wwPDB X-ray Structure Validation Summary Report (i)

Sep 17, 2023 – 09:37 PM EDT

PDB ID	:	4YZV
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.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

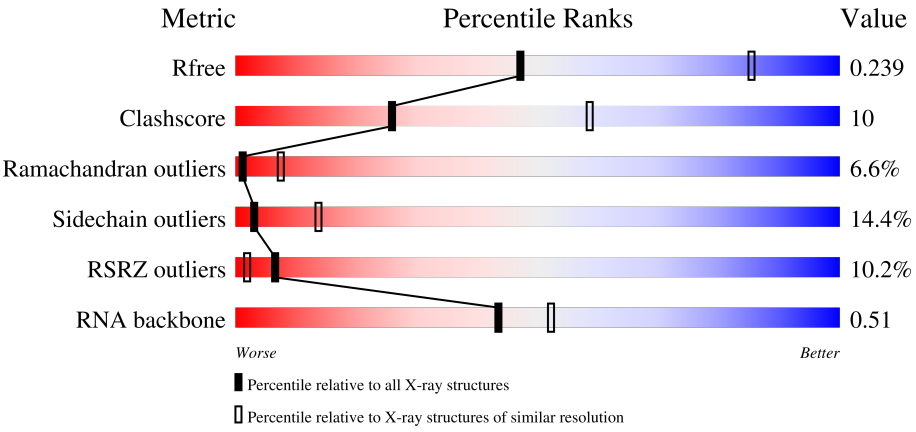
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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 <=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	12% 57% 31% 11% ••
1	XA	1522	7% 58% 32% 8% ••
2	QB	256	34% 52% 32% 8% • 8%
2	XB	256	19% 50% 34% 8% 8%

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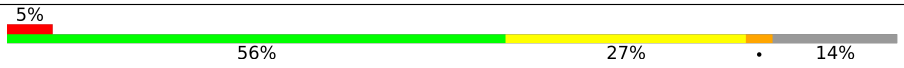
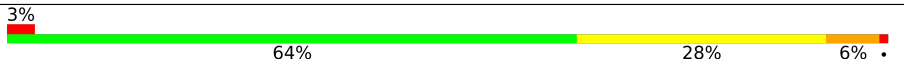
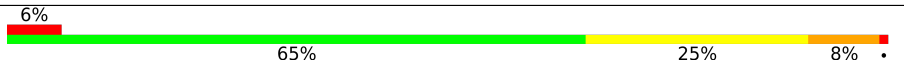
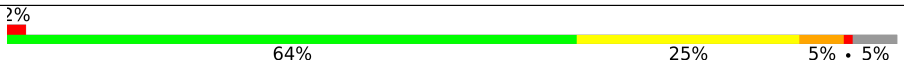
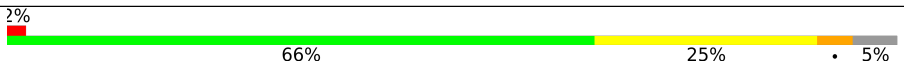
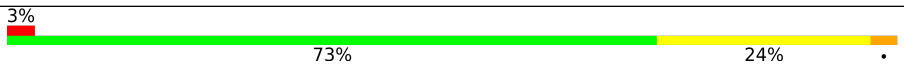
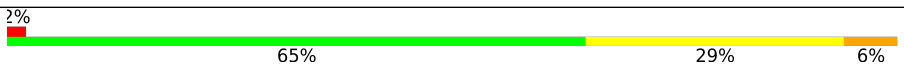
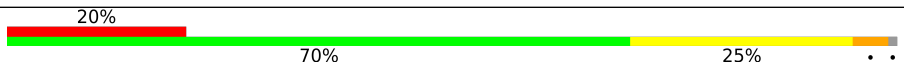
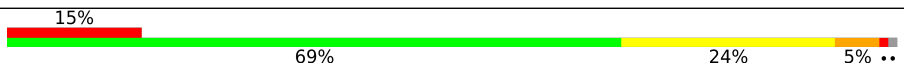
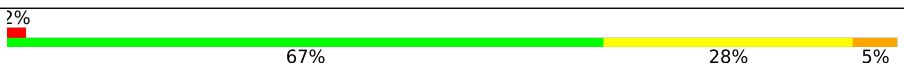
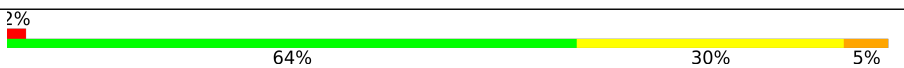
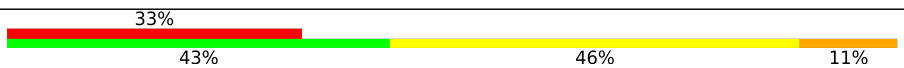
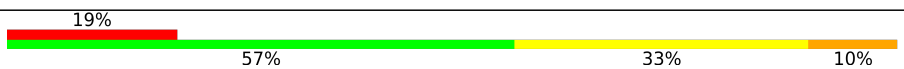
Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
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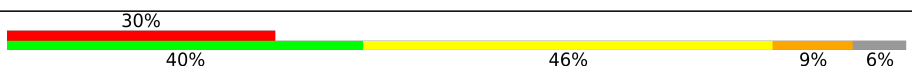
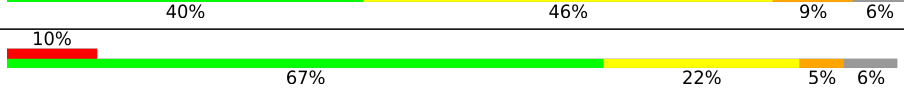
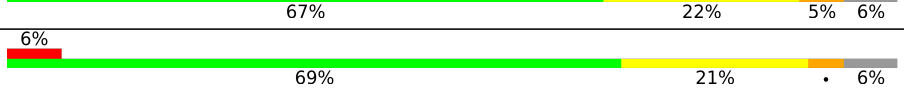
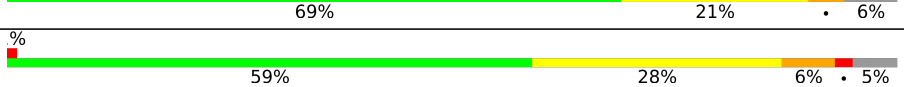
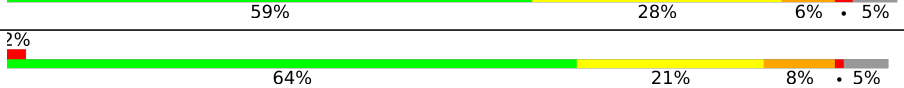
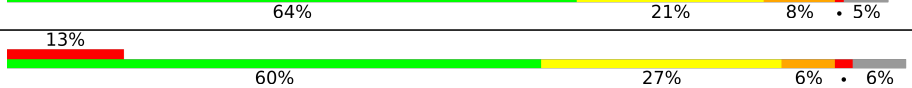
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
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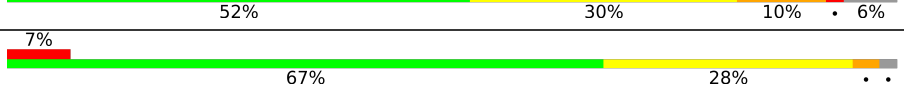
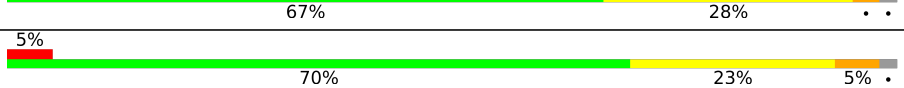
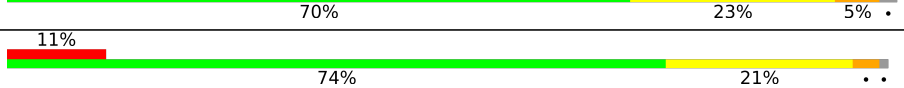
14	QN	61	
14	XN	61	
15	QO	89	

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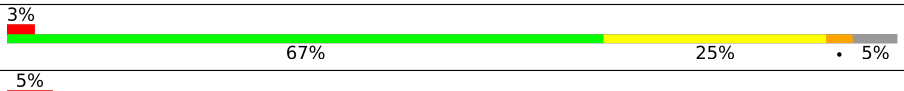
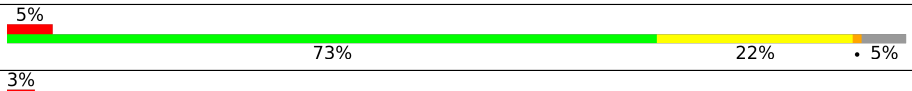
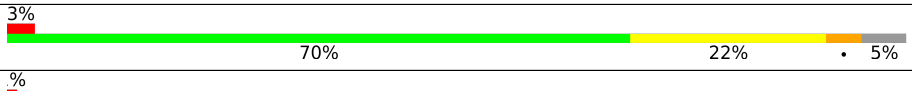
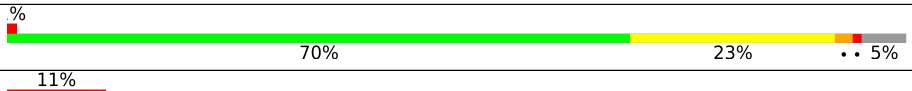
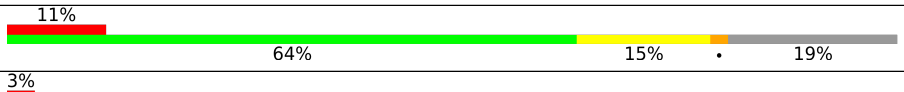
Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
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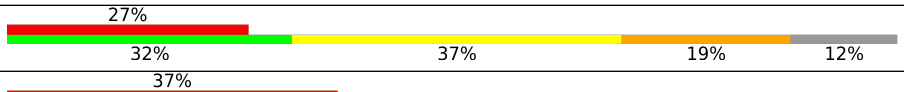
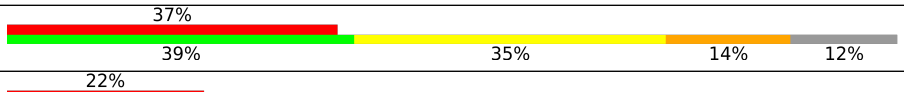
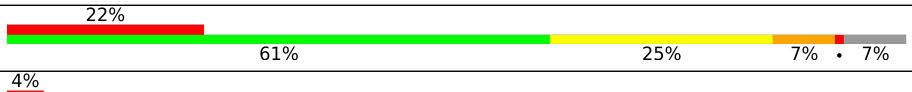
19	QS	93	
19	XS	93	
20	QT	106	
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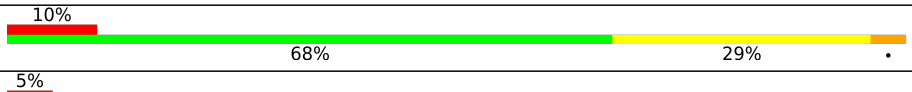
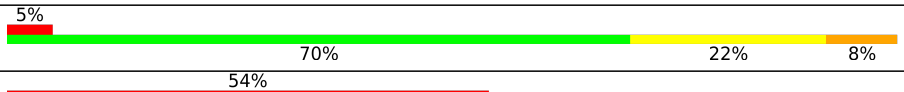
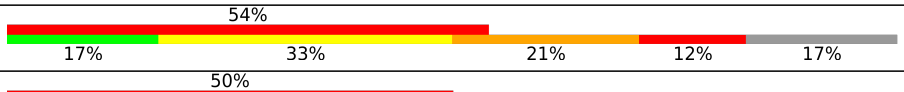
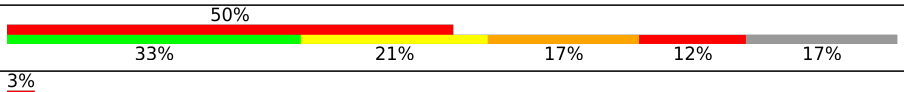
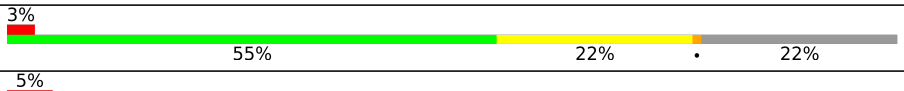
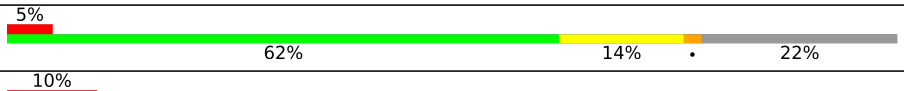
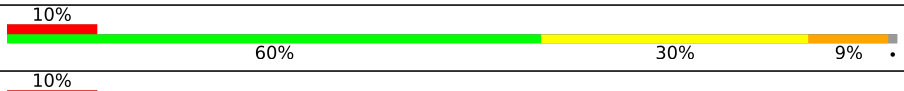
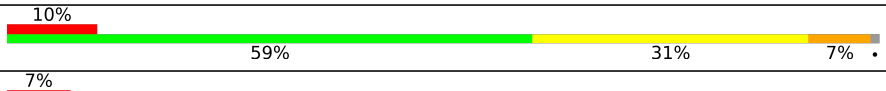
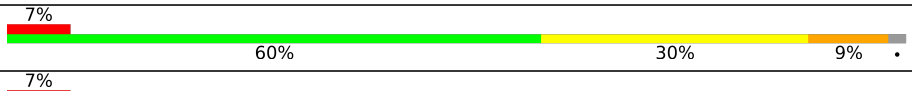
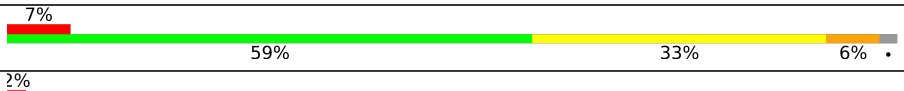
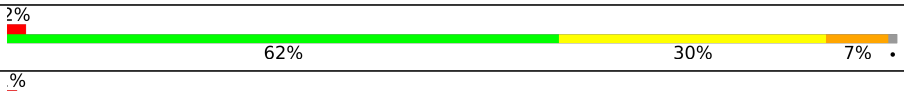
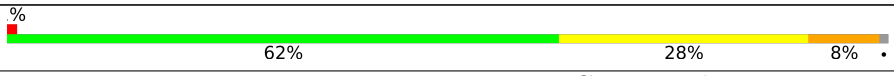
22	QV	77	
22	XV	77	
23	QX	24	
23	XX	24	
24	QY	117	
24	XY	117	
25	RA	2916	
25	YA	2916	
26	RB	124	
26	YB	124	
27	RD	276	
27	YD	276	

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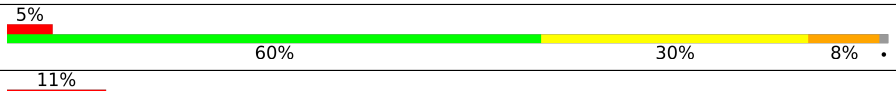
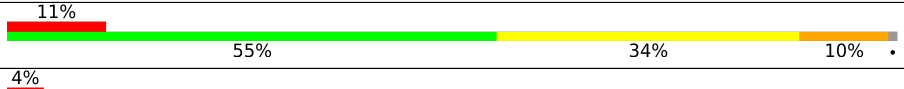
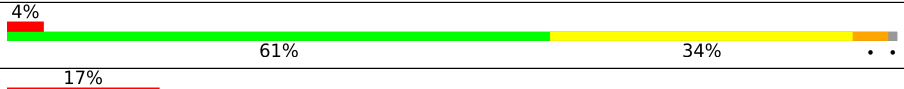
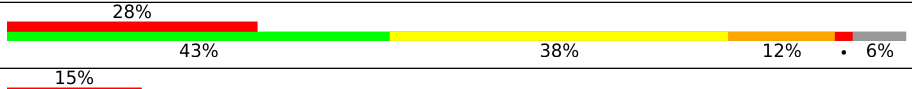
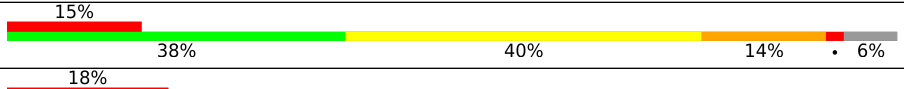
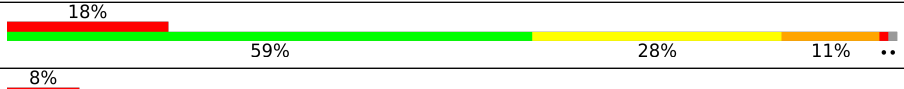
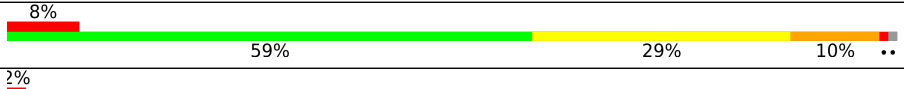
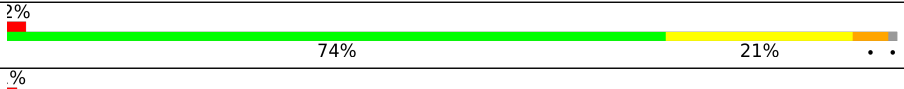
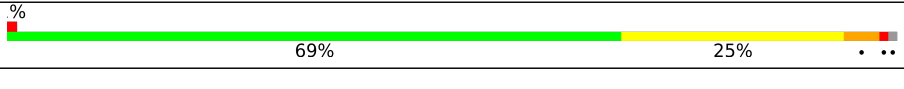
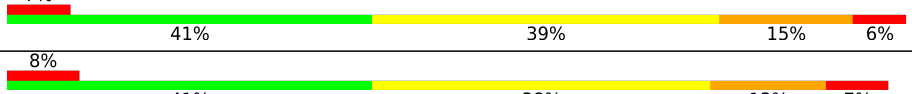
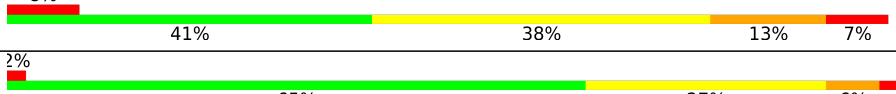
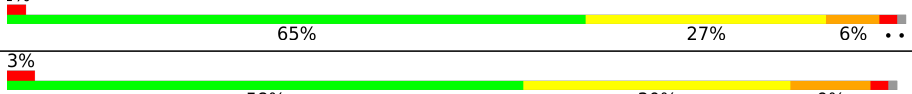
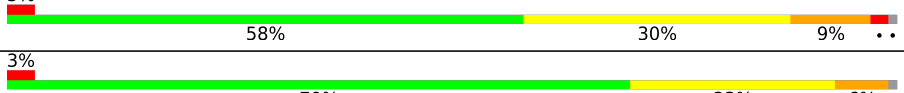
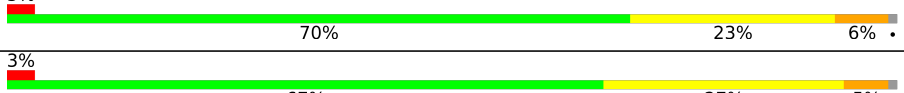
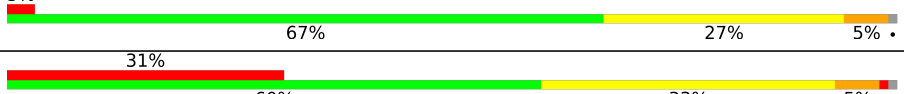
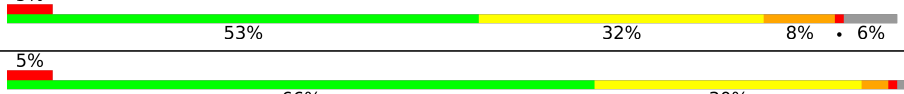
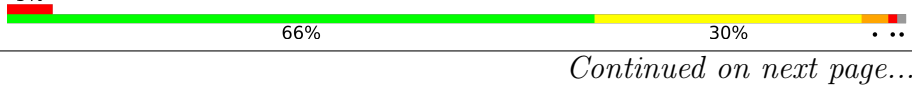
28	YE	206	
29	RF	210	
29	YF	210	
30	RG	182	
30	YG	182	
31	RH	180	
31	YH	180	
32	RI	148	
32	YI	148	
33	RN	140	
33	YN	140	
34	RO	122	
34	YO	122	
35	RP	150	
35	YP	150	
36	RQ	141	
36	YQ	141	
37	RR	118	
37	YR	118	
38	RS	112	
38	YS	112	
39	RT	146	
39	YT	146	
40	RU	118	

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Mol	Chain	Length	Quality of chain
40	YU	118	4% 68% 27%
41	RV	101	6% 40% 45% 12%
41	YV	101	11% 42% 45% 11%
42	RW	113	% 66% 29%
42	YW	113	65% 27% 8%
43	RX	96	3% 73% 20%
43	YX	96	67% 27%
44	RY	110	18% 34% 39% 14% 6% 7%
44	YY	110	19% 33% 40% 18% 7%
45	RZ	206	19% 41% 31% 14% 15%
45	YZ	206	9% 48% 30% 10% 11%
46	R0	85	% 64% 31%
46	Y0	85	6% 56% 36% 5%
47	R1	98	6% 50% 38% 9%
47	Y1	98	5% 59% 35%
48	R2	72	6% 53% 31% 10%
48	Y2	72	7% 61% 25% 7%
49	R3	60	70% 22% 7%
49	Y3	60	67% 28%
50	R4	71	37% 45% 35% 18%
50	Y4	71	28% 32% 45% 20%
51	R5	60	12% 70% 23%
51	Y5	60	8% 55% 33% 5% 5%
52	R6	54	59% 24% 37% 28% 11%
52	Y6	54	56% 22% 31% 31% 11%

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Mol	Chain	Length	Quality of chain
53	R7	49	4% 69% 27%
53	Y7	49	2% 61% 31% 8%
54	R8	65	8% 35% 45% 15%
54	Y8	65	8% 45% 42% 9%
55	R9	37	57% 68% 27% 5%
55	Y9	37	11% 70% 27%
56	Z6	3	33% 33% 33%
56	Z7	3	33% 33% 33%

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	1697	-	-	-	X
57	MG	QA	1751	-	-	-	X
57	MG	R0	102	-	-	-	X
57	MG	RA	3075	-	-	-	X
57	MG	RA	3092	-	-	-	X
57	MG	RA	3102	-	-	-	X
57	MG	RA	3146	-	-	-	X
57	MG	RA	3176	-	-	-	X
57	MG	RA	3182	-	-	-	X
57	MG	RA	3188	-	-	-	X
57	MG	RA	3210	-	-	-	X
57	MG	RA	3292	-	-	-	X
57	MG	RA	3298	-	-	-	X
57	MG	RA	3300	-	-	-	X
57	MG	RA	3302	-	-	-	X
57	MG	RA	3322	-	-	-	X
57	MG	RA	3323	-	-	-	X
57	MG	RA	3329	-	-	-	X
57	MG	RA	3338	-	-	-	X
57	MG	RA	3341	-	-	-	X
57	MG	RA	3351	-	-	-	X
57	MG	RA	3353	-	-	-	X
57	MG	RA	3361	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3370	-	-	-	X
57	MG	RA	3376	-	-	-	X
57	MG	RA	3387	-	-	-	X
57	MG	RA	3392	-	-	-	X
57	MG	RA	3438	-	-	-	X
57	MG	RY	202	-	-	-	X
57	MG	XA	1639	-	-	-	X
57	MG	XA	1646	-	-	-	X
57	MG	XA	1669	-	-	-	X
57	MG	XA	1685	-	-	-	X
57	MG	XA	1702	-	-	-	X
57	MG	XA	1704	-	-	-	X
57	MG	XA	1725	-	-	-	X
57	MG	XA	1756	-	-	-	X
57	MG	YA	3001	-	-	-	X
57	MG	YA	3100	-	-	-	X
57	MG	YA	3104	-	-	-	X
57	MG	YA	3111	-	-	-	X
57	MG	YA	3134	-	-	-	X
57	MG	YA	3147	-	-	-	X
57	MG	YA	3186	-	-	-	X
57	MG	YA	3197	-	-	-	X
57	MG	YA	3215	-	-	-	X
57	MG	YA	3255	-	-	-	X
57	MG	YA	3268	-	-	-	X
57	MG	YA	3283	-	-	-	X
57	MG	YA	3287	-	-	-	X
57	MG	YA	3297	-	-	-	X
57	MG	YA	3300	-	-	-	X
57	MG	YA	3327	-	-	-	X
57	MG	YA	3340	-	-	-	X
57	MG	YA	3348	-	-	-	X
57	MG	YA	3353	-	-	-	X
57	MG	YA	3362	-	-	-	X
57	MG	YA	3365	-	-	-	X
57	MG	YA	3371	-	-	-	X
57	MG	YA	3374	-	-	-	X
57	MG	YA	3391	-	-	-	X
57	MG	YA	3444	-	-	-	X
57	MG	YA	3448	-	-	-	X
57	MG	YA	3490	-	-	-	X
57	MG	YA	3499	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3502	-	-	-	X
57	MG	YU	201	-	-	-	X

2 Entry composition (i)

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 217	C 134	N 52	O 31	0	0	0
21	XU	25	Total 217	C 134	N 52	O 31	0	0	0

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

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

- Molecule 23 is a RNA chain called messenger RNA.

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

- Molecule 24 is a protein called Killer protein.

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

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 (three-letter code: 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 Mg 3 3	0	0
57	XA	164	Total Mg 164 164	0	0
57	XD	1	Total Mg 1 1	0	0
57	XE	1	Total Mg 1 1	0	0
57	XF	1	Total Mg 1 1	0	0
57	XK	1	Total Mg 1 1	0	0
57	XL	1	Total Mg 1 1	0	0
57	XN	1	Total Mg 1 1	0	0
57	XS	1	Total Mg 1 1	0	0
57	XV	4	Total Mg 4 4	0	0
57	YA	504	Total Mg 504 504	0	0
57	YB	6	Total Mg 6 6	0	0
57	YD	1	Total Mg 1 1	0	0
57	YE	2	Total Mg 2 2	0	0
57	YF	2	Total Mg 2 2	0	0
57	YG	1	Total Mg 1 1	0	0
57	YH	2	Total Mg 2 2	0	0
57	YN	1	Total Mg 1 1	0	0
57	YO	1	Total Mg 1 1	0	0
57	YP	2	Total Mg 2 2	0	0
57	YQ	2	Total Mg 2 2	0	0

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

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

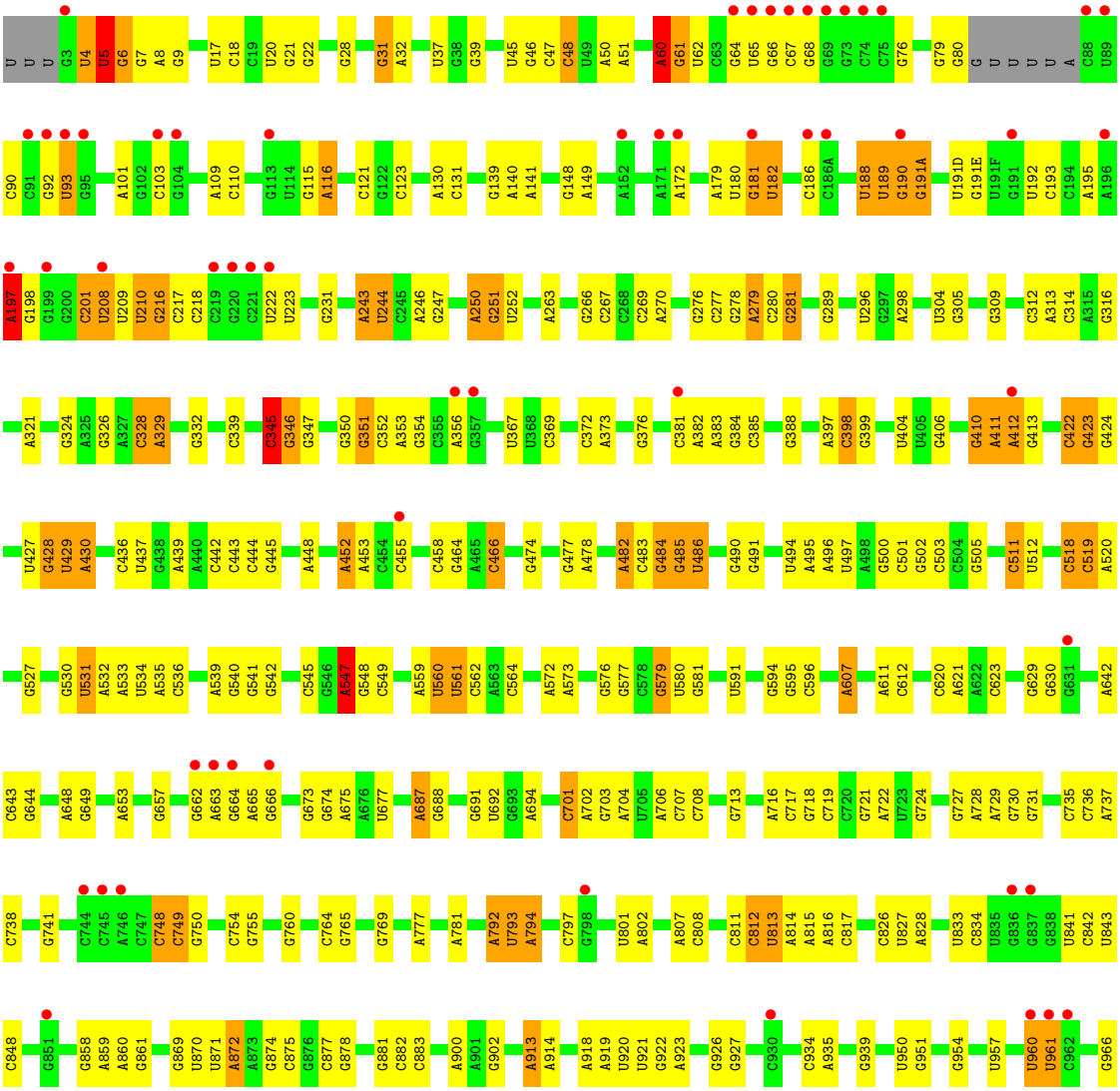
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	QD	1	Total Zn 1 1	0	0
58	QN	1	Total Zn 1 1	0	0
58	XD	1	Total Zn 1 1	0	0
58	XN	1	Total Zn 1 1	0	0

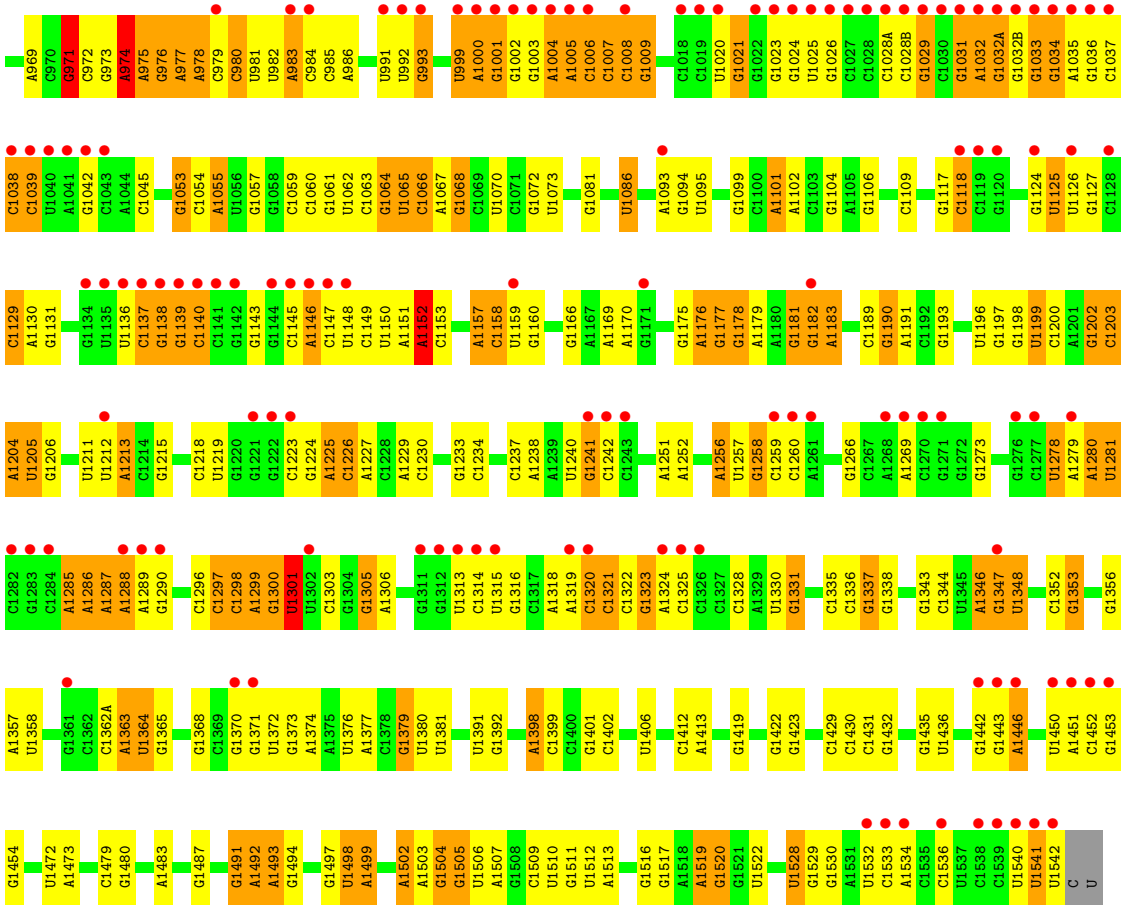
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

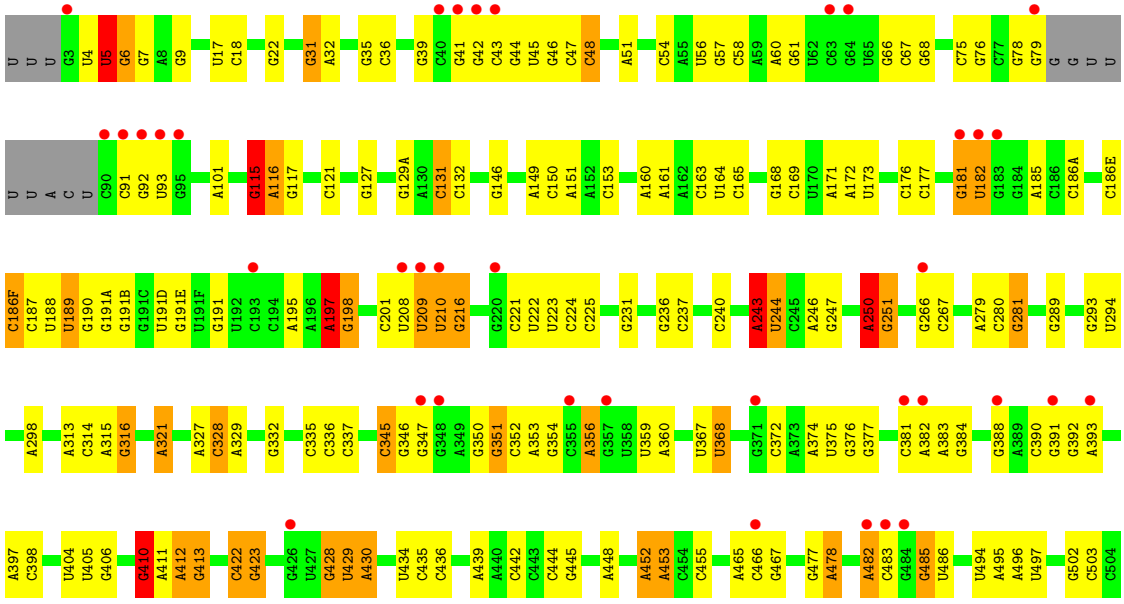
Chain QA:

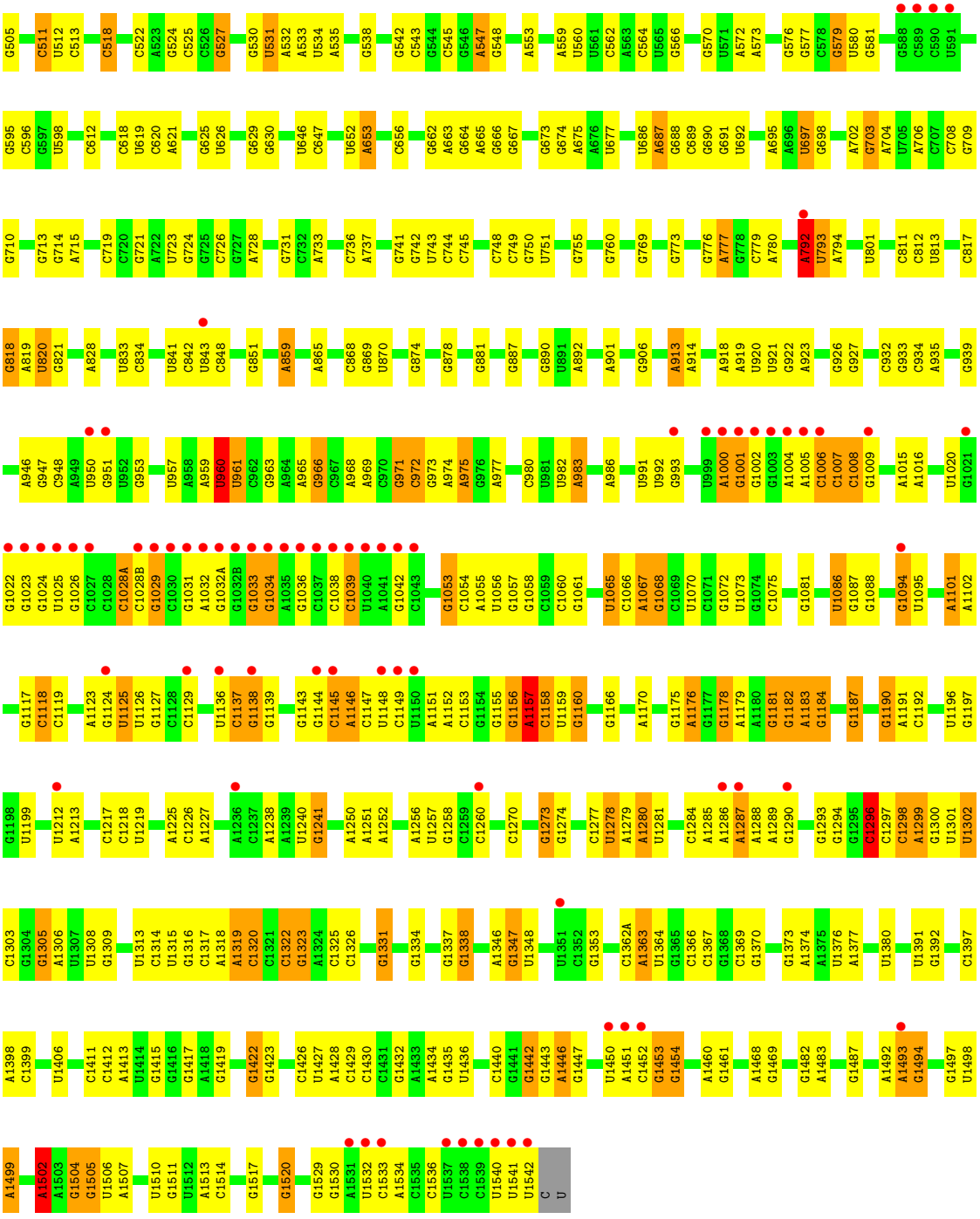




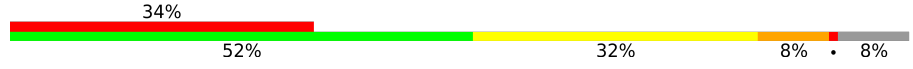
• Molecule 1: 16S rRNA

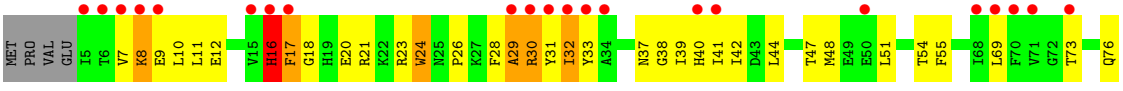
Chain XA:

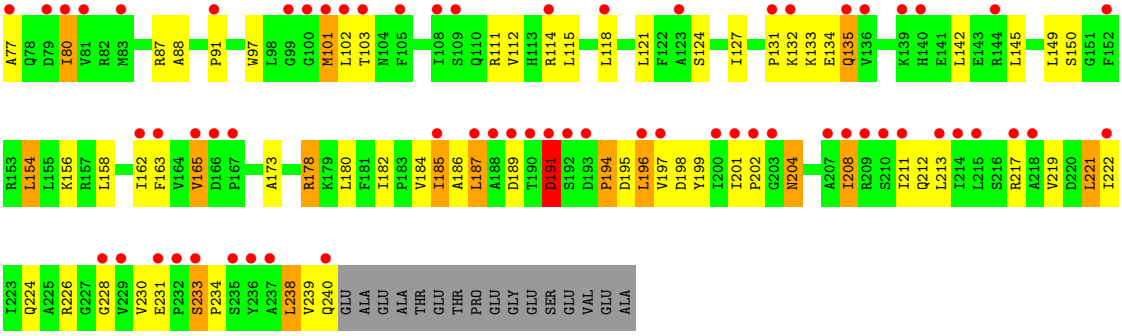




• Molecule 2: 30S ribosomal protein S2

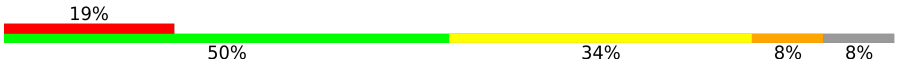


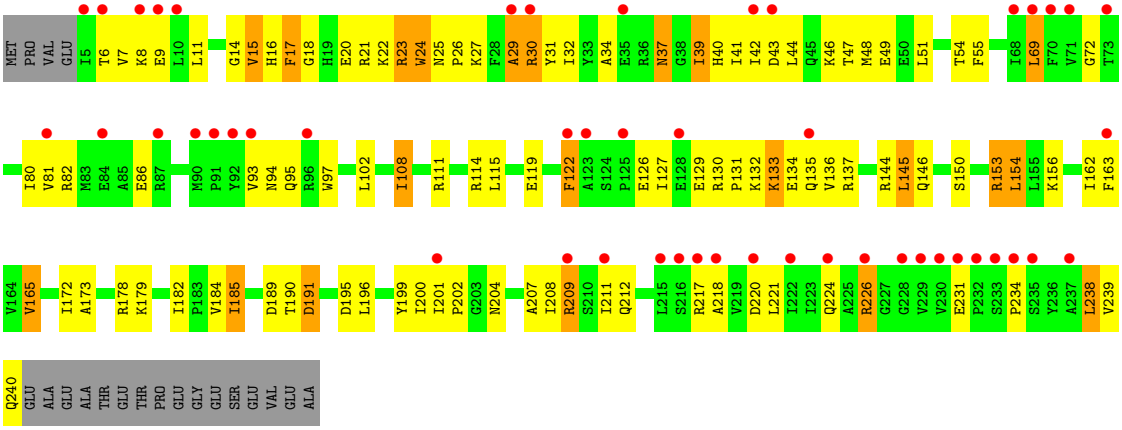




• Molecule 2: 30S ribosomal protein S2

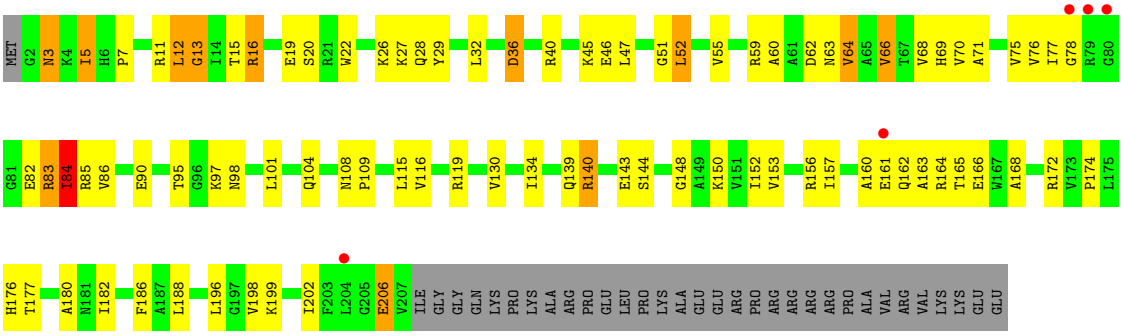
Chain XB:





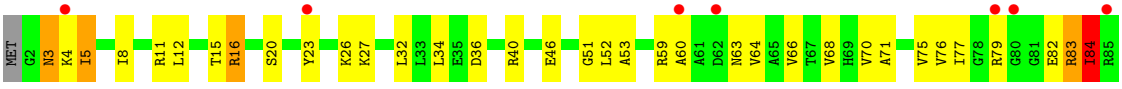
• Molecule 3: 30S ribosomal protein S3

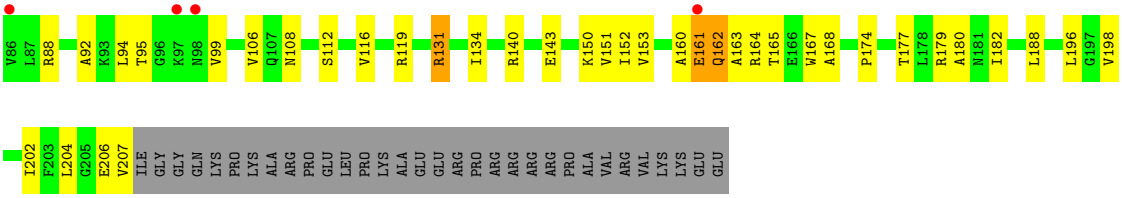
Chain QC:



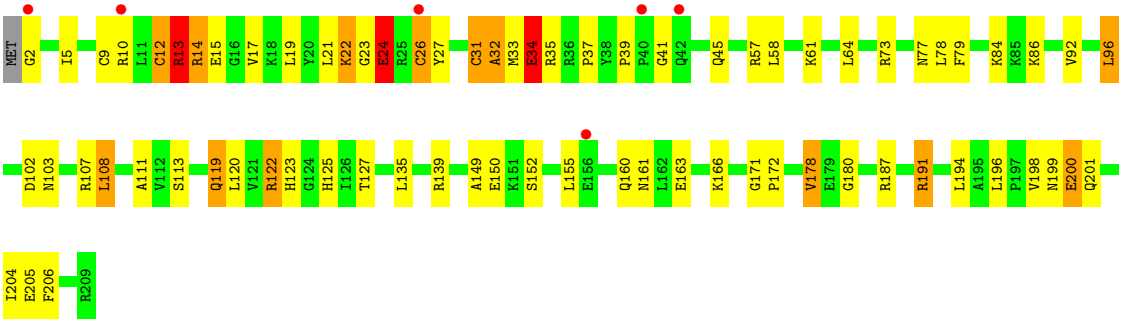
• Molecule 3: 30S ribosomal protein S3

Chain XC:

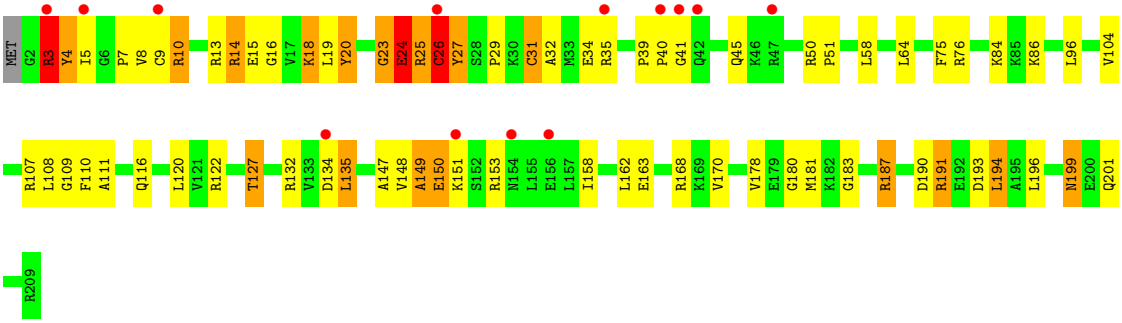




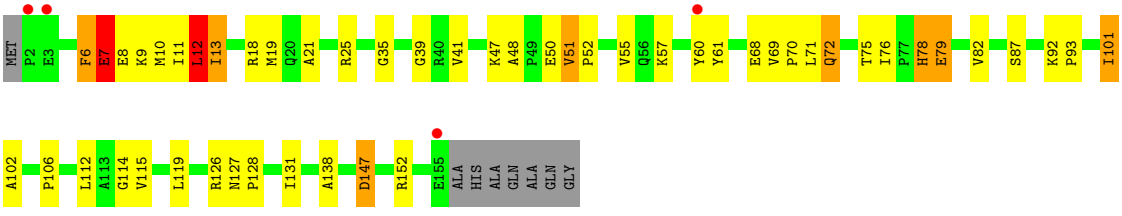
• Molecule 4: 30S ribosomal protein S4



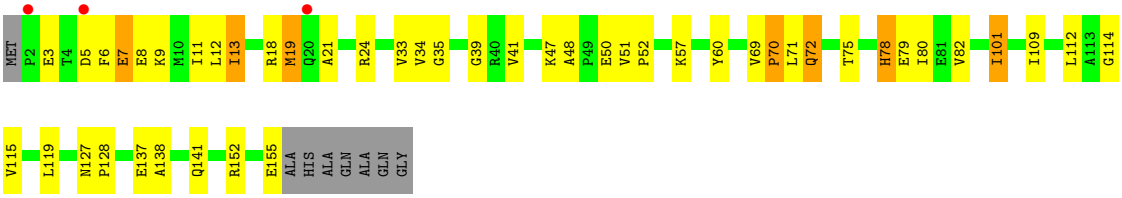
• Molecule 4: 30S ribosomal protein S4



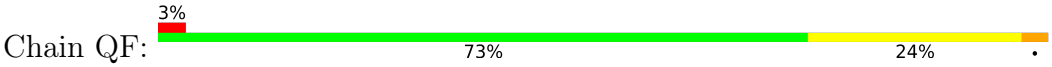
• Molecule 5: 30S ribosomal protein S5

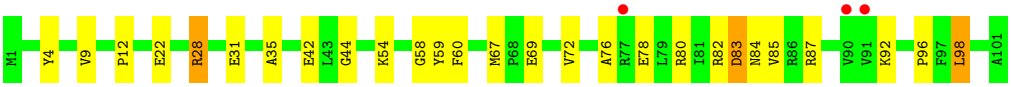


• Molecule 5: 30S ribosomal protein S5

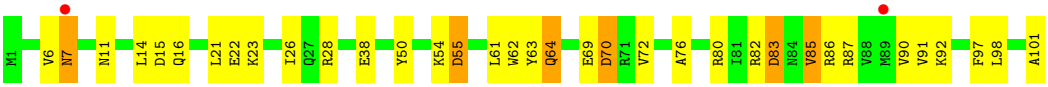


• Molecule 6: 30S ribosomal protein S6

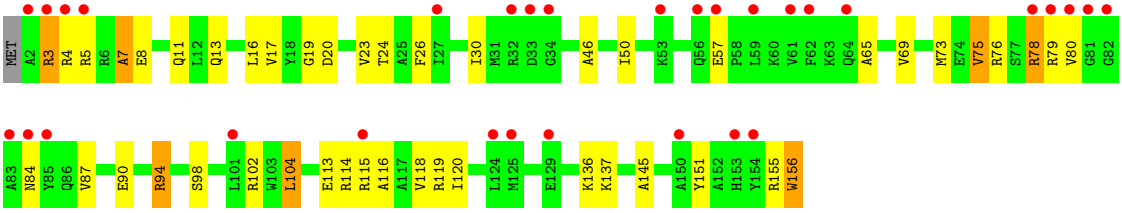




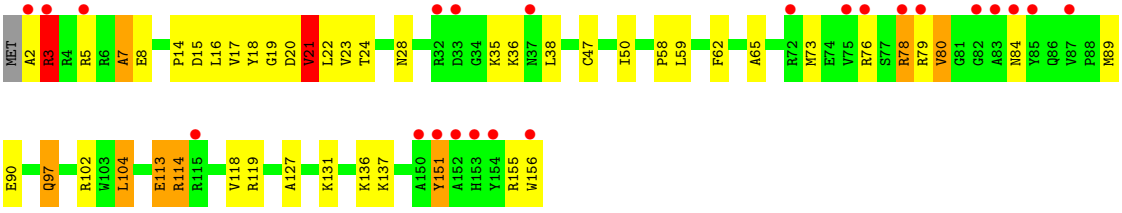
• Molecule 6: 30S ribosomal protein S6



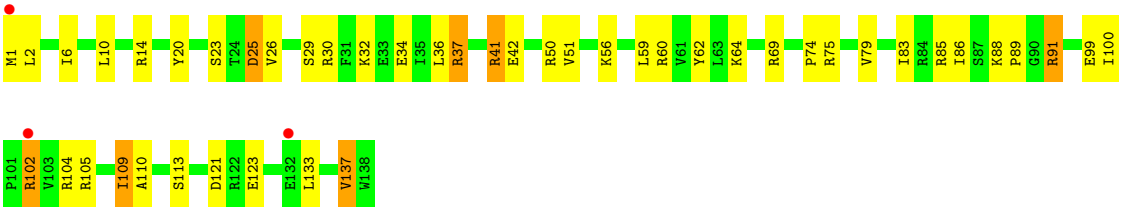
• Molecule 7: 30S ribosomal protein S7



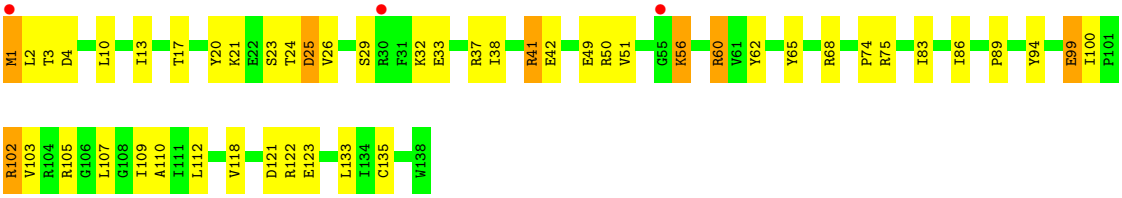
• Molecule 7: 30S ribosomal protein S7



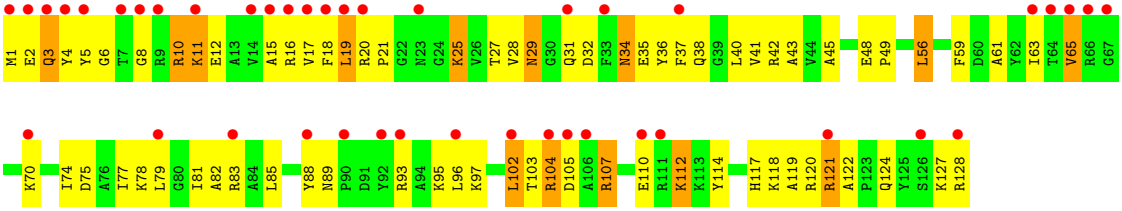
• Molecule 8: 30S ribosomal protein S8



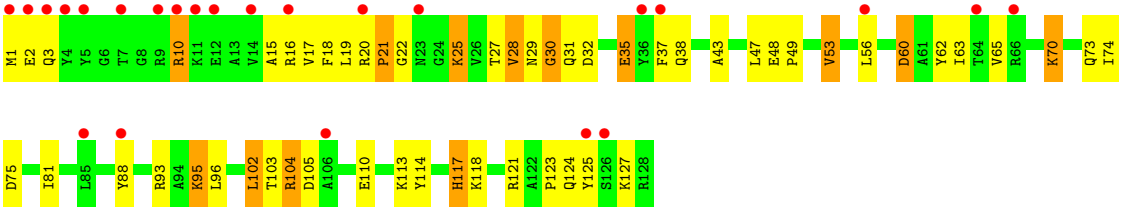
• Molecule 8: 30S ribosomal protein S8



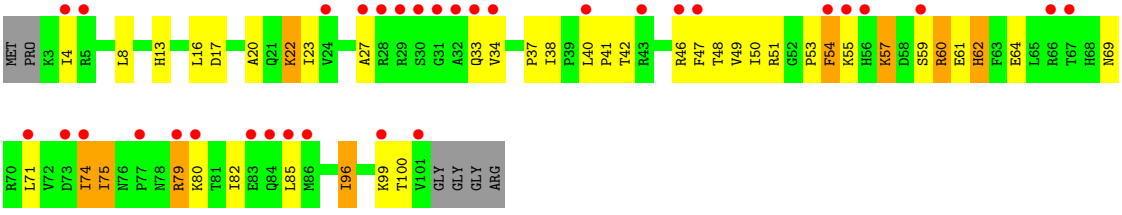
• Molecule 9: 30S ribosomal protein S9



• Molecule 9: 30S ribosomal protein S9

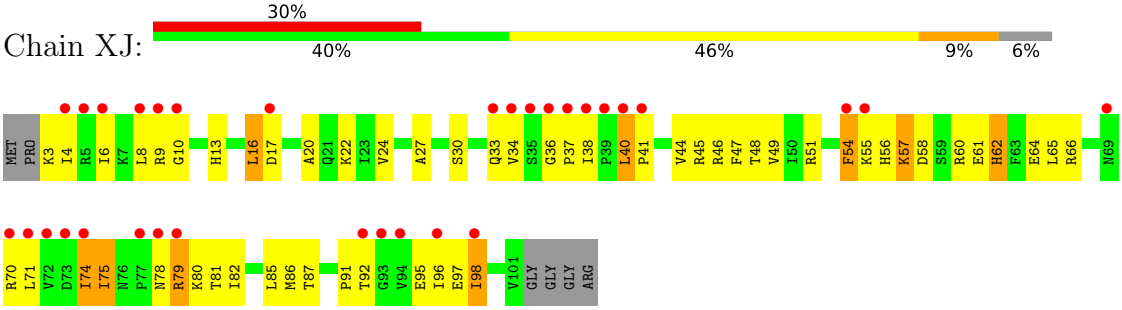


• Molecule 10: 30S ribosomal protein S10



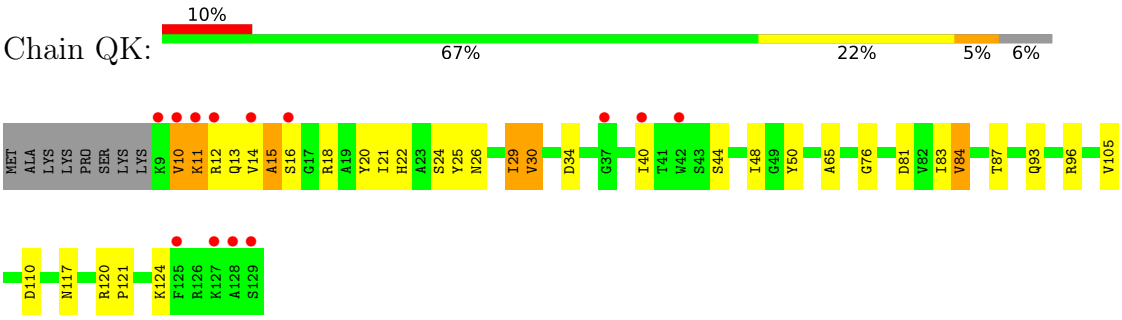
• Molecule 10: 30S ribosomal protein S10

Chain XJ:



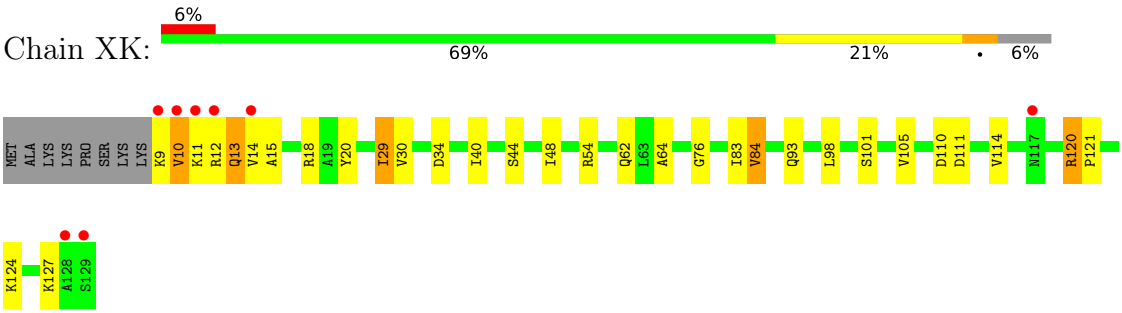
• Molecule 11: 30S ribosomal protein S11

Chain QK:



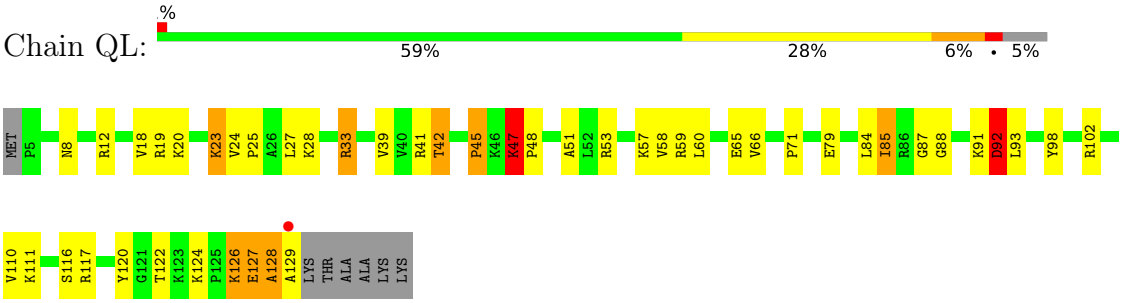
• Molecule 11: 30S ribosomal protein S11

Chain XK:



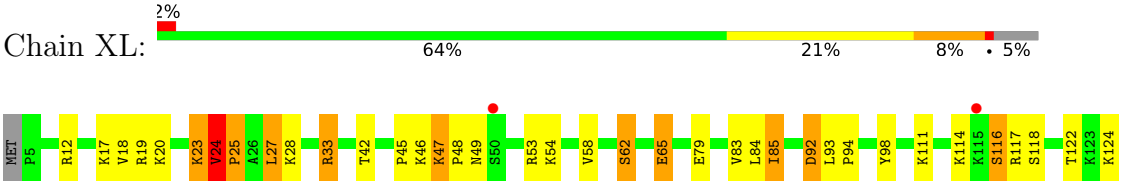
• Molecule 12: 30S ribosomal protein S12

Chain QL:



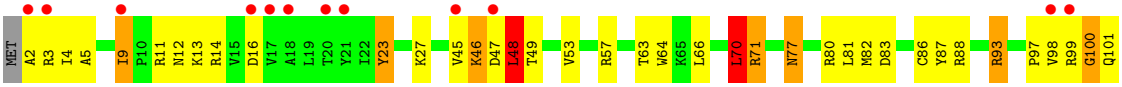
• Molecule 12: 30S ribosomal protein S12

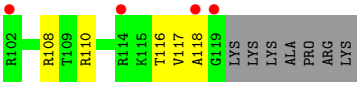
Chain XL:



• Molecule 13: 30S ribosomal protein S13

Chain QM:





• Molecule 13: 30S ribosomal protein S13

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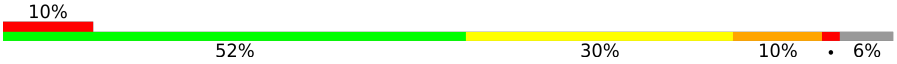
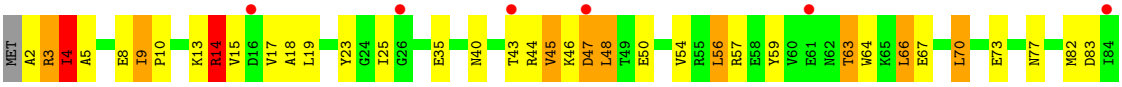
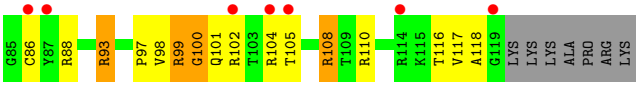
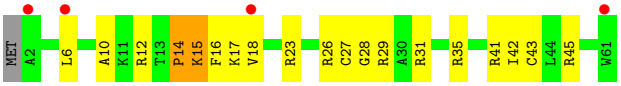






• Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:



• Molecule 14: 30S ribosomal protein S14 type Z

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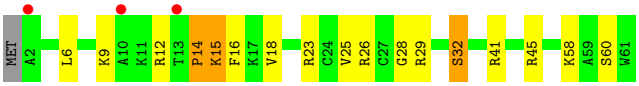
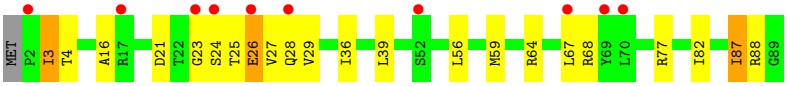


• Molecule 15: 30S ribosomal protein S15

Chain QO:



• Molecule 15: 30S ribosomal protein S15

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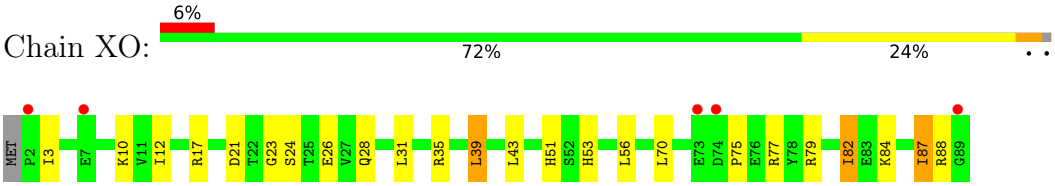
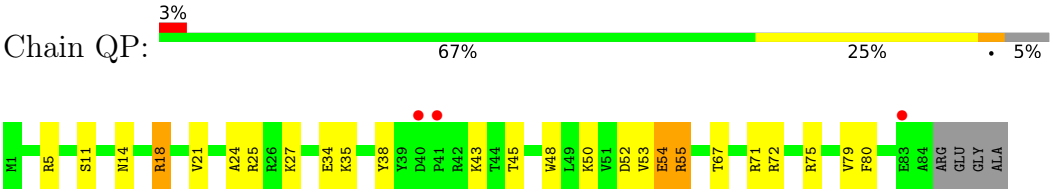


• Molecule 16: 30S ribosomal protein S16

Chain QP:



• Molecule 16: 30S ribosomal protein S16

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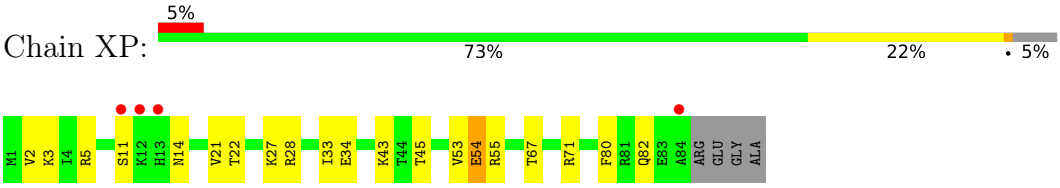

• Molecule 17: 30S ribosomal protein S17

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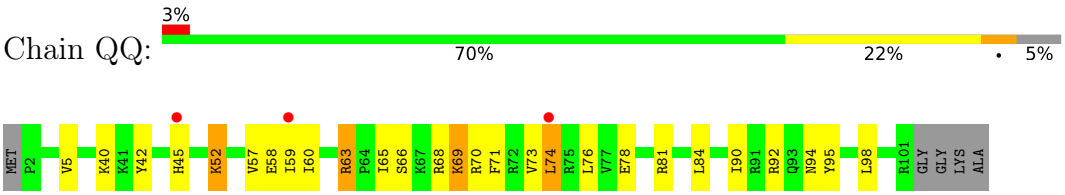
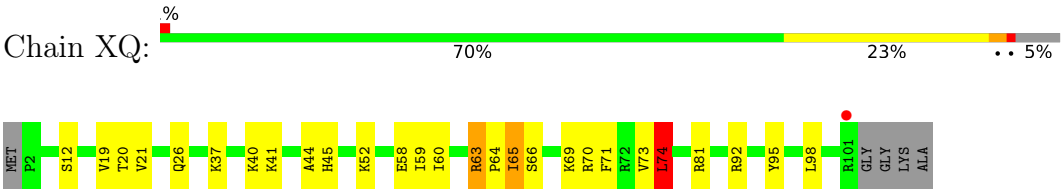


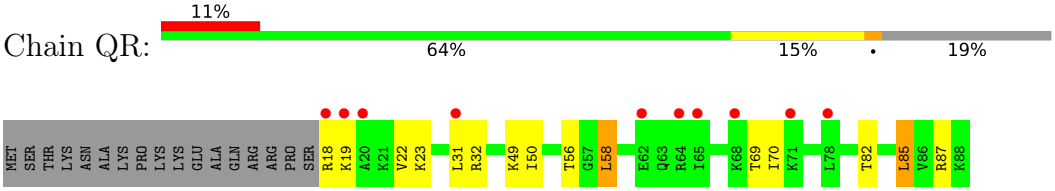
• Molecule 17: 30S ribosomal protein S17

Chain XQ:



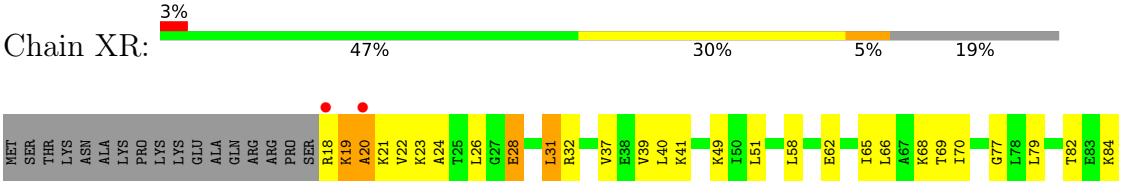
• Molecule 18: 30S ribosomal protein S18

Chain QR:



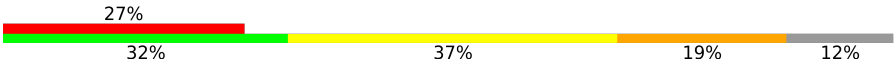
• Molecule 18: 30S ribosomal protein S18

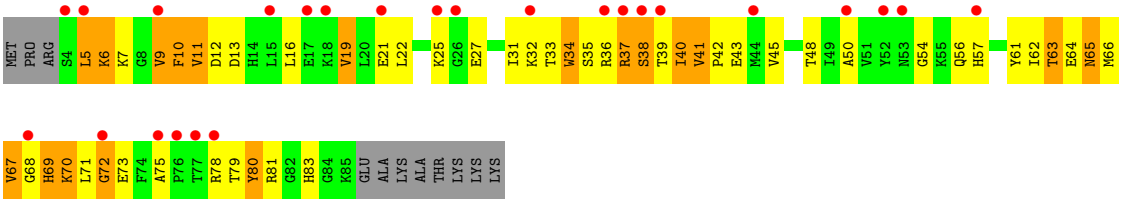
Chain XR:



• Molecule 19: 30S ribosomal protein S19

Chain QS:





• Molecule 19: 30S ribosomal protein S19

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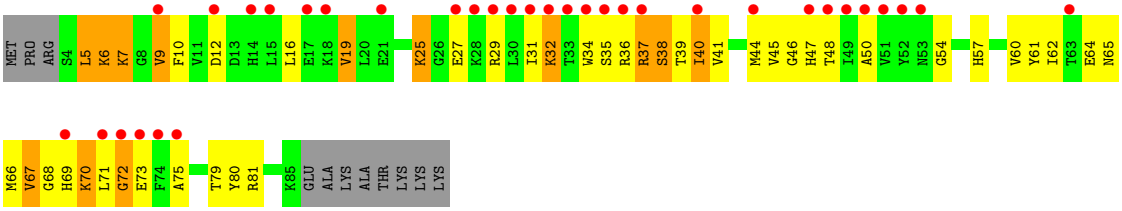
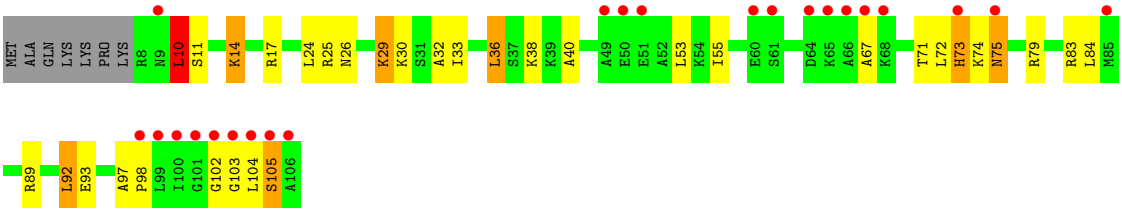


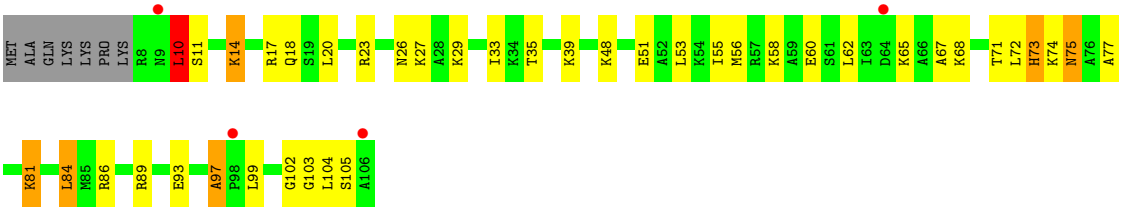
• Molecule 20: 30S ribosomal protein S20

Chain QT:



• Molecule 20: 30S ribosomal protein S20

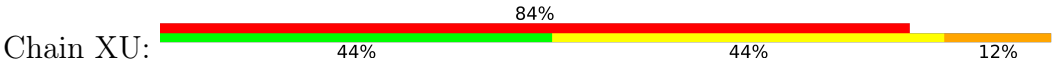
Chain XT:



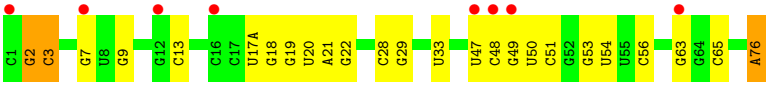
• Molecule 21: 30S ribosomal protein Thx

Chain QU:

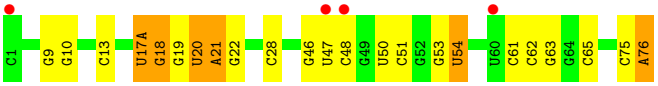
• Molecule 21: 30S ribosomal protein Thx



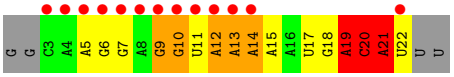
• Molecule 22: P-site tRNA-fMet



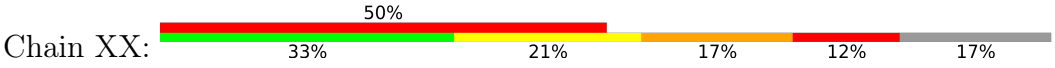
• Molecule 22: P-site tRNA-fMet

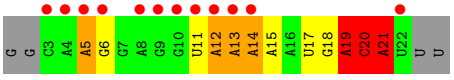


• Molecule 23: messenger RNA

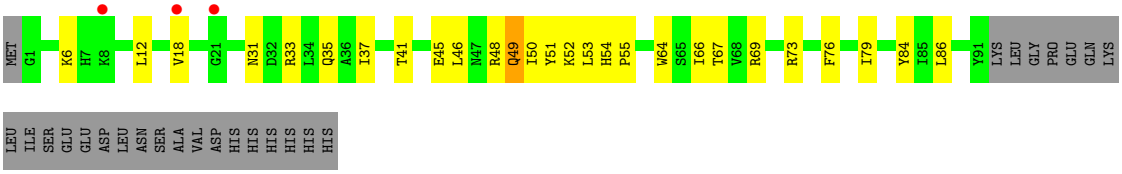


• Molecule 23: messenger RNA



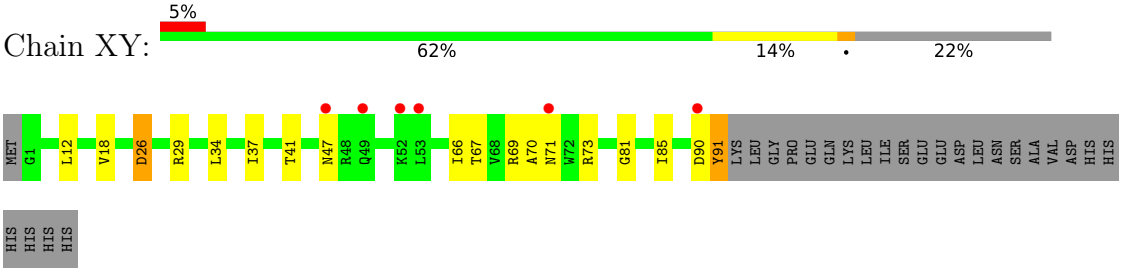


• Molecule 24: Killer protein



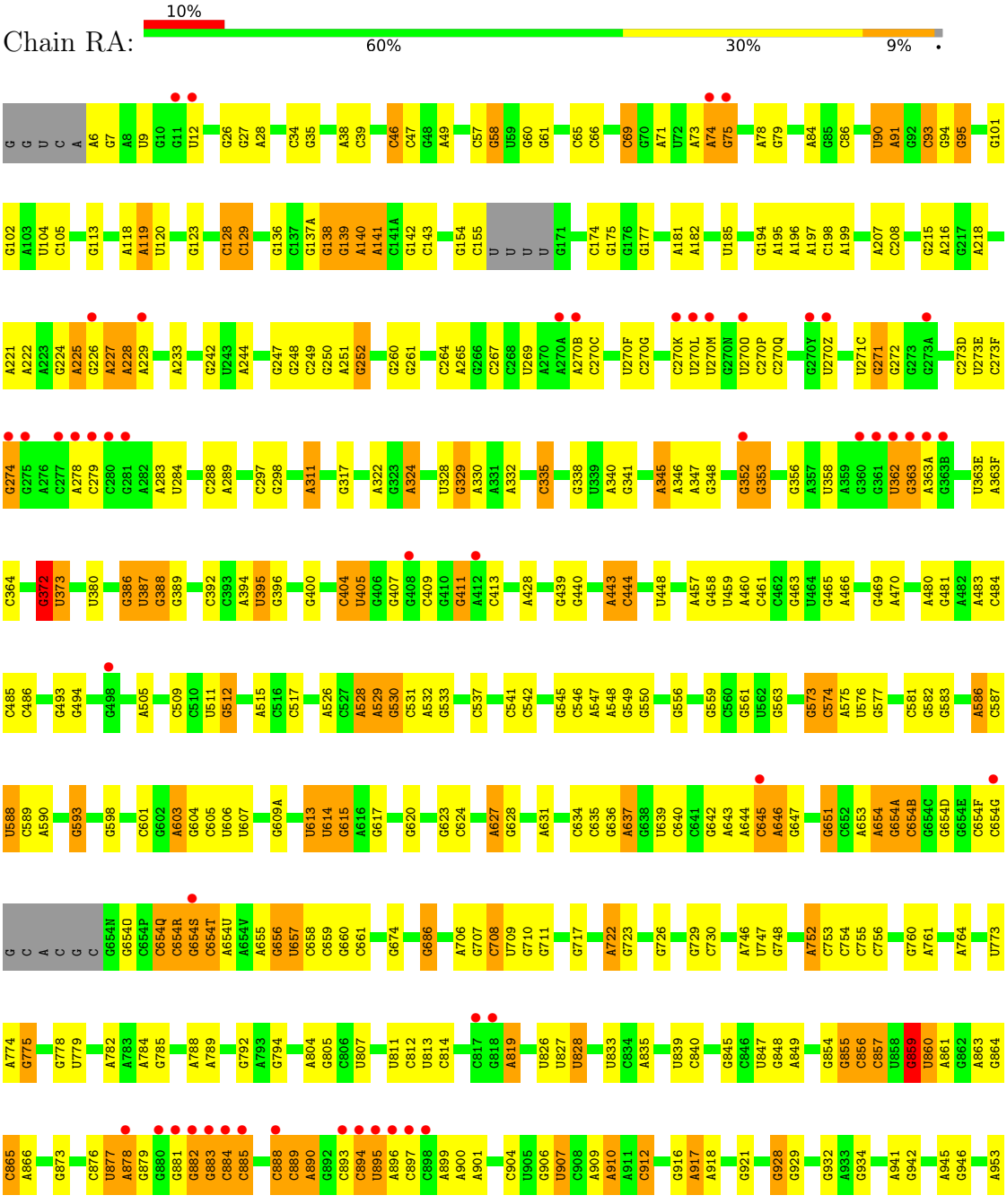
• Molecule 24: Killer protein

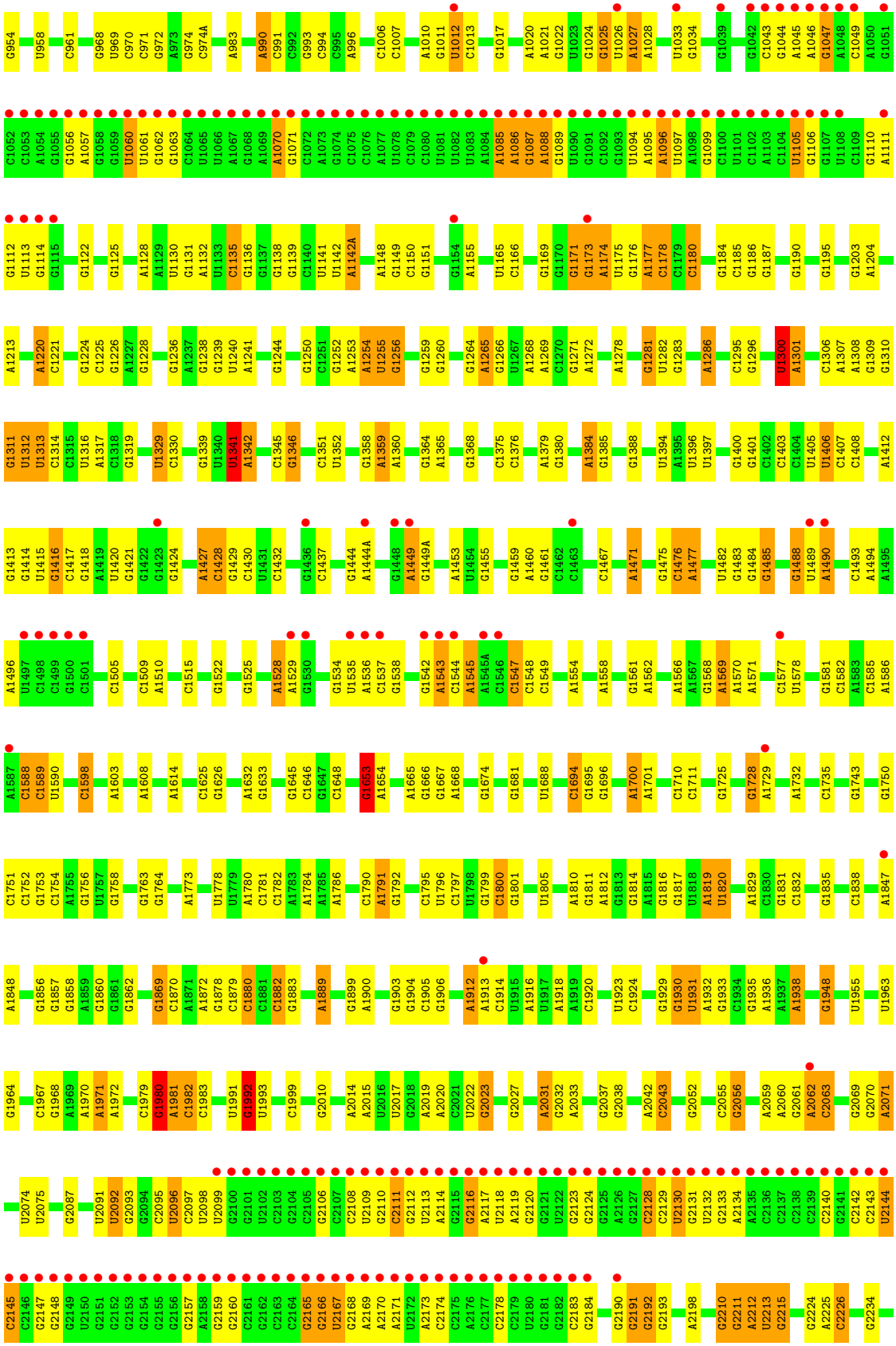
Chain XY:



• Molecule 25: 23S rRNA

Chain RA:

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C1052 C1053 A1054 G1055 G1056 A1057 G1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 C1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 G1089 U1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108 C1109 G1110 A1111
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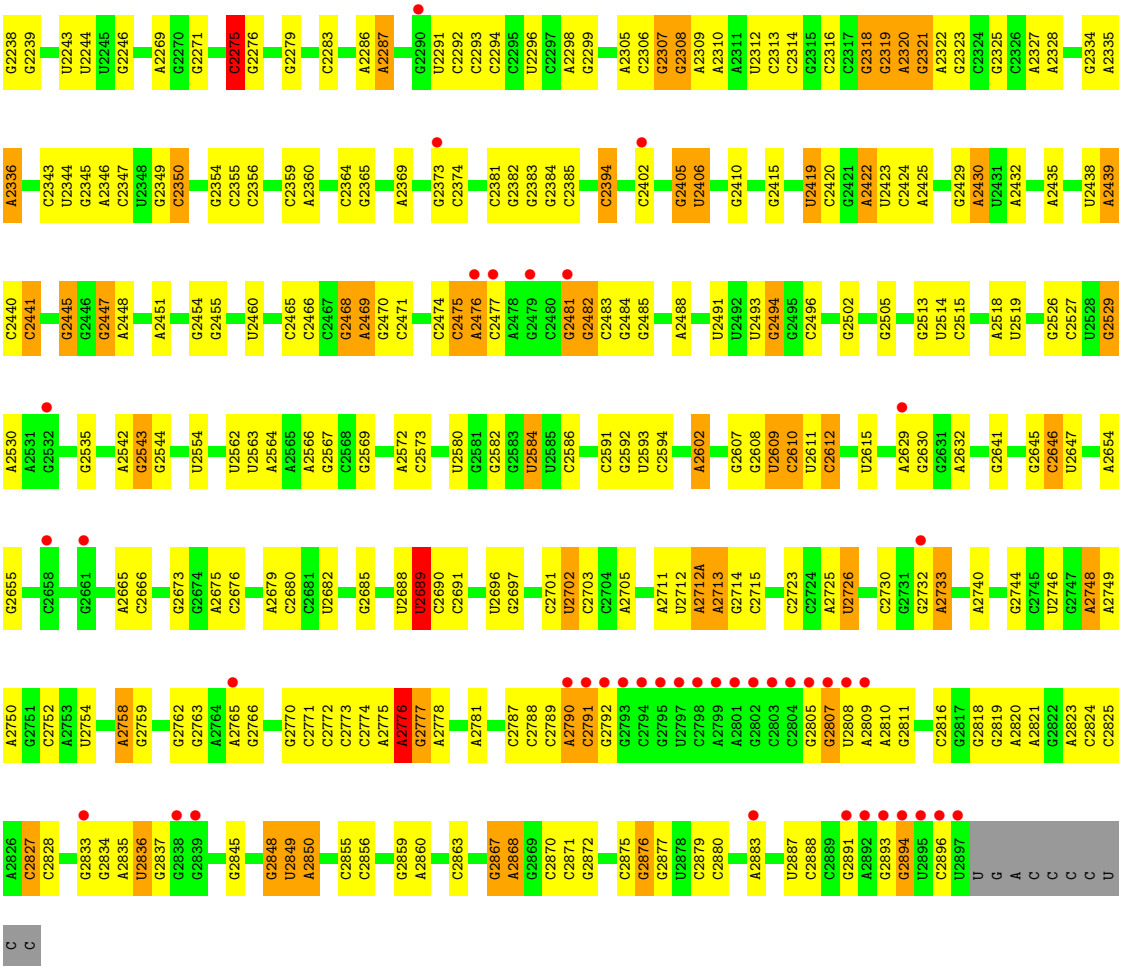
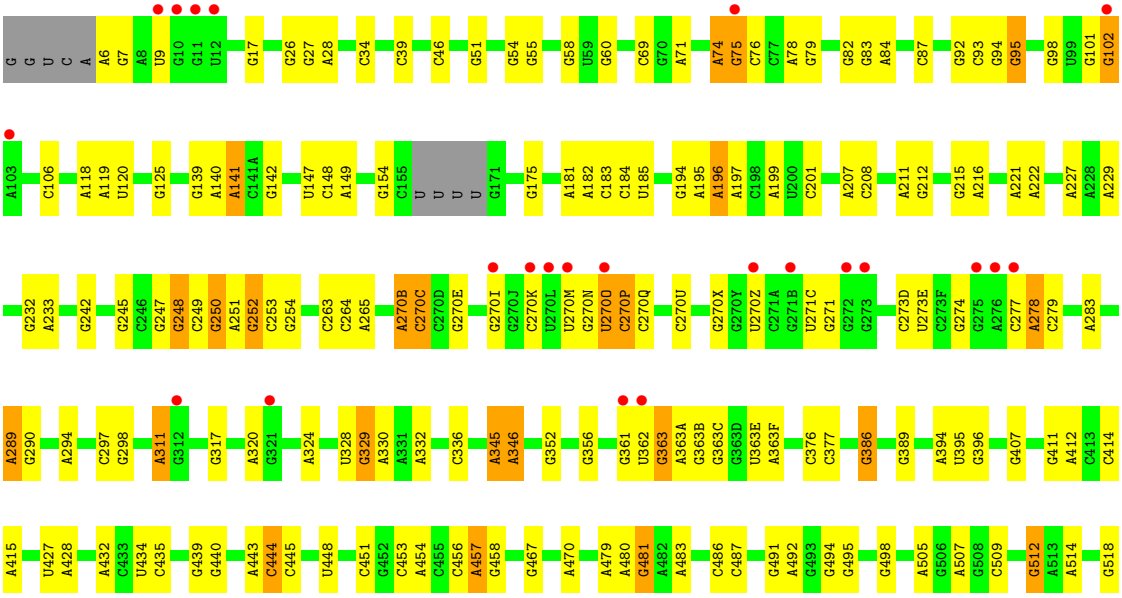
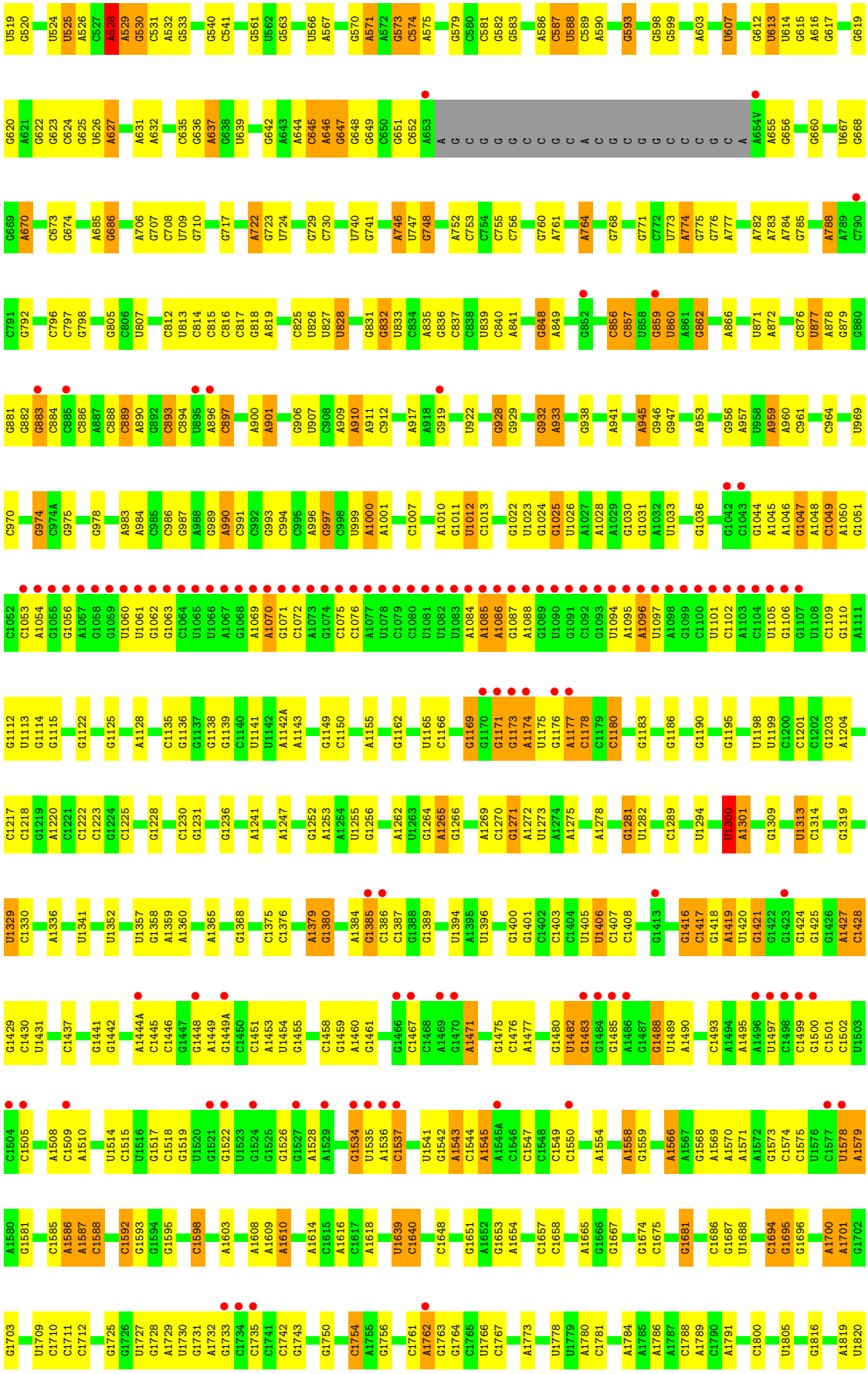


• Molecule 25: 23S rRNA

Chain YA:

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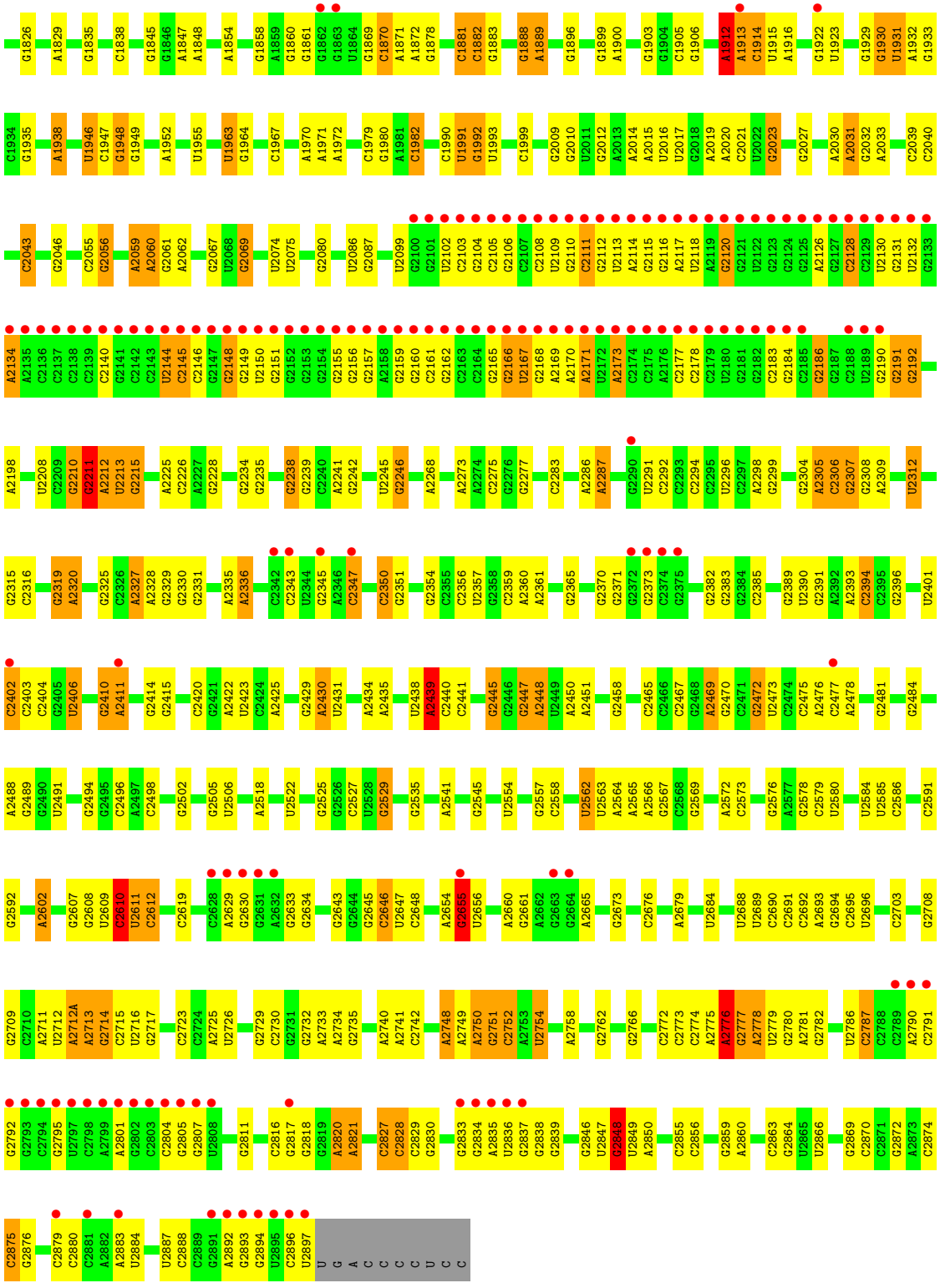
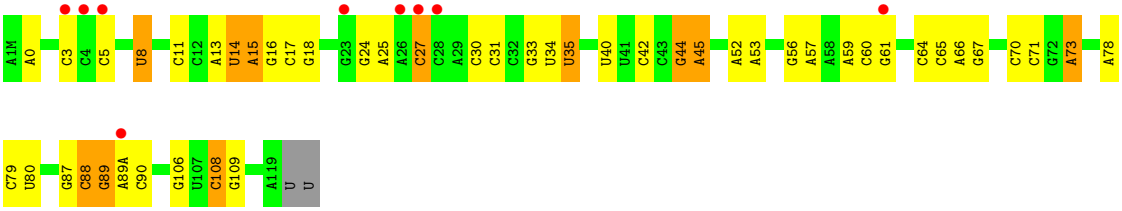
G1703 U1709 C1710 C1711 C1712 G1725 G1726 U1727 G1728 A1729 U1730 G1731 A1732 G1733 C1734 C1735 C1741 C1742 G1743 G1750 C1754 A1755 G1756 C1761 A1762 G1763 G1764 C1765 U1766 C1767 A1773 U1778 U1779 A1780 C1781 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 C1800 U1805 G1816 A1819 U1820



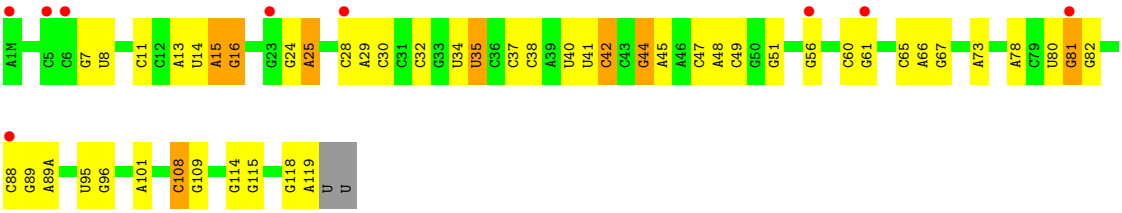
• Molecule 26: 5S rRNA

Chain RB:



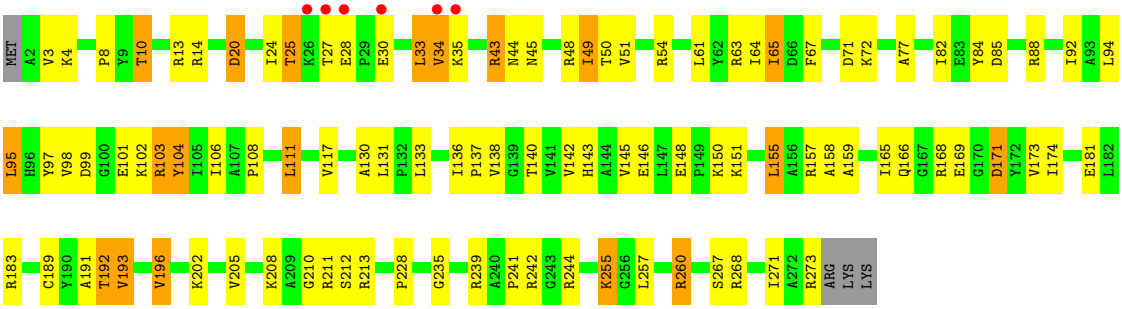
• Molecule 26: 5S rRNA

Chain YB:



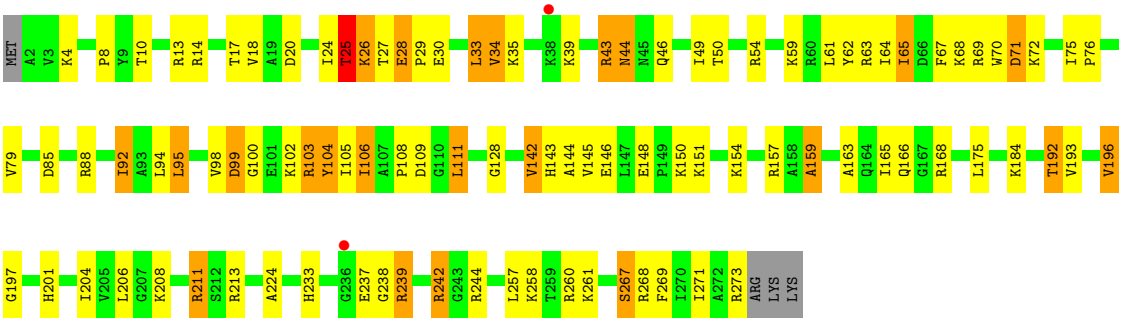
• Molecule 27: 50S ribosomal protein L2

Chain RD:



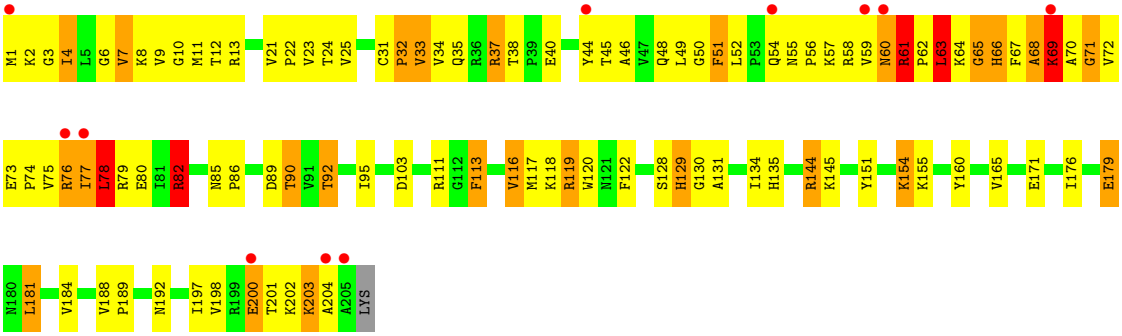
• Molecule 27: 50S ribosomal protein L2

Chain YD:

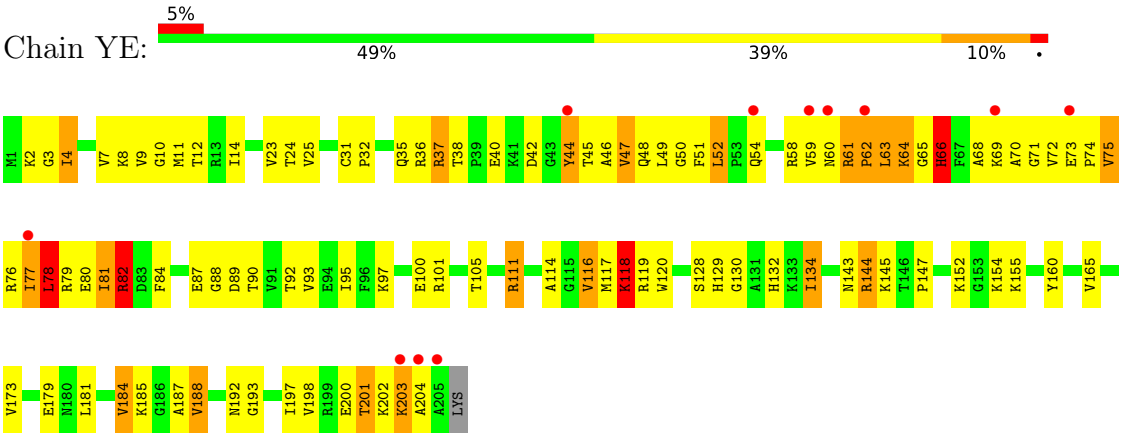


• Molecule 28: 50S ribosomal protein L3

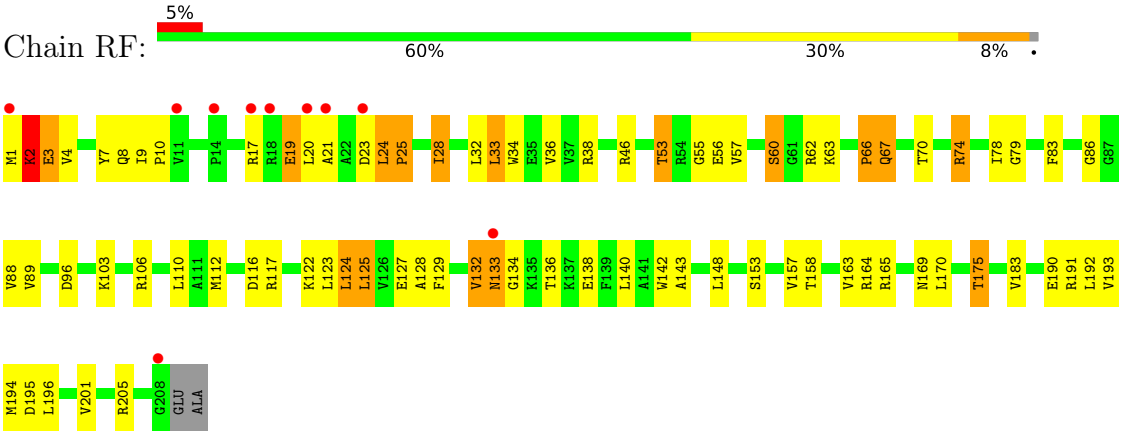
Chain RE:



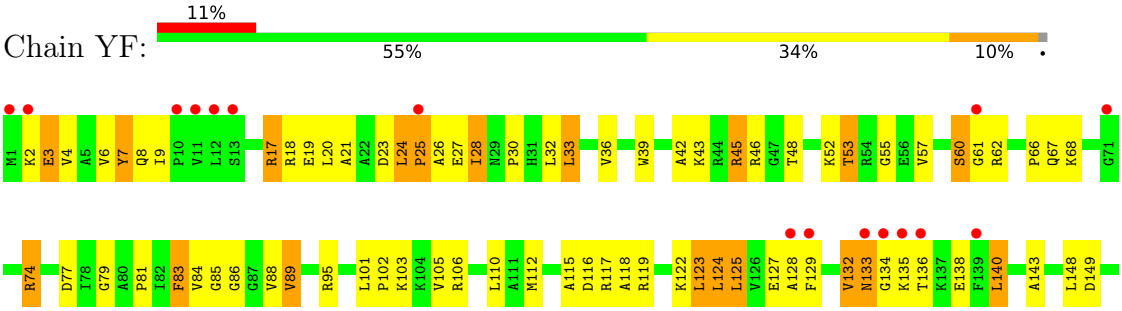
• Molecule 28: 50S ribosomal protein L3

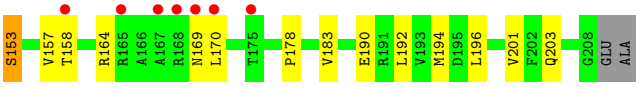


• Molecule 29: 50S ribosomal protein L4



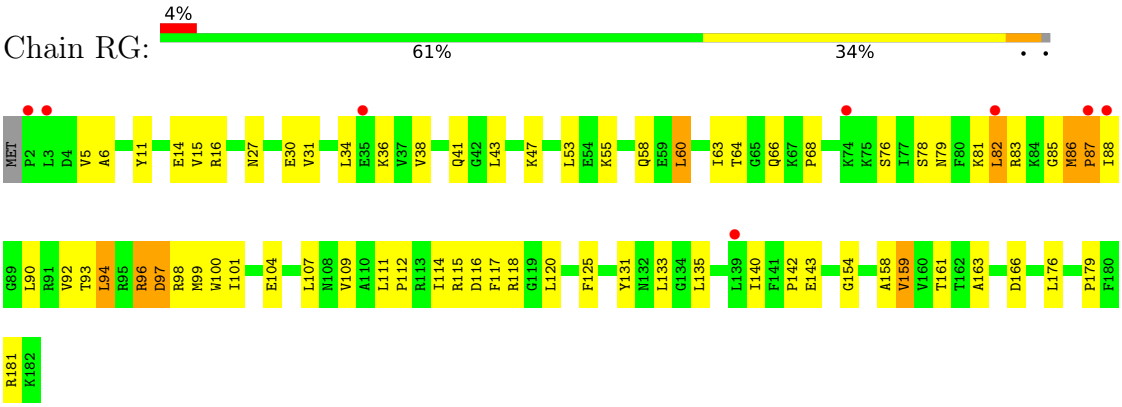
• Molecule 29: 50S ribosomal protein L4





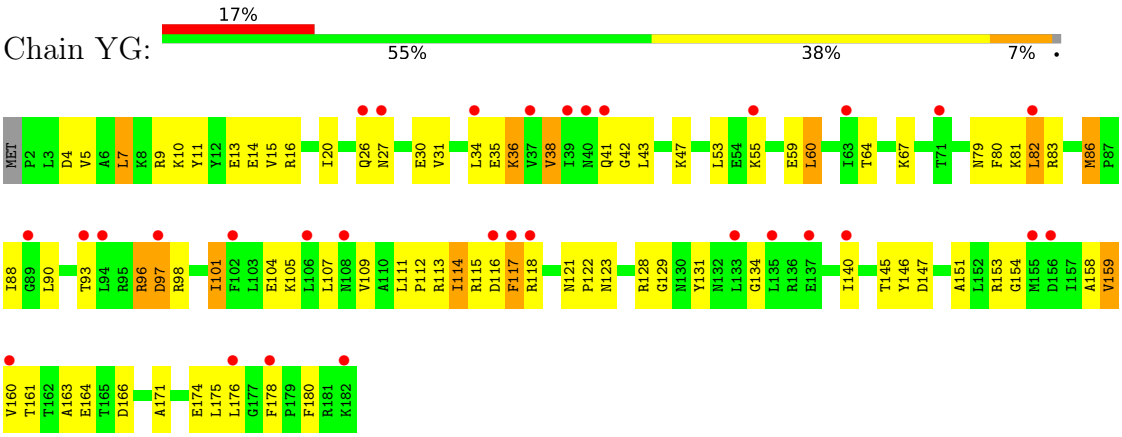
• Molecule 30: 50S ribosomal protein L5

Chain RG:



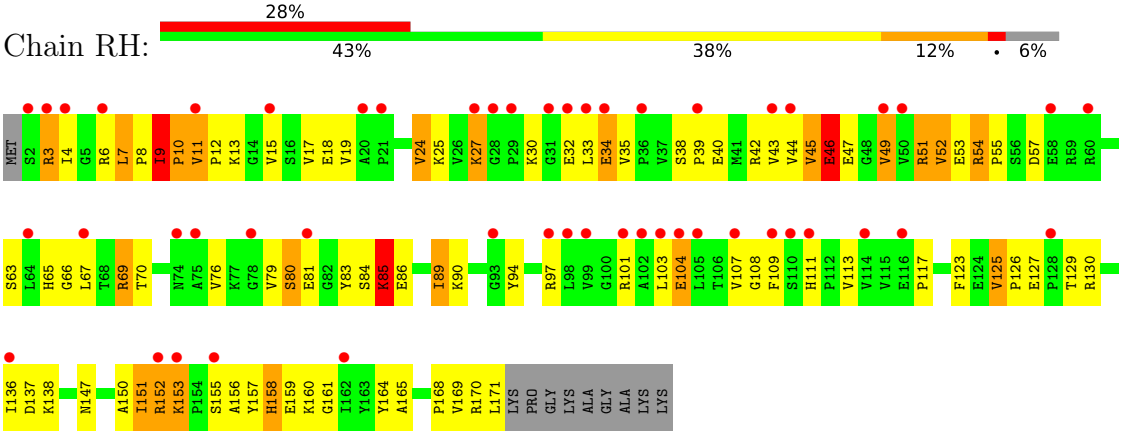
• Molecule 30: 50S ribosomal protein L5

Chain YG:



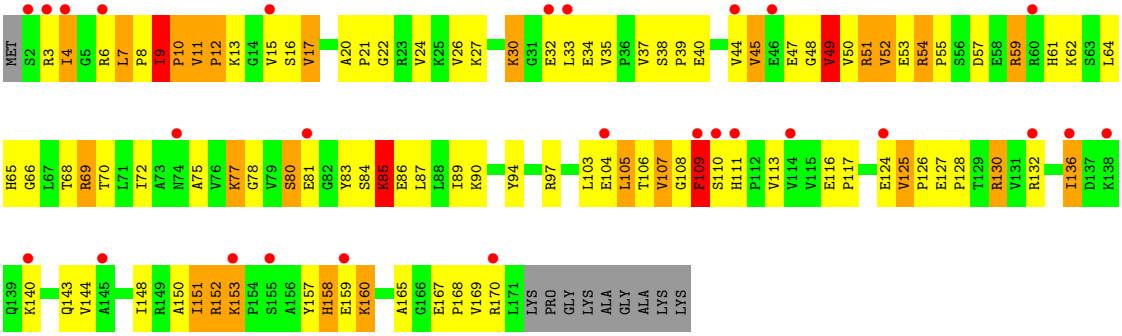
• Molecule 31: 50S ribosomal protein L6

Chain RH:



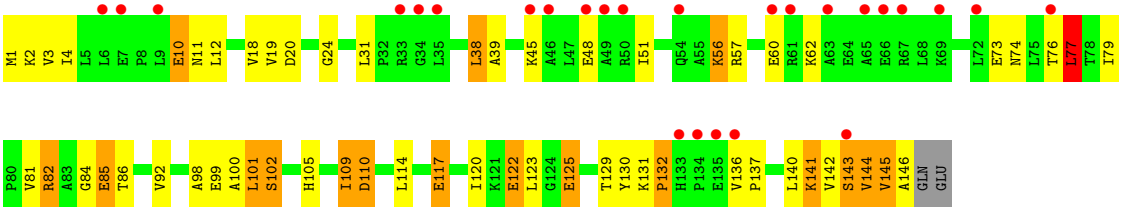
• Molecule 31: 50S ribosomal protein L6

Chain YH:



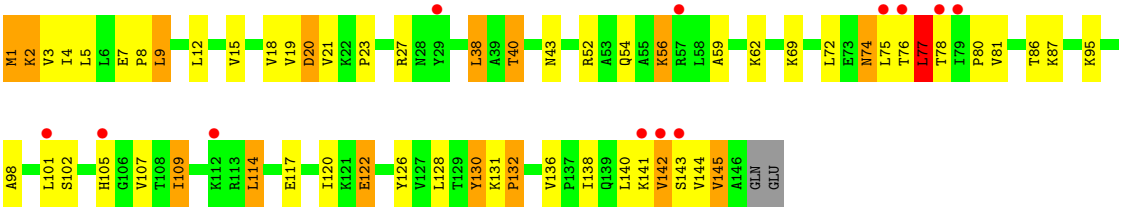
• Molecule 32: 50S ribosomal protein L9

Chain RI:



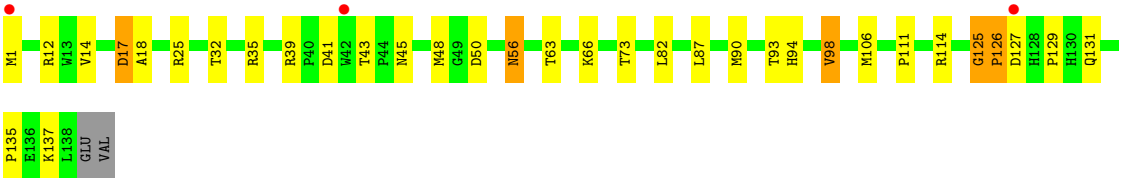
• Molecule 32: 50S ribosomal protein L9

Chain YI:



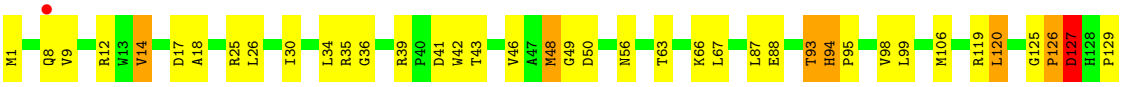
• Molecule 33: 50S ribosomal protein L13

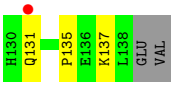
Chain RN:



• Molecule 33: 50S ribosomal protein L13

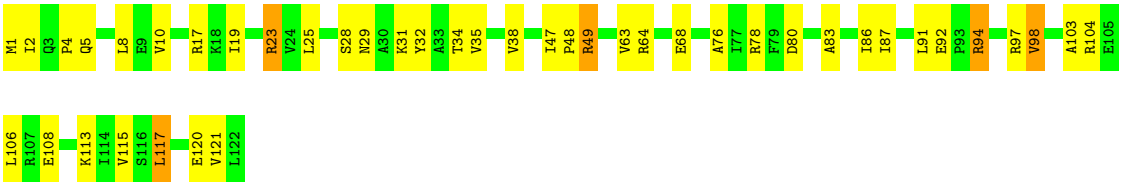
Chain YN:





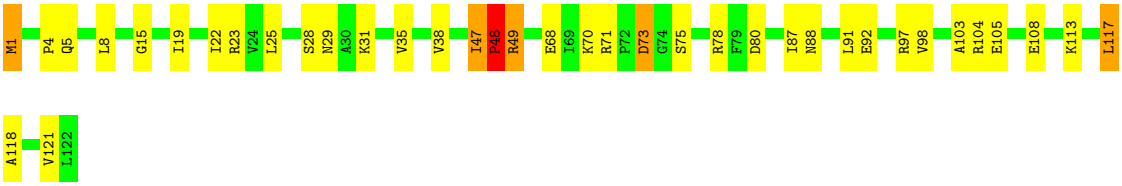
• Molecule 34: 50S ribosomal protein L14

Chain RO:



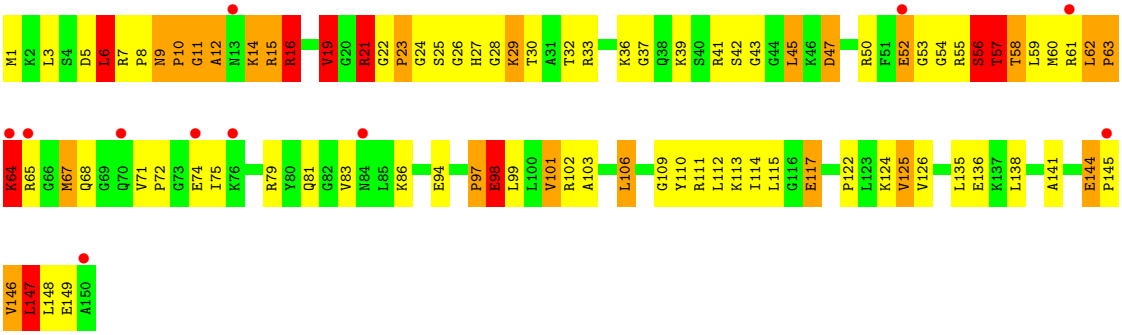
• Molecule 34: 50S ribosomal protein L14

Chain YO:



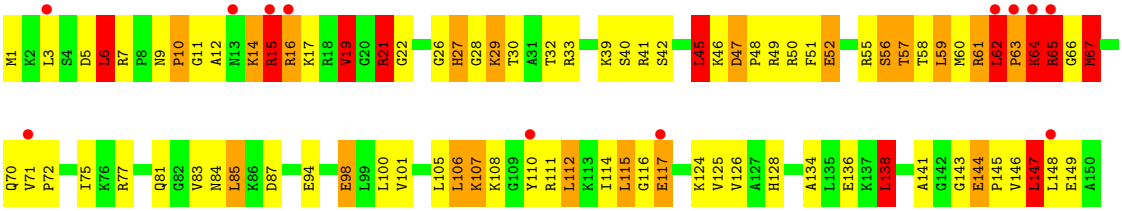
• Molecule 35: 50S ribosomal protein L15

Chain RP:



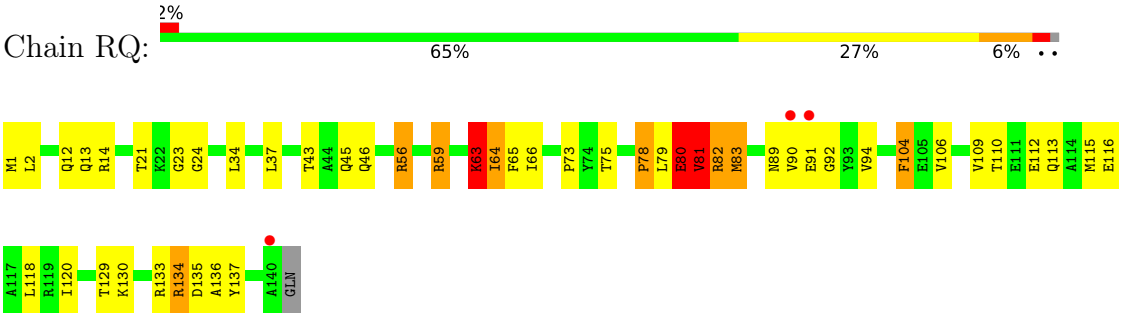
• Molecule 35: 50S ribosomal protein L15

Chain YP:



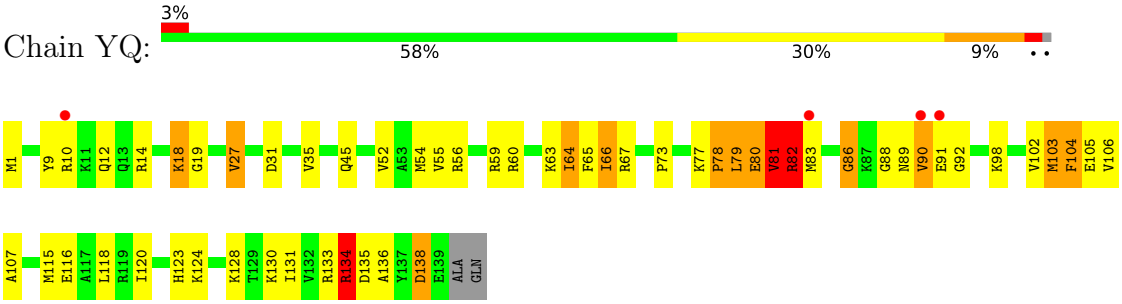
• Molecule 36: 50S ribosomal protein L16

Chain RQ:



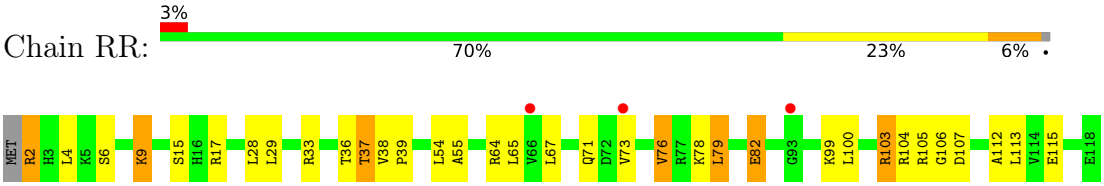
• Molecule 36: 50S ribosomal protein L16

Chain YQ:



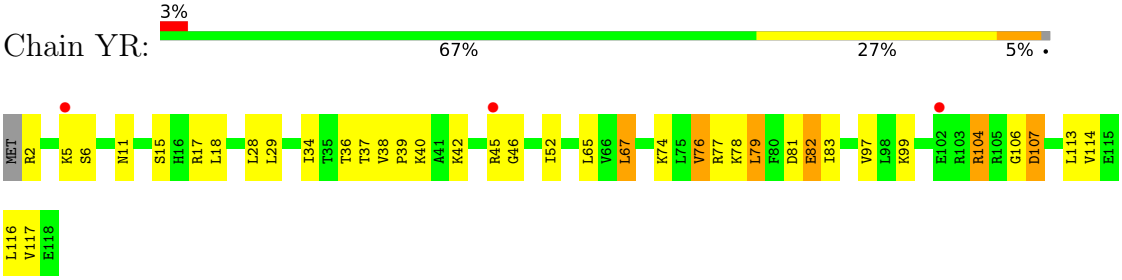
• Molecule 37: 50S ribosomal protein L17

Chain RR:



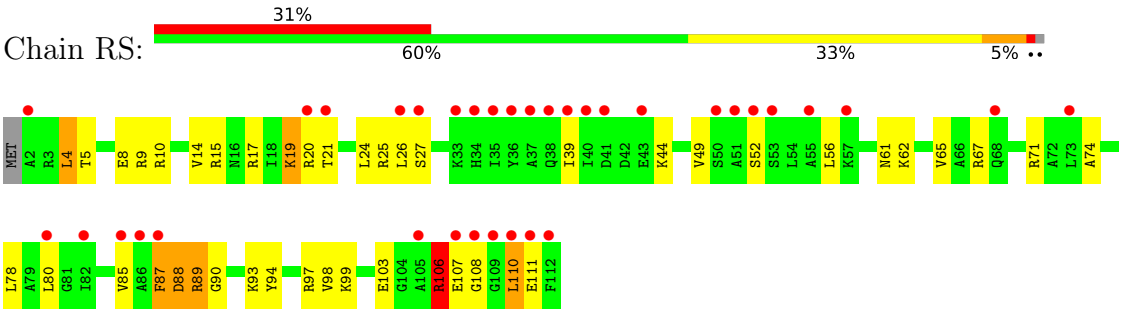
• Molecule 37: 50S ribosomal protein L17

Chain YR:



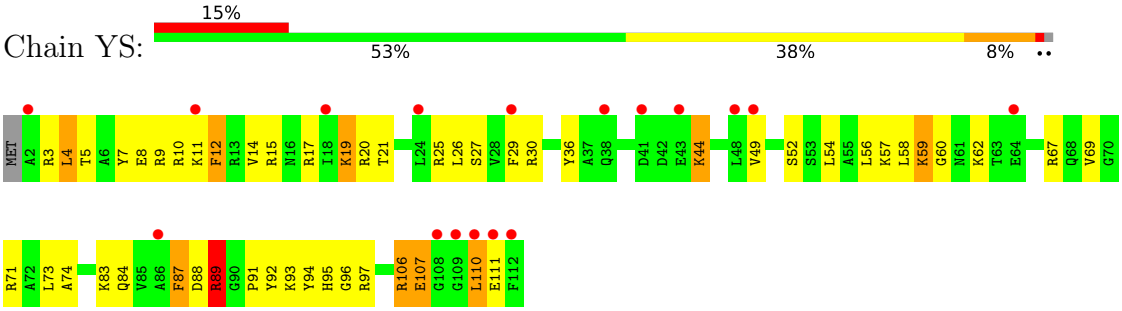
• Molecule 38: 50S ribosomal protein L18

Chain RS:



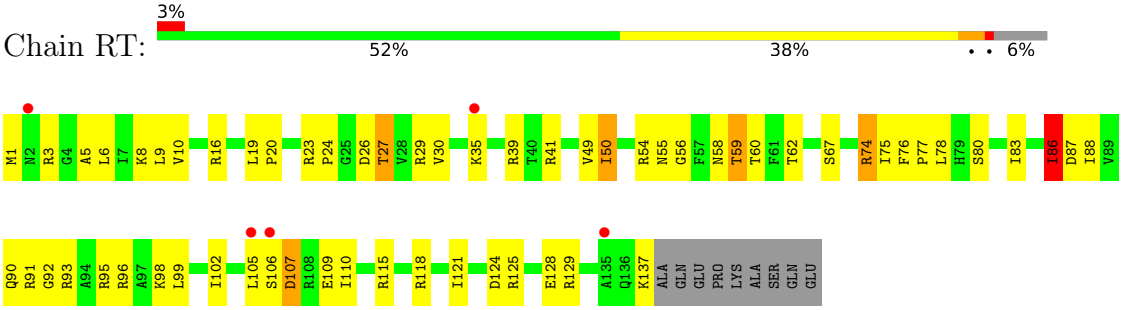
• Molecule 38: 50S ribosomal protein L18

Chain YS:



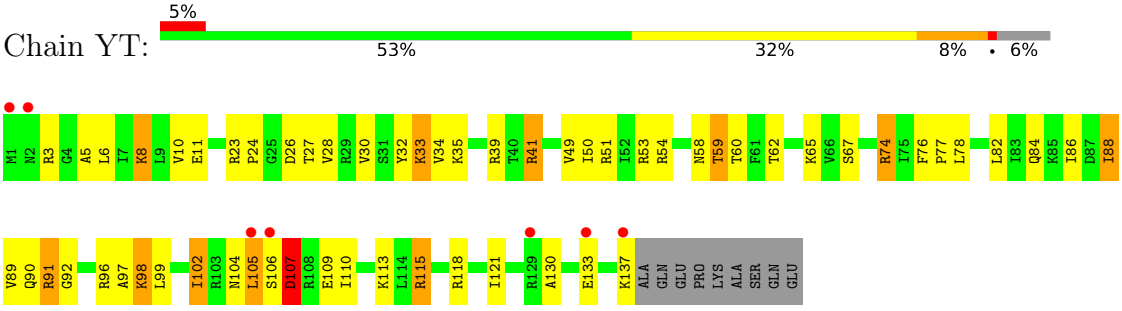
• Molecule 39: 50S ribosomal protein L19

Chain RT:



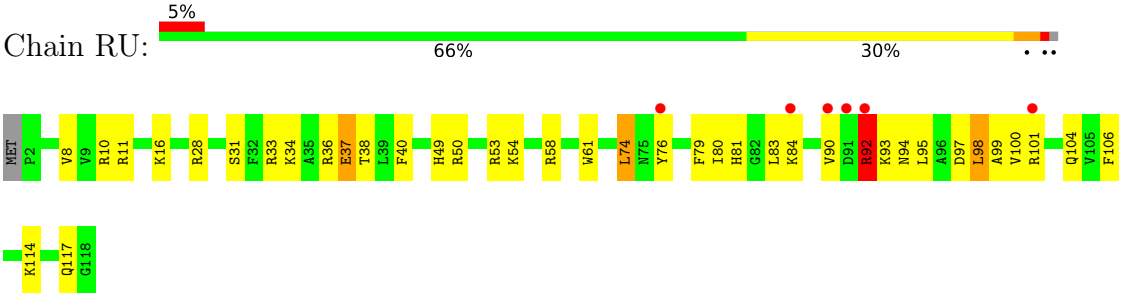
• Molecule 39: 50S ribosomal protein L19

Chain YT:



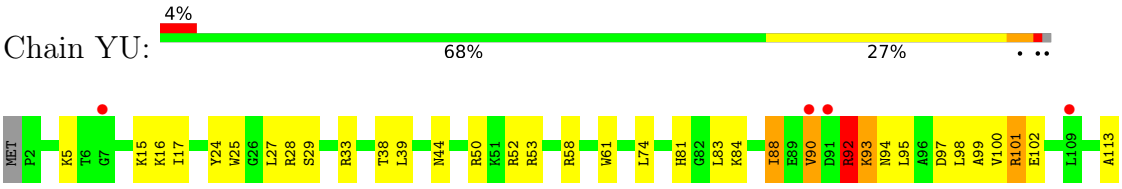
• Molecule 40: 50S ribosomal protein L20

Chain RU:



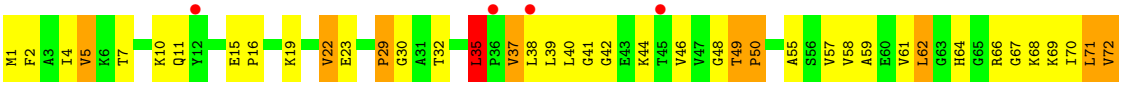
• Molecule 40: 50S ribosomal protein L20

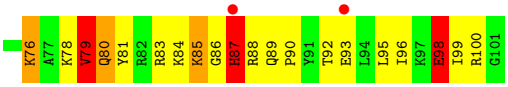
Chain YU:



• Molecule 41: 50S ribosomal protein L21

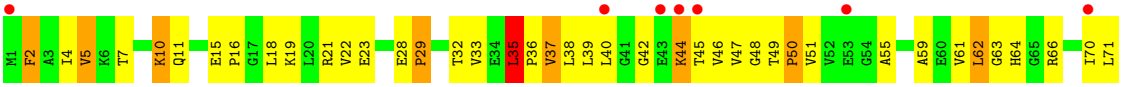
Chain RV:

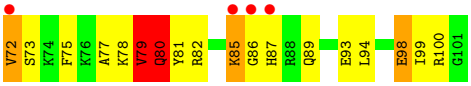




• Molecule 41: 50S ribosomal protein L21

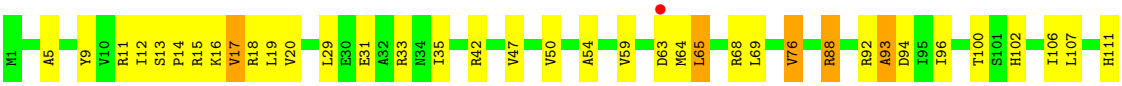
Chain YV:





• Molecule 42: 50S ribosomal protein L22

Chain RW:

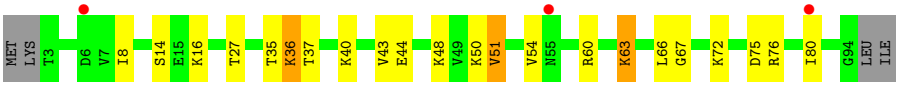


• Molecule 42: 50S ribosomal protein L22

Chain YW:

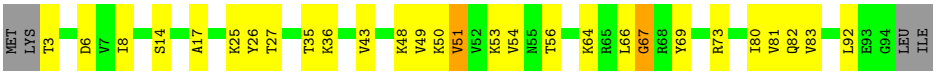
• Molecule 43: 50S ribosomal protein L23

Chain RX:



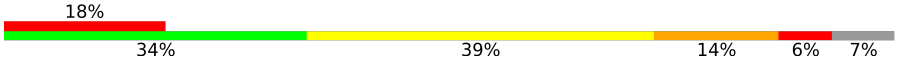
• Molecule 43: 50S ribosomal protein L23

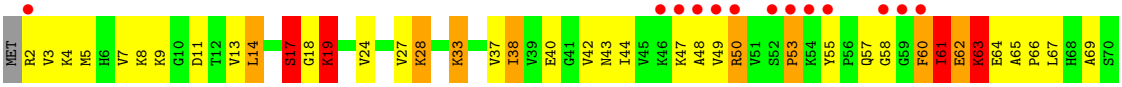
Chain YX:

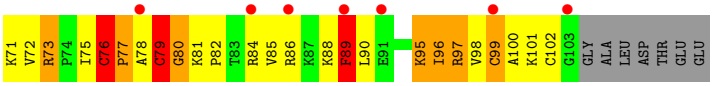


• Molecule 44: 50S ribosomal protein L24

Chain RY:

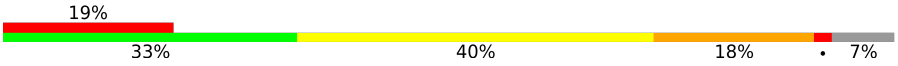


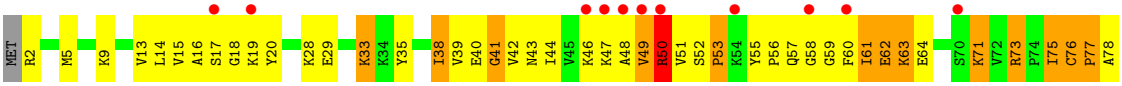


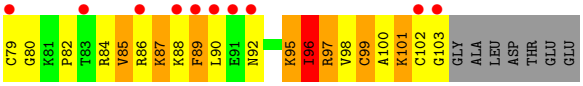


• Molecule 44: 50S ribosomal protein L24

Chain YY:

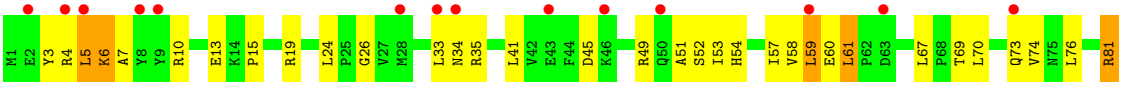


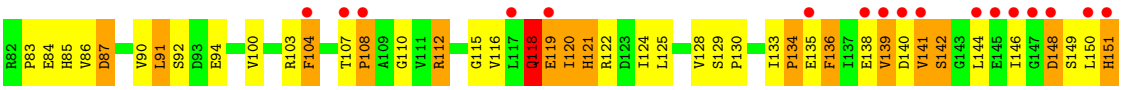


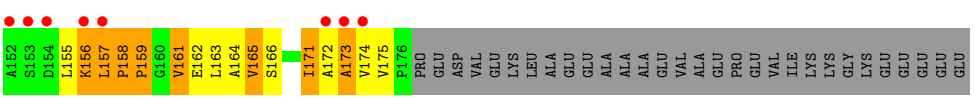


• Molecule 45: 50S ribosomal protein L25

Chain RZ:

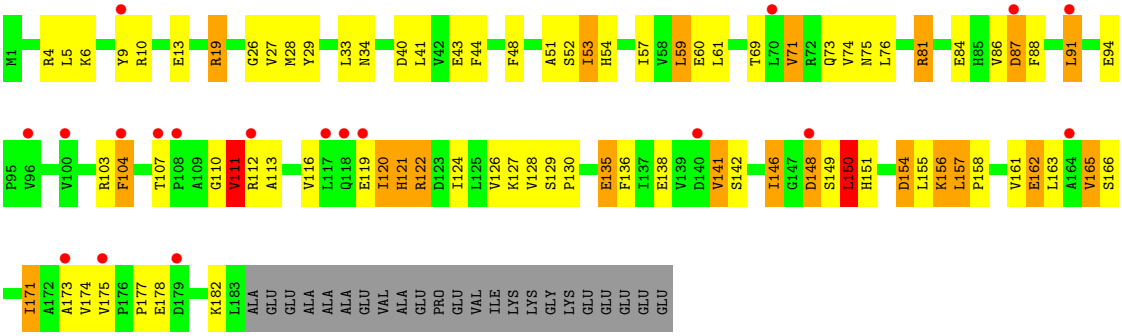






• Molecule 45: 50S ribosomal protein L25

Chain YZ:

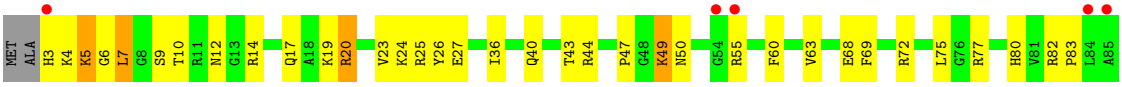


• Molecule 46: 50S ribosomal protein L27

Chain R0:

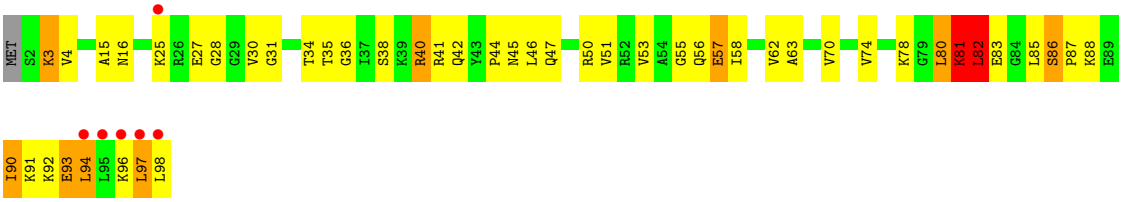
• Molecule 46: 50S ribosomal protein L27

Chain Y0:



• Molecule 47: 50S ribosomal protein L28

Chain R1:

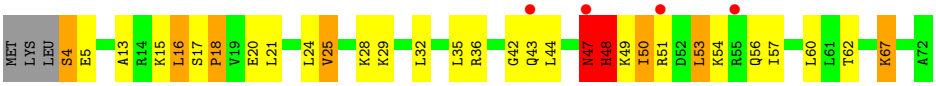


• Molecule 47: 50S ribosomal protein L28

Chain Y1:

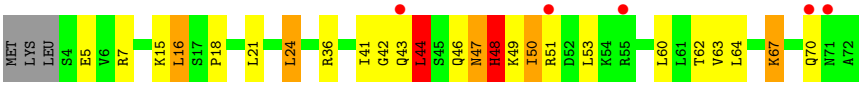
• Molecule 48: 50S ribosomal protein L29

Chain R2:



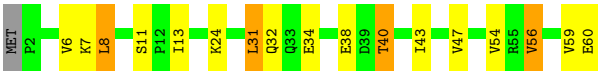
• Molecule 48: 50S ribosomal protein L29

Chain Y2:



• Molecule 49: 50S ribosomal protein L30

Chain R3:

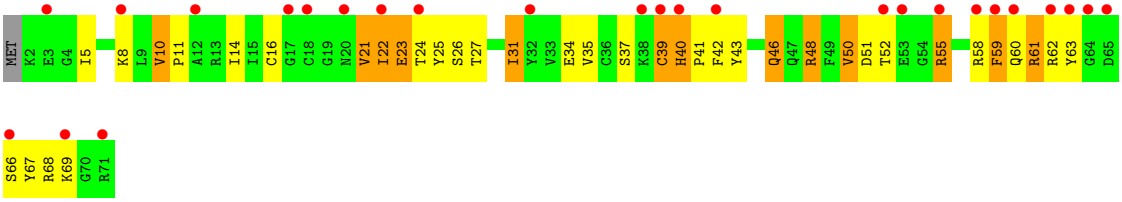


• Molecule 49: 50S ribosomal protein L30

Chain Y3:

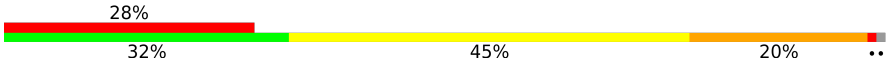
• Molecule 50: 50S ribosomal protein L31

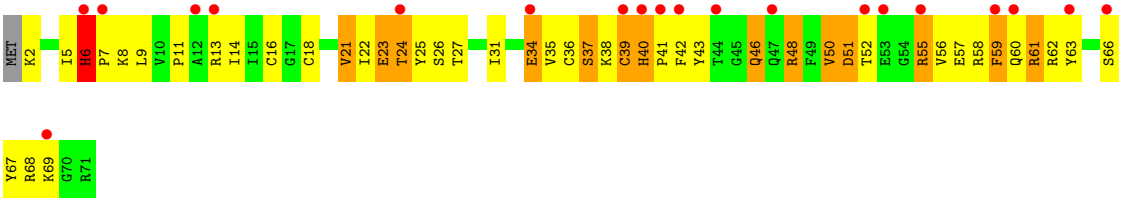
Chain R4:



• Molecule 50: 50S ribosomal protein L31

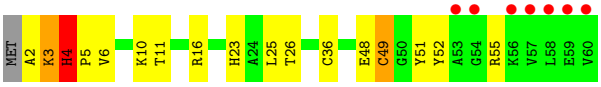
Chain Y4:



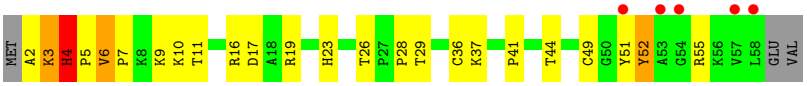


• Molecule 51: 50S ribosomal protein L32

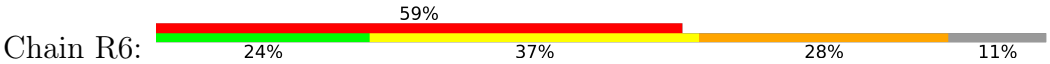
Chain R5:



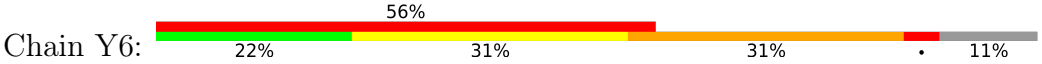
• Molecule 51: 50S ribosomal protein L32



• Molecule 52: 50S ribosomal protein L33

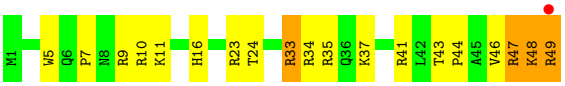


• Molecule 52: 50S ribosomal protein L33

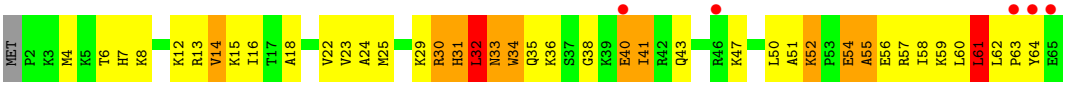


• Molecule 53: 50S ribosomal protein L34

• Molecule 53: 50S ribosomal protein L34

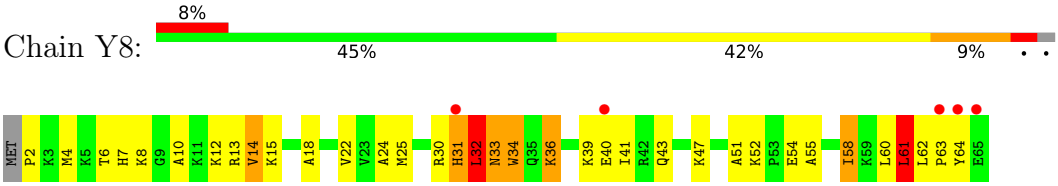


• Molecule 54: 50S ribosomal protein L35



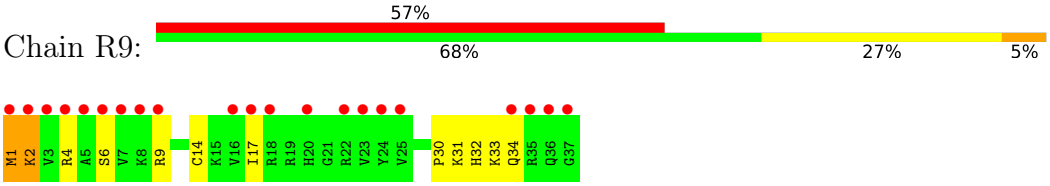
• Molecule 54: 50S ribosomal protein L35

Chain Y8:



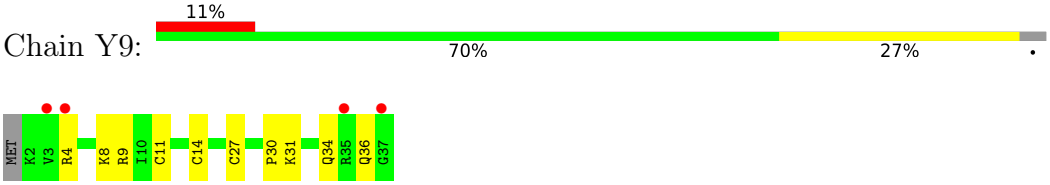
• Molecule 55: 50S ribosomal protein L36

Chain R9:



• Molecule 55: 50S ribosomal protein L36

Chain Y9:



• Molecule 56: CC-puromycin

Chain Z6:

• Molecule 56: CC-puromycin

Chain Z7:

4 Data and refinement statistics (i)

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 96.01 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (34.93-3.10) 99.3 (96.01-3.10)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 3.13Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.203 , 0.237 0.206 , 0.239	Depositor DCC
R_{free} test set	49438 reflections (4.69%)	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)	0.28 , 70.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: A2M, ZN, OMC, MG, PPU

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	0.31	0/36346	0.80	17/56724 (0.0%)
1	XA	0.34	2/36276 (0.0%)	0.81	23/56615 (0.0%)
2	QB	0.25	0/1950	0.49	0/2630
2	XB	0.25	0/1950	0.49	1/2630 (0.0%)
3	QC	0.24	0/1636	0.47	0/2205
3	XC	0.27	0/1636	0.48	0/2205
4	QD	0.28	0/1733	0.50	0/2318
4	XD	0.28	0/1733	0.50	0/2318
5	QE	0.28	0/1195	0.48	0/1609
5	XE	0.29	0/1195	0.48	0/1609
6	QF	0.25	0/856	0.44	0/1154
6	XF	0.28	0/856	0.45	0/1154
7	QG	0.23	0/1276	0.45	0/1709
7	XG	0.26	0/1276	0.46	0/1709
8	QH	0.24	0/1136	0.47	0/1527
8	XH	0.27	0/1136	0.45	0/1527
9	QI	0.24	0/1037	0.48	0/1389
9	XI	0.26	0/1037	0.48	0/1389
10	QJ	0.24	0/814	0.45	0/1095
10	XJ	0.24	0/814	0.46	0/1095
11	QK	0.24	0/916	0.44	0/1234
11	XK	0.28	0/916	0.48	0/1234
12	QL	0.31	0/991	0.52	1/1327 (0.1%)
12	XL	0.36	1/991 (0.1%)	0.56	1/1327 (0.1%)
13	QM	0.26	0/947	0.53	1/1270 (0.1%)
13	XM	0.25	0/947	0.53	0/1270
14	QN	0.25	0/501	0.47	0/664
14	XN	0.29	0/501	0.49	0/664
15	QO	0.24	0/745	0.39	0/992
15	XO	0.26	0/745	0.43	0/992
16	QP	0.26	0/721	0.46	0/970
16	XP	0.25	0/721	0.45	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	QQ	0.26	0/847	0.46	0/1131
17	XQ	0.30	0/847	0.47	0/1131
18	QR	0.25	0/590	0.48	0/782
18	XR	0.26	0/590	0.51	0/782
19	QS	0.27	0/670	0.53	0/901
19	XS	0.29	0/670	0.52	0/901
20	QT	0.24	0/765	0.49	1/1007 (0.1%)
20	XT	0.25	0/765	0.48	0/1007
21	QU	0.23	0/221	0.47	0/288
21	XU	0.24	0/221	0.45	0/288
22	QV	0.31	0/1832	0.79	0/2855
22	XV	0.32	0/1832	0.76	0/2855
23	QX	0.36	0/414	0.77	0/645
23	XX	0.35	0/414	0.86	0/645
24	QY	0.31	0/762	0.45	0/1028
24	XY	0.25	0/762	0.42	0/1028
25	RA	0.40	1/69742 (0.0%)	0.86	33/108874 (0.0%)
25	YA	0.42	1/69356 (0.0%)	0.87	27/108271 (0.0%)
26	RB	0.30	0/2928	0.81	0/4568
26	YB	0.31	0/2928	0.81	0/4568
27	RD	0.34	0/2165	0.56	0/2919
27	YD	0.37	0/2165	0.60	0/2919
28	RE	0.30	0/1601	0.55	0/2160
28	YE	0.34	0/1601	0.58	0/2160
29	RF	0.35	0/1662	0.58	0/2249
29	YF	0.31	0/1662	0.57	0/2249
30	RG	0.24	0/1499	0.46	0/2016
30	YG	0.25	0/1499	0.46	0/2016
31	RH	0.25	0/1332	0.60	1/1802 (0.1%)
31	YH	0.27	0/1332	0.61	1/1802 (0.1%)
32	RI	0.24	0/1151	0.54	0/1558
32	YI	0.28	0/1151	0.58	0/1558
33	RN	0.28	0/1131	0.50	0/1525
33	YN	0.29	0/1131	0.50	0/1525
34	RO	0.32	0/943	0.51	0/1269
34	YO	0.33	0/943	0.53	0/1269
35	RP	0.34	0/1162	0.66	0/1544
35	YP	0.35	0/1162	0.69	2/1544 (0.1%)
36	RQ	0.34	0/1133	0.57	0/1515
36	YQ	0.35	0/1128	0.58	1/1508 (0.1%)
37	RR	0.27	0/974	0.51	0/1302
37	YR	0.30	0/974	0.53	0/1302
38	RS	0.25	0/892	0.48	0/1187

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	YS	0.29	0/892	0.54	0/1187
39	RT	0.27	0/1155	0.46	0/1542
39	YT	0.30	0/1155	0.47	0/1542
40	RU	0.32	0/982	0.53	0/1306
40	YU	0.33	0/982	0.52	0/1306
41	RV	0.38	0/790	0.69	1/1057 (0.1%)
41	YV	0.35	0/790	0.67	1/1057 (0.1%)
42	RW	0.30	0/911	0.51	0/1220
42	YW	0.30	0/911	0.52	0/1220
43	RX	0.32	0/739	0.51	0/993
43	YX	0.35	0/739	0.52	0/993
44	RY	0.33	0/798	0.59	0/1064
44	YY	0.32	0/798	0.59	0/1064
45	RZ	0.28	0/1435	0.56	0/1947
45	YZ	0.30	0/1493	0.60	0/2026
46	R0	0.32	0/666	0.52	0/885
46	Y0	0.32	0/666	0.58	0/885
47	R1	0.31	0/770	0.57	0/1022
47	Y1	0.36	0/770	0.59	0/1022
48	R2	0.28	0/583	0.58	0/771
48	Y2	0.33	0/583	0.59	1/771 (0.1%)
49	R3	0.29	0/474	0.44	0/635
49	Y3	0.28	0/474	0.47	0/635
50	R4	0.24	0/586	0.46	0/785
50	Y4	0.30	0/586	0.51	0/785
51	R5	0.30	0/473	0.58	1/639 (0.2%)
51	Y5	0.50	1/456 (0.2%)	0.71	2/617 (0.3%)
52	R6	0.29	0/424	0.67	0/565
52	Y6	0.44	0/424	0.82	0/565
53	R7	0.33	0/438	0.49	0/575
53	Y7	0.34	0/438	0.53	0/575
54	R8	0.42	0/525	0.75	0/691
54	Y8	0.38	0/525	0.66	0/691
55	R9	0.26	0/310	0.42	0/407
55	Y9	0.24	0/302	0.41	0/397
56	Z6	0.53	0/40	0.56	0/60
56	Z7	0.38	0/40	0.62	0/60
All	All	0.36	6/318202 (0.0%)	0.77	116/475540 (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)

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	RA	1983	C	O3'-P	-5.65	1.54	1.61
25	YA	2643	G	O3'-P	-5.59	1.54	1.61
1	XA	1296	C	O3'-P	-5.42	1.54	1.61
1	XA	1156	G	O3'-P	-5.28	1.54	1.61
51	Y5	7	PRO	N-CD	5.26	1.55	1.47

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	XA	1157	A	P-O3'-C3'	8.78	130.23	119.70
1	XA	115	G	P-O3'-C3'	8.69	130.12	119.70
25	YA	1912	A	P-O3'-C3'	6.44	127.43	119.70
1	XA	1156	G	P-O3'-C3'	-6.17	112.29	119.70
1	QA	345	C	P-O3'-C3'	6.01	126.91	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	410	0
1	XA	32409	0	16361	373	0
2	QB	1915	0	1969	57	0
2	XB	1915	0	1969	60	0
3	QC	1612	0	1677	51	0
3	XC	1612	0	1677	34	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	24	0
6	QF	843	0	857	16	0
6	XF	843	0	857	19	0
7	QG	1257	0	1296	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	31	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	19	0
11	XK	901	0	926	19	0
12	QL	975	0	1062	26	0
12	XL	975	0	1062	22	0
13	QM	937	0	994	29	0
13	XM	937	0	994	59	0
14	QN	492	0	529	17	0
14	XN	492	0	529	11	0
15	QO	734	0	771	14	0
15	XO	734	0	771	16	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	15	0
18	QR	585	0	657	9	0
18	XR	585	0	657	19	0
19	QS	656	0	678	46	0
19	XS	656	0	678	40	0
20	QT	763	0	861	21	0
20	XT	763	0	861	27	0
21	QU	217	0	234	9	0
21	XU	217	0	234	13	0
22	QV	1640	0	837	11	0
22	XV	1640	0	837	12	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	12	0
25	RA	62269	0	31392	690	0
25	YA	61924	0	31214	645	0
26	RB	2617	0	1328	27	0
26	YB	2617	0	1328	25	0
27	RD	2115	0	2195	66	0
27	YD	2115	0	2195	71	0
28	RE	1568	0	1634	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	YE	1568	0	1634	75	0
29	RF	1627	0	1680	52	0
29	YF	1627	0	1680	55	0
30	RG	1474	0	1535	43	0
30	YG	1474	0	1535	46	0
31	RH	1307	0	1382	95	0
31	YH	1307	0	1381	82	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	28	0
35	RP	1145	0	1228	113	0
35	YP	1145	0	1228	141	0
36	RQ	1112	0	1170	32	0
36	YQ	1107	0	1165	36	0
37	RR	960	0	1021	15	0
37	YR	960	0	1021	25	0
38	RS	882	0	943	29	0
38	YS	882	0	943	34	0
39	RT	1141	0	1202	44	0
39	YT	1141	0	1202	38	0
40	RU	964	0	1022	36	0
40	YU	964	0	1022	34	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	17	0
43	YX	725	0	778	17	0
44	RY	785	0	877	68	0
44	YY	785	0	878	47	0
45	RZ	1404	0	1437	90	0
45	YZ	1461	0	1493	47	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	22	0
48	R2	581	0	629	17	0
48	Y2	581	0	629	16	0
49	R3	469	0	518	9	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	22	0
50	Y4	573	0	565	37	0
51	R5	459	0	480	10	0
51	Y5	442	0	465	22	0
52	R6	417	0	441	24	0
52	Y6	417	0	441	51	0
53	R7	430	0	480	8	0
53	Y7	430	0	480	12	0
54	R8	517	0	582	49	0
54	Y8	517	0	582	69	0
55	R9	307	0	338	8	0
55	Y9	299	0	326	6	0
56	Z6	74	0	51	8	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	4997	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 10.

The worst 5 of 4997 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 (i)

5.3.1 Protein backbone (i)

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
14	XN	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	2 12
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%)	15 49
17	XQ	98/105 (93%)	89 (91%)	7 (7%)	2 (2%)	7 31
18	QR	69/88 (78%)	61 (88%)	8 (12%)	0	100 100
18	XR	69/88 (78%)	62 (90%)	6 (9%)	1 (1%)	11 40
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%)	4 23
20	XT	97/106 (92%)	80 (82%)	14 (14%)	3 (3%)	4 23
21	QU	23/25 (92%)	16 (70%)	6 (26%)	1 (4%)	2 16
21	XU	23/25 (92%)	18 (78%)	3 (13%)	2 (9%)	1 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%)	4 23
27	YD	270/276 (98%)	228 (84%)	32 (12%)	10 (4%)	3 19
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 8
29	YF	206/210 (98%)	168 (82%)	22 (11%)	16 (8%)	1 5
30	RG	179/182 (98%)	141 (79%)	26 (14%)	12 (7%)	1 7
30	YG	179/182 (98%)	147 (82%)	21 (12%)	11 (6%)	1 9
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%)	2 14
32	YI	144/148 (97%)	116 (81%)	24 (17%)	4 (3%)	5 25
33	RN	136/140 (97%)	116 (85%)	13 (10%)	7 (5%)	2 13
33	YN	136/140 (97%)	110 (81%)	19 (14%)	7 (5%)	2 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
34	RO	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	19 54
34	YO	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	19 54
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 5
36	YQ	137/141 (97%)	111 (81%)	15 (11%)	11 (8%)	1 5
37	RR	115/118 (98%)	107 (93%)	4 (4%)	4 (4%)	3 20
37	YR	115/118 (98%)	109 (95%)	3 (3%)	3 (3%)	5 26
38	RS	109/112 (97%)	84 (77%)	17 (16%)	8 (7%)	1 6
38	YS	109/112 (97%)	85 (78%)	13 (12%)	11 (10%)	0 3
39	RT	135/146 (92%)	109 (81%)	24 (18%)	2 (2%)	10 39
39	YT	135/146 (92%)	113 (84%)	17 (13%)	5 (4%)	3 19
40	RU	115/118 (98%)	107 (93%)	6 (5%)	2 (2%)	9 36
40	YU	115/118 (98%)	103 (90%)	9 (8%)	3 (3%)	5 26
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%)	5 25
42	YW	111/113 (98%)	104 (94%)	3 (3%)	4 (4%)	3 20
43	RX	90/96 (94%)	76 (84%)	12 (13%)	2 (2%)	6 29
43	YX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	6 29
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%)	3 19
46	Y0	81/85 (95%)	67 (83%)	11 (14%)	3 (4%)	3 19
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 8
48	R2	67/72 (93%)	54 (81%)	8 (12%)	5 (8%)	1 6
48	Y2	67/72 (93%)	56 (84%)	5 (8%)	6 (9%)	1 4
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 20
51	Y5	55/60 (92%)	48 (87%)	4 (7%)	3 (6%)	2 11
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%)	4 24
55	Y9	34/37 (92%)	33 (97%)	1 (3%)	0	100 100
All	All	11647/12358 (94%)	9391 (81%)	1489 (13%)	767 (7%)	1 7

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 (i)

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%)	174 (85%)	30 (15%)	3 13
2	XB	204/220 (93%)	176 (86%)	28 (14%)	3 16
3	QC	160/188 (85%)	142 (89%)	18 (11%)	6 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	XC	160/188 (85%)	141 (88%)	19 (12%)	5 20
4	QD	180/181 (99%)	157 (87%)	23 (13%)	4 18
4	XD	180/181 (99%)	155 (86%)	25 (14%)	3 15
5	QE	119/123 (97%)	101 (85%)	18 (15%)	3 12
5	XE	119/123 (97%)	106 (89%)	13 (11%)	6 25
6	QF	90/90 (100%)	85 (94%)	5 (6%)	21 52
6	XF	90/90 (100%)	77 (86%)	13 (14%)	3 14
7	QG	126/127 (99%)	112 (89%)	14 (11%)	6 24
7	XG	126/127 (99%)	109 (86%)	17 (14%)	4 16
8	QH	119/119 (100%)	109 (92%)	10 (8%)	11 38
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6 25
9	QI	99/99 (100%)	79 (80%)	20 (20%)	1 5
9	XI	99/99 (100%)	80 (81%)	19 (19%)	1 6
10	QJ	89/92 (97%)	77 (86%)	12 (14%)	4 16
10	XJ	89/92 (97%)	75 (84%)	14 (16%)	2 11
11	QK	92/99 (93%)	82 (89%)	10 (11%)	6 25
11	XK	92/99 (93%)	84 (91%)	8 (9%)	10 36
12	QL	104/109 (95%)	89 (86%)	15 (14%)	3 14
12	XL	104/109 (95%)	87 (84%)	17 (16%)	2 10
13	QM	94/101 (93%)	80 (85%)	14 (15%)	3 13
13	XM	94/101 (93%)	82 (87%)	12 (13%)	4 18
14	QN	49/50 (98%)	48 (98%)	1 (2%)	55 80
14	XN	49/50 (98%)	44 (90%)	5 (10%)	7 27
15	QO	79/80 (99%)	74 (94%)	5 (6%)	18 48
15	XO	79/80 (99%)	74 (94%)	5 (6%)	18 48
16	QP	72/74 (97%)	64 (89%)	8 (11%)	6 24
16	XP	72/74 (97%)	64 (89%)	8 (11%)	6 24
17	QQ	95/97 (98%)	90 (95%)	5 (5%)	22 54
17	XQ	95/97 (98%)	88 (93%)	7 (7%)	13 42
18	QR	62/77 (80%)	56 (90%)	6 (10%)	8 30
18	XR	62/77 (80%)	54 (87%)	8 (13%)	4 18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	QS	71/80 (89%)	54 (76%)	17 (24%)	0 2
19	XS	71/80 (89%)	58 (82%)	13 (18%)	1 7
20	QT	76/82 (93%)	62 (82%)	14 (18%)	1 7
20	XT	76/82 (93%)	66 (87%)	10 (13%)	4 17
21	QU	20/20 (100%)	18 (90%)	2 (10%)	7 28
21	XU	20/20 (100%)	18 (90%)	2 (10%)	7 28
24	QY	78/102 (76%)	75 (96%)	3 (4%)	33 66
24	XY	78/102 (76%)	74 (95%)	4 (5%)	24 56
27	RD	214/218 (98%)	178 (83%)	36 (17%)	2 9
27	YD	214/218 (98%)	179 (84%)	35 (16%)	2 10
28	RE	165/166 (99%)	137 (83%)	28 (17%)	2 9
28	YE	165/166 (99%)	138 (84%)	27 (16%)	2 10
29	RF	165/166 (99%)	139 (84%)	26 (16%)	2 11
29	YF	165/166 (99%)	142 (86%)	23 (14%)	3 15
30	RG	155/156 (99%)	147 (95%)	8 (5%)	23 55
30	YG	155/156 (99%)	138 (89%)	17 (11%)	6 25
31	RH	142/148 (96%)	123 (87%)	19 (13%)	4 16
31	YH	142/148 (96%)	115 (81%)	27 (19%)	1 6
32	RI	122/124 (98%)	98 (80%)	24 (20%)	1 6
32	YI	122/124 (98%)	99 (81%)	23 (19%)	1 6
33	RN	117/119 (98%)	107 (92%)	10 (8%)	10 37
33	YN	117/119 (98%)	104 (89%)	13 (11%)	6 24
34	RO	100/100 (100%)	91 (91%)	9 (9%)	9 34
34	YO	100/100 (100%)	90 (90%)	10 (10%)	7 28
35	RP	116/116 (100%)	81 (70%)	35 (30%)	0 0
35	YP	116/116 (100%)	83 (72%)	33 (28%)	0 1
36	RQ	110/111 (99%)	93 (84%)	17 (16%)	2 11
36	YQ	110/111 (99%)	93 (84%)	17 (16%)	2 11
37	RR	100/101 (99%)	82 (82%)	18 (18%)	1 7
37	YR	100/101 (99%)	87 (87%)	13 (13%)	4 18
38	RS	87/88 (99%)	80 (92%)	7 (8%)	12 40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
38	YS	87/88 (99%)	73 (84%)	14 (16%)	2 10
39	RT	120/127 (94%)	100 (83%)	20 (17%)	2 9
39	YT	120/127 (94%)	98 (82%)	22 (18%)	1 7
40	RU	93/94 (99%)	85 (91%)	8 (9%)	10 37
40	YU	93/94 (99%)	85 (91%)	8 (9%)	10 37
41	RV	82/82 (100%)	66 (80%)	16 (20%)	1 6
41	YV	82/82 (100%)	63 (77%)	19 (23%)	1 3
42	RW	92/92 (100%)	82 (89%)	10 (11%)	6 25
42	YW	92/92 (100%)	79 (86%)	13 (14%)	3 15
43	RX	74/78 (95%)	65 (88%)	9 (12%)	5 19
43	YX	74/78 (95%)	68 (92%)	6 (8%)	11 39
44	RY	85/91 (93%)	63 (74%)	22 (26%)	0 1
44	YY	85/91 (93%)	61 (72%)	24 (28%)	0 1
45	RZ	155/179 (87%)	129 (83%)	26 (17%)	2 9
45	YZ	162/179 (90%)	134 (83%)	28 (17%)	2 9
46	R0	66/67 (98%)	62 (94%)	4 (6%)	18 49
46	Y0	66/67 (98%)	58 (88%)	8 (12%)	5 20
47	R1	82/83 (99%)	68 (83%)	14 (17%)	2 9
47	Y1	82/83 (99%)	72 (88%)	10 (12%)	5 19
48	R2	64/67 (96%)	52 (81%)	12 (19%)	1 6
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	6 25
49	R3	51/52 (98%)	44 (86%)	7 (14%)	3 16
49	Y3	51/52 (98%)	47 (92%)	4 (8%)	12 40
50	R4	62/63 (98%)	47 (76%)	15 (24%)	0 2
50	Y4	62/63 (98%)	44 (71%)	18 (29%)	0 1
51	R5	51/52 (98%)	40 (78%)	11 (22%)	1 4
51	Y5	49/52 (94%)	42 (86%)	7 (14%)	3 14
52	R6	47/52 (90%)	32 (68%)	15 (32%)	0 0
52	Y6	47/52 (90%)	30 (64%)	17 (36%)	0 0
53	R7	42/42 (100%)	35 (83%)	7 (17%)	2 9
53	Y7	42/42 (100%)	35 (83%)	7 (17%)	2 9

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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 7
55	R9	34/34 (100%)	32 (94%)	2 (6%)	19 50
55	Y9	33/34 (97%)	33 (100%)	0	100 100
All	All	9854/10266 (96%)	8438 (86%)	1416 (14%)	3 14

5 of 1416 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	XR	87	ARG
35	YP	65	ARG
24	XY	47	ASN
18	XR	85	LEU
29	YF	192	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
24	XY	54	HIS
9	XI	117	HIS
3	XC	108	ASN
45	RZ	118	GLN
7	XG	97	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1509/1522 (99%)	309 (20%)	50 (3%)
1	XA	1506/1522 (98%)	306 (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%)	599 (20%)	54 (1%)
25	YA	2872/2916 (98%)	584 (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%)	1891 (20%)	191 (2%)

5 of 1891 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 (i)

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	56,25	32,40,41	0.90	1 (3%)	33,57,60	1.73	7 (21%)
23	A2M	QX	19	23,22	18,25,26	1.05	1 (5%)	18,36,39	1.53	4 (22%)
56	PPU	Z7	76	56,25	32,40,41	0.93	1 (3%)	33,57,60	1.46	8 (24%)
23	A2M	QX	21	23,1	18,25,26	1.13	2 (11%)	18,36,39	1.40	2 (11%)
23	A2M	XX	21	23,1	18,25,26	1.07	1 (5%)	18,36,39	1.42	2 (11%)
23	OMC	XX	20	23	19,22,23	0.82	0	26,31,34	0.94	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	OMC	QX	20	23	19,22,23	0.84	0	26,31,34	0.96	1 (3%)
23	A2M	XX	19	23,22	18,25,26	0.88	0	18,36,39	1.59	4 (22%)

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	56,25	-	1/21/43/44	0/4/4/4
23	A2M	QX	19	23,22	-	0/5/27/28	0/3/3/3
56	PPU	Z7	76	56,25	-	3/21/43/44	0/4/4/4
23	A2M	QX	21	23,1	-	4/5/27/28	0/3/3/3
23	A2M	XX	21	23,1	-	3/5/27/28	0/3/3/3
23	OMC	XX	20	23	-	2/9/27/28	0/2/2/2
23	OMC	QX	20	23	-	3/9/27/28	0/2/2/2
23	A2M	XX	19	23,22	-	1/5/27/28	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	QX	21	A2M	C5-C4	2.68	1.48	1.40
23	XX	21	A2M	C5-C4	2.64	1.47	1.40
23	QX	19	A2M	C5-C4	2.56	1.47	1.40
56	Z7	76	PPU	C5-C4	2.11	1.46	1.40
56	Z6	76	PPU	C5-C4	2.04	1.46	1.40

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	Z6	76	PPU	N1-C6-N6	6.33	123.72	117.06
56	Z7	76	PPU	N1-C6-N6	3.89	121.15	117.06
23	XX	19	A2M	N3-C2-N1	-3.75	122.82	128.68
56	Z6	76	PPU	C9-N6-C6	-3.58	108.68	119.51
23	QX	19	A2M	N3-C2-N1	-3.45	123.29	128.68

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	QX	21	A2M	C3'-C2'-O2'-CM'
23	XX	21	A2M	C3'-C4'-C5'-O5'
23	XX	21	A2M	C3'-C2'-O2'-CM'
56	Z7	76	PPU	C5-C6-N6-C9
56	Z7	76	PPU	C5-C6-N6-C10

There are no ring outliers.

8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z6	76	PPU	7	0
23	QX	19	A2M	1	0
56	Z7	76	PPU	9	0
23	QX	21	A2M	1	0
23	XX	21	A2M	4	0
23	XX	20	OMC	1	0
23	QX	20	OMC	1	0
23	XX	19	A2M	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.84	178 (11%) 4 2	34, 73, 167, 323	0
1	XA	1508/1522 (99%)	0.70	110 (7%) 15 6	27, 64, 152, 309	0
2	QB	236/256 (92%)	1.63	86 (36%) 0 0	56, 114, 192, 239	0
2	XB	236/256 (92%)	1.13	49 (20%) 1 0	51, 99, 182, 208	0
3	QC	206/239 (86%)	0.16	5 (2%) 59 37	42, 97, 183, 230	0
3	XC	206/239 (86%)	0.23	11 (5%) 26 12	48, 84, 156, 235	0
4	QD	208/209 (99%)	0.25	6 (2%) 51 28	37, 65, 105, 184	0
4	XD	208/209 (99%)	0.30	13 (6%) 20 8	39, 67, 113, 170	0
5	QE	154/162 (95%)	0.08	4 (2%) 56 33	38, 64, 127, 212	0
5	XE	154/162 (95%)	0.07	3 (1%) 66 46	33, 60, 127, 229	0
6	QF	101/101 (100%)	0.34	3 (2%) 50 27	51, 87, 129, 142	0
6	XF	101/101 (100%)	0.12	2 (1%) 65 44	34, 64, 107, 165	0
7	QG	155/156 (99%)	0.96	31 (20%) 1 0	71, 109, 182, 224	0
7	XG	155/156 (99%)	0.66	23 (14%) 2 1	49, 89, 156, 201	0
8	QH	138/138 (100%)	-0.00	3 (2%) 62 41	48, 72, 106, 156	0
8	XH	138/138 (100%)	0.24	3 (2%) 62 41	41, 64, 110, 142	0
9	QI	128/128 (100%)	1.67	42 (32%) 0 0	69, 127, 198, 231	0
9	XI	128/128 (100%)	1.20	24 (18%) 1 0	46, 97, 172, 248	0
10	QJ	99/105 (94%)	1.57	33 (33%) 0 0	67, 123, 200, 249	0
10	XJ	99/105 (94%)	1.44	32 (32%) 0 0	45, 109, 178, 237	0
11	QK	121/129 (93%)	0.98	13 (10%) 6 2	42, 85, 170, 226	0
11	XK	121/129 (93%)	0.31	8 (6%) 18 7	33, 65, 157, 195	0
12	QL	125/132 (94%)	0.12	1 (0%) 86 72	34, 58, 110, 215	0
12	XL	125/132 (94%)	0.26	2 (1%) 72 51	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%)	0.79	16 (13%) 3 1	66, 113, 181, 242	0
13	XM	118/126 (93%)	0.86	13 (11%) 5 2	52, 97, 150, 259	0
14	QN	60/61 (98%)	0.55	4 (6%) 17 7	63, 95, 133, 188	0
14	XN	60/61 (98%)	0.38	3 (5%) 28 13	50, 77, 123, 190	0
15	QO	88/89 (98%)	0.73	10 (11%) 5 2	42, 75, 119, 154	0
15	XO	88/89 (98%)	0.68	5 (5%) 23 11	30, 63, 104, 120	0
16	QP	84/88 (95%)	0.36	3 (3%) 42 22	46, 66, 101, 182	0
16	XP	84/88 (95%)	0.35	4 (4%) 30 14	50, 70, 104, 198	0
17	QQ	100/105 (95%)	0.36	3 (3%) 50 27	44, 74, 105, 120	0
17	XQ	100/105 (95%)	0.06	1 (1%) 82 67	41, 67, 103, 183	0
18	QR	71/88 (80%)	0.85	10 (14%) 2 1	59, 91, 157, 210	0
18	XR	71/88 (80%)	0.23	3 (4%) 36 18	36, 63, 144, 203	0
19	QS	82/93 (88%)	1.38	25 (30%) 0 0	64, 120, 198, 256	0
19	XS	82/93 (88%)	1.80	34 (41%) 0 0	52, 100, 182, 224	0
20	QT	99/106 (93%)	1.41	23 (23%) 0 0	47, 80, 163, 206	0
20	XT	99/106 (93%)	0.47	4 (4%) 38 19	47, 80, 163, 198	0
21	QU	25/25 (100%)	3.11	16 (64%) 0 0	68, 98, 172, 193	0
21	XU	25/25 (100%)	3.49	21 (84%) 0 0	65, 95, 117, 174	0
22	QV	77/77 (100%)	0.78	8 (10%) 6 2	29, 71, 129, 189	0
22	XV	77/77 (100%)	0.42	4 (5%) 27 12	29, 68, 106, 175	0
23	QX	17/24 (70%)	4.93	13 (76%) 0 0	51, 206, 281, 292	0
23	XX	17/24 (70%)	4.33	12 (70%) 0 0	37, 216, 350, 357	0
24	QY	91/117 (77%)	0.07	3 (3%) 46 24	53, 81, 111, 140	0
24	XY	91/117 (77%)	0.31	6 (6%) 18 7	50, 78, 103, 123	0
25	RA	2891/2916 (99%)	0.91	285 (9%) 7 2	21, 50, 223, 352	0
25	YA	2875/2916 (98%)	0.97	282 (9%) 7 2	19, 45, 231, 375	0
26	RB	122/124 (98%)	0.63	9 (7%) 14 5	40, 82, 126, 193	0
26	YB	122/124 (98%)	0.67	9 (7%) 14 5	41, 72, 121, 208	0
27	RD	272/276 (98%)	0.07	6 (2%) 62 41	16, 46, 89, 168	0
27	YD	272/276 (98%)	-0.00	2 (0%) 87 75	10, 36, 80, 191	0
28	RE	205/206 (99%)	0.34	11 (5%) 25 12	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%)	0.41	11 (5%) 25 12	23, 58, 148, 254	0
29	RF	208/210 (99%)	0.23	10 (4%) 30 14	18, 44, 142, 240	0
29	YF	208/210 (99%)	0.73	23 (11%) 5 2	21, 51, 167, 229	0
30	RG	181/182 (99%)	0.43	8 (4%) 34 17	56, 92, 150, 174	0
30	YG	181/182 (99%)	1.00	31 (17%) 1 0	45, 81, 134, 169	0
31	RH	170/180 (94%)	1.70	50 (29%) 0 0	53, 125, 218, 256	0
31	YH	170/180 (94%)	1.14	27 (15%) 1 1	54, 104, 201, 250	0
32	RI	146/148 (98%)	0.88	26 (17%) 1 0	46, 96, 156, 246	0
32	YI	146/148 (98%)	0.49	12 (8%) 11 4	30, 84, 153, 224	0
33	RN	138/140 (98%)	0.17	3 (2%) 62 41	30, 65, 114, 163	0
33	YN	138/140 (98%)	-0.04	2 (1%) 75 56	30, 61, 121, 149	0
34	RO	122/122 (100%)	-0.06	0 100 100	32, 55, 86, 131	0
34	YO	122/122 (100%)	-0.11	0 100 100	25, 46, 77, 97	0
35	RP	150/150 (100%)	0.64	11 (7%) 15 6	17, 63, 133, 211	0
35	YP	150/150 (100%)	0.45	12 (8%) 12 5	19, 54, 139, 202	0
36	RQ	140/141 (99%)	0.22	3 (2%) 63 43	28, 59, 104, 202	0
36	YQ	139/141 (98%)	0.08	4 (2%) 51 28	31, 55, 114, 204	0
37	RR	117/118 (99%)	0.20	3 (2%) 56 33	24, 56, 91, 123	0
37	YR	117/118 (99%)	0.31	3 (2%) 56 33	25, 51, 87, 124	0
38	RS	111/112 (99%)	1.40	35 (31%) 0 0	50, 83, 148, 217	0
38	YS	111/112 (99%)	0.89	17 (15%) 2 1	38, 67, 122, 171	0
39	RT	137/146 (93%)	0.23	5 (3%) 42 22	34, 67, 146, 241	0
39	YT	137/146 (93%)	0.22	7 (5%) 28 13	29, 59, 155, 214	0
40	RU	117/118 (99%)	0.39	6 (5%) 28 13	24, 48, 105, 151	0
40	YU	117/118 (99%)	0.31	5 (4%) 35 17	29, 54, 101, 169	0
41	RV	101/101 (100%)	0.24	6 (5%) 22 10	20, 65, 123, 222	0
41	YV	101/101 (100%)	0.67	11 (10%) 5 2	28, 75, 133, 247	0
42	RW	113/113 (100%)	0.11	1 (0%) 84 69	24, 49, 94, 175	0
42	YW	113/113 (100%)	0.03	0 100 100	25, 46, 99, 194	0
43	RX	92/96 (95%)	0.26	3 (3%) 46 24	39, 62, 87, 135	0
43	YX	92/96 (95%)	0.16	0 100 100	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%)	1.14	20 (19%) 1 0	40, 75, 179, 238	0
44	YY	102/110 (92%)	1.28	21 (20%) 1 0	33, 79, 184, 214	0
45	RZ	176/206 (85%)	1.11	39 (22%) 0 0	49, 93, 187, 286	0
45	YZ	183/206 (88%)	0.71	19 (10%) 6 2	41, 92, 163, 211	0
46	R0	83/85 (97%)	0.06	1 (1%) 79 61	27, 50, 94, 200	0
46	Y0	83/85 (97%)	0.30	5 (6%) 21 10	24, 50, 81, 189	0
47	R1	97/98 (98%)	0.51	6 (6%) 20 9	29, 58, 172, 241	0
47	Y1	97/98 (98%)	0.28	5 (5%) 27 12	22, 46, 176, 235	0
48	R2	69/72 (95%)	0.30	4 (5%) 23 10	39, 79, 141, 190	0
48	Y2	69/72 (95%)	0.50	5 (7%) 15 6	29, 60, 106, 196	0
49	R3	59/60 (98%)	0.11	0 100 100	33, 53, 103, 126	0
49	Y3	59/60 (98%)	0.28	0 100 100	35, 61, 112, 167	0
50	R4	70/71 (98%)	2.04	26 (37%) 0 0	79, 165, 243, 284	0
50	Y4	70/71 (98%)	1.80	20 (28%) 0 0	79, 143, 226, 269	0
51	R5	59/60 (98%)	0.56	7 (11%) 4 2	23, 53, 179, 237	0
51	Y5	57/60 (95%)	0.31	5 (8%) 10 4	21, 53, 161, 284	0
52	R6	48/54 (88%)	3.82	32 (66%) 0 0	73, 134, 213, 253	0
52	Y6	48/54 (88%)	3.20	30 (62%) 0 0	73, 129, 207, 245	0
53	R7	49/49 (100%)	0.18	2 (4%) 37 18	21, 33, 127, 192	0
53	Y7	49/49 (100%)	0.08	1 (2%) 65 44	18, 29, 82, 193	0
54	R8	64/65 (98%)	0.59	5 (7%) 13 5	19, 47, 122, 180	0
54	Y8	64/65 (98%)	0.61	5 (7%) 13 5	16, 44, 72, 174	0
55	R9	37/37 (100%)	2.77	21 (56%) 0 0	52, 78, 134, 165	0
55	Y9	36/37 (97%)	0.93	4 (11%) 5 2	36, 76, 110, 130	0
56	Z6	2/3 (66%)	0.14	0 100 100	29, 29, 29, 38	0
56	Z7	2/3 (66%)	0.23	0 100 100	30, 30, 30, 43	0
All	All	21068/21690 (97%)	0.72	2151 (10%) 6 2	10, 65, 171, 375	0

The worst 5 of 2151 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	YA	1087	G	23.1
31	YH	2	SER	22.8

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Mol	Chain	Res	Type	RSRZ
25	YA	2138	C	22.0
20	QT	106	ALA	18.7
25	YA	2137	C	18.6

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, 95^{th} 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	0.74	0.36	44,130,130,130	0
23	A2M	XX	21	23/24	0.82	0.38	44,118,118,118	0
23	OMC	XX	20	21/22	0.92	0.21	44,74,74,74	0
23	OMC	QX	20	21/22	0.93	0.20	44,77,77,77	0
23	A2M	QX	19	23/24	0.94	0.20	39,73,73,73	0
23	A2M	XX	19	23/24	0.96	0.18	62,62,104,137	0
56	PPU	Z6	76	37/38	0.96	0.25	26,33,40,43	0
56	PPU	Z7	76	37/38	0.96	0.27	27,32,49,62	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	YA	3228	1/1	0.21	0.25	69,69,69,69	0
57	MG	YA	3448	1/1	0.30	0.76	82,82,82,82	0
57	MG	RA	3345	1/1	0.31	0.38	73,73,73,73	0
57	MG	YA	3294	1/1	0.34	0.32	45,45,45,45	0
57	MG	XA	1690	1/1	0.39	0.34	52,52,52,52	0
57	MG	QA	1720	1/1	0.40	0.30	67,67,67,67	0
57	MG	YA	3374	1/1	0.44	0.47	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3414	1/1	0.47	0.12	42,42,42,42	0
57	MG	QA	1630	1/1	0.47	0.34	63,63,63,63	0
57	MG	RA	3075	1/1	0.48	0.55	42,42,42,42	0
57	MG	YA	3495	1/1	0.49	0.36	63,63,63,63	0
57	MG	XA	1743	1/1	0.50	0.24	56,56,56,56	0
57	MG	RA	3292	1/1	0.50	0.55	67,67,67,67	0
57	MG	YA	3186	1/1	0.51	0.49	48,48,48,48	0
57	MG	RA	3372	1/1	0.52	0.36	74,74,74,74	0
57	MG	XA	1763	1/1	0.53	0.33	59,59,59,59	0
57	MG	RA	3036	1/1	0.53	0.28	51,51,51,51	0
57	MG	YA	3335	1/1	0.53	0.29	52,52,52,52	0
57	MG	YA	3001	1/1	0.54	0.73	68,68,68,68	0
57	MG	RA	3371	1/1	0.55	0.36	70,70,70,70	0
57	MG	RA	3261	1/1	0.55	0.38	79,79,79,79	0
57	MG	YA	3104	1/1	0.56	0.42	76,76,76,76	0
57	MG	YA	3128	1/1	0.56	0.36	38,38,38,38	0
57	MG	RA	3366	1/1	0.56	0.19	71,71,71,71	0
57	MG	XA	1732	1/1	0.57	0.28	56,56,56,56	0
57	MG	RA	3397	1/1	0.57	0.21	52,52,52,52	0
57	MG	YA	3082	1/1	0.57	0.24	24,24,24,24	0
57	MG	RA	3083	1/1	0.58	0.28	30,30,30,30	0
57	MG	QA	1672	1/1	0.58	0.38	71,71,71,71	0
57	MG	QA	1637	1/1	0.58	0.34	74,74,74,74	0
57	MG	YA	3501	1/1	0.58	0.39	31,31,31,31	0
57	MG	YA	3287	1/1	0.59	0.46	58,58,58,58	0
57	MG	QA	1671	1/1	0.59	0.39	49,49,49,49	0
57	MG	YA	3394	1/1	0.59	0.34	56,56,56,56	0
57	MG	RA	3361	1/1	0.60	0.55	65,65,65,65	0
57	MG	RA	3102	1/1	0.60	0.54	28,28,28,28	0
57	MG	YA	3183	1/1	0.60	0.28	45,45,45,45	0
57	MG	YA	3392	1/1	0.60	0.37	51,51,51,51	0
57	MG	YA	3300	1/1	0.61	0.53	51,51,51,51	0
57	MG	XD	302	1/1	0.61	0.17	51,51,51,51	0
57	MG	YA	3362	1/1	0.61	0.47	61,61,61,61	0
57	MG	YA	3118	1/1	0.62	0.32	40,40,40,40	0
57	MG	RA	3198	1/1	0.62	0.34	50,50,50,50	0
57	MG	RA	3069	1/1	0.63	0.27	18,18,18,18	0
57	MG	YU	201	1/1	0.63	0.42	45,45,45,45	0
57	MG	XA	1646	1/1	0.64	0.58	87,87,87,87	0
57	MG	QA	1734	1/1	0.64	0.28	55,55,55,55	0
57	MG	RA	3392	1/1	0.64	0.51	42,42,42,42	0
57	MG	YA	3488	1/1	0.64	0.36	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3342	1/1	0.64	0.19	52,52,52,52	0
57	MG	YA	3371	1/1	0.64	0.51	64,64,64,64	0
57	MG	RA	3173	1/1	0.64	0.27	28,28,28,28	0
57	MG	YA	3398	1/1	0.65	0.20	67,67,67,67	0
57	MG	YA	3255	1/1	0.65	0.41	64,64,64,64	0
57	MG	YA	3451	1/1	0.65	0.27	66,66,66,66	0
57	MG	QA	1719	1/1	0.65	0.31	60,60,60,60	0
57	MG	RA	3431	1/1	0.65	0.35	53,53,53,53	0
57	MG	RA	3376	1/1	0.65	0.40	66,66,66,66	0
57	MG	YA	3120	1/1	0.65	0.24	41,41,41,41	0
57	MG	RA	3274	1/1	0.66	0.34	68,68,68,68	0
57	MG	RA	3387	1/1	0.66	0.43	56,56,56,56	0
57	MG	YA	3421	1/1	0.66	0.29	38,38,38,38	0
57	MG	YA	3444	1/1	0.66	0.43	48,48,48,48	0
57	MG	RA	3323	1/1	0.66	1.69	87,87,87,87	0
57	MG	RA	3210	1/1	0.67	0.51	64,64,64,64	0
57	MG	YA	3281	1/1	0.67	0.28	52,52,52,52	0
57	MG	RA	3449	1/1	0.67	0.33	32,32,32,32	0
57	MG	YO	201	1/1	0.67	0.24	66,66,66,66	0
57	MG	XA	1628	1/1	0.67	0.15	52,52,52,52	0
57	MG	YA	3470	1/1	0.68	0.23	50,50,50,50	0
57	MG	RA	3321	1/1	0.68	0.32	53,53,53,53	0
57	MG	YA	3493	1/1	0.68	0.33	63,63,63,63	0
57	MG	YA	3068	1/1	0.68	0.18	32,32,32,32	0
57	MG	RD	302	1/1	0.68	0.40	29,29,29,29	0
57	MG	RA	3333	1/1	0.68	0.11	55,55,55,55	0
57	MG	YA	3352	1/1	0.68	0.15	84,84,84,84	0
57	MG	XA	1744	1/1	0.69	0.31	33,33,33,33	0
57	MG	RA	3364	1/1	0.69	0.34	64,64,64,64	0
57	MG	XA	1634	1/1	0.69	0.19	41,41,41,41	0
57	MG	QA	1727	1/1	0.69	0.19	57,57,57,57	0
57	MG	YA	3215	1/1	0.69	0.49	33,33,33,33	0
57	MG	RA	3146	1/1	0.69	0.57	37,37,37,37	0
57	MG	XA	1723	1/1	0.69	0.31	55,55,55,55	0
57	MG	YA	3377	1/1	0.69	0.32	43,43,43,43	0
57	MG	YA	3268	1/1	0.69	0.42	55,55,55,55	0
57	MG	RA	3298	1/1	0.69	0.40	62,62,62,62	0
57	MG	R0	102	1/1	0.69	0.49	57,57,57,57	0
57	MG	XA	1624	1/1	0.70	0.24	39,39,39,39	0
57	MG	QV	103	1/1	0.70	0.28	52,52,52,52	0
57	MG	YA	3499	1/1	0.70	0.47	67,67,67,67	0
57	MG	QA	1722	1/1	0.70	0.34	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3297	1/1	0.70	0.64	49,49,49,49	0
57	MG	QA	1741	1/1	0.70	0.18	46,46,46,46	0
57	MG	RB	205	1/1	0.71	0.32	59,59,59,59	0
57	MG	RA	3353	1/1	0.71	0.42	46,46,46,46	0
57	MG	YA	3437	1/1	0.71	0.24	37,37,37,37	0
57	MG	RA	3106	1/1	0.71	0.29	41,41,41,41	0
57	MG	R2	101	1/1	0.71	0.22	68,68,68,68	0
57	MG	YA	3348	1/1	0.71	0.47	77,77,77,77	0
57	MG	RA	3368	1/1	0.71	0.26	55,55,55,55	0
57	MG	XA	1700	1/1	0.72	0.24	47,47,47,47	0
57	MG	RA	3092	1/1	0.72	0.45	56,56,56,56	0
57	MG	RA	3300	1/1	0.72	0.45	37,37,37,37	0
57	MG	QA	1738	1/1	0.72	0.17	43,43,43,43	0
57	MG	QA	1693	1/1	0.72	0.34	63,63,63,63	0
57	MG	QA	1744	1/1	0.72	0.15	54,54,54,54	0
57	MG	YA	3147	1/1	0.72	0.48	25,25,25,25	0
57	MG	YA	3179	1/1	0.72	0.17	63,63,63,63	0
57	MG	XA	1685	1/1	0.72	0.54	62,62,62,62	0
57	MG	YB	206	1/1	0.72	0.29	49,49,49,49	0
57	MG	YA	3328	1/1	0.72	0.31	47,47,47,47	0
57	MG	QA	1669	1/1	0.72	0.25	53,53,53,53	0
57	MG	RA	3450	1/1	0.73	0.29	25,25,25,25	0
57	MG	XA	1756	1/1	0.73	0.48	45,45,45,45	0
57	MG	QA	1745	1/1	0.73	0.23	52,52,52,52	0
57	MG	XA	1712	1/1	0.73	0.12	61,61,61,61	0
57	MG	YA	3402	1/1	0.73	0.24	56,56,56,56	0
57	MG	RA	3214	1/1	0.73	0.38	57,57,57,57	0
57	MG	YA	3428	1/1	0.73	0.39	32,32,32,32	0
57	MG	RA	3438	1/1	0.73	0.51	58,58,58,58	0
57	MG	RA	3229	1/1	0.73	0.17	30,30,30,30	0
57	MG	YA	3100	1/1	0.73	0.43	20,20,20,20	0
57	MG	RA	3302	1/1	0.74	0.55	59,59,59,59	0
57	MG	QA	1631	1/1	0.74	0.33	55,55,55,55	0
57	MG	XA	1704	1/1	0.74	0.50	62,62,62,62	0
57	MG	YA	3452	1/1	0.74	0.30	49,49,49,49	0
57	MG	YA	3391	1/1	0.74	0.60	49,49,49,49	0
57	MG	RA	3351	1/1	0.74	0.60	58,58,58,58	0
57	MG	YA	3133	1/1	0.74	0.31	38,38,38,38	0
57	MG	RA	3341	1/1	0.74	1.00	73,73,73,73	0
57	MG	YA	3158	1/1	0.74	0.18	30,30,30,30	0
57	MG	YA	3409	1/1	0.74	0.28	47,47,47,47	0
57	MG	YA	3160	1/1	0.74	0.31	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YH	202	1/1	0.74	0.26	47,47,47,47	0
57	MG	YA	3283	1/1	0.74	0.45	52,52,52,52	0
57	MG	YA	3365	1/1	0.74	0.48	39,39,39,39	0
57	MG	XA	1725	1/1	0.75	0.43	54,54,54,54	0
57	MG	QN	102	1/1	0.75	0.13	61,61,61,61	0
57	MG	QA	1743	1/1	0.75	0.20	52,52,52,52	0
57	MG	QA	1704	1/1	0.75	0.27	59,59,59,59	0
57	MG	XA	1656	1/1	0.75	0.17	65,65,65,65	0
57	MG	YA	3134	1/1	0.75	0.93	47,47,47,47	0
57	MG	YA	3387	1/1	0.75	0.24	71,71,71,71	0
57	MG	QA	1697	1/1	0.75	0.43	76,76,76,76	0
57	MG	YA	3291	1/1	0.75	0.29	54,54,54,54	0
57	MG	RA	3218	1/1	0.75	0.21	35,35,35,35	0
57	MG	RE	303	1/1	0.75	0.23	51,51,51,51	0
57	MG	YA	3502	1/1	0.75	0.47	32,32,32,32	0
57	MG	RA	3118	1/1	0.75	0.28	55,55,55,55	0
57	MG	QA	1751	1/1	0.75	0.49	84,84,84,84	0
57	MG	RA	3168	1/1	0.75	0.30	48,48,48,48	0
57	MG	YA	3197	1/1	0.75	0.77	38,38,38,38	0
57	MG	XA	1625	1/1	0.76	0.23	37,37,37,37	0
57	MG	QA	1713	1/1	0.76	0.17	58,58,58,58	0
57	MG	QD	303	1/1	0.76	0.11	48,48,48,48	0
57	MG	YA	3172	1/1	0.76	0.32	52,52,52,52	0
57	MG	YA	3231	1/1	0.76	0.28	35,35,35,35	0
57	MG	YA	3236	1/1	0.76	0.24	40,40,40,40	0
57	MG	YA	3249	1/1	0.76	0.27	42,42,42,42	0
57	MG	YA	3176	1/1	0.76	0.18	57,57,57,57	0
57	MG	RA	3277	1/1	0.76	0.31	57,57,57,57	0
57	MG	XA	1703	1/1	0.76	0.21	55,55,55,55	0
57	MG	RY	202	1/1	0.77	0.48	50,50,50,50	0
57	MG	RA	3442	1/1	0.77	0.38	41,41,41,41	0
57	MG	YA	3489	1/1	0.77	0.30	59,59,59,59	0
57	MG	XA	1682	1/1	0.77	0.33	42,42,42,42	0
57	MG	RA	3394	1/1	0.77	0.15	31,31,31,31	0
57	MG	RA	3143	1/1	0.77	0.25	61,61,61,61	0
57	MG	QA	1678	1/1	0.77	0.18	70,70,70,70	0
57	MG	QA	1686	1/1	0.77	0.24	43,43,43,43	0
57	MG	XA	1758	1/1	0.77	0.36	46,46,46,46	0
57	MG	YA	3265	1/1	0.77	0.30	45,45,45,45	0
57	MG	RA	3232	1/1	0.77	0.38	53,53,53,53	0
57	MG	YP	202	1/1	0.77	0.30	45,45,45,45	0
57	MG	YR	201	1/1	0.77	0.29	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3457	1/1	0.77	0.27	24,24,24,24	0
57	MG	RY	201	1/1	0.78	0.18	37,37,37,37	0
57	MG	QA	1737	1/1	0.78	0.35	56,56,56,56	0
57	MG	XA	1748	1/1	0.78	0.40	62,62,62,62	0
57	MG	YA	3324	1/1	0.78	0.25	53,53,53,53	0
57	MG	RA	3182	1/1	0.78	0.49	78,78,78,78	0
57	MG	QA	1650	1/1	0.78	0.29	36,36,36,36	0
57	MG	RA	3358	1/1	0.78	0.15	46,46,46,46	0
57	MG	RA	3332	1/1	0.78	0.12	67,67,67,67	0
57	MG	RA	3294	1/1	0.78	0.33	63,63,63,63	0
57	MG	XA	1629	1/1	0.78	0.33	54,54,54,54	0
57	MG	RA	3205	1/1	0.78	0.20	30,30,30,30	0
57	MG	XA	1639	1/1	0.78	0.88	74,74,74,74	0
57	MG	QA	1684	1/1	0.78	0.37	54,54,54,54	0
57	MG	YA	3111	1/1	0.78	0.50	57,57,57,57	0
57	MG	XA	1752	1/1	0.79	0.31	56,56,56,56	0
57	MG	XA	1702	1/1	0.79	0.75	69,69,69,69	0
57	MG	RA	3041	1/1	0.79	0.21	23,23,23,23	0
57	MG	YA	3289	1/1	0.79	0.19	38,38,38,38	0
57	MG	YA	3198	1/1	0.79	0.12	54,54,54,54	0
57	MG	YA	3201	1/1	0.79	0.37	35,35,35,35	0
57	MG	YA	3490	1/1	0.79	0.69	63,63,63,63	0
57	MG	QA	1666	1/1	0.79	0.12	42,42,42,42	0
57	MG	RA	3336	1/1	0.79	0.16	33,33,33,33	0
57	MG	RA	3338	1/1	0.79	0.63	70,70,70,70	0
57	MG	XA	1669	1/1	0.79	0.48	48,48,48,48	0
57	MG	YA	3404	1/1	0.79	0.31	63,63,63,63	0
57	MG	RA	3422	1/1	0.79	0.21	41,41,41,41	0
57	MG	YA	3340	1/1	0.79	0.50	54,54,54,54	0
57	MG	QA	1668	1/1	0.79	0.20	44,44,44,44	0
57	MG	RA	3329	1/1	0.79	0.75	65,65,65,65	0
57	MG	YA	3353	1/1	0.79	0.59	53,53,53,53	0
57	MG	XA	1630	1/1	0.79	0.20	75,75,75,75	0
57	MG	RA	3399	1/1	0.80	0.24	40,40,40,40	0
57	MG	RA	3370	1/1	0.80	0.51	65,65,65,65	0
57	MG	YA	3467	1/1	0.80	0.20	43,43,43,43	0
57	MG	RA	3157	1/1	0.80	0.16	40,40,40,40	0
57	MG	XA	1708	1/1	0.80	0.14	39,39,39,39	0
57	MG	YA	3310	1/1	0.80	0.29	54,54,54,54	0
57	MG	RA	3357	1/1	0.80	0.88	61,61,61,61	0
57	MG	YA	3327	1/1	0.80	0.45	69,69,69,69	0
57	MG	YA	3152	1/1	0.80	0.39	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1716	1/1	0.80	0.39	51,51,51,51	0
57	MG	YA	3059	1/1	0.80	0.18	28,28,28,28	0
57	MG	YA	3410	1/1	0.80	0.16	62,62,62,62	0
57	MG	RA	3433	1/1	0.80	0.31	49,49,49,49	0
57	MG	RA	3322	1/1	0.80	0.42	84,84,84,84	0
57	MG	RA	3188	1/1	0.80	0.40	58,58,58,58	0
57	MG	RA	3167	1/1	0.80	0.28	31,31,31,31	0
57	MG	RA	3176	1/1	0.80	0.44	57,57,57,57	0
57	MG	RA	3285	1/1	0.80	0.36	35,35,35,35	0
57	MG	Y0	101	1/1	0.80	0.36	52,52,52,52	0
57	MG	QA	1708	1/1	0.81	0.36	60,60,60,60	0
57	MG	RA	3315	1/1	0.81	0.23	27,27,27,27	0
57	MG	YA	3360	1/1	0.81	0.55	61,61,61,61	0
57	MG	QA	1735	1/1	0.81	0.34	73,73,73,73	0
57	MG	RA	3347	1/1	0.81	0.50	65,65,65,65	0
57	MG	RA	3014	1/1	0.81	0.35	17,17,17,17	0
57	MG	XA	1709	1/1	0.81	0.54	54,54,54,54	0
57	MG	YA	3476	1/1	0.81	0.14	53,53,53,53	0
57	MG	YA	3482	1/1	0.81	0.26	54,54,54,54	0
57	MG	RA	3383	1/1	0.81	0.12	75,75,75,75	0
57	MG	QA	1742	1/1	0.81	0.22	44,44,44,44	0
57	MG	RA	3291	1/1	0.81	0.62	48,48,48,48	0
57	MG	RD	301	1/1	0.81	0.30	28,28,28,28	0
57	MG	YA	3393	1/1	0.81	0.18	56,56,56,56	0
57	MG	YA	3498	1/1	0.81	0.55	57,57,57,57	0
57	MG	RA	3147	1/1	0.81	0.23	48,48,48,48	0
57	MG	YA	3308	1/1	0.81	0.71	54,54,54,54	0
57	MG	RA	3221	1/1	0.81	0.78	43,43,43,43	0
57	MG	YA	3218	1/1	0.81	0.63	40,40,40,40	0
57	MG	RA	3187	1/1	0.81	0.55	55,55,55,55	0
57	MG	RA	3408	1/1	0.81	0.27	38,38,38,38	0
57	MG	YA	3234	1/1	0.81	0.51	50,50,50,50	0
57	MG	YA	3425	1/1	0.81	0.12	33,33,33,33	0
57	MG	XA	1686	1/1	0.81	0.25	39,39,39,39	0
57	MG	QA	1633	1/1	0.81	0.37	57,57,57,57	0
57	MG	YA	3329	1/1	0.82	0.76	50,50,50,50	0
57	MG	YA	3142	1/1	0.82	0.67	65,65,65,65	0
57	MG	YA	3145	1/1	0.82	0.22	50,50,50,50	0
57	MG	XA	1707	1/1	0.82	0.51	54,54,54,54	0
57	MG	YA	3149	1/1	0.82	0.42	34,34,34,34	0
57	MG	RA	3217	1/1	0.82	0.41	50,50,50,50	0
57	MG	YA	3461	1/1	0.82	0.31	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3262	1/1	0.82	0.22	41,41,41,41	0
57	MG	XA	1666	1/1	0.82	0.36	52,52,52,52	0
57	MG	YA	3475	1/1	0.82	0.82	40,40,40,40	0
57	MG	RA	3446	1/1	0.82	0.50	33,33,33,33	0
57	MG	YA	3366	1/1	0.82	0.93	57,57,57,57	0
57	MG	YA	3272	1/1	0.82	0.22	48,48,48,48	0
57	MG	YA	3274	1/1	0.82	0.42	48,48,48,48	0
57	MG	YA	3162	1/1	0.82	0.28	46,46,46,46	0
57	MG	YA	3167	1/1	0.82	0.28	43,43,43,43	0
57	MG	YA	3285	1/1	0.82	0.17	52,52,52,52	0
57	MG	RA	3183	1/1	0.82	0.13	65,65,65,65	0
57	MG	XA	1684	1/1	0.82	0.26	55,55,55,55	0
57	MG	YA	3090	1/1	0.82	0.25	46,46,46,46	0
57	MG	QA	1679	1/1	0.82	0.25	37,37,37,37	0
57	MG	YA	3503	1/1	0.82	0.21	45,45,45,45	0
57	MG	RA	3111	1/1	0.82	0.17	45,45,45,45	0
57	MG	XA	1687	1/1	0.82	0.14	55,55,55,55	0
57	MG	QA	1680	1/1	0.82	0.40	58,58,58,58	0
57	MG	QA	1711	1/1	0.82	0.11	55,55,55,55	0
57	MG	RA	3093	1/1	0.82	0.34	38,38,38,38	0
57	MG	RA	3002	1/1	0.82	0.27	55,55,55,55	0
57	MG	RA	3319	1/1	0.82	0.24	51,51,51,51	0
57	MG	QA	1670	1/1	0.83	0.38	54,54,54,54	0
57	MG	YA	3140	1/1	0.83	0.11	32,32,32,32	0
57	MG	YA	3336	1/1	0.83	0.22	52,52,52,52	0
57	MG	XA	1761	1/1	0.83	0.20	53,53,53,53	0
57	MG	RA	3059	1/1	0.83	0.11	27,27,27,27	0
57	MG	RA	3254	1/1	0.83	0.09	47,47,47,47	0
57	MG	RA	3325	1/1	0.83	0.43	41,41,41,41	0
57	MG	YA	3354	1/1	0.83	0.20	41,41,41,41	0
57	MG	YA	3022	1/1	0.83	0.31	72,72,72,72	0
57	MG	YA	3031	1/1	0.83	0.28	19,19,19,19	0
57	MG	RA	3296	1/1	0.83	0.31	51,51,51,51	0
57	MG	YA	3063	1/1	0.83	0.21	21,21,21,21	0
57	MG	YA	3369	1/1	0.83	0.19	49,49,49,49	0
57	MG	RA	3356	1/1	0.83	0.71	46,46,46,46	0
57	MG	QA	1625	1/1	0.83	0.10	47,47,47,47	0
57	MG	YA	3173	1/1	0.83	0.36	28,28,28,28	0
57	MG	RA	3388	1/1	0.83	0.14	56,56,56,56	0
57	MG	YA	3288	1/1	0.83	0.48	51,51,51,51	0
57	MG	YA	3097	1/1	0.83	0.25	20,20,20,20	0
57	MG	XA	1727	1/1	0.83	0.38	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3447	1/1	0.83	0.20	32,32,32,32	0
57	MG	YA	3187	1/1	0.83	0.56	64,64,64,64	0
57	MG	YA	3110	1/1	0.83	0.33	42,42,42,42	0
57	MG	RA	3264	1/1	0.83	0.17	41,41,41,41	0
57	MG	YA	3406	1/1	0.83	0.37	49,49,49,49	0
57	MG	XA	1699	1/1	0.83	0.19	52,52,52,52	0
57	MG	RA	3128	1/1	0.83	0.18	35,35,35,35	0
57	MG	YQ	202	1/1	0.83	0.19	39,39,39,39	0
57	MG	YA	3420	1/1	0.83	0.29	65,65,65,65	0
57	MG	RA	3138	1/1	0.83	0.31	40,40,40,40	0
57	MG	YV	201	1/1	0.83	0.29	17,17,17,17	0
57	MG	QD	302	1/1	0.83	0.36	67,67,67,67	0
57	MG	QA	1640	1/1	0.84	0.71	60,60,60,60	0
57	MG	YA	3232	1/1	0.84	0.16	35,35,35,35	0
57	MG	YA	3471	1/1	0.84	0.27	44,44,44,44	0
57	MG	RA	3418	1/1	0.84	0.18	43,43,43,43	0
57	MG	RA	3148	1/1	0.84	0.39	19,19,19,19	0
57	MG	YA	3477	1/1	0.84	0.25	44,44,44,44	0
57	MG	YA	3480	1/1	0.84	0.22	50,50,50,50	0
57	MG	YA	3246	1/1	0.84	0.10	38,38,38,38	0
57	MG	RA	3426	1/1	0.84	0.13	56,56,56,56	0
57	MG	RA	3348	1/1	0.84	0.32	47,47,47,47	0
57	MG	YA	3399	1/1	0.84	0.20	47,47,47,47	0
57	MG	YA	3261	1/1	0.84	0.21	33,33,33,33	0
57	MG	RA	3211	1/1	0.84	0.18	31,31,31,31	0
57	MG	RQ	201	1/1	0.84	0.29	34,34,34,34	0
57	MG	XA	1728	1/1	0.84	0.57	59,59,59,59	0
57	MG	YA	3182	1/1	0.84	0.23	52,52,52,52	0
57	MG	QA	1749	1/1	0.84	0.33	57,57,57,57	0
57	MG	YA	3275	1/1	0.84	0.25	59,59,59,59	0
57	MG	YA	3136	1/1	0.84	0.37	33,33,33,33	0
57	MG	XA	1742	1/1	0.84	0.39	50,50,50,50	0
57	MG	YA	3361	1/1	0.84	0.35	48,48,48,48	0
57	MG	QA	1603	1/1	0.84	0.27	53,53,53,53	0
57	MG	XA	1657	1/1	0.84	0.37	37,37,37,37	0
57	MG	QA	1724	1/1	0.84	0.37	63,63,63,63	0
57	MG	QA	1677	1/1	0.84	0.15	50,50,50,50	0
57	MG	YA	3099	1/1	0.84	0.18	53,53,53,53	0
57	MG	YA	3155	1/1	0.84	0.34	44,44,44,44	0
57	MG	YA	3345	1/1	0.85	0.32	70,70,70,70	0
57	MG	YA	3443	1/1	0.85	0.22	43,43,43,43	0
57	MG	XA	1654	1/1	0.85	0.39	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3327	1/1	0.85	0.28	67,67,67,67	0
57	MG	YA	3450	1/1	0.85	0.34	50,50,50,50	0
57	MG	QA	1723	1/1	0.85	0.20	74,74,74,74	0
57	MG	RE	301	1/1	0.85	0.37	41,41,41,41	0
57	MG	YA	3356	1/1	0.85	0.21	54,54,54,54	0
57	MG	YA	3458	1/1	0.85	0.39	28,28,28,28	0
57	MG	RA	3424	1/1	0.85	0.18	54,54,54,54	0
57	MG	YA	3466	1/1	0.85	0.43	48,48,48,48	0
57	MG	QA	1661	1/1	0.85	0.15	52,52,52,52	0
57	MG	YA	3273	1/1	0.85	0.34	50,50,50,50	0
57	MG	QA	1665	1/1	0.85	0.30	54,54,54,54	0
57	MG	XA	1736	1/1	0.85	0.19	56,56,56,56	0
57	MG	YA	3367	1/1	0.85	0.21	70,70,70,70	0
57	MG	XA	1739	1/1	0.85	0.18	48,48,48,48	0
57	MG	RA	3308	1/1	0.85	0.28	53,53,53,53	0
57	MG	RA	3434	1/1	0.85	0.31	46,46,46,46	0
57	MG	RA	3279	1/1	0.85	0.18	29,29,29,29	0
57	MG	YA	3384	1/1	0.85	0.28	65,65,65,65	0
57	MG	XA	1747	1/1	0.85	0.24	64,64,64,64	0
57	MG	XA	1620	1/1	0.85	0.14	27,27,27,27	0
57	MG	RA	3439	1/1	0.85	0.33	54,54,54,54	0
57	MG	RA	3441	1/1	0.85	0.77	59,59,59,59	0
57	MG	YA	3204	1/1	0.85	0.86	68,68,68,68	0
57	MG	YA	3207	1/1	0.85	0.21	20,20,20,20	0
57	MG	YA	3302	1/1	0.85	0.29	61,61,61,61	0
57	MG	XA	1757	1/1	0.85	0.16	68,68,68,68	0
57	MG	RA	3066	1/1	0.85	0.07	35,35,35,35	0
57	MG	YG	201	1/1	0.85	0.07	51,51,51,51	0
57	MG	QA	1688	1/1	0.85	0.14	56,56,56,56	0
57	MG	RA	3249	1/1	0.85	0.29	48,48,48,48	0
57	MG	RA	3401	1/1	0.85	0.26	58,58,58,58	0
57	MG	YQ	201	1/1	0.85	0.20	54,54,54,54	0
57	MG	XV	103	1/1	0.85	0.29	45,45,45,45	0
57	MG	YA	3148	1/1	0.85	0.38	59,59,59,59	0
57	MG	RA	3107	1/1	0.85	0.35	26,26,26,26	0
57	MG	QA	1648	1/1	0.85	0.12	56,56,56,56	0
57	MG	YA	3429	1/1	0.85	0.26	14,14,14,14	0
57	MG	RA	3334	1/1	0.86	0.97	71,71,71,71	0
57	MG	RA	3097	1/1	0.86	0.92	53,53,53,53	0
57	MG	RA	3267	1/1	0.86	0.56	41,41,41,41	0
57	MG	RA	3309	1/1	0.86	0.17	60,60,60,60	0
57	MG	YA	3380	1/1	0.86	0.20	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	QA	1696	1/1	0.86	0.20	58,58,58,58	0
57	MG	XK	201	1/1	0.86	0.31	37,37,37,37	0
57	MG	QA	1746	1/1	0.86	0.28	40,40,40,40	0
57	MG	YA	3309	1/1	0.86	0.65	73,73,73,73	0
57	MG	XA	1722	1/1	0.86	0.37	42,42,42,42	0
57	MG	YA	3323	1/1	0.86	0.19	42,42,42,42	0
57	MG	QA	1728	1/1	0.86	0.17	45,45,45,45	0
57	MG	RA	3003	1/1	0.86	0.39	22,22,22,22	0
57	MG	YA	3239	1/1	0.86	0.13	24,24,24,24	0
57	MG	XA	1677	1/1	0.86	0.34	65,65,65,65	0
57	MG	XA	1680	1/1	0.86	0.24	50,50,50,50	0
57	MG	RA	3158	1/1	0.86	0.40	57,57,57,57	0
57	MG	RA	3240	1/1	0.86	0.26	28,28,28,28	0
57	MG	YA	3088	1/1	0.86	0.35	21,21,21,21	0
57	MG	YA	3169	1/1	0.86	0.48	46,46,46,46	0
57	MG	YA	3349	1/1	0.86	0.25	62,62,62,62	0
57	MG	RA	3244	1/1	0.86	0.23	33,33,33,33	0
57	MG	R5	103	1/1	0.86	0.08	40,40,40,40	0
57	MG	QA	1639	1/1	0.86	0.27	76,76,76,76	0
57	MG	QA	1638	1/1	0.86	0.13	48,48,48,48	0
57	MG	RA	3398	1/1	0.86	0.14	24,24,24,24	0
57	MG	RA	3359	1/1	0.86	0.20	51,51,51,51	0
57	MG	XA	1749	1/1	0.86	0.34	52,52,52,52	0
57	MG	RA	3448	1/1	0.86	0.33	27,27,27,27	0
57	MG	XA	1755	1/1	0.86	0.15	58,58,58,58	0
57	MG	YA	3453	1/1	0.86	0.55	54,54,54,54	0
57	MG	QA	1707	1/1	0.86	0.61	45,45,45,45	0
57	MG	Y7	101	1/1	0.86	0.60	55,55,55,55	0
57	MG	YA	3192	1/1	0.87	0.34	34,34,34,34	0
57	MG	RA	3310	1/1	0.87	0.23	52,52,52,52	0
57	MG	YA	3370	1/1	0.87	0.93	50,50,50,50	0
57	MG	RA	3337	1/1	0.87	0.37	40,40,40,40	0
57	MG	RA	3362	1/1	0.87	0.10	56,56,56,56	0
57	MG	YA	3295	1/1	0.87	0.09	39,39,39,39	0
57	MG	RA	3108	1/1	0.87	0.28	56,56,56,56	0
57	MG	QA	1732	1/1	0.87	0.23	44,44,44,44	0
57	MG	RA	3412	1/1	0.87	0.21	41,41,41,41	0
57	MG	RA	3216	1/1	0.87	0.16	32,32,32,32	0
57	MG	RA	3415	1/1	0.87	0.48	23,23,23,23	0
57	MG	XN	102	1/1	0.87	0.17	52,52,52,52	0
57	MG	RA	3117	1/1	0.87	0.67	39,39,39,39	0
57	MG	YA	3395	1/1	0.87	0.50	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3396	1/1	0.87	0.23	48,48,48,48	0
57	MG	RA	3419	1/1	0.87	0.31	40,40,40,40	0
57	MG	YA	3010	1/1	0.87	0.49	22,22,22,22	0
57	MG	YA	3237	1/1	0.87	0.14	54,54,54,54	0
57	MG	YA	3019	1/1	0.87	0.33	21,21,21,21	0
57	MG	RA	3047	1/1	0.87	0.23	16,16,16,16	0
57	MG	YA	3408	1/1	0.87	0.36	47,47,47,47	0
57	MG	RA	3265	1/1	0.87	0.65	57,57,57,57	0
57	MG	RA	3126	1/1	0.87	0.25	34,34,34,34	0
57	MG	QA	1705	1/1	0.87	0.46	30,30,30,30	0
57	MG	RA	3354	1/1	0.87	0.17	65,65,65,65	0
57	MG	RA	3307	1/1	0.87	0.45	64,64,64,64	0
57	MG	RA	3091	1/1	0.87	0.31	24,24,24,24	0
57	MG	R5	102	1/1	0.87	0.26	40,40,40,40	0
57	MG	QA	1614	1/1	0.87	0.18	39,39,39,39	0
57	MG	XA	1617	1/1	0.87	0.19	42,42,42,42	0
57	MG	YA	3181	1/1	0.87	0.26	50,50,50,50	0
57	MG	RA	3440	1/1	0.87	0.37	53,53,53,53	0
57	MG	XA	1692	1/1	0.87	0.14	36,36,36,36	0
57	MG	XA	1694	1/1	0.87	0.20	43,43,43,43	0
57	MG	XA	1622	1/1	0.87	0.37	40,40,40,40	0
58	ZN	XD	301	1/1	0.87	0.41	60,60,60,60	0
57	MG	RA	3234	1/1	0.88	0.49	49,49,49,49	0
57	MG	RA	3303	1/1	0.88	0.14	42,42,42,42	0
57	MG	YA	3427	1/1	0.88	0.27	29,29,29,29	0
57	MG	XA	1724	1/1	0.88	0.60	54,54,54,54	0
57	MG	QA	1655	1/1	0.88	0.36	46,46,46,46	0
57	MG	YA	3433	1/1	0.88	0.35	46,46,46,46	0
57	MG	XA	1648	1/1	0.88	0.21	55,55,55,55	0
57	MG	YA	3439	1/1	0.88	0.33	42,42,42,42	0
57	MG	XA	1651	1/1	0.88	0.40	32,32,32,32	0
57	MG	RA	3349	1/1	0.88	0.20	41,41,41,41	0
57	MG	QV	105	1/1	0.88	0.34	31,31,31,31	0
57	MG	YA	3219	1/1	0.88	0.26	46,46,46,46	0
57	MG	RA	3186	1/1	0.88	0.22	54,54,54,54	0
57	MG	YA	3230	1/1	0.88	0.29	56,56,56,56	0
57	MG	QA	1681	1/1	0.88	0.21	68,68,68,68	0
57	MG	YA	3456	1/1	0.88	0.25	47,47,47,47	0
57	MG	QA	1674	1/1	0.88	0.17	54,54,54,54	0
57	MG	XA	1676	1/1	0.88	0.22	33,33,33,33	0
57	MG	RA	3413	1/1	0.88	0.31	41,41,41,41	0
57	MG	RA	3191	1/1	0.88	0.14	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3005	1/1	0.88	0.46	21,21,21,21	0
57	MG	YA	3244	1/1	0.88	0.54	57,57,57,57	0
57	MG	RV	201	1/1	0.88	0.27	14,14,14,14	0
57	MG	QA	1747	1/1	0.88	0.10	57,57,57,57	0
57	MG	RA	3272	1/1	0.88	0.23	26,26,26,26	0
57	MG	RA	3420	1/1	0.88	0.17	49,49,49,49	0
57	MG	RA	3206	1/1	0.88	0.20	18,18,18,18	0
57	MG	XA	1760	1/1	0.88	0.13	77,77,77,77	0
57	MG	YA	3266	1/1	0.88	0.40	31,31,31,31	0
57	MG	YA	3372	1/1	0.88	0.41	55,55,55,55	0
57	MG	XA	1691	1/1	0.88	0.20	46,46,46,46	0
57	MG	RA	3023	1/1	0.88	0.28	55,55,55,55	0
57	MG	QA	1610	1/1	0.88	0.10	76,76,76,76	0
57	MG	YA	3383	1/1	0.88	0.15	51,51,51,51	0
57	MG	XA	1608	1/1	0.88	0.41	47,47,47,47	0
57	MG	QA	1623	1/1	0.88	0.36	34,34,34,34	0
57	MG	XS	300	1/1	0.88	0.20	46,46,46,46	0
57	MG	RA	3288	1/1	0.88	0.17	61,61,61,61	0
57	MG	RA	3163	1/1	0.88	0.10	55,55,55,55	0
57	MG	YA	3005	1/1	0.88	0.44	24,24,24,24	0
57	MG	XA	1623	1/1	0.88	0.25	36,36,36,36	0
57	MG	YA	3175	1/1	0.88	0.12	27,27,27,27	0
57	MG	QA	1653	1/1	0.88	0.59	50,50,50,50	0
57	MG	YA	3292	1/1	0.88	0.26	32,32,32,32	0
57	MG	YA	3177	1/1	0.88	0.26	59,59,59,59	0
57	MG	QA	1710	1/1	0.88	0.19	50,50,50,50	0
57	MG	QA	1694	1/1	0.88	0.17	55,55,55,55	0
57	MG	YA	3038	1/1	0.88	0.22	45,45,45,45	0
57	MG	YW	201	1/1	0.88	0.33	32,32,32,32	0
57	MG	YA	3048	1/1	0.88	0.30	33,33,33,33	0
57	MG	Y5	102	1/1	0.88	0.29	50,50,50,50	0
57	MG	Y5	103	1/1	0.88	0.29	23,23,23,23	0
57	MG	RA	3175	1/1	0.88	0.16	31,31,31,31	0
57	MG	QV	101	1/1	0.88	0.29	15,15,15,15	0
57	MG	RA	3432	1/1	0.89	0.26	39,39,39,39	0
57	MG	QA	1706	1/1	0.89	0.23	47,47,47,47	0
57	MG	RA	3120	1/1	0.89	0.14	42,42,42,42	0
57	MG	RA	3343	1/1	0.89	0.63	56,56,56,56	0
57	MG	YA	3417	1/1	0.89	0.12	55,55,55,55	0
57	MG	YA	3418	1/1	0.89	0.28	24,24,24,24	0
57	MG	RA	3314	1/1	0.89	0.12	62,62,62,62	0
57	MG	RA	3385	1/1	0.89	0.25	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3298	1/1	0.89	0.28	52,52,52,52	0
57	MG	YA	3013	1/1	0.89	0.57	27,27,27,27	0
57	MG	RA	3124	1/1	0.89	0.23	40,40,40,40	0
57	MG	RA	3230	1/1	0.89	0.22	42,42,42,42	0
57	MG	XA	1710	1/1	0.89	0.20	58,58,58,58	0
57	MG	YA	3035	1/1	0.89	0.23	39,39,39,39	0
57	MG	YA	3320	1/1	0.89	0.35	48,48,48,48	0
57	MG	XA	1633	1/1	0.89	0.37	28,28,28,28	0
57	MG	YA	3189	1/1	0.89	0.26	52,52,52,52	0
57	MG	YA	3326	1/1	0.89	0.67	46,46,46,46	0
57	MG	XA	1714	1/1	0.89	0.20	41,41,41,41	0
57	MG	QA	1729	1/1	0.89	0.17	30,30,30,30	0
57	MG	XA	1636	1/1	0.89	0.25	46,46,46,46	0
57	MG	YA	3199	1/1	0.89	0.45	54,54,54,54	0
57	MG	RA	3350	1/1	0.89	0.99	54,54,54,54	0
57	MG	QA	1731	1/1	0.89	0.27	45,45,45,45	0
57	MG	RA	3203	1/1	0.89	0.33	18,18,18,18	0
57	MG	RA	3324	1/1	0.89	0.44	40,40,40,40	0
57	MG	YA	3216	1/1	0.89	0.24	30,30,30,30	0
57	MG	YA	3091	1/1	0.89	0.30	40,40,40,40	0
57	MG	RA	3451	1/1	0.89	0.45	23,23,23,23	0
57	MG	YA	3226	1/1	0.89	0.36	48,48,48,48	0
57	MG	YA	3472	1/1	0.89	0.41	66,66,66,66	0
57	MG	RA	3133	1/1	0.89	0.50	59,59,59,59	0
57	MG	YA	3359	1/1	0.89	0.20	36,36,36,36	0
57	MG	XA	1734	1/1	0.89	0.21	16,16,16,16	0
57	MG	YA	3478	1/1	0.89	0.48	81,81,81,81	0
57	MG	RA	3172	1/1	0.89	0.17	47,47,47,47	0
57	MG	YA	3106	1/1	0.89	0.28	42,42,42,42	0
57	MG	XA	1738	1/1	0.89	0.24	43,43,43,43	0
57	MG	XA	1663	1/1	0.89	0.34	42,42,42,42	0
57	MG	YA	3114	1/1	0.89	0.35	26,26,26,26	0
57	MG	XA	1740	1/1	0.89	0.28	56,56,56,56	0
57	MG	RA	3134	1/1	0.89	0.85	46,46,46,46	0
57	MG	RA	3255	1/1	0.89	0.54	43,43,43,43	0
57	MG	QA	1627	1/1	0.89	0.14	42,42,42,42	0
57	MG	RF	301	1/1	0.89	0.15	34,34,34,34	0
57	MG	YA	3256	1/1	0.89	0.29	57,57,57,57	0
57	MG	QL	201	1/1	0.89	0.21	58,58,58,58	0
57	MG	YA	3382	1/1	0.89	0.28	55,55,55,55	0
57	MG	XA	1681	1/1	0.89	0.17	38,38,38,38	0
57	MG	RA	3416	1/1	0.89	0.25	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3385	1/1	0.89	0.37	50,50,50,50	0
57	MG	RA	3051	1/1	0.89	0.35	26,26,26,26	0
57	MG	RA	3365	1/1	0.89	0.24	51,51,51,51	0
57	MG	QA	1699	1/1	0.89	0.28	58,58,58,58	0
57	MG	RA	3367	1/1	0.89	0.45	31,31,31,31	0
57	MG	RA	3270	1/1	0.89	0.45	42,42,42,42	0
57	MG	RA	3369	1/1	0.89	0.58	40,40,40,40	0
57	MG	XA	1762	1/1	0.89	0.09	33,33,33,33	0
57	MG	RA	3428	1/1	0.89	0.45	37,37,37,37	0
57	MG	Y5	101	1/1	0.89	0.28	27,27,27,27	0
57	MG	RA	3339	1/1	0.89	0.13	52,52,52,52	0
57	MG	YA	3400	1/1	0.89	0.13	42,42,42,42	0
57	MG	XA	1698	1/1	0.89	0.12	75,75,75,75	0
57	MG	YA	3168	1/1	0.89	0.24	31,31,31,31	0
57	MG	YA	3293	1/1	0.90	0.35	33,33,33,33	0
57	MG	YA	3061	1/1	0.90	0.51	27,27,27,27	0
57	MG	RA	3268	1/1	0.90	0.18	42,42,42,42	0
57	MG	QA	1673	1/1	0.90	0.12	60,60,60,60	0
57	MG	RA	3355	1/1	0.90	0.68	81,81,81,81	0
57	MG	RA	3094	1/1	0.90	0.42	43,43,43,43	0
57	MG	YA	3301	1/1	0.90	0.17	55,55,55,55	0
57	MG	YA	3188	1/1	0.90	0.37	38,38,38,38	0
57	MG	RA	3185	1/1	0.90	0.12	32,32,32,32	0
57	MG	XA	1671	1/1	0.90	0.39	41,41,41,41	0
57	MG	YA	3092	1/1	0.90	0.45	37,37,37,37	0
57	MG	YA	3313	1/1	0.90	0.59	37,37,37,37	0
57	MG	YA	3316	1/1	0.90	0.29	42,42,42,42	0
57	MG	YA	3095	1/1	0.90	0.36	42,42,42,42	0
57	MG	YA	3436	1/1	0.90	0.66	38,38,38,38	0
57	MG	XA	1675	1/1	0.90	0.33	47,47,47,47	0
57	MG	RA	3276	1/1	0.90	0.19	50,50,50,50	0
57	MG	RA	3222	1/1	0.90	0.46	50,50,50,50	0
57	MG	RA	3227	1/1	0.90	0.12	42,42,42,42	0
57	MG	RA	3283	1/1	0.90	0.35	36,36,36,36	0
57	MG	YA	3108	1/1	0.90	0.23	25,25,25,25	0
57	MG	RA	3151	1/1	0.90	0.21	54,54,54,54	0
57	MG	RA	3330	1/1	0.90	0.25	49,49,49,49	0
57	MG	RA	3331	1/1	0.90	0.66	34,34,34,34	0
57	MG	YA	3117	1/1	0.90	0.53	34,34,34,34	0
57	MG	QA	1613	1/1	0.90	0.28	53,53,53,53	0
57	MG	RA	3427	1/1	0.90	0.34	48,48,48,48	0
57	MG	YA	3459	1/1	0.90	0.22	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3125	1/1	0.90	0.23	23,23,23,23	0
57	MG	XA	1613	1/1	0.90	0.14	24,24,24,24	0
57	MG	RA	3006	1/1	0.90	0.17	12,12,12,12	0
57	MG	YA	3355	1/1	0.90	0.51	33,33,33,33	0
57	MG	XA	1693	1/1	0.90	0.47	89,89,89,89	0
57	MG	RA	3237	1/1	0.90	0.45	34,34,34,34	0
57	MG	RA	3192	1/1	0.90	0.22	36,36,36,36	0
57	MG	YA	3245	1/1	0.90	0.49	40,40,40,40	0
57	MG	YA	3143	1/1	0.90	0.43	48,48,48,48	0
57	MG	YA	3363	1/1	0.90	0.56	59,59,59,59	0
57	MG	YA	3364	1/1	0.90	0.10	33,33,33,33	0
57	MG	YA	3481	1/1	0.90	0.46	53,53,53,53	0
57	MG	YA	3248	1/1	0.90	0.28	61,61,61,61	0
57	MG	YA	3483	1/1	0.90	0.20	51,51,51,51	0
57	MG	YA	3487	1/1	0.90	0.19	27,27,27,27	0
57	MG	RA	3242	1/1	0.90	0.09	40,40,40,40	0
57	MG	YA	3251	1/1	0.90	0.63	33,33,33,33	0
57	MG	RA	3435	1/1	0.90	0.27	57,57,57,57	0
57	MG	XA	1701	1/1	0.90	0.46	41,41,41,41	0
57	MG	RA	3166	1/1	0.90	0.14	27,27,27,27	0
57	MG	YA	3496	1/1	0.90	0.43	55,55,55,55	0
57	MG	RA	3301	1/1	0.90	0.28	34,34,34,34	0
57	MG	YA	3264	1/1	0.90	0.24	29,29,29,29	0
57	MG	YA	3153	1/1	0.90	0.47	41,41,41,41	0
57	MG	RA	3105	1/1	0.90	0.17	33,33,33,33	0
57	MG	YA	3157	1/1	0.90	0.15	34,34,34,34	0
57	MG	XA	1705	1/1	0.90	0.47	47,47,47,47	0
57	MG	QA	1609	1/1	0.90	0.45	61,61,61,61	0
57	MG	XA	1631	1/1	0.90	0.30	24,24,24,24	0
57	MG	RA	3170	1/1	0.90	0.23	47,47,47,47	0
57	MG	YA	3390	1/1	0.90	0.32	45,45,45,45	0
57	MG	YA	3276	1/1	0.90	0.39	43,43,43,43	0
57	MG	YA	3280	1/1	0.90	0.39	41,41,41,41	0
57	MG	QA	1739	1/1	0.90	0.30	52,52,52,52	0
57	MG	RA	3393	1/1	0.90	0.58	23,23,23,23	0
57	MG	QA	1715	1/1	0.90	0.28	33,33,33,33	0
57	MG	QA	1733	1/1	0.90	0.17	42,42,42,42	0
57	MG	YA	3397	1/1	0.90	0.25	62,62,62,62	0
57	MG	XA	1719	1/1	0.90	0.22	43,43,43,43	0
57	MG	RA	3312	1/1	0.90	0.14	47,47,47,47	0
57	MG	QA	1601	1/1	0.90	0.29	39,39,39,39	0
57	MG	RB	203	1/1	0.90	0.31	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3403	1/1	0.90	0.21	46,46,46,46	0
57	MG	YA	3286	1/1	0.91	0.49	56,56,56,56	0
57	MG	XA	1696	1/1	0.91	0.20	53,53,53,53	0
57	MG	RA	3049	1/1	0.91	0.31	23,23,23,23	0
57	MG	YA	3401	1/1	0.91	0.53	38,38,38,38	0
57	MG	RA	3305	1/1	0.91	0.32	41,41,41,41	0
57	MG	RA	3239	1/1	0.91	0.25	60,60,60,60	0
57	MG	QA	1643	1/1	0.91	0.09	40,40,40,40	0
57	MG	RA	3053	1/1	0.91	0.28	40,40,40,40	0
57	MG	QA	1683	1/1	0.91	0.35	59,59,59,59	0
57	MG	RA	3246	1/1	0.91	0.25	39,39,39,39	0
57	MG	YA	3029	1/1	0.91	0.28	33,33,33,33	0
57	MG	RA	3247	1/1	0.91	0.42	37,37,37,37	0
57	MG	XA	1626	1/1	0.91	0.32	37,37,37,37	0
57	MG	YA	3037	1/1	0.91	0.33	27,27,27,27	0
57	MG	QA	1647	1/1	0.91	0.32	60,60,60,60	0
57	MG	YA	3306	1/1	0.91	0.36	42,42,42,42	0
57	MG	YA	3040	1/1	0.91	0.27	26,26,26,26	0
57	MG	YA	3046	1/1	0.91	0.21	14,14,14,14	0
57	MG	YA	3047	1/1	0.91	0.51	18,18,18,18	0
57	MG	YA	3311	1/1	0.91	0.34	77,77,77,77	0
57	MG	RA	3316	1/1	0.91	0.86	40,40,40,40	0
57	MG	YA	3315	1/1	0.91	0.13	34,34,34,34	0
57	MG	YA	3438	1/1	0.91	0.16	26,26,26,26	0
57	MG	RA	3317	1/1	0.91	0.40	36,36,36,36	0
57	MG	YA	3193	1/1	0.91	0.45	43,43,43,43	0
57	MG	YA	3322	1/1	0.91	0.19	48,48,48,48	0
57	MG	RA	3253	1/1	0.91	0.47	53,53,53,53	0
57	MG	XA	1632	1/1	0.91	0.33	49,49,49,49	0
57	MG	QA	1662	1/1	0.91	0.17	27,27,27,27	0
57	MG	RA	3071	1/1	0.91	0.28	12,12,12,12	0
57	MG	QA	1687	1/1	0.91	0.10	52,52,52,52	0
57	MG	XA	1637	1/1	0.91	0.28	57,57,57,57	0
57	MG	YA	3333	1/1	0.91	0.18	53,53,53,53	0
57	MG	QA	1628	1/1	0.91	0.12	65,65,65,65	0
57	MG	RA	3137	1/1	0.91	0.16	55,55,55,55	0
57	MG	YA	3217	1/1	0.91	0.20	35,35,35,35	0
57	MG	YA	3343	1/1	0.91	0.51	48,48,48,48	0
57	MG	RA	3444	1/1	0.91	0.14	52,52,52,52	0
57	MG	YA	3469	1/1	0.91	0.39	45,45,45,45	0
57	MG	RA	3445	1/1	0.91	0.54	18,18,18,18	0
57	MG	XA	1730	1/1	0.91	0.44	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3350	1/1	0.91	0.37	55,55,55,55	0
57	MG	YA	3351	1/1	0.91	0.34	50,50,50,50	0
57	MG	QA	1690	1/1	0.91	0.24	49,49,49,49	0
57	MG	RA	3141	1/1	0.91	0.07	34,34,34,34	0
57	MG	YA	3105	1/1	0.91	0.19	56,56,56,56	0
57	MG	XA	1735	1/1	0.91	0.33	44,44,44,44	0
57	MG	YA	3107	1/1	0.91	0.18	33,33,33,33	0
57	MG	QA	1730	1/1	0.91	0.09	69,69,69,69	0
57	MG	QA	1619	1/1	0.91	0.44	31,31,31,31	0
57	MG	QA	1712	1/1	0.91	0.19	58,58,58,58	0
57	MG	QA	1651	1/1	0.91	0.30	39,39,39,39	0
57	MG	RA	3099	1/1	0.91	0.29	13,13,13,13	0
57	MG	RA	3278	1/1	0.91	0.27	39,39,39,39	0
57	MG	RA	3154	1/1	0.91	0.53	42,42,42,42	0
57	MG	RA	3156	1/1	0.91	0.13	42,42,42,42	0
57	MG	YA	3130	1/1	0.91	0.26	34,34,34,34	0
57	MG	YA	3132	1/1	0.91	0.15	29,29,29,29	0
57	MG	RA	3032	1/1	0.91	0.28	17,17,17,17	0
57	MG	YA	3500	1/1	0.91	0.35	71,71,71,71	0
57	MG	YA	3258	1/1	0.91	0.48	58,58,58,58	0
57	MG	QA	1642	1/1	0.91	0.15	50,50,50,50	0
57	MG	RA	3161	1/1	0.91	0.15	36,36,36,36	0
57	MG	YA	3376	1/1	0.91	0.34	63,63,63,63	0
57	MG	YE	301	1/1	0.91	0.20	40,40,40,40	0
57	MG	XA	1754	1/1	0.91	0.40	61,61,61,61	0
57	MG	XA	1683	1/1	0.91	0.17	38,38,38,38	0
57	MG	RA	3407	1/1	0.91	0.14	60,60,60,60	0
57	MG	RQ	202	1/1	0.91	0.11	58,58,58,58	0
57	MG	RA	3162	1/1	0.91	0.55	34,34,34,34	0
57	MG	XA	1759	1/1	0.91	0.71	60,60,60,60	0
57	MG	QA	1654	1/1	0.91	0.47	41,41,41,41	0
57	MG	YA	3388	1/1	0.91	0.12	52,52,52,52	0
57	MG	RA	3044	1/1	0.91	0.54	27,27,27,27	0
57	MG	RA	3046	1/1	0.91	0.38	16,16,16,16	0
57	MG	YA	3278	1/1	0.91	0.61	55,55,55,55	0
57	MG	QA	1736	1/1	0.91	0.13	47,47,47,47	0
57	MG	RA	3114	1/1	0.91	0.29	30,30,30,30	0
57	MG	RA	3171	1/1	0.91	0.71	69,69,69,69	0
57	MG	YA	3284	1/1	0.91	0.37	54,54,54,54	0
57	MG	XA	1695	1/1	0.91	0.30	40,40,40,40	0
57	MG	YA	3206	1/1	0.92	0.23	38,38,38,38	0
57	MG	YA	3411	1/1	0.92	0.35	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3314	1/1	0.92	0.48	49,49,49,49	0
57	MG	RA	3252	1/1	0.92	0.21	43,43,43,43	0
57	MG	YA	3211	1/1	0.92	0.35	43,43,43,43	0
57	MG	YA	3212	1/1	0.92	0.12	28,28,28,28	0
57	MG	RA	3209	1/1	0.92	0.38	30,30,30,30	0
57	MG	XA	1745	1/1	0.92	0.19	36,36,36,36	0
57	MG	RA	3306	1/1	0.92	0.35	39,39,39,39	0
57	MG	YA	3109	1/1	0.92	0.49	40,40,40,40	0
57	MG	RA	3135	1/1	0.92	0.40	44,44,44,44	0
57	MG	YA	3224	1/1	0.92	0.31	35,35,35,35	0
57	MG	RA	3411	1/1	0.92	0.27	49,49,49,49	0
57	MG	YA	3227	1/1	0.92	0.44	51,51,51,51	0
57	MG	YA	3334	1/1	0.92	0.23	35,35,35,35	0
57	MG	YA	3442	1/1	0.92	0.30	61,61,61,61	0
57	MG	QA	1612	1/1	0.92	0.24	48,48,48,48	0
57	MG	YA	3229	1/1	0.92	0.33	29,29,29,29	0
57	MG	YA	3115	1/1	0.92	0.91	45,45,45,45	0
57	MG	RA	3256	1/1	0.92	0.60	67,67,67,67	0
57	MG	RA	3212	1/1	0.92	0.38	30,30,30,30	0
57	MG	RA	3262	1/1	0.92	0.17	40,40,40,40	0
57	MG	RA	3263	1/1	0.92	0.54	42,42,42,42	0
57	MG	RA	3018	1/1	0.92	0.48	20,20,20,20	0
57	MG	RA	3140	1/1	0.92	0.26	18,18,18,18	0
57	MG	YA	3242	1/1	0.92	0.22	25,25,25,25	0
57	MG	QE	201	1/1	0.92	0.13	42,42,42,42	0
57	MG	RA	3070	1/1	0.92	0.30	28,28,28,28	0
57	MG	YA	3135	1/1	0.92	0.26	31,31,31,31	0
57	MG	RA	3220	1/1	0.92	0.89	53,53,53,53	0
57	MG	QA	1721	1/1	0.92	0.28	52,52,52,52	0
57	MG	RA	3363	1/1	0.92	0.50	39,39,39,39	0
57	MG	RA	3033	1/1	0.92	0.52	25,25,25,25	0
57	MG	RA	3430	1/1	0.92	0.19	52,52,52,52	0
57	MG	YA	3473	1/1	0.92	0.24	39,39,39,39	0
57	MG	RA	3223	1/1	0.92	0.55	38,38,38,38	0
57	MG	QA	1700	1/1	0.92	0.56	51,51,51,51	0
57	MG	XV	104	1/1	0.92	0.21	15,15,15,15	0
57	MG	XA	1627	1/1	0.92	0.12	71,71,71,71	0
57	MG	YA	3479	1/1	0.92	0.09	42,42,42,42	0
57	MG	RA	3087	1/1	0.92	0.19	31,31,31,31	0
57	MG	YA	3368	1/1	0.92	0.28	49,49,49,49	0
57	MG	RA	3328	1/1	0.92	0.55	61,61,61,61	0
57	MG	RA	3152	1/1	0.92	0.68	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3484	1/1	0.92	0.18	47,47,47,47	0
57	MG	RA	3436	1/1	0.92	0.20	51,51,51,51	0
57	MG	RA	3437	1/1	0.92	0.29	52,52,52,52	0
57	MG	YA	3373	1/1	0.92	0.36	61,61,61,61	0
57	MG	RA	3281	1/1	0.92	0.27	53,53,53,53	0
57	MG	YA	3164	1/1	0.92	0.08	50,50,50,50	0
57	MG	YA	3166	1/1	0.92	0.18	41,41,41,41	0
57	MG	RA	3153	1/1	0.92	0.24	23,23,23,23	0
57	MG	YA	3497	1/1	0.92	0.11	55,55,55,55	0
57	MG	XA	1713	1/1	0.92	0.42	48,48,48,48	0
57	MG	RA	3119	1/1	0.92	0.35	23,23,23,23	0
57	MG	YA	3170	1/1	0.92	0.31	38,38,38,38	0
57	MG	RA	3374	1/1	0.92	0.79	44,44,44,44	0
57	MG	XA	1718	1/1	0.92	0.26	47,47,47,47	0
57	MG	YA	3041	1/1	0.92	0.40	23,23,23,23	0
57	MG	XA	1638	1/1	0.92	0.28	59,59,59,59	0
57	MG	RA	3375	1/1	0.92	0.60	61,61,61,61	0
57	MG	QA	1702	1/1	0.92	0.19	54,54,54,54	0
57	MG	RA	3380	1/1	0.92	0.36	15,15,15,15	0
57	MG	QA	1621	1/1	0.92	0.17	45,45,45,45	0
57	MG	XA	1726	1/1	0.92	0.26	54,54,54,54	0
57	MG	RA	3335	1/1	0.92	0.18	43,43,43,43	0
57	MG	QA	1629	1/1	0.92	0.29	53,53,53,53	0
57	MG	RA	3196	1/1	0.92	0.49	33,33,33,33	0
57	MG	RA	3391	1/1	0.92	0.12	24,24,24,24	0
57	MG	YA	3190	1/1	0.92	0.62	25,25,25,25	0
57	MG	QA	1675	1/1	0.92	0.37	48,48,48,48	0
57	MG	XA	1668	1/1	0.92	0.26	35,35,35,35	0
57	MG	RA	3245	1/1	0.92	0.20	34,34,34,34	0
57	MG	QA	1718	1/1	0.92	0.31	51,51,51,51	0
57	MG	XA	1672	1/1	0.92	0.14	52,52,52,52	0
57	MG	QA	1676	1/1	0.92	0.20	46,46,46,46	0
57	MG	QA	1740	1/1	0.92	0.53	46,46,46,46	0
57	MG	RA	3340	1/1	0.93	0.18	40,40,40,40	0
57	MG	YA	3412	1/1	0.93	0.20	25,25,25,25	0
57	MG	YA	3414	1/1	0.93	0.77	60,60,60,60	0
57	MG	XA	1602	1/1	0.93	0.31	32,32,32,32	0
57	MG	XA	1603	1/1	0.93	0.12	29,29,29,29	0
57	MG	RA	3086	1/1	0.93	0.23	27,27,27,27	0
57	MG	YA	3213	1/1	0.93	0.22	14,14,14,14	0
57	MG	YA	3423	1/1	0.93	0.44	57,57,57,57	0
57	MG	QA	1691	1/1	0.93	0.25	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1615	1/1	0.93	0.38	38,38,38,38	0
57	MG	RA	3378	1/1	0.93	0.09	49,49,49,49	0
57	MG	XA	1618	1/1	0.93	0.28	24,24,24,24	0
57	MG	YA	3431	1/1	0.93	0.08	31,31,31,31	0
57	MG	YA	3432	1/1	0.93	0.32	47,47,47,47	0
57	MG	YA	3119	1/1	0.93	0.32	32,32,32,32	0
57	MG	YA	3434	1/1	0.93	0.23	45,45,45,45	0
57	MG	RA	3144	1/1	0.93	0.42	44,44,44,44	0
57	MG	YA	3125	1/1	0.93	0.31	22,22,22,22	0
57	MG	RA	3381	1/1	0.93	0.79	43,43,43,43	0
57	MG	QA	1618	1/1	0.93	0.13	44,44,44,44	0
57	MG	YA	3440	1/1	0.93	0.34	49,49,49,49	0
57	MG	YA	3441	1/1	0.93	0.23	35,35,35,35	0
57	MG	RA	3384	1/1	0.93	0.24	28,28,28,28	0
57	MG	RA	3346	1/1	0.93	0.21	38,38,38,38	0
57	MG	RA	3241	1/1	0.93	0.18	35,35,35,35	0
57	MG	RA	3275	1/1	0.93	0.95	51,51,51,51	0
57	MG	QA	1703	1/1	0.93	0.33	86,86,86,86	0
57	MG	YA	3139	1/1	0.93	0.38	29,29,29,29	0
57	MG	RA	3243	1/1	0.93	0.29	48,48,48,48	0
57	MG	YA	3238	1/1	0.93	0.24	28,28,28,28	0
57	MG	RA	3318	1/1	0.93	0.34	51,51,51,51	0
57	MG	YA	3241	1/1	0.93	0.21	29,29,29,29	0
57	MG	YA	3002	1/1	0.93	0.49	11,11,11,11	0
57	MG	RA	3443	1/1	0.93	0.29	56,56,56,56	0
57	MG	RA	3029	1/1	0.93	0.27	28,28,28,28	0
57	MG	YA	3462	1/1	0.93	0.25	36,36,36,36	0
57	MG	RA	3030	1/1	0.93	0.34	15,15,15,15	0
57	MG	RA	3095	1/1	0.93	0.19	38,38,38,38	0
57	MG	YA	3468	1/1	0.93	0.21	41,41,41,41	0
57	MG	YA	3151	1/1	0.93	0.29	28,28,28,28	0
57	MG	QA	1748	1/1	0.93	0.12	46,46,46,46	0
57	MG	YA	3253	1/1	0.93	0.16	48,48,48,48	0
57	MG	RA	3067	1/1	0.93	0.18	32,32,32,32	0
57	MG	RA	3403	1/1	0.93	0.26	54,54,54,54	0
57	MG	YA	3156	1/1	0.93	0.23	29,29,29,29	0
57	MG	RA	3250	1/1	0.93	0.31	56,56,56,56	0
57	MG	QA	1646	1/1	0.93	0.09	52,52,52,52	0
57	MG	RA	3409	1/1	0.93	0.40	43,43,43,43	0
57	MG	RB	204	1/1	0.93	0.07	47,47,47,47	0
57	MG	XA	1653	1/1	0.93	0.28	29,29,29,29	0
57	MG	RA	3360	1/1	0.93	0.12	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3269	1/1	0.93	0.27	60,60,60,60	0
57	MG	YA	3271	1/1	0.93	0.38	42,42,42,42	0
57	MG	XA	1655	1/1	0.93	0.32	53,53,53,53	0
57	MG	QA	1664	1/1	0.93	0.19	39,39,39,39	0
57	MG	QA	1714	1/1	0.93	0.35	46,46,46,46	0
57	MG	QA	1620	1/1	0.93	0.16	40,40,40,40	0
57	MG	RA	3077	1/1	0.93	0.26	24,24,24,24	0
57	MG	RA	3299	1/1	0.93	0.35	49,49,49,49	0
57	MG	YA	3381	1/1	0.93	0.54	54,54,54,54	0
57	MG	YA	3069	1/1	0.93	0.27	19,19,19,19	0
57	MG	YA	3073	1/1	0.93	0.21	25,25,25,25	0
57	MG	YA	3282	1/1	0.93	0.32	31,31,31,31	0
57	MG	YA	3074	1/1	0.93	0.36	23,23,23,23	0
57	MG	YA	3076	1/1	0.93	0.29	27,27,27,27	0
57	MG	YA	3079	1/1	0.93	0.30	31,31,31,31	0
57	MG	YA	3389	1/1	0.93	0.35	51,51,51,51	0
57	MG	RP	201	1/1	0.93	0.20	31,31,31,31	0
57	MG	YB	203	1/1	0.93	0.25	31,31,31,31	0
57	MG	YA	3086	1/1	0.93	0.21	23,23,23,23	0
57	MG	YA	3184	1/1	0.93	0.20	46,46,46,46	0
57	MG	XA	1670	1/1	0.93	0.17	16,16,16,16	0
57	MG	YH	201	1/1	0.93	0.32	58,58,58,58	0
57	MG	RA	3257	1/1	0.93	0.23	42,42,42,42	0
57	MG	YN	201	1/1	0.93	0.24	38,38,38,38	0
57	MG	RA	3259	1/1	0.93	0.23	51,51,51,51	0
57	MG	XA	1674	1/1	0.93	0.24	43,43,43,43	0
57	MG	RA	3139	1/1	0.93	0.16	44,44,44,44	0
57	MG	RA	3165	1/1	0.93	0.12	57,57,57,57	0
57	MG	YA	3296	1/1	0.93	0.26	52,52,52,52	0
57	MG	RA	3197	1/1	0.93	0.29	24,24,24,24	0
57	MG	YA	3194	1/1	0.93	0.25	33,33,33,33	0
57	MG	R0	101	1/1	0.93	0.32	16,16,16,16	0
57	MG	RA	3425	1/1	0.93	0.34	46,46,46,46	0
57	MG	RA	3231	1/1	0.93	0.16	41,41,41,41	0
57	MG	YA	3305	1/1	0.93	0.36	34,34,34,34	0
57	MG	YA	3200	1/1	0.93	0.21	32,32,32,32	0
57	MG	R5	101	1/1	0.93	0.29	17,17,17,17	0
58	ZN	QD	301	1/1	0.93	0.39	49,49,49,49	0
57	MG	QA	1658	1/1	0.93	0.50	34,34,34,34	0
57	MG	RA	3405	1/1	0.94	0.26	48,48,48,48	0
57	MG	XA	1697	1/1	0.94	0.15	62,62,62,62	0
57	MG	RA	3287	1/1	0.94	0.29	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3251	1/1	0.94	0.11	24,24,24,24	0
57	MG	YA	3223	1/1	0.94	0.09	30,30,30,30	0
57	MG	XA	1764	1/1	0.94	0.07	45,45,45,45	0
57	MG	YA	3225	1/1	0.94	0.26	16,16,16,16	0
57	MG	RA	3181	1/1	0.94	0.12	56,56,56,56	0
57	MG	YA	3121	1/1	0.94	0.12	27,27,27,27	0
57	MG	RA	3410	1/1	0.94	0.19	43,43,43,43	0
57	MG	YA	3126	1/1	0.94	0.31	22,22,22,22	0
57	MG	XL	201	1/1	0.94	0.15	39,39,39,39	0
57	MG	RB	201	1/1	0.94	0.29	32,32,32,32	0
57	MG	RB	202	1/1	0.94	0.36	33,33,33,33	0
57	MG	RA	3127	1/1	0.94	0.39	60,60,60,60	0
57	MG	RA	3072	1/1	0.94	0.15	32,32,32,32	0
57	MG	RA	3017	1/1	0.94	0.23	16,16,16,16	0
57	MG	QA	1657	1/1	0.94	0.59	42,42,42,42	0
57	MG	YA	3445	1/1	0.94	0.20	38,38,38,38	0
57	MG	RA	3226	1/1	0.94	0.56	35,35,35,35	0
57	MG	RA	3022	1/1	0.94	0.52	22,22,22,22	0
57	MG	YA	3011	1/1	0.94	0.52	22,22,22,22	0
57	MG	XA	1647	1/1	0.94	0.09	45,45,45,45	0
57	MG	YA	3144	1/1	0.94	0.61	42,42,42,42	0
57	MG	RE	302	1/1	0.94	0.45	15,15,15,15	0
57	MG	YA	3247	1/1	0.94	0.47	47,47,47,47	0
57	MG	YA	3357	1/1	0.94	0.13	50,50,50,50	0
57	MG	RA	3260	1/1	0.94	0.32	45,45,45,45	0
57	MG	YA	3028	1/1	0.94	0.20	14,14,14,14	0
57	MG	QV	104	1/1	0.94	0.18	56,56,56,56	0
57	MG	RA	3109	1/1	0.94	0.30	25,25,25,25	0
57	MG	YA	3032	1/1	0.94	0.35	26,26,26,26	0
57	MG	QA	1602	1/1	0.94	0.32	33,33,33,33	0
57	MG	YA	3154	1/1	0.94	0.29	24,24,24,24	0
57	MG	RA	3423	1/1	0.94	0.20	51,51,51,51	0
57	MG	RR	201	1/1	0.94	0.36	33,33,33,33	0
57	MG	XA	1661	1/1	0.94	0.52	43,43,43,43	0
57	MG	RA	3164	1/1	0.94	0.17	41,41,41,41	0
57	MG	YA	3474	1/1	0.94	0.58	37,37,37,37	0
57	MG	RA	3089	1/1	0.94	0.30	21,21,21,21	0
57	MG	YA	3267	1/1	0.94	0.12	43,43,43,43	0
57	MG	RA	3235	1/1	0.94	0.22	48,48,48,48	0
57	MG	RA	3379	1/1	0.94	0.52	36,36,36,36	0
57	MG	YA	3049	1/1	0.94	0.41	13,13,13,13	0
57	MG	YA	3375	1/1	0.94	0.65	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3052	1/1	0.94	0.57	9,9,9,9	0
57	MG	XA	1729	1/1	0.94	0.14	24,24,24,24	0
57	MG	YA	3060	1/1	0.94	0.50	12,12,12,12	0
57	MG	RA	3344	1/1	0.94	0.19	47,47,47,47	0
57	MG	YA	3485	1/1	0.94	0.18	52,52,52,52	0
57	MG	YA	3171	1/1	0.94	0.27	39,39,39,39	0
57	MG	YA	3277	1/1	0.94	0.14	44,44,44,44	0
57	MG	QA	1645	1/1	0.94	0.10	44,44,44,44	0
57	MG	XA	1733	1/1	0.94	0.24	18,18,18,18	0
57	MG	YA	3492	1/1	0.94	0.22	55,55,55,55	0
57	MG	YA	3386	1/1	0.94	0.37	58,58,58,58	0
57	MG	RA	3269	1/1	0.94	0.39	50,50,50,50	0
57	MG	YA	3070	1/1	0.94	0.32	28,28,28,28	0
57	MG	YA	3071	1/1	0.94	0.11	33,33,33,33	0
57	MG	RA	3202	1/1	0.94	0.08	49,49,49,49	0
57	MG	RA	3271	1/1	0.94	0.07	27,27,27,27	0
57	MG	XA	1737	1/1	0.94	0.38	34,34,34,34	0
57	MG	RA	3062	1/1	0.94	0.40	30,30,30,30	0
57	MG	QA	1652	1/1	0.94	0.22	34,34,34,34	0
57	MG	YA	3185	1/1	0.94	0.19	21,21,21,21	0
57	MG	YA	3083	1/1	0.94	0.31	30,30,30,30	0
57	MG	XA	1679	1/1	0.94	0.11	35,35,35,35	0
57	MG	YD	301	1/1	0.94	0.32	26,26,26,26	0
57	MG	XA	1606	1/1	0.94	0.38	18,18,18,18	0
57	MG	YF	301	1/1	0.94	0.17	27,27,27,27	0
57	MG	YF	302	1/1	0.94	0.26	35,35,35,35	0
57	MG	XA	1607	1/1	0.94	0.21	35,35,35,35	0
57	MG	RA	3390	1/1	0.94	0.35	19,19,19,19	0
57	MG	XA	1612	1/1	0.94	0.26	43,43,43,43	0
57	MG	XA	1746	1/1	0.94	0.26	46,46,46,46	0
57	MG	YA	3096	1/1	0.94	0.62	41,41,41,41	0
57	MG	QA	1615	1/1	0.94	0.30	38,38,38,38	0
57	MG	RA	3121	1/1	0.94	0.12	31,31,31,31	0
57	MG	QA	1634	1/1	0.94	0.22	45,45,45,45	0
57	MG	RA	3150	1/1	0.94	0.27	40,40,40,40	0
57	MG	XA	1753	1/1	0.94	0.18	51,51,51,51	0
57	MG	RA	3012	1/1	0.94	0.48	11,11,11,11	0
57	MG	QA	1622	1/1	0.94	0.52	50,50,50,50	0
57	MG	YA	3413	1/1	0.94	0.38	53,53,53,53	0
57	MG	RA	3282	1/1	0.94	0.24	36,36,36,36	0
57	MG	YA	3415	1/1	0.94	0.08	62,62,62,62	0
57	MG	RA	3177	1/1	0.94	0.35	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3179	1/1	0.94	0.18	47,47,47,47	0
57	MG	Z7	101	1/1	0.94	0.31	35,35,35,35	0
57	MG	RA	3404	1/1	0.94	0.24	46,46,46,46	0
57	MG	YA	3112	1/1	0.94	0.18	19,19,19,19	0
57	MG	YA	3021	1/1	0.95	0.48	33,33,33,33	0
57	MG	YA	3321	1/1	0.95	0.19	67,67,67,67	0
57	MG	RA	3131	1/1	0.95	0.17	43,43,43,43	0
57	MG	YA	3131	1/1	0.95	0.20	40,40,40,40	0
57	MG	YA	3025	1/1	0.95	0.49	34,34,34,34	0
57	MG	YA	3325	1/1	0.95	0.50	51,51,51,51	0
57	MG	RA	3295	1/1	0.95	0.39	32,32,32,32	0
57	MG	XA	1601	1/1	0.95	0.33	36,36,36,36	0
57	MG	RA	3213	1/1	0.95	0.24	13,13,13,13	0
57	MG	RA	3050	1/1	0.95	0.28	12,12,12,12	0
57	MG	RA	3215	1/1	0.95	0.57	53,53,53,53	0
57	MG	YA	3036	1/1	0.95	0.45	21,21,21,21	0
57	MG	YA	3233	1/1	0.95	0.26	38,38,38,38	0
57	MG	QA	1611	1/1	0.95	0.44	31,31,31,31	0
57	MG	YA	3337	1/1	0.95	0.45	39,39,39,39	0
57	MG	YA	3339	1/1	0.95	0.13	31,31,31,31	0
57	MG	RA	3020	1/1	0.95	0.50	24,24,24,24	0
57	MG	YA	3039	1/1	0.95	0.41	11,11,11,11	0
57	MG	YA	3446	1/1	0.95	0.32	37,37,37,37	0
57	MG	XA	1611	1/1	0.95	0.18	43,43,43,43	0
57	MG	YA	3449	1/1	0.95	0.16	36,36,36,36	0
57	MG	YA	3346	1/1	0.95	0.37	47,47,47,47	0
57	MG	RA	3136	1/1	0.95	0.46	40,40,40,40	0
57	MG	QA	1682	1/1	0.95	0.26	49,49,49,49	0
57	MG	QA	1632	1/1	0.95	0.15	58,58,58,58	0
57	MG	YA	3455	1/1	0.95	0.22	52,52,52,52	0
57	MG	YA	3243	1/1	0.95	0.50	46,46,46,46	0
57	MG	RA	3064	1/1	0.95	0.30	26,26,26,26	0
57	MG	RA	3103	1/1	0.95	0.36	52,52,52,52	0
57	MG	XA	1619	1/1	0.95	0.32	28,28,28,28	0
57	MG	YA	3460	1/1	0.95	0.11	37,37,37,37	0
57	MG	YA	3056	1/1	0.95	0.35	5,5,5,5	0
57	MG	XA	1741	1/1	0.95	0.32	44,44,44,44	0
57	MG	YA	3465	1/1	0.95	0.27	43,43,43,43	0
57	MG	RA	3028	1/1	0.95	0.44	12,12,12,12	0
57	MG	RA	3142	1/1	0.95	0.34	28,28,28,28	0
57	MG	RA	3400	1/1	0.95	0.32	44,44,44,44	0
57	MG	YA	3254	1/1	0.95	0.24	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1689	1/1	0.95	0.18	46,46,46,46	0
57	MG	YA	3161	1/1	0.95	0.32	29,29,29,29	0
57	MG	YA	3257	1/1	0.95	0.34	29,29,29,29	0
57	MG	QA	1726	1/1	0.95	0.12	38,38,38,38	0
57	MG	YA	3259	1/1	0.95	0.26	35,35,35,35	0
57	MG	QA	1624	1/1	0.95	0.30	36,36,36,36	0
57	MG	YA	3165	1/1	0.95	0.25	14,14,14,14	0
57	MG	RA	3145	1/1	0.95	0.29	22,22,22,22	0
57	MG	QA	1604	1/1	0.95	0.24	33,33,33,33	0
57	MG	XA	1750	1/1	0.95	0.07	44,44,44,44	0
57	MG	RA	3406	1/1	0.95	0.10	50,50,50,50	0
57	MG	QA	1717	1/1	0.95	0.09	53,53,53,53	0
57	MG	YA	3080	1/1	0.95	0.59	21,21,21,21	0
57	MG	YA	3270	1/1	0.95	0.49	32,32,32,32	0
57	MG	RA	3035	1/1	0.95	0.27	21,21,21,21	0
57	MG	RA	3113	1/1	0.95	0.22	32,32,32,32	0
57	MG	YA	3379	1/1	0.95	0.07	42,42,42,42	0
57	MG	YA	3174	1/1	0.95	0.57	29,29,29,29	0
57	MG	YA	3084	1/1	0.95	0.15	20,20,20,20	0
57	MG	QA	1626	1/1	0.95	0.11	21,21,21,21	0
57	MG	YA	3491	1/1	0.95	0.31	37,37,37,37	0
57	MG	RA	3320	1/1	0.95	0.12	44,44,44,44	0
57	MG	YA	3178	1/1	0.95	0.19	18,18,18,18	0
57	MG	YA	3089	1/1	0.95	0.40	8,8,8,8	0
57	MG	RA	3116	1/1	0.95	0.43	20,20,20,20	0
57	MG	RA	3040	1/1	0.95	0.34	18,18,18,18	0
57	MG	RA	3078	1/1	0.95	0.54	22,22,22,22	0
57	MG	YA	3093	1/1	0.95	0.21	17,17,17,17	0
57	MG	RA	3079	1/1	0.95	0.58	26,26,26,26	0
57	MG	RA	3008	1/1	0.95	0.86	34,34,34,34	0
57	MG	XA	1643	1/1	0.95	0.50	35,35,35,35	0
57	MG	RA	3326	1/1	0.95	0.13	46,46,46,46	0
57	MG	YB	201	1/1	0.95	0.40	32,32,32,32	0
57	MG	YB	202	1/1	0.95	0.27	19,19,19,19	0
57	MG	RA	3085	1/1	0.95	0.12	15,15,15,15	0
57	MG	YB	204	1/1	0.95	0.11	69,69,69,69	0
57	MG	RA	3043	1/1	0.95	0.30	36,36,36,36	0
57	MG	RA	3011	1/1	0.95	0.42	23,23,23,23	0
57	MG	XA	1652	1/1	0.95	0.43	46,46,46,46	0
57	MG	RA	3286	1/1	0.95	0.35	43,43,43,43	0
57	MG	XV	101	1/1	0.95	0.29	23,23,23,23	0
57	MG	RA	3248	1/1	0.95	0.52	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	QA	1644	1/1	0.95	0.42	27,27,27,27	0
57	MG	XA	1717	1/1	0.95	0.15	37,37,37,37	0
57	MG	RA	3289	1/1	0.95	0.17	39,39,39,39	0
57	MG	YA	3003	1/1	0.95	0.39	14,14,14,14	0
57	MG	YA	3004	1/1	0.95	0.49	13,13,13,13	0
57	MG	RA	3290	1/1	0.95	0.10	52,52,52,52	0
57	MG	YA	3210	1/1	0.95	0.30	32,32,32,32	0
57	MG	YA	3006	1/1	0.95	0.36	17,17,17,17	0
57	MG	XA	1720	1/1	0.95	0.18	44,44,44,44	0
57	MG	QA	1709	1/1	0.95	0.34	36,36,36,36	0
57	MG	QA	1689	1/1	0.95	0.36	28,28,28,28	0
57	MG	YA	3122	1/1	0.95	0.39	19,19,19,19	0
57	MG	YA	3312	1/1	0.95	0.54	24,24,24,24	0
57	MG	YA	3124	1/1	0.95	0.32	27,27,27,27	0
57	MG	YA	3016	1/1	0.95	0.17	8,8,8,8	0
57	MG	RA	3293	1/1	0.95	0.44	25,25,25,25	0
57	MG	YA	3220	1/1	0.95	0.23	39,39,39,39	0
57	MG	YA	3422	1/1	0.95	0.39	29,29,29,29	0
57	MG	YA	3317	1/1	0.95	0.68	51,51,51,51	0
58	ZN	XN	101	1/1	0.95	0.17	69,69,69,69	0
57	MG	QA	1636	1/1	0.96	0.20	48,48,48,48	0
57	MG	RA	3088	1/1	0.96	0.31	23,23,23,23	0
57	MG	RA	3038	1/1	0.96	0.40	23,23,23,23	0
57	MG	RA	3065	1/1	0.96	0.53	31,31,31,31	0
57	MG	YA	3087	1/1	0.96	0.45	25,25,25,25	0
57	MG	RA	3352	1/1	0.96	0.49	44,44,44,44	0
57	MG	RA	3402	1/1	0.96	0.54	36,36,36,36	0
57	MG	RA	3180	1/1	0.96	0.50	23,23,23,23	0
57	MG	XE	201	1/1	0.96	0.37	32,32,32,32	0
57	MG	YA	3454	1/1	0.96	0.35	45,45,45,45	0
57	MG	XF	201	1/1	0.96	0.12	31,31,31,31	0
57	MG	QA	1616	1/1	0.96	0.19	45,45,45,45	0
57	MG	YA	3094	1/1	0.96	0.05	45,45,45,45	0
57	MG	RA	3224	1/1	0.96	0.22	31,31,31,31	0
57	MG	RA	3225	1/1	0.96	0.12	67,67,67,67	0
57	MG	RA	3019	1/1	0.96	0.35	20,20,20,20	0
57	MG	YA	3098	1/1	0.96	0.37	24,24,24,24	0
57	MG	RA	3042	1/1	0.96	0.35	14,14,14,14	0
57	MG	XV	102	1/1	0.96	0.55	26,26,26,26	0
57	MG	XA	1640	1/1	0.96	0.20	36,36,36,36	0
57	MG	XA	1641	1/1	0.96	0.07	51,51,51,51	0
57	MG	XA	1642	1/1	0.96	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3184	1/1	0.96	0.28	40,40,40,40	0
57	MG	YA	3378	1/1	0.96	0.22	56,56,56,56	0
57	MG	XA	1645	1/1	0.96	0.11	37,37,37,37	0
57	MG	RA	3122	1/1	0.96	0.41	29,29,29,29	0
57	MG	RA	3123	1/1	0.96	0.12	28,28,28,28	0
57	MG	QA	1659	1/1	0.96	0.43	43,43,43,43	0
57	MG	YA	3007	1/1	0.96	0.68	40,40,40,40	0
57	MG	YA	3113	1/1	0.96	0.28	34,34,34,34	0
57	MG	RA	3096	1/1	0.96	0.09	45,45,45,45	0
57	MG	RA	3189	1/1	0.96	0.40	18,18,18,18	0
57	MG	RA	3236	1/1	0.96	0.44	38,38,38,38	0
57	MG	RA	3190	1/1	0.96	0.47	18,18,18,18	0
57	MG	RA	3417	1/1	0.96	0.15	53,53,53,53	0
57	MG	RA	3280	1/1	0.96	0.28	24,24,24,24	0
57	MG	RA	3238	1/1	0.96	0.29	28,28,28,28	0
57	MG	RA	3155	1/1	0.96	0.24	30,30,30,30	0
57	MG	YA	3027	1/1	0.96	0.33	14,14,14,14	0
57	MG	YA	3486	1/1	0.96	0.17	38,38,38,38	0
57	MG	XA	1662	1/1	0.96	0.69	40,40,40,40	0
57	MG	YA	3304	1/1	0.96	0.28	47,47,47,47	0
57	MG	RA	3421	1/1	0.96	0.30	51,51,51,51	0
57	MG	QA	1641	1/1	0.96	0.20	33,33,33,33	0
57	MG	XA	1667	1/1	0.96	0.29	40,40,40,40	0
57	MG	YA	3221	1/1	0.96	0.45	32,32,32,32	0
57	MG	RA	3195	1/1	0.96	0.37	30,30,30,30	0
57	MG	QA	1698	1/1	0.96	0.32	47,47,47,47	0
57	MG	RA	3100	1/1	0.96	0.35	18,18,18,18	0
57	MG	RA	3160	1/1	0.96	0.16	30,30,30,30	0
57	MG	RA	3200	1/1	0.96	0.74	37,37,37,37	0
57	MG	YA	3405	1/1	0.96	0.32	57,57,57,57	0
57	MG	XA	1673	1/1	0.96	0.25	24,24,24,24	0
57	MG	RA	3377	1/1	0.96	0.17	38,38,38,38	0
57	MG	YA	3045	1/1	0.96	0.39	11,11,11,11	0
57	MG	YA	3141	1/1	0.96	0.57	37,37,37,37	0
57	MG	RA	3429	1/1	0.96	0.14	66,66,66,66	0
57	MG	QA	1606	1/1	0.96	0.23	19,19,19,19	0
57	MG	RA	3132	1/1	0.96	0.19	17,17,17,17	0
57	MG	YA	3235	1/1	0.96	0.55	51,51,51,51	0
57	MG	RA	3076	1/1	0.96	0.23	25,25,25,25	0
57	MG	YA	3416	1/1	0.96	0.30	10,10,10,10	0
57	MG	YA	3050	1/1	0.96	0.23	23,23,23,23	0
57	MG	XA	1609	1/1	0.96	0.05	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3419	1/1	0.96	0.11	37,37,37,37	0
57	MG	YA	3053	1/1	0.96	0.33	24,24,24,24	0
57	MG	RA	3104	1/1	0.96	0.40	28,28,28,28	0
57	MG	RA	3382	1/1	0.96	0.33	21,21,21,21	0
57	MG	RA	3208	1/1	0.96	0.39	32,32,32,32	0
57	MG	RA	3009	1/1	0.96	0.23	18,18,18,18	0
57	MG	YP	201	1/1	0.96	0.19	11,11,11,11	0
57	MG	YA	3426	1/1	0.96	0.78	23,23,23,23	0
57	MG	QA	1685	1/1	0.96	0.23	28,28,28,28	0
57	MG	YA	3066	1/1	0.96	0.21	33,33,33,33	0
57	MG	QA	1716	1/1	0.96	0.25	76,76,76,76	0
57	MG	QA	1750	1/1	0.96	0.07	45,45,45,45	0
57	MG	XA	1688	1/1	0.96	0.30	26,26,26,26	0
57	MG	RA	3084	1/1	0.96	0.41	33,33,33,33	0
57	MG	YA	3252	1/1	0.96	0.10	28,28,28,28	0
57	MG	YA	3347	1/1	0.96	0.19	40,40,40,40	0
57	MG	RA	3110	1/1	0.96	0.74	33,33,33,33	0
57	MG	RA	3016	1/1	0.96	0.38	15,15,15,15	0
57	MG	RA	3061	1/1	0.96	0.54	28,28,28,28	0
57	MG	YA	3077	1/1	0.96	0.43	16,16,16,16	0
57	MG	YA	3078	1/1	0.96	0.49	17,17,17,17	0
57	MG	RA	3304	1/1	0.96	0.09	45,45,45,45	0
57	MG	RA	3395	1/1	0.96	0.31	45,45,45,45	0
57	MG	XA	1604	1/1	0.97	0.27	36,36,36,36	0
57	MG	YA	3435	1/1	0.97	0.10	27,27,27,27	0
57	MG	XA	1711	1/1	0.97	0.09	27,27,27,27	0
57	MG	YA	3075	1/1	0.97	0.32	13,13,13,13	0
57	MG	XA	1605	1/1	0.97	0.33	18,18,18,18	0
57	MG	XA	1659	1/1	0.97	0.39	31,31,31,31	0
57	MG	YA	3342	1/1	0.97	0.33	27,27,27,27	0
57	MG	XA	1660	1/1	0.97	0.17	38,38,38,38	0
57	MG	YA	3344	1/1	0.97	0.70	28,28,28,28	0
57	MG	QA	1667	1/1	0.97	0.23	43,43,43,43	0
57	MG	RA	3174	1/1	0.97	0.56	19,19,19,19	0
57	MG	YA	3081	1/1	0.97	0.41	19,19,19,19	0
57	MG	QA	1635	1/1	0.97	0.26	29,29,29,29	0
57	MG	YA	3447	1/1	0.97	0.16	44,44,44,44	0
57	MG	YA	3163	1/1	0.97	0.18	25,25,25,25	0
57	MG	YA	3250	1/1	0.97	0.84	45,45,45,45	0
57	MG	RA	3004	1/1	0.97	0.42	17,17,17,17	0
57	MG	QA	1663	1/1	0.97	0.38	49,49,49,49	0
57	MG	XA	1721	1/1	0.97	0.22	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	QA	1695	1/1	0.97	0.22	42,42,42,42	0
57	MG	RA	3098	1/1	0.97	0.54	44,44,44,44	0
57	MG	QA	1725	1/1	0.97	0.11	44,44,44,44	0
57	MG	RA	3284	1/1	0.97	0.21	38,38,38,38	0
57	MG	YA	3358	1/1	0.97	0.31	35,35,35,35	0
57	MG	RA	3045	1/1	0.97	0.54	19,19,19,19	0
57	MG	RA	3024	1/1	0.97	0.47	18,18,18,18	0
57	MG	YA	3260	1/1	0.97	0.40	49,49,49,49	0
57	MG	YA	3008	1/1	0.97	0.13	19,19,19,19	0
57	MG	RA	3027	1/1	0.97	0.34	9,9,9,9	0
57	MG	YA	3463	1/1	0.97	0.47	39,39,39,39	0
57	MG	YA	3464	1/1	0.97	0.24	43,43,43,43	0
57	MG	YA	3263	1/1	0.97	0.30	44,44,44,44	0
57	MG	RA	3130	1/1	0.97	0.17	28,28,28,28	0
57	MG	YA	3012	1/1	0.97	0.37	19,19,19,19	0
57	MG	RA	3219	1/1	0.97	0.21	20,20,20,20	0
57	MG	XA	1731	1/1	0.97	0.21	41,41,41,41	0
57	MG	YA	3017	1/1	0.97	0.28	16,16,16,16	0
57	MG	YA	3018	1/1	0.97	0.32	9,9,9,9	0
57	MG	YA	3101	1/1	0.97	0.44	35,35,35,35	0
57	MG	YA	3103	1/1	0.97	0.19	25,25,25,25	0
57	MG	QV	102	1/1	0.97	0.46	25,25,25,25	0
57	MG	XA	1678	1/1	0.97	0.14	28,28,28,28	0
57	MG	RA	3010	1/1	0.97	0.53	20,20,20,20	0
57	MG	YA	3024	1/1	0.97	0.40	18,18,18,18	0
57	MG	RA	3159	1/1	0.97	0.67	17,17,17,17	0
57	MG	QA	1608	1/1	0.97	0.24	39,39,39,39	0
57	MG	RA	3080	1/1	0.97	0.35	36,36,36,36	0
57	MG	YA	3279	1/1	0.97	0.40	20,20,20,20	0
57	MG	YA	3191	1/1	0.97	0.32	30,30,30,30	0
57	MG	RA	3373	1/1	0.97	0.24	49,49,49,49	0
57	MG	RA	3052	1/1	0.97	0.49	13,13,13,13	0
57	MG	QA	1660	1/1	0.97	0.25	32,32,32,32	0
57	MG	YA	3195	1/1	0.97	0.35	23,23,23,23	0
57	MG	YA	3196	1/1	0.97	0.39	24,24,24,24	0
57	MG	YA	3034	1/1	0.97	0.39	22,22,22,22	0
57	MG	RA	3297	1/1	0.97	0.12	27,27,27,27	0
57	MG	YA	3116	1/1	0.97	0.48	16,16,16,16	0
57	MG	RA	3194	1/1	0.97	0.41	9,9,9,9	0
57	MG	RA	3228	1/1	0.97	0.36	27,27,27,27	0
57	MG	YA	3202	1/1	0.97	0.28	22,22,22,22	0
57	MG	YA	3203	1/1	0.97	0.43	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3054	1/1	0.97	0.35	27,27,27,27	0
57	MG	YA	3205	1/1	0.97	0.35	21,21,21,21	0
57	MG	RP	202	1/1	0.97	0.18	28,28,28,28	0
57	MG	RA	3056	1/1	0.97	0.33	23,23,23,23	0
57	MG	YA	3208	1/1	0.97	0.51	35,35,35,35	0
57	MG	YA	3299	1/1	0.97	0.44	28,28,28,28	0
57	MG	YA	3209	1/1	0.97	0.09	14,14,14,14	0
57	MG	RA	3112	1/1	0.97	0.29	24,24,24,24	0
57	MG	YA	3123	1/1	0.97	0.26	30,30,30,30	0
57	MG	YA	3044	1/1	0.97	0.62	28,28,28,28	0
57	MG	RA	3266	1/1	0.97	0.29	37,37,37,37	0
57	MG	QA	1607	1/1	0.97	0.23	15,15,15,15	0
57	MG	YB	205	1/1	0.97	0.14	52,52,52,52	0
57	MG	YA	3307	1/1	0.97	0.40	68,68,68,68	0
57	MG	YA	3407	1/1	0.97	0.13	45,45,45,45	0
57	MG	RA	3233	1/1	0.97	0.27	38,38,38,38	0
57	MG	XA	1751	1/1	0.97	0.07	46,46,46,46	0
57	MG	RA	3060	1/1	0.97	0.28	9,9,9,9	0
57	MG	XA	1644	1/1	0.97	0.18	40,40,40,40	0
57	MG	RA	3201	1/1	0.97	0.44	27,27,27,27	0
57	MG	RA	3015	1/1	0.97	0.49	31,31,31,31	0
57	MG	YA	3222	1/1	0.97	0.54	32,32,32,32	0
57	MG	RA	3001	1/1	0.97	0.15	43,43,43,43	0
57	MG	YA	3057	1/1	0.97	0.19	17,17,17,17	0
57	MG	YA	3137	1/1	0.97	0.35	34,34,34,34	0
57	MG	RA	3273	1/1	0.97	0.39	41,41,41,41	0
57	MG	XA	1649	1/1	0.97	0.29	23,23,23,23	0
57	MG	XA	1650	1/1	0.97	0.45	23,23,23,23	0
57	MG	RA	3311	1/1	0.97	0.41	24,24,24,24	0
57	MG	RA	3204	1/1	0.97	0.58	39,39,39,39	0
57	MG	YA	3067	1/1	0.97	0.44	25,25,25,25	0
57	MG	XA	1706	1/1	0.97	0.28	31,31,31,31	0
57	MG	RA	3313	1/1	0.97	0.69	25,25,25,25	0
57	MG	RA	3037	1/1	0.97	0.48	10,10,10,10	0
57	MG	RA	3396	1/1	0.97	0.37	31,31,31,31	0
57	MG	YA	3331	1/1	0.97	0.57	18,18,18,18	0
57	MG	YA	3430	1/1	0.97	0.06	43,43,43,43	0
57	MG	YA	3332	1/1	0.97	0.13	42,42,42,42	0
57	MG	YA	3150	1/1	0.97	0.53	15,15,15,15	0
57	MG	YA	3072	1/1	0.97	0.26	19,19,19,19	0
57	MG	YA	3341	1/1	0.98	0.53	20,20,20,20	0
57	MG	RA	3193	1/1	0.98	0.45	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1635	1/1	0.98	0.22	43,43,43,43	0
57	MG	YA	3009	1/1	0.98	0.60	17,17,17,17	0
57	MG	QA	1701	1/1	0.98	0.21	47,47,47,47	0
57	MG	RA	3073	1/1	0.98	0.24	22,22,22,22	0
57	MG	YA	3062	1/1	0.98	0.40	17,17,17,17	0
57	MG	QA	1656	1/1	0.98	0.51	41,41,41,41	0
57	MG	YA	3065	1/1	0.98	0.16	16,16,16,16	0
57	MG	RA	3169	1/1	0.98	0.39	19,19,19,19	0
57	MG	YA	3014	1/1	0.98	0.36	19,19,19,19	0
57	MG	YA	3015	1/1	0.98	0.51	13,13,13,13	0
57	MG	RA	3258	1/1	0.98	0.57	39,39,39,39	0
57	MG	YA	3290	1/1	0.98	0.16	38,38,38,38	0
57	MG	RA	3057	1/1	0.98	0.42	13,13,13,13	0
57	MG	RA	3199	1/1	0.98	0.29	23,23,23,23	0
57	MG	RA	3058	1/1	0.98	0.37	24,24,24,24	0
57	MG	YA	3180	1/1	0.98	0.55	11,11,11,11	0
57	MG	YA	3020	1/1	0.98	0.55	23,23,23,23	0
57	MG	YA	3424	1/1	0.98	0.12	1,1,1,1	0
57	MG	RA	3013	1/1	0.98	0.29	16,16,16,16	0
57	MG	RA	3031	1/1	0.98	0.54	10,10,10,10	0
57	MG	YA	3240	1/1	0.98	0.74	34,34,34,34	0
57	MG	YA	3127	1/1	0.98	0.18	41,41,41,41	0
57	MG	RA	3389	1/1	0.98	0.17	9,9,9,9	0
57	MG	XA	1610	1/1	0.98	0.34	33,33,33,33	0
57	MG	YA	3026	1/1	0.98	0.33	9,9,9,9	0
57	MG	YA	3303	1/1	0.98	0.07	41,41,41,41	0
57	MG	RA	3101	1/1	0.98	0.30	44,44,44,44	0
57	MG	RA	3149	1/1	0.98	0.58	21,21,21,21	0
57	MG	RA	3021	1/1	0.98	0.59	33,33,33,33	0
57	MG	YA	3030	1/1	0.98	0.55	15,15,15,15	0
57	MG	XA	1614	1/1	0.98	0.31	22,22,22,22	0
57	MG	YA	3504	1/1	0.98	0.40	18,18,18,18	0
57	MG	RA	3081	1/1	0.98	0.47	14,14,14,14	0
57	MG	YA	3138	1/1	0.98	0.20	39,39,39,39	0
57	MG	YA	3085	1/1	0.98	0.27	24,24,24,24	0
57	MG	YA	3033	1/1	0.98	0.37	16,16,16,16	0
57	MG	XA	1616	1/1	0.98	0.31	46,46,46,46	0
57	MG	RA	3207	1/1	0.98	0.59	26,26,26,26	0
57	MG	RA	3178	1/1	0.98	0.28	15,15,15,15	0
57	MG	RA	3082	1/1	0.98	0.38	5,5,5,5	0
57	MG	YE	302	1/1	0.98	0.37	18,18,18,18	0
57	MG	RA	3007	1/1	0.98	0.46	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3318	1/1	0.98	0.19	54,54,54,54	0
57	MG	YA	3319	1/1	0.98	0.26	57,57,57,57	0
57	MG	RA	3129	1/1	0.98	0.21	12,12,12,12	0
57	MG	RA	3063	1/1	0.98	0.34	10,10,10,10	0
57	MG	QA	1617	1/1	0.98	0.30	41,41,41,41	0
57	MG	YA	3042	1/1	0.98	0.19	23,23,23,23	0
57	MG	YA	3043	1/1	0.98	0.40	19,19,19,19	0
57	MG	RA	3048	1/1	0.98	0.54	13,13,13,13	0
57	MG	QA	1605	1/1	0.98	0.21	36,36,36,36	0
57	MG	RA	3025	1/1	0.98	0.42	19,19,19,19	0
57	MG	RA	3068	1/1	0.98	0.45	14,14,14,14	0
57	MG	RA	3090	1/1	0.98	0.38	11,11,11,11	0
57	MG	YA	3330	1/1	0.98	0.38	11,11,11,11	0
57	MG	YA	3102	1/1	0.98	0.44	40,40,40,40	0
57	MG	RA	3026	1/1	0.98	0.33	16,16,16,16	0
57	MG	YA	3214	1/1	0.98	0.50	19,19,19,19	0
57	MG	YA	3159	1/1	0.98	0.48	13,13,13,13	0
57	MG	RA	3039	1/1	0.98	0.24	34,34,34,34	0
57	MG	YA	3051	1/1	0.98	0.51	30,30,30,30	0
57	MG	RA	3115	1/1	0.98	0.56	52,52,52,52	0
57	MG	YA	3338	1/1	0.98	0.44	25,25,25,25	0
58	ZN	QN	101	1/1	0.98	0.17	79,79,79,79	0
57	MG	QA	1692	1/1	0.98	0.27	26,26,26,26	0
57	MG	YA	3055	1/1	0.98	0.34	14,14,14,14	0
57	MG	RA	3074	1/1	0.99	0.20	37,37,37,37	0
57	MG	QA	1649	1/1	0.99	0.41	32,32,32,32	0
57	MG	XA	1715	1/1	0.99	0.17	40,40,40,40	0
57	MG	YA	3054	1/1	0.99	0.53	20,20,20,20	0
57	MG	RA	3034	1/1	0.99	0.40	20,20,20,20	0
57	MG	RA	3055	1/1	0.99	0.52	25,25,25,25	0
57	MG	YA	3494	1/1	0.99	0.28	49,49,49,49	0
57	MG	YA	3023	1/1	0.99	0.40	14,14,14,14	0
57	MG	YA	3058	1/1	0.99	0.27	55,55,55,55	0
57	MG	YA	3129	1/1	0.99	0.20	19,19,19,19	0
57	MG	RA	3386	1/1	0.99	0.52	24,24,24,24	0
57	MG	YA	3146	1/1	0.99	0.45	29,29,29,29	0
57	MG	XA	1664	1/1	0.99	0.45	31,31,31,31	0
57	MG	XA	1665	1/1	0.99	0.28	29,29,29,29	0
57	MG	XA	1621	1/1	0.99	0.41	46,46,46,46	0
57	MG	XA	1658	1/1	0.99	0.13	34,34,34,34	0
57	MG	YA	3064	1/1	0.99	0.53	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.