	1/1	0.89	0.31	50,50,50,50	0
57	MG	QA	1684	1/1	0.89	0.18	54,54,54,54	0
57	MG	YA	3038	1/1	0.89	0.27	45,45,45,45	0
57	MG	YA	3460	1/1	0.89	0.12	37,37,37,37	0
57	MG	YA	3461	1/1	0.89	0.11	39,39,39,39	0
57	MG	YA	3467	1/1	0.89	0.10	43,43,43,43	0
57	MG	YA	3247	1/1	0.89	0.26	47,47,47,47	0
57	MG	RA	3282	1/1	0.89	0.15	36,36,36,36	0
57	MG	RA	3164	1/1	0.89	0.20	41,41,41,41	0
57	MG	YA	3257	1/1	0.89	0.17	29,29,29,29	0
57	MG	YA	3258	1/1	0.89	0.36	58,58,58,58	0
57	MG	YA	3058	1/1	0.89	0.27	55,55,55,55	0
57	MG	RA	3354	1/1	0.89	0.15	65,65,65,65	0
57	MG	YA	3080	1/1	0.89	0.30	21,21,21,21	0
57	MG	YA	3269	1/1	0.89	0.25	60,60,60,60	0
57	MG	QA	1624	1/1	0.89	0.18	36,36,36,36	0
57	MG	YA	3280	1/1	0.89	0.25	41,41,41,41	0
57	MG	RA	3113	1/1	0.89	0.16	32,32,32,32	0
57	MG	RA	3450	1/1	0.89	0.18	25,25,25,25	0
57	MG	RA	3301	1/1	0.89	0.17	34,34,34,34	0
57	MG	XA	1685	1/1	0.89	0.36	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3227	1/1	0.89	0.12	42,42,42,42	0
57	MG	RE	302	1/1	0.89	0.19	15,15,15,15	0
57	MG	RA	3303	1/1	0.89	0.06	42,42,42,42	0
57	MG	YA	3108	1/1	0.89	0.16	25,25,25,25	0
57	MG	RA	3306	1/1	0.89	0.20	39,39,39,39	0
57	MG	RA	3229	1/1	0.89	0.11	30,30,30,30	0
57	MG	YA	3303	1/1	0.89	0.15	41,41,41,41	0
57	MG	RR	201	1/1	0.89	0.26	33,33,33,33	0
57	MG	YA	3125	1/1	0.89	0.13	22,22,22,22	0
57	MG	YA	3310	1/1	0.89	0.36	54,54,54,54	0
57	MG	YA	3311	1/1	0.89	0.47	77,77,77,77	0
57	MG	YQ	201	1/1	0.89	0.23	54,54,54,54	0
57	MG	RY	201	1/1	0.89	0.15	37,37,37,37	0
57	MG	YA	3316	1/1	0.89	0.13	42,42,42,42	0
57	MG	YW	201	1/1	0.89	0.11	32,32,32,32	0
57	MG	RA	3175	1/1	0.89	0.09	31,31,31,31	0
57	MG	RA	3291	1/1	0.90	0.33	48,48,48,48	0
57	MG	YA	3012	1/1	0.90	0.21	19,19,19,19	0
57	MG	RA	3344	1/1	0.90	0.17	47,47,47,47	0
57	MG	YA	3408	1/1	0.90	0.16	47,47,47,47	0
57	MG	XA	1692	1/1	0.90	0.09	36,36,36,36	0
57	MG	RA	3412	1/1	0.90	0.13	41,41,41,41	0
57	MG	YA	3286	1/1	0.90	0.41	56,56,56,56	0
57	MG	QA	1604	1/1	0.90	0.21	33,33,33,33	0
57	MG	YA	3031	1/1	0.90	0.21	19,19,19,19	0
57	MG	YA	3289	1/1	0.90	0.09	38,38,38,38	0
57	MG	YA	3170	1/1	0.90	0.21	38,38,38,38	0
57	MG	XA	1619	1/1	0.90	0.32	28,28,28,28	0
57	MG	YA	3295	1/1	0.90	0.22	39,39,39,39	0
57	MG	YA	3434	1/1	0.90	0.29	45,45,45,45	0
57	MG	RA	3116	1/1	0.90	0.24	20,20,20,20	0
57	MG	YA	3037	1/1	0.90	0.19	27,27,27,27	0
57	MG	QA	1623	1/1	0.90	0.32	34,34,34,34	0
57	MG	YA	3441	1/1	0.90	0.12	35,35,35,35	0
57	MG	YA	3444	1/1	0.90	0.23	48,48,48,48	0
57	MG	RA	3120	1/1	0.90	0.17	42,42,42,42	0
57	MG	RA	3304	1/1	0.90	0.12	45,45,45,45	0
57	MG	YA	3048	1/1	0.90	0.17	33,33,33,33	0
57	MG	QA	1650	1/1	0.90	0.29	36,36,36,36	0
57	MG	RA	3125	1/1	0.90	0.14	23,23,23,23	0
57	MG	RA	3250	1/1	0.90	0.25	56,56,56,56	0
57	MG	RA	3165	1/1	0.90	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3325	1/1	0.90	0.30	51,51,51,51	0
57	MG	RA	3435	1/1	0.90	0.20	57,57,57,57	0
57	MG	YA	3468	1/1	0.90	0.12	41,41,41,41	0
57	MG	YA	3204	1/1	0.90	0.36	68,68,68,68	0
57	MG	QA	1674	1/1	0.90	0.23	54,54,54,54	0
57	MG	YA	3095	1/1	0.90	0.09	42,42,42,42	0
57	MG	QA	1641	1/1	0.90	0.19	33,33,33,33	0
57	MG	RA	3262	1/1	0.90	0.19	40,40,40,40	0
57	MG	QA	1601	1/1	0.90	0.31	39,39,39,39	0
57	MG	YA	3350	1/1	0.90	0.29	55,55,55,55	0
57	MG	RA	3267	1/1	0.90	0.23	41,41,41,41	0
57	MG	YA	3221	1/1	0.90	0.25	32,32,32,32	0
57	MG	RA	3370	1/1	0.90	0.10	65,65,65,65	0
57	MG	QA	1696	1/1	0.90	0.25	58,58,58,58	0
57	MG	RA	3177	1/1	0.90	0.21	44,44,44,44	0
57	MG	XA	1651	1/1	0.90	0.17	32,32,32,32	0
57	MG	YA	3231	1/1	0.90	0.24	35,35,35,35	0
57	MG	RA	3224	1/1	0.90	0.15	31,31,31,31	0
57	MG	YA	3233	1/1	0.90	0.28	38,38,38,38	0
57	MG	RA	3329	1/1	0.90	0.34	65,65,65,65	0
57	MG	RA	3383	1/1	0.90	0.09	75,75,75,75	0
57	MG	RA	3078	1/1	0.90	0.25	22,22,22,22	0
57	MG	XA	1758	1/1	0.90	0.19	46,46,46,46	0
57	MG	YB	205	1/1	0.90	0.21	52,52,52,52	0
57	MG	RA	3107	1/1	0.90	0.25	26,26,26,26	0
57	MG	RA	3108	1/1	0.90	0.40	56,56,56,56	0
57	MG	YG	201	1/1	0.90	0.14	51,51,51,51	0
57	MG	RA	3337	1/1	0.90	0.18	40,40,40,40	0
57	MG	XA	1762	1/1	0.90	0.10	33,33,33,33	0
57	MG	RA	3150	1/1	0.90	0.17	40,40,40,40	0
57	MG	XA	1682	1/1	0.90	0.16	42,42,42,42	0
57	MG	QE	201	1/1	0.90	0.10	42,42,42,42	0
57	MG	RA	3290	1/1	0.90	0.11	52,52,52,52	0
57	MG	YA	3395	1/1	0.90	0.09	37,37,37,37	0
57	MG	YV	201	1/1	0.90	0.10	17,17,17,17	0
57	MG	YA	3153	1/1	0.90	0.28	41,41,41,41	0
57	MG	RA	3399	1/1	0.90	0.11	40,40,40,40	0
57	MG	YA	3358	1/1	0.91	0.11	35,35,35,35	0
57	MG	YA	3175	1/1	0.91	0.11	27,27,27,27	0
57	MG	QD	303	1/1	0.91	0.07	48,48,48,48	0
57	MG	RA	3104	1/1	0.91	0.23	28,28,28,28	0
57	MG	YA	3364	1/1	0.91	0.08	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3212	1/1	0.91	0.26	30,30,30,30	0
57	MG	YA	3181	1/1	0.91	0.20	50,50,50,50	0
57	MG	RA	3351	1/1	0.91	0.25	58,58,58,58	0
57	MG	YA	3369	1/1	0.91	0.22	49,49,49,49	0
57	MG	XS	300	1/1	0.91	0.19	46,46,46,46	0
57	MG	XV	101	1/1	0.91	0.19	23,23,23,23	0
57	MG	YA	3374	1/1	0.91	0.24	57,57,57,57	0
57	MG	YA	3187	1/1	0.91	0.31	64,64,64,64	0
57	MG	XV	104	1/1	0.91	0.08	15,15,15,15	0
57	MG	RA	3436	1/1	0.91	0.18	51,51,51,51	0
57	MG	RA	3213	1/1	0.91	0.17	13,13,13,13	0
57	MG	QA	1702	1/1	0.91	0.17	54,54,54,54	0
57	MG	XA	1661	1/1	0.91	0.26	43,43,43,43	0
57	MG	YA	3019	1/1	0.91	0.18	21,21,21,21	0
57	MG	RA	3441	1/1	0.91	0.35	59,59,59,59	0
57	MG	XA	1666	1/1	0.91	0.23	52,52,52,52	0
57	MG	XA	1669	1/1	0.91	0.26	48,48,48,48	0
57	MG	RA	3049	1/1	0.91	0.15	23,23,23,23	0
57	MG	YA	3218	1/1	0.91	0.27	40,40,40,40	0
57	MG	RA	3059	1/1	0.91	0.16	27,27,27,27	0
57	MG	RA	3062	1/1	0.91	0.29	30,30,30,30	0
57	MG	RA	3298	1/1	0.91	0.28	62,62,62,62	0
57	MG	RA	3220	1/1	0.91	0.27	53,53,53,53	0
57	MG	RA	3221	1/1	0.91	0.24	43,43,43,43	0
57	MG	YA	3409	1/1	0.91	0.28	47,47,47,47	0
57	MG	YA	3044	1/1	0.91	0.32	28,28,28,28	0
57	MG	RB	202	1/1	0.91	0.32	33,33,33,33	0
57	MG	YA	3413	1/1	0.91	0.35	53,53,53,53	0
57	MG	YA	3230	1/1	0.91	0.37	56,56,56,56	0
57	MG	YA	3417	1/1	0.91	0.13	55,55,55,55	0
57	MG	RA	3064	1/1	0.91	0.19	26,26,26,26	0
57	MG	RA	3367	1/1	0.91	0.22	31,31,31,31	0
57	MG	YA	3065	1/1	0.91	0.13	16,16,16,16	0
57	MG	RA	3066	1/1	0.91	0.17	35,35,35,35	0
57	MG	XA	1691	1/1	0.91	0.18	46,46,46,46	0
57	MG	RP	201	1/1	0.91	0.09	31,31,31,31	0
57	MG	YA	3429	1/1	0.91	0.10	14,14,14,14	0
57	MG	YA	3430	1/1	0.91	0.11	43,43,43,43	0
57	MG	YA	3086	1/1	0.91	0.15	23,23,23,23	0
57	MG	YA	3088	1/1	0.91	0.17	21,21,21,21	0
57	MG	RA	3171	1/1	0.91	0.46	69,69,69,69	0
57	MG	YA	3253	1/1	0.91	0.23	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3254	1/1	0.91	0.15	19,19,19,19	0
57	MG	RA	3172	1/1	0.91	0.29	47,47,47,47	0
57	MG	YA	3446	1/1	0.91	0.13	37,37,37,37	0
57	MG	QA	1653	1/1	0.91	0.29	50,50,50,50	0
57	MG	RV	201	1/1	0.91	0.13	14,14,14,14	0
57	MG	XA	1700	1/1	0.91	0.29	47,47,47,47	0
57	MG	QA	1687	1/1	0.91	0.23	52,52,52,52	0
57	MG	YA	3267	1/1	0.91	0.20	43,43,43,43	0
57	MG	YA	3101	1/1	0.91	0.34	35,35,35,35	0
57	MG	QV	103	1/1	0.91	0.19	52,52,52,52	0
57	MG	QA	1730	1/1	0.91	0.18	69,69,69,69	0
57	MG	YA	3277	1/1	0.91	0.20	44,44,44,44	0
57	MG	YA	3105	1/1	0.91	0.25	56,56,56,56	0
57	MG	RA	3126	1/1	0.91	0.15	34,34,34,34	0
57	MG	R5	102	1/1	0.91	0.14	40,40,40,40	0
57	MG	YA	3110	1/1	0.91	0.20	42,42,42,42	0
57	MG	RA	3243	1/1	0.91	0.26	48,48,48,48	0
57	MG	XA	1716	1/1	0.91	0.17	51,51,51,51	0
57	MG	RA	3244	1/1	0.91	0.24	33,33,33,33	0
57	MG	QA	1731	1/1	0.91	0.18	45,45,45,45	0
57	MG	QA	1718	1/1	0.91	0.38	51,51,51,51	0
57	MG	XA	1724	1/1	0.91	0.31	54,54,54,54	0
57	MG	YA	3480	1/1	0.91	0.16	50,50,50,50	0
57	MG	YA	3292	1/1	0.91	0.09	32,32,32,32	0
57	MG	XA	1612	1/1	0.91	0.22	43,43,43,43	0
57	MG	XA	1727	1/1	0.91	0.21	51,51,51,51	0
57	MG	RA	3005	1/1	0.91	0.24	21,21,21,21	0
57	MG	RA	3087	1/1	0.91	0.15	31,31,31,31	0
57	MG	YA	3140	1/1	0.91	0.09	32,32,32,32	0
57	MG	YA	3142	1/1	0.91	0.28	65,65,65,65	0
57	MG	RA	3188	1/1	0.91	0.29	58,58,58,58	0
57	MG	YA	3145	1/1	0.91	0.16	50,50,50,50	0
57	MG	RA	3189	1/1	0.91	0.21	18,18,18,18	0
57	MG	RA	3402	1/1	0.91	0.16	36,36,36,36	0
57	MG	RA	3406	1/1	0.91	0.30	50,50,50,50	0
57	MG	XA	1745	1/1	0.91	0.09	36,36,36,36	0
57	MG	YA	3154	1/1	0.91	0.18	24,24,24,24	0
57	MG	RA	3407	1/1	0.91	0.40	60,60,60,60	0
57	MG	QA	1723	1/1	0.91	0.32	74,74,74,74	0
57	MG	RA	3019	1/1	0.91	0.20	20,20,20,20	0
57	MG	RA	3202	1/1	0.91	0.15	49,49,49,49	0
57	MG	QA	1747	1/1	0.91	0.25	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3268	1/1	0.91	0.14	42,42,42,42	0
57	MG	YA	3166	1/1	0.91	0.28	41,41,41,41	0
57	MG	RA	3148	1/1	0.91	0.12	19,19,19,19	0
57	MG	QA	1724	1/1	0.91	0.42	63,63,63,63	0
57	MG	RA	3425	1/1	0.91	0.20	46,46,46,46	0
57	MG	QD	302	1/1	0.91	0.18	67,67,67,67	0
57	MG	Y7	101	1/1	0.91	0.21	55,55,55,55	0
57	MG	YA	3353	1/1	0.92	0.22	53,53,53,53	0
57	MG	XA	1647	1/1	0.92	0.11	45,45,45,45	0
57	MG	RA	3275	1/1	0.92	0.36	51,51,51,51	0
57	MG	QA	1608	1/1	0.92	0.34	39,39,39,39	0
57	MG	RA	3057	1/1	0.92	0.27	13,13,13,13	0
57	MG	RA	3349	1/1	0.92	0.05	41,41,41,41	0
57	MG	QA	1680	1/1	0.92	0.31	58,58,58,58	0
57	MG	YA	3004	1/1	0.92	0.21	13,13,13,13	0
57	MG	YA	3365	1/1	0.92	0.14	39,39,39,39	0
57	MG	YA	3005	1/1	0.92	0.32	24,24,24,24	0
57	MG	QV	104	1/1	0.92	0.23	56,56,56,56	0
57	MG	QA	1681	1/1	0.92	0.20	68,68,68,68	0
57	MG	XA	1665	1/1	0.92	0.20	29,29,29,29	0
57	MG	RA	3286	1/1	0.92	0.23	43,43,43,43	0
57	MG	RA	3065	1/1	0.92	0.31	31,31,31,31	0
57	MG	YA	3373	1/1	0.92	0.39	61,61,61,61	0
57	MG	RA	3447	1/1	0.92	0.12	32,32,32,32	0
57	MG	YA	3197	1/1	0.92	0.27	38,38,38,38	0
57	MG	RA	3170	1/1	0.92	0.16	47,47,47,47	0
57	MG	QA	1715	1/1	0.92	0.18	33,33,33,33	0
57	MG	RA	3292	1/1	0.92	0.36	67,67,67,67	0
57	MG	QA	1744	1/1	0.92	0.13	54,54,54,54	0
57	MG	XA	1683	1/1	0.92	0.12	38,38,38,38	0
57	MG	YA	3209	1/1	0.92	0.10	14,14,14,14	0
57	MG	QA	1613	1/1	0.92	0.25	53,53,53,53	0
57	MG	RA	3228	1/1	0.92	0.22	27,27,27,27	0
57	MG	RD	302	1/1	0.92	0.20	29,29,29,29	0
57	MG	YA	3217	1/1	0.92	0.09	35,35,35,35	0
57	MG	YA	3045	1/1	0.92	0.20	11,11,11,11	0
57	MG	YA	3046	1/1	0.92	0.14	14,14,14,14	0
57	MG	YA	3400	1/1	0.92	0.18	42,42,42,42	0
57	MG	RA	3122	1/1	0.92	0.26	29,29,29,29	0
57	MG	RA	3230	1/1	0.92	0.27	42,42,42,42	0
57	MG	QA	1646	1/1	0.92	0.16	52,52,52,52	0
57	MG	YA	3061	1/1	0.92	0.30	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3017	1/1	0.92	0.13	16,16,16,16	0
57	MG	RA	3018	1/1	0.92	0.33	20,20,20,20	0
57	MG	YA	3070	1/1	0.92	0.30	28,28,28,28	0
57	MG	XA	1694	1/1	0.92	0.11	43,43,43,43	0
57	MG	YA	3081	1/1	0.92	0.24	19,19,19,19	0
57	MG	XA	1696	1/1	0.92	0.18	53,53,53,53	0
57	MG	YA	3235	1/1	0.92	0.30	51,51,51,51	0
57	MG	RA	3308	1/1	0.92	0.25	53,53,53,53	0
57	MG	RA	3379	1/1	0.92	0.17	36,36,36,36	0
57	MG	YA	3241	1/1	0.92	0.28	29,29,29,29	0
57	MG	QA	1748	1/1	0.92	0.13	46,46,46,46	0
57	MG	RA	3239	1/1	0.92	0.21	60,60,60,60	0
57	MG	XA	1702	1/1	0.92	0.44	69,69,69,69	0
57	MG	R0	101	1/1	0.92	0.12	16,16,16,16	0
57	MG	YA	3249	1/1	0.92	0.08	42,42,42,42	0
57	MG	RA	3021	1/1	0.92	0.27	33,33,33,33	0
57	MG	RA	3315	1/1	0.92	0.08	27,27,27,27	0
57	MG	RA	3391	1/1	0.92	0.08	24,24,24,24	0
57	MG	RA	3086	1/1	0.92	0.13	27,27,27,27	0
57	MG	YA	3443	1/1	0.92	0.08	43,43,43,43	0
57	MG	YA	3103	1/1	0.92	0.21	25,25,25,25	0
57	MG	RA	3135	1/1	0.92	0.22	44,44,44,44	0
57	MG	XA	1603	1/1	0.92	0.17	29,29,29,29	0
57	MG	QA	1614	1/1	0.92	0.10	39,39,39,39	0
57	MG	RA	3037	1/1	0.92	0.26	10,10,10,10	0
57	MG	RA	3248	1/1	0.92	0.19	33,33,33,33	0
57	MG	YA	3111	1/1	0.92	0.27	57,57,57,57	0
57	MG	YA	3276	1/1	0.92	0.26	43,43,43,43	0
57	MG	YA	3459	1/1	0.92	0.09	24,24,24,24	0
57	MG	YA	3117	1/1	0.92	0.23	34,34,34,34	0
57	MG	YA	3278	1/1	0.92	0.27	55,55,55,55	0
57	MG	XA	1723	1/1	0.92	0.21	55,55,55,55	0
57	MG	YA	3119	1/1	0.92	0.19	32,32,32,32	0
57	MG	RA	3142	1/1	0.92	0.15	28,28,28,28	0
57	MG	RA	3143	1/1	0.92	0.29	61,61,61,61	0
57	MG	YA	3284	1/1	0.92	0.25	54,54,54,54	0
57	MG	XA	1620	1/1	0.92	0.05	27,27,27,27	0
57	MG	XA	1621	1/1	0.92	0.27	46,46,46,46	0
57	MG	YA	3132	1/1	0.92	0.11	29,29,29,29	0
57	MG	RA	3040	1/1	0.92	0.16	18,18,18,18	0
57	MG	QA	1676	1/1	0.92	0.13	46,46,46,46	0
57	MG	RA	3204	1/1	0.92	0.36	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3136	1/1	0.92	0.18	33,33,33,33	0
57	MG	YA	3481	1/1	0.92	0.33	53,53,53,53	0
57	MG	YA	3485	1/1	0.92	0.21	52,52,52,52	0
57	MG	YA	3488	1/1	0.92	0.18	53,53,53,53	0
57	MG	YA	3489	1/1	0.92	0.23	59,59,59,59	0
57	MG	QA	1706	1/1	0.92	0.22	47,47,47,47	0
57	MG	XA	1742	1/1	0.92	0.28	50,50,50,50	0
57	MG	YA	3298	1/1	0.92	0.30	52,52,52,52	0
57	MG	RA	3335	1/1	0.92	0.23	43,43,43,43	0
57	MG	YA	3497	1/1	0.92	0.12	55,55,55,55	0
57	MG	RA	3263	1/1	0.92	0.33	42,42,42,42	0
57	MG	XA	1746	1/1	0.92	0.18	46,46,46,46	0
57	MG	QA	1691	1/1	0.92	0.15	38,38,38,38	0
57	MG	RA	3416	1/1	0.92	0.21	44,44,44,44	0
57	MG	RA	3099	1/1	0.92	0.07	13,13,13,13	0
57	MG	RA	3418	1/1	0.92	0.07	43,43,43,43	0
57	MG	YA	3151	1/1	0.92	0.14	28,28,28,28	0
57	MG	XA	1755	1/1	0.92	0.15	58,58,58,58	0
57	MG	YA	3320	1/1	0.92	0.26	48,48,48,48	0
57	MG	YD	301	1/1	0.92	0.20	26,26,26,26	0
57	MG	XA	1756	1/1	0.92	0.07	45,45,45,45	0
57	MG	QA	1648	1/1	0.92	0.14	56,56,56,56	0
57	MG	YA	3332	1/1	0.92	0.21	42,42,42,42	0
57	MG	RA	3154	1/1	0.92	0.28	42,42,42,42	0
57	MG	XA	1640	1/1	0.92	0.26	36,36,36,36	0
57	MG	RA	3272	1/1	0.92	0.15	26,26,26,26	0
57	MG	RA	3429	1/1	0.92	0.10	66,66,66,66	0
57	MG	YA	3342	1/1	0.92	0.15	27,27,27,27	0
57	MG	YA	3161	1/1	0.92	0.24	29,29,29,29	0
57	MG	YA	3163	1/1	0.92	0.18	25,25,25,25	0
57	MG	RA	3103	1/1	0.92	0.33	52,52,52,52	0
57	MG	XA	1645	1/1	0.92	0.19	37,37,37,37	0
57	MG	RA	3432	1/1	0.92	0.06	39,39,39,39	0
58	ZN	XD	301	1/1	0.92	0.28	60,60,60,60	0
57	MG	XA	1643	1/1	0.93	0.20	35,35,35,35	0
57	MG	QA	1705	1/1	0.93	0.18	30,30,30,30	0
57	MG	RA	3020	1/1	0.93	0.26	24,24,24,24	0
57	MG	RA	3310	1/1	0.93	0.16	52,52,52,52	0
57	MG	YA	3381	1/1	0.93	0.28	54,54,54,54	0
57	MG	YA	3234	1/1	0.93	0.34	50,50,50,50	0
57	MG	RA	3105	1/1	0.93	0.26	33,33,33,33	0
57	MG	YA	3385	1/1	0.93	0.23	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1679	1/1	0.93	0.13	37,37,37,37	0
57	MG	XA	1750	1/1	0.93	0.13	44,44,44,44	0
57	MG	YA	3390	1/1	0.93	0.21	45,45,45,45	0
57	MG	XA	1650	1/1	0.93	0.28	23,23,23,23	0
57	MG	RA	3067	1/1	0.93	0.22	32,32,32,32	0
57	MG	YA	3123	1/1	0.93	0.22	30,30,30,30	0
57	MG	YA	3124	1/1	0.93	0.22	27,27,27,27	0
57	MG	RB	201	1/1	0.93	0.25	32,32,32,32	0
57	MG	RA	3025	1/1	0.93	0.13	19,19,19,19	0
57	MG	RB	204	1/1	0.93	0.11	47,47,47,47	0
57	MG	XA	1660	1/1	0.93	0.18	38,38,38,38	0
57	MG	RA	3259	1/1	0.93	0.28	51,51,51,51	0
57	MG	YA	3405	1/1	0.93	0.21	57,57,57,57	0
57	MG	RA	3110	1/1	0.93	0.42	33,33,33,33	0
57	MG	RE	301	1/1	0.93	0.23	41,41,41,41	0
57	MG	QA	1645	1/1	0.93	0.06	44,44,44,44	0
57	MG	YA	3264	1/1	0.93	0.08	29,29,29,29	0
57	MG	RA	3071	1/1	0.93	0.19	12,12,12,12	0
57	MG	YA	3412	1/1	0.93	0.18	25,25,25,25	0
57	MG	RA	3158	1/1	0.93	0.30	57,57,57,57	0
57	MG	XA	1671	1/1	0.93	0.14	41,41,41,41	0
57	MG	RA	3327	1/1	0.93	0.36	67,67,67,67	0
57	MG	XA	1676	1/1	0.93	0.20	33,33,33,33	0
57	MG	YA	3275	1/1	0.93	0.38	59,59,59,59	0
57	MG	XA	1677	1/1	0.93	0.20	65,65,65,65	0
57	MG	RA	3266	1/1	0.93	0.16	37,37,37,37	0
57	MG	QA	1607	1/1	0.93	0.15	15,15,15,15	0
57	MG	YA	3427	1/1	0.93	0.09	29,29,29,29	0
57	MG	YA	3279	1/1	0.93	0.21	20,20,20,20	0
57	MG	RA	3038	1/1	0.93	0.23	23,23,23,23	0
57	MG	RA	3119	1/1	0.93	0.22	23,23,23,23	0
57	MG	QA	1733	1/1	0.93	0.08	42,42,42,42	0
57	MG	RA	3082	1/1	0.93	0.22	5,5,5,5	0
57	MG	RA	3403	1/1	0.93	0.13	54,54,54,54	0
57	MG	RA	3404	1/1	0.93	0.26	46,46,46,46	0
57	MG	YA	3021	1/1	0.93	0.33	33,33,33,33	0
57	MG	RA	3336	1/1	0.93	0.13	33,33,33,33	0
57	MG	QA	1602	1/1	0.93	0.33	33,33,33,33	0
57	MG	YA	3445	1/1	0.93	0.20	38,38,38,38	0
57	MG	QA	1619	1/1	0.93	0.28	31,31,31,31	0
57	MG	YA	3162	1/1	0.93	0.35	46,46,46,46	0
57	MG	RA	3410	1/1	0.93	0.15	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3450	1/1	0.93	0.19	50,50,50,50	0
57	MG	YA	3293	1/1	0.93	0.18	33,33,33,33	0
57	MG	RA	3044	1/1	0.93	0.24	27,27,27,27	0
57	MG	YA	3455	1/1	0.93	0.17	52,52,52,52	0
57	MG	RA	3279	1/1	0.93	0.19	29,29,29,29	0
57	MG	YA	3167	1/1	0.93	0.12	43,43,43,43	0
57	MG	XA	1609	1/1	0.93	0.11	67,67,67,67	0
57	MG	XA	1611	1/1	0.93	0.20	43,43,43,43	0
57	MG	RA	3127	1/1	0.93	0.38	60,60,60,60	0
57	MG	YA	3304	1/1	0.93	0.27	47,47,47,47	0
57	MG	RA	3045	1/1	0.93	0.24	19,19,19,19	0
57	MG	XA	1616	1/1	0.93	0.27	46,46,46,46	0
57	MG	QA	1658	1/1	0.93	0.26	34,34,34,34	0
57	MG	RA	3008	1/1	0.93	0.34	34,34,34,34	0
57	MG	RA	3180	1/1	0.93	0.27	23,23,23,23	0
57	MG	YA	3314	1/1	0.93	0.28	49,49,49,49	0
57	MG	YA	3053	1/1	0.93	0.25	24,24,24,24	0
57	MG	XA	1708	1/1	0.93	0.17	39,39,39,39	0
57	MG	YA	3321	1/1	0.93	0.18	67,67,67,67	0
57	MG	YA	3322	1/1	0.93	0.29	48,48,48,48	0
57	MG	YA	3323	1/1	0.93	0.21	42,42,42,42	0
57	MG	XA	1623	1/1	0.93	0.18	36,36,36,36	0
57	MG	YA	3482	1/1	0.93	0.24	54,54,54,54	0
57	MG	YA	3484	1/1	0.93	0.29	47,47,47,47	0
57	MG	RA	3012	1/1	0.93	0.27	11,11,11,11	0
57	MG	YA	3326	1/1	0.93	0.29	46,46,46,46	0
57	MG	YA	3328	1/1	0.93	0.20	47,47,47,47	0
57	MG	RA	3424	1/1	0.93	0.23	54,54,54,54	0
57	MG	YA	3189	1/1	0.93	0.22	52,52,52,52	0
57	MG	QA	1625	1/1	0.93	0.15	47,47,47,47	0
57	MG	YA	3071	1/1	0.93	0.16	33,33,33,33	0
57	MG	YA	3496	1/1	0.93	0.14	55,55,55,55	0
57	MG	YA	3076	1/1	0.93	0.20	27,27,27,27	0
57	MG	YA	3079	1/1	0.93	0.24	31,31,31,31	0
57	MG	RA	3350	1/1	0.93	0.23	54,54,54,54	0
57	MG	YA	3347	1/1	0.93	0.25	40,40,40,40	0
57	MG	YA	3200	1/1	0.93	0.11	32,32,32,32	0
57	MG	RA	3184	1/1	0.93	0.24	40,40,40,40	0
57	MG	YA	3203	1/1	0.93	0.28	35,35,35,35	0
57	MG	YB	202	1/1	0.93	0.22	19,19,19,19	0
57	MG	RA	3293	1/1	0.93	0.31	25,25,25,25	0
57	MG	RA	3140	1/1	0.93	0.18	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3296	1/1	0.93	0.19	51,51,51,51	0
57	MG	YA	3355	1/1	0.93	0.14	33,33,33,33	0
57	MG	YA	3210	1/1	0.93	0.19	32,32,32,32	0
57	MG	YF	301	1/1	0.93	0.07	27,27,27,27	0
57	MG	RA	3236	1/1	0.93	0.25	38,38,38,38	0
57	MG	YA	3213	1/1	0.93	0.19	14,14,14,14	0
57	MG	QA	1621	1/1	0.93	0.07	45,45,45,45	0
57	MG	YA	3092	1/1	0.93	0.37	37,37,37,37	0
57	MG	RA	3240	1/1	0.93	0.07	28,28,28,28	0
57	MG	YP	202	1/1	0.93	0.12	45,45,45,45	0
57	MG	YA	3096	1/1	0.93	0.33	41,41,41,41	0
57	MG	RA	3098	1/1	0.93	0.31	44,44,44,44	0
57	MG	YR	201	1/1	0.93	0.17	34,34,34,34	0
57	MG	XA	1731	1/1	0.93	0.11	41,41,41,41	0
57	MG	RA	3061	1/1	0.93	0.26	28,28,28,28	0
57	MG	XA	1735	1/1	0.93	0.38	44,44,44,44	0
57	MG	Y0	101	1/1	0.93	0.34	52,52,52,52	0
57	MG	RA	3190	1/1	0.93	0.30	18,18,18,18	0
57	MG	XA	1739	1/1	0.93	0.14	48,48,48,48	0
57	MG	Z7	101	1/1	0.93	0.12	35,35,35,35	0
57	MG	QA	1739	1/1	0.93	0.29	52,52,52,52	0
57	MG	XA	1607	1/1	0.94	0.39	35,35,35,35	0
57	MG	QA	1629	1/1	0.94	0.29	53,53,53,53	0
57	MG	RA	3252	1/1	0.94	0.23	43,43,43,43	0
57	MG	YA	3393	1/1	0.94	0.28	56,56,56,56	0
57	MG	XA	1610	1/1	0.94	0.20	33,33,33,33	0
57	MG	QA	1740	1/1	0.94	0.29	46,46,46,46	0
57	MG	YA	3002	1/1	0.94	0.21	11,11,11,11	0
57	MG	YA	3261	1/1	0.94	0.06	33,33,33,33	0
57	MG	RA	3423	1/1	0.94	0.19	51,51,51,51	0
57	MG	RA	3255	1/1	0.94	0.25	43,43,43,43	0
57	MG	YA	3141	1/1	0.94	0.27	37,37,37,37	0
57	MG	YA	3266	1/1	0.94	0.20	31,31,31,31	0
57	MG	QA	1682	1/1	0.94	0.31	49,49,49,49	0
57	MG	YA	3407	1/1	0.94	0.07	45,45,45,45	0
57	MG	XA	1618	1/1	0.94	0.27	24,24,24,24	0
57	MG	YA	3144	1/1	0.94	0.31	42,42,42,42	0
57	MG	YA	3270	1/1	0.94	0.25	32,32,32,32	0
57	MG	YA	3271	1/1	0.94	0.25	42,42,42,42	0
57	MG	RA	3359	1/1	0.94	0.16	51,51,51,51	0
57	MG	RA	3428	1/1	0.94	0.11	37,37,37,37	0
57	MG	RA	3022	1/1	0.94	0.33	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1622	1/1	0.94	0.31	40,40,40,40	0
57	MG	QA	1717	1/1	0.94	0.20	53,53,53,53	0
57	MG	RA	3139	1/1	0.94	0.16	44,44,44,44	0
57	MG	RA	3365	1/1	0.94	0.26	51,51,51,51	0
57	MG	YA	3034	1/1	0.94	0.17	22,22,22,22	0
57	MG	RA	3313	1/1	0.94	0.17	25,25,25,25	0
57	MG	RA	3029	1/1	0.94	0.16	28,28,28,28	0
57	MG	RA	3219	1/1	0.94	0.07	20,20,20,20	0
57	MG	RA	3033	1/1	0.94	0.28	25,25,25,25	0
57	MG	XA	1633	1/1	0.94	0.23	28,28,28,28	0
57	MG	YA	3432	1/1	0.94	0.17	47,47,47,47	0
57	MG	YA	3433	1/1	0.94	0.34	46,46,46,46	0
57	MG	QA	1683	1/1	0.94	0.34	59,59,59,59	0
57	MG	YA	3435	1/1	0.94	0.07	27,27,27,27	0
57	MG	XA	1713	1/1	0.94	0.33	48,48,48,48	0
57	MG	XA	1714	1/1	0.94	0.29	41,41,41,41	0
57	MG	YA	3165	1/1	0.94	0.11	14,14,14,14	0
57	MG	RA	3319	1/1	0.94	0.19	51,51,51,51	0
57	MG	XA	1718	1/1	0.94	0.22	47,47,47,47	0
57	MG	YA	3049	1/1	0.94	0.21	13,13,13,13	0
57	MG	YA	3051	1/1	0.94	0.27	30,30,30,30	0
57	MG	RA	3442	1/1	0.94	0.14	41,41,41,41	0
57	MG	YA	3171	1/1	0.94	0.13	39,39,39,39	0
57	MG	YA	3054	1/1	0.94	0.31	20,20,20,20	0
57	MG	RA	3373	1/1	0.94	0.21	49,49,49,49	0
57	MG	YA	3059	1/1	0.94	0.08	28,28,28,28	0
57	MG	YA	3306	1/1	0.94	0.28	42,42,42,42	0
57	MG	YA	3454	1/1	0.94	0.20	45,45,45,45	0
57	MG	YA	3060	1/1	0.94	0.21	12,12,12,12	0
57	MG	YA	3456	1/1	0.94	0.25	47,47,47,47	0
57	MG	RA	3222	1/1	0.94	0.30	50,50,50,50	0
57	MG	YA	3180	1/1	0.94	0.25	11,11,11,11	0
57	MG	QA	1707	1/1	0.94	0.27	45,45,45,45	0
57	MG	YA	3066	1/1	0.94	0.16	33,33,33,33	0
57	MG	YA	3067	1/1	0.94	0.28	25,25,25,25	0
57	MG	YA	3463	1/1	0.94	0.21	39,39,39,39	0
57	MG	RA	3181	1/1	0.94	0.21	56,56,56,56	0
57	MG	YA	3319	1/1	0.94	0.17	57,57,57,57	0
57	MG	YA	3469	1/1	0.94	0.30	45,45,45,45	0
57	MG	RA	3380	1/1	0.94	0.16	15,15,15,15	0
57	MG	YA	3471	1/1	0.94	0.17	44,44,44,44	0
57	MG	RA	3273	1/1	0.94	0.16	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3190	1/1	0.94	0.23	25,25,25,25	0
57	MG	YA	3074	1/1	0.94	0.15	23,23,23,23	0
57	MG	RA	3226	1/1	0.94	0.24	35,35,35,35	0
57	MG	QA	1620	1/1	0.94	0.32	40,40,40,40	0
57	MG	QA	1746	1/1	0.94	0.21	40,40,40,40	0
57	MG	RA	3388	1/1	0.94	0.32	56,56,56,56	0
57	MG	YA	3329	1/1	0.94	0.36	50,50,50,50	0
57	MG	XA	1733	1/1	0.94	0.17	18,18,18,18	0
57	MG	YA	3083	1/1	0.94	0.20	30,30,30,30	0
57	MG	YA	3334	1/1	0.94	0.28	35,35,35,35	0
57	MG	XA	1734	1/1	0.94	0.11	16,16,16,16	0
57	MG	YA	3087	1/1	0.94	0.21	25,25,25,25	0
57	MG	YA	3487	1/1	0.94	0.11	27,27,27,27	0
57	MG	RA	3330	1/1	0.94	0.20	49,49,49,49	0
57	MG	QA	1709	1/1	0.94	0.27	36,36,36,36	0
57	MG	YA	3343	1/1	0.94	0.24	48,48,48,48	0
57	MG	YA	3491	1/1	0.94	0.14	37,37,37,37	0
57	MG	RA	3079	1/1	0.94	0.21	26,26,26,26	0
57	MG	YA	3211	1/1	0.94	0.20	43,43,43,43	0
57	MG	RA	3395	1/1	0.94	0.33	45,45,45,45	0
57	MG	XA	1741	1/1	0.94	0.22	44,44,44,44	0
57	MG	RA	3007	1/1	0.94	0.20	19,19,19,19	0
57	MG	RA	3117	1/1	0.94	0.30	39,39,39,39	0
57	MG	QA	1616	1/1	0.94	0.12	45,45,45,45	0
57	MG	XA	1659	1/1	0.94	0.33	31,31,31,31	0
57	MG	RA	3011	1/1	0.94	0.13	23,23,23,23	0
57	MG	QA	1750	1/1	0.94	0.09	45,45,45,45	0
57	MG	XA	1749	1/1	0.94	0.27	52,52,52,52	0
57	MG	YB	201	1/1	0.94	0.32	32,32,32,32	0
57	MG	YA	3222	1/1	0.94	0.19	32,32,32,32	0
57	MG	YA	3224	1/1	0.94	0.22	35,35,35,35	0
57	MG	XA	1662	1/1	0.94	0.31	40,40,40,40	0
57	MG	YA	3363	1/1	0.94	0.26	59,59,59,59	0
57	MG	RA	3013	1/1	0.94	0.16	16,16,16,16	0
57	MG	RA	3200	1/1	0.94	0.36	37,37,37,37	0
57	MG	XA	1753	1/1	0.94	0.18	51,51,51,51	0
57	MG	QA	1606	1/1	0.94	0.19	19,19,19,19	0
57	MG	RA	3160	1/1	0.94	0.08	30,30,30,30	0
57	MG	YA	3115	1/1	0.94	0.19	45,45,45,45	0
57	MG	YA	3116	1/1	0.94	0.18	16,16,16,16	0
57	MG	RA	3161	1/1	0.94	0.21	36,36,36,36	0
57	MG	QA	1649	1/1	0.94	0.19	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3297	1/1	0.94	0.11	27,27,27,27	0
57	MG	RA	3058	1/1	0.94	0.21	24,24,24,24	0
57	MG	YA	3238	1/1	0.94	0.10	28,28,28,28	0
57	MG	RA	3299	1/1	0.94	0.05	49,49,49,49	0
57	MG	YA	3242	1/1	0.94	0.09	25,25,25,25	0
57	MG	YA	3244	1/1	0.94	0.35	57,57,57,57	0
57	MG	XA	1602	1/1	0.94	0.35	32,32,32,32	0
57	MG	QA	1689	1/1	0.94	0.20	28,28,28,28	0
57	MG	Y5	103	1/1	0.94	0.11	23,23,23,23	0
57	MG	RA	3167	1/1	0.94	0.18	31,31,31,31	0
57	MG	XA	1606	1/1	0.94	0.20	18,18,18,18	0
57	MG	YA	3388	1/1	0.94	0.12	52,52,52,52	0
57	MG	YA	3389	1/1	0.95	0.17	51,51,51,51	0
57	MG	XA	1688	1/1	0.95	0.17	26,26,26,26	0
57	MG	RA	3238	1/1	0.95	0.18	28,28,28,28	0
57	MG	RA	3193	1/1	0.95	0.23	16,16,16,16	0
57	MG	RA	3196	1/1	0.95	0.35	33,33,33,33	0
57	MG	XA	1613	1/1	0.95	0.09	24,24,24,24	0
57	MG	YA	3256	1/1	0.95	0.20	57,57,57,57	0
57	MG	YA	3010	1/1	0.95	0.16	22,22,22,22	0
57	MG	YA	3398	1/1	0.95	0.20	67,67,67,67	0
57	MG	RA	3421	1/1	0.95	0.26	51,51,51,51	0
57	MG	YA	3259	1/1	0.95	0.16	35,35,35,35	0
57	MG	XA	1695	1/1	0.95	0.18	40,40,40,40	0
57	MG	YA	3262	1/1	0.95	0.23	41,41,41,41	0
57	MG	RA	3422	1/1	0.95	0.09	41,41,41,41	0
57	MG	YA	3015	1/1	0.95	0.21	13,13,13,13	0
57	MG	YA	3016	1/1	0.95	0.08	8,8,8,8	0
57	MG	RA	3241	1/1	0.95	0.26	35,35,35,35	0
57	MG	YA	3020	1/1	0.95	0.26	23,23,23,23	0
57	MG	RA	3197	1/1	0.95	0.25	24,24,24,24	0
57	MG	RA	3300	1/1	0.95	0.06	37,37,37,37	0
57	MG	RA	3004	1/1	0.95	0.25	17,17,17,17	0
57	MG	XA	1701	1/1	0.95	0.25	41,41,41,41	0
57	MG	YA	3272	1/1	0.95	0.11	48,48,48,48	0
57	MG	YA	3415	1/1	0.95	0.41	62,62,62,62	0
57	MG	YA	3273	1/1	0.95	0.18	50,50,50,50	0
57	MG	YA	3030	1/1	0.95	0.23	15,15,15,15	0
57	MG	RA	3427	1/1	0.95	0.26	48,48,48,48	0
57	MG	YA	3150	1/1	0.95	0.33	15,15,15,15	0
57	MG	YA	3032	1/1	0.95	0.18	26,26,26,26	0
57	MG	YA	3152	1/1	0.95	0.21	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3199	1/1	0.95	0.20	23,23,23,23	0
57	MG	RA	3121	1/1	0.95	0.13	31,31,31,31	0
57	MG	RA	3201	1/1	0.95	0.14	27,27,27,27	0
57	MG	XA	1707	1/1	0.95	0.36	54,54,54,54	0
57	MG	RA	3028	1/1	0.95	0.21	12,12,12,12	0
57	MG	RA	3159	1/1	0.95	0.27	17,17,17,17	0
57	MG	YA	3041	1/1	0.95	0.19	23,23,23,23	0
57	MG	YA	3042	1/1	0.95	0.18	23,23,23,23	0
57	MG	RA	3123	1/1	0.95	0.12	28,28,28,28	0
57	MG	QA	1612	1/1	0.95	0.19	48,48,48,48	0
57	MG	XA	1631	1/1	0.95	0.14	24,24,24,24	0
57	MG	XA	1632	1/1	0.95	0.27	49,49,49,49	0
57	MG	YA	3442	1/1	0.95	0.13	61,61,61,61	0
57	MG	RA	3162	1/1	0.95	0.08	34,34,34,34	0
57	MG	XA	1717	1/1	0.95	0.22	37,37,37,37	0
57	MG	RA	3060	1/1	0.95	0.12	9,9,9,9	0
57	MG	YA	3052	1/1	0.95	0.24	9,9,9,9	0
57	MG	RA	3369	1/1	0.95	0.24	40,40,40,40	0
57	MG	RA	3209	1/1	0.95	0.24	30,30,30,30	0
57	MG	QA	1695	1/1	0.95	0.20	42,42,42,42	0
57	MG	YA	3174	1/1	0.95	0.33	29,29,29,29	0
57	MG	RA	3035	1/1	0.95	0.13	21,21,21,21	0
57	MG	YA	3305	1/1	0.95	0.23	34,34,34,34	0
57	MG	RA	3166	1/1	0.95	0.14	27,27,27,27	0
57	MG	XA	1725	1/1	0.95	0.15	54,54,54,54	0
57	MG	YA	3178	1/1	0.95	0.12	18,18,18,18	0
57	MG	RA	3375	1/1	0.95	0.31	61,61,61,61	0
57	MG	QA	1617	1/1	0.95	0.16	41,41,41,41	0
57	MG	RA	3097	1/1	0.95	0.34	53,53,53,53	0
57	MG	RA	3320	1/1	0.95	0.16	44,44,44,44	0
57	MG	YA	3069	1/1	0.95	0.14	19,19,19,19	0
57	MG	YA	3464	1/1	0.95	0.13	43,43,43,43	0
57	MG	YA	3466	1/1	0.95	0.22	48,48,48,48	0
57	MG	YA	3318	1/1	0.95	0.11	54,54,54,54	0
57	MG	QA	1697	1/1	0.95	0.42	76,76,76,76	0
57	MG	QA	1615	1/1	0.95	0.14	38,38,38,38	0
57	MG	YA	3188	1/1	0.95	0.16	38,38,38,38	0
57	MG	YA	3073	1/1	0.95	0.16	25,25,25,25	0
57	MG	RA	3136	1/1	0.95	0.35	40,40,40,40	0
57	MG	RA	3324	1/1	0.95	0.22	40,40,40,40	0
57	MG	YA	3077	1/1	0.95	0.25	16,16,16,16	0
57	MG	YA	3078	1/1	0.95	0.22	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3327	1/1	0.95	0.16	69,69,69,69	0
57	MG	QA	1712	1/1	0.95	0.25	58,58,58,58	0
57	MG	RA	3270	1/1	0.95	0.27	42,42,42,42	0
57	MG	YA	3330	1/1	0.95	0.18	11,11,11,11	0
57	MG	YA	3331	1/1	0.95	0.29	18,18,18,18	0
57	MG	XA	1737	1/1	0.95	0.22	34,34,34,34	0
57	MG	QA	1628	1/1	0.95	0.08	65,65,65,65	0
57	MG	XA	1652	1/1	0.95	0.33	46,46,46,46	0
57	MG	YA	3085	1/1	0.95	0.18	24,24,24,24	0
57	MG	YA	3205	1/1	0.95	0.15	21,21,21,21	0
57	MG	YA	3338	1/1	0.95	0.23	25,25,25,25	0
57	MG	YA	3206	1/1	0.95	0.32	38,38,38,38	0
57	MG	QA	1701	1/1	0.95	0.30	47,47,47,47	0
57	MG	RA	3393	1/1	0.95	0.19	23,23,23,23	0
57	MG	RF	301	1/1	0.95	0.05	34,34,34,34	0
57	MG	YA	3346	1/1	0.95	0.40	47,47,47,47	0
57	MG	YA	3089	1/1	0.95	0.21	8,8,8,8	0
57	MG	QA	1662	1/1	0.95	0.09	27,27,27,27	0
57	MG	RA	3331	1/1	0.95	0.17	34,34,34,34	0
57	MG	YA	3214	1/1	0.95	0.22	19,19,19,19	0
57	MG	RA	3223	1/1	0.95	0.27	38,38,38,38	0
57	MG	YA	3094	1/1	0.95	0.16	45,45,45,45	0
57	MG	QA	1663	1/1	0.95	0.34	49,49,49,49	0
57	MG	QA	1690	1/1	0.95	0.25	49,49,49,49	0
57	MG	RA	3400	1/1	0.95	0.27	44,44,44,44	0
57	MG	YA	3504	1/1	0.95	0.25	18,18,18,18	0
57	MG	RA	3278	1/1	0.95	0.21	39,39,39,39	0
57	MG	XA	1668	1/1	0.95	0.19	35,35,35,35	0
57	MG	RA	3144	1/1	0.95	0.25	44,44,44,44	0
57	MG	RA	3077	1/1	0.95	0.15	24,24,24,24	0
57	MG	YA	3225	1/1	0.95	0.15	16,16,16,16	0
57	MG	QA	1654	1/1	0.95	0.26	41,41,41,41	0
57	MG	RA	3283	1/1	0.95	0.22	36,36,36,36	0
57	MG	RA	3341	1/1	0.95	0.36	73,73,73,73	0
57	MG	YA	3106	1/1	0.95	0.37	42,42,42,42	0
57	MG	QA	1644	1/1	0.95	0.20	27,27,27,27	0
57	MG	XA	1679	1/1	0.95	0.20	35,35,35,35	0
57	MG	RA	3149	1/1	0.95	0.34	21,21,21,21	0
57	MG	RA	3411	1/1	0.95	0.15	49,49,49,49	0
57	MG	YA	3113	1/1	0.95	0.22	34,34,34,34	0
57	MG	YA	3114	1/1	0.95	0.16	26,26,26,26	0
57	MG	RA	3080	1/1	0.95	0.25	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1764	1/1	0.95	0.06	45,45,45,45	0
57	MG	XA	1605	1/1	0.95	0.23	18,18,18,18	0
57	MG	RA	3050	1/1	0.95	0.15	12,12,12,12	0
57	MG	RA	3053	1/1	0.95	0.16	40,40,40,40	0
57	MG	YA	3243	1/1	0.95	0.24	46,46,46,46	0
57	MG	YA	3384	1/1	0.95	0.12	65,65,65,65	0
57	MG	RA	3054	1/1	0.95	0.29	27,27,27,27	0
57	MG	YA	3121	1/1	0.95	0.10	27,27,27,27	0
57	MG	RA	3085	1/1	0.95	0.08	15,15,15,15	0
58	ZN	QD	301	1/1	0.95	0.24	49,49,49,49	0
57	MG	XV	102	1/1	0.95	0.20	26,26,26,26	0
57	MG	RA	3382	1/1	0.96	0.20	21,21,21,21	0
57	MG	YA	3359	1/1	0.96	0.06	36,36,36,36	0
57	MG	XA	1754	1/1	0.96	0.07	61,61,61,61	0
57	MG	XA	1673	1/1	0.96	0.16	24,24,24,24	0
57	MG	RA	3444	1/1	0.96	0.37	52,52,52,52	0
57	MG	RA	3305	1/1	0.96	0.17	41,41,41,41	0
57	MG	YA	3093	1/1	0.96	0.17	17,17,17,17	0
57	MG	RA	3257	1/1	0.96	0.07	42,42,42,42	0
57	MG	RA	3051	1/1	0.96	0.19	26,26,26,26	0
57	MG	RA	3016	1/1	0.96	0.21	15,15,15,15	0
57	MG	QA	1634	1/1	0.96	0.18	45,45,45,45	0
57	MG	RA	3419	1/1	0.96	0.18	40,40,40,40	0
57	MG	YA	3370	1/1	0.96	0.23	50,50,50,50	0
57	MG	YA	3223	1/1	0.96	0.16	30,30,30,30	0
57	MG	YA	3290	1/1	0.96	0.22	38,38,38,38	0
57	MG	YA	3159	1/1	0.96	0.16	13,13,13,13	0
57	MG	RA	3094	1/1	0.96	0.43	43,43,43,43	0
57	MG	YA	3465	1/1	0.96	0.17	43,43,43,43	0
57	MG	YA	3375	1/1	0.96	0.10	35,35,35,35	0
57	MG	QA	1635	1/1	0.96	0.16	29,29,29,29	0
57	MG	RA	3081	1/1	0.96	0.22	14,14,14,14	0
57	MG	YA	3379	1/1	0.96	0.16	42,42,42,42	0
57	MG	RB	203	1/1	0.96	0.29	45,45,45,45	0
57	MG	RA	3132	1/1	0.96	0.07	17,17,17,17	0
57	MG	XA	1729	1/1	0.96	0.07	24,24,24,24	0
57	MG	RA	3114	1/1	0.96	0.11	30,30,30,30	0
57	MG	YA	3107	1/1	0.96	0.28	33,33,33,33	0
57	MG	RA	3115	1/1	0.96	0.16	52,52,52,52	0
57	MG	XV	103	1/1	0.96	0.28	45,45,45,45	0
57	MG	YA	3056	1/1	0.96	0.21	5,5,5,5	0
57	MG	YA	3057	1/1	0.96	0.13	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3308	1/1	0.96	0.36	54,54,54,54	0
57	MG	YA	3172	1/1	0.96	0.37	52,52,52,52	0
57	MG	YA	3112	1/1	0.96	0.07	19,19,19,19	0
57	MG	YA	3239	1/1	0.96	0.09	24,24,24,24	0
57	MG	YA	3483	1/1	0.96	0.22	51,51,51,51	0
57	MG	YA	3240	1/1	0.96	0.30	34,34,34,34	0
57	MG	XA	1649	1/1	0.96	0.19	23,23,23,23	0
57	MG	RA	3340	1/1	0.96	0.10	40,40,40,40	0
57	MG	YA	3317	1/1	0.96	0.40	51,51,51,51	0
57	MG	QA	1685	1/1	0.96	0.12	28,28,28,28	0
57	MG	RA	3247	1/1	0.96	0.40	37,37,37,37	0
57	MG	YA	3063	1/1	0.96	0.13	21,21,21,21	0
57	MG	YA	3064	1/1	0.96	0.29	26,26,26,26	0
57	MG	YA	3403	1/1	0.96	0.22	46,46,46,46	0
57	MG	RA	3001	1/1	0.96	0.09	43,43,43,43	0
57	MG	QA	1618	1/1	0.96	0.22	44,44,44,44	0
57	MG	QA	1698	1/1	0.96	0.27	47,47,47,47	0
57	MG	YA	3250	1/1	0.96	0.29	45,45,45,45	0
57	MG	YA	3251	1/1	0.96	0.20	33,33,33,33	0
57	MG	QA	1656	1/1	0.96	0.36	41,41,41,41	0
57	MG	YA	3184	1/1	0.96	0.08	46,46,46,46	0
57	MG	RA	3374	1/1	0.96	0.30	44,44,44,44	0
57	MG	RA	3215	1/1	0.96	0.42	53,53,53,53	0
57	MG	XA	1626	1/1	0.96	0.31	37,37,37,37	0
57	MG	YA	3129	1/1	0.96	0.13	19,19,19,19	0
57	MG	YA	3072	1/1	0.96	0.21	19,19,19,19	0
57	MG	YA	3260	1/1	0.96	0.34	49,49,49,49	0
57	MG	YA	3017	1/1	0.96	0.19	16,16,16,16	0
57	MG	RA	3076	1/1	0.96	0.16	25,25,25,25	0
57	MG	YA	3420	1/1	0.96	0.29	65,65,65,65	0
57	MG	YA	3337	1/1	0.96	0.11	39,39,39,39	0
57	MG	YA	3193	1/1	0.96	0.33	43,43,43,43	0
57	MG	YF	302	1/1	0.96	0.09	35,35,35,35	0
57	MG	YA	3194	1/1	0.96	0.26	33,33,33,33	0
57	MG	XA	1664	1/1	0.96	0.28	31,31,31,31	0
57	MG	RA	3326	1/1	0.96	0.17	46,46,46,46	0
57	MG	RA	3089	1/1	0.96	0.16	21,21,21,21	0
57	MG	YA	3023	1/1	0.96	0.22	14,14,14,14	0
57	MG	YA	3431	1/1	0.96	0.09	31,31,31,31	0
57	MG	YA	3138	1/1	0.96	0.21	39,39,39,39	0
57	MG	YA	3024	1/1	0.96	0.18	18,18,18,18	0
57	MG	RA	3439	1/1	0.96	0.30	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3026	1/1	0.96	0.17	9,9,9,9	0
57	MG	YA	3436	1/1	0.96	0.20	38,38,38,38	0
57	MG	YA	3351	1/1	0.96	0.21	50,50,50,50	0
57	MG	YA	3438	1/1	0.96	0.07	26,26,26,26	0
57	MG	Y5	101	1/1	0.96	0.11	27,27,27,27	0
57	MG	YA	3028	1/1	0.96	0.16	14,14,14,14	0
57	MG	YA	3084	1/1	0.96	0.06	20,20,20,20	0
57	MG	RA	3440	1/1	0.96	0.19	53,53,53,53	0
57	MG	R5	101	1/1	0.96	0.11	17,17,17,17	0
57	MG	RA	3280	1/1	0.96	0.16	24,24,24,24	0
57	MG	YA	3357	1/1	0.96	0.17	50,50,50,50	0
57	MG	RA	3027	1/1	0.97	0.15	9,9,9,9	0
57	MG	RA	3356	1/1	0.97	0.28	46,46,46,46	0
57	MG	QA	1611	1/1	0.97	0.19	31,31,31,31	0
57	MG	XA	1738	1/1	0.97	0.24	43,43,43,43	0
57	MG	XA	1667	1/1	0.97	0.35	40,40,40,40	0
57	MG	YA	3050	1/1	0.97	0.15	23,23,23,23	0
57	MG	QA	1664	1/1	0.97	0.17	39,39,39,39	0
57	MG	RA	3174	1/1	0.97	0.32	19,19,19,19	0
57	MG	RA	3030	1/1	0.97	0.14	15,15,15,15	0
57	MG	RA	3260	1/1	0.97	0.30	45,45,45,45	0
57	MG	XA	1744	1/1	0.97	0.05	33,33,33,33	0
57	MG	RA	3109	1/1	0.97	0.27	25,25,25,25	0
57	MG	RA	3311	1/1	0.97	0.23	24,24,24,24	0
57	MG	XA	1674	1/1	0.97	0.29	43,43,43,43	0
57	MG	XA	1675	1/1	0.97	0.13	47,47,47,47	0
57	MG	YA	3341	1/1	0.97	0.31	20,20,20,20	0
57	MG	RA	3052	1/1	0.97	0.17	13,13,13,13	0
57	MG	YA	3062	1/1	0.97	0.16	17,17,17,17	0
57	MG	RA	3178	1/1	0.97	0.16	15,15,15,15	0
57	MG	XA	1678	1/1	0.97	0.09	28,28,28,28	0
57	MG	YA	3449	1/1	0.97	0.20	36,36,36,36	0
57	MG	RA	3031	1/1	0.97	0.21	10,10,10,10	0
57	MG	RA	3265	1/1	0.97	0.30	57,57,57,57	0
57	MG	RA	3145	1/1	0.97	0.14	22,22,22,22	0
57	MG	YA	3453	1/1	0.97	0.22	54,54,54,54	0
57	MG	RA	3430	1/1	0.97	0.05	52,52,52,52	0
57	MG	YA	3252	1/1	0.97	0.16	28,28,28,28	0
57	MG	XA	1617	1/1	0.97	0.26	42,42,42,42	0
57	MG	RA	3032	1/1	0.97	0.17	17,17,17,17	0
57	MG	RA	3055	1/1	0.97	0.33	25,25,25,25	0
57	MG	RA	3056	1/1	0.97	0.20	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1626	1/1	0.97	0.05	21,21,21,21	0
57	MG	RA	3271	1/1	0.97	0.04	27,27,27,27	0
57	MG	RA	3034	1/1	0.97	0.13	20,20,20,20	0
57	MG	RA	3186	1/1	0.97	0.29	54,54,54,54	0
57	MG	RA	3151	1/1	0.97	0.33	54,54,54,54	0
57	MG	QA	1725	1/1	0.97	0.06	44,44,44,44	0
57	MG	XF	201	1/1	0.97	0.09	31,31,31,31	0
57	MG	RA	3381	1/1	0.97	0.36	43,43,43,43	0
57	MG	XL	201	1/1	0.97	0.06	39,39,39,39	0
57	MG	QA	1726	1/1	0.97	0.04	38,38,38,38	0
57	MG	QA	1660	1/1	0.97	0.31	32,32,32,32	0
57	MG	RA	3191	1/1	0.97	0.17	24,24,24,24	0
57	MG	RA	3006	1/1	0.97	0.03	12,12,12,12	0
57	MG	RA	3386	1/1	0.97	0.26	24,24,24,24	0
57	MG	RA	3233	1/1	0.97	0.06	38,38,38,38	0
57	MG	RA	3039	1/1	0.97	0.24	34,34,34,34	0
57	MG	RA	3389	1/1	0.97	0.04	9,9,9,9	0
57	MG	YA	3003	1/1	0.97	0.22	14,14,14,14	0
57	MG	RA	3390	1/1	0.97	0.27	19,19,19,19	0
57	MG	RA	3195	1/1	0.97	0.17	30,30,30,30	0
57	MG	YA	3006	1/1	0.97	0.18	17,17,17,17	0
57	MG	YA	3185	1/1	0.97	0.16	21,21,21,21	0
57	MG	YA	3378	1/1	0.97	0.12	56,56,56,56	0
57	MG	YA	3008	1/1	0.97	0.12	19,19,19,19	0
57	MG	YA	3009	1/1	0.97	0.20	17,17,17,17	0
57	MG	QA	1636	1/1	0.97	0.21	48,48,48,48	0
57	MG	YA	3098	1/1	0.97	0.19	24,24,24,24	0
57	MG	XA	1706	1/1	0.97	0.21	31,31,31,31	0
57	MG	RA	3237	1/1	0.97	0.10	34,34,34,34	0
57	MG	QA	1692	1/1	0.97	0.22	26,26,26,26	0
57	MG	YA	3014	1/1	0.97	0.21	19,19,19,19	0
57	MG	RA	3042	1/1	0.97	0.14	14,14,14,14	0
57	MG	RA	3288	1/1	0.97	0.29	61,61,61,61	0
57	MG	XA	1711	1/1	0.97	0.19	27,27,27,27	0
57	MG	YA	3018	1/1	0.97	0.12	9,9,9,9	0
57	MG	RA	3289	1/1	0.97	0.11	39,39,39,39	0
57	MG	RA	3068	1/1	0.97	0.17	14,14,14,14	0
57	MG	YA	3202	1/1	0.97	0.20	22,22,22,22	0
57	MG	RA	3010	1/1	0.97	0.22	20,20,20,20	0
57	MG	XA	1715	1/1	0.97	0.20	40,40,40,40	0
57	MG	YA	3396	1/1	0.97	0.19	48,48,48,48	0
57	MG	YA	3296	1/1	0.97	0.24	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3297	1/1	0.97	0.35	49,49,49,49	0
57	MG	RA	3023	1/1	0.97	0.24	55,55,55,55	0
57	MG	RA	3131	1/1	0.97	0.14	43,43,43,43	0
57	MG	RA	3024	1/1	0.97	0.31	18,18,18,18	0
57	MG	YA	3302	1/1	0.97	0.35	61,61,61,61	0
57	MG	RA	3295	1/1	0.97	0.15	32,32,32,32	0
57	MG	YA	3027	1/1	0.97	0.17	14,14,14,14	0
57	MG	RA	3405	1/1	0.97	0.33	48,48,48,48	0
57	MG	RA	3101	1/1	0.97	0.27	44,44,44,44	0
57	MG	QA	1627	1/1	0.97	0.26	42,42,42,42	0
57	MG	XA	1653	1/1	0.97	0.15	29,29,29,29	0
57	MG	XA	1654	1/1	0.97	0.23	23,23,23,23	0
57	MG	YA	3033	1/1	0.97	0.14	16,16,16,16	0
57	MG	RA	3073	1/1	0.97	0.19	22,22,22,22	0
57	MG	RA	3409	1/1	0.97	0.16	43,43,43,43	0
57	MG	RA	3207	1/1	0.97	0.22	26,26,26,26	0
57	MG	YA	3315	1/1	0.97	0.22	34,34,34,34	0
57	MG	YA	3416	1/1	0.97	0.13	10,10,10,10	0
57	MG	YA	3126	1/1	0.97	0.23	22,22,22,22	0
57	MG	YA	3127	1/1	0.97	0.19	41,41,41,41	0
57	MG	XA	1658	1/1	0.97	0.07	34,34,34,34	0
57	MG	RA	3074	1/1	0.97	0.13	37,37,37,37	0
57	MG	YA	3039	1/1	0.97	0.18	11,11,11,11	0
57	MG	YA	3422	1/1	0.97	0.25	29,29,29,29	0
57	MG	RA	3169	1/1	0.97	0.10	19,19,19,19	0
57	MG	RA	3352	1/1	0.97	0.24	44,44,44,44	0
57	MG	YA	3426	1/1	0.97	0.25	23,23,23,23	0
57	MG	RA	3251	1/1	0.97	0.05	24,24,24,24	0
57	MG	RA	3137	1/1	0.97	0.37	55,55,55,55	0
58	ZN	XN	101	1/1	0.97	0.06	69,69,69,69	0
57	MG	YA	3312	1/1	0.98	0.18	24,24,24,24	0
57	MG	YA	3122	1/1	0.98	0.27	19,19,19,19	0
57	MG	RA	3090	1/1	0.98	0.19	11,11,11,11	0
57	MG	XE	201	1/1	0.98	0.19	32,32,32,32	0
57	MG	XA	1720	1/1	0.98	0.12	44,44,44,44	0
57	MG	YA	3424	1/1	0.98	0.04	1,1,1,1	0
57	MG	YA	3043	1/1	0.98	0.19	19,19,19,19	0
57	MG	RA	3026	1/1	0.98	0.18	16,16,16,16	0
57	MG	XA	1614	1/1	0.98	0.13	22,22,22,22	0
57	MG	RA	3129	1/1	0.98	0.10	12,12,12,12	0
57	MG	RA	3377	1/1	0.98	0.26	38,38,38,38	0
57	MG	YB	203	1/1	0.98	0.30	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3131	1/1	0.98	0.19	40,40,40,40	0
57	MG	RA	3360	1/1	0.98	0.04	32,32,32,32	0
57	MG	RA	3284	1/1	0.98	0.11	38,38,38,38	0
57	MG	RA	3130	1/1	0.98	0.16	28,28,28,28	0
57	MG	YA	3195	1/1	0.98	0.25	23,23,23,23	0
57	MG	YE	302	1/1	0.98	0.18	18,18,18,18	0
57	MG	YA	3196	1/1	0.98	0.27	24,24,24,24	0
57	MG	RA	3363	1/1	0.98	0.09	39,39,39,39	0
57	MG	RB	205	1/1	0.98	0.22	59,59,59,59	0
57	MG	YA	3401	1/1	0.98	0.17	38,38,38,38	0
57	MG	RA	3100	1/1	0.98	0.18	18,18,18,18	0
57	MG	RA	3258	1/1	0.98	0.21	39,39,39,39	0
57	MG	YA	3055	1/1	0.98	0.18	14,14,14,14	0
57	MG	YA	3299	1/1	0.98	0.21	28,28,28,28	0
57	MG	RA	3047	1/1	0.98	0.06	16,16,16,16	0
57	MG	QA	1749	1/1	0.98	0.33	57,57,57,57	0
57	MG	XA	1689	1/1	0.98	0.05	46,46,46,46	0
57	MG	YA	3007	1/1	0.98	0.36	40,40,40,40	0
57	MG	RA	3194	1/1	0.98	0.15	9,9,9,9	0
57	MG	YA	3486	1/1	0.98	0.05	38,38,38,38	0
57	MG	YA	3339	1/1	0.98	0.08	31,31,31,31	0
57	MG	RA	3112	1/1	0.98	0.13	24,24,24,24	0
57	MG	YA	3146	1/1	0.98	0.17	29,29,29,29	0
57	MG	RA	3015	1/1	0.98	0.32	31,31,31,31	0
57	MG	RP	202	1/1	0.98	0.10	28,28,28,28	0
57	MG	QL	201	1/1	0.98	0.09	58,58,58,58	0
57	MG	RA	3088	1/1	0.98	0.10	23,23,23,23	0
58	ZN	QN	101	1/1	0.98	0.06	79,79,79,79	0
57	MG	YA	3494	1/1	0.98	0.21	49,49,49,49	0
57	MG	QV	102	1/1	0.98	0.22	25,25,25,25	0
57	MG	RA	3443	1/1	0.99	0.09	56,56,56,56	0
57	MG	YA	3208	1/1	0.99	0.28	35,35,35,35	0
57	MG	YP	201	1/1	0.99	0.05	11,11,11,11	0
57	MG	YA	3075	1/1	0.99	0.14	13,13,13,13	0
57	MG	RA	3253	1/1	0.99	0.39	53,53,53,53	0
57	MG	RA	3063	1/1	0.99	0.12	10,10,10,10	0
57	MG	RA	3009	1/1	0.99	0.11	18,18,18,18	0
57	MG	YA	3462	1/1	0.99	0.06	36,36,36,36	0
57	MG	RA	3396	1/1	0.99	0.10	31,31,31,31	0
57	MG	RA	3316	1/1	0.99	0.26	40,40,40,40	0
57	MG	YA	3344	1/1	1.00	0.31	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.