



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 08:14 pm BST

PDB ID : 4LT8
Title : Crystal Structure of tRNA Proline (CGG) Bound to Codon CCC-G on the Ribosome
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-07-23
Resolution : 3.14 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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	:	2.11
buster-report	:	1.1.7 (2018)
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)	:	2.11

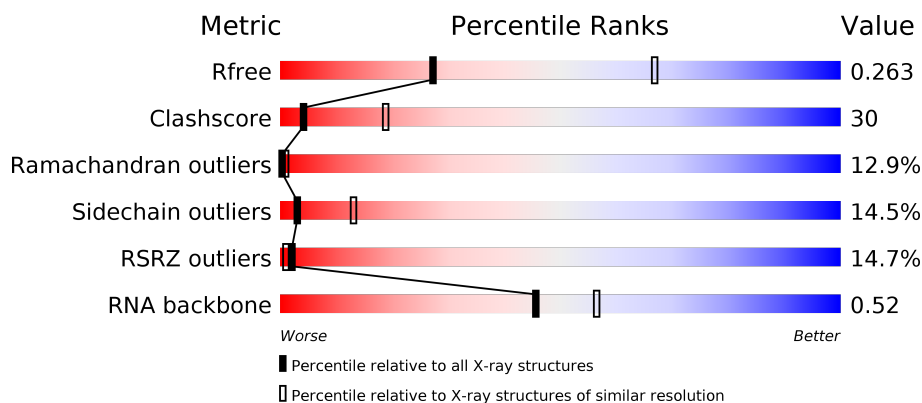
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.14 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	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)
RNA backbone	3102	1000 (3.46-2.82)

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

Mol	Chain	Length	Quality of chain
1	QA	1522	<div> <div>17%</div> <div> <div>50%</div> <div>37%</div> <div>10%</div> <div>..</div> </div> </div>
1	XA	1522	<div> <div>19%</div> <div> <div>50%</div> <div>37%</div> <div>11%</div> <div>..</div> </div> </div>
2	QB	256	<div> <div>17%</div> <div> <div>17%</div> <div>58%</div> <div>16%</div> <div>• 7%</div> </div> </div>
2	XB	256	<div> <div>9%</div> <div> <div>17%</div> <div>59%</div> <div>16%</div> <div>• 7%</div> </div> </div>

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

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Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QY	17	
23	XY	17	
24	QX	25	
24	XX	25	
25	RA	2916	
25	YA	2916	
26	RB	122	
26	YB	122	
27	RD	276	
27	YD	276	

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

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

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Mol	Chain	Length	Quality of chain
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	
56	Z6	3	
56	Z8	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3002	-	-	-	X
57	MG	RA	3091	-	-	-	X
57	MG	RA	3221	-	-	-	X
57	MG	RA	3222	-	-	-	X
57	MG	YA	3120	-	-	-	X
57	MG	YA	3164	-	-	-	X
57	MG	YA	3207	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291998 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1500	Total	C	N	O	P	0	0	0
			32247	14353	5981	10414	1499			
1	XA	1500	Total	C	N	O	P	0	0	0
			32249	14354	5984	10412	1499			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
2	XB	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	QC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	XC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	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	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	XE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	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	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	XI	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- 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	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	XK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	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	121	Total	C	N	O	S	0	0	0
			964	597	199	166	2			
13	XM	121	Total	C	N	O	S	0	0	0
			964	597	199	166	2			

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

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	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	XR	70	Total	C	N	O	0	0	0
			574	367	112	95			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			
19	XS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	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 S21.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	XV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QY	15	Total	C	N	O	P	0	0	0
			323	144	58	106	15			
23	XY	15	Total	C	N	O	P	0	0	0
			323	144	58	106	15			

- Molecule 24 is a RNA chain called A-site ASL Pro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QX	8	Total	C	N	O	P	0	0	0
			170	76	31	55	8			
24	XX	8	Total	C	N	O	P	0	0	0
			170	76	31	55	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	RA	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			
25	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	RB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	YB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- 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	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
29	YF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- 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 L11.

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 L13.

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 L14.

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 L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
36	YQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
37	YR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 38 is a protein called 50S ribosomal protein L17.

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

- Molecule 39 is a protein called 50S ribosomal protein L18.

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 L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
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 L20.

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 L21.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 L22.

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 L23.

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 L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	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 L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			
46	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 47 is a protein called 50S ribosomal protein L27.

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 L28.

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 L29.

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 L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	R4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			
50	Y4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

- 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	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	R6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			
52	Y6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	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	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 56 is a RNA chain called tRNA acceptor end mimic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	Z6	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
56	Z8	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).

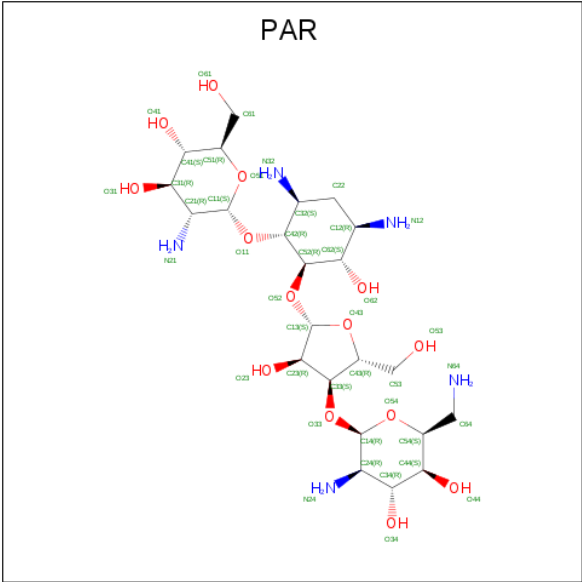
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	69	Total	Mg	0	0
			69	69		
57	RP	1	Total	Mg	0	0
			1	1		
57	YA	265	Total	Mg	0	0
			265	265		
57	QM	1	Total	Mg	0	0
			1	1		
57	XX	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QV	1	Total 1	Mg 1	0	0
57	XA	74	Total 74	Mg 74	0	0
57	R0	1	Total 1	Mg 1	0	0
57	QH	1	Total 1	Mg 1	0	0
57	YQ	1	Total 1	Mg 1	0	0
57	RR	2	Total 2	Mg 2	0	0
57	RD	1	Total 1	Mg 1	0	0
57	Y7	1	Total 1	Mg 1	0	0
57	QF	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	Y0	1	Total 1	Mg 1	0	0
57	RA	240	Total 240	Mg 240	0	0
57	YP	1	Total 1	Mg 1	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	RE	2	Total 2	Mg 2	0	0
57	YB	3	Total 3	Mg 3	0	0
57	XV	2	Total 2	Mg 2	0	0
57	RB	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0
57	YE	2	Total 2	Mg 2	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	QA	1	Total	C	N	O	0	0
			42	23	5	14		
58	XA	1	Total	C	N	O	0	0
			42	23	5	14		

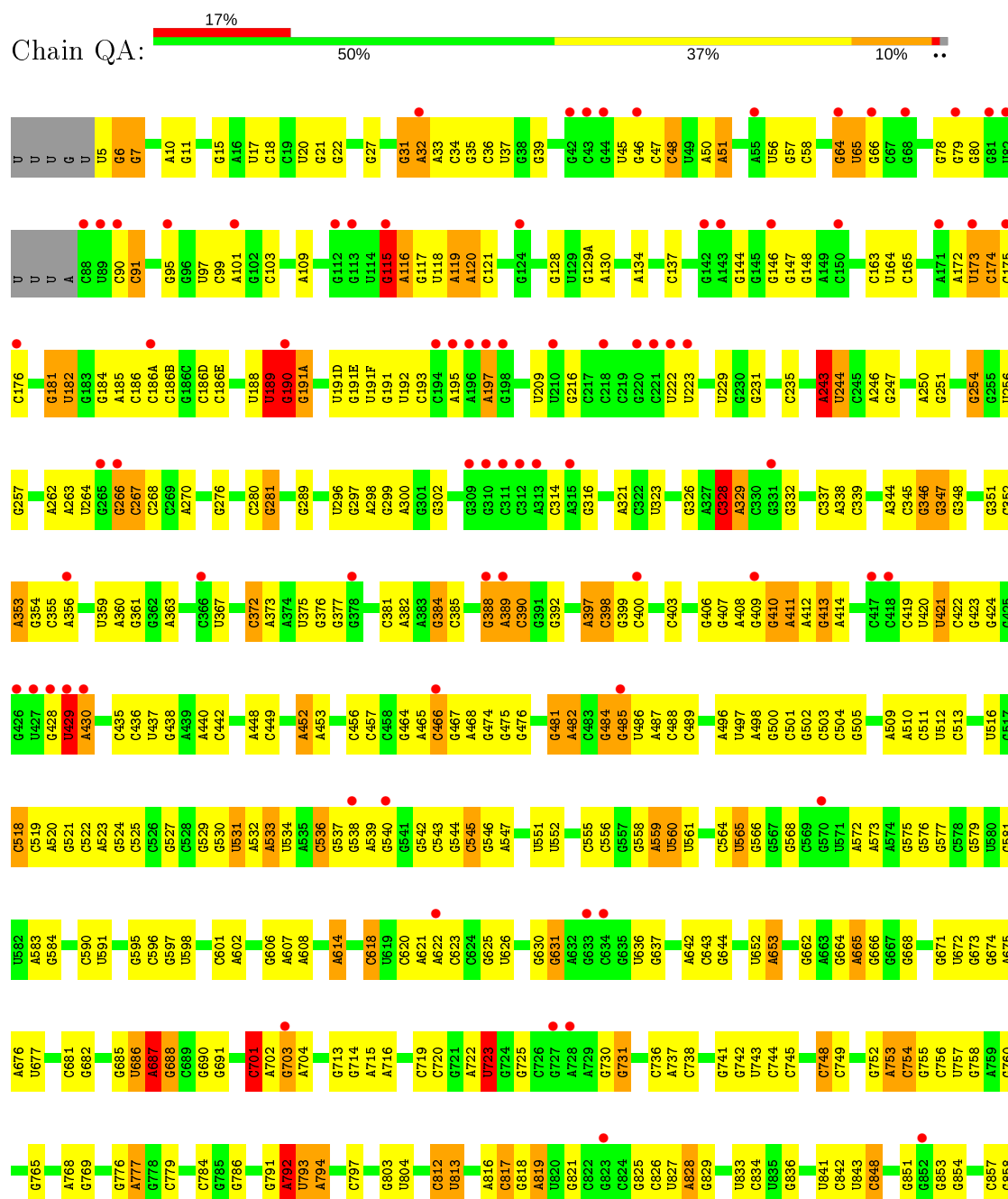
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

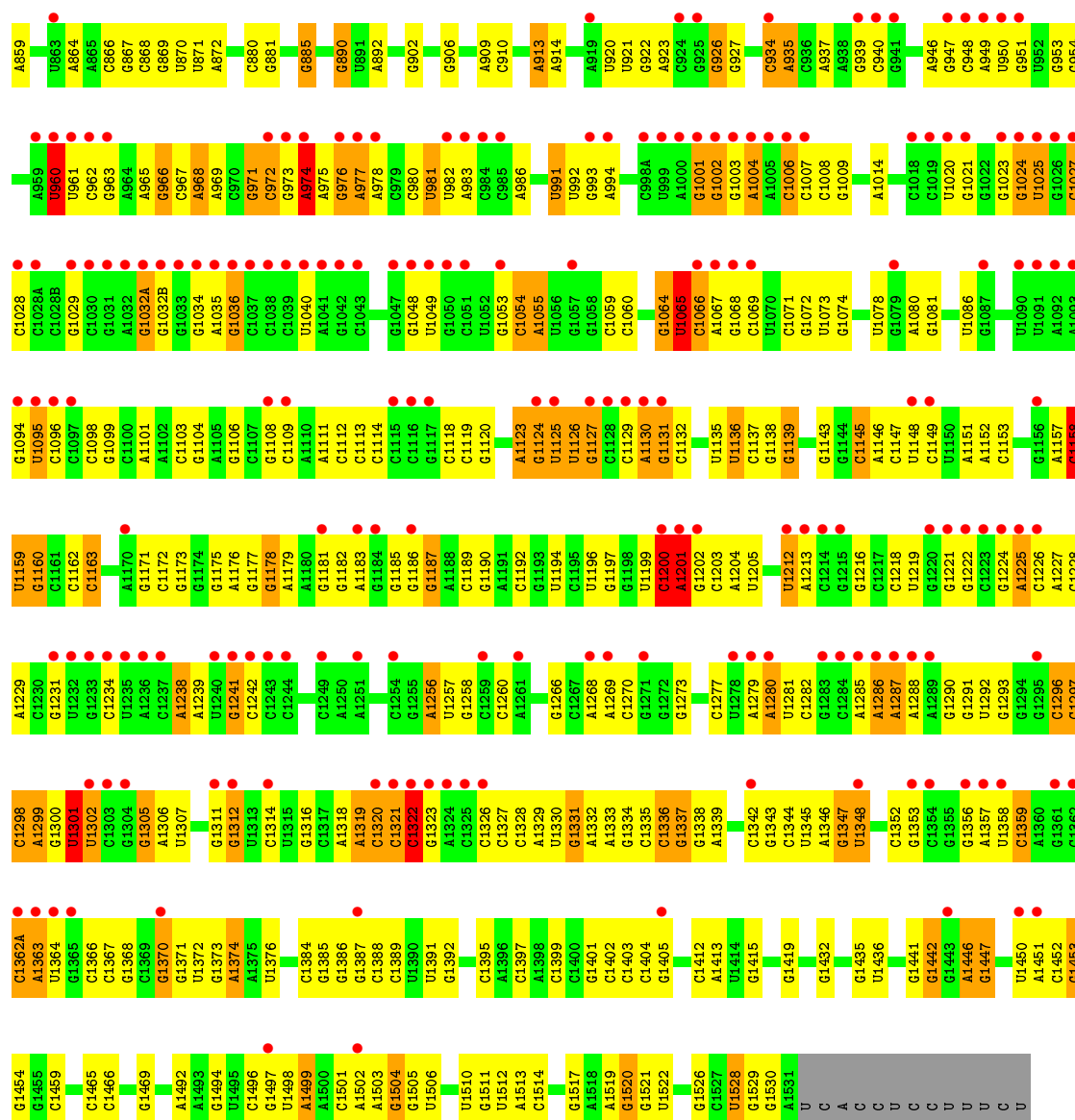
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	XD	1	Total	Zn	0	0
			1	1		
59	QD	1	Total	Zn	0	0
			1	1		
59	QN	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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

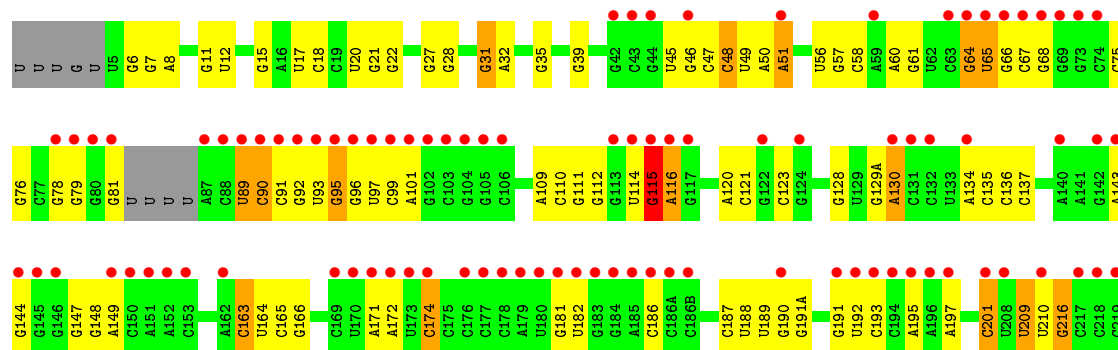




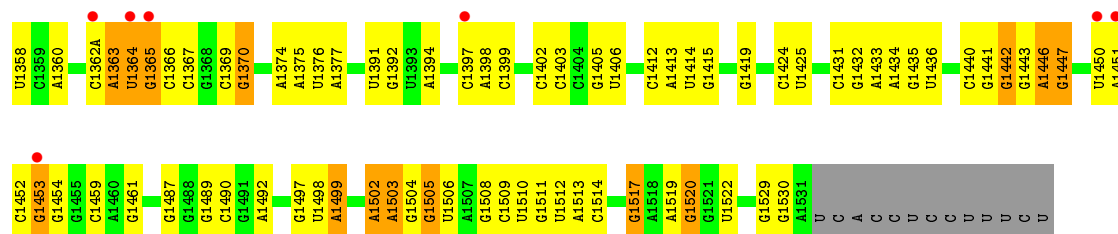
• Molecule 1: 16S rRNA



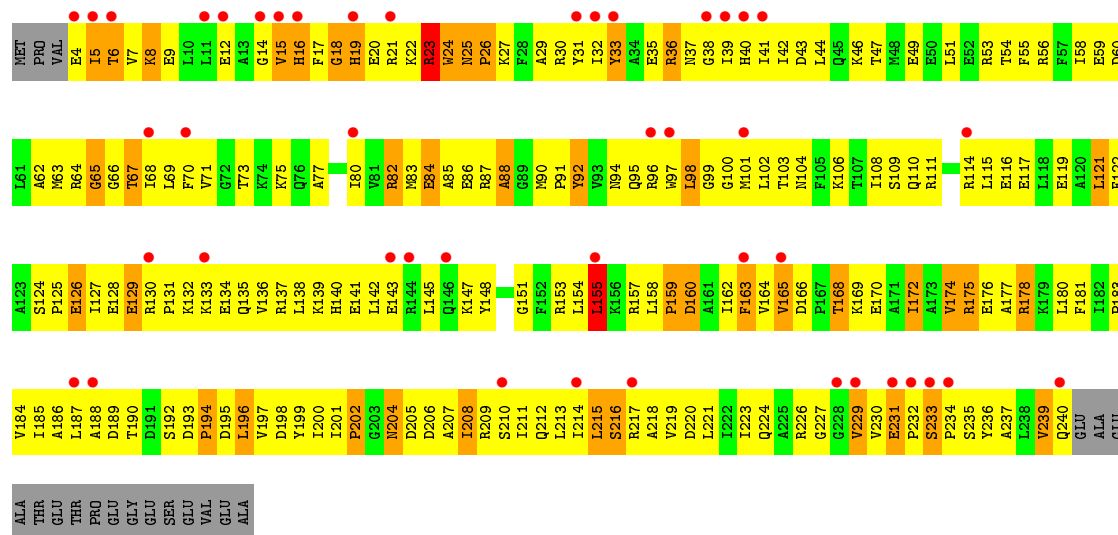
Chain XA:



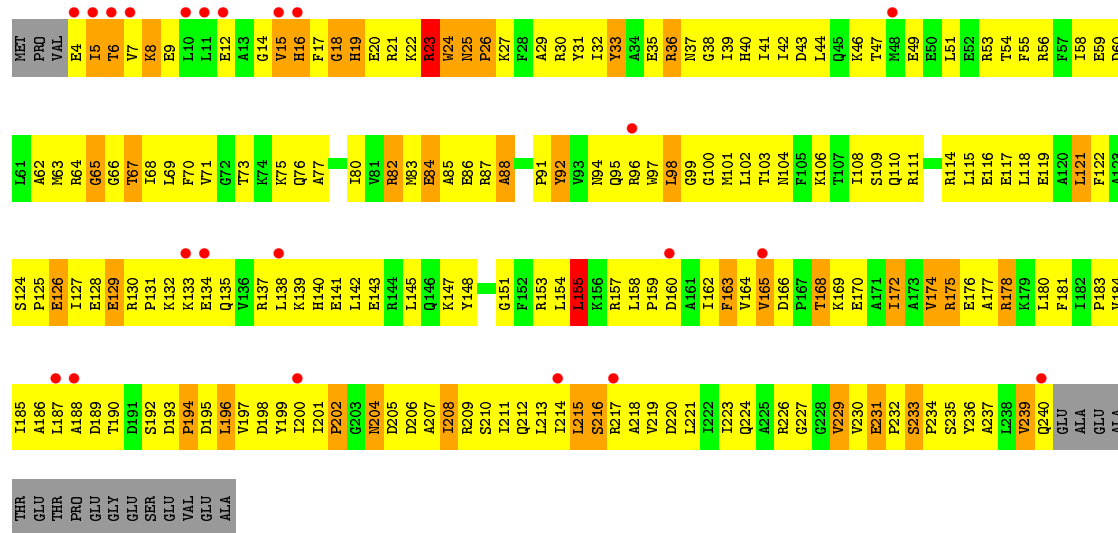




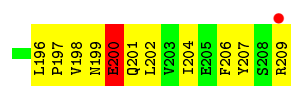
• Molecule 2: 30S ribosomal protein S2



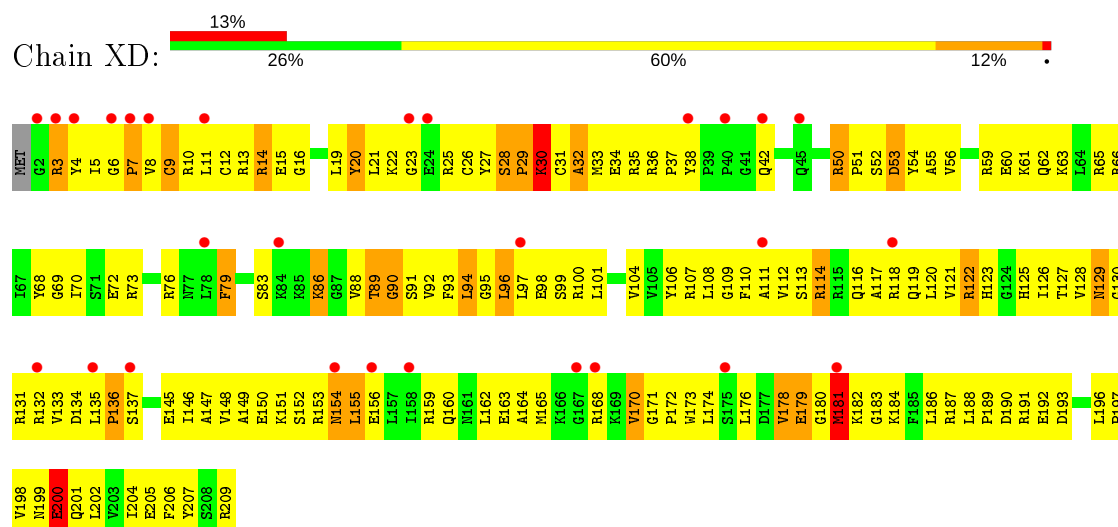
• Molecule 2: 30S ribosomal protein S2



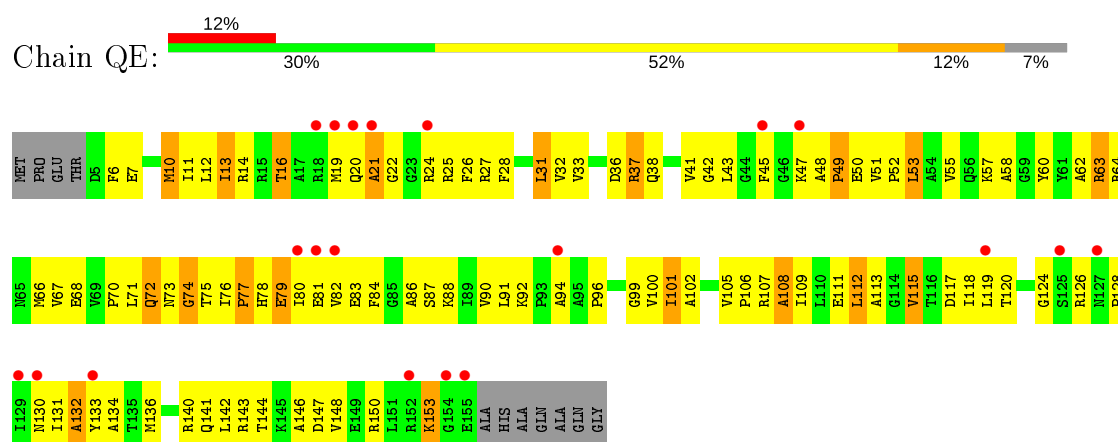
• Molecule 3: 30S ribosomal protein S3



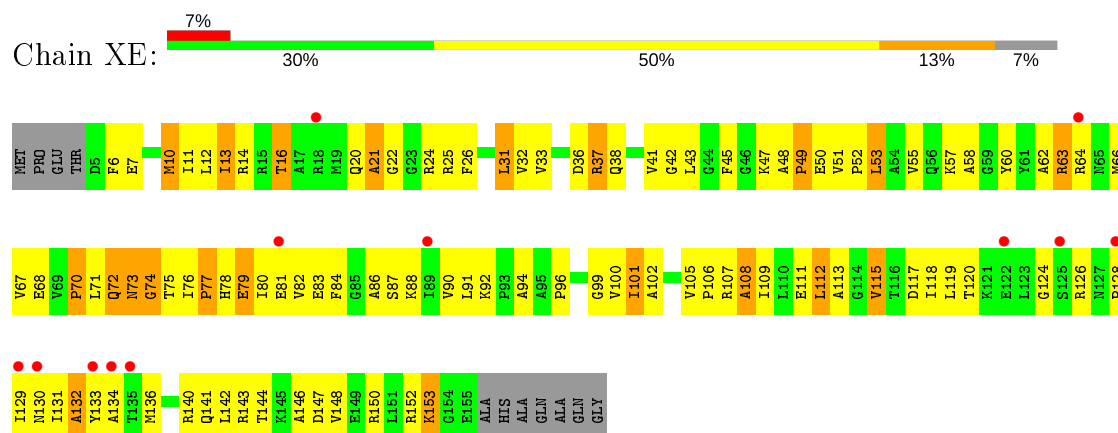
• Molecule 4: 30S ribosomal protein S4



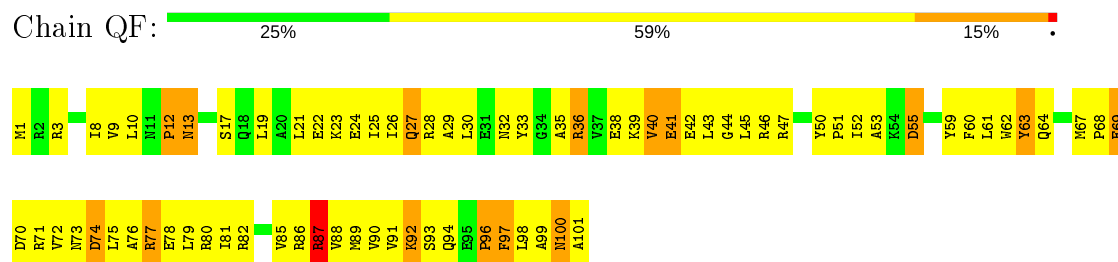
• Molecule 5: 30S ribosomal protein S5



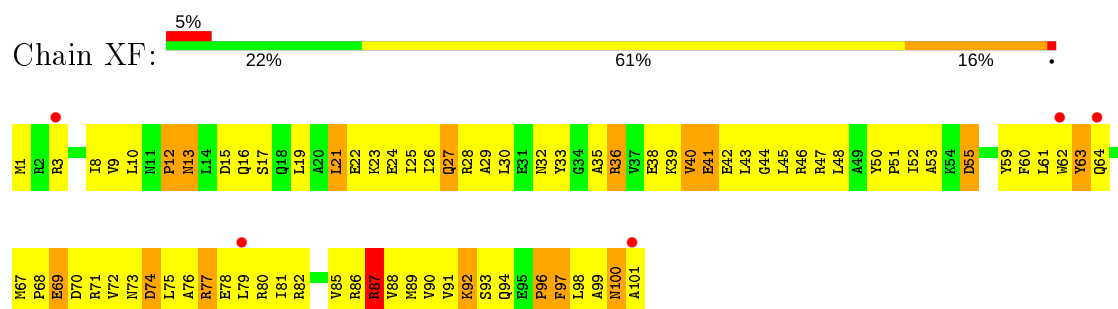
• Molecule 5: 30S ribosomal protein S5



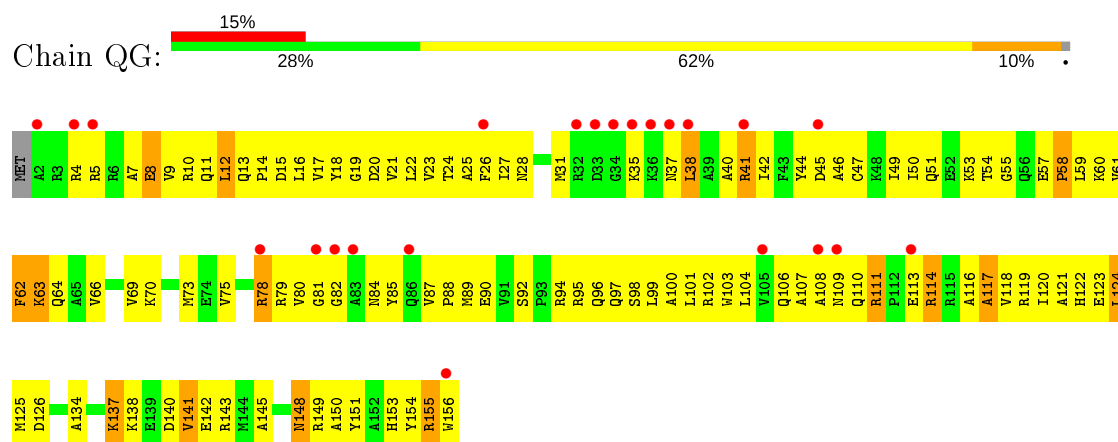
- Molecule 6: 30S ribosomal protein S6



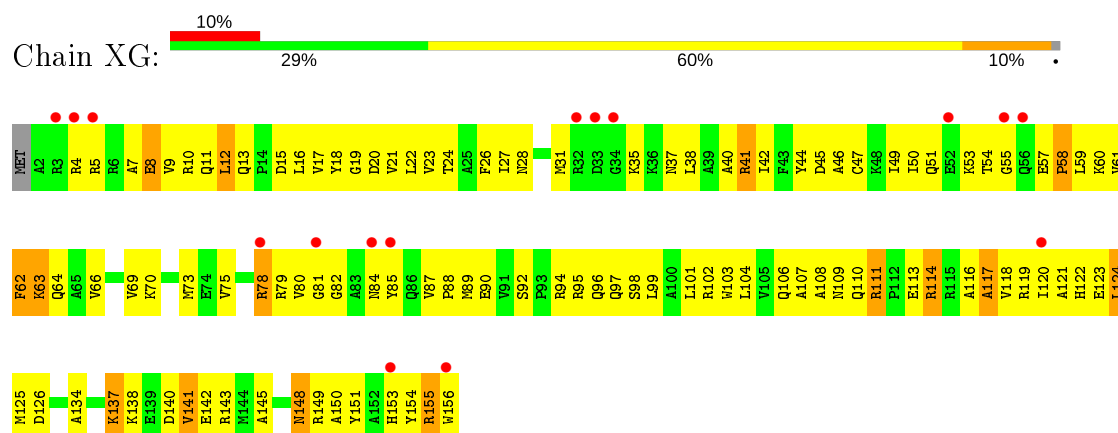
- Molecule 6: 30S ribosomal protein S6



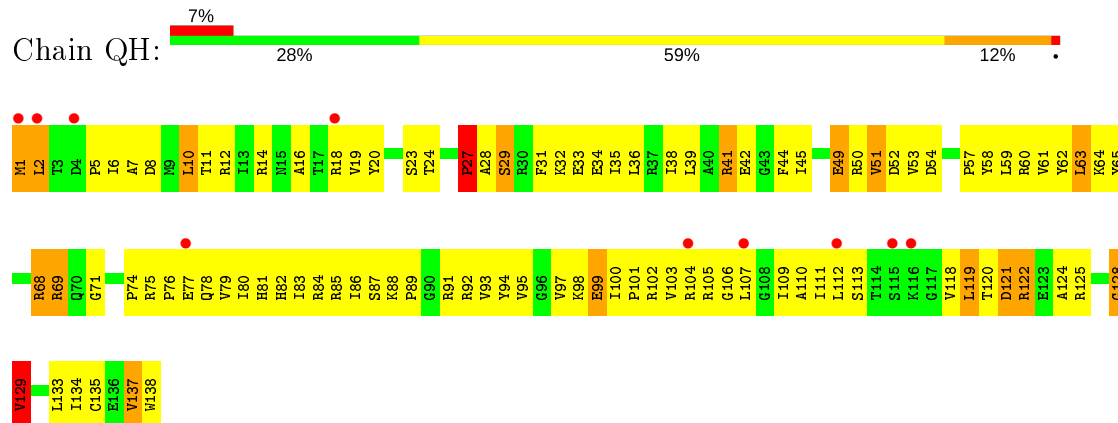
- Molecule 7: 30S ribosomal protein S7



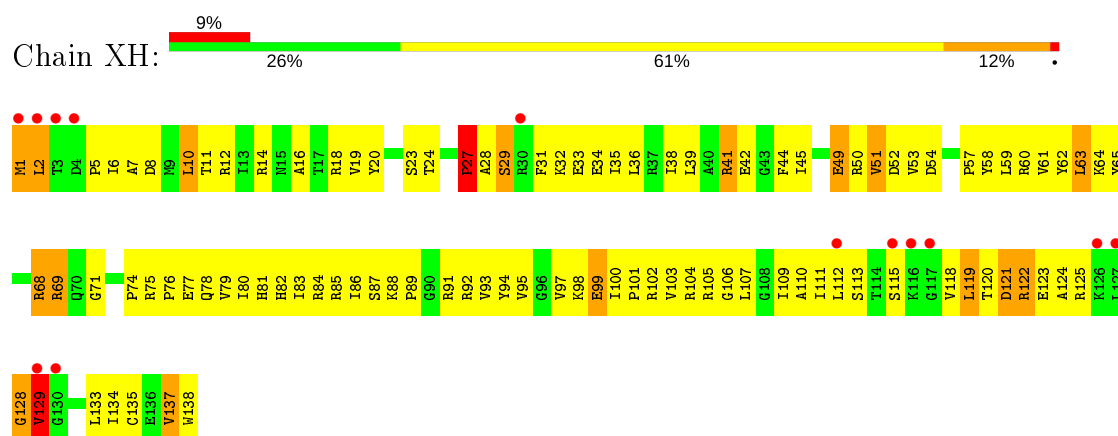
- Molecule 7: 30S ribosomal protein S7



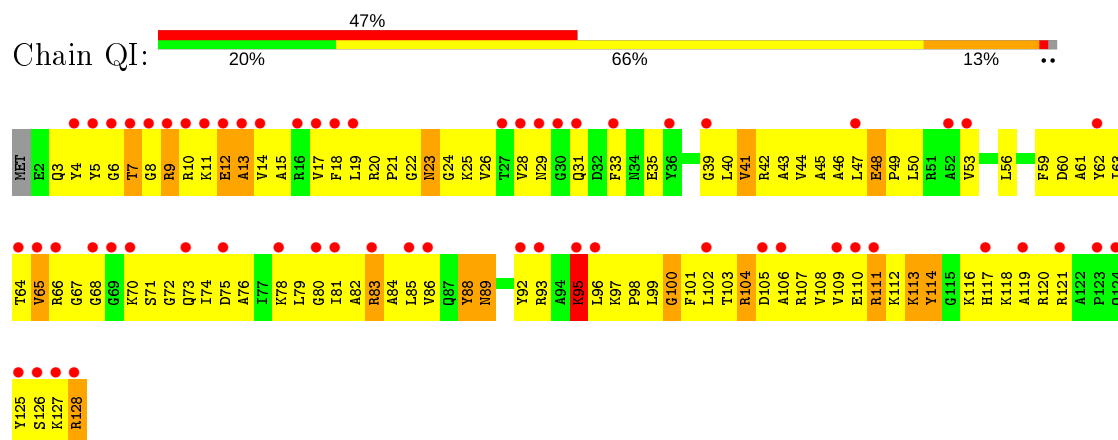
- Molecule 8: 30S ribosomal protein S8



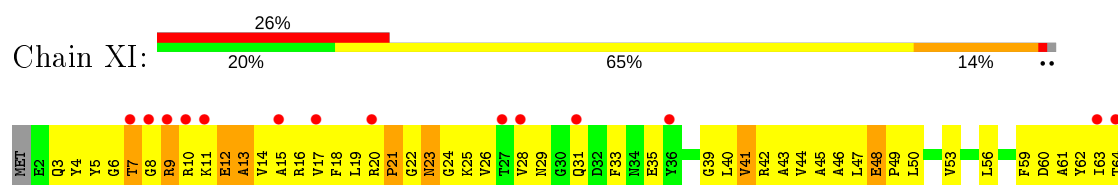
- Molecule 8: 30S ribosomal protein S8

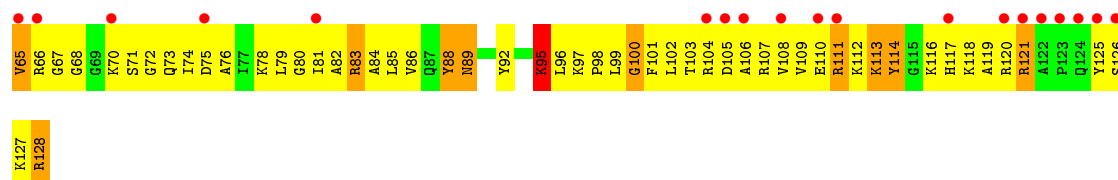


- Molecule 9: 30S ribosomal protein S9

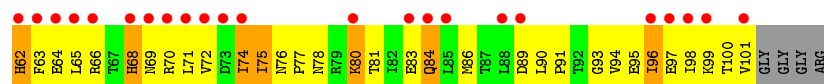
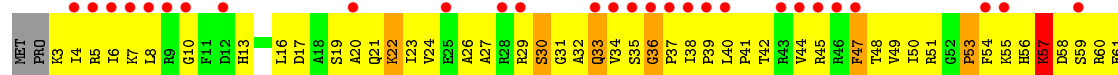


- Molecule 9: 30S ribosomal protein S9

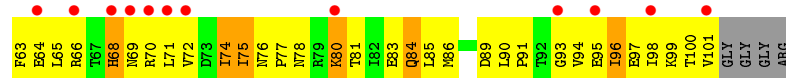
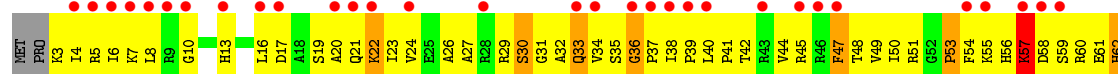




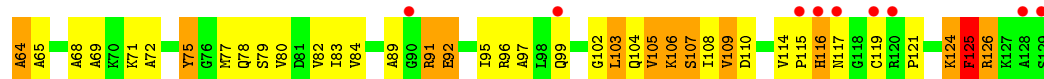
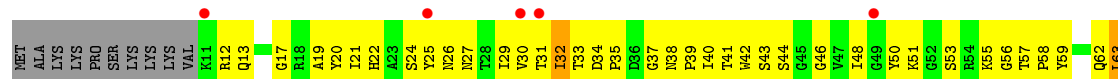
• Molecule 10: 30S ribosomal protein S10



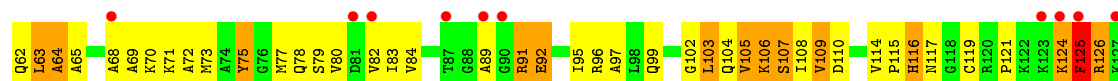
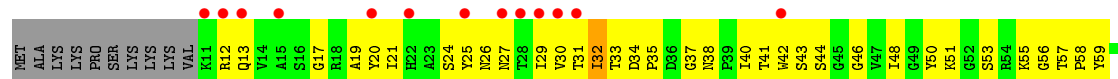
• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11



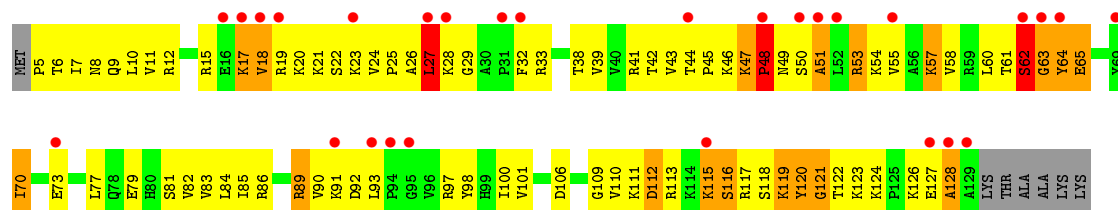
• Molecule 11: 30S ribosomal protein S11



A128
S129

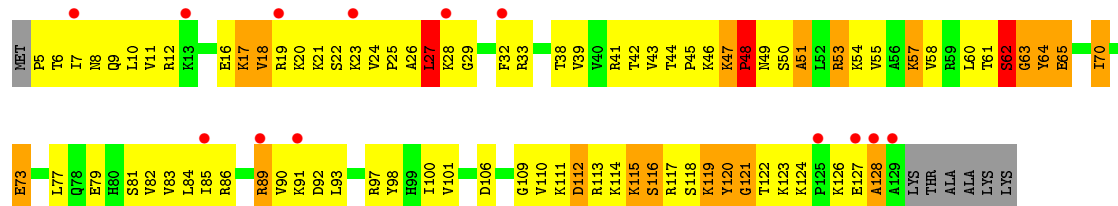
• Molecule 12: 30S ribosomal protein S12

Chain QL: 21% 30% 49% 14% 5%



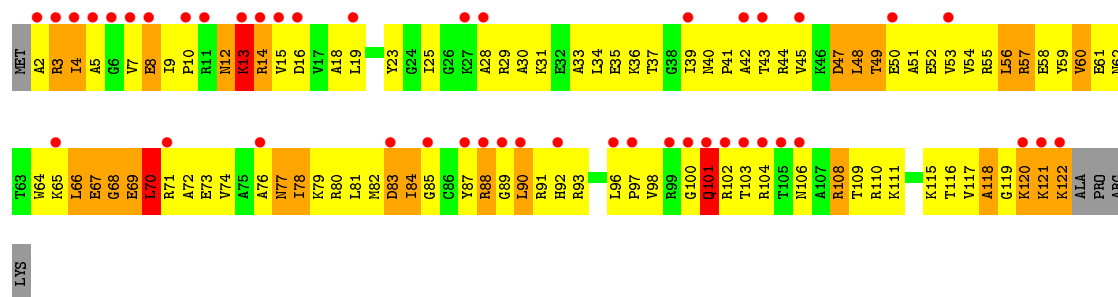
• Molecule 12: 30S ribosomal protein S12

Chain XL: 10% 29% 49% 14% 5%



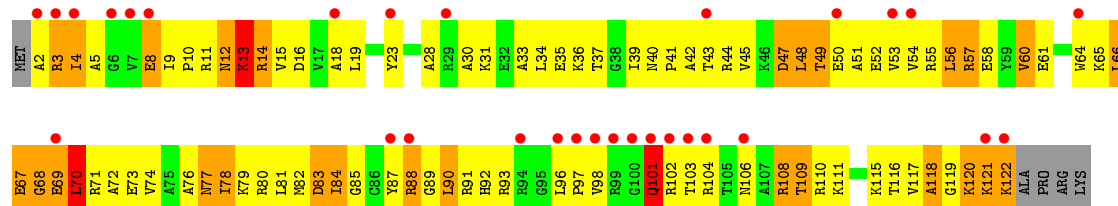
• Molecule 13: 30S ribosomal protein S13

Chain QM: 36% 18% 55% 21%

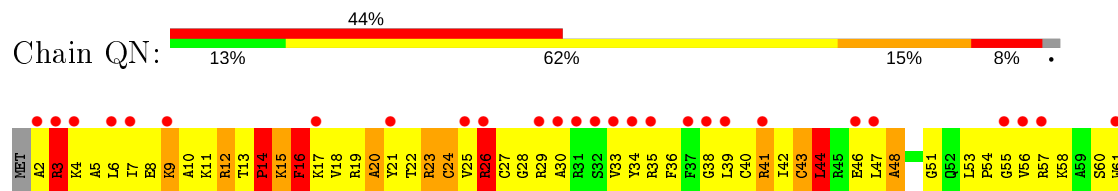


• Molecule 13: 30S ribosomal protein S13

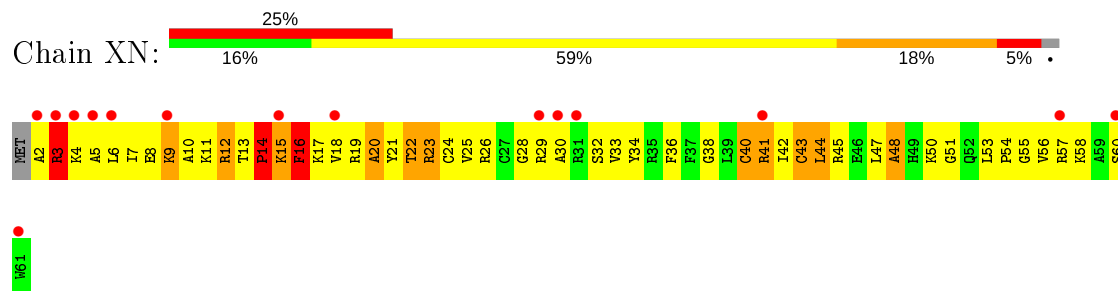
Chain XM: 24% 22% 50% 21%



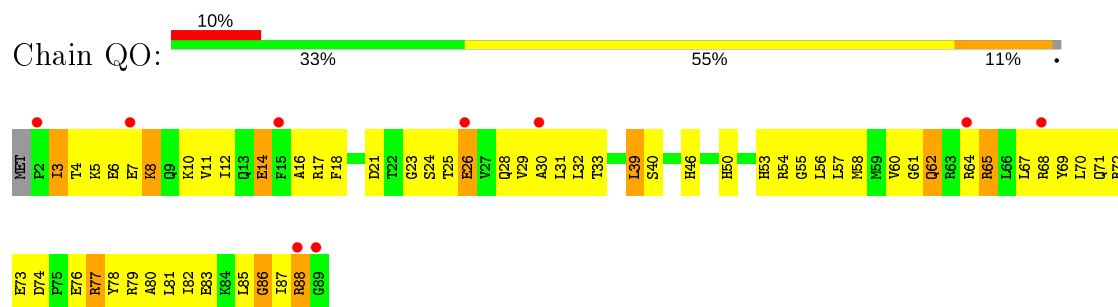
- Molecule 14: 30S ribosomal protein S14



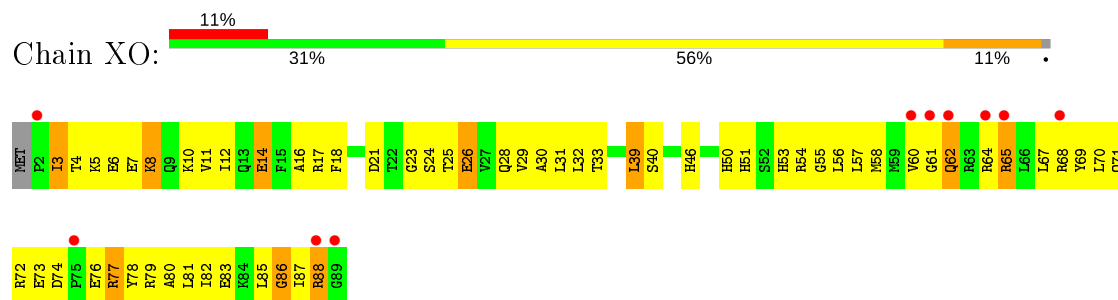
- Molecule 14: 30S ribosomal protein S14



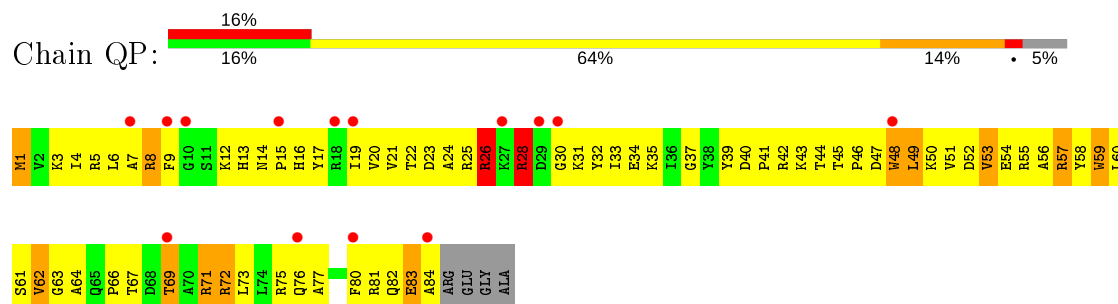
- Molecule 15: 30S ribosomal protein S15



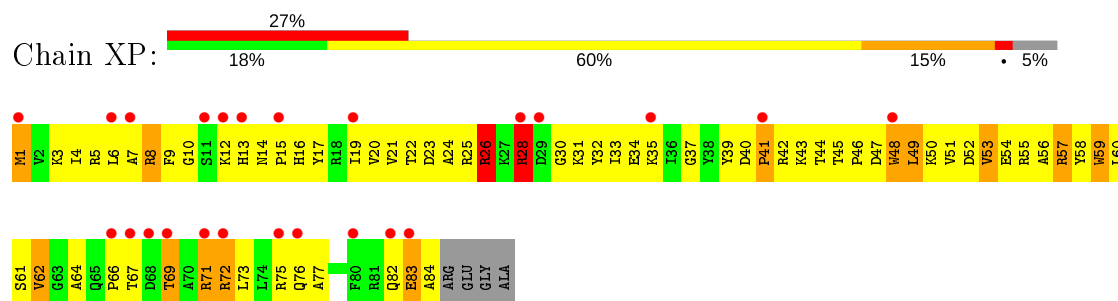
- Molecule 15: 30S ribosomal protein S15



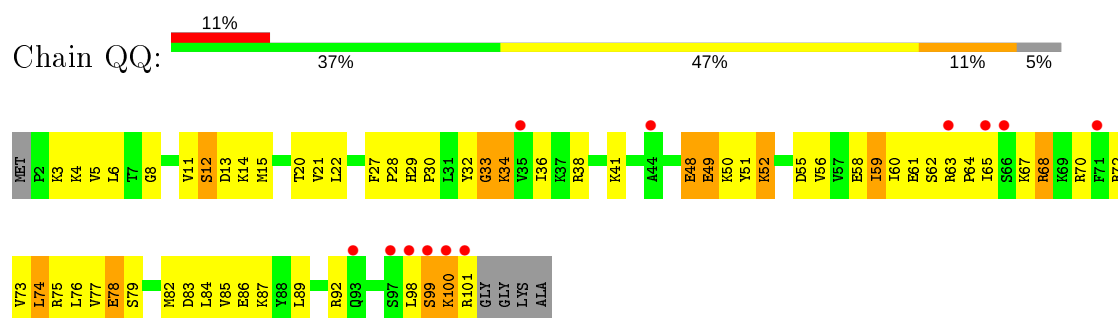
- Molecule 16: 30S ribosomal protein S16



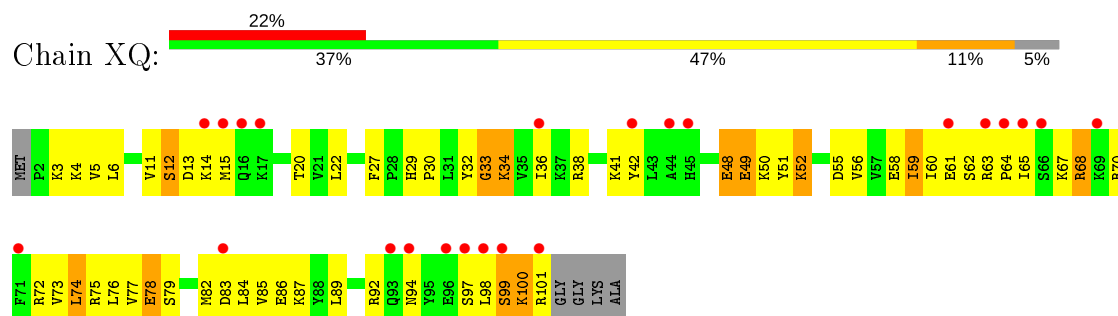
- Molecule 16: 30S ribosomal protein S16



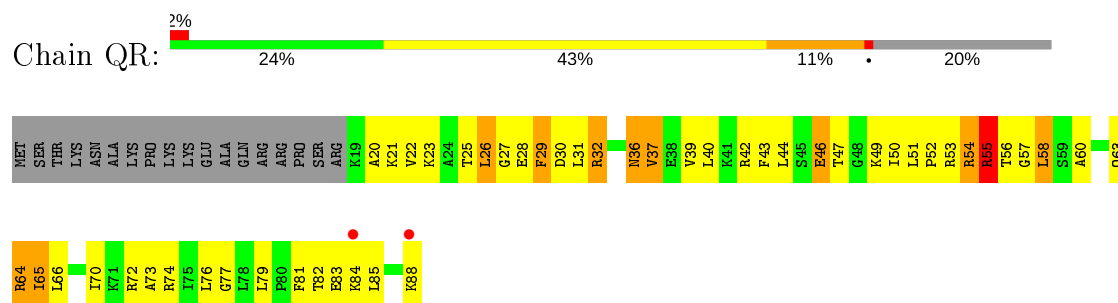
- Molecule 17: 30S ribosomal protein S17



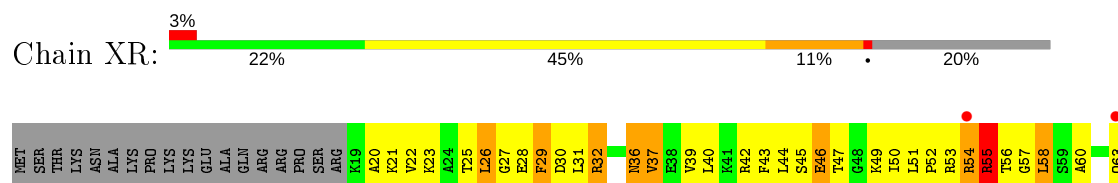
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

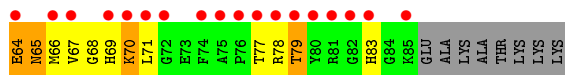
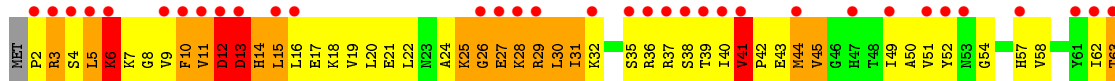
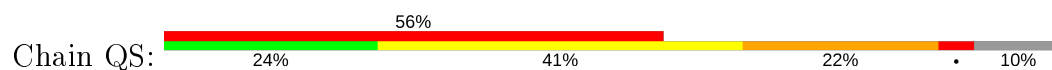


- Molecule 18: 30S ribosomal protein S18

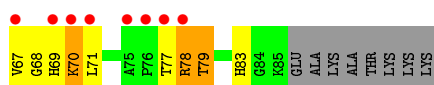
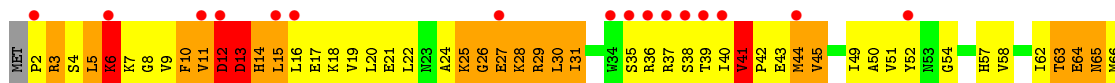
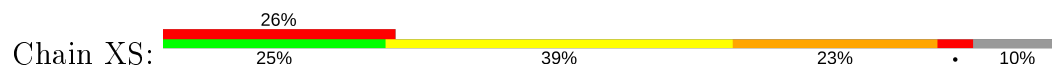




• Molecule 19: 30S ribosomal protein S19



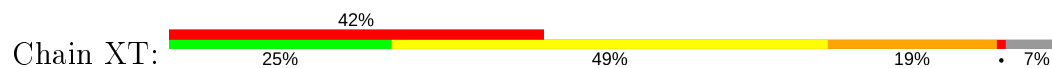
• Molecule 19: 30S ribosomal protein S19



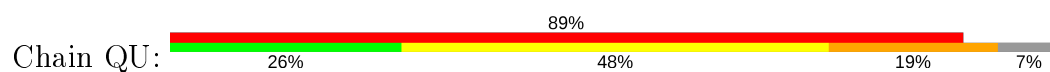
• Molecule 20: 30S ribosomal protein S20



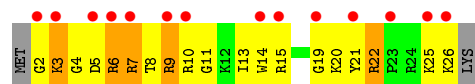
• Molecule 20: 30S ribosomal protein S20



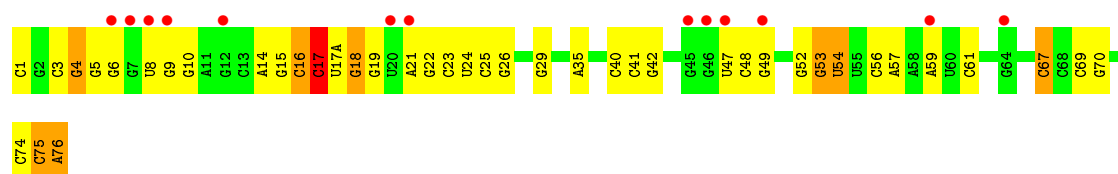
• Molecule 21: 30S ribosomal protein S21



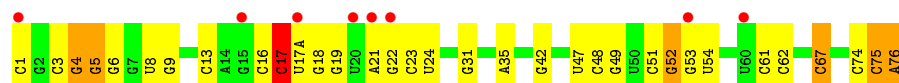
- Molecule 21: 30S ribosomal protein S21



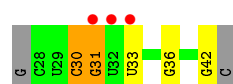
- Molecule 22: P-site tRNA fMet



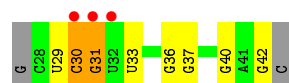
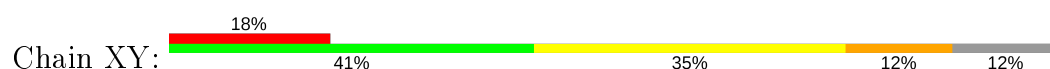
- Molecule 22: P-site tRNA fMet



- Molecule 23: messenger RNA



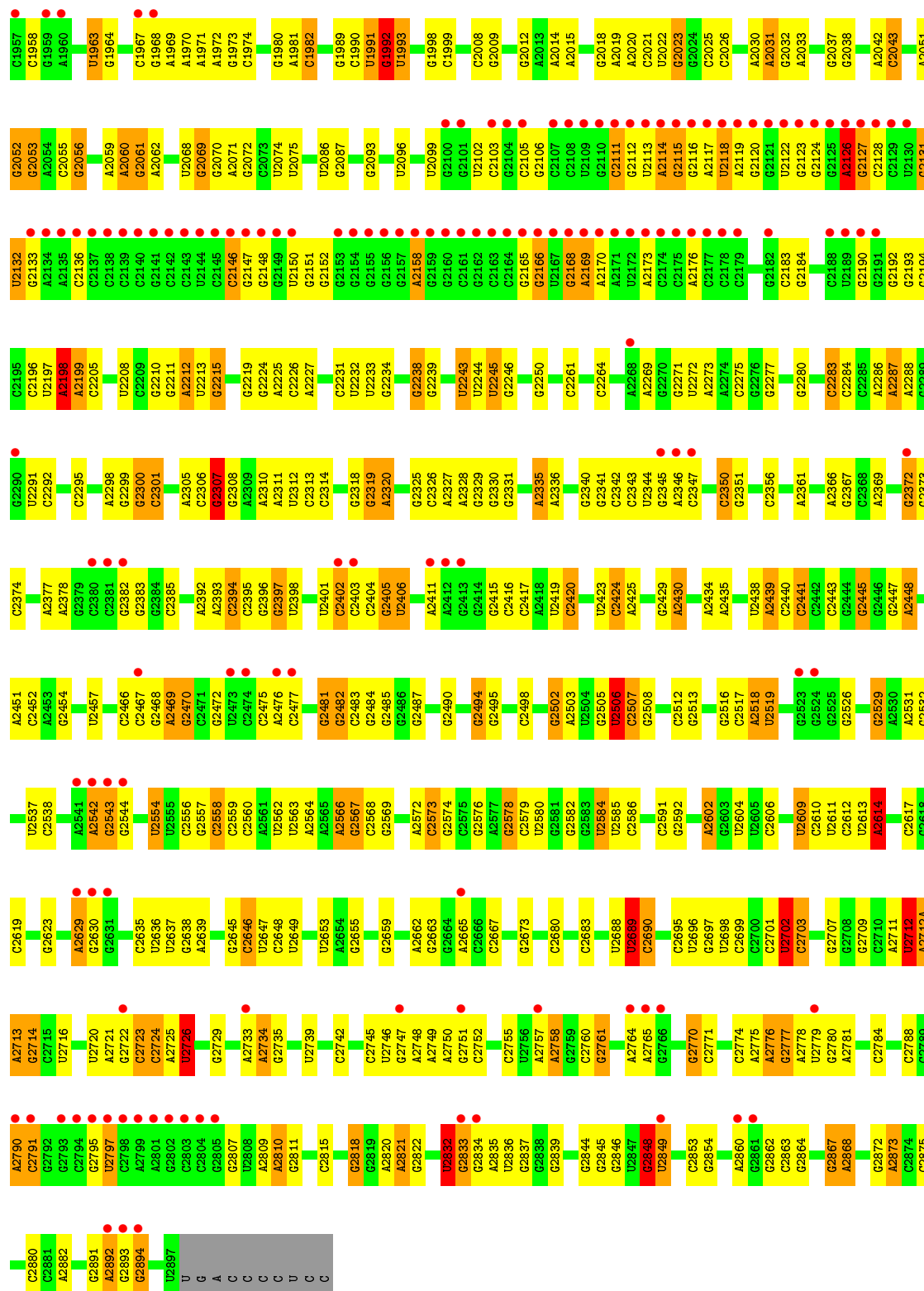
- Molecule 23: messenger RNA



- Molecule 24: A-site ASL Pro





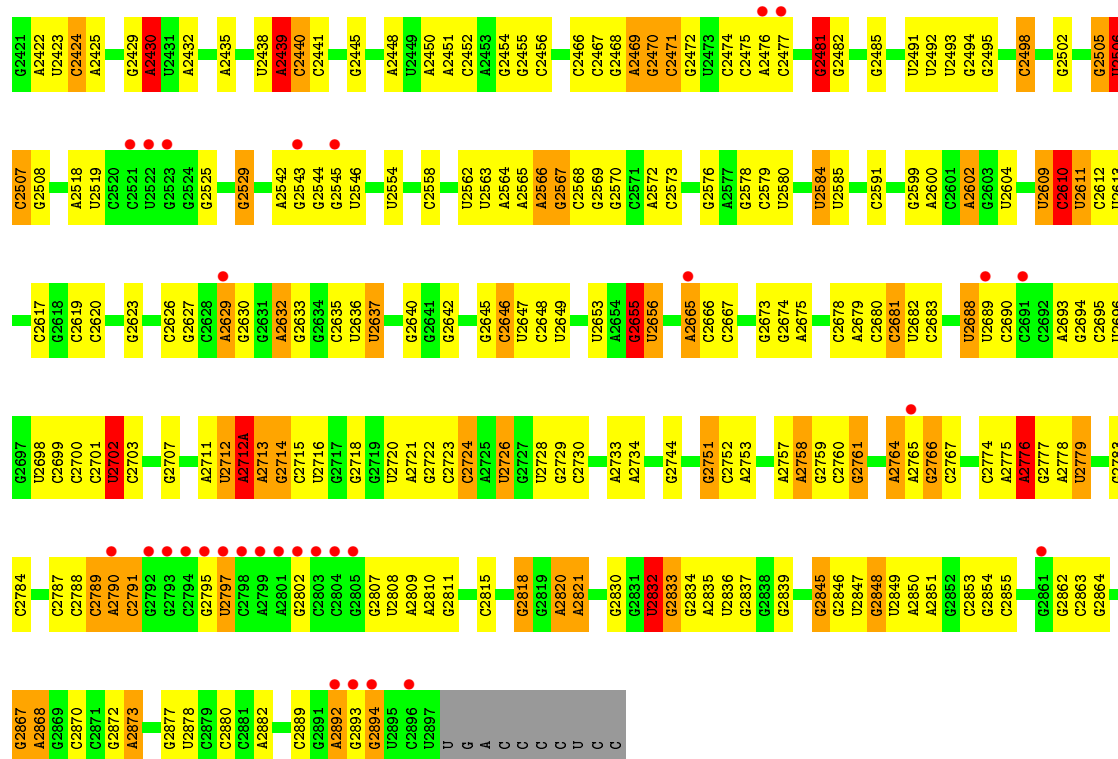


• Molecule 25: 23S rRNA





G2343	U2232	G2148	U2074	G1992	C1902	U1798	U1706	C1592	C1506	G1418	A1336	G1239
U2344	U2233	G2149	U2075	U1993	G1903	G1799	G1707	C1592	A1507	A1419	G1337	U1240
G2345	G2234	U2150	G2076	C1994	G1906	G1800	C1708	A1597	C1508	G1421	G1338	A1241
A2346	G2238	G2152	G2087	G1998	G1906	G1801	U1709	C1599	C1509	U1340	G1339	G1244
G2347	G2243	G2153	G2088	A2001	A1913	A1803	G1717	C1600	A1510	A1427	U1341	G1244
U2348	U2244	G2154	G2093	G2002	C1914	A1809	G1718	C1600	G1512	C1428	G1250	G1250
G2349	U2245	G2155	G2096	G2002	U1915	G1813	G1718	C1600	C1513	C1429	C1251	C1251
G2350	G2246	G2156	U2096	G2009	A1916	G1814	G1725	A1603	C1515	C1430	A1349	G1252
U2357	G2250	A2158	G2096	G2009	A1917	G1815	G1725	A1603	C1515	U1431	A1253	A1253
A2360	G2251	G2159	U2099	G2012	A1918	G1816	G1728	C1607	U1520	A1434	G1352	G1256
A2361	G2271	G2160	G2100	A2013	A1919	G1817	A1729	A1608	A1353	G1354	A1354	C1257
C2364	C2275	G2162	G2101	A2014	U1923	G1818	U1730	A1609	G1355	G1348	G1348	C1257
G2365	G2276	G2163	U2102	A2015	C1924	G1819	G1731	A1610	G1355	C1349	A1349	G1252
A2369	G2277	G2164	G2103	G2018	U1927	G1820	G1732	C1617	U1520	U1434	U1352	G1256
C2383	C2283	G2165	G2104	G2019	A1928	G1821	G1733	A1618	A1528	G1441	A1354	C1257
C2384	C2284	G2166	G2105	A2020	A1929	G1822	C1742	A1637	A1529	G1442	A1354	C1257
G2372	C2285	U2167	G2106	C2021	G1930	G1823	G1743	C1640	G1530	A1444A	A1359	A1262
G2373	C2286	A2169	U2109	G2022	U1931	G1824	G1743	C1640	G1532	G1448	G1363	U1263
A2286	A2286	A2170	G2110	G2023	A1932	G1825	G1750	C1640	G1533	A1449	G1364	G1264
A2287	A2287	G2171	G2111	G2024	G1933	G1826	G1751	G1647	U1535	G1449	A1268	G1266
A2288	A2288	U2172	G2112	C2025	G1936	A1829	C1752	C1648	A1536	U1454	G1369	U1267
U2291	U2291	A2173	U2113	C2026	A1937	G1835	G1753	C1653	C1537	G1455	G1370	G1271
C2292	C2292	G2174	A2114	A2030	A1937	G1836	C1754	A1654	G1538	C1458	G1371	A1272
G2293	C2293	C2175	G2115	A2031	A1938	G1837	G1756	A1654	G1542	G1459	U1372	U1273
C2294	C2294	A2176	G2116	G2032	U1939	G1838	G1756	A1654	G1543	A1460	A1373	G1279
C2295	C2295	G2177	A2117	A2033	U1939	G1839	G1756	A1654	A1544	G1461	G1280	G1280
C2296	C2296	C2178	U2118	U2034	G1950	G1842	A1759	C1657	C1544	G1462	G1281	G1281
C2297	C2297	G2179	A2119	G2035	U1951	C1843	A1762	U1659	A1545	C1463	U1282	U1282
U2298	U2298	U2180	G2120	G2036	A1952	C1844	G1763	G1667	A1545A	C1464	G1385	A1287
G2299	G2299	G2181	U2122	G2037	A1953	G1845	G1764	A1668	C1546	G1465	G1386	G1386
G2303	G2303	C2183	G2123	C2039	U1956	A1847	G1769	A1669	C1547	C1466	G1387	C1291
C2306	C2306	G2188	G2124	A2042	U1957	A1848	G1770	G1674	C1550	A1471	U1390	U1292
G2307	G2307	U2189	G2125	C2043	C1958	G1852	C1771	C1675	C1551	C1477	U1391	C1293
A2309	A2309	G2190	A2126	G2049	U1959	G1858	G1772	A1676	A1554	C1478	U1394	U1300
A2310	A2310	G2191	C2128	G2049	A1960	A1859	A1773	A1677	A1558	A1479	A1395	A1301
A2311	A2311	G2192	G2129	C2050	U1963	U1864	U1778	G1681	G1559	G1479	U1396	A1302
G2318	G2318	A2198	U2130	A2051	U1964	G1869	U1779	U1688	A1567	G1480	G1398	A1308
G2319	G2319	U2208	U2132	C2055	C1965	C1870	A1780	U1688	G1568	U1482	C1399	G1309
G2320	A2320	G2209	A2133	G2056	A1966	A1871	C1782	A1689	A1569	G1483	G1400	U1313
G2325	G2325	G2210	A2134	A2057	G1968	A1872	A1783	U1693	A1570	G1484	G1401	C1314
C2327	C2327	G2211	A2135	A2058	A1969	G1878	A1784	C1694	A1571	G1485	C1402	G1319
A2328	A2328	G2212	C2136	A2059	A1970	A1785	A1785	C1694	C1577	A1490	C1403	C1320
G2329	G2329	A2212	G2137	A2060	A1971	A1786	A1786	G1695	U1578	G1491	C1404	G1320
G2330	G2330	G2213	C2138	G2061	A1972	A1787	A1787	G1696	A1579	G1492	U1405	A1321
G2331	G2331	G2214	C2139	C2062	G1973	G1883	C1788	G1697	A1580	C1493	U1406	A1322
G2334	G2334	G2215	C2140	C2063	G1980	A1884	A1789	A1698	A1581	C1496	C1408	U1329
A2335	A2335	G2219	G2141	C2064	U1981	G1888	C1790	A1699	U1497	A1496	G1411	C1330
U2418	U2418	G2220	C2142	C2065	A1981	A1889	A1791	A1700	C1585	U1497	A1331	A1331
A2419	A2419	A2225	C2143	C2066	C1982	G1896	A1794	G1702	A1586	G1500	G1332	G1332
G2420	G2420	A2226	U2144	G2067	G1989	G1899	C1795	G1703	A1587	C1505	G1416	G1334
A2336	A2336	A2227	C2145	G2068	C1990	G1899	U1796	G1704	C1588			U1335
			G2147	G2069	U1991		C1797		C1589			



• Molecule 26: 5S rRNA

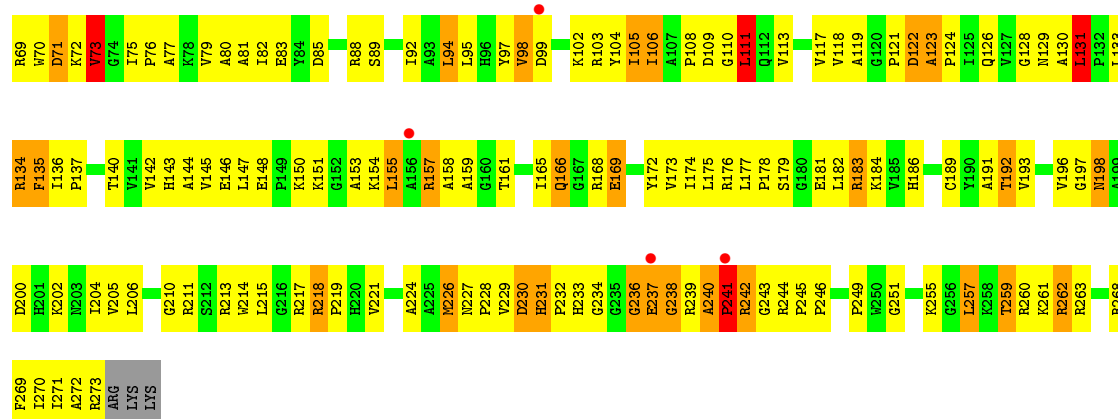


• Molecule 26: 5S rRNA

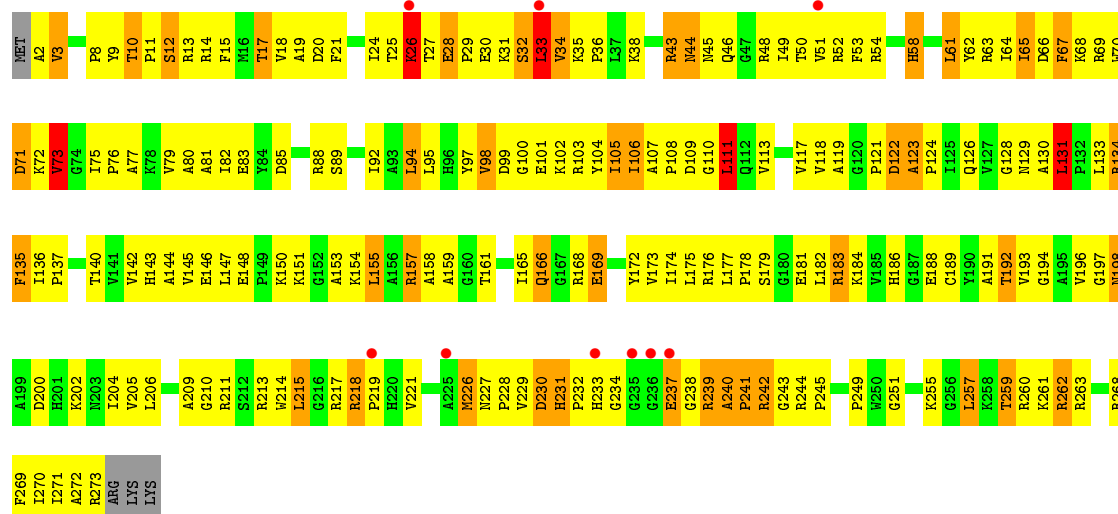


• Molecule 27: 50S ribosomal protein L2

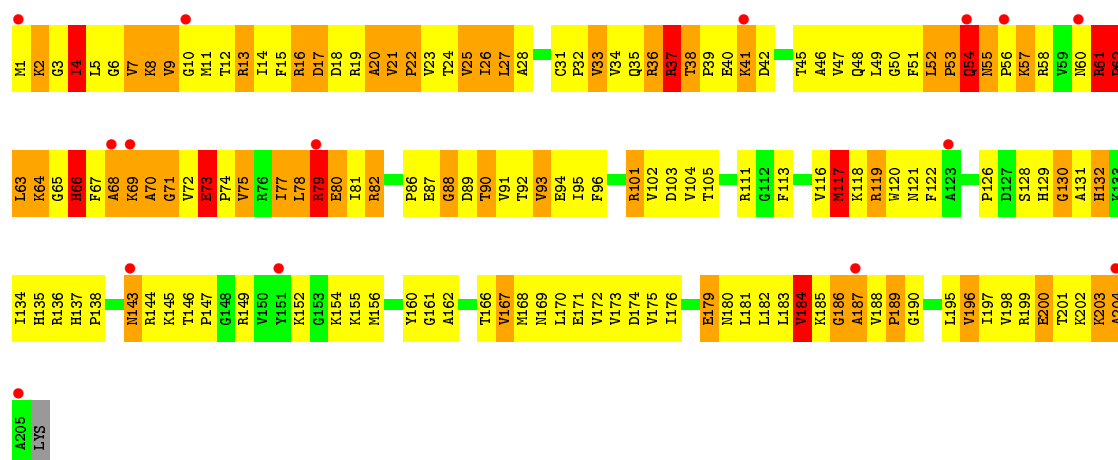




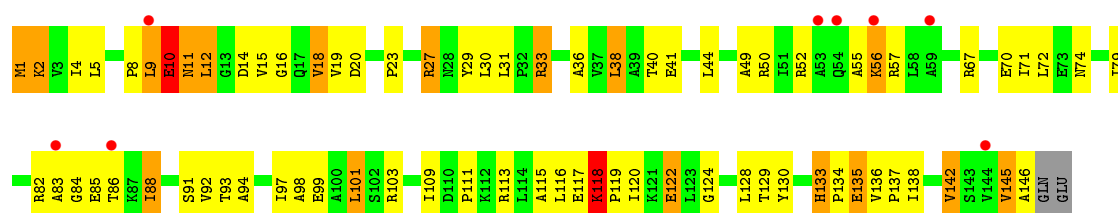
• Molecule 27: 50S ribosomal protein L2



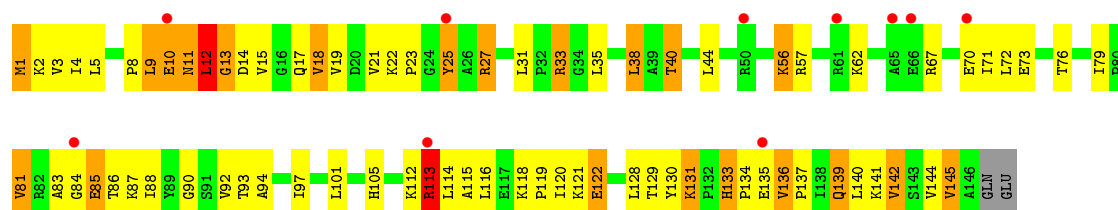
• Molecule 28: 50S ribosomal protein L3



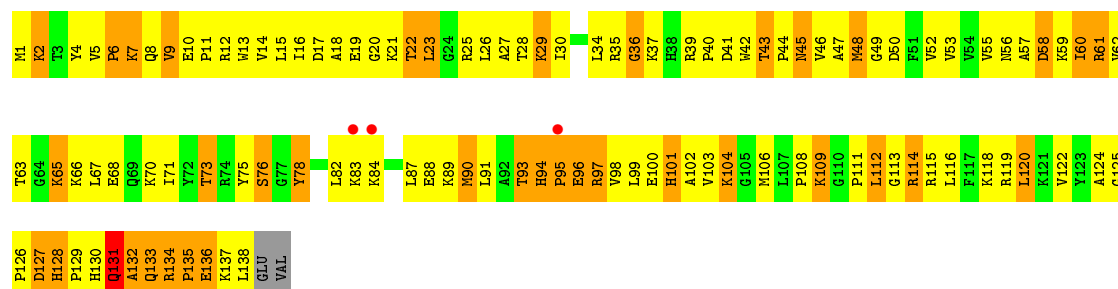
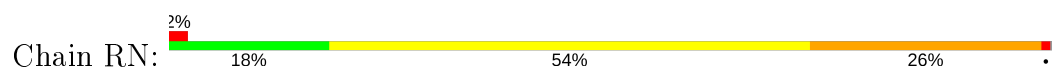
- Molecule 32: 50S ribosomal protein L9



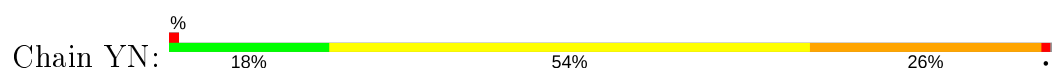
- Molecule 32: 50S ribosomal protein L9

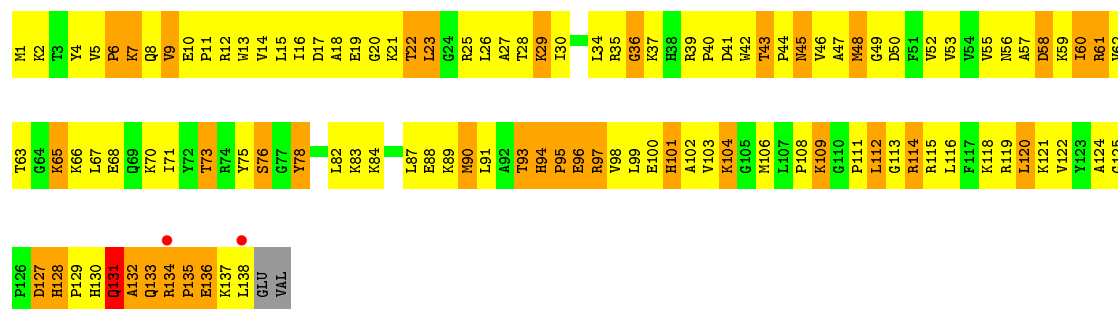


- Molecule 33: 50S ribosomal protein L11

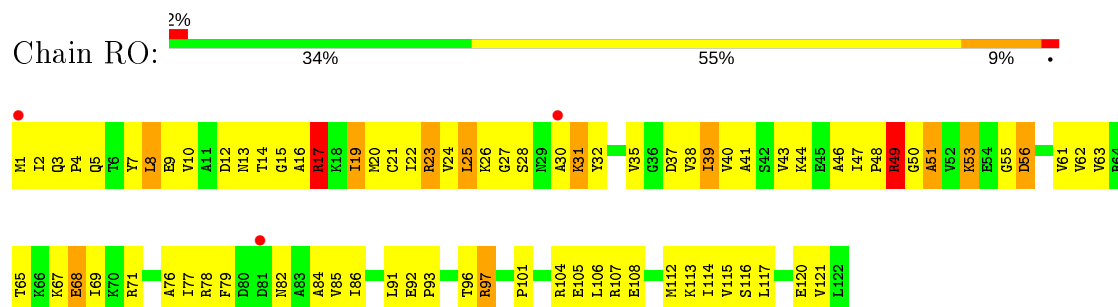


- Molecule 33: 50S ribosomal protein L11

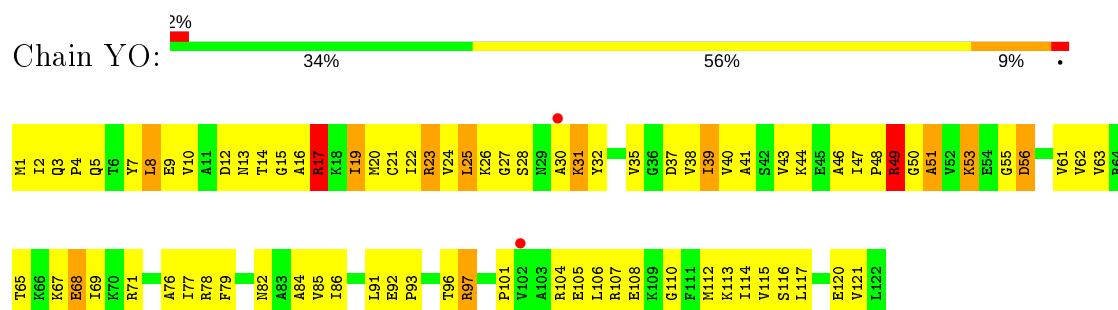




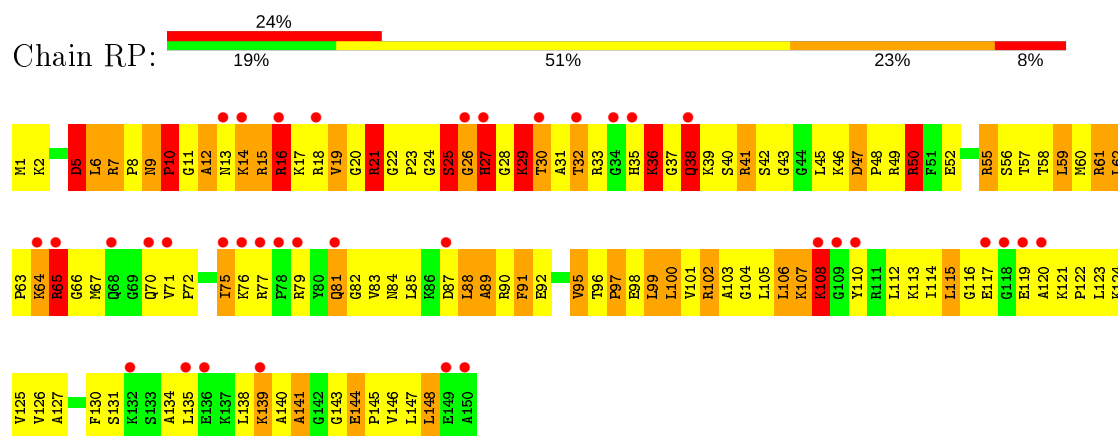
• Molecule 34: 50S ribosomal protein L13



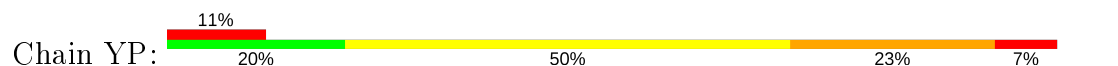
• Molecule 34: 50S ribosomal protein L13

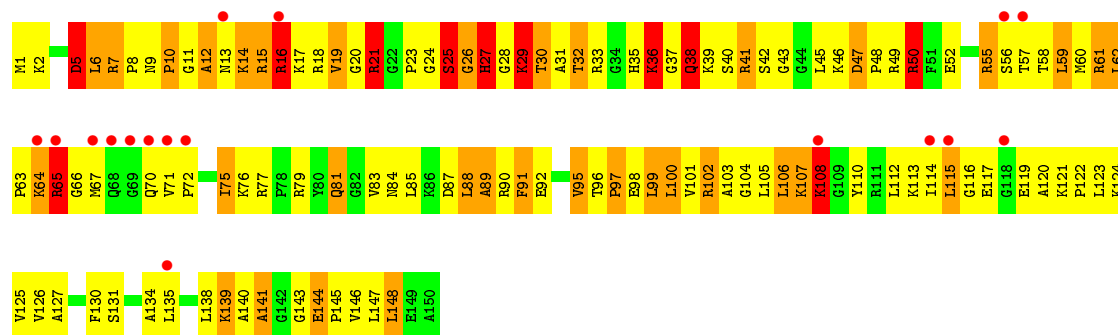


• Molecule 35: 50S ribosomal protein L14

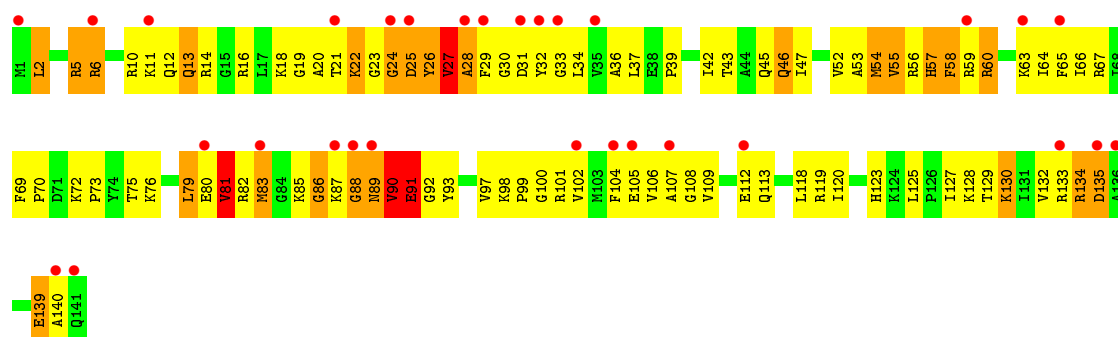


• Molecule 35: 50S ribosomal protein L14

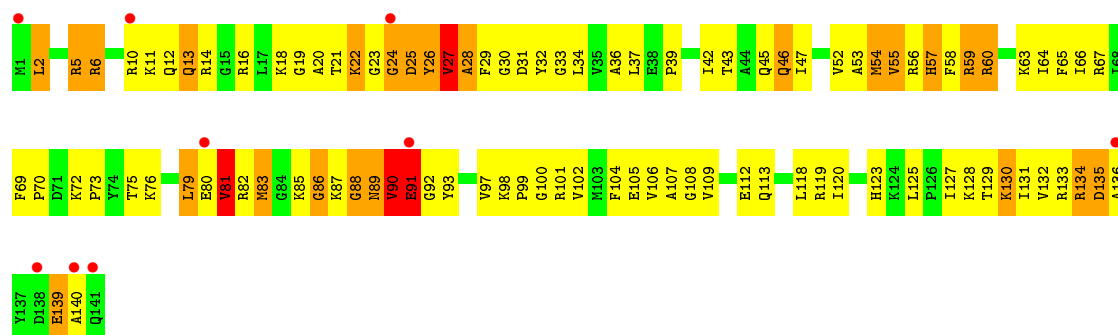




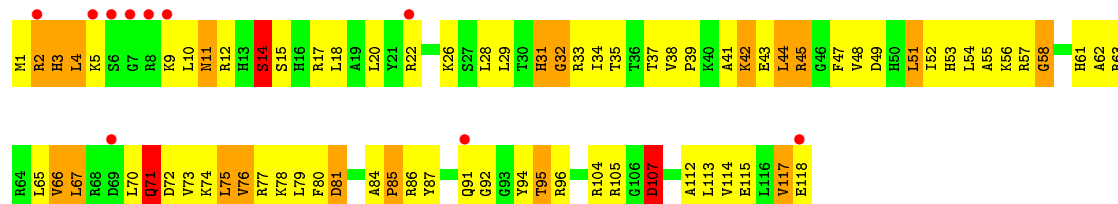
• Molecule 36: 50S ribosomal protein L15



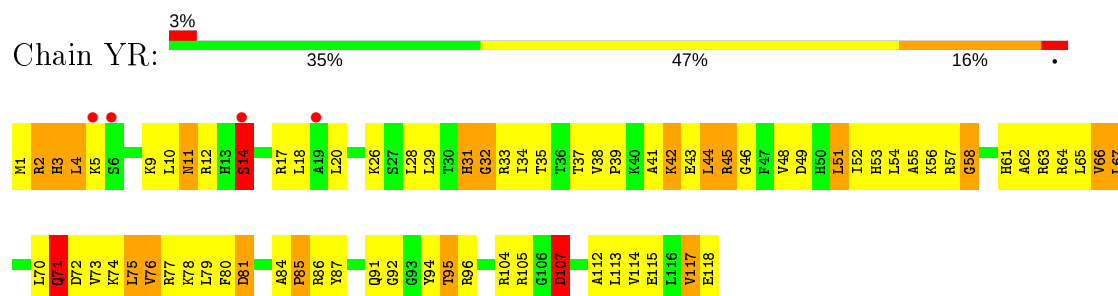
• Molecule 36: 50S ribosomal protein L15



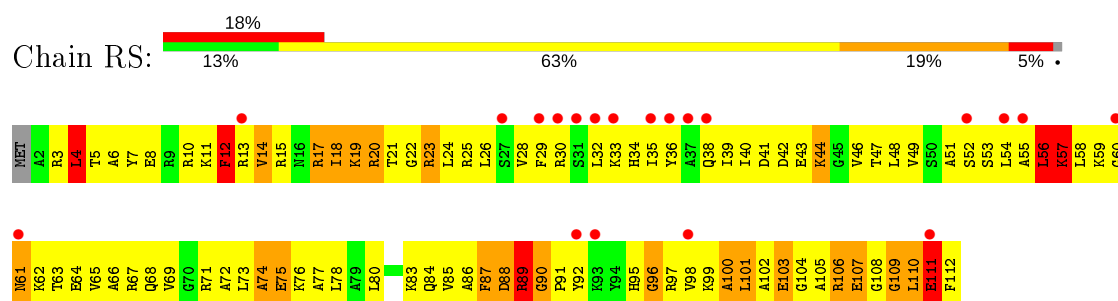
• Molecule 37: 50S ribosomal protein L16



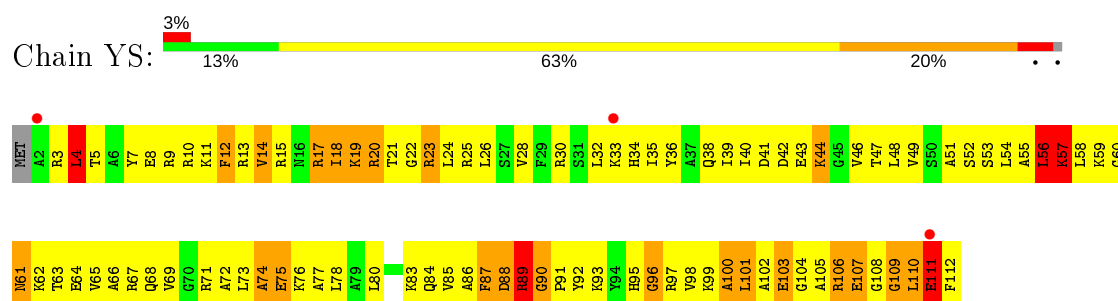
- Molecule 37: 50S ribosomal protein L16



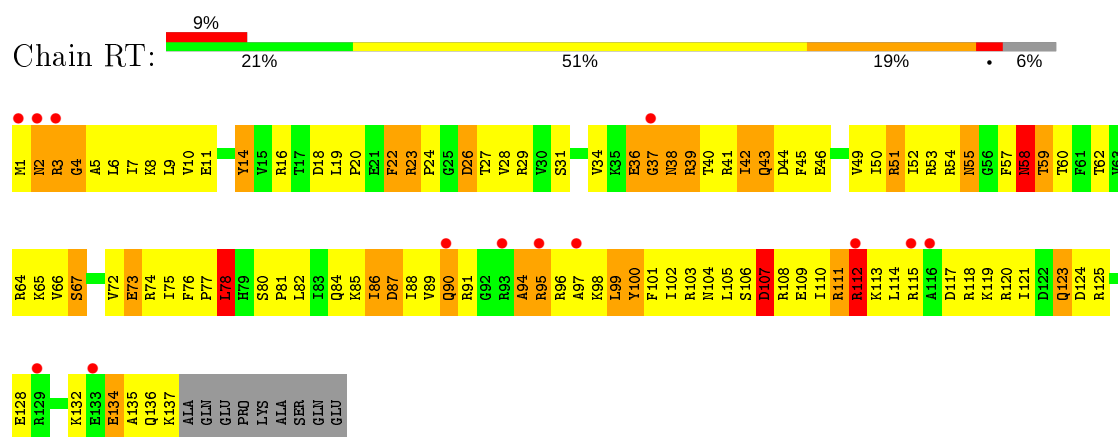
- Molecule 38: 50S ribosomal protein L17



- Molecule 38: 50S ribosomal protein L17

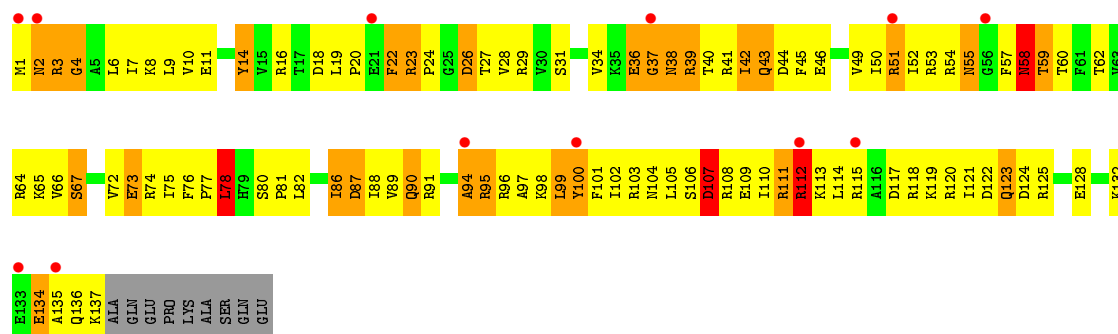


- Molecule 39: 50S ribosomal protein L18

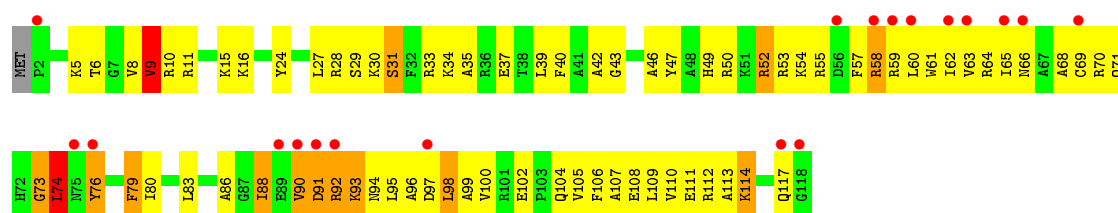


- Molecule 39: 50S ribosomal protein L18

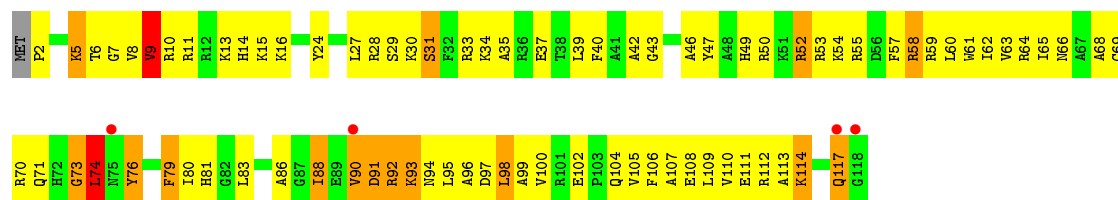




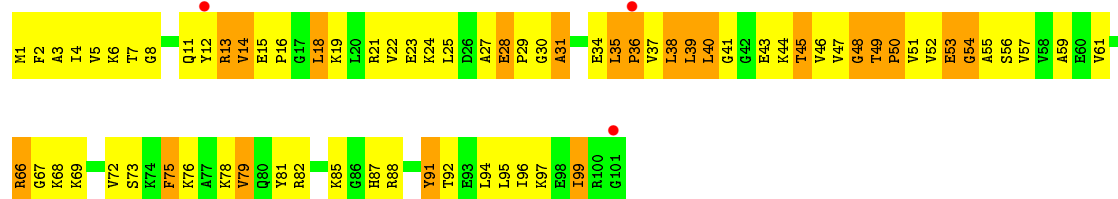
• Molecule 40: 50S ribosomal protein L19



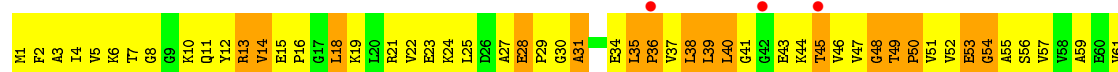
• Molecule 40: 50S ribosomal protein L19

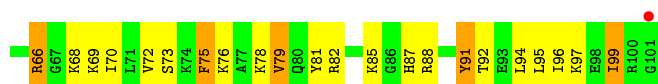


• Molecule 41: 50S ribosomal protein L20

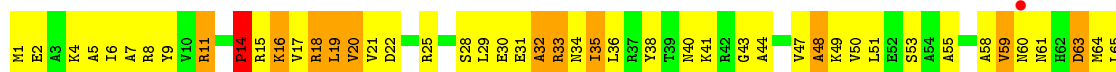


• Molecule 41: 50S ribosomal protein L20

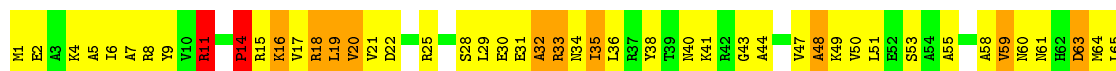




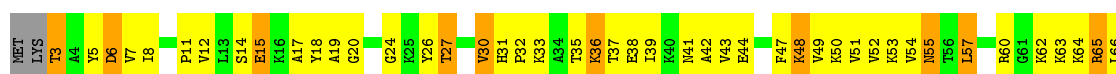
- Molecule 42: 50S ribosomal protein L21



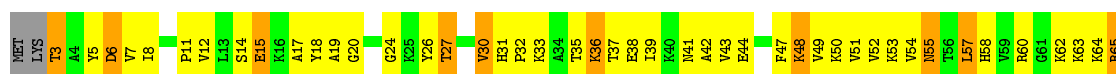
- Molecule 42: 50S ribosomal protein L21



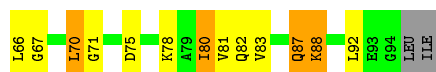
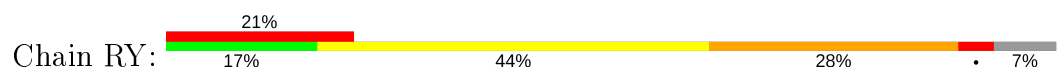
- Molecule 43: 50S ribosomal protein L22



- Molecule 43: 50S ribosomal protein L22



- Molecule 44: 50S ribosomal protein L23

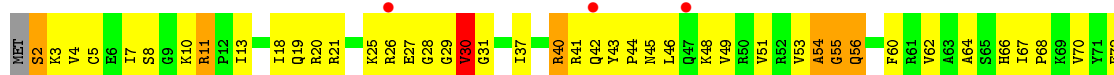




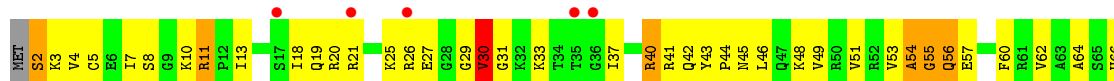
- Molecule 46: 50S ribosomal protein L25



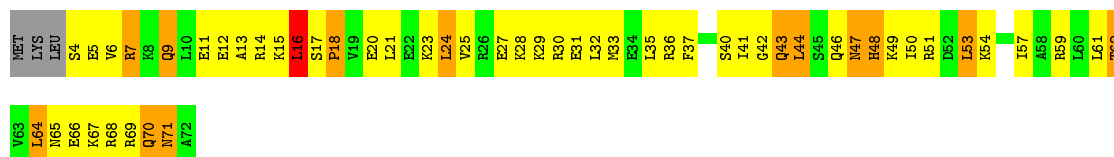
- Molecule 47: 50S ribosomal protein L27



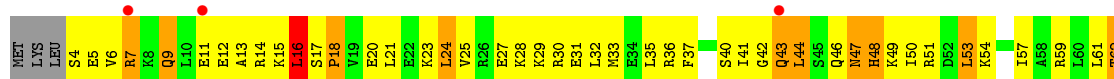
- Molecule 47: 50S ribosomal protein L27



- Molecule 48: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L28

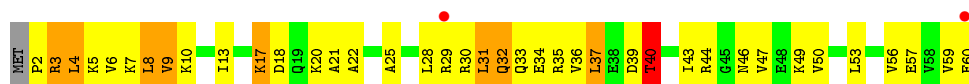




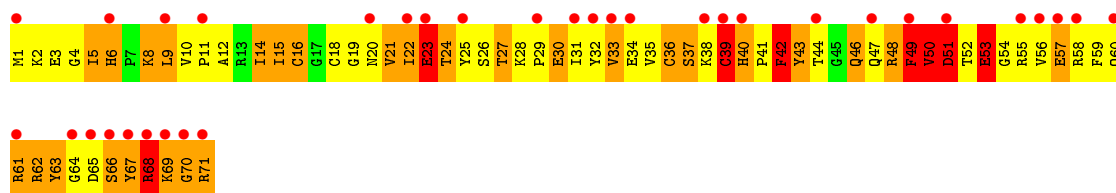
- Molecule 49: 50S ribosomal protein L29



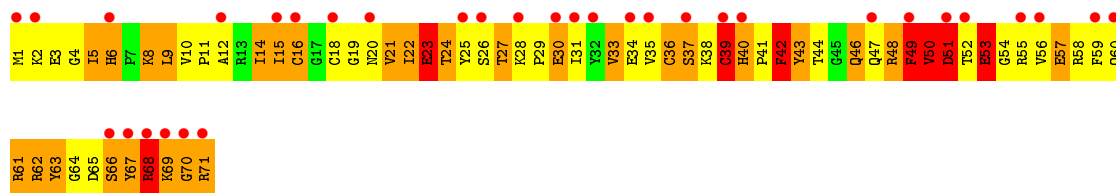
- Molecule 49: 50S ribosomal protein L29



- Molecule 50: 50S ribosomal protein L30



- Molecule 50: 50S ribosomal protein L30

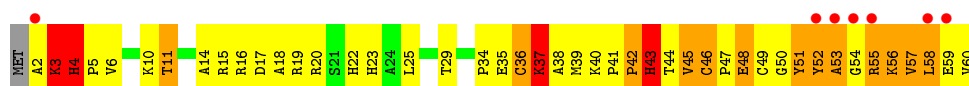


- Molecule 51: 50S ribosomal protein L32

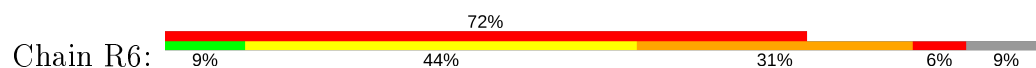


- Molecule 51: 50S ribosomal protein L32

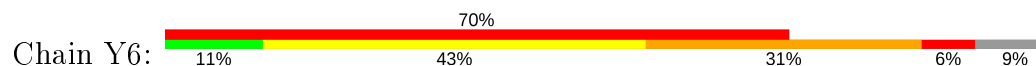




- Molecule 52: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L33



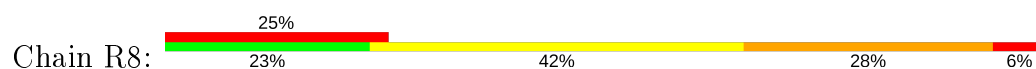
- Molecule 53: 50S ribosomal protein L34



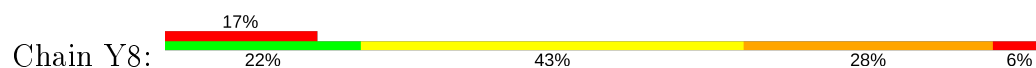
- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L35

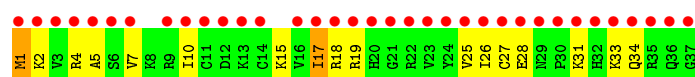


E65

- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: tRNA acceptor end mimic



C74
C75
A76

- Molecule 56: tRNA acceptor end mimic



C74
C75
A76

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.21Å 448.45Å 619.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	189.60 – 3.14 189.60 – 3.09	Depositor EDS
% Data completeness (in resolution range)	99.6 (189.60-3.14) 99.5 (189.60-3.09)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.230 , 0.262 0.231 , 0.263	Depositor DCC
R_{free} test set	49008 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 65.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	291998	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PAR, 1MG, 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	0.37	0/36098	0.89	48/56341 (0.1%)
1	XA	0.37	0/36101	0.89	50/56346 (0.1%)
2	QB	0.35	0/1959	0.65	0/2642
2	XB	0.35	0/1959	0.65	0/2642
3	QC	0.36	0/1629	0.60	0/2195
3	XC	0.36	0/1629	0.60	0/2195
4	QD	0.41	0/1733	0.68	1/2318 (0.0%)
4	XD	0.44	0/1733	0.68	1/2318 (0.0%)
5	QE	0.38	0/1171	0.66	0/1576
5	XE	0.38	0/1171	0.66	0/1576
6	QF	0.43	0/856	0.68	0/1154
6	XF	0.43	0/856	0.68	0/1154
7	QG	0.37	0/1276	0.61	0/1709
7	XG	0.37	0/1276	0.60	0/1709
8	QH	0.40	0/1136	0.69	0/1527
8	XH	0.40	0/1136	0.69	0/1527
9	QI	0.36	0/1029	0.67	0/1379
9	XI	0.36	0/1029	0.67	0/1379
10	QJ	0.35	0/814	0.61	0/1095
10	XJ	0.36	0/814	0.61	0/1095
11	QK	0.40	0/900	0.67	0/1213
11	XK	0.40	0/900	0.67	0/1213
12	QL	0.45	0/991	1.00	4/1327 (0.3%)
12	XL	0.46	0/991	1.00	4/1327 (0.3%)
13	QM	0.34	0/974	0.66	0/1303
13	XM	0.35	0/974	0.66	0/1303
14	QN	0.42	0/501	0.68	0/664
14	XN	0.52	0/501	0.67	0/664
15	QO	0.39	0/745	0.67	0/992
15	XO	0.39	0/745	0.67	0/992
16	QP	0.36	0/721	0.67	0/970
16	XP	0.37	0/721	0.67	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.37	0/847	0.68	0/1131
17	XQ	0.37	0/847	0.68	0/1131
18	QR	0.39	0/579	0.72	0/768
18	XR	0.39	0/579	0.72	0/768
19	QS	0.36	0/689	0.84	2/926 (0.2%)
19	XS	0.36	0/689	0.84	2/926 (0.2%)
20	QT	0.33	0/765	0.70	0/1007
20	XT	0.34	0/765	0.69	0/1007
21	QU	0.37	0/221	0.63	0/288
21	XU	0.37	0/221	0.63	0/288
22	QV	0.39	1/1836 (0.1%)	0.81	3/2859 (0.1%)
22	XV	0.42	1/1836 (0.1%)	0.84	4/2859 (0.1%)
23	QY	0.24	0/333	0.81	0/517
23	XY	0.24	0/333	0.74	0/517
24	QX	0.65	0/189	1.41	5/292 (1.7%)
24	XX	0.39	0/189	1.08	2/292 (0.7%)
25	RA	0.39	0/69521	0.88	70/108529 (0.1%)
25	YA	0.43	1/69543 (0.0%)	0.92	116/108563 (0.1%)
26	RB	0.32	0/2878	0.84	0/4490
26	YB	0.36	0/2878	0.88	1/4490 (0.0%)
27	RD	0.60	2/2165 (0.1%)	0.90	4/2919 (0.1%)
27	YD	0.56	0/2165	0.90	4/2919 (0.1%)
28	RE	0.52	0/1601	0.91	2/2160 (0.1%)
28	YE	0.52	0/1601	0.91	2/2160 (0.1%)
29	RF	0.50	0/1620	0.76	0/2194
29	YF	0.50	0/1620	0.76	0/2194
30	RG	0.40	0/1499	0.66	0/2016
30	YG	0.40	0/1499	0.66	0/2016
31	RH	0.45	0/1332	0.85	3/1802 (0.2%)
31	YH	0.45	0/1332	0.85	4/1802 (0.2%)
32	RI	0.28	0/1151	0.56	0/1558
32	YI	0.27	0/1151	0.58	0/1558
33	RN	0.46	0/1131	0.78	1/1525 (0.1%)
33	YN	0.46	0/1131	0.78	1/1525 (0.1%)
34	RO	0.54	0/943	0.71	0/1269
34	YO	0.53	0/943	0.71	0/1269
35	RP	0.50	0/1162	0.95	3/1544 (0.2%)
35	YP	0.50	0/1162	0.95	3/1544 (0.2%)
36	RQ	0.54	0/1143	0.91	3/1527 (0.2%)
36	YQ	0.54	0/1143	0.89	3/1527 (0.2%)
37	RR	0.45	0/982	0.80	1/1312 (0.1%)
37	YR	0.45	0/982	0.80	1/1312 (0.1%)
38	RS	0.46	0/892	0.82	1/1187 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YS	0.45	0/892	0.83	1/1187 (0.1%)
39	RT	0.47	0/1155	0.73	2/1542 (0.1%)
39	YT	0.46	0/1155	0.73	2/1542 (0.1%)
40	RU	0.48	0/982	0.78	0/1306
40	YU	0.48	0/982	0.77	0/1306
41	RV	0.47	0/790	0.82	0/1057
41	YV	0.47	0/790	0.82	0/1057
42	RW	0.45	0/911	0.75	0/1220
42	YW	0.45	0/911	0.75	0/1220
43	RX	0.56	0/739	0.77	0/993
43	YX	0.56	0/739	0.77	0/993
44	RY	0.52	0/798	0.80	0/1064
44	YY	0.52	0/798	0.80	0/1064
45	RZ	0.27	0/1493	0.52	0/2026
45	YZ	0.28	0/1493	0.54	0/2026
46	R0	0.30	0/657	0.54	0/874
46	Y0	0.34	0/657	0.53	0/874
47	R1	0.49	0/770	0.85	1/1022 (0.1%)
47	Y1	0.49	0/770	0.85	1/1022 (0.1%)
48	R2	0.51	0/583	0.83	1/771 (0.1%)
48	Y2	0.50	0/583	0.83	1/771 (0.1%)
49	R3	0.47	0/474	0.72	0/635
49	Y3	0.43	0/474	0.71	0/635
50	R4	0.38	0/594	0.78	1/795 (0.1%)
50	Y4	0.38	0/594	0.78	1/795 (0.1%)
51	R5	0.51	0/473	0.74	0/639
51	Y5	0.51	0/473	0.74	0/639
52	R6	0.42	0/431	0.76	0/575
52	Y6	0.42	0/431	0.76	0/575
53	R7	0.56	0/438	0.76	0/575
53	Y7	0.56	0/438	0.76	0/575
54	R8	0.62	0/525	0.93	1/691 (0.1%)
54	Y8	0.62	0/525	0.93	1/691 (0.1%)
55	R9	0.35	0/310	0.59	0/407
55	Y9	0.37	0/310	0.61	0/407
56	Z6	0.79	0/40	1.81	1/60 (1.7%)
56	Z8	0.77	0/40	1.81	1/60 (1.7%)
All	All	0.41	5/316375 (0.0%)	0.86	364/472993 (0.1%)

All (5) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	1	C	OP3-P	-10.56	1.48	1.61
22	XV	1	C	OP3-P	-10.53	1.48	1.61
27	RD	236	GLY	C-N	8.57	1.53	1.34
25	YA	774	A	N9-C4	-5.56	1.34	1.37
27	RD	241	PRO	N-CD	5.19	1.55	1.47

The worst 5 of 364 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	XL	47	LYS	C-N-CD	-20.45	75.61	120.60
12	QL	47	LYS	C-N-CD	-20.44	75.62	120.60
25	YA	2506	U	N3-C2-O2	-10.56	114.81	122.20
28	YE	21	VAL	C-N-CD	-10.11	98.35	120.60
28	RE	21	VAL	C-N-CD	-10.09	98.41	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	576	0
1	XA	32249	0	16279	575	1
2	QB	1924	0	1975	287	0
2	XB	1924	0	1975	293	0
3	QC	1605	0	1668	212	0
3	XC	1605	0	1668	215	2
4	QD	1703	0	1765	261	0
4	XD	1703	0	1764	217	0
5	QE	1155	0	1213	140	0
5	XE	1155	0	1213	141	0
6	QF	843	0	857	97	0
6	XF	843	0	857	101	0
7	QG	1257	0	1296	148	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	143	0
8	QH	1116	0	1175	148	0
8	XH	1116	0	1177	154	0
9	QI	1010	0	1037	145	0
9	XI	1010	0	1037	153	0
10	QJ	801	0	849	152	0
10	XJ	801	0	849	141	0
11	QK	885	0	904	103	2
11	XK	885	0	904	109	0
12	QL	975	0	1062	107	0
12	XL	975	0	1062	110	0
13	QM	964	0	1034	163	0
13	XM	964	0	1034	150	0
14	QN	492	0	529	100	0
14	XN	492	0	529	94	0
15	QO	734	0	771	73	0
15	XO	734	0	771	72	0
16	QP	705	0	725	115	0
16	XP	705	0	725	113	0
17	QQ	834	0	904	85	0
17	XQ	834	0	904	78	0
18	QR	574	0	644	66	0
18	XR	574	0	644	69	0
19	QS	674	0	699	103	0
19	XS	674	0	699	136	0
20	QT	763	0	860	108	0
20	XT	763	0	861	103	0
21	QU	217	0	234	27	0
21	XU	217	0	234	28	0
22	QV	1644	0	836	22	0
22	XV	1644	0	836	15	0
23	QY	323	0	165	2	0
23	XY	323	0	165	6	0
24	QX	170	0	88	2	0
24	XX	170	0	88	1	0
25	RA	62071	0	31288	992	0
25	YA	62091	0	31296	935	0
26	RB	2573	0	1306	62	0
26	YB	2573	0	1306	26	0
27	RD	2115	0	2195	319	0
27	YD	2115	0	2195	332	0
28	RE	1568	0	1634	270	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	YE	1568	0	1634	265	0
29	RF	1585	0	1632	181	0
29	YF	1585	0	1632	180	0
30	RG	1474	0	1535	211	0
30	YG	1474	0	1535	193	0
31	RH	1307	0	1382	225	0
31	YH	1307	0	1382	221	0
32	RI	1136	0	1223	42	1
32	YI	1136	0	1223	40	0
33	RN	1104	0	1180	191	0
33	YN	1104	0	1180	183	0
34	RO	933	0	996	123	0
34	YO	933	0	996	123	0
35	RP	1145	0	1228	250	0
35	YP	1145	0	1228	245	0
36	RQ	1122	0	1179	159	0
36	YQ	1122	0	1179	158	0
37	RR	968	0	1033	113	0
37	YR	968	0	1033	113	0
38	RS	882	0	943	165	0
38	YS	882	0	943	159	0
39	RT	1141	0	1202	154	0
39	YT	1141	0	1202	153	0
40	RU	964	0	1022	131	0
40	YU	964	0	1022	137	0
41	RV	779	0	852	129	0
41	YV	779	0	852	136	3
42	RW	900	0	964	99	0
42	YW	900	0	964	100	0
43	RX	725	0	778	69	0
43	YX	725	0	778	74	0
44	RY	785	0	878	163	0
44	YY	785	0	878	151	0
45	RZ	1461	0	1493	46	0
45	YZ	1461	0	1493	57	0
46	R0	648	0	672	20	0
46	Y0	648	0	672	28	0
47	R1	763	0	848	146	0
47	Y1	763	0	848	142	0
48	R2	581	0	629	81	0
48	Y2	581	0	629	77	0
49	R3	469	0	518	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Y3	469	0	518	41	0
50	R4	581	0	574	153	0
50	Y4	581	0	574	164	0
51	R5	459	0	480	77	0
51	Y5	459	0	480	75	3
52	R6	424	0	450	92	0
52	Y6	424	0	450	89	0
53	R7	430	0	480	43	0
53	Y7	430	0	480	44	0
54	R8	517	0	582	106	0
54	Y8	517	0	582	103	0
55	R9	307	0	338	18	0
55	Y9	307	0	338	18	0
56	Z6	74	0	51	6	0
56	Z8	74	0	51	7	0
57	QA	69	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	1	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	RA	240	0	0	0	0
57	RB	2	0	0	0	0
57	RD	1	0	0	0	0
57	RE	2	0	0	0	0
57	RF	1	0	0	0	0
57	RP	1	0	0	0	0
57	RR	2	0	0	0	0
57	XA	74	0	0	0	0
57	XV	2	0	0	0	0
57	XX	1	0	0	0	0
57	Y0	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y7	1	0	0	0	0
57	YA	265	0	0	0	0
57	YB	3	0	0	0	0
57	YE	2	0	0	0	0
57	YP	1	0	0	0	0
57	YQ	1	0	0	0	0
58	QA	42	0	45	3	0
58	XA	42	0	45	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	QD	1	0	0	0	0
59	QN	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
All	All	291998	0	198367	14453	6

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 30.

The worst 5 of 14453 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)
14:XN:32:SER:CB	14:XN:41:ARG:HB3	1.23	1.55
14:XN:32:SER:HB3	14:XN:41:ARG:CB	1.28	1.54
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.35	1.53
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.35	1.52
4:XD:22:LYS:CG	4:XD:26:CYS:SG	2.01	1.49

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:QK:99:GLN:NE2	3:XC:79:ARG:NH2[4_555]	1.49	0.71
41:YV:51:VAL:N	51:Y5:60:VAL:O[4_445]	1.70	0.50
11:QK:99:GLN:OE1	3:XC:79:ARG:NE[4_555]	2.04	0.16
41:YV:50:PRO:CG	51:Y5:60:VAL:O[4_445]	2.14	0.06
32:RI:91:SER:OG	1:XA:368:U:OP1[4_555]	2.15	0.05

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	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	1
2	XB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	1
3	QC	203/239 (85%)	129 (64%)	55 (27%)	19 (9%)	0	3
3	XC	203/239 (85%)	129 (64%)	55 (27%)	19 (9%)	0	3
4	QD	206/209 (99%)	136 (66%)	50 (24%)	20 (10%)	0	3
4	XD	206/209 (99%)	135 (66%)	49 (24%)	22 (11%)	0	2
5	QE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	0	3
5	XE	149/162 (92%)	103 (69%)	30 (20%)	16 (11%)	0	2
6	QF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	3
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	3
7	QG	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	0	3
7	XG	153/156 (98%)	103 (67%)	36 (24%)	14 (9%)	1	3
8	QH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	2
8	XH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	2
9	QI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	1
9	XI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	1
10	QJ	97/105 (92%)	68 (70%)	20 (21%)	9 (9%)	0	3
10	XJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	0	2
11	QK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	5
11	XK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	5
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	1
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	1
13	QM	119/126 (94%)	71 (60%)	27 (23%)	21 (18%)	0	0
13	XM	119/126 (94%)	71 (60%)	26 (22%)	22 (18%)	0	0
14	QN	58/61 (95%)	31 (53%)	15 (26%)	12 (21%)	0	0
14	XN	58/61 (95%)	32 (55%)	14 (24%)	12 (21%)	0	0
15	QO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	6
15	XO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	6
16	QP	82/88 (93%)	48 (58%)	24 (29%)	10 (12%)	0	1
16	XP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	1
17	QQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	4
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	QR	68/88 (77%)	45 (66%)	15 (22%)	8 (12%)	0	1
18	XR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	1
19	QS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	0
19	XS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	0
20	QT	97/106 (92%)	63 (65%)	16 (16%)	18 (19%)	0	0
20	XT	97/106 (92%)	63 (65%)	15 (16%)	19 (20%)	0	0
21	QU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	0
21	XU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	0
27	RD	270/276 (98%)	203 (75%)	48 (18%)	19 (7%)	1	6
27	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	1	6
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	0
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	0
29	RF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0	3
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0	3
30	RG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	1
30	YG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	1
31	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	0
31	YH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	0
32	RI	144/148 (97%)	102 (71%)	27 (19%)	15 (10%)	0	2
32	YI	144/148 (97%)	103 (72%)	25 (17%)	16 (11%)	0	2
33	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	0
33	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	0
34	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	5
34	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	5
35	RP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	0
35	YP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	0
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	0	3
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	0	3
37	RR	116/118 (98%)	83 (72%)	19 (16%)	14 (12%)	0	1
37	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	1
38	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	YS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	0
39	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	0
39	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	0
40	RU	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	5
40	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	5
41	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	3
41	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	3
42	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	1
42	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	1
43	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	10
43	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	10
44	RY	100/110 (91%)	58 (58%)	16 (16%)	26 (26%)	0	0
44	YY	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0	0
45	RZ	181/206 (88%)	126 (70%)	35 (19%)	20 (11%)	0	2
45	YZ	181/206 (88%)	135 (75%)	28 (16%)	18 (10%)	0	3
46	R0	80/85 (94%)	71 (89%)	7 (9%)	2 (2%)	5	25
46	Y0	80/85 (94%)	72 (90%)	6 (8%)	2 (2%)	5	25
47	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	1
47	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	1
48	R2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	1
48	Y2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	1
49	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	11
49	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	11
50	R4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
50	Y4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
51	R5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	0
51	Y5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	0
52	R6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
52	Y6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
53	R7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	7
53	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	R8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	0
54	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	0
55	R9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11470/12128 (95%)	7666 (67%)	2321 (20%)	1483 (13%)	0	1

5 of 1483 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	6	THR
2	QB	15	VAL
2	QB	26	PRO
2	QB	84	GLU
2	QB	88	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	181 (88%)	24 (12%)	5	21
2	XB	205/220 (93%)	181 (88%)	24 (12%)	5	21
3	QC	159/188 (85%)	143 (90%)	16 (10%)	7	26
3	XC	159/188 (85%)	143 (90%)	16 (10%)	7	26
4	QD	180/181 (99%)	160 (89%)	20 (11%)	6	23
4	XD	180/181 (99%)	165 (92%)	15 (8%)	11	36
5	QE	116/123 (94%)	108 (93%)	8 (7%)	15	43
5	XE	116/123 (94%)	107 (92%)	9 (8%)	12	38
6	QF	90/90 (100%)	76 (84%)	14 (16%)	2	11
6	XF	90/90 (100%)	76 (84%)	14 (16%)	2	11
7	QG	126/127 (99%)	114 (90%)	12 (10%)	8	29
7	XG	126/127 (99%)	115 (91%)	11 (9%)	10	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	QH	119/119 (100%)	106 (89%)	13 (11%)	6	23
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	23
9	QI	98/99 (99%)	87 (89%)	11 (11%)	6	22
9	XI	98/99 (99%)	87 (89%)	11 (11%)	6	22
10	QJ	89/92 (97%)	81 (91%)	8 (9%)	9	32
10	XJ	89/92 (97%)	81 (91%)	8 (9%)	9	32
11	QK	90/99 (91%)	81 (90%)	9 (10%)	7	27
11	XK	90/99 (91%)	81 (90%)	9 (10%)	7	27
12	QL	104/109 (95%)	90 (86%)	14 (14%)	4	15
12	XL	104/109 (95%)	90 (86%)	14 (14%)	4	15
13	QM	97/101 (96%)	81 (84%)	16 (16%)	2	9
13	XM	97/101 (96%)	81 (84%)	16 (16%)	2	9
14	QN	49/50 (98%)	40 (82%)	9 (18%)	1	7
14	XN	49/50 (98%)	44 (90%)	5 (10%)	7	25
15	QO	79/80 (99%)	73 (92%)	6 (8%)	13	39
15	XO	79/80 (99%)	73 (92%)	6 (8%)	13	39
16	QP	72/74 (97%)	63 (88%)	9 (12%)	4	18
16	XP	72/74 (97%)	63 (88%)	9 (12%)	4	18
17	QQ	95/97 (98%)	89 (94%)	6 (6%)	18	46
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	18	46
18	QR	61/77 (79%)	54 (88%)	7 (12%)	5	21
18	XR	61/77 (79%)	54 (88%)	7 (12%)	5	21
19	QS	73/80 (91%)	62 (85%)	11 (15%)	3	12
19	XS	73/80 (91%)	62 (85%)	11 (15%)	3	12
20	QT	76/82 (93%)	68 (90%)	8 (10%)	7	24
20	XT	76/82 (93%)	68 (90%)	8 (10%)	7	24
21	QU	20/22 (91%)	19 (95%)	1 (5%)	24	55
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	55
27	RD	214/218 (98%)	177 (83%)	37 (17%)	2	8
27	YD	214/218 (98%)	177 (83%)	37 (17%)	2	8
28	RE	165/166 (99%)	128 (78%)	37 (22%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	3
29	RF	161/166 (97%)	140 (87%)	21 (13%)	4	17
29	YF	161/166 (97%)	140 (87%)	21 (13%)	4	17
30	RG	155/156 (99%)	130 (84%)	25 (16%)	2	10
30	YG	155/156 (99%)	130 (84%)	25 (16%)	2	10
31	RH	142/148 (96%)	114 (80%)	28 (20%)	1	6
31	YH	142/148 (96%)	114 (80%)	28 (20%)	1	6
32	RI	122/124 (98%)	100 (82%)	22 (18%)	1	7
32	YI	122/124 (98%)	98 (80%)	24 (20%)	1	6
33	RN	117/119 (98%)	98 (84%)	19 (16%)	2	10
33	YN	117/119 (98%)	98 (84%)	19 (16%)	2	10
34	RO	100/100 (100%)	90 (90%)	10 (10%)	7	27
34	YO	100/100 (100%)	90 (90%)	10 (10%)	7	27
35	RP	116/116 (100%)	89 (77%)	27 (23%)	1	3
35	YP	116/116 (100%)	89 (77%)	27 (23%)	1	3
36	RQ	111/111 (100%)	93 (84%)	18 (16%)	2	10
36	YQ	111/111 (100%)	93 (84%)	18 (16%)	2	10
37	RR	101/101 (100%)	84 (83%)	17 (17%)	2	9
37	YR	101/101 (100%)	84 (83%)	17 (17%)	2	9
38	RS	87/88 (99%)	74 (85%)	13 (15%)	3	12
38	YS	87/88 (99%)	74 (85%)	13 (15%)	3	12
39	RT	120/127 (94%)	97 (81%)	23 (19%)	1	6
39	YT	120/127 (94%)	97 (81%)	23 (19%)	1	6
40	RU	93/94 (99%)	80 (86%)	13 (14%)	3	14
40	YU	93/94 (99%)	80 (86%)	13 (14%)	3	14
41	RV	82/82 (100%)	71 (87%)	11 (13%)	4	16
41	YV	82/82 (100%)	71 (87%)	11 (13%)	4	16
42	RW	92/92 (100%)	77 (84%)	15 (16%)	2	10
42	YW	92/92 (100%)	77 (84%)	15 (16%)	2	10
43	RX	74/78 (95%)	63 (85%)	11 (15%)	3	12
43	YX	74/78 (95%)	63 (85%)	11 (15%)	3	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	RY	85/91 (93%)	70 (82%)	15 (18%)	2	8
44	YY	85/91 (93%)	70 (82%)	15 (18%)	2	8
45	RZ	162/179 (90%)	138 (85%)	24 (15%)	3	12
45	YZ	162/179 (90%)	142 (88%)	20 (12%)	4	18
46	R0	65/67 (97%)	58 (89%)	7 (11%)	6	24
46	Y0	65/67 (97%)	63 (97%)	2 (3%)	40	69
47	R1	82/83 (99%)	67 (82%)	15 (18%)	1	7
47	Y1	82/83 (99%)	67 (82%)	15 (18%)	1	7
48	R2	64/67 (96%)	57 (89%)	7 (11%)	6	23
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	6	23
49	R3	51/52 (98%)	40 (78%)	11 (22%)	1	4
49	Y3	51/52 (98%)	40 (78%)	11 (22%)	1	4
50	R4	63/63 (100%)	44 (70%)	19 (30%)	0	1
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	1
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	3
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	3
52	R6	48/52 (92%)	38 (79%)	10 (21%)	1	5
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	5
53	R7	42/42 (100%)	39 (93%)	3 (7%)	14	42
53	Y7	42/42 (100%)	39 (93%)	3 (7%)	14	42
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	1
54	Y8	54/55 (98%)	39 (72%)	15 (28%)	0	1
55	R9	34/34 (100%)	32 (94%)	2 (6%)	19	48
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	19	48
All	All	9702/10066 (96%)	8299 (86%)	1403 (14%)	3	13

5 of 1403 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	R2	53	LEU
6	XF	97	PHE
45	YZ	76	LEU
50	R4	39	CYS
2	XB	23	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
47	R1	56	GLN
5	XE	78	HIS
43	YX	87	GLN
48	R2	47	ASN
2	XB	95	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	293 (19%)	45 (3%)
1	XA	1498/1522 (98%)	299 (19%)	47 (3%)
22	QV	76/77 (98%)	21 (27%)	1 (1%)
22	XV	76/77 (98%)	21 (27%)	1 (1%)
23	QY	14/17 (82%)	4 (28%)	1 (7%)
23	XY	14/17 (82%)	4 (28%)	1 (7%)
24	QX	7/25 (28%)	4 (57%)	0
24	XX	7/25 (28%)	3 (42%)	2 (28%)
25	RA	2879/2916 (98%)	618 (21%)	67 (2%)
25	YA	2880/2916 (98%)	612 (21%)	64 (2%)
26	RB	119/122 (97%)	24 (20%)	2 (1%)
26	YB	119/122 (97%)	29 (24%)	1 (0%)
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9190/9364 (98%)	1932 (21%)	232 (2%)

5 of 1932 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	7	G
1	QA	32	A
1	QA	39	G
1	QA	47	C

5 of 232 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2566	A
1	XA	345	C
25	YA	1955	U

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Mol	Chain	Res	Type
25	RA	2723	C
1	XA	60	A

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

4 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	Z8	76	25,56	32,40,41	2.54	6 (18%)	33,57,60	2.15	5 (15%)
56	PPU	Z6	76	25,56	32,40,41	2.55	6 (18%)	33,57,60	2.16	5 (15%)
23	1MG	QY	37	23	18,26,27	2.82	3 (16%)	19,39,42	1.65	2 (10%)
23	1MG	XY	37	23	18,26,27	2.77	3 (16%)	19,39,42	1.56	3 (15%)

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	Z8	76	25,56	-	2/21/43/44	0/4/4/4
56	PPU	Z6	76	25,56	-	2/21/43/44	0/4/4/4
23	1MG	QY	37	23	-	0/3/25/26	0/3/3/3
23	1MG	XY	37	23	-	0/3/25/26	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z6	76	PPU	O-C	9.29	1.41	1.23
56	Z8	76	PPU	O-C	9.21	1.41	1.23
23	QY	37	1MG	C4-N3	8.81	1.49	1.35
23	XY	37	1MG	C4-N3	8.71	1.49	1.35
23	QY	37	1MG	C2-N2	6.89	1.47	1.33

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z6	76	PPU	C3'-N3'-C	-8.64	110.18	123.21
56	Z8	76	PPU	C3'-N3'-C	-8.63	110.19	123.21
56	Z8	76	PPU	N3-C2-N1	-4.66	121.40	128.68
56	Z6	76	PPU	N3-C2-N1	-4.63	121.45	128.68
23	QY	37	1MG	N2-C2-N1	4.61	124.27	118.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	Z8	76	PPU	O-C-CA-N
56	Z6	76	PPU	O-C-CA-N
56	Z8	76	PPU	N3'-C-CA-N
56	Z6	76	PPU	N3'-C-CA-N

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z8	76	PPU	7	0
56	Z6	76	PPU	5	0
23	XY	37	1MG	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 682 ligands modelled in this entry, 680 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	PAR	QA	1670	-	45,45,45	1.47	7 (15%)	64,67,67	1.39	8 (12%)
58	PAR	XA	1675	-	45,45,45	1.50	7 (15%)	64,67,67	1.34	5 (7%)

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
58	PAR	QA	1670	-	-	8/18/94/94	0/4/4/4
58	PAR	XA	1675	-	-	6/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	QA	1670	PAR	C64-C54	5.09	1.59	1.52
58	XA	1675	PAR	C64-C54	4.86	1.58	1.52
58	QA	1670	PAR	C52-C42	3.12	1.58	1.52
58	XA	1675	PAR	C52-C42	3.02	1.58	1.52
58	QA	1670	PAR	O54-C14	2.93	1.49	1.41

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	XA	1675	PAR	O33-C14-C24	4.67	116.26	108.22
58	XA	1675	PAR	C14-O54-C54	4.31	122.16	113.69
58	QA	1670	PAR	O52-C13-C23	3.84	115.92	107.96
58	QA	1670	PAR	C14-O54-C54	3.81	121.16	113.69
58	QA	1670	PAR	O33-C14-C24	3.76	114.69	108.22

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

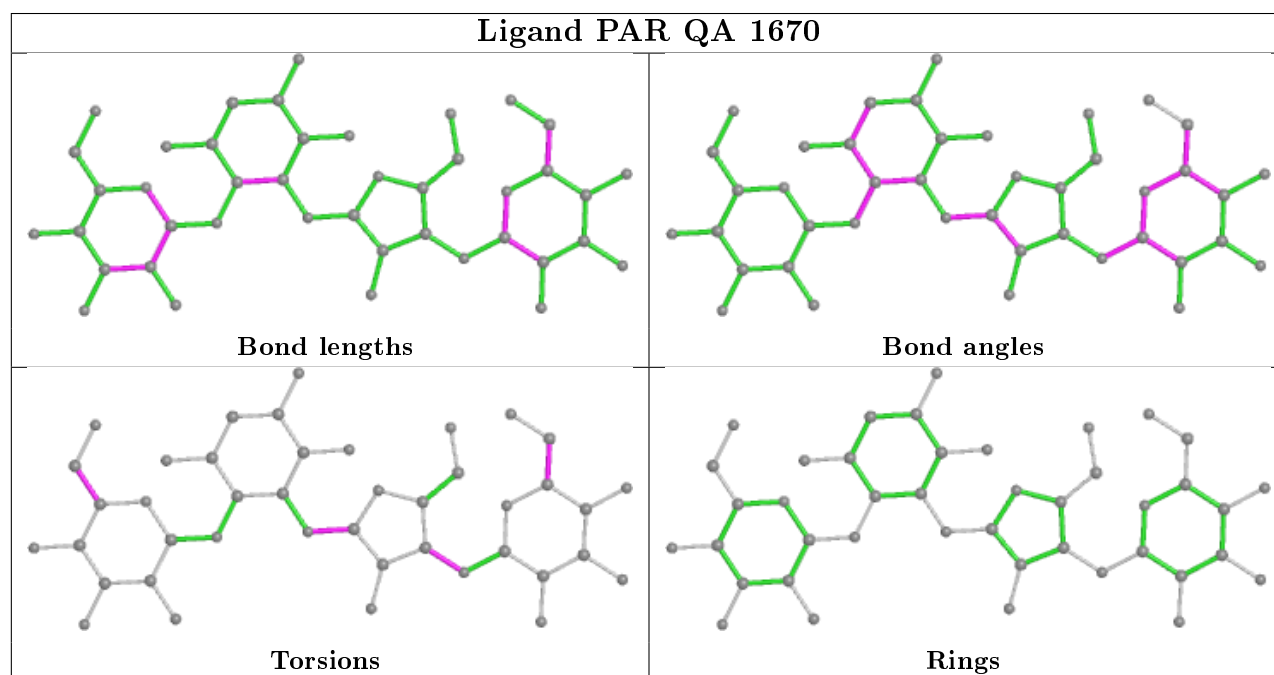
Mol	Chain	Res	Type	Atoms
58	QA	1670	PAR	C44-C54-C64-N64
58	QA	1670	PAR	O54-C54-C64-N64
58	XA	1675	PAR	O51-C51-C61-O61
58	QA	1670	PAR	O51-C51-C61-O61
58	XA	1675	PAR	C41-C51-C61-O61

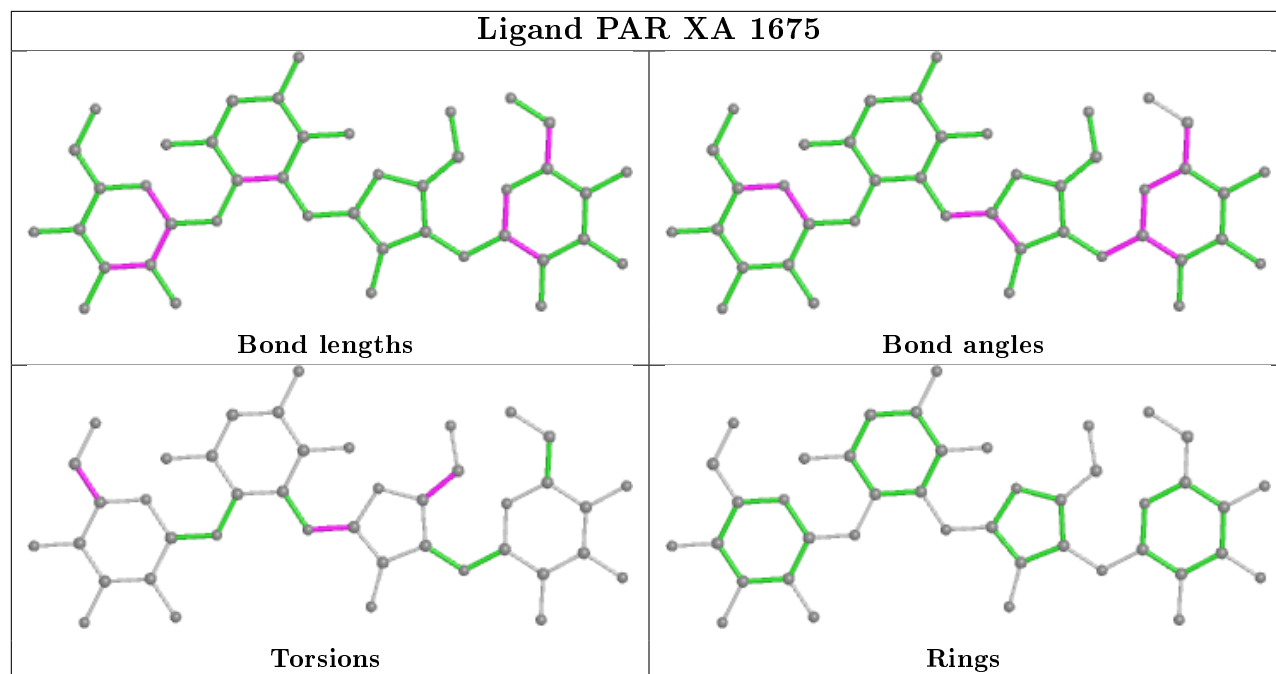
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	QA	1670	PAR	3	0
58	XA	1675	PAR	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1500/1522 (98%)	1.17	266 (17%) 1 0	27, 67, 148, 352	0
1	XA	1500/1522 (98%)	1.28	291 (19%) 1 0	18, 55, 149, 326	0
2	QB	237/256 (92%)	1.03	44 (18%) 1 0	54, 126, 215, 288	0
2	XB	237/256 (92%)	0.69	22 (9%) 8 3	43, 102, 177, 293	0
3	QC	205/239 (85%)	0.68	26 (12%) 3 1	56, 108, 175, 255	0
3	XC	205/239 (85%)	0.46	9 (4%) 34 17	30, 78, 132, 181	0
4	QD	208/209 (99%)	1.23	52 (25%) 0 0	41, 79, 136, 185	0
4	XD	208/209 (99%)	0.89	28 (13%) 3 1	30, 74, 134, 231	0
5	QE	151/162 (93%)	0.82	20 (13%) 3 1	42, 85, 148, 260	0
5	XE	151/162 (93%)	0.63	12 (7%) 12 5	23, 61, 121, 196	0
6	QF	101/101 (100%)	0.34	0 100 100	30, 74, 112, 155	0
6	XF	101/101 (100%)	0.46	5 (4%) 28 13	26, 69, 110, 146	0
7	QG	155/156 (99%)	0.87	23 (14%) 2 1	46, 97, 158, 302	0
7	XG	155/156 (99%)	0.72	16 (10%) 6 2	35, 82, 149, 230	0
8	QH	138/138 (100%)	0.74	10 (7%) 15 6	39, 83, 130, 174	0
8	XH	138/138 (100%)	0.73	13 (9%) 8 3	34, 68, 117, 169	0
9	QI	127/128 (99%)	2.28	60 (47%) 0 0	48, 117, 170, 243	0
9	XI	127/128 (99%)	1.25	33 (25%) 0 0	33, 91, 152, 203	0
10	QJ	99/105 (94%)	2.53	51 (51%) 0 0	53, 140, 243, 283	0
10	XJ	99/105 (94%)	1.87	43 (43%) 0 0	21, 100, 169, 213	0
11	QK	119/129 (92%)	0.93	14 (11%) 4 2	42, 77, 149, 228	0
11	XK	119/129 (92%)	1.23	24 (20%) 1 0	28, 70, 134, 196	0
12	QL	125/132 (94%)	1.19	28 (22%) 0 0	35, 69, 140, 262	0
12	XL	125/132 (94%)	0.84	13 (10%) 6 2	22, 51, 113, 282	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	2.08	45 (37%)	0	0	43, 108, 185, 410	0
13	XM	121/126 (96%)	1.36	30 (24%)	0	0	36, 86, 141, 273	0
14	QN	60/61 (98%)	2.07	27 (45%)	0	0	59, 101, 150, 166	0
14	XN	60/61 (98%)	1.14	15 (25%)	0	0	36, 67, 127, 143	0
15	QO	88/89 (98%)	0.74	9 (10%)	6	2	32, 78, 150, 180	0
15	XO	88/89 (98%)	0.78	10 (11%)	5	2	27, 62, 111, 129	0
16	QP	84/88 (95%)	1.07	14 (16%)	1	1	38, 71, 115, 186	0
16	XP	84/88 (95%)	1.38	24 (28%)	0	0	39, 73, 119, 211	0
17	QQ	100/105 (95%)	0.87	12 (12%)	4	2	44, 79, 131, 161	0
17	XQ	100/105 (95%)	1.35	23 (23%)	0	0	35, 75, 127, 166	0
18	QR	70/88 (79%)	0.54	2 (2%)	51	30	28, 73, 141, 149	0
18	XR	70/88 (79%)	0.38	3 (4%)	35	17	27, 66, 118, 171	0
19	QS	84/93 (90%)	2.59	52 (61%)	0	0	80, 119, 195, 275	0
19	XS	84/93 (90%)	1.45	24 (28%)	0	0	47, 88, 168, 219	0
20	QT	99/106 (93%)	1.53	33 (33%)	0	0	37, 82, 140, 220	0
20	XT	99/106 (93%)	1.80	44 (44%)	0	0	28, 86, 149, 177	0
21	QU	25/27 (92%)	5.65	24 (96%)	0	0	45, 98, 150, 185	0
21	XU	25/27 (92%)	3.12	14 (56%)	0	0	43, 69, 139, 153	0
22	QV	77/77 (100%)	0.95	13 (16%)	1	1	27, 73, 146, 212	0
22	XV	77/77 (100%)	0.72	8 (10%)	6	2	17, 59, 103, 207	0
23	QY	14/17 (82%)	1.43	3 (21%)	0	0	69, 116, 169, 189	0
23	XY	14/17 (82%)	1.51	3 (21%)	0	0	41, 102, 143, 157	0
24	QX	8/25 (32%)	1.22	2 (25%)	0	0	49, 58, 151, 164	0
24	XX	8/25 (32%)	2.15	2 (25%)	0	0	32, 38, 89, 104	0
25	RA	2882/2916 (98%)	1.12	339 (11%)	4	2	13, 44, 212, 472	0
25	YA	2883/2916 (98%)	0.99	232 (8%)	12	5	7, 35, 201, 461	0
26	RB	120/122 (98%)	0.98	18 (15%)	2	1	43, 69, 105, 120	0
26	YB	120/122 (98%)	0.38	0	100	100	29, 51, 71, 110	0
27	RD	272/276 (98%)	0.53	8 (2%)	51	30	9, 42, 81, 176	0
27	YD	272/276 (98%)	0.52	9 (3%)	46	25	5, 35, 71, 188	0
28	RE	205/206 (99%)	0.75	15 (7%)	15	6	11, 56, 123, 335	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YE	205/206 (99%)	0.62	8 (3%) 39 20	2, 52, 123, 250	0
29	RF	202/210 (96%)	0.50	10 (4%) 28 13	15, 62, 132, 185	0
29	YF	202/210 (96%)	0.50	8 (3%) 38 20	8, 45, 121, 194	0
30	RG	181/182 (99%)	3.16	111 (61%) 0 0	79, 156, 284, 386	0
30	YG	181/182 (99%)	1.52	58 (32%) 0 0	30, 89, 155, 309	0
31	RH	170/180 (94%)	2.71	106 (62%) 0 0	79, 145, 235, 306	0
31	YH	170/180 (94%)	0.81	12 (7%) 16 6	31, 79, 122, 167	0
32	RI	146/148 (98%)	0.42	8 (5%) 25 11	25, 87, 178, 297	0
32	YI	146/148 (98%)	0.51	10 (6%) 17 7	22, 83, 152, 183	0
33	RN	138/140 (98%)	0.40	3 (2%) 62 42	26, 64, 124, 179	0
33	YN	138/140 (98%)	0.40	2 (1%) 75 59	16, 54, 108, 166	0
34	RO	122/122 (100%)	0.45	3 (2%) 57 37	22, 55, 103, 142	0
34	YO	122/122 (100%)	0.55	2 (1%) 72 53	16, 48, 78, 126	0
35	RP	150/150 (100%)	1.18	36 (24%) 0 0	18, 68, 154, 247	0
35	YP	150/150 (100%)	0.81	17 (11%) 5 2	9, 53, 126, 253	0
36	RQ	141/141 (100%)	1.23	30 (21%) 0 0	28, 67, 128, 178	0
36	YQ	141/141 (100%)	0.52	9 (6%) 19 8	14, 47, 124, 154	0
37	RR	118/118 (100%)	0.62	10 (8%) 10 4	18, 48, 81, 170	0
37	YR	118/118 (100%)	0.55	4 (3%) 45 24	20, 46, 85, 137	0
38	RS	111/112 (99%)	1.05	20 (18%) 1 0	38, 76, 131, 184	0
38	YS	111/112 (99%)	0.62	3 (2%) 54 32	28, 58, 106, 195	0
39	RT	137/146 (93%)	0.84	13 (9%) 8 3	29, 67, 161, 259	0
39	YT	137/146 (93%)	0.75	12 (8%) 10 4	27, 61, 152, 303	0
40	RU	117/118 (99%)	0.97	19 (16%) 1 1	20, 54, 114, 221	0
40	YU	117/118 (99%)	0.63	4 (3%) 45 24	19, 39, 97, 221	0
41	RV	101/101 (100%)	0.59	3 (2%) 50 29	21, 77, 140, 320	0
41	YV	101/101 (100%)	0.54	4 (3%) 38 20	13, 63, 124, 304	0
42	RW	113/113 (100%)	0.34	3 (2%) 54 32	19, 41, 99, 220	0
42	YW	113/113 (100%)	0.14	1 (0%) 84 72	15, 41, 95, 193	0
43	RX	92/96 (95%)	0.47	0 100 100	26, 53, 87, 135	0
43	YX	92/96 (95%)	0.44	0 100 100	12, 39, 76, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RY	102/110 (92%)	1.36	23 (22%) 0 0	40, 99, 177, 285	0
44	YY	102/110 (92%)	0.85	12 (11%) 4 2	31, 73, 155, 210	0
45	RZ	183/206 (88%)	1.11	33 (18%) 1 0	41, 93, 178, 292	0
45	YZ	183/206 (88%)	0.63	14 (7%) 13 5	32, 71, 179, 271	0
46	R0	82/85 (96%)	0.63	6 (7%) 15 6	18, 49, 71, 179	0
46	Y0	82/85 (96%)	0.47	4 (4%) 29 14	11, 34, 60, 87	0
47	R1	97/98 (98%)	0.80	6 (6%) 20 9	21, 51, 160, 335	0
47	Y1	97/98 (98%)	0.83	9 (9%) 8 3	16, 49, 139, 210	0
48	R2	69/72 (95%)	0.35	0 100 100	28, 69, 143, 169	0
48	Y2	69/72 (95%)	0.61	3 (4%) 35 17	19, 59, 119, 177	0
49	R3	59/60 (98%)	0.64	3 (5%) 28 13	31, 71, 112, 169	0
49	Y3	59/60 (98%)	0.37	2 (3%) 45 24	22, 49, 91, 198	0
50	R4	71/71 (100%)	3.01	34 (47%) 0 0	107, 211, 311, 396	0
50	Y4	71/71 (100%)	2.42	33 (46%) 0 0	66, 156, 274, 384	0
51	R5	59/60 (98%)	0.90	6 (10%) 6 2	8, 49, 223, 238	0
51	Y5	59/60 (98%)	0.72	7 (11%) 4 2	11, 49, 223, 335	0
52	R6	49/54 (90%)	5.55	39 (79%) 0 0	86, 175, 268, 291	0
52	Y6	49/54 (90%)	4.62	38 (77%) 0 0	76, 163, 229, 312	0
53	R7	49/49 (100%)	0.49	4 (8%) 11 5	16, 29, 87, 168	0
53	Y7	49/49 (100%)	0.35	3 (6%) 21 9	8, 23, 87, 176	0
54	R8	64/65 (98%)	1.44	16 (25%) 0 0	20, 53, 102, 208	0
54	Y8	64/65 (98%)	1.16	11 (17%) 1 1	16, 44, 97, 214	0
55	R9	37/37 (100%)	8.29	37 (100%) 0 0	82, 138, 203, 344	0
55	Y9	37/37 (100%)	5.92	35 (94%) 0 0	57, 119, 223, 246	0
56	Z6	2/3 (66%)	1.44	0 100 100	33, 33, 33, 47	0
56	Z8	2/3 (66%)	1.72	0 100 100	24, 24, 24, 36	0
All	All	20873/21492 (97%)	1.06	3067 (14%) 2 1	2, 61, 174, 472	0

The worst 5 of 3067 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	YA	2117	A	23.8
25	YA	1061	U	20.2

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Mol	Chain	Res	Type	RSRZ
13	QM	7	VAL	20.1
25	YA	2112	G	20.1
25	YA	2136	C	19.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	PPU	Z8	76	37/38	0.88	0.42	37,37,37,37	0
56	PPU	Z6	76	37/38	0.89	0.43	41,41,41,41	0
23	1MG	QY	37	24/25	0.93	0.27	63,63,63,63	0
23	1MG	XY	37	24/25	0.95	0.25	45,45,45,45	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	YA	3105	1/1	0.12	0.26	21,21,21,21	0
57	MG	QA	1626	1/1	0.14	0.20	59,59,59,59	0
57	MG	RA	3120	1/1	0.22	0.34	60,60,60,60	0
57	MG	YA	3165	1/1	0.30	0.32	54,54,54,54	0
57	MG	YA	3139	1/1	0.36	0.26	70,70,70,70	0
57	MG	RA	3222	1/1	0.37	0.42	93,93,93,93	0
57	MG	QA	1629	1/1	0.38	0.33	43,43,43,43	0
57	MG	RA	3192	1/1	0.44	0.34	79,79,79,79	0
57	MG	YA	3120	1/1	0.45	0.62	63,63,63,63	0
57	MG	RA	3204	1/1	0.48	0.38	82,82,82,82	0
57	MG	RA	3226	1/1	0.48	0.27	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3221	1/1	0.52	0.40	62,62,62,62	0
57	MG	XA	1655	1/1	0.56	0.23	81,81,81,81	0
57	MG	YA	3241	1/1	0.59	0.25	46,46,46,46	0
57	MG	YA	3164	1/1	0.59	0.41	36,36,36,36	0
57	MG	QA	1657	1/1	0.60	0.30	58,58,58,58	0
57	MG	QA	1650	1/1	0.62	0.18	49,49,49,49	0
57	MG	YA	3207	1/1	0.64	0.69	80,80,80,80	0
57	MG	XA	1672	1/1	0.65	0.20	40,40,40,40	0
57	MG	YA	3127	1/1	0.67	0.30	26,26,26,26	0
57	MG	RA	3200	1/1	0.68	0.28	38,38,38,38	0
57	MG	RA	3091	1/1	0.68	0.47	73,73,73,73	0
57	MG	QA	1656	1/1	0.68	0.26	52,52,52,52	0
57	MG	YA	3158	1/1	0.73	0.19	24,24,24,24	0
57	MG	RA	3139	1/1	0.73	0.20	49,49,49,49	0
57	MG	XA	1656	1/1	0.73	0.12	31,31,31,31	0
57	MG	RA	3084	1/1	0.74	0.16	9,9,9,9	0
59	ZN	XN	101	1/1	0.74	0.23	65,65,65,65	0
57	MG	RA	3227	1/1	0.74	0.24	73,73,73,73	0
57	MG	RA	3050	1/1	0.74	0.26	31,31,31,31	0
57	MG	RB	202	1/1	0.75	0.09	54,54,54,54	0
57	MG	RA	3130	1/1	0.75	0.23	46,46,46,46	0
57	MG	RA	3115	1/1	0.75	0.20	7,7,7,7	0
57	MG	YA	3198	1/1	0.76	0.34	59,59,59,59	0
57	MG	YA	3172	1/1	0.76	0.18	43,43,43,43	0
57	MG	RA	3207	1/1	0.76	0.36	47,47,47,47	0
57	MG	YA	3153	1/1	0.76	0.15	21,21,21,21	0
57	MG	RA	3177	1/1	0.76	0.40	38,38,38,38	0
57	MG	XA	1609	1/1	0.76	0.21	22,22,22,22	0
57	MG	YA	3189	1/1	0.76	0.27	23,23,23,23	0
57	MG	RA	3155	1/1	0.76	0.30	24,24,24,24	0
57	MG	RA	3101	1/1	0.76	0.22	7,7,7,7	0
57	MG	RA	3199	1/1	0.77	0.14	29,29,29,29	0
57	MG	YA	3170	1/1	0.77	0.15	38,38,38,38	0
57	MG	QH	201	1/1	0.77	0.09	58,58,58,58	0
57	MG	QA	1637	1/1	0.77	0.23	57,57,57,57	0
57	MG	XA	1610	1/1	0.77	0.23	42,42,42,42	0
57	MG	QA	1609	1/1	0.78	0.16	34,34,34,34	0
57	MG	RA	3209	1/1	0.78	0.32	50,50,50,50	0
57	MG	RA	3195	1/1	0.78	0.37	31,31,31,31	0
57	MG	YA	3196	1/1	0.78	0.30	28,28,28,28	0
57	MG	RA	3220	1/1	0.78	0.27	56,56,56,56	0
57	MG	YA	3222	1/1	0.78	0.18	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3235	1/1	0.78	0.26	29,29,29,29	0
57	MG	RA	3002	1/1	0.78	0.54	36,36,36,36	0
57	MG	YA	3144	1/1	0.79	0.24	35,35,35,35	0
57	MG	YA	3160	1/1	0.79	0.16	12,12,12,12	0
57	MG	XA	1653	1/1	0.79	0.15	60,60,60,60	0
57	MG	RA	3232	1/1	0.79	0.18	30,30,30,30	0
57	MG	YA	3259	1/1	0.80	0.42	43,43,43,43	0
57	MG	XA	1631	1/1	0.80	0.19	35,35,35,35	0
57	MG	XA	1630	1/1	0.80	0.15	16,16,16,16	0
57	MG	YA	3204	1/1	0.80	0.17	19,19,19,19	0
57	MG	RA	3194	1/1	0.80	0.22	44,44,44,44	0
57	MG	XA	1647	1/1	0.81	0.15	49,49,49,49	0
57	MG	YA	3130	1/1	0.81	0.25	17,17,17,17	0
59	ZN	XD	301	1/1	0.81	0.36	45,45,45,45	0
57	MG	RA	3026	1/1	0.81	0.16	8,8,8,8	0
57	MG	RA	3212	1/1	0.81	0.19	42,42,42,42	0
57	MG	YA	3220	1/1	0.81	0.32	52,52,52,52	0
57	MG	RA	3176	1/1	0.81	0.14	24,24,24,24	0
57	MG	QA	1645	1/1	0.81	0.28	53,53,53,53	0
57	MG	YA	3208	1/1	0.82	0.15	55,55,55,55	0
57	MG	XA	1621	1/1	0.82	0.15	29,29,29,29	0
57	MG	RA	3217	1/1	0.82	0.10	28,28,28,28	0
57	MG	RA	3055	1/1	0.82	0.17	7,7,7,7	0
57	MG	RA	3134	1/1	0.82	0.27	44,44,44,44	0
57	MG	RA	3143	1/1	0.82	0.27	40,40,40,40	0
57	MG	YA	3237	1/1	0.82	0.21	44,44,44,44	0
57	MG	QA	1638	1/1	0.83	0.25	27,27,27,27	0
57	MG	YA	3192	1/1	0.83	0.25	30,30,30,30	0
57	MG	YA	3045	1/1	0.83	0.18	2,2,2,2	0
57	MG	QA	1644	1/1	0.83	0.33	40,40,40,40	0
57	MG	YA	3244	1/1	0.83	0.28	25,25,25,25	0
57	MG	R0	101	1/1	0.83	0.19	11,11,11,11	0
57	MG	RA	3043	1/1	0.83	0.16	4,4,4,4	0
57	MG	XA	1665	1/1	0.83	0.21	44,44,44,44	0
57	MG	RA	3210	1/1	0.83	0.18	30,30,30,30	0
57	MG	YA	3052	1/1	0.84	0.23	21,21,21,21	0
57	MG	YA	3146	1/1	0.84	0.32	57,57,57,57	0
57	MG	RA	3188	1/1	0.84	0.22	39,39,39,39	0
57	MG	RA	3211	1/1	0.84	0.40	43,43,43,43	0
57	MG	XA	1652	1/1	0.84	0.25	32,32,32,32	0
57	MG	YA	3071	1/1	0.84	0.25	10,10,10,10	0
57	MG	RA	3180	1/1	0.84	0.17	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3193	1/1	0.84	0.30	51,51,51,51	0
57	MG	QA	1664	1/1	0.84	0.15	40,40,40,40	0
57	MG	YA	3173	1/1	0.84	0.21	43,43,43,43	0
57	MG	RA	3201	1/1	0.84	0.20	24,24,24,24	0
57	MG	YA	3116	1/1	0.84	0.19	36,36,36,36	0
57	MG	YA	3016	1/1	0.84	0.13	8,8,8,8	0
57	MG	YA	3229	1/1	0.85	0.16	24,24,24,24	0
57	MG	XA	1649	1/1	0.85	0.20	30,30,30,30	0
57	MG	YA	3084	1/1	0.85	0.21	10,10,10,10	0
57	MG	RA	3131	1/1	0.85	0.39	41,41,41,41	0
57	MG	RA	3138	1/1	0.85	0.32	12,12,12,12	0
57	MG	QA	1631	1/1	0.85	0.52	46,46,46,46	0
57	MG	RA	3197	1/1	0.85	0.18	55,55,55,55	0
57	MG	YA	3221	1/1	0.85	0.23	19,19,19,19	0
57	MG	RA	3228	1/1	0.85	0.67	58,58,58,58	0
57	MG	RA	3137	1/1	0.85	0.20	10,10,10,10	0
57	MG	RA	3179	1/1	0.85	0.23	15,15,15,15	0
57	MG	RA	3124	1/1	0.85	0.18	23,23,23,23	0
57	MG	RA	3219	1/1	0.86	0.27	63,63,63,63	0
57	MG	RA	3215	1/1	0.86	0.14	48,48,48,48	0
57	MG	YA	3177	1/1	0.86	0.10	20,20,20,20	0
57	MG	YB	203	1/1	0.86	0.17	37,37,37,37	0
57	MG	QA	1632	1/1	0.86	0.22	35,35,35,35	0
57	MG	RA	3069	1/1	0.86	0.11	21,21,21,21	0
57	MG	QA	1665	1/1	0.86	0.14	18,18,18,18	0
57	MG	RA	3127	1/1	0.86	0.21	23,23,23,23	0
57	MG	YA	3155	1/1	0.86	0.17	53,53,53,53	0
57	MG	RA	3181	1/1	0.86	0.33	48,48,48,48	0
57	MG	YA	3210	1/1	0.86	0.21	37,37,37,37	0
57	MG	YA	3194	1/1	0.86	0.23	41,41,41,41	0
57	MG	RA	3119	1/1	0.86	0.24	56,56,56,56	0
57	MG	YA	3174	1/1	0.86	0.12	19,19,19,19	0
57	MG	RA	3142	1/1	0.86	0.24	39,39,39,39	0
57	MG	RA	3171	1/1	0.86	0.18	33,33,33,33	0
57	MG	RA	3145	1/1	0.86	0.15	27,27,27,27	0
57	MG	RA	3187	1/1	0.86	0.24	63,63,63,63	0
57	MG	XA	1633	1/1	0.86	0.16	37,37,37,37	0
57	MG	XA	1654	1/1	0.86	0.27	53,53,53,53	0
57	MG	XA	1671	1/1	0.86	0.16	71,71,71,71	0
57	MG	Y0	101	1/1	0.87	0.22	7,7,7,7	0
57	MG	YA	3183	1/1	0.87	0.18	30,30,30,30	0
57	MG	YA	3074	1/1	0.87	0.09	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3063	1/1	0.87	0.14	13,13,13,13	0
57	MG	RA	3183	1/1	0.87	0.17	19,19,19,19	0
57	MG	RA	3010	1/1	0.87	0.26	78,78,78,78	0
57	MG	XA	1635	1/1	0.87	0.16	41,41,41,41	0
57	MG	YE	301	1/1	0.87	0.18	7,7,7,7	0
57	MG	RA	3068	1/1	0.87	0.18	21,21,21,21	0
57	MG	RA	3135	1/1	0.87	0.17	16,16,16,16	0
57	MG	XA	1664	1/1	0.87	0.24	51,51,51,51	0
57	MG	QA	1620	1/1	0.87	0.17	28,28,28,28	0
57	MG	YE	302	1/1	0.87	0.20	10,10,10,10	0
57	MG	QA	1651	1/1	0.87	0.21	35,35,35,35	0
57	MG	RA	3216	1/1	0.87	0.24	43,43,43,43	0
57	MG	YA	3107	1/1	0.87	0.22	11,11,11,11	0
57	MG	YA	3171	1/1	0.87	0.37	32,32,32,32	0
57	MG	YA	3239	1/1	0.87	0.28	46,46,46,46	0
57	MG	Y7	101	1/1	0.87	0.40	38,38,38,38	0
57	MG	YA	3255	1/1	0.88	0.31	13,13,13,13	0
57	MG	YA	3182	1/1	0.88	0.21	24,24,24,24	0
57	MG	XA	1661	1/1	0.88	0.22	48,48,48,48	0
58	PAR	QA	1670	42/42	0.88	0.39	56,56,56,56	0
57	MG	YA	3152	1/1	0.88	0.23	51,51,51,51	0
57	MG	RA	3225	1/1	0.88	0.10	27,27,27,27	0
57	MG	YA	3060	1/1	0.88	0.17	4,4,4,4	0
57	MG	RA	3088	1/1	0.88	0.33	19,19,19,19	0
57	MG	YA	3200	1/1	0.88	0.19	26,26,26,26	0
57	MG	YA	3216	1/1	0.88	0.20	59,59,59,59	0
57	MG	YA	3166	1/1	0.88	0.30	58,58,58,58	0
57	MG	QA	1668	1/1	0.88	0.14	42,42,42,42	0
57	MG	YA	3191	1/1	0.88	0.25	24,24,24,24	0
57	MG	QA	1655	1/1	0.88	0.14	51,51,51,51	0
57	MG	XA	1673	1/1	0.88	0.32	26,26,26,26	0
57	MG	YA	3039	1/1	0.88	0.12	19,19,19,19	0
57	MG	RA	3173	1/1	0.88	0.16	15,15,15,15	0
57	MG	RA	3163	1/1	0.88	0.16	38,38,38,38	0
57	MG	XA	1663	1/1	0.88	0.09	44,44,44,44	0
57	MG	RA	3049	1/1	0.89	0.10	8,8,8,8	0
57	MG	RA	3081	1/1	0.89	0.07	30,30,30,30	0
57	MG	QA	1647	1/1	0.89	0.10	23,23,23,23	0
57	MG	RA	3190	1/1	0.89	0.17	38,38,38,38	0
57	MG	RD	301	1/1	0.89	0.23	41,41,41,41	0
57	MG	YA	3205	1/1	0.89	0.18	38,38,38,38	0
57	MG	RA	3198	1/1	0.89	0.12	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3201	1/1	0.89	0.13	14,14,14,14	0
57	MG	RA	3141	1/1	0.89	0.16	33,33,33,33	0
57	MG	QA	1640	1/1	0.89	0.14	51,51,51,51	0
57	MG	YA	3018	1/1	0.89	0.32	13,13,13,13	0
57	MG	RA	3235	1/1	0.89	0.25	22,22,22,22	0
57	MG	RA	3238	1/1	0.89	0.32	32,32,32,32	0
57	MG	XA	1660	1/1	0.89	0.12	30,30,30,30	0
57	MG	RA	3008	1/1	0.89	0.20	27,27,27,27	0
57	MG	YA	3150	1/1	0.89	0.23	61,61,61,61	0
57	MG	YA	3195	1/1	0.89	0.20	35,35,35,35	0
57	MG	YA	3179	1/1	0.89	0.23	35,35,35,35	0
57	MG	RA	3165	1/1	0.89	0.09	19,19,19,19	0
57	MG	YA	3206	1/1	0.89	0.14	15,15,15,15	0
57	MG	RA	3013	1/1	0.89	0.29	20,20,20,20	0
57	MG	YA	3129	1/1	0.89	0.19	27,27,27,27	0
57	MG	RA	3205	1/1	0.89	0.24	46,46,46,46	0
57	MG	YA	3128	1/1	0.89	0.27	26,26,26,26	0
57	MG	QA	1618	1/1	0.89	0.19	42,42,42,42	0
57	MG	YA	3072	1/1	0.89	0.23	17,17,17,17	0
57	MG	R5	101	1/1	0.89	0.19	19,19,19,19	0
57	MG	RA	3153	1/1	0.90	0.28	51,51,51,51	0
57	MG	YA	3156	1/1	0.90	0.26	33,33,33,33	0
57	MG	YA	3243	1/1	0.90	0.21	42,42,42,42	0
57	MG	YA	3215	1/1	0.90	0.31	25,25,25,25	0
57	MG	XA	1648	1/1	0.90	0.11	39,39,39,39	0
57	MG	QA	1633	1/1	0.90	0.26	44,44,44,44	0
57	MG	YA	3217	1/1	0.90	0.15	29,29,29,29	0
57	MG	XA	1645	1/1	0.90	0.13	29,29,29,29	0
57	MG	RA	3160	1/1	0.90	0.21	51,51,51,51	0
57	MG	YA	3227	1/1	0.90	0.19	13,13,13,13	0
57	MG	YA	3199	1/1	0.90	0.31	18,18,18,18	0
57	MG	RA	3161	1/1	0.90	0.15	27,27,27,27	0
57	MG	RA	3150	1/1	0.90	0.13	25,25,25,25	0
57	MG	YA	3137	1/1	0.90	0.15	6,6,6,6	0
57	MG	RA	3158	1/1	0.90	0.33	51,51,51,51	0
57	MG	RA	3208	1/1	0.90	0.15	19,19,19,19	0
57	MG	RA	3159	1/1	0.90	0.17	30,30,30,30	0
57	MG	QF	201	1/1	0.90	0.21	39,39,39,39	0
57	MG	RA	3213	1/1	0.90	0.29	29,29,29,29	0
57	MG	RA	3086	1/1	0.91	0.23	14,14,14,14	0
57	MG	RR	202	1/1	0.91	0.23	19,19,19,19	0
57	MG	QA	1616	1/1	0.91	0.07	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3251	1/1	0.91	0.29	20,20,20,20	0
57	MG	XA	1659	1/1	0.91	0.30	34,34,34,34	0
57	MG	XA	1643	1/1	0.91	0.15	29,29,29,29	0
57	MG	RA	3184	1/1	0.91	0.24	13,13,13,13	0
57	MG	XA	1638	1/1	0.91	0.11	16,16,16,16	0
57	MG	QA	1669	1/1	0.91	0.23	45,45,45,45	0
57	MG	YA	3262	1/1	0.91	0.17	38,38,38,38	0
57	MG	YA	3046	1/1	0.91	0.25	8,8,8,8	0
57	MG	YA	3008	1/1	0.91	0.22	9,9,9,9	0
58	PAR	XA	1675	42/42	0.91	0.32	49,49,49,49	0
57	MG	RA	3191	1/1	0.91	0.10	21,21,21,21	0
57	MG	RA	3062	1/1	0.91	0.10	56,56,56,56	0
57	MG	QA	1615	1/1	0.91	0.25	23,23,23,23	0
57	MG	QA	1646	1/1	0.91	0.09	39,39,39,39	0
57	MG	RA	3009	1/1	0.91	0.10	9,9,9,9	0
57	MG	QA	1660	1/1	0.91	0.21	35,35,35,35	0
57	MG	YA	3145	1/1	0.91	0.23	11,11,11,11	0
57	MG	QA	1662	1/1	0.91	0.11	53,53,53,53	0
57	MG	XA	1639	1/1	0.91	0.09	35,35,35,35	0
59	ZN	QN	101	1/1	0.91	0.12	80,80,80,80	0
57	MG	RA	3170	1/1	0.91	0.11	25,25,25,25	0
57	MG	YA	3143	1/1	0.91	0.18	17,17,17,17	0
57	MG	YA	3228	1/1	0.91	0.19	22,22,22,22	0
57	MG	RA	3175	1/1	0.91	0.20	21,21,21,21	0
57	MG	YA	3022	1/1	0.91	0.28	7,7,7,7	0
57	MG	XA	1666	1/1	0.91	0.34	43,43,43,43	0
57	MG	YA	3188	1/1	0.91	0.14	32,32,32,32	0
57	MG	XA	1636	1/1	0.91	0.13	5,5,5,5	0
57	MG	RA	3164	1/1	0.91	0.29	36,36,36,36	0
57	MG	YA	3209	1/1	0.91	0.17	27,27,27,27	0
57	MG	RA	3218	1/1	0.91	0.18	29,29,29,29	0
57	MG	RA	3151	1/1	0.91	0.11	18,18,18,18	0
57	MG	XA	1632	1/1	0.91	0.18	17,17,17,17	0
57	MG	RA	3044	1/1	0.91	0.21	24,24,24,24	0
57	MG	YA	3236	1/1	0.92	0.22	40,40,40,40	0
57	MG	YA	3218	1/1	0.92	0.10	10,10,10,10	0
57	MG	QA	1625	1/1	0.92	0.09	36,36,36,36	0
57	MG	YB	202	1/1	0.92	0.23	20,20,20,20	0
57	MG	YA	3247	1/1	0.92	0.13	30,30,30,30	0
57	MG	QA	1617	1/1	0.92	0.16	19,19,19,19	0
57	MG	XA	1674	1/1	0.92	0.12	25,25,25,25	0
57	MG	RA	3126	1/1	0.92	0.34	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3135	1/1	0.92	0.14	21,21,21,21	0
57	MG	RA	3196	1/1	0.92	0.20	15,15,15,15	0
57	MG	RA	3118	1/1	0.92	0.10	33,33,33,33	0
57	MG	YA	3082	1/1	0.92	0.14	8,8,8,8	0
57	MG	RA	3110	1/1	0.92	0.21	9,9,9,9	0
57	MG	QA	1658	1/1	0.92	0.20	63,63,63,63	0
57	MG	XA	1625	1/1	0.92	0.12	16,16,16,16	0
57	MG	RA	3178	1/1	0.92	0.16	22,22,22,22	0
57	MG	QA	1666	1/1	0.92	0.19	36,36,36,36	0
57	MG	YA	3234	1/1	0.92	0.14	21,21,21,21	0
57	MG	XA	1622	1/1	0.92	0.16	26,26,26,26	0
57	MG	XA	1657	1/1	0.92	0.19	31,31,31,31	0
57	MG	QA	1603	1/1	0.92	0.16	7,7,7,7	0
57	MG	YP	201	1/1	0.92	0.12	23,23,23,23	0
57	MG	RA	3058	1/1	0.92	0.25	37,37,37,37	0
57	MG	RA	3214	1/1	0.92	0.17	18,18,18,18	0
57	MG	YA	3126	1/1	0.92	0.15	22,22,22,22	0
57	MG	RA	3185	1/1	0.92	0.33	25,25,25,25	0
57	MG	XA	1613	1/1	0.93	0.27	13,13,13,13	0
57	MG	RA	3182	1/1	0.93	0.18	10,10,10,10	0
57	MG	RA	3059	1/1	0.93	0.16	2,2,2,2	0
57	MG	YA	3238	1/1	0.93	0.12	24,24,24,24	0
57	MG	XA	1668	1/1	0.93	0.33	19,19,19,19	0
57	MG	RA	3052	1/1	0.93	0.25	4,4,4,4	0
57	MG	YA	3233	1/1	0.93	0.12	34,34,34,34	0
57	MG	QA	1605	1/1	0.93	0.32	30,30,30,30	0
57	MG	RA	3168	1/1	0.93	0.26	22,22,22,22	0
57	MG	XA	1624	1/1	0.93	0.10	55,55,55,55	0
57	MG	QA	1614	1/1	0.93	0.12	26,26,26,26	0
57	MG	RA	3056	1/1	0.93	0.31	17,17,17,17	0
57	MG	XA	1616	1/1	0.93	0.11	17,17,17,17	0
57	MG	YA	3041	1/1	0.93	0.23	5,5,5,5	0
57	MG	YB	201	1/1	0.93	0.33	35,35,35,35	0
57	MG	YA	3024	1/1	0.93	0.19	16,16,16,16	0
57	MG	RA	3148	1/1	0.93	0.27	36,36,36,36	0
57	MG	QA	1623	1/1	0.93	0.16	37,37,37,37	0
57	MG	RA	3051	1/1	0.93	0.16	3,3,3,3	0
57	MG	YA	3181	1/1	0.93	0.21	34,34,34,34	0
57	MG	YA	3211	1/1	0.93	0.27	14,14,14,14	0
57	MG	YA	3240	1/1	0.93	0.44	43,43,43,43	0
57	MG	YA	3224	1/1	0.93	0.15	24,24,24,24	0
57	MG	RA	3234	1/1	0.93	0.17	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3142	1/1	0.93	0.22	28,28,28,28	0
57	MG	YA	3202	1/1	0.93	0.21	59,59,59,59	0
57	MG	YA	3029	1/1	0.93	0.23	12,12,12,12	0
57	MG	YA	3134	1/1	0.93	0.18	21,21,21,21	0
57	MG	XA	1611	1/1	0.93	0.21	23,23,23,23	0
57	MG	RA	3133	1/1	0.93	0.18	28,28,28,28	0
57	MG	YA	3133	1/1	0.93	0.12	18,18,18,18	0
57	MG	QA	1627	1/1	0.93	0.10	26,26,26,26	0
57	MG	YA	3214	1/1	0.93	0.16	35,35,35,35	0
57	MG	QA	1602	1/1	0.93	0.20	18,18,18,18	0
57	MG	YA	3159	1/1	0.93	0.21	18,18,18,18	0
57	MG	RA	3070	1/1	0.93	0.24	26,26,26,26	0
57	MG	RA	3167	1/1	0.93	0.14	29,29,29,29	0
57	MG	XA	1637	1/1	0.93	0.34	24,24,24,24	0
57	MG	RA	3223	1/1	0.93	0.17	23,23,23,23	0
57	MG	YA	3161	1/1	0.93	0.10	25,25,25,25	0
57	MG	QA	1661	1/1	0.93	0.09	38,38,38,38	0
57	MG	YA	3148	1/1	0.93	0.16	14,14,14,14	0
57	MG	YA	3088	1/1	0.93	0.18	1,1,1,1	0
57	MG	YA	3219	1/1	0.93	0.90	52,52,52,52	0
57	MG	YA	3101	1/1	0.93	0.30	8,8,8,8	0
57	MG	RA	3174	1/1	0.93	0.10	38,38,38,38	0
57	MG	QA	1639	1/1	0.93	0.11	36,36,36,36	0
57	MG	RA	3001	1/1	0.93	0.24	11,11,11,11	0
57	MG	RA	3162	1/1	0.93	0.14	18,18,18,18	0
57	MG	YA	3154	1/1	0.93	0.22	9,9,9,9	0
57	MG	YA	3242	1/1	0.93	0.17	72,72,72,72	0
57	MG	QA	1613	1/1	0.93	0.19	21,21,21,21	0
57	MG	RA	3149	1/1	0.93	0.16	32,32,32,32	0
57	MG	QA	1641	1/1	0.93	0.17	24,24,24,24	0
57	MG	YA	3104	1/1	0.94	0.25	24,24,24,24	0
57	MG	RA	3156	1/1	0.94	0.23	44,44,44,44	0
57	MG	YA	3185	1/1	0.94	0.14	10,10,10,10	0
57	MG	XA	1650	1/1	0.94	0.09	26,26,26,26	0
57	MG	XA	1607	1/1	0.94	0.28	31,31,31,31	0
57	MG	YA	3079	1/1	0.94	0.13	12,12,12,12	0
57	MG	QA	1663	1/1	0.94	0.10	82,82,82,82	0
57	MG	YA	3068	1/1	0.94	0.23	17,17,17,17	0
57	MG	RA	3072	1/1	0.94	0.24	13,13,13,13	0
57	MG	YA	3065	1/1	0.94	0.14	8,8,8,8	0
57	MG	QA	1667	1/1	0.94	0.13	32,32,32,32	0
57	MG	QA	1601	1/1	0.94	0.17	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3123	1/1	0.94	0.18	9,9,9,9	0
57	MG	QA	1653	1/1	0.94	0.15	36,36,36,36	0
57	MG	YA	3186	1/1	0.94	0.16	39,39,39,39	0
57	MG	RA	3066	1/1	0.94	0.20	24,24,24,24	0
57	MG	YA	3131	1/1	0.94	0.14	35,35,35,35	0
57	MG	YA	3223	1/1	0.94	0.15	25,25,25,25	0
57	MG	YA	3032	1/1	0.94	0.21	4,4,4,4	0
57	MG	RA	3064	1/1	0.94	0.24	5,5,5,5	0
57	MG	YA	3106	1/1	0.94	0.13	9,9,9,9	0
57	MG	YA	3263	1/1	0.94	0.17	33,33,33,33	0
57	MG	RA	3092	1/1	0.94	0.12	9,9,9,9	0
57	MG	RA	3023	1/1	0.94	0.21	14,14,14,14	0
57	MG	RA	3054	1/1	0.94	0.11	0,0,0,0	0
57	MG	QA	1659	1/1	0.94	0.11	39,39,39,39	0
57	MG	RA	3099	1/1	0.94	0.34	24,24,24,24	0
57	MG	YA	3178	1/1	0.94	0.19	35,35,35,35	0
57	MG	RA	3082	1/1	0.94	0.18	42,42,42,42	0
57	MG	XA	1658	1/1	0.94	0.24	46,46,46,46	0
57	MG	YA	3117	1/1	0.94	0.12	18,18,18,18	0
57	MG	YA	3033	1/1	0.94	0.28	4,4,4,4	0
57	MG	XV	101	1/1	0.94	0.19	9,9,9,9	0
57	MG	YA	3246	1/1	0.94	0.24	21,21,21,21	0
57	MG	YA	3151	1/1	0.94	0.17	25,25,25,25	0
57	MG	YA	3054	1/1	0.94	0.22	49,49,49,49	0
57	MG	QA	1643	1/1	0.94	0.12	22,22,22,22	0
57	MG	YA	3163	1/1	0.94	0.14	28,28,28,28	0
57	MG	YA	3103	1/1	0.94	0.22	31,31,31,31	0
57	MG	YA	3075	1/1	0.94	0.25	28,28,28,28	0
57	MG	RA	3011	1/1	0.94	0.49	32,32,32,32	0
57	MG	RA	3166	1/1	0.94	0.12	43,43,43,43	0
57	MG	RA	3103	1/1	0.94	0.12	8,8,8,8	0
57	MG	YA	3140	1/1	0.94	0.28	20,20,20,20	0
57	MG	YA	3083	1/1	0.94	0.20	7,7,7,7	0
57	MG	YA	3132	1/1	0.94	0.14	18,18,18,18	0
57	MG	YA	3113	1/1	0.94	0.19	19,19,19,19	0
57	MG	RA	3071	1/1	0.94	0.18	19,19,19,19	0
57	MG	QA	1622	1/1	0.94	0.07	32,32,32,32	0
57	MG	YA	3119	1/1	0.94	0.23	31,31,31,31	0
57	MG	RA	3098	1/1	0.94	0.25	10,10,10,10	0
57	MG	YA	3030	1/1	0.94	0.38	20,20,20,20	0
57	MG	QA	1621	1/1	0.95	0.08	14,14,14,14	0
57	MG	YA	3197	1/1	0.95	0.13	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	XA	1601	1/1	0.95	0.20	4,4,4,4	0
57	MG	RA	3087	1/1	0.95	0.14	34,34,34,34	0
57	MG	YA	3004	1/1	0.95	0.17	5,5,5,5	0
57	MG	YA	3053	1/1	0.95	0.23	5,5,5,5	0
57	MG	YA	3149	1/1	0.95	0.13	16,16,16,16	0
57	MG	RA	3121	1/1	0.95	0.20	29,29,29,29	0
57	MG	QA	1654	1/1	0.95	0.11	79,79,79,79	0
57	MG	RA	3096	1/1	0.95	0.28	23,23,23,23	0
57	MG	YA	3102	1/1	0.95	0.26	12,12,12,12	0
57	MG	YA	3253	1/1	0.95	0.30	18,18,18,18	0
57	MG	RA	3140	1/1	0.95	0.38	26,26,26,26	0
57	MG	RA	3132	1/1	0.95	0.31	22,22,22,22	0
57	MG	QA	1634	1/1	0.95	0.23	20,20,20,20	0
57	MG	QA	1648	1/1	0.95	0.16	12,12,12,12	0
57	MG	YA	3049	1/1	0.95	0.28	14,14,14,14	0
57	MG	YA	3175	1/1	0.95	0.21	37,37,37,37	0
57	MG	RF	301	1/1	0.95	0.10	40,40,40,40	0
57	MG	RA	3102	1/1	0.95	0.23	14,14,14,14	0
57	MG	XA	1640	1/1	0.95	0.30	31,31,31,31	0
57	MG	QA	1628	1/1	0.95	0.28	25,25,25,25	0
57	MG	XA	1646	1/1	0.95	0.25	45,45,45,45	0
57	MG	RA	3157	1/1	0.95	0.23	49,49,49,49	0
57	MG	YA	3187	1/1	0.95	0.09	29,29,29,29	0
57	MG	YA	3099	1/1	0.95	0.35	7,7,7,7	0
57	MG	RA	3097	1/1	0.95	0.27	14,14,14,14	0
57	MG	XA	1641	1/1	0.95	0.11	40,40,40,40	0
57	MG	YA	3036	1/1	0.95	0.22	5,5,5,5	0
57	MG	YA	3180	1/1	0.95	0.25	49,49,49,49	0
57	MG	RA	3146	1/1	0.95	0.14	33,33,33,33	0
57	MG	RA	3035	1/1	0.95	0.31	11,11,11,11	0
57	MG	XA	1606	1/1	0.95	0.25	17,17,17,17	0
57	MG	XA	1670	1/1	0.95	0.11	29,29,29,29	0
57	MG	YA	3147	1/1	0.95	0.14	8,8,8,8	0
57	MG	YA	3061	1/1	0.95	0.11	15,15,15,15	0
57	MG	RA	3144	1/1	0.95	0.26	17,17,17,17	0
57	MG	RA	3076	1/1	0.95	0.26	15,15,15,15	0
57	MG	RA	3030	1/1	0.95	0.27	12,12,12,12	0
57	MG	RA	3024	1/1	0.95	0.21	5,5,5,5	0
57	MG	RA	3203	1/1	0.95	0.14	35,35,35,35	0
57	MG	YA	3193	1/1	0.95	0.20	27,27,27,27	0
57	MG	RA	3172	1/1	0.95	0.12	23,23,23,23	0
57	MG	RA	3189	1/1	0.95	0.10	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	QA	1619	1/1	0.95	0.11	33,33,33,33	0
57	MG	RA	3117	1/1	0.95	0.19	3,3,3,3	0
57	MG	RA	3078	1/1	0.95	0.21	22,22,22,22	0
57	MG	YA	3213	1/1	0.95	0.27	29,29,29,29	0
57	MG	YA	3038	1/1	0.95	0.12	6,6,6,6	0
57	MG	RA	3080	1/1	0.95	0.23	19,19,19,19	0
57	MG	YA	3250	1/1	0.95	0.12	40,40,40,40	0
57	MG	RA	3034	1/1	0.95	0.34	30,30,30,30	0
57	MG	RA	3093	1/1	0.95	0.25	9,9,9,9	0
57	MG	YA	3258	1/1	0.95	0.36	11,11,11,11	0
57	MG	YA	3048	1/1	0.95	0.22	10,10,10,10	0
57	MG	YA	3231	1/1	0.95	0.10	19,19,19,19	0
57	MG	XX	101	1/1	0.95	0.18	22,22,22,22	0
57	MG	YA	3230	1/1	0.95	0.18	32,32,32,32	0
57	MG	YA	3249	1/1	0.95	0.18	26,26,26,26	0
57	MG	RA	3045	1/1	0.95	0.24	16,16,16,16	0
57	MG	YA	3162	1/1	0.95	0.15	20,20,20,20	0
57	MG	RA	3085	1/1	0.95	0.18	16,16,16,16	0
59	ZN	QD	301	1/1	0.95	0.26	47,47,47,47	0
57	MG	YA	3226	1/1	0.95	0.19	3,3,3,3	0
57	MG	RA	3036	1/1	0.95	0.21	4,4,4,4	0
57	MG	RB	201	1/1	0.95	0.12	59,59,59,59	0
57	MG	RA	3202	1/1	0.95	0.10	21,21,21,21	0
57	MG	RA	3006	1/1	0.95	0.34	18,18,18,18	0
57	MG	YA	3157	1/1	0.95	0.10	30,30,30,30	0
57	MG	YA	3056	1/1	0.96	0.14	8,8,8,8	0
57	MG	RA	3231	1/1	0.96	0.37	9,9,9,9	0
57	MG	RA	3105	1/1	0.96	0.26	18,18,18,18	0
57	MG	YA	3168	1/1	0.96	0.08	13,13,13,13	0
57	MG	XA	1644	1/1	0.96	0.19	27,27,27,27	0
57	MG	YA	3225	1/1	0.96	0.19	9,9,9,9	0
57	MG	RA	3240	1/1	0.96	0.33	25,25,25,25	0
57	MG	RA	3108	1/1	0.96	0.14	24,24,24,24	0
57	MG	YA	3094	1/1	0.96	0.18	2,2,2,2	0
57	MG	RA	3019	1/1	0.96	0.31	19,19,19,19	0
57	MG	YA	3062	1/1	0.96	0.12	9,9,9,9	0
57	MG	YA	3012	1/1	0.96	0.38	9,9,9,9	0
57	MG	RA	3053	1/1	0.96	0.37	16,16,16,16	0
57	MG	QA	1607	1/1	0.96	0.10	40,40,40,40	0
57	MG	RA	3113	1/1	0.96	0.11	32,32,32,32	0
57	MG	YA	3058	1/1	0.96	0.18	12,12,12,12	0
57	MG	YA	3115	1/1	0.96	0.15	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3125	1/1	0.96	0.18	11,11,11,11	0
57	MG	XA	1642	1/1	0.96	0.19	23,23,23,23	0
57	MG	XA	1617	1/1	0.96	0.16	14,14,14,14	0
57	MG	XA	1634	1/1	0.96	0.10	15,15,15,15	0
57	MG	YA	3169	1/1	0.96	0.20	20,20,20,20	0
57	MG	RA	3239	1/1	0.96	0.23	19,19,19,19	0
57	MG	YA	3069	1/1	0.96	0.31	15,15,15,15	0
57	MG	RA	3060	1/1	0.96	0.29	8,8,8,8	0
57	MG	RA	3112	1/1	0.96	0.10	25,25,25,25	0
57	MG	YA	3095	1/1	0.96	0.21	7,7,7,7	0
57	MG	XA	1603	1/1	0.96	0.14	38,38,38,38	0
57	MG	RA	3033	1/1	0.96	0.27	3,3,3,3	0
57	MG	RA	3136	1/1	0.96	0.10	9,9,9,9	0
57	MG	QA	1624	1/1	0.96	0.19	27,27,27,27	0
57	MG	RA	3206	1/1	0.96	0.33	15,15,15,15	0
57	MG	RA	3107	1/1	0.96	0.17	25,25,25,25	0
57	MG	YA	3118	1/1	0.96	0.28	25,25,25,25	0
57	MG	RA	3128	1/1	0.96	0.25	31,31,31,31	0
57	MG	RA	3073	1/1	0.96	0.21	24,24,24,24	0
57	MG	YA	3111	1/1	0.96	0.15	34,34,34,34	0
57	MG	YA	3138	1/1	0.96	0.10	10,10,10,10	0
57	MG	YA	3264	1/1	0.96	0.13	24,24,24,24	0
57	MG	QA	1630	1/1	0.96	0.17	48,48,48,48	0
57	MG	YA	3014	1/1	0.96	0.17	3,3,3,3	0
57	MG	YA	3013	1/1	0.96	0.22	1,1,1,1	0
57	MG	QA	1652	1/1	0.96	0.20	37,37,37,37	0
57	MG	QA	1608	1/1	0.96	0.06	13,13,13,13	0
57	MG	YA	3025	1/1	0.96	0.19	8,8,8,8	0
57	MG	QA	1612	1/1	0.96	0.21	13,13,13,13	0
57	MG	RA	3083	1/1	0.96	0.20	11,11,11,11	0
57	MG	YA	3252	1/1	0.96	0.38	25,25,25,25	0
57	MG	RA	3236	1/1	0.96	0.28	33,33,33,33	0
57	MG	XA	1629	1/1	0.96	0.19	29,29,29,29	0
57	MG	YA	3040	1/1	0.96	0.26	8,8,8,8	0
57	MG	QA	1611	1/1	0.96	0.26	14,14,14,14	0
57	MG	RA	3047	1/1	0.96	0.34	9,9,9,9	0
57	MG	YA	3265	1/1	0.96	0.29	27,27,27,27	0
57	MG	YA	3001	1/1	0.96	0.22	9,9,9,9	0
57	MG	RA	3074	1/1	0.96	0.18	4,4,4,4	0
57	MG	RA	3237	1/1	0.96	0.27	26,26,26,26	0
57	MG	QA	1649	1/1	0.96	0.17	39,39,39,39	0
57	MG	YA	3044	1/1	0.96	0.29	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3032	1/1	0.96	0.26	15,15,15,15	0
57	MG	YA	3110	1/1	0.96	0.10	15,15,15,15	0
57	MG	YA	3070	1/1	0.96	0.18	8,8,8,8	0
57	MG	RE	302	1/1	0.96	0.26	23,23,23,23	0
57	MG	RA	3122	1/1	0.96	0.15	29,29,29,29	0
57	MG	YA	3047	1/1	0.96	0.28	6,6,6,6	0
57	MG	YA	3089	1/1	0.97	0.27	8,8,8,8	0
57	MG	RA	3109	1/1	0.97	0.09	8,8,8,8	0
57	MG	XA	1667	1/1	0.97	0.32	32,32,32,32	0
57	MG	XA	1662	1/1	0.97	0.08	11,11,11,11	0
57	MG	YA	3017	1/1	0.97	0.18	2,2,2,2	0
57	MG	RA	3057	1/1	0.97	0.27	11,11,11,11	0
57	MG	XA	1612	1/1	0.97	0.12	13,13,13,13	0
57	MG	XA	1651	1/1	0.97	0.15	12,12,12,12	0
57	MG	QA	1635	1/1	0.97	0.08	33,33,33,33	0
57	MG	RA	3041	1/1	0.97	0.21	2,2,2,2	0
57	MG	YA	3011	1/1	0.97	0.27	20,20,20,20	0
57	MG	XA	1608	1/1	0.97	0.34	23,23,23,23	0
57	MG	XA	1627	1/1	0.97	0.09	7,7,7,7	0
57	MG	YA	3260	1/1	0.97	0.17	14,14,14,14	0
57	MG	RA	3230	1/1	0.97	0.32	18,18,18,18	0
57	MG	XA	1604	1/1	0.97	0.14	15,15,15,15	0
57	MG	YA	3073	1/1	0.97	0.21	7,7,7,7	0
57	MG	YA	3037	1/1	0.97	0.19	1,1,1,1	0
57	MG	RA	3233	1/1	0.97	0.27	24,24,24,24	0
57	MG	YA	3254	1/1	0.97	0.19	7,7,7,7	0
57	MG	XV	102	1/1	0.97	0.21	0,0,0,0	0
57	MG	XA	1623	1/1	0.97	0.27	40,40,40,40	0
57	MG	YA	3077	1/1	0.97	0.23	16,16,16,16	0
57	MG	YA	3245	1/1	0.97	0.14	38,38,38,38	0
57	MG	RA	3003	1/1	0.97	0.30	14,14,14,14	0
57	MG	YA	3093	1/1	0.97	0.16	13,13,13,13	0
57	MG	RA	3111	1/1	0.97	0.35	22,22,22,22	0
57	MG	XA	1614	1/1	0.97	0.17	7,7,7,7	0
57	MG	RA	3061	1/1	0.97	0.28	9,9,9,9	0
57	MG	RA	3106	1/1	0.97	0.16	11,11,11,11	0
57	MG	YA	3232	1/1	0.97	0.13	23,23,23,23	0
57	MG	YA	3121	1/1	0.97	0.11	18,18,18,18	0
57	MG	YA	3114	1/1	0.97	0.19	8,8,8,8	0
57	MG	YA	3090	1/1	0.97	0.23	5,5,5,5	0
57	MG	RA	3040	1/1	0.97	0.30	21,21,21,21	0
57	MG	QA	1642	1/1	0.97	0.10	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3026	1/1	0.97	0.29	8,8,8,8	0
57	MG	YA	3100	1/1	0.97	0.31	13,13,13,13	0
57	MG	YA	3097	1/1	0.97	0.21	19,19,19,19	0
57	MG	RA	3075	1/1	0.97	0.09	15,15,15,15	0
57	MG	YQ	201	1/1	0.97	0.14	25,25,25,25	0
57	MG	RP	201	1/1	0.97	0.29	30,30,30,30	0
57	MG	XA	1605	1/1	0.97	0.21	16,16,16,16	0
57	MG	RA	3129	1/1	0.97	0.12	21,21,21,21	0
57	MG	YA	3141	1/1	0.97	0.10	16,16,16,16	0
57	MG	RA	3063	1/1	0.97	0.41	6,6,6,6	0
57	MG	RA	3152	1/1	0.97	0.17	14,14,14,14	0
57	MG	YA	3064	1/1	0.97	0.08	39,39,39,39	0
57	MG	RE	301	1/1	0.97	0.11	1,1,1,1	0
57	MG	RA	3018	1/1	0.97	0.12	9,9,9,9	0
57	MG	RA	3015	1/1	0.97	0.17	2,2,2,2	0
57	MG	RA	3154	1/1	0.97	0.20	22,22,22,22	0
57	MG	YA	3020	1/1	0.97	0.37	7,7,7,7	0
57	MG	QA	1606	1/1	0.97	0.10	22,22,22,22	0
57	MG	YA	3023	1/1	0.97	0.26	16,16,16,16	0
57	MG	RA	3090	1/1	0.97	0.17	23,23,23,23	0
57	MG	RA	3046	1/1	0.97	0.15	12,12,12,12	0
57	MG	RA	3048	1/1	0.97	0.16	1,1,1,1	0
57	MG	YA	3019	1/1	0.97	0.25	1,1,1,1	0
57	MG	YA	3035	1/1	0.97	0.20	5,5,5,5	0
57	MG	RA	3039	1/1	0.97	0.24	2,2,2,2	0
57	MG	RA	3004	1/1	0.97	0.32	15,15,15,15	0
57	MG	XA	1620	1/1	0.97	0.23	17,17,17,17	0
57	MG	YA	3078	1/1	0.97	0.24	19,19,19,19	0
57	MG	YA	3015	1/1	0.97	0.32	8,8,8,8	0
57	MG	RA	3094	1/1	0.97	0.14	9,9,9,9	0
57	MG	RA	3123	1/1	0.97	0.18	28,28,28,28	0
57	MG	RA	3020	1/1	0.97	0.24	1,1,1,1	0
57	MG	XA	1669	1/1	0.97	0.16	41,41,41,41	0
57	MG	YA	3096	1/1	0.97	0.21	10,10,10,10	0
57	MG	YA	3055	1/1	0.97	0.24	10,10,10,10	0
57	MG	YA	3098	1/1	0.97	0.16	16,16,16,16	0
57	MG	YA	3034	1/1	0.97	0.33	9,9,9,9	0
57	MG	YA	3010	1/1	0.97	0.21	4,4,4,4	0
57	MG	RA	3169	1/1	0.97	0.44	35,35,35,35	0
57	MG	YA	3086	1/1	0.97	0.22	6,6,6,6	0
57	MG	RA	3037	1/1	0.98	0.21	11,11,11,11	0
57	MG	YA	3087	1/1	0.98	0.27	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3027	1/1	0.98	0.28	0,0,0,0	0
57	MG	RA	3007	1/1	0.98	0.24	6,6,6,6	0
57	MG	YA	3002	1/1	0.98	0.27	9,9,9,9	0
57	MG	XA	1602	1/1	0.98	0.12	30,30,30,30	0
57	MG	RA	3021	1/1	0.98	0.29	2,2,2,2	0
57	MG	YA	3043	1/1	0.98	0.33	15,15,15,15	0
57	MG	YA	3006	1/1	0.98	0.28	9,9,9,9	0
57	MG	YA	3136	1/1	0.98	0.17	18,18,18,18	0
57	MG	XA	1619	1/1	0.98	0.11	18,18,18,18	0
57	MG	RA	3095	1/1	0.98	0.26	14,14,14,14	0
57	MG	YA	3109	1/1	0.98	0.30	10,10,10,10	0
57	MG	YA	3042	1/1	0.98	0.19	19,19,19,19	0
57	MG	RA	3016	1/1	0.98	0.24	1,1,1,1	0
57	MG	YA	3261	1/1	0.98	0.29	8,8,8,8	0
57	MG	YA	3050	1/1	0.98	0.33	9,9,9,9	0
57	MG	RA	3025	1/1	0.98	0.17	15,15,15,15	0
57	MG	YA	3076	1/1	0.98	0.34	7,7,7,7	0
57	MG	RA	3042	1/1	0.98	0.24	3,3,3,3	0
57	MG	YA	3081	1/1	0.98	0.19	5,5,5,5	0
57	MG	RA	3022	1/1	0.98	0.22	16,16,16,16	0
57	MG	YA	3167	1/1	0.98	0.09	21,21,21,21	0
57	MG	QA	1604	1/1	0.98	0.25	12,12,12,12	0
57	MG	RA	3116	1/1	0.98	0.22	1,1,1,1	0
57	MG	YA	3124	1/1	0.98	0.27	9,9,9,9	0
57	MG	RR	201	1/1	0.98	0.22	7,7,7,7	0
57	MG	YA	3059	1/1	0.98	0.12	6,6,6,6	0
57	MG	YA	3009	1/1	0.98	0.27	12,12,12,12	0
57	MG	YA	3021	1/1	0.98	0.30	9,9,9,9	0
57	MG	RA	3089	1/1	0.98	0.15	8,8,8,8	0
57	MG	RA	3104	1/1	0.98	0.19	16,16,16,16	0
57	MG	YA	3091	1/1	0.98	0.19	21,21,21,21	0
57	MG	RA	3029	1/1	0.98	0.32	2,2,2,2	0
57	MG	RA	3114	1/1	0.98	0.25	20,20,20,20	0
57	MG	QA	1610	1/1	0.98	0.13	11,11,11,11	0
57	MG	XA	1615	1/1	0.98	0.08	15,15,15,15	0
57	MG	RA	3012	1/1	0.98	0.26	8,8,8,8	0
57	MG	RA	3224	1/1	0.98	0.11	52,52,52,52	0
57	MG	YA	3003	1/1	0.98	0.22	10,10,10,10	0
57	MG	YA	3112	1/1	0.98	0.06	15,15,15,15	0
57	MG	XA	1628	1/1	0.98	0.16	27,27,27,27	0
57	MG	RA	3125	1/1	0.98	0.24	28,28,28,28	0
57	MG	YA	3005	1/1	0.98	0.06	1,1,1,1	0

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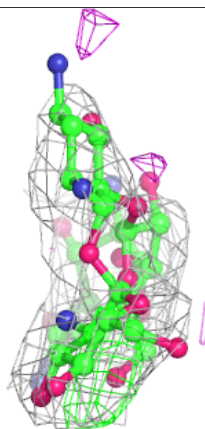
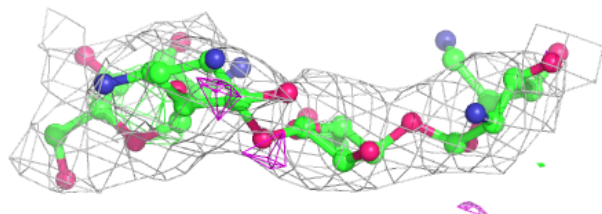
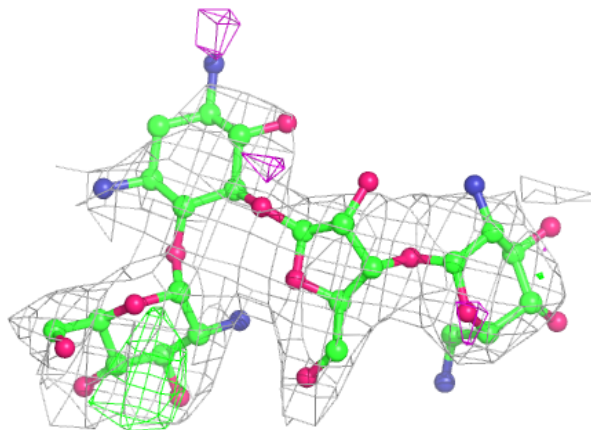
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	Y5	101	1/1	0.98	0.16	26,26,26,26	0
57	MG	YA	3085	1/1	0.98	0.15	71,71,71,71	0
57	MG	YA	3212	1/1	0.98	0.11	9,9,9,9	0
57	MG	YA	3080	1/1	0.98	0.18	10,10,10,10	0
57	MG	YA	3203	1/1	0.98	0.18	27,27,27,27	0
57	MG	YA	3176	1/1	0.98	0.16	6,6,6,6	0
57	MG	RA	3229	1/1	0.98	0.30	5,5,5,5	0
57	MG	YA	3184	1/1	0.98	0.20	20,20,20,20	0
57	MG	RA	3005	1/1	0.98	0.37	13,13,13,13	0
57	MG	RA	3079	1/1	0.98	0.20	17,17,17,17	0
57	MG	YA	3028	1/1	0.98	0.19	9,9,9,9	0
57	MG	RA	3028	1/1	0.98	0.23	4,4,4,4	0
57	MG	XA	1618	1/1	0.98	0.17	7,7,7,7	0
57	MG	YA	3031	1/1	0.98	0.22	2,2,2,2	0
57	MG	RA	3100	1/1	0.98	0.34	9,9,9,9	0
57	MG	YA	3248	1/1	0.98	0.23	26,26,26,26	0
57	MG	RA	3014	1/1	0.98	0.30	9,9,9,9	0
57	MG	RA	3186	1/1	0.98	0.07	20,20,20,20	0
57	MG	RA	3147	1/1	0.98	0.18	21,21,21,21	0
57	MG	QA	1636	1/1	0.99	0.09	16,16,16,16	0
57	MG	YA	3066	1/1	0.99	0.22	16,16,16,16	0
57	MG	YA	3190	1/1	0.99	0.07	2,2,2,2	0
57	MG	YA	3067	1/1	0.99	0.20	22,22,22,22	0
57	MG	RA	3017	1/1	0.99	0.28	8,8,8,8	0
57	MG	YA	3122	1/1	0.99	0.17	9,9,9,9	0
57	MG	RA	3038	1/1	0.99	0.31	9,9,9,9	0
57	MG	QV	101	1/1	0.99	0.15	26,26,26,26	0
57	MG	XA	1626	1/1	0.99	0.19	19,19,19,19	0
57	MG	RA	3031	1/1	0.99	0.18	16,16,16,16	0
57	MG	YA	3057	1/1	0.99	0.22	6,6,6,6	0
57	MG	YA	3256	1/1	0.99	0.28	7,7,7,7	0
57	MG	RA	3065	1/1	0.99	0.14	16,16,16,16	0
57	MG	YA	3092	1/1	0.99	0.18	30,30,30,30	0
57	MG	YA	3051	1/1	0.99	0.18	2,2,2,2	0
57	MG	QM	201	1/1	0.99	0.04	55,55,55,55	0
57	MG	RA	3027	1/1	0.99	0.23	3,3,3,3	0
57	MG	RA	3077	1/1	0.99	0.30	6,6,6,6	0
57	MG	RA	3067	1/1	0.99	0.20	9,9,9,9	0
57	MG	YA	3108	1/1	0.99	0.17	3,3,3,3	0
57	MG	YA	3257	1/1	0.99	0.24	3,3,3,3	0
57	MG	YA	3007	1/1	0.99	0.20	9,9,9,9	0

The following is a graphical depiction of the model fit to experimental electron density of all

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

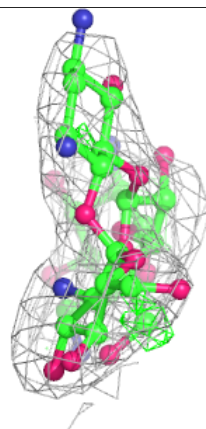
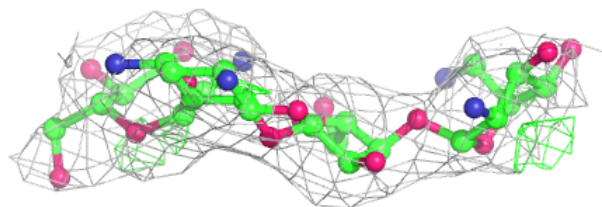
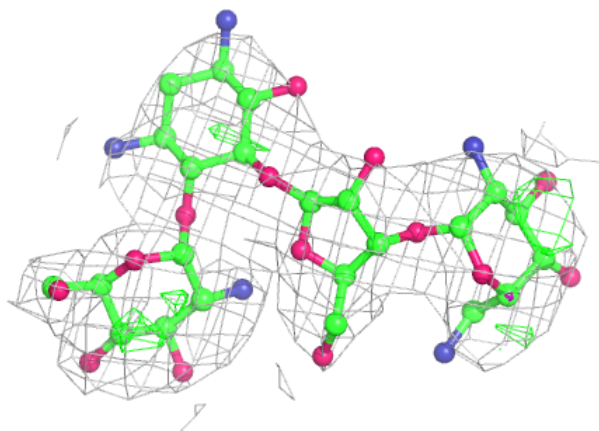
Electron density around PAR QA 1670:

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



Electron density around PAR XA 1675:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.