



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 08:53 AM UTC

PDB ID : 4TUD / pdb_00004tud
Title : Crystal structure of ASL-SufJ bound to Codon ACC-C on the Ribosome
Authors : Fagan, C.E.; Dunham, C.M.
Deposited on : 2014-06-24
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

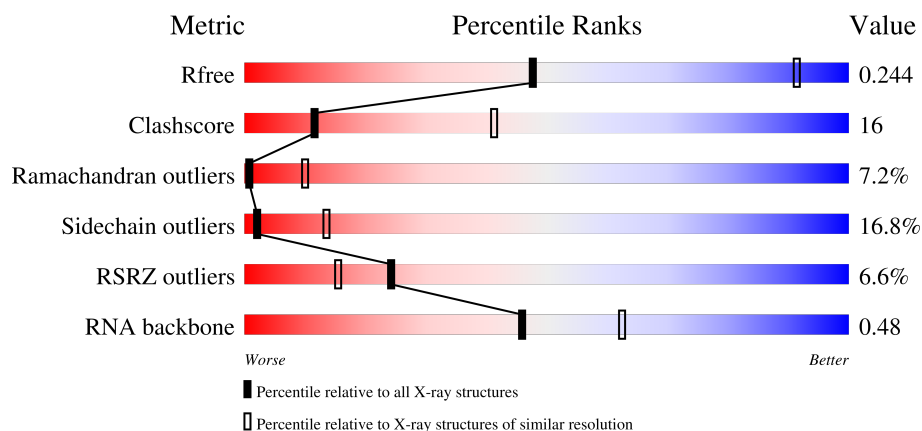
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

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

Mol	Chain	Length	Quality of chain
1	QA	1522	3% 55% 36% 8%
1	XA	1522	3% 55% 34% 9%
2	QB	256	5% 46% 38% 8% 7%
2	XB	256	2% 44% 39% 9% 7%

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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	QX	25	
23	XX	25	
24	QY	18	
24	XY	18	
25	RA	2915	
25	YA	2915	
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	Z5	3	
56	Z6	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	QA	1667	-	-	-	X
57	MG	R8	101	-	-	-	X
57	MG	YA	3232	-	-	-	X
57	MG	YA	3260	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 292106 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 type Z.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	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 Thx.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			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	QX	9	Total	C	N	O	P	0	0	0
			173	76	31	57	9			
23	XX	9	Total	C	N	O	P	0	0	0
			173	76	31	57	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	15	Total	C	N	O	P	0	0	0
			319	142	55	107	15			
24	XY	15	Total	C	N	O	P	0	0	0
			319	142	55	107	15			

- 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	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			

- 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 L13.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RQ	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 L17.

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 L18.

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 L19.

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

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

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

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

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

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

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

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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 L23.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RZ	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 L27.

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 L28.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	R4	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	58	Total	C	N	O	S	0	0	0
			454	285	89	75	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 CC-Puro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	Z5	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
56	Z6	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	90	Total	Mg	0	0
			90	90		
57	QF	1	Total	Mg	0	0
			1	1		
57	QK	1	Total	Mg	0	0
			1	1		
57	QM	1	Total	Mg	0	0
			1	1		
57	QT	1	Total	Mg	0	0
			1	1		

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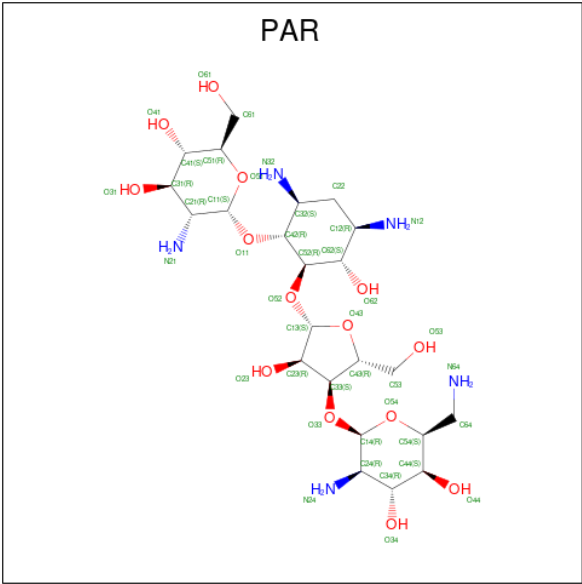
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QV	2	Total 2	Mg 2	0	0
57	QY	1	Total 1	Mg 1	0	0
57	RA	281	Total 281	Mg 281	0	0
57	RB	3	Total 3	Mg 3	0	0
57	RD	1	Total 1	Mg 1	0	0
57	RE	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0
57	RQ	1	Total 1	Mg 1	0	0
57	RR	2	Total 2	Mg 2	0	0
57	R0	2	Total 2	Mg 2	0	0
57	R3	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	XA	104	Total 104	Mg 104	0	0
57	XD	1	Total 1	Mg 1	0	0
57	XV	3	Total 3	Mg 3	0	0
57	XX	1	Total 1	Mg 1	0	0
57	XY	1	Total 1	Mg 1	0	0
57	YA	291	Total 291	Mg 291	0	0
57	YB	3	Total 3	Mg 3	0	0
57	YD	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YE	2	Total	Mg	0	0
			2	2		
57	YP	3	Total	Mg	0	0
			3	3		
57	YR	2	Total	Mg	0	0
			2	2		
57	YY	1	Total	Mg	0	0
			1	1		
57	Y0	1	Total	Mg	0	0
			1	1		
57	Y1	1	Total	Mg	0	0
			1	1		
57	Y3	1	Total	Mg	0	0
			1	1		
57	Y5	1	Total	Mg	0	0
			1	1		
57	Y7	1	Total	Mg	0	0
			1	1		

- Molecule 58 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).



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		

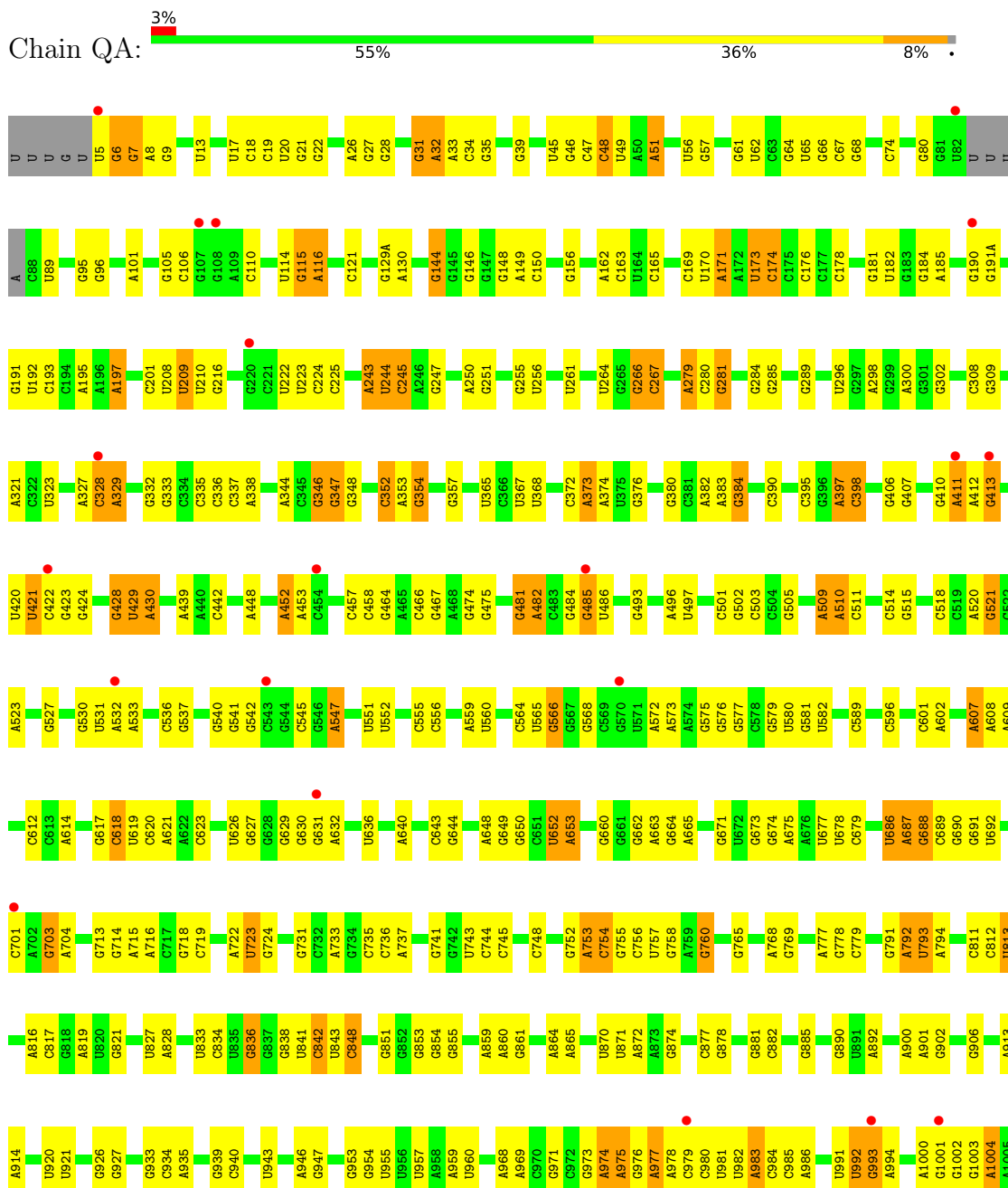
- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

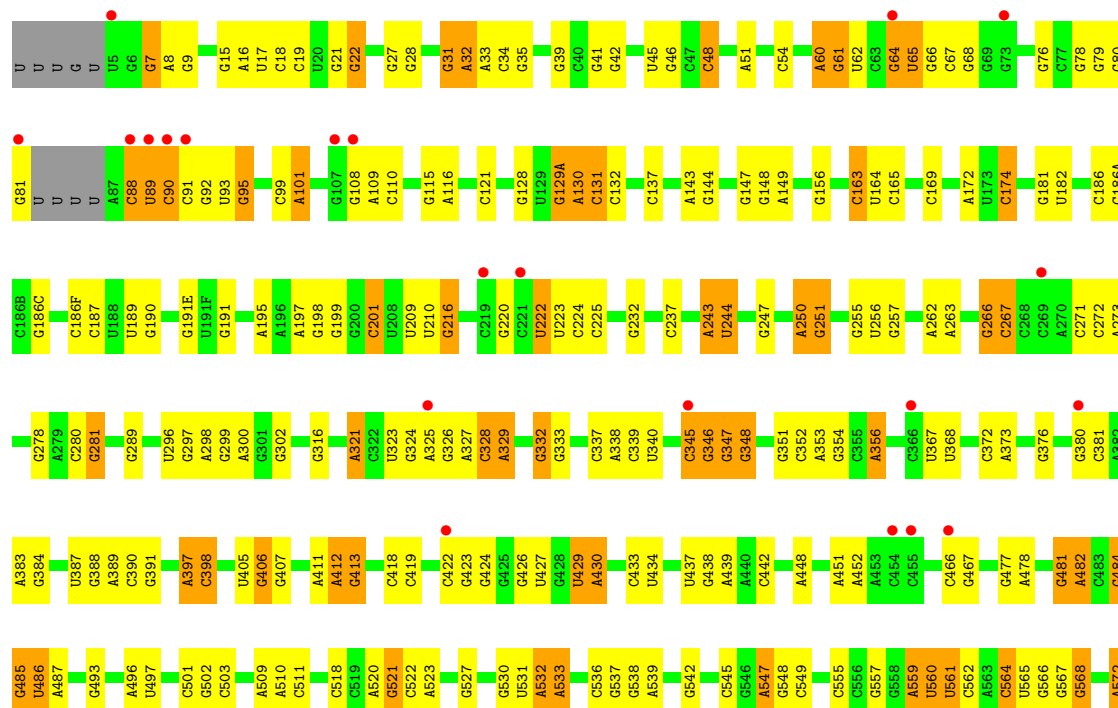
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	QD	1	Total 1	Zn 1	0	0
59	QN	1	Total 1	Zn 1	0	0
59	XD	1	Total 1	Zn 1	0	0
59	XN	1	Total 1	Zn 1	0	0

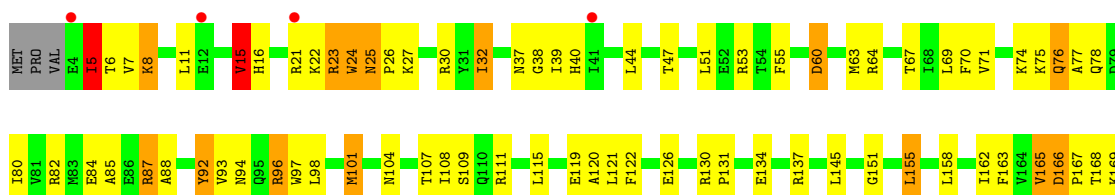
3 Residue-property plots

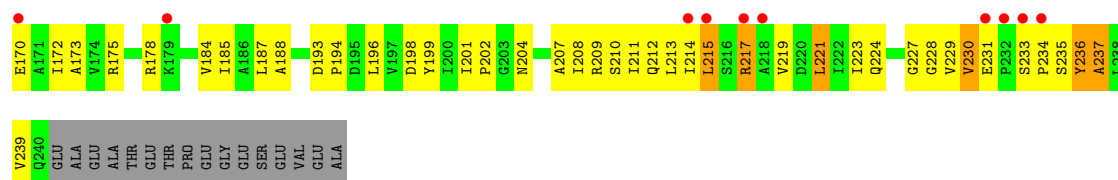
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

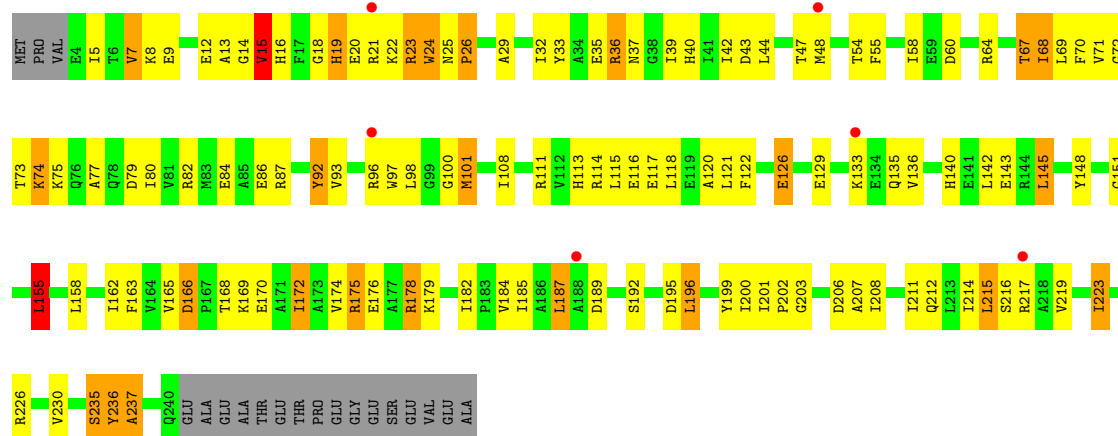




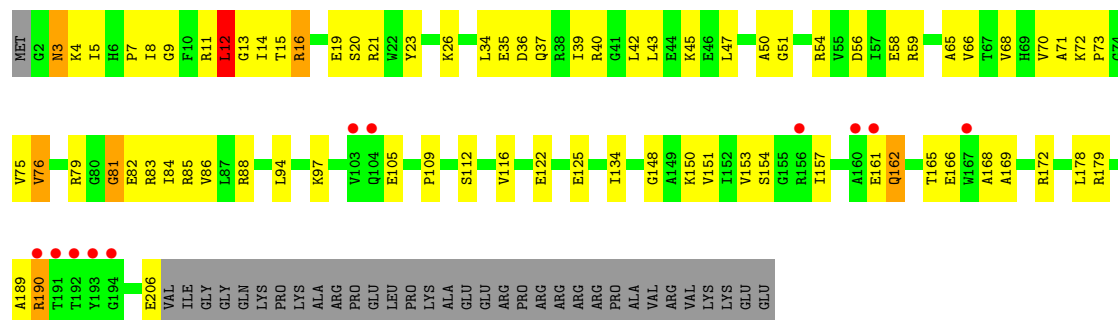




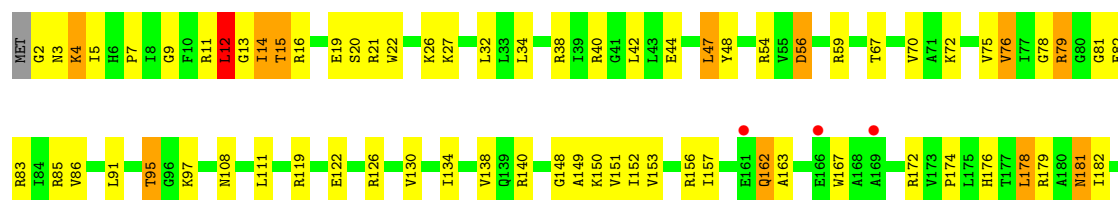
• Molecule 2: 30S ribosomal protein S2

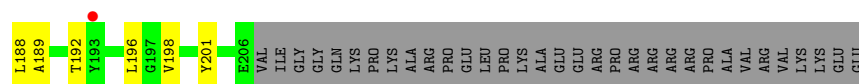


• Molecule 3: 30S ribosomal protein S3

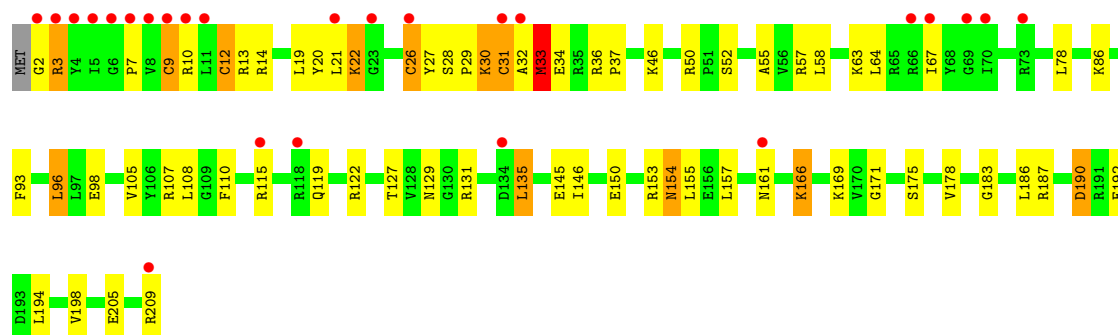


• Molecule 3: 30S ribosomal protein S3

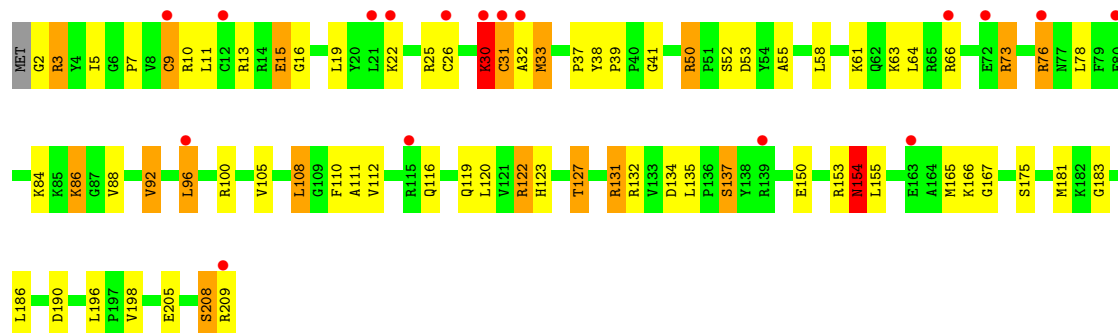




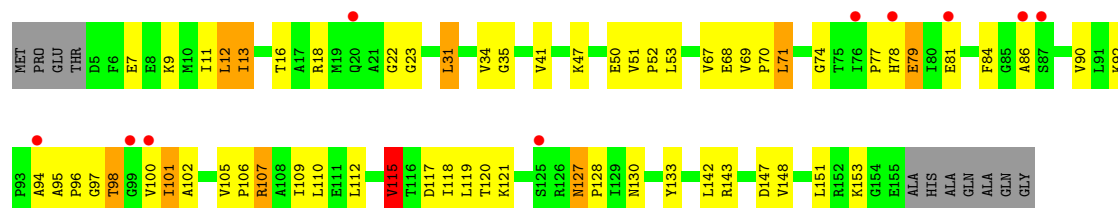
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

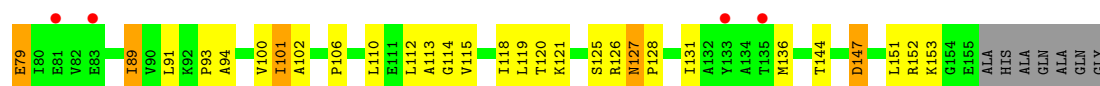


• Molecule 5: 30S ribosomal protein S5

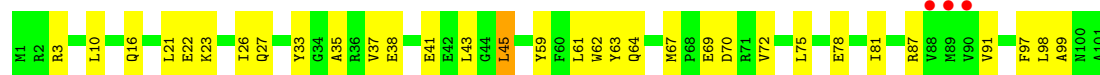


• Molecule 5: 30S ribosomal protein S5

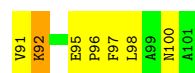
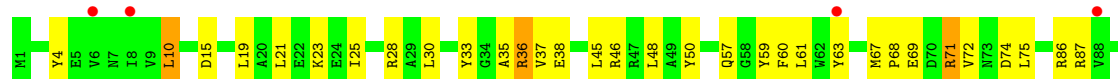




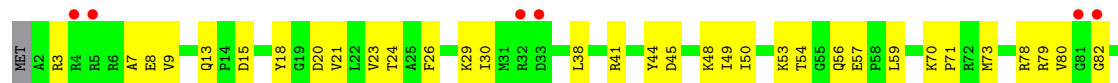
- Molecule 6: 30S ribosomal protein S6



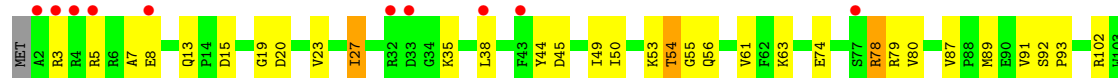
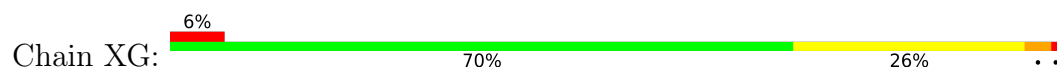
- Molecule 6: 30S ribosomal protein S6



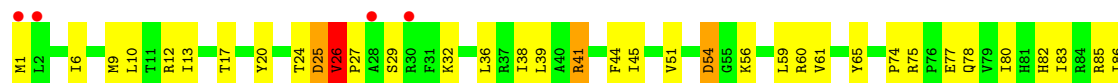
- Molecule 7: 30S ribosomal protein S7



- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8

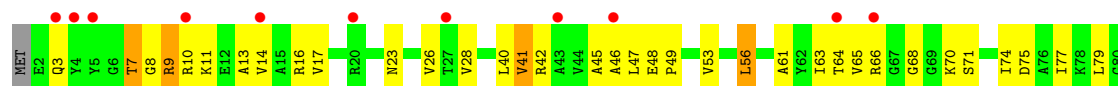




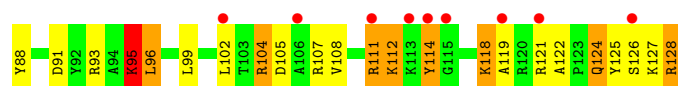
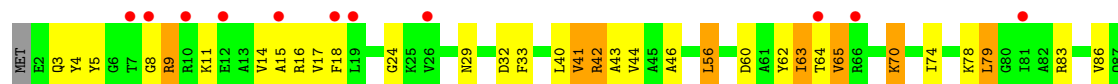
- Molecule 8: 30S ribosomal protein S8



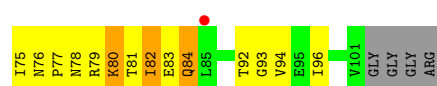
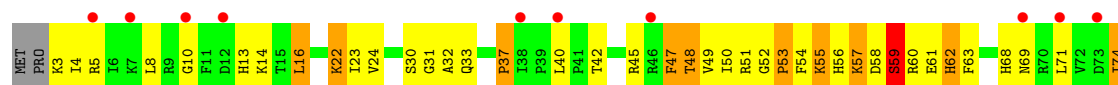
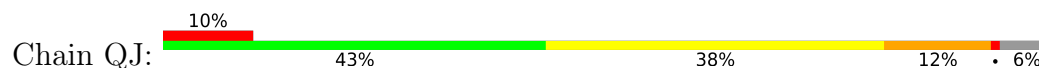
- Molecule 9: 30S ribosomal protein S9



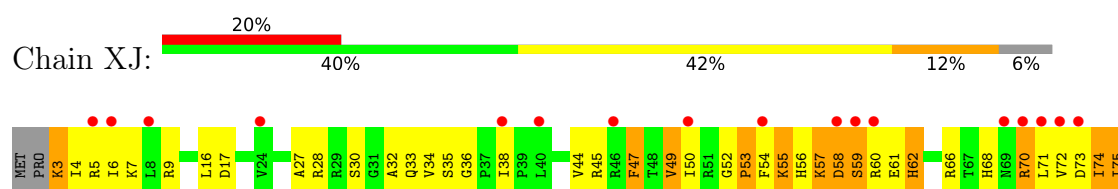
- Molecule 9: 30S ribosomal protein S9



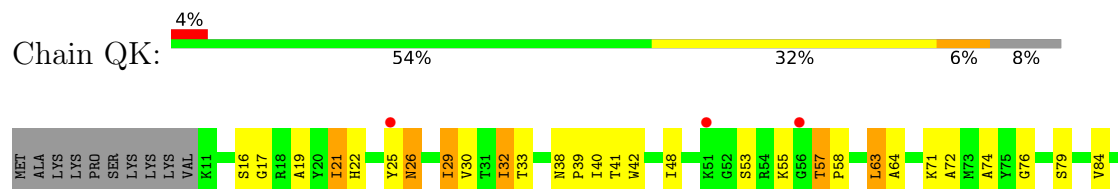
- Molecule 10: 30S ribosomal protein S10



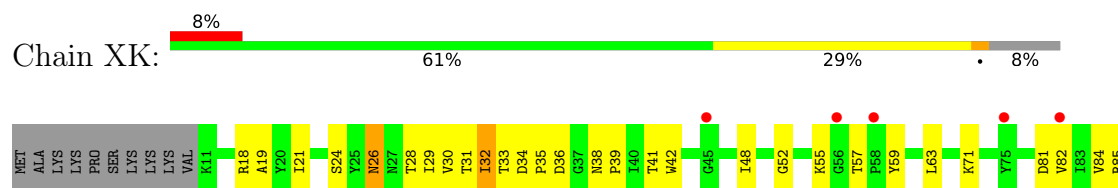
- Molecule 10: 30S ribosomal protein S10



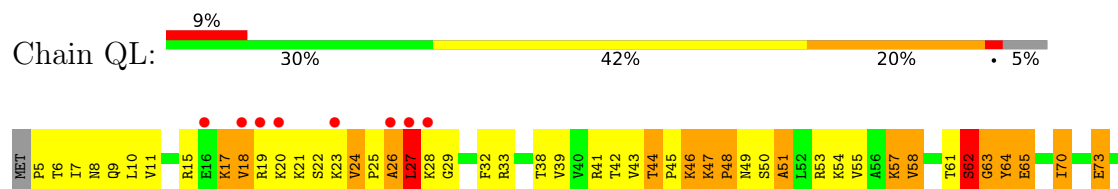
- Molecule 11: 30S ribosomal protein S11



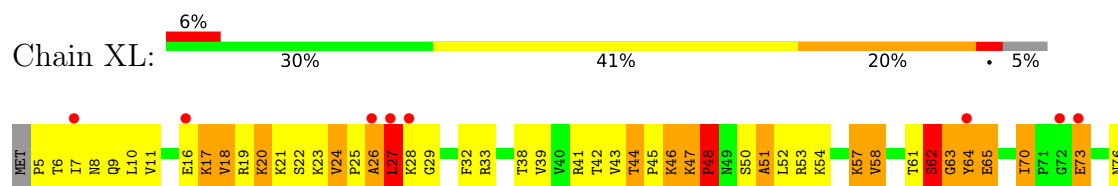
- Molecule 11: 30S ribosomal protein S11

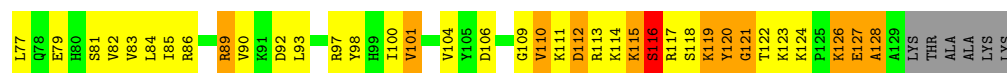


- Molecule 12: 30S ribosomal protein S12

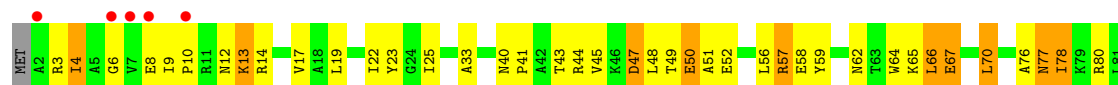


- Molecule 12: 30S ribosomal protein S12





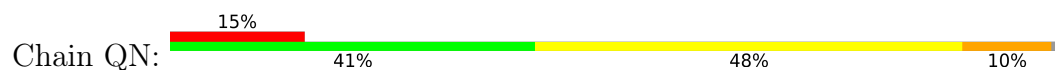
- Molecule 13: 30S ribosomal protein S13



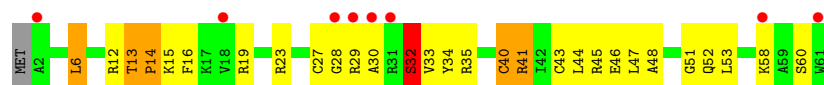
- Molecule 13: 30S ribosomal protein S13



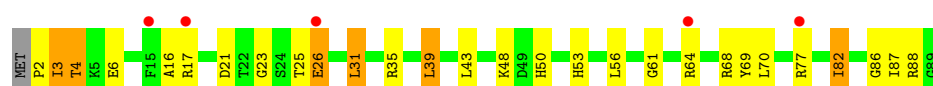
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15



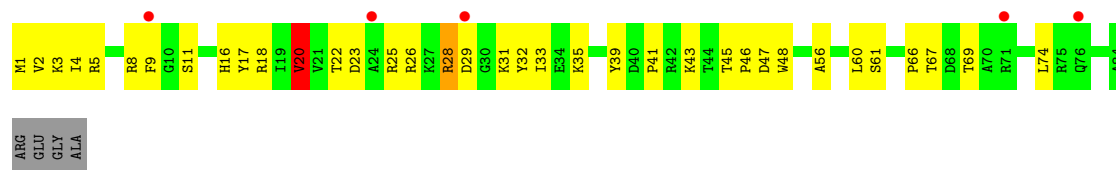
- Molecule 15: 30S ribosomal protein S15



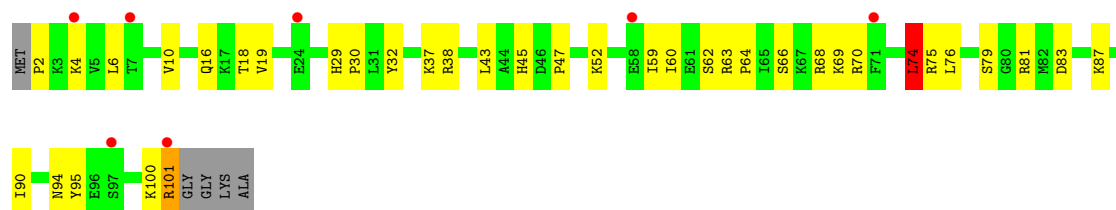
• Molecule 16: 30S ribosomal protein S16



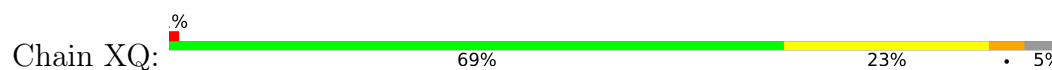
• Molecule 16: 30S ribosomal protein S16



• Molecule 17: 30S ribosomal protein S17



• Molecule 17: 30S ribosomal protein S17



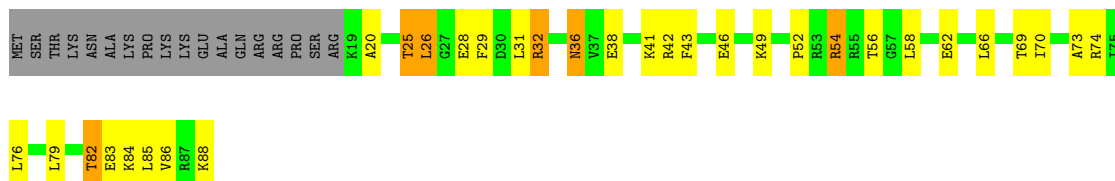
• Molecule 18: 30S ribosomal protein S18





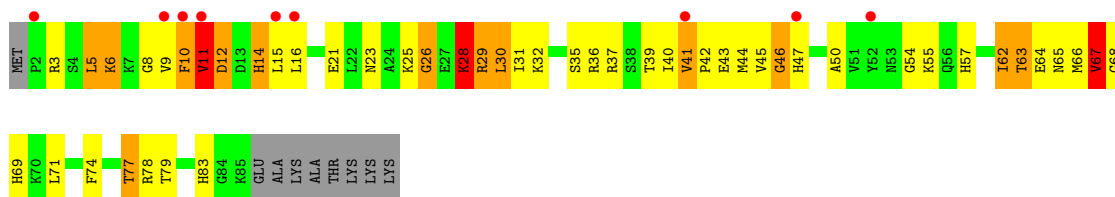
- Molecule 18: 30S ribosomal protein S18

Chain XR: 43% 30% 7% 20%



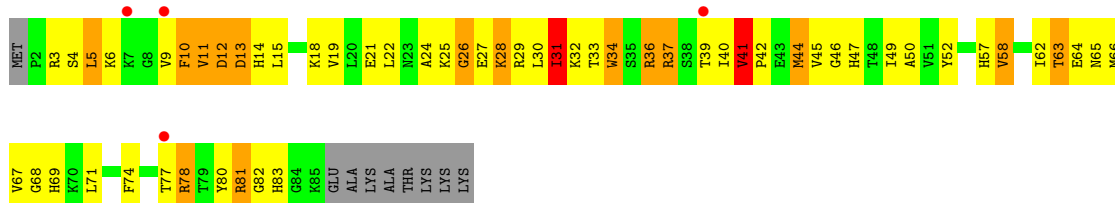
- Molecule 19: 30S ribosomal protein S19

Chain QS: 10% 37% 37% 14% 10%



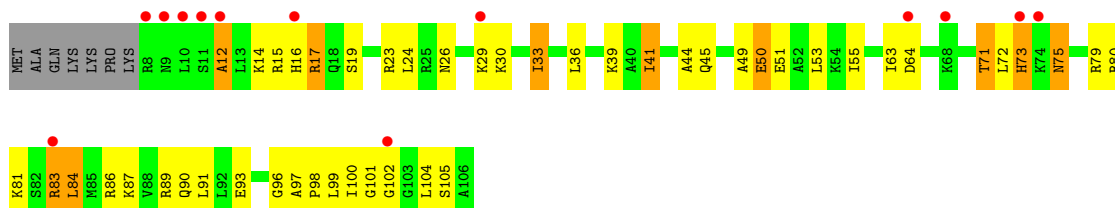
- Molecule 19: 30S ribosomal protein S19

Chain XS: 4% 29% 43% 16% 10%



- Molecule 20: 30S ribosomal protein S20

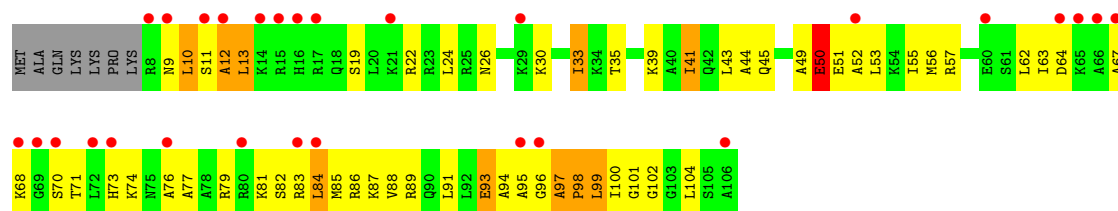
Chain QT: 12% 48% 36% 9% 7%



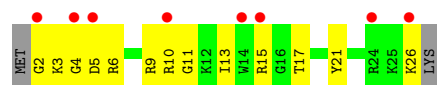
- Molecule 20: 30S ribosomal protein S20

Chain XT: 26% 39% 44% 9% 7%

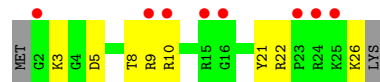




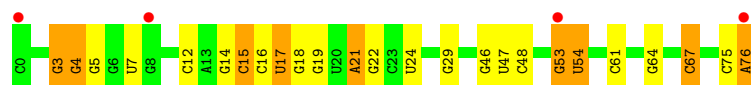
- Molecule 21: 30S ribosomal protein Thx



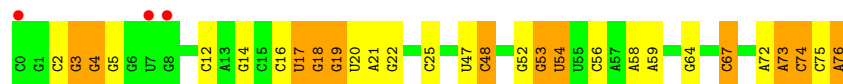
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: P-site tRNA-fMet



- Molecule 22: P-site tRNA-fMet



- Molecule 23: messenger RNA



- Molecule 23: messenger RNA

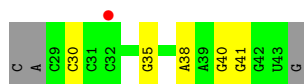




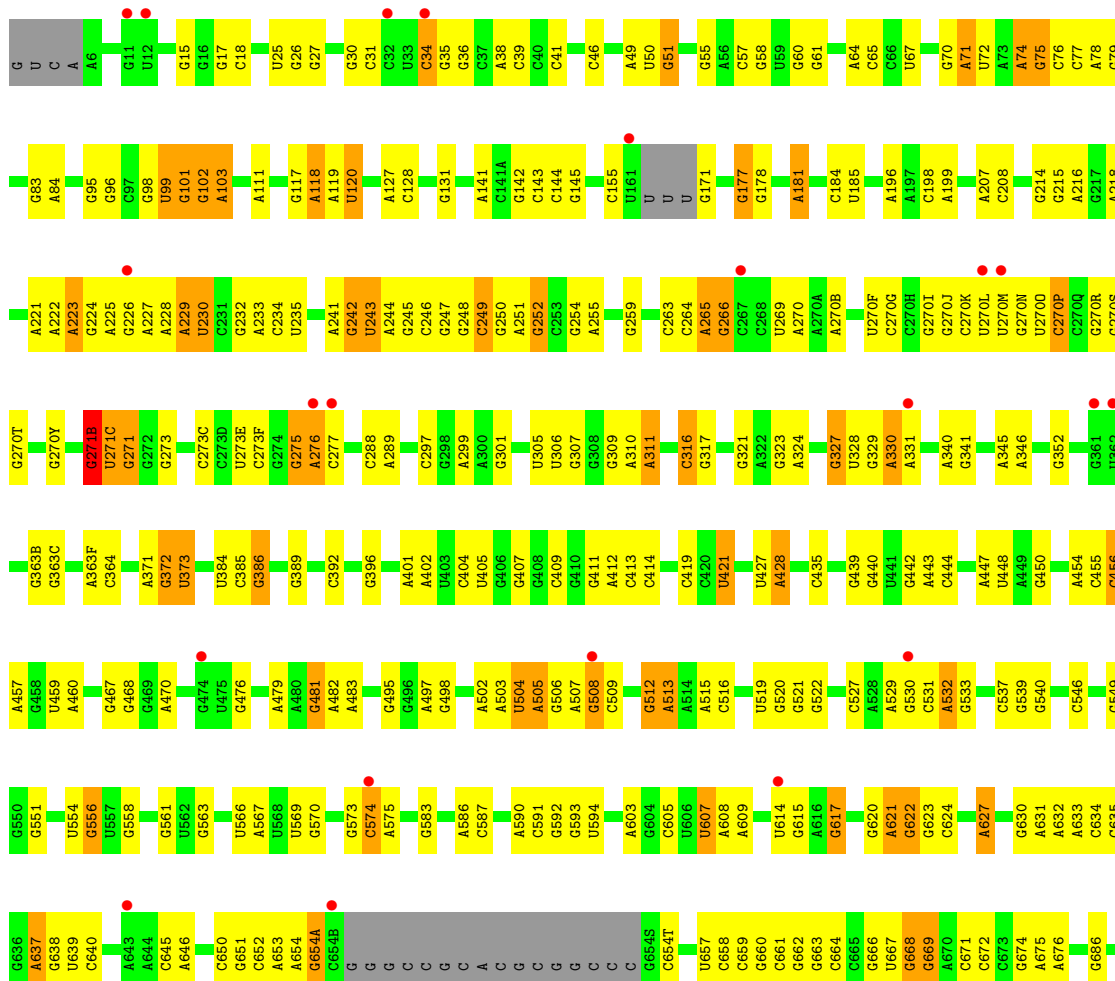
● Molecule 24: A-site ASL-SufJ



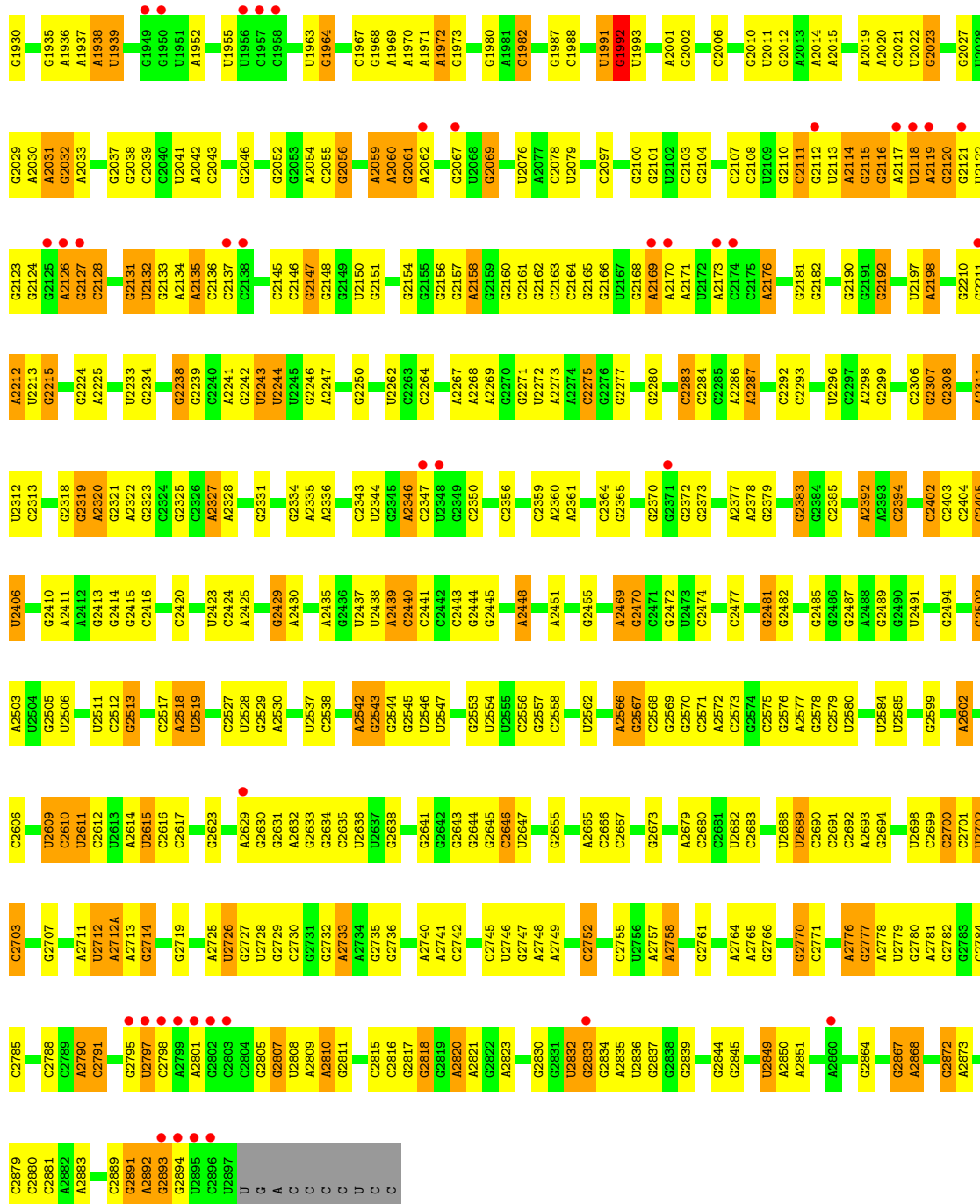
● Molecule 24: A-site ASL-SufJ



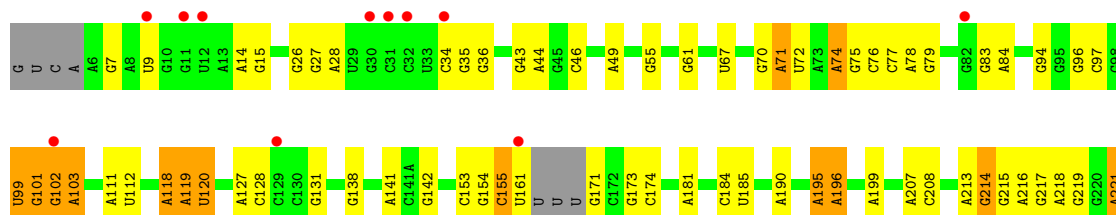
● Molecule 25: 23S rRNA

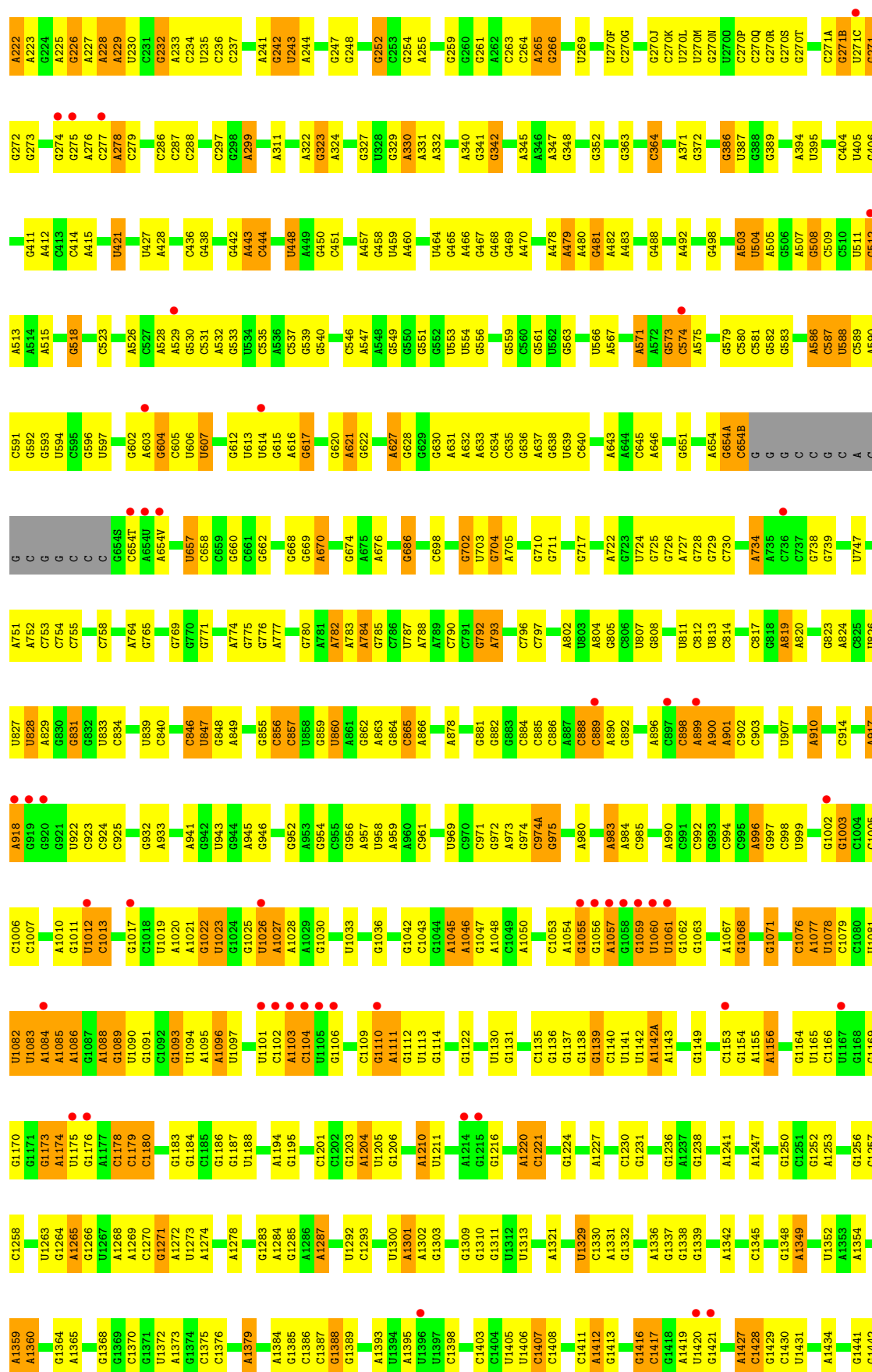


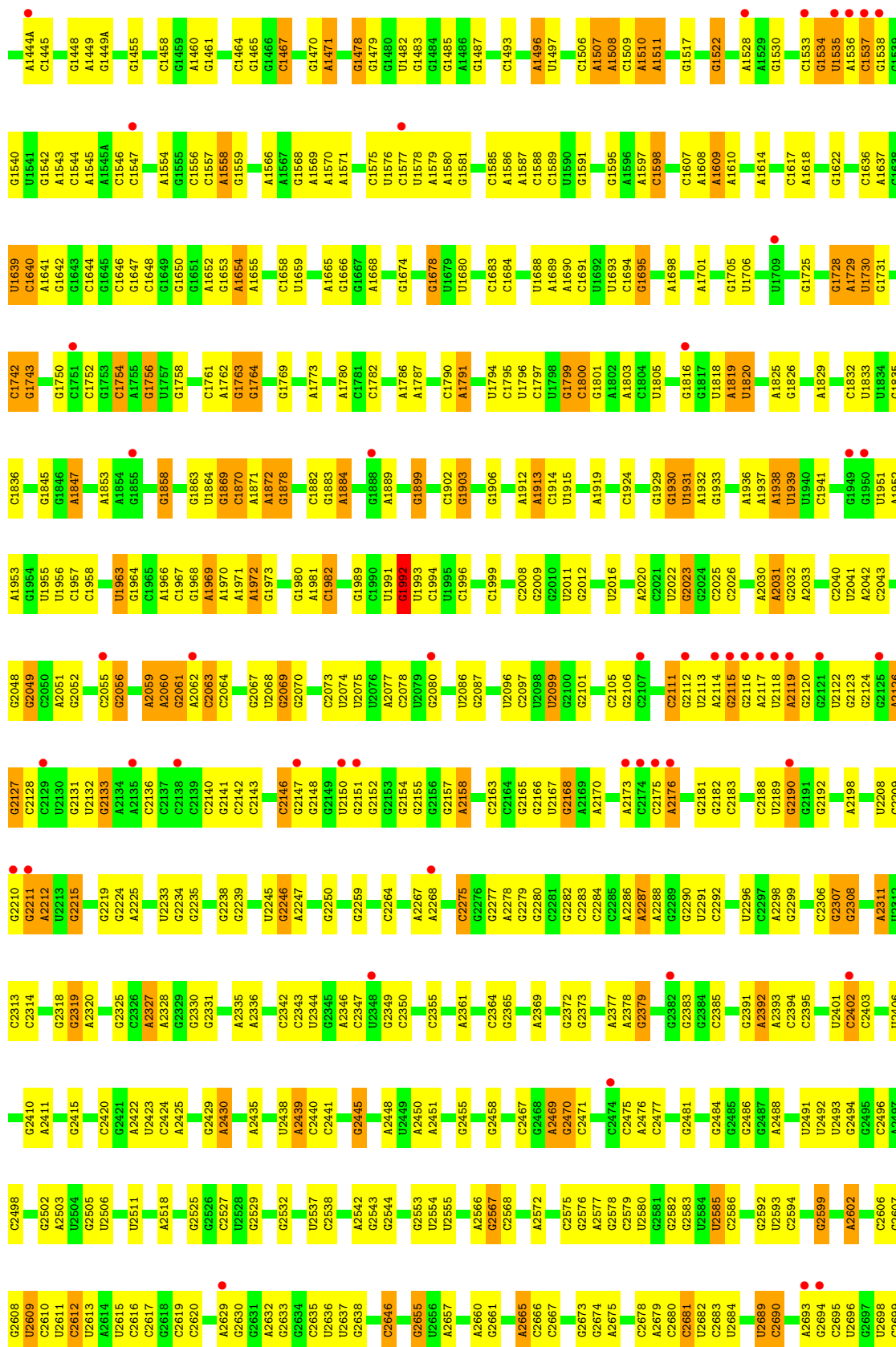


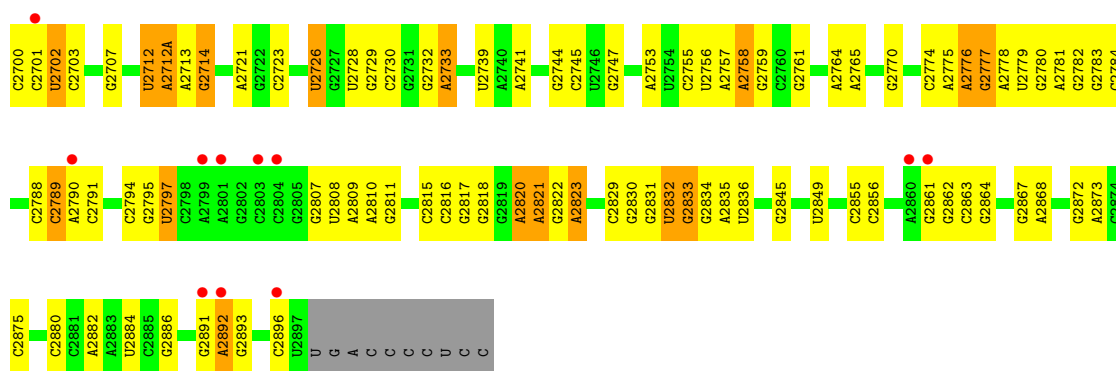


• Molecule 25: 23S rRNA

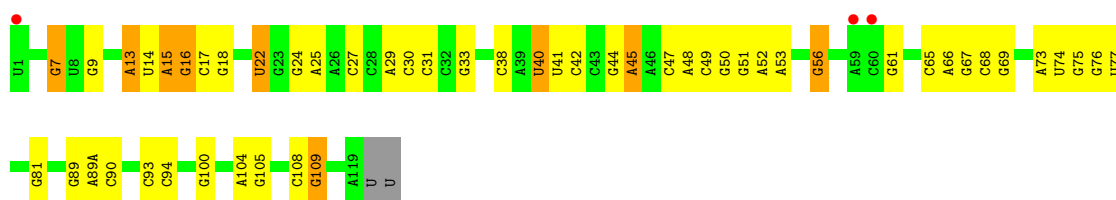




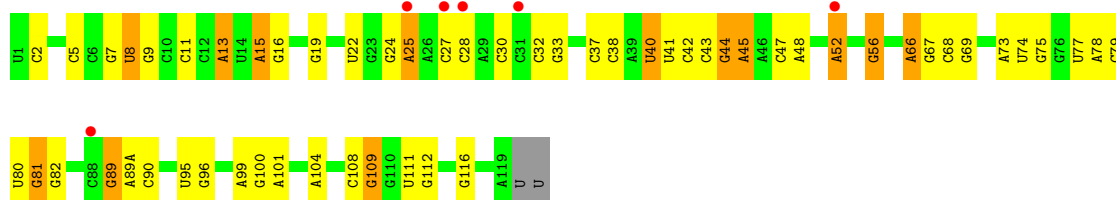




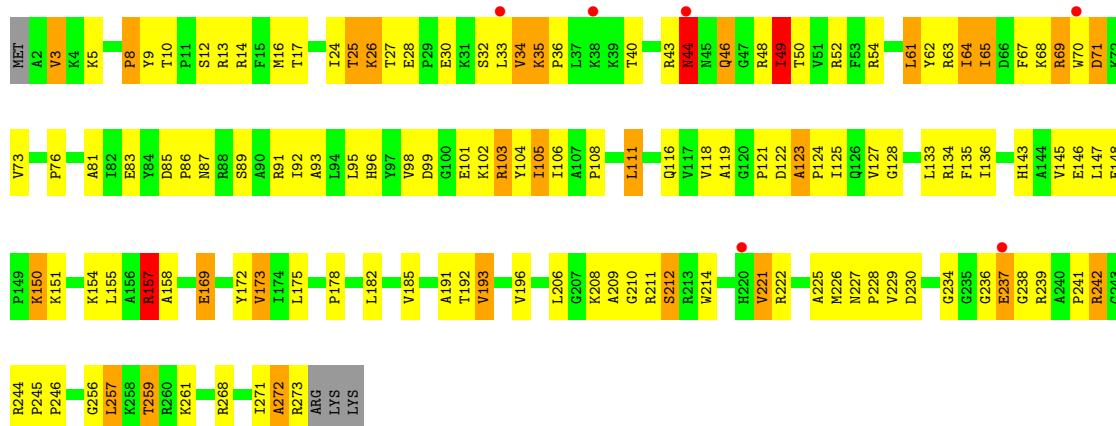
• Molecule 26: 5S rRNA



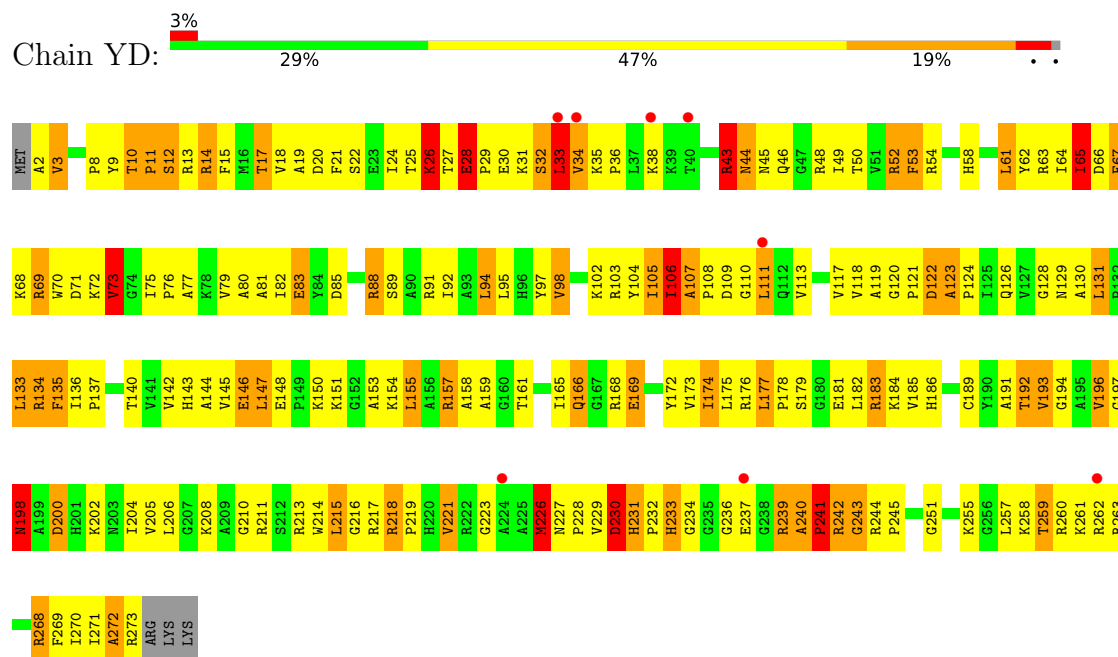
• Molecule 26: 5S rRNA



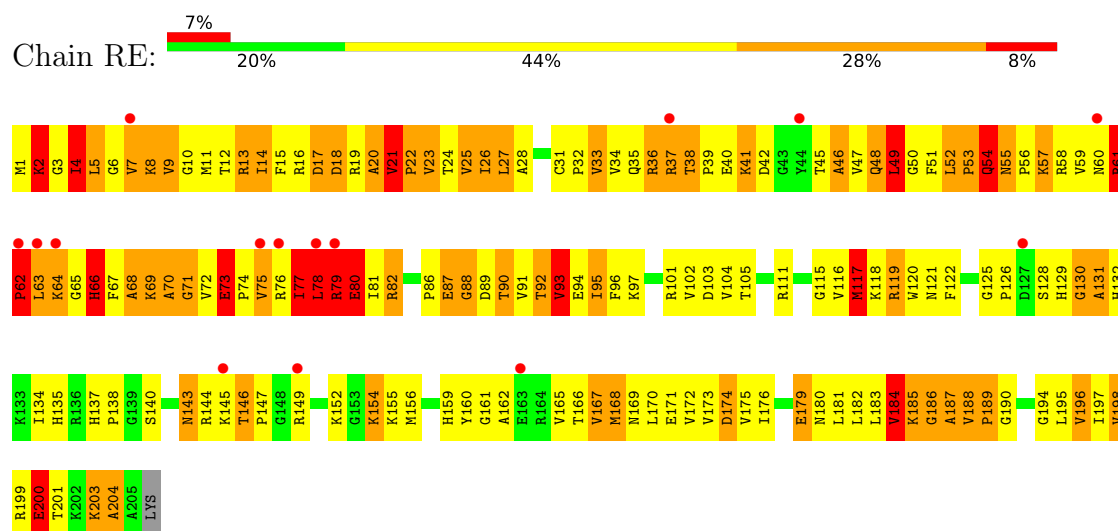
• Molecule 27: 50S ribosomal protein L2



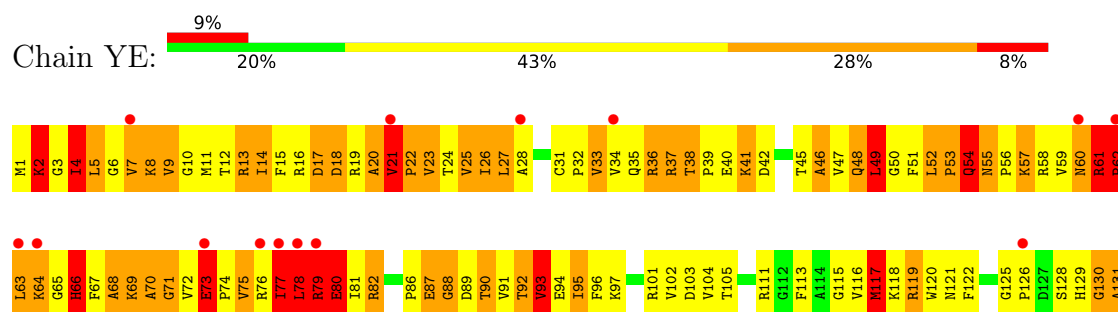
• Molecule 27: 50S ribosomal protein L2

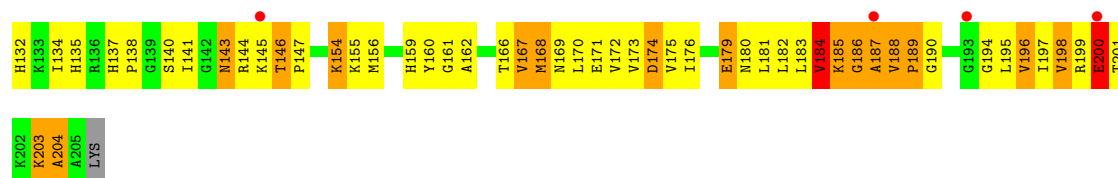


• Molecule 28: 50S ribosomal protein L3

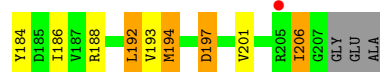
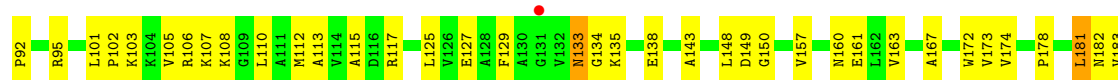
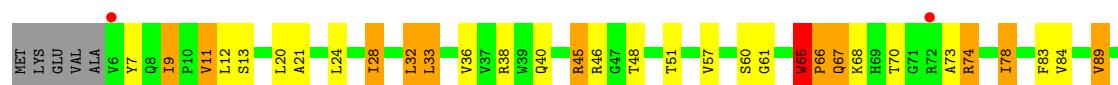


• Molecule 28: 50S ribosomal protein L3

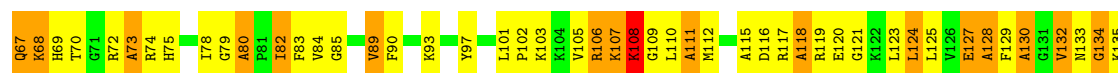
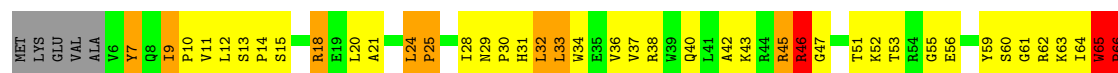




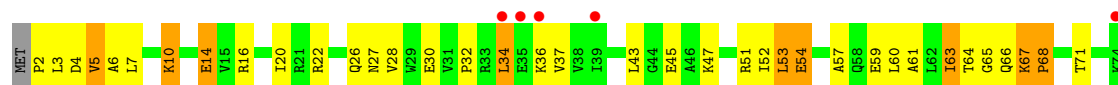
• Molecule 29: 50S ribosomal protein L4



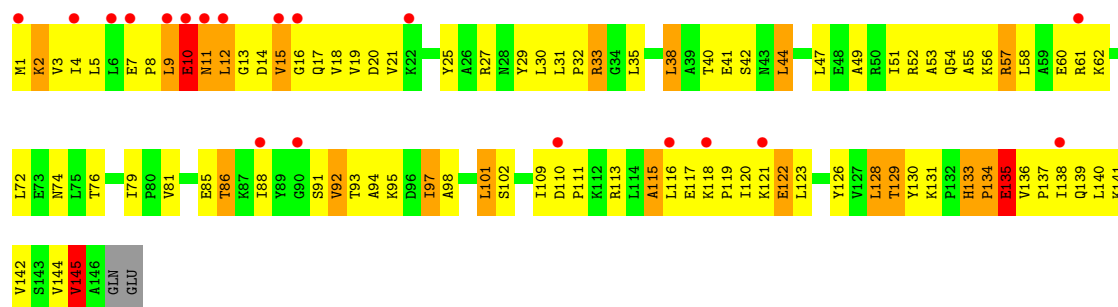
• Molecule 29: 50S ribosomal protein L4



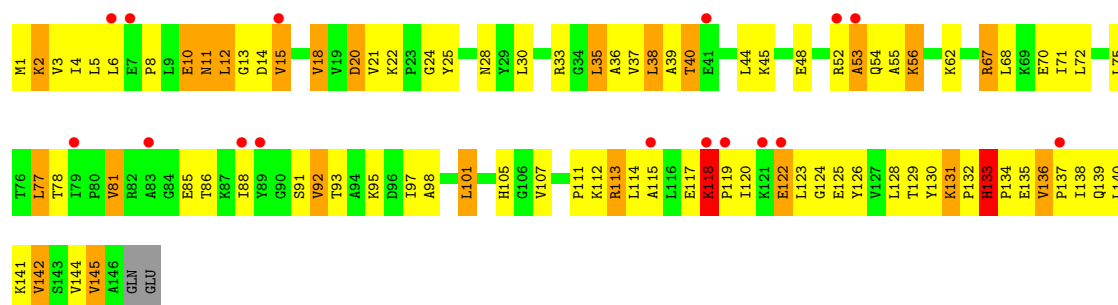
• Molecule 30: 50S ribosomal protein L5



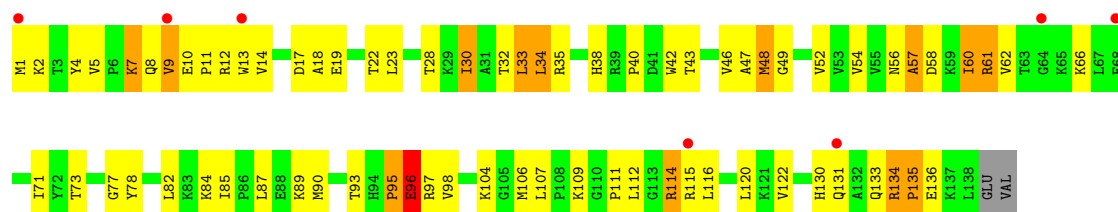




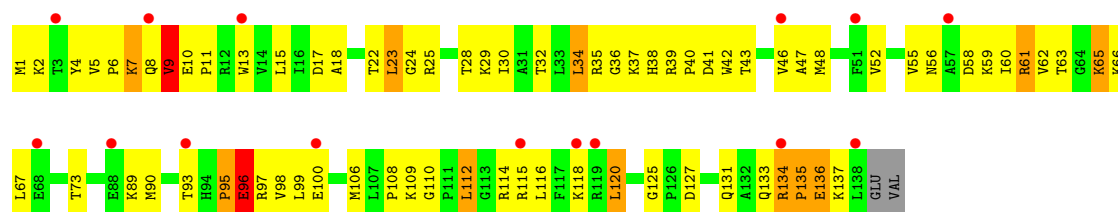
• Molecule 32: 50S ribosomal protein L9



• Molecule 33: 50S ribosomal protein L13

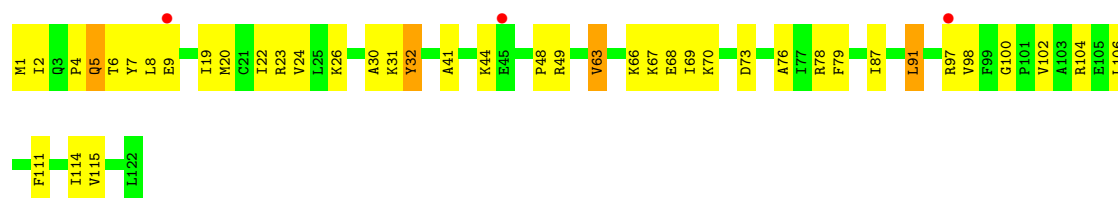


• Molecule 33: 50S ribosomal protein L13



• Molecule 34: 50S ribosomal protein L14

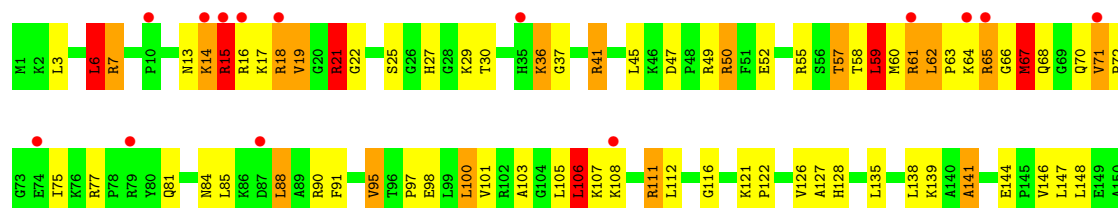




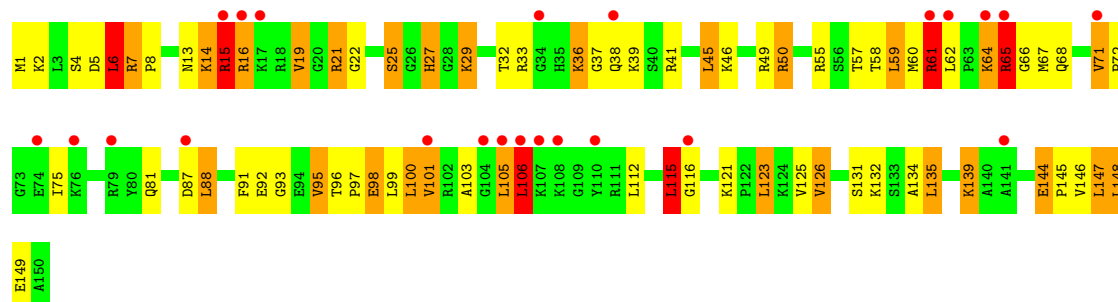
• Molecule 34: 50S ribosomal protein L14



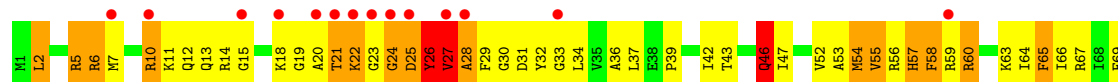
• Molecule 35: 50S ribosomal protein L15

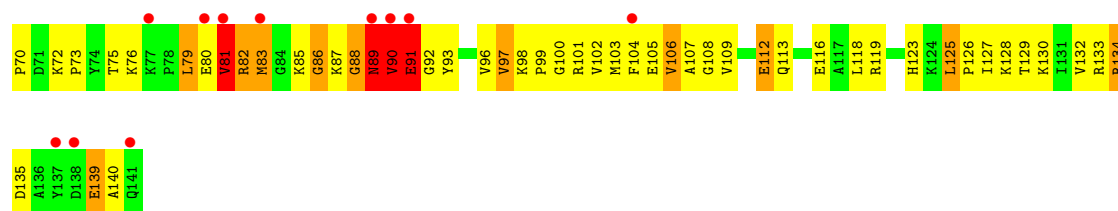


• Molecule 35: 50S ribosomal protein L15

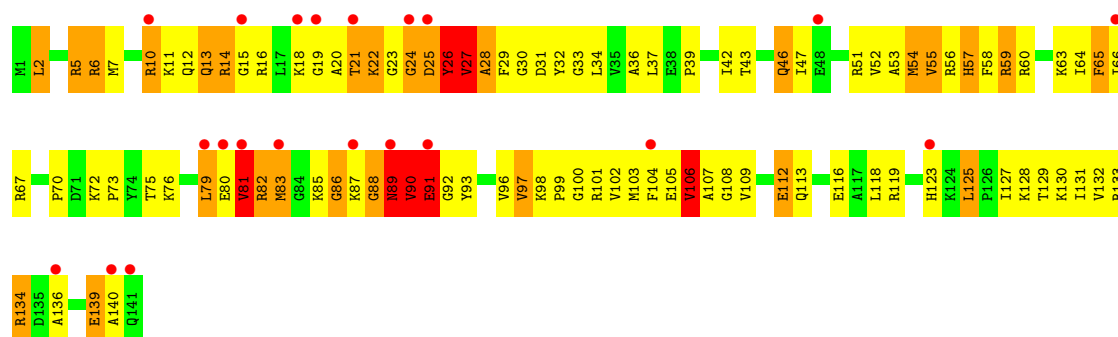


• Molecule 36: 50S ribosomal protein L16

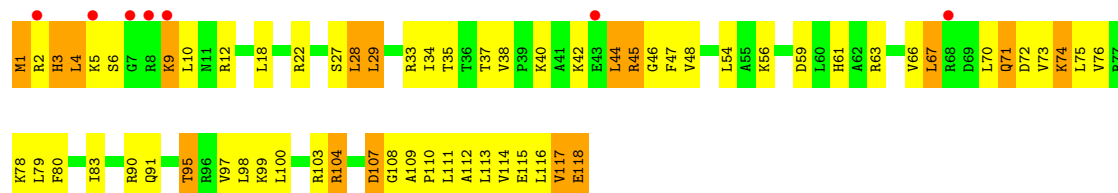




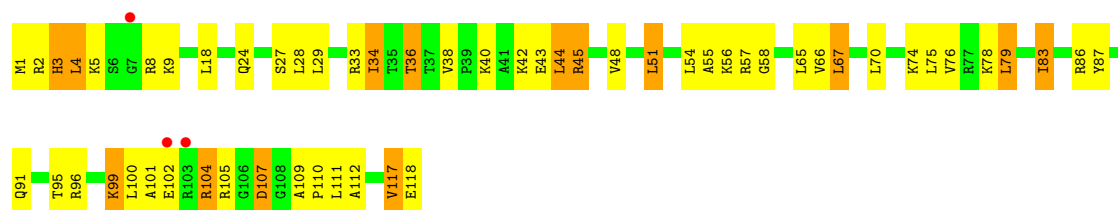
• Molecule 36: 50S ribosomal protein L16



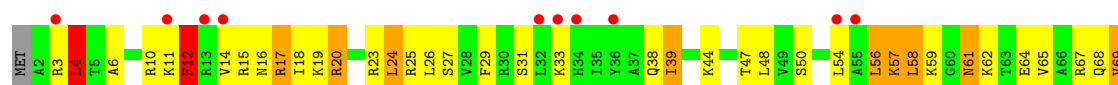
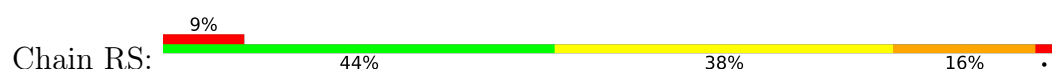
• Molecule 37: 50S ribosomal protein L17



• Molecule 37: 50S ribosomal protein L17

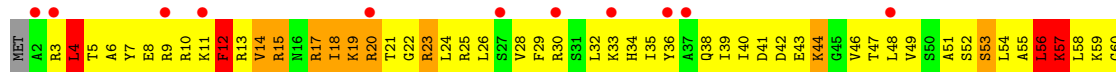
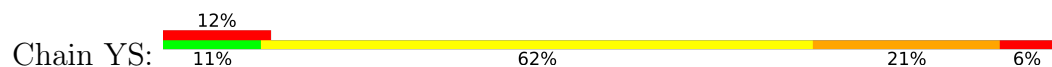


• Molecule 38: 50S ribosomal protein L18





- Molecule 38: 50S ribosomal protein L18



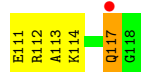
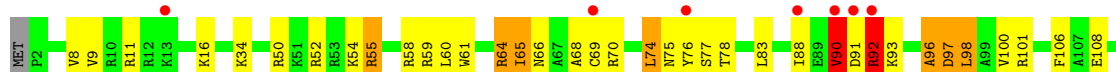
- Molecule 39: 50S ribosomal protein L19



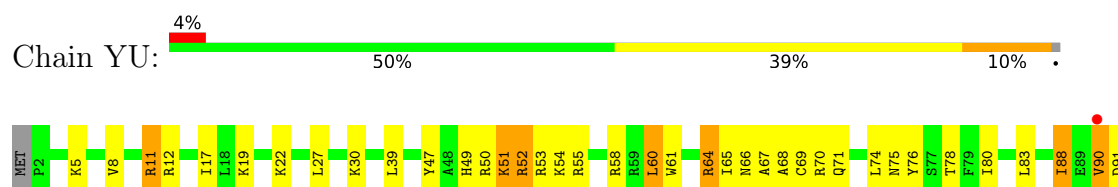
- Molecule 39: 50S ribosomal protein L19



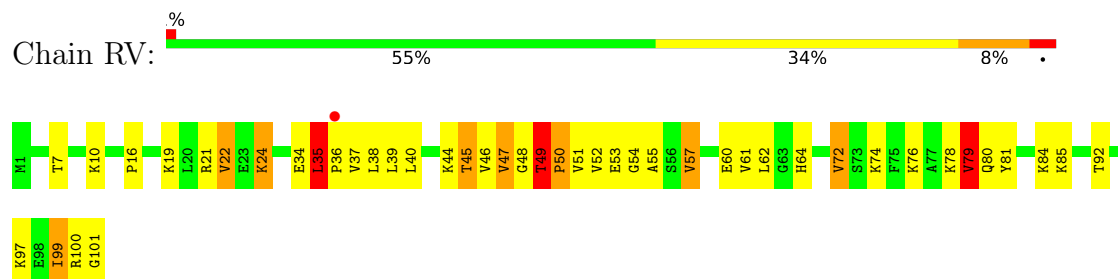
- Molecule 40: 50S ribosomal protein L20



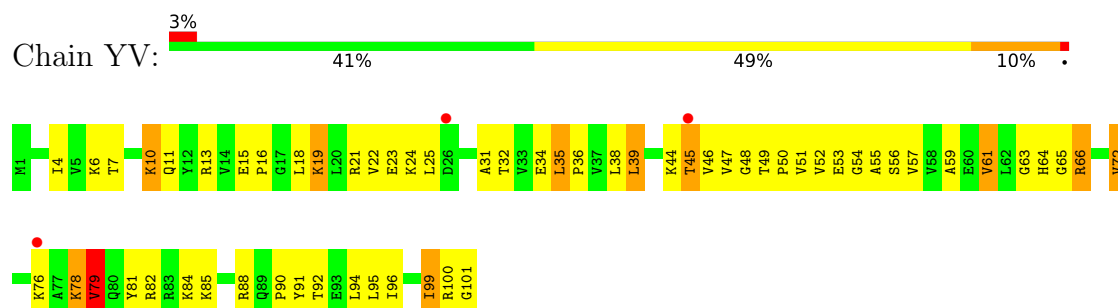
- Molecule 40: 50S ribosomal protein L20



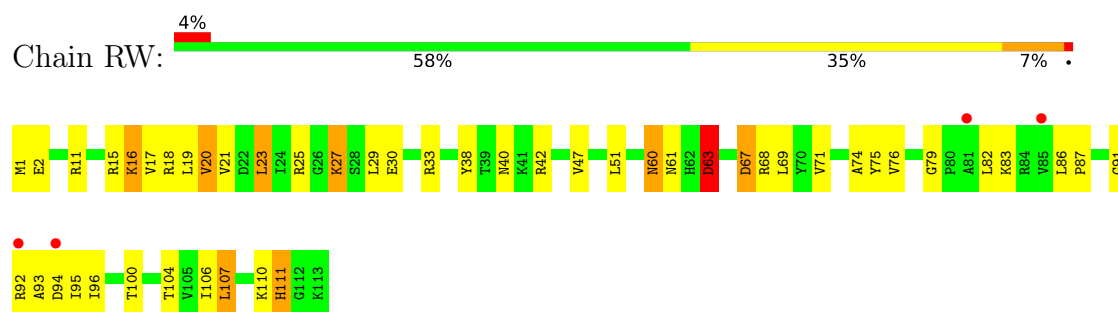
• Molecule 41: 50S ribosomal protein L21



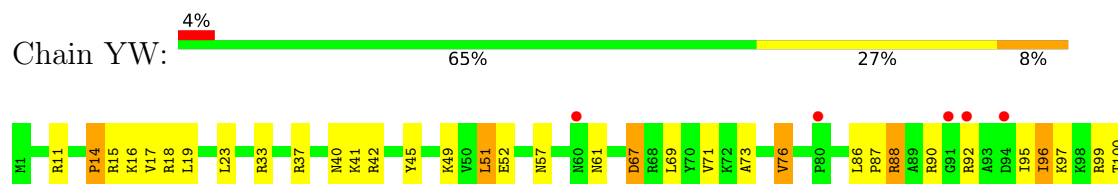
• Molecule 41: 50S ribosomal protein L21



• Molecule 42: 50S ribosomal protein L22

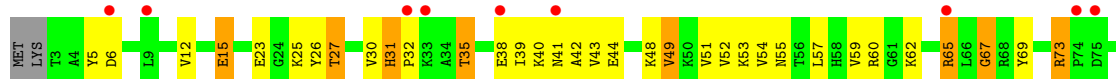


• Molecule 42: 50S ribosomal protein L22

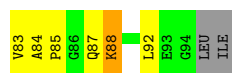




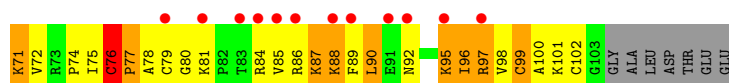
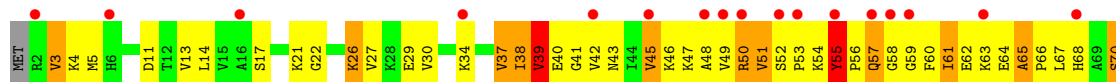
- Molecule 43: 50S ribosomal protein L23



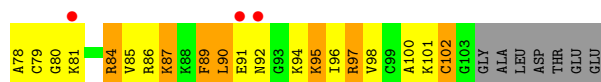
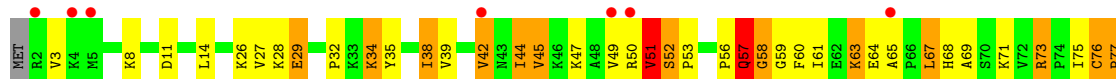
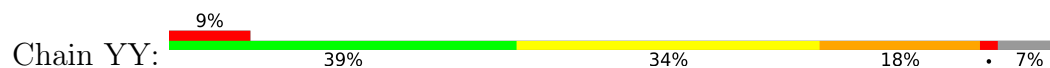
- Molecule 43: 50S ribosomal protein L23



- Molecule 44: 50S ribosomal protein L24

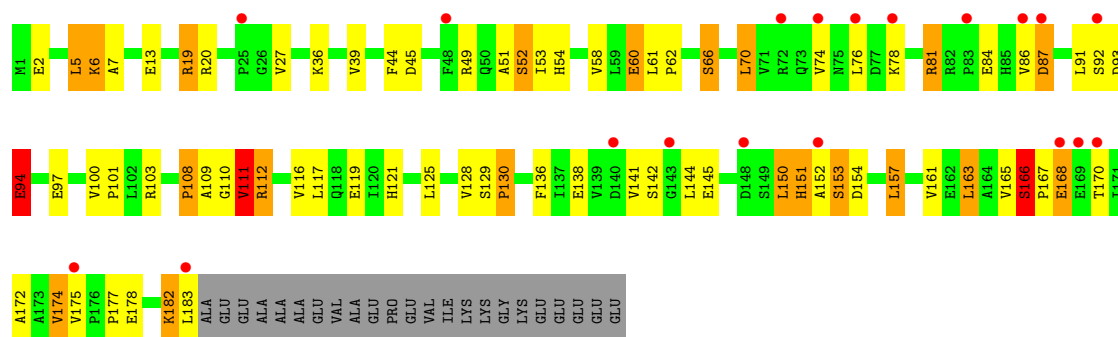


- Molecule 44: 50S ribosomal protein L24

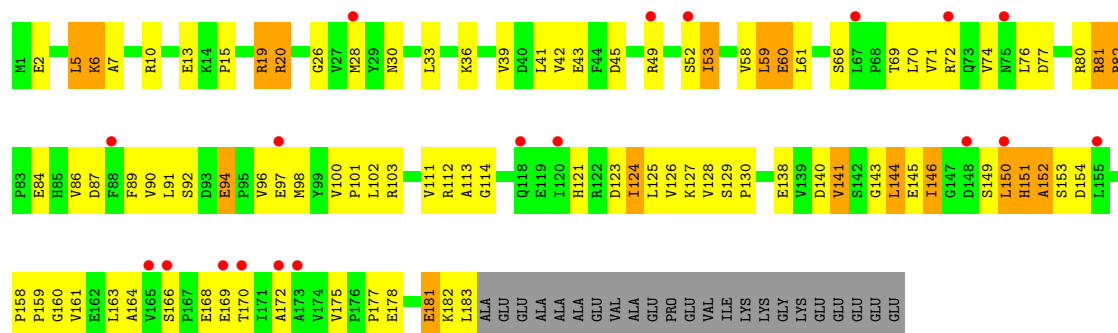
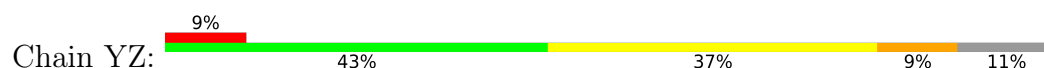


- Molecule 45: 50S ribosomal protein L25

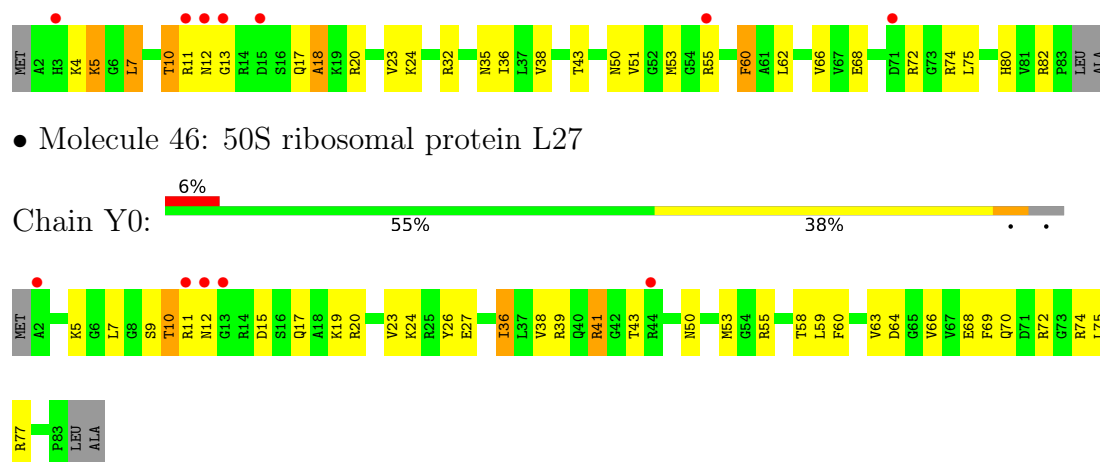




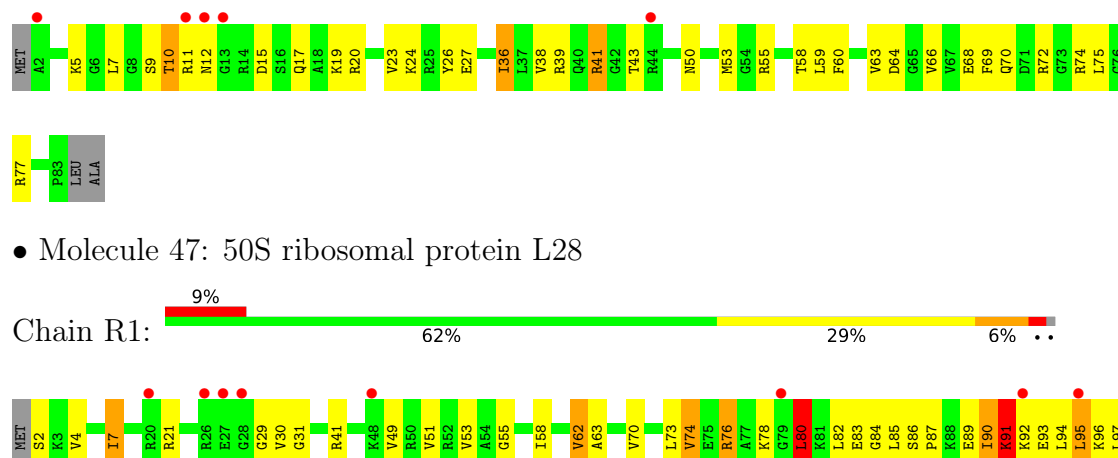
• Molecule 45: 50S ribosomal protein L25



• Molecule 46: 50S ribosomal protein L27



• Molecule 46: 50S ribosomal protein L27



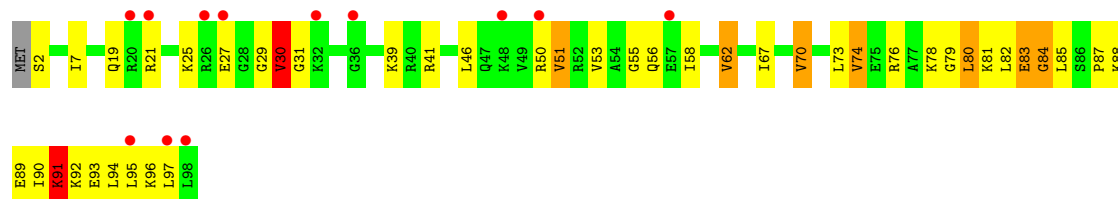
• Molecule 47: 50S ribosomal protein L28





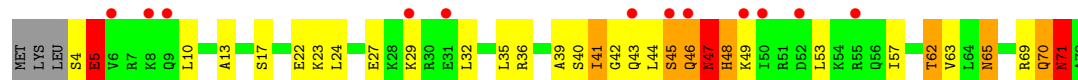
- Molecule 47: 50S ribosomal protein L28

Chain Y1: 12% 55% 35% 7% ..



- Molecule 48: 50S ribosomal protein L29

Chain R2: 17% 51% 31% 10% . .



- Molecule 48: 50S ribosomal protein L29

Chain Y2: 6% 19% 51% 24% . .



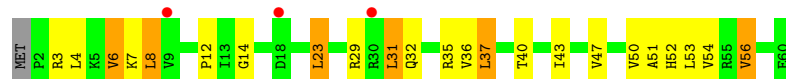
- Molecule 49: 50S ribosomal protein L30

Chain R3: 5% 68% 25% 5% .



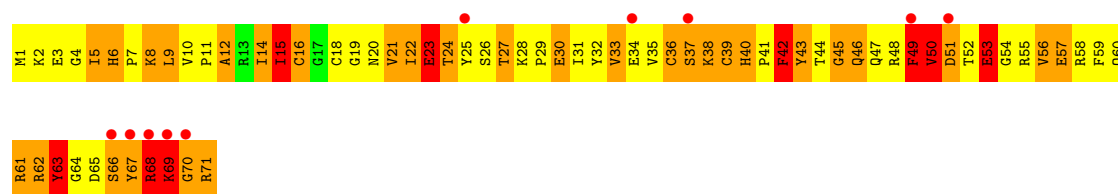
- Molecule 49: 50S ribosomal protein L30

Chain Y3: 5% 60% 28% 10% .

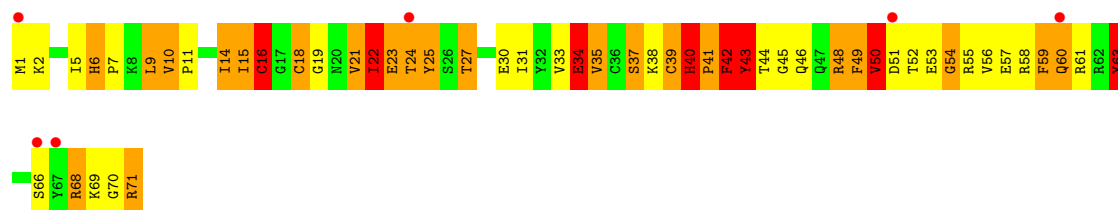
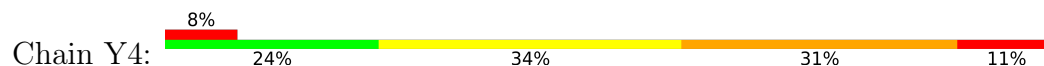


- Molecule 50: 50S ribosomal protein L31

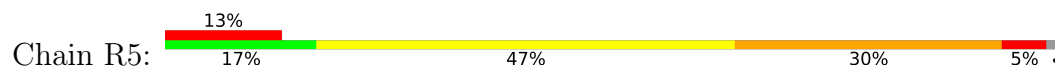
Chain R4: 14% 42% 42% 13%



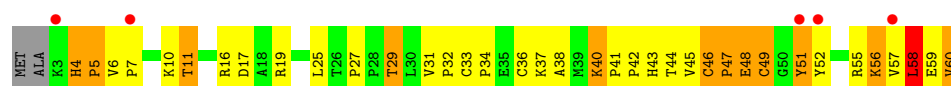
• Molecule 50: 50S ribosomal protein L31



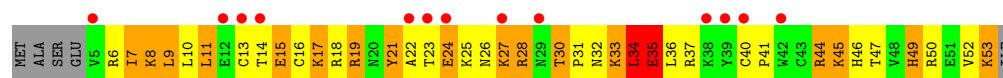
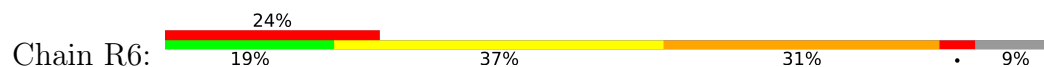
• Molecule 51: 50S ribosomal protein L32



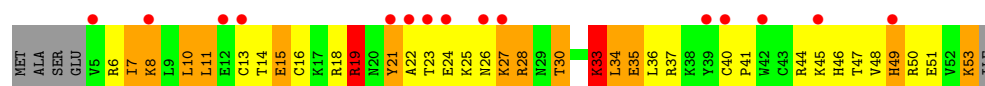
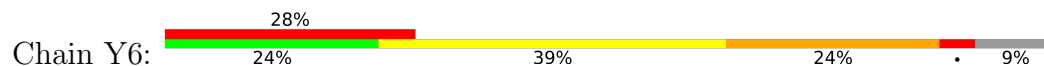
• Molecule 51: 50S ribosomal protein L32



• Molecule 52: 50S ribosomal protein L33

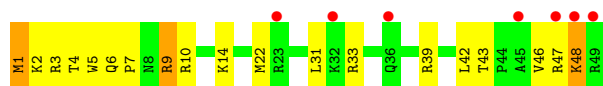


• Molecule 52: 50S ribosomal protein L33



• Molecule 53: 50S ribosomal protein L34

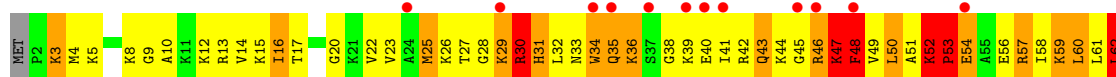
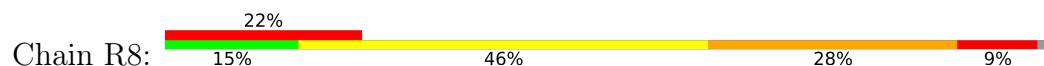




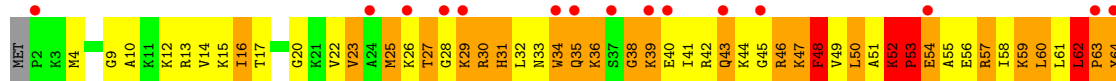
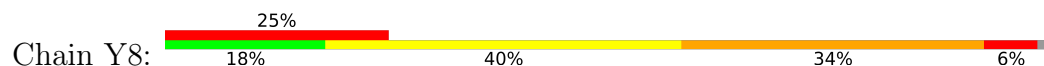
- Molecule 53: 50S ribosomal protein L34



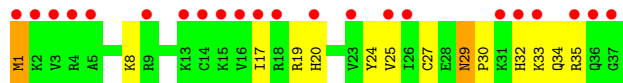
- Molecule 54: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: CC-Puro





- Molecule 56: CC-Puro

Chain Z6:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.46Å 450.70Å 621.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 3.60 49.85 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.85-3.60) 99.9 (49.85-3.60)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.205 , 0.244 0.206 , 0.244	Depositor DCC
R_{free} test set	36000 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	102.3	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 128.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	292106	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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, PPU, PAR, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	QA	0.18	0/36098	0.37	0/56341
1	XA	0.18	0/36101	0.37	2/56346 (0.0%)
2	QB	0.40	0/1959	0.87	4/2642 (0.2%)
2	XB	0.41	0/1959	0.89	4/2642 (0.2%)
3	QC	0.44	0/1629	0.87	0/2195
3	XC	0.48	0/1629	0.85	1/2195 (0.0%)
4	QD	0.34	0/1733	0.81	4/2318 (0.2%)
4	XD	0.51	0/1733	0.96	5/2318 (0.2%)
5	QE	0.50	1/1171 (0.1%)	0.97	6/1576 (0.4%)
5	XE	0.54	0/1171	0.94	2/1576 (0.1%)
6	QF	0.46	0/856	0.80	0/1154
6	XF	0.52	0/856	0.87	0/1154
7	QG	0.43	0/1276	0.85	0/1709
7	XG	0.47	0/1276	0.88	2/1709 (0.1%)
8	QH	0.44	0/1136	0.93	2/1527 (0.1%)
8	XH	0.47	0/1136	0.92	4/1527 (0.3%)
9	QI	0.42	0/1029	0.90	1/1379 (0.1%)
9	XI	0.43	0/1029	0.90	2/1379 (0.1%)
10	QJ	0.56	1/814 (0.1%)	0.99	6/1095 (0.5%)
10	XJ	0.52	2/814 (0.2%)	1.03	6/1095 (0.5%)
11	QK	0.50	0/900	0.94	3/1213 (0.2%)
11	XK	0.52	0/900	0.94	0/1213
12	QL	0.59	1/991 (0.1%)	1.23	9/1327 (0.7%)
12	XL	0.59	0/991	1.27	12/1327 (0.9%)
13	QM	0.43	0/974	0.97	1/1303 (0.1%)
13	XM	0.47	0/974	0.97	1/1303 (0.1%)
14	QN	0.50	0/501	0.96	1/664 (0.2%)
14	XN	0.57	0/501	1.04	3/664 (0.5%)
15	QO	0.46	0/745	0.80	0/992
15	XO	0.50	0/745	0.90	0/992
16	QP	0.48	0/721	0.94	2/970 (0.2%)
16	XP	0.48	0/721	0.88	1/970 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.42	0/847	0.85	0/1131
17	XQ	0.43	0/847	0.83	0/1131
18	QR	0.45	0/579	0.89	0/768
18	XR	0.47	0/579	0.85	1/768 (0.1%)
19	QS	0.46	0/689	0.99	3/926 (0.3%)
19	XS	0.48	0/689	1.01	6/926 (0.6%)
20	QT	0.53	1/765 (0.1%)	1.03	3/1007 (0.3%)
20	XT	0.45	0/765	1.06	4/1007 (0.4%)
21	QU	0.39	0/221	0.80	0/288
21	XU	0.38	0/221	0.82	0/288
22	QV	0.19	0/1836	0.35	0/2859
22	XV	0.20	0/1836	0.38	0/2859
23	QX	0.13	0/192	0.24	0/297
23	XX	0.16	0/192	0.25	0/297
24	QY	0.12	0/355	0.22	0/551
24	XY	0.16	0/355	0.32	0/551
25	RA	0.22	0/69521	0.41	3/108529 (0.0%)
25	YA	0.23	0/69521	0.42	2/108529 (0.0%)
26	RB	0.20	0/2878	0.40	0/4490
26	YB	0.20	0/2878	0.40	0/4490
27	RD	0.64	0/2165	1.07	10/2919 (0.3%)
27	YD	0.72	1/2165 (0.0%)	1.30	30/2919 (1.0%)
28	RE	0.62	0/1601	1.35	29/2160 (1.3%)
28	YE	0.62	0/1601	1.35	29/2160 (1.3%)
29	RF	0.38	0/1620	0.83	2/2194 (0.1%)
29	YF	0.62	0/1620	1.20	20/2194 (0.9%)
30	RG	0.41	0/1499	0.91	0/2016
30	YG	0.51	0/1499	0.91	2/2016 (0.1%)
31	RH	0.58	0/1332	1.22	14/1802 (0.8%)
31	YH	0.57	0/1332	1.22	15/1802 (0.8%)
32	RI	0.41	0/1151	0.90	2/1558 (0.1%)
32	YI	0.42	0/1151	0.92	4/1558 (0.3%)
33	RN	0.52	0/1131	1.01	2/1525 (0.1%)
33	YN	0.56	0/1131	0.95	1/1525 (0.1%)
34	RO	0.56	0/943	0.98	3/1269 (0.2%)
34	YO	0.60	0/943	0.98	0/1269
35	RP	0.40	0/1162	0.90	2/1544 (0.1%)
35	YP	0.44	0/1162	0.96	2/1544 (0.1%)
36	RQ	0.71	0/1143	1.36	19/1527 (1.2%)
36	YQ	0.71	0/1143	1.35	19/1527 (1.2%)
37	RR	0.55	0/982	0.99	1/1312 (0.1%)
37	YR	0.57	0/982	1.04	3/1312 (0.2%)
38	RS	0.43	0/892	0.88	0/1187

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YS	0.53	0/892	1.14	7/1187 (0.6%)
39	RT	0.54	0/1155	0.98	3/1542 (0.2%)
39	YT	0.57	0/1155	1.05	7/1542 (0.5%)
40	RU	0.54	0/982	1.04	6/1306 (0.5%)
40	YU	0.65	0/982	1.07	2/1306 (0.2%)
41	RV	0.47	0/790	0.97	4/1057 (0.4%)
41	YV	0.58	0/790	1.01	2/1057 (0.2%)
42	RW	0.65	0/911	0.98	1/1220 (0.1%)
42	YW	0.60	0/911	1.01	0/1220
43	RX	0.59	0/739	0.95	4/993 (0.4%)
43	YX	0.60	0/739	1.00	1/993 (0.1%)
44	RY	0.54	0/798	1.07	6/1064 (0.6%)
44	YY	0.59	0/798	1.09	5/1064 (0.5%)
45	RZ	0.37	0/1493	0.88	7/2026 (0.3%)
45	YZ	0.38	0/1493	0.93	4/2026 (0.2%)
46	R0	0.56	0/657	1.04	5/874 (0.6%)
46	Y0	0.61	0/657	0.98	1/874 (0.1%)
47	R1	0.56	0/770	0.97	0/1022
47	Y1	0.59	0/770	0.96	1/1022 (0.1%)
48	R2	0.47	0/583	1.00	2/771 (0.3%)
48	Y2	0.60	0/583	1.32	8/771 (1.0%)
49	R3	0.47	0/474	0.91	0/635
49	Y3	0.53	0/474	0.87	0/635
50	R4	0.47	0/594	1.24	10/795 (1.3%)
50	Y4	0.53	0/594	1.16	6/795 (0.8%)
51	R5	0.64	0/473	1.21	6/639 (0.9%)
51	Y5	0.67	0/468	1.15	4/632 (0.6%)
52	R6	0.53	0/431	1.01	2/575 (0.3%)
52	Y6	0.56	0/431	1.00	2/575 (0.3%)
53	R7	0.63	0/438	1.05	2/575 (0.3%)
53	Y7	0.69	0/438	1.02	3/575 (0.5%)
54	R8	0.79	0/525	1.39	9/691 (1.3%)
54	Y8	0.80	0/525	1.41	9/691 (1.3%)
55	R9	0.36	0/310	0.81	0/407
55	Y9	0.46	0/310	0.81	0/407
56	Z5	0.45	0/40	0.62	0/60
56	Z6	0.46	0/40	0.62	0/60
All	All	0.34	7/316398 (0.0%)	0.63	444/473030 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	QJ	59	SER	C-N	-8.64	1.25	1.33
5	QE	70	PRO	N-CD	5.47	1.55	1.47
12	QL	48	PRO	N-CD	5.45	1.55	1.47
10	XJ	53	PRO	N-CD	5.28	1.55	1.47
20	QT	83	ARG	C-N	-5.20	1.26	1.33

The worst 5 of 444 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	R4	39	CYS	N-CA-C	-13.57	95.98	112.54
28	YE	58	ARG	N-CA-C	-11.81	95.23	113.89
28	RE	58	ARG	N-CA-C	-11.79	95.26	113.89
48	Y2	5	GLU	N-CA-C	-11.59	99.63	113.88
12	XL	119	LYS	N-CA-C	-10.38	95.16	110.52

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	450	0
1	XA	32249	0	16279	450	1
2	QB	1924	0	1975	66	0
2	XB	1924	0	1975	91	0
3	QC	1605	0	1668	51	0
3	XC	1605	0	1668	60	0
4	QD	1703	0	1764	60	0
4	XD	1703	0	1762	55	0
5	QE	1155	0	1213	48	0
5	XE	1155	0	1213	52	0
6	QF	843	0	857	17	0
6	XF	843	0	857	26	0
7	QG	1257	0	1296	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	22	0
8	QH	1116	0	1177	40	0
8	XH	1116	0	1177	29	0
9	QI	1010	0	1037	37	0
9	XI	1010	0	1037	43	0
10	QJ	801	0	849	65	0
10	XJ	801	0	849	56	0
11	QK	885	0	903	31	0
11	XK	885	0	904	27	0
12	QL	975	0	1062	95	0
12	XL	975	0	1062	105	0
13	QM	964	0	1034	51	0
13	XM	964	0	1034	45	0
14	QN	492	0	529	23	0
14	XN	492	0	529	21	0
15	QO	734	0	771	20	0
15	XO	734	0	771	16	0
16	QP	705	0	725	13	0
16	XP	705	0	725	24	0
17	QQ	834	0	904	21	0
17	XQ	834	0	904	19	0
18	QR	574	0	644	12	0
18	XR	574	0	644	21	0
19	QS	674	0	699	77	0
19	XS	674	0	699	54	0
20	QT	763	0	861	36	0
20	XT	763	0	861	65	0
21	QU	217	0	234	12	0
21	XU	217	0	234	6	0
22	QV	1644	0	836	12	0
22	XV	1644	0	836	21	0
23	QX	173	0	87	0	0
23	XX	173	0	87	1	0
24	QY	319	0	162	1	0
24	XY	319	0	162	3	0
25	RA	62071	0	31287	844	0
25	YA	62071	0	31287	873	0
26	RB	2573	0	1306	38	0
26	YB	2573	0	1306	46	0
27	RD	2115	0	2195	102	0
27	YD	2115	0	2195	321	0
28	RE	1568	0	1634	288	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	YE	1568	0	1634	302	0
29	RF	1585	0	1632	57	0
29	YF	1585	0	1632	192	0
30	RG	1474	0	1535	101	0
30	YG	1474	0	1535	73	0
31	RH	1307	0	1382	230	0
31	YH	1307	0	1382	237	0
32	RI	1136	0	1223	64	1
32	YI	1136	0	1223	53	0
33	RN	1104	0	1180	44	0
33	YN	1104	0	1180	58	0
34	RO	933	0	996	31	0
34	YO	933	0	996	32	0
35	RP	1145	0	1228	75	0
35	YP	1145	0	1227	81	0
36	RQ	1122	0	1179	167	0
36	YQ	1122	0	1179	171	0
37	RR	968	0	1033	49	0
37	YR	968	0	1033	34	0
38	RS	882	0	943	49	0
38	YS	882	0	943	167	0
39	RT	1141	0	1202	63	0
39	YT	1141	0	1202	57	0
40	RU	964	0	1022	30	0
40	YU	964	0	1022	61	0
41	RV	779	0	852	22	0
41	YV	779	0	852	49	0
42	RW	900	0	964	26	0
42	YW	900	0	964	28	0
43	RX	725	0	778	31	0
43	YX	725	0	778	25	0
44	RY	785	0	878	53	0
44	YY	785	0	878	45	0
45	RZ	1461	0	1493	44	0
45	YZ	1461	0	1493	60	0
46	R0	648	0	672	26	0
46	Y0	648	0	672	36	0
47	R1	763	0	848	24	0
47	Y1	763	0	848	31	0
48	R2	581	0	629	21	0
48	Y2	581	0	629	81	0
49	R3	469	0	518	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Y3	469	0	518	16	0
50	R4	581	0	575	218	0
50	Y4	581	0	577	102	0
51	R5	459	0	480	84	0
51	Y5	454	0	475	40	0
52	R6	424	0	450	29	0
52	Y6	424	0	450	31	0
53	R7	430	0	480	21	0
53	Y7	430	0	480	22	0
54	R8	517	0	582	96	0
54	Y8	517	0	582	112	0
55	R9	307	0	338	11	0
55	Y9	307	0	338	14	0
56	Z5	74	0	51	6	0
56	Z6	74	0	51	11	0
57	QA	90	0	0	0	0
57	QF	1	0	0	0	0
57	QK	1	0	0	0	0
57	QM	1	0	0	0	0
57	QT	1	0	0	0	0
57	QV	2	0	0	0	0
57	QY	1	0	0	0	0
57	R0	2	0	0	0	0
57	R3	1	0	0	0	0
57	R5	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	281	0	0	0	0
57	RB	3	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	RQ	1	0	0	0	0
57	RR	2	0	0	0	0
57	XA	104	0	0	0	0
57	XD	1	0	0	0	0
57	XV	3	0	0	0	0
57	XX	1	0	0	0	0
57	XY	1	0	0	0	0
57	Y0	1	0	0	0	0
57	Y1	1	0	0	0	0
57	Y3	1	0	0	0	0
57	Y5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	Y7	1	0	0	0	0
57	YA	291	0	0	0	0
57	YB	3	0	0	0	0
57	YD	1	0	0	0	0
57	YE	2	0	0	0	0
57	YP	3	0	0	0	0
57	YR	2	0	0	0	0
57	YY	1	0	0	0	0
58	QA	42	0	45	1	0
58	XA	42	0	45	0	0
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	292106	0	198346	7806	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 7806 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)
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.35	1.54
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.36	1.52
30:RG:112:PRO:HB3	50:R4:37:SER:CB	1.45	1.45
30:RG:112:PRO:CB	50:R4:37:SER:HB2	1.46	1.42
19:QS:68:GLY:CA	50:R4:68:ARG:HG2	1.51	1.38

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:RI:91:SER:OG	1:XA:368:U:OP1[4_555]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	174 (74%)	44 (19%)	17 (7%)	1	10
2	XB	235/256 (92%)	177 (75%)	43 (18%)	15 (6%)	1	12
3	QC	203/239 (85%)	164 (81%)	33 (16%)	6 (3%)	3	25
3	XC	203/239 (85%)	172 (85%)	28 (14%)	3 (2%)	8	37
4	QD	206/209 (99%)	186 (90%)	17 (8%)	3 (2%)	8	37
4	XD	206/209 (99%)	176 (85%)	25 (12%)	5 (2%)	4	29
5	QE	149/162 (92%)	136 (91%)	9 (6%)	4 (3%)	4	27
5	XE	149/162 (92%)	134 (90%)	13 (9%)	2 (1%)	9	39
6	QF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
6	XF	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	QG	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	9	39
7	XG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	9	39
8	QH	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	18	51
8	XH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	3	26
9	QI	125/128 (98%)	103 (82%)	17 (14%)	5 (4%)	2	20
9	XI	125/128 (98%)	97 (78%)	24 (19%)	4 (3%)	3	24
10	QJ	97/105 (92%)	77 (79%)	16 (16%)	4 (4%)	2	19
10	XJ	97/105 (92%)	79 (81%)	13 (13%)	5 (5%)	1	15
11	QK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	7	35
11	XK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	7	35
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	4
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	4
13	QM	119/126 (94%)	95 (80%)	15 (13%)	9 (8%)	1	9
13	XM	119/126 (94%)	94 (79%)	16 (13%)	9 (8%)	1	9
14	QN	58/61 (95%)	50 (86%)	4 (7%)	4 (7%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	XN	58/61 (95%)	46 (79%)	6 (10%)	6 (10%)	0	5
15	QO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	10	41
15	XO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	5	30
16	QP	82/88 (93%)	73 (89%)	8 (10%)	1 (1%)	10	41
16	XP	82/88 (93%)	72 (88%)	9 (11%)	1 (1%)	10	41
17	QQ	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	6	32
17	XQ	98/105 (93%)	88 (90%)	10 (10%)	0	100	100
18	QR	68/88 (77%)	56 (82%)	9 (13%)	3 (4%)	2	18
18	XR	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	8	37
19	QS	82/93 (88%)	55 (67%)	16 (20%)	11 (13%)	0	3
19	XS	82/93 (88%)	54 (66%)	18 (22%)	10 (12%)	0	4
20	QT	97/106 (92%)	76 (78%)	15 (16%)	6 (6%)	1	12
20	XT	97/106 (92%)	77 (79%)	16 (16%)	4 (4%)	2	19
21	QU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	2	18
21	XU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	2	18
27	RD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	2	18
27	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	1	10
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	1
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	1
29	RF	200/210 (95%)	181 (90%)	13 (6%)	6 (3%)	3	25
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0	5
30	RG	179/182 (98%)	139 (78%)	25 (14%)	15 (8%)	0	7
30	YG	179/182 (98%)	142 (79%)	25 (14%)	12 (7%)	1	11
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%)	109 (76%)	24 (17%)	11 (8%)	1	9
32	YI	144/148 (97%)	108 (75%)	23 (16%)	13 (9%)	0	6
33	RN	136/140 (97%)	104 (76%)	20 (15%)	12 (9%)	0	7
33	YN	136/140 (97%)	107 (79%)	16 (12%)	13 (10%)	0	6
34	RO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	7	35
34	YO	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	7	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	RP	148/150 (99%)	109 (74%)	26 (18%)	13 (9%)	0	7
35	YP	148/150 (99%)	101 (68%)	35 (24%)	12 (8%)	1	8
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	0	5
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	0	5
37	RR	116/118 (98%)	106 (91%)	5 (4%)	5 (4%)	2	18
37	YR	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	1	15
38	RS	109/112 (97%)	76 (70%)	22 (20%)	11 (10%)	0	5
38	YS	109/112 (97%)	62 (57%)	29 (27%)	18 (16%)	0	2
39	RT	135/146 (92%)	108 (80%)	15 (11%)	12 (9%)	0	7
39	YT	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	1	9
40	RU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	3	23
40	YU	115/118 (98%)	102 (89%)	11 (10%)	2 (2%)	7	35
41	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	1	13
41	YV	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	8
42	RW	111/113 (98%)	99 (89%)	8 (7%)	4 (4%)	2	22
42	YW	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	6	34
43	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	5	30
43	YX	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	5	30
44	RY	100/110 (91%)	71 (71%)	13 (13%)	16 (16%)	0	2
44	YY	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	0	4
45	RZ	181/206 (88%)	127 (70%)	34 (19%)	20 (11%)	0	5
45	YZ	181/206 (88%)	135 (75%)	28 (16%)	18 (10%)	0	6
46	R0	80/85 (94%)	66 (82%)	13 (16%)	1 (1%)	9	39
46	Y0	80/85 (94%)	73 (91%)	7 (9%)	0	100	100
47	R1	95/98 (97%)	75 (79%)	11 (12%)	9 (10%)	0	6
47	Y1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	1	12
48	R2	67/72 (93%)	54 (81%)	9 (13%)	4 (6%)	1	13
48	Y2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	3
49	R3	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	3	23
49	Y3	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	6	34
50	R4	69/71 (97%)	22 (32%)	21 (30%)	26 (38%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	Y4	69/71 (97%)	34 (49%)	14 (20%)	21 (30%)	0	0
51	R5	57/60 (95%)	33 (58%)	10 (18%)	14 (25%)	0	0
51	Y5	56/60 (93%)	46 (82%)	8 (14%)	2 (4%)	2	22
52	R6	47/54 (87%)	23 (49%)	13 (28%)	11 (23%)	0	0
52	Y6	47/54 (87%)	22 (47%)	17 (36%)	8 (17%)	0	2
53	R7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	5	31
53	Y7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	5	31
54	R8	62/65 (95%)	36 (58%)	14 (23%)	12 (19%)	0	1
54	Y8	62/65 (95%)	38 (61%)	15 (24%)	9 (14%)	0	3
55	R9	35/37 (95%)	35 (100%)	0	0	100	100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11469/12128 (95%)	9030 (79%)	1608 (14%)	831 (7%)	1	10

5 of 831 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	236	TYR
3	QC	12	LEU
3	QC	190	ARG
4	QD	33	MET
12	QL	18	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	170 (83%)	35 (17%)	2	13
2	XB	205/220 (93%)	180 (88%)	25 (12%)	5	23
3	QC	159/188 (85%)	146 (92%)	13 (8%)	10	36
3	XC	159/188 (85%)	145 (91%)	14 (9%)	9	33
4	QD	180/181 (99%)	161 (89%)	19 (11%)	6	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	XD	180/181 (99%)	155 (86%)	25 (14%)	3	19
5	QE	116/123 (94%)	100 (86%)	16 (14%)	3	20
5	XE	116/123 (94%)	100 (86%)	16 (14%)	3	20
6	QF	90/90 (100%)	79 (88%)	11 (12%)	5	23
6	XF	90/90 (100%)	79 (88%)	11 (12%)	5	23
7	QG	126/127 (99%)	116 (92%)	10 (8%)	11	37
7	XG	126/127 (99%)	112 (89%)	14 (11%)	6	27
8	QH	119/119 (100%)	105 (88%)	14 (12%)	5	24
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	27
9	QI	98/99 (99%)	80 (82%)	18 (18%)	1	10
9	XI	98/99 (99%)	77 (79%)	21 (21%)	1	7
10	QJ	89/92 (97%)	77 (86%)	12 (14%)	4	21
10	XJ	89/92 (97%)	74 (83%)	15 (17%)	2	13
11	QK	90/99 (91%)	79 (88%)	11 (12%)	5	23
11	XK	90/99 (91%)	82 (91%)	8 (9%)	9	33
12	QL	104/109 (95%)	87 (84%)	17 (16%)	2	15
12	XL	104/109 (95%)	86 (83%)	18 (17%)	2	12
13	QM	97/101 (96%)	73 (75%)	24 (25%)	1	4
13	XM	97/101 (96%)	79 (81%)	18 (19%)	1	10
14	QN	49/50 (98%)	40 (82%)	9 (18%)	1	10
14	XN	49/50 (98%)	42 (86%)	7 (14%)	3	19
15	QO	79/80 (99%)	72 (91%)	7 (9%)	9	33
15	XO	79/80 (99%)	68 (86%)	11 (14%)	3	19
16	QP	72/74 (97%)	62 (86%)	10 (14%)	3	19
16	XP	72/74 (97%)	66 (92%)	6 (8%)	10	35
17	QQ	95/97 (98%)	86 (90%)	9 (10%)	8	32
17	XQ	95/97 (98%)	88 (93%)	7 (7%)	13	39
18	QR	61/77 (79%)	50 (82%)	11 (18%)	2	11
18	XR	61/77 (79%)	50 (82%)	11 (18%)	2	11
19	QS	73/80 (91%)	58 (80%)	15 (20%)	1	8
19	XS	73/80 (91%)	56 (77%)	17 (23%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	QT	76/82 (93%)	66 (87%)	10 (13%)	4	21
20	XT	76/82 (93%)	66 (87%)	10 (13%)	4	21
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
27	RD	214/218 (98%)	170 (79%)	44 (21%)	1	8
27	YD	214/218 (98%)	173 (81%)	41 (19%)	1	9
28	RE	165/166 (99%)	125 (76%)	40 (24%)	1	5
28	YE	165/166 (99%)	125 (76%)	40 (24%)	1	5
29	RF	161/166 (97%)	138 (86%)	23 (14%)	3	19
29	YF	161/166 (97%)	138 (86%)	23 (14%)	3	19
30	RG	155/156 (99%)	135 (87%)	20 (13%)	4	22
30	YG	155/156 (99%)	131 (84%)	24 (16%)	2	16
31	RH	142/148 (96%)	111 (78%)	31 (22%)	1	7
31	YH	142/148 (96%)	112 (79%)	30 (21%)	1	7
32	RI	122/124 (98%)	99 (81%)	23 (19%)	1	9
32	YI	122/124 (98%)	93 (76%)	29 (24%)	1	5
33	RN	117/119 (98%)	94 (80%)	23 (20%)	1	8
33	YN	117/119 (98%)	94 (80%)	23 (20%)	1	8
34	RO	100/100 (100%)	91 (91%)	9 (9%)	9	33
34	YO	100/100 (100%)	85 (85%)	15 (15%)	3	17
35	RP	116/116 (100%)	85 (73%)	31 (27%)	0	3
35	YP	116/116 (100%)	78 (67%)	38 (33%)	0	2
36	RQ	111/111 (100%)	95 (86%)	16 (14%)	3	18
36	YQ	111/111 (100%)	95 (86%)	16 (14%)	3	18
37	RR	101/101 (100%)	81 (80%)	20 (20%)	1	8
37	YR	101/101 (100%)	80 (79%)	21 (21%)	1	7
38	RS	87/88 (99%)	67 (77%)	20 (23%)	1	6
38	YS	87/88 (99%)	73 (84%)	14 (16%)	2	15
39	RT	120/127 (94%)	101 (84%)	19 (16%)	2	15
39	YT	120/127 (94%)	94 (78%)	26 (22%)	1	7
40	RU	93/94 (99%)	79 (85%)	14 (15%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	YU	93/94 (99%)	79 (85%)	14 (15%)	3	17
41	RV	82/82 (100%)	63 (77%)	19 (23%)	1	5
41	YV	82/82 (100%)	66 (80%)	16 (20%)	1	9
42	RW	92/92 (100%)	73 (79%)	19 (21%)	1	7
42	YW	92/92 (100%)	76 (83%)	16 (17%)	2	12
43	RX	74/78 (95%)	61 (82%)	13 (18%)	2	12
43	YX	74/78 (95%)	59 (80%)	15 (20%)	1	8
44	RY	85/91 (93%)	56 (66%)	29 (34%)	0	1
44	YY	85/91 (93%)	62 (73%)	23 (27%)	0	3
45	RZ	162/179 (90%)	141 (87%)	21 (13%)	4	21
45	YZ	162/179 (90%)	141 (87%)	21 (13%)	4	21
46	R0	65/67 (97%)	58 (89%)	7 (11%)	6	28
46	Y0	65/67 (97%)	57 (88%)	8 (12%)	4	23
47	R1	82/83 (99%)	74 (90%)	8 (10%)	7	31
47	Y1	82/83 (99%)	69 (84%)	13 (16%)	2	15
48	R2	64/67 (96%)	48 (75%)	16 (25%)	0	4
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	6	27
49	R3	51/52 (98%)	43 (84%)	8 (16%)	2	15
49	Y3	51/52 (98%)	44 (86%)	7 (14%)	3	20
50	R4	63/63 (100%)	48 (76%)	15 (24%)	1	5
50	Y4	63/63 (100%)	43 (68%)	20 (32%)	0	2
51	R5	51/52 (98%)	40 (78%)	11 (22%)	1	7
51	Y5	51/52 (98%)	37 (72%)	14 (28%)	0	3
52	R6	48/52 (92%)	32 (67%)	16 (33%)	0	2
52	Y6	48/52 (92%)	34 (71%)	14 (29%)	0	2
53	R7	42/42 (100%)	35 (83%)	7 (17%)	2	14
53	Y7	42/42 (100%)	35 (83%)	7 (17%)	2	14
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	3
54	Y8	54/55 (98%)	38 (70%)	16 (30%)	0	2
55	R9	34/34 (100%)	30 (88%)	4 (12%)	5	24
55	Y9	34/34 (100%)	31 (91%)	3 (9%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9702/10066 (96%)	8069 (83%)	1633 (17%)	2 13

5 of 1633 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	XH	109	ILE
28	YE	79	ARG
52	Y6	23	THR
10	XJ	45	ARG
8	XH	80	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
11	XK	38	ASN
30	YG	132	ASN
13	XM	77	ASN
27	YD	164	GLN
33	YN	133	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	260 (17%)	40 (2%)
1	XA	1498/1522 (98%)	283 (18%)	33 (2%)
22	QV	76/77 (98%)	18 (23%)	1 (1%)
22	XV	76/77 (98%)	18 (23%)	1 (1%)
23	QX	7/25 (28%)	1 (14%)	0
23	XX	7/25 (28%)	1 (14%)	0
24	QY	14/18 (77%)	2 (14%)	0
24	XY	14/18 (77%)	1 (7%)	0
25	RA	2879/2915 (98%)	571 (19%)	49 (1%)
25	YA	2879/2915 (98%)	581 (20%)	49 (1%)
26	RB	119/122 (97%)	18 (15%)	1 (0%)
26	YB	119/122 (97%)	25 (21%)	1 (0%)
56	Z5	1/3 (33%)	0	0
56	Z6	1/3 (33%)	0	0
All	All	9189/9364 (98%)	1779 (19%)	175 (1%)

5 of 1779 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	7	G
1	QA	9	G
1	QA	32	A
1	QA	39	G

5 of 175 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	992	U
25	YA	856	C
1	XA	1336	C
25	YA	229	A
25	YA	1084	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	PPU	Z6	101	56,25	37,40,41	2.58	8 (21%)	47,57,60	2.56	15 (31%)
56	PPU	Z5	101	56,25	37,40,41	2.58	8 (21%)	47,57,60	2.56	15 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PPU	Z6	101	56,25	-	2/25/43/44	0/4/4/4
56	PPU	Z5	101	56,25	-	2/25/43/44	0/4/4/4

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z6	101	PPU	O-C	9.65	1.41	1.23
56	Z5	101	PPU	O-C	9.60	1.41	1.23
56	Z6	101	PPU	C9-N6	-6.26	1.31	1.45
56	Z5	101	PPU	C9-N6	-6.23	1.31	1.45
56	Z5	101	PPU	C-N3'	5.89	1.46	1.34

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z5	101	PPU	C3'-N3'-C	-8.57	110.16	123.20
56	Z6	101	PPU	C3'-N3'-C	-8.48	110.30	123.20
56	Z6	101	PPU	C2'-C1'-N9	-5.96	98.50	113.30
56	Z5	101	PPU	C2'-C1'-N9	-5.94	98.55	113.30
56	Z6	101	PPU	C5-C4-N3	-5.03	119.79	126.72

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	Z5	101	PPU	O-C-CA-N
56	Z6	101	PPU	O-C-CA-N
56	Z5	101	PPU	N3'-C-CA-N
56	Z6	101	PPU	N3'-C-CA-N

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z6	101	PPU	9	0
56	Z5	101	PPU	6	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 817 ligands modelled in this entry, 815 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	XA	1705	-	44,45,45	1.58	8 (18%)	63,67,67	1.24	6 (9%)
58	PAR	QA	1691	-	44,45,45	1.58	7 (15%)	63,67,67	1.29	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	XA	1705	-	-	6/18/94/94	0/4/4/4
58	PAR	QA	1691	-	-	6/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	XA	1705	PAR	O54-C14	3.67	1.51	1.41
58	XA	1705	PAR	C14-C24	3.53	1.59	1.52
58	XA	1705	PAR	O51-C11	3.32	1.50	1.41
58	QA	1691	PAR	C52-C42	3.24	1.58	1.52
58	QA	1691	PAR	O51-C11	3.20	1.50	1.41

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	QA	1691	PAR	C14-O54-C54	5.19	123.86	113.72
58	XA	1705	PAR	O33-C14-C24	4.69	115.76	108.08
58	XA	1705	PAR	C14-O54-C54	3.12	119.81	113.72
58	XA	1705	PAR	O54-C54-C64	3.02	111.88	106.07
58	QA	1691	PAR	O54-C54-C64	2.95	111.74	106.07

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	XA	1705	PAR	O43-C43-C53-O53

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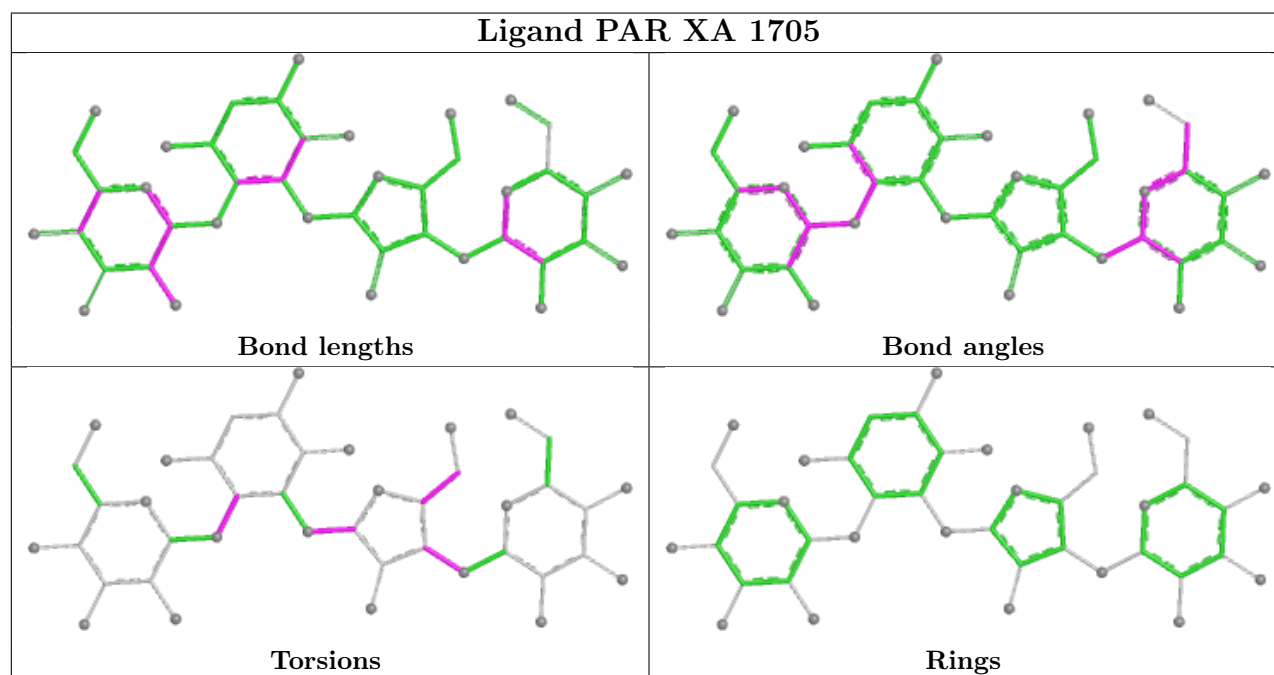
Mol	Chain	Res	Type	Atoms
58	QA	1691	PAR	O51-C51-C61-O61
58	QA	1691	PAR	O43-C43-C53-O53
58	QA	1691	PAR	C33-C43-C53-O53
58	XA	1705	PAR	C33-C43-C53-O53

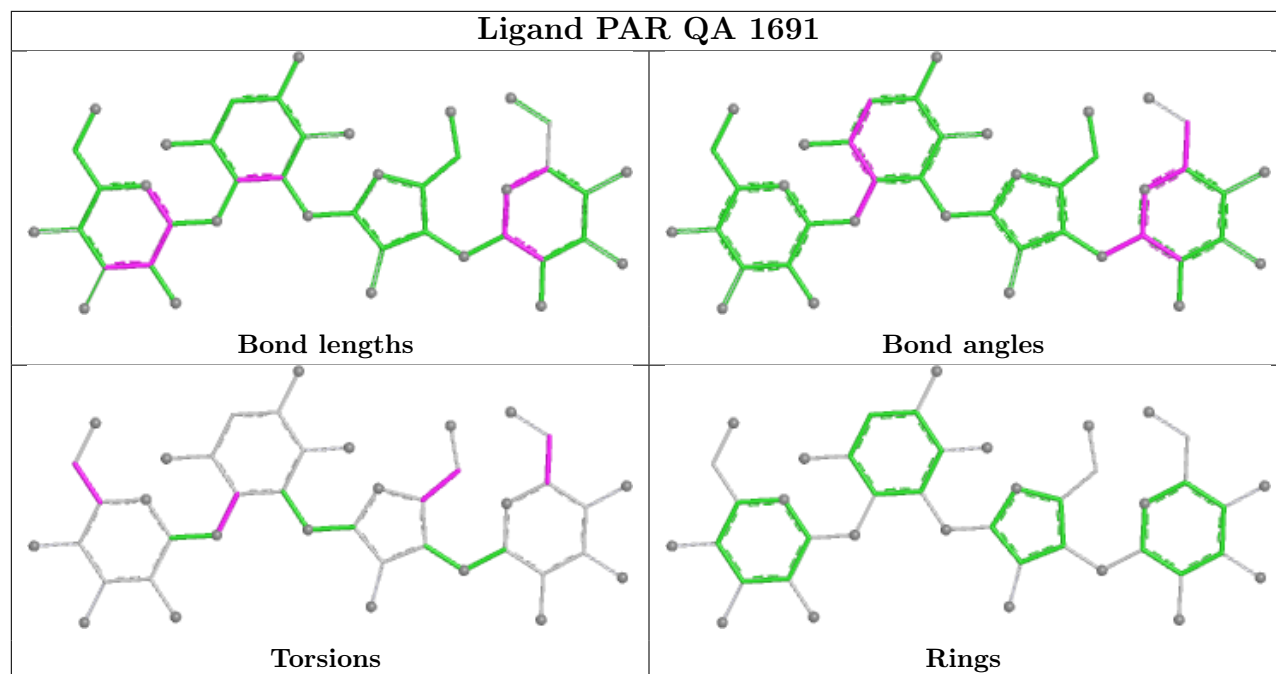
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	QA	1691	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	QA	1500/1522 (98%)	0.22	47 (3%)	51	29	57, 104, 185, 383	0
1	XA	1500/1522 (98%)	0.29	53 (3%)	47	27	51, 103, 207, 434	0
2	QB	237/256 (92%)	0.64	14 (5%)	28	17	84, 155, 246, 386	0
2	XB	237/256 (92%)	0.43	6 (2%)	58	34	81, 153, 230, 296	0
3	QC	205/239 (85%)	0.46	11 (5%)	31	18	87, 140, 198, 246	0
3	XC	205/239 (85%)	0.23	4 (1%)	65	38	74, 125, 191, 265	0
4	QD	208/209 (99%)	0.72	25 (12%)	9	7	67, 119, 174, 208	0
4	XD	208/209 (99%)	0.56	17 (8%)	17	12	59, 102, 153, 201	0
5	QE	151/162 (93%)	0.53	10 (6%)	24	15	67, 121, 174, 270	0
5	XE	151/162 (93%)	0.38	5 (3%)	49	28	64, 99, 154, 224	0
6	QF	101/101 (100%)	0.25	3 (2%)	52	30	61, 101, 141, 186	0
6	XF	101/101 (100%)	0.30	4 (3%)	42	24	62, 117, 176, 247	0
7	QG	155/156 (99%)	0.47	8 (5%)	33	19	68, 122, 169, 283	0
7	XG	155/156 (99%)	0.57	10 (6%)	25	16	90, 141, 199, 237	0
8	QH	138/138 (100%)	0.52	10 (7%)	21	14	79, 122, 158, 186	0
8	XH	138/138 (100%)	0.49	10 (7%)	21	14	68, 110, 153, 210	0
9	QI	127/128 (99%)	1.04	26 (20%)	2	3	91, 148, 201, 230	0
9	XI	127/128 (99%)	0.92	20 (15%)	5	5	84, 175, 244, 299	0
10	QJ	99/105 (94%)	0.97	11 (11%)	10	8	82, 161, 241, 373	0
10	XJ	99/105 (94%)	1.29	21 (21%)	2	3	79, 163, 228, 273	0
11	QK	119/129 (92%)	0.45	5 (4%)	40	22	56, 101, 162, 256	0
11	XK	119/129 (92%)	0.70	10 (8%)	17	12	67, 110, 177, 274	0
12	QL	125/132 (94%)	0.80	12 (9%)	13	10	69, 104, 168, 283	0
12	XL	125/132 (94%)	0.62	8 (6%)	25	16	53, 84, 144, 324	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	0.52	10 (8%)	17	12	71, 128, 203, 279	0
13	XM	121/126 (96%)	0.61	12 (9%)	13	10	86, 136, 197, 303	0
14	QN	60/61 (98%)	0.85	9 (15%)	5	5	91, 134, 169, 183	0
14	XN	60/61 (98%)	0.99	8 (13%)	7	6	72, 118, 153, 169	0
15	QO	88/89 (98%)	0.42	5 (5%)	29	17	67, 104, 163, 177	0
15	XO	88/89 (98%)	0.39	3 (3%)	48	27	68, 104, 164, 190	0
16	QP	84/88 (95%)	0.69	12 (14%)	6	6	73, 105, 160, 205	0
16	XP	84/88 (95%)	0.73	5 (5%)	27	17	82, 111, 164, 246	0
17	QQ	100/105 (95%)	0.56	7 (7%)	22	15	70, 112, 153, 202	0
17	XQ	100/105 (95%)	0.47	1 (1%)	79	54	66, 107, 155, 172	0
18	QR	70/88 (79%)	0.15	1 (1%)	73	46	65, 103, 146, 201	0
18	XR	70/88 (79%)	0.22	0	100	100	71, 117, 165, 215	0
19	QS	84/93 (90%)	0.75	9 (10%)	11	9	94, 147, 213, 259	0
19	XS	84/93 (90%)	0.70	4 (4%)	35	20	78, 146, 191, 257	0
20	QT	99/106 (93%)	0.96	13 (13%)	7	6	74, 119, 177, 200	0
20	XT	99/106 (93%)	1.43	28 (28%)	1	1	77, 138, 193, 294	0
21	QU	25/27 (92%)	1.44	8 (32%)	1	1	75, 120, 182, 217	0
21	XU	25/27 (92%)	1.77	8 (32%)	1	1	87, 134, 191, 194	0
22	QV	77/77 (100%)	0.52	4 (5%)	33	19	55, 115, 175, 233	0
22	XV	77/77 (100%)	0.45	3 (3%)	43	24	49, 105, 172, 220	0
23	QX	9/25 (36%)	0.34	1 (11%)	10	8	75, 96, 133, 165	0
23	XX	9/25 (36%)	0.54	1 (11%)	10	8	71, 83, 133, 180	0
24	QY	15/18 (83%)	0.26	0	100	100	95, 123, 212, 232	0
24	XY	15/18 (83%)	0.49	1 (6%)	24	15	84, 117, 186, 205	0
25	RA	2882/2915 (98%)	0.08	101 (3%)	47	27	39, 80, 234, 425	0
25	YA	2882/2915 (98%)	0.15	119 (4%)	41	23	34, 77, 235, 417	0
26	RB	120/122 (98%)	0.27	3 (2%)	58	34	84, 112, 143, 194	0
26	YB	120/122 (98%)	0.65	6 (5%)	34	19	77, 126, 164, 215	0
27	RD	272/276 (98%)	0.19	6 (2%)	62	36	39, 71, 108, 261	0
27	YD	272/276 (98%)	0.30	8 (2%)	53	30	35, 71, 111, 288	0
28	RE	205/206 (99%)	0.70	15 (7%)	21	14	52, 98, 171, 310	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
28	YE	205/206 (99%)	0.73	18 (8%)	15 11	34, 95, 173, 258	0
29	RF	202/210 (96%)	0.34	4 (1%)	65 38	40, 88, 154, 206	0
29	YF	202/210 (96%)	0.26	2 (0%)	79 54	29, 81, 144, 195	0
30	RG	181/182 (99%)	0.77	17 (9%)	14 10	72, 122, 179, 230	0
30	YG	181/182 (99%)	0.63	17 (9%)	14 10	89, 136, 196, 248	0
31	RH	170/180 (94%)	0.74	16 (9%)	14 10	106, 194, 282, 354	0
31	YH	170/180 (94%)	0.82	18 (10%)	11 9	73, 117, 176, 235	0
32	RI	146/148 (98%)	0.81	19 (13%)	7 6	60, 141, 186, 279	0
32	YI	146/148 (98%)	0.85	16 (10%)	10 9	83, 154, 200, 232	0
33	RN	138/140 (98%)	0.50	7 (5%)	33 19	67, 100, 163, 207	0
33	YN	138/140 (98%)	0.66	15 (10%)	10 9	63, 99, 168, 191	0
34	RO	122/122 (100%)	0.39	3 (2%)	58 34	52, 95, 138, 173	0
34	YO	122/122 (100%)	0.32	3 (2%)	58 34	42, 74, 109, 166	0
35	RP	150/150 (100%)	0.64	14 (9%)	14 10	45, 96, 164, 244	0
35	YP	150/150 (100%)	0.94	23 (15%)	5 5	30, 89, 148, 315	0
36	RQ	141/141 (100%)	0.86	25 (17%)	4 4	57, 103, 163, 249	0
36	YQ	141/141 (100%)	1.01	21 (14%)	5 5	51, 95, 157, 272	0
37	RR	118/118 (100%)	0.43	7 (5%)	28 17	54, 81, 120, 145	0
37	YR	118/118 (100%)	0.45	3 (2%)	58 34	51, 86, 126, 180	0
38	RS	111/112 (99%)	0.77	10 (9%)	15 11	67, 115, 168, 265	0
38	YS	111/112 (99%)	0.82	13 (11%)	9 8	85, 134, 190, 269	0
39	RT	137/146 (93%)	0.56	10 (7%)	21 14	64, 107, 210, 292	0
39	YT	137/146 (93%)	0.62	11 (8%)	18 13	60, 93, 177, 240	0
40	RU	117/118 (99%)	0.57	8 (6%)	23 15	48, 83, 146, 225	0
40	YU	117/118 (99%)	0.55	5 (4%)	40 22	43, 87, 148, 282	0
41	RV	101/101 (100%)	0.42	1 (0%)	79 54	51, 108, 171, 279	0
41	YV	101/101 (100%)	0.40	3 (2%)	52 30	55, 115, 179, 318	0
42	RW	113/113 (100%)	0.26	4 (3%)	47 27	42, 71, 130, 212	0
42	YW	113/113 (100%)	0.26	5 (4%)	39 22	47, 74, 140, 251	0
43	RX	92/96 (95%)	0.47	9 (9%)	13 10	52, 83, 125, 147	0
43	YX	92/96 (95%)	0.56	7 (7%)	20 13	51, 78, 122, 171	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RY	102/110 (92%)	1.54	29 (28%) 1 1	55, 114, 227, 327	0
44	YY	102/110 (92%)	0.83	10 (9%) 13 10	59, 104, 184, 353	0
45	RZ	183/206 (88%)	0.77	19 (10%) 11 9	82, 141, 220, 276	0
45	YZ	183/206 (88%)	0.90	19 (10%) 11 9	77, 141, 224, 346	0
46	R0	82/85 (96%)	0.52	7 (8%) 16 12	62, 84, 115, 132	0
46	Y0	82/85 (96%)	0.75	5 (6%) 27 16	57, 93, 121, 148	0
47	R1	97/98 (98%)	0.71	9 (9%) 14 10	44, 83, 188, 262	0
47	Y1	97/98 (98%)	0.63	12 (12%) 8 7	43, 85, 163, 203	0
48	R2	69/72 (95%)	1.06	12 (17%) 4 4	64, 110, 179, 234	0
48	Y2	69/72 (95%)	0.54	4 (5%) 29 17	51, 91, 147, 262	0
49	R3	59/60 (98%)	0.28	3 (5%) 33 19	61, 99, 152, 191	0
49	Y3	59/60 (98%)	0.36	3 (5%) 33 19	56, 99, 165, 237	0
50	R4	71/71 (100%)	1.09	10 (14%) 6 6	114, 191, 338, 387	0
50	Y4	71/71 (100%)	0.80	6 (8%) 16 12	122, 190, 287, 387	0
51	R5	59/60 (98%)	0.84	8 (13%) 7 6	46, 92, 234, 303	0
51	Y5	58/60 (96%)	0.82	5 (8%) 16 12	43, 97, 260, 296	0
52	R6	49/54 (90%)	1.64	13 (26%) 1 2	109, 153, 219, 278	0
52	Y6	49/54 (90%)	1.58	15 (30%) 1 1	117, 165, 246, 359	0
53	R7	49/49 (100%)	0.60	7 (14%) 6 6	39, 61, 133, 189	0
53	Y7	49/49 (100%)	0.43	4 (8%) 17 12	34, 55, 138, 211	0
54	R8	64/65 (98%)	1.33	14 (21%) 2 2	49, 83, 154, 240	0
54	Y8	64/65 (98%)	1.22	16 (25%) 2 2	53, 84, 145, 225	0
55	R9	37/37 (100%)	2.24	22 (59%) 0 0	152, 197, 266, 308	0
55	Y9	37/37 (100%)	2.96	23 (62%) 0 0	121, 172, 251, 289	0
56	Z5	2/3 (66%)	0.59	0 100 100	66, 66, 66, 77	0
56	Z6	2/3 (66%)	1.19	0 100 100	74, 74, 74, 74	0
All	All	20875/21492 (97%)	0.44	1370 (6%) 24 15	29, 102, 206, 434	0

The worst 5 of 1370 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	YA	1536	A	12.9
7	XG	5	ARG	11.5

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Mol	Chain	Res	Type	RSRZ
14	XN	2	ALA	8.2
25	RA	2799	A	8.0
52	Y6	42	TRP	7.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	PPU	Z5	101	37/38	0.95	0.13	68,69,69,69	0
56	PPU	Z6	101	37/38	0.95	0.12	54,60,68,70	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	YA	3172	1/1	0.01	0.27	151,151,151,151	0
57	MG	RA	3101	1/1	0.12	0.33	53,53,53,53	0
57	MG	QA	1626	1/1	0.17	0.21	124,124,124,124	0
57	MG	Y0	101	1/1	0.21	0.27	72,72,72,72	0
57	MG	YA	3185	1/1	0.28	0.22	84,84,84,84	0
57	MG	YA	3083	1/1	0.29	0.35	47,47,47,47	0
57	MG	QA	1618	1/1	0.36	0.40	70,70,70,70	0
57	MG	RA	3149	1/1	0.36	0.18	41,41,41,41	0
57	MG	QA	1667	1/1	0.37	0.50	75,75,75,75	0
57	MG	RA	3166	1/1	0.45	0.22	93,93,93,93	0
57	MG	YA	3260	1/1	0.46	0.62	145,145,145,145	0
57	MG	R0	101	1/1	0.46	0.20	41,41,41,41	0
57	MG	YA	3155	1/1	0.47	0.30	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3071	1/1	0.48	0.18	39,39,39,39	0
57	MG	RA	3116	1/1	0.51	0.22	66,66,66,66	0
57	MG	RA	3134	1/1	0.51	0.24	68,68,68,68	0
57	MG	RA	3025	1/1	0.51	0.23	50,50,50,50	0
57	MG	RA	3131	1/1	0.52	0.18	68,68,68,68	0
57	MG	YA	3232	1/1	0.52	0.45	46,46,46,46	0
57	MG	RA	3111	1/1	0.52	0.23	42,42,42,42	0
57	MG	RA	3099	1/1	0.52	0.23	40,40,40,40	0
57	MG	QA	1637	1/1	0.53	0.39	92,92,92,92	0
57	MG	YA	3194	1/1	0.54	0.26	85,85,85,85	0
57	MG	RA	3160	1/1	0.54	0.26	74,74,74,74	0
57	MG	YA	3133	1/1	0.56	0.21	48,48,48,48	0
57	MG	YA	3066	1/1	0.57	0.24	26,26,26,26	0
57	MG	RA	3135	1/1	0.59	0.28	79,79,79,79	0
57	MG	RA	3126	1/1	0.59	0.17	84,84,84,84	0
57	MG	YA	3157	1/1	0.59	0.14	53,53,53,53	0
57	MG	RA	3185	1/1	0.60	0.21	45,45,45,45	0
57	MG	R8	101	1/1	0.61	0.42	86,86,86,86	0
57	MG	YA	3171	1/1	0.61	0.39	55,55,55,55	0
57	MG	RA	3164	1/1	0.61	0.16	56,56,56,56	0
57	MG	YA	3281	1/1	0.61	0.28	72,72,72,72	0
57	MG	QA	1686	1/1	0.61	0.34	80,80,80,80	0
57	MG	QA	1636	1/1	0.62	0.23	87,87,87,87	0
57	MG	XA	1644	1/1	0.63	0.18	100,100,100,100	0
57	MG	YA	3283	1/1	0.63	0.34	75,75,75,75	0
57	MG	XA	1659	1/1	0.63	0.23	89,89,89,89	0
57	MG	YA	3196	1/1	0.64	0.16	65,65,65,65	0
57	MG	YA	3128	1/1	0.64	0.25	51,51,51,51	0
57	MG	RA	3022	1/1	0.64	0.39	36,36,36,36	0
57	MG	YA	3046	1/1	0.65	0.27	30,30,30,30	0
57	MG	XA	1629	1/1	0.66	0.15	62,62,62,62	0
57	MG	YA	3038	1/1	0.66	0.12	21,21,21,21	0
57	MG	YA	3204	1/1	0.67	0.19	75,75,75,75	0
57	MG	RA	3067	1/1	0.67	0.13	39,39,39,39	0
57	MG	YA	3182	1/1	0.68	0.17	63,63,63,63	0
57	MG	YP	201	1/1	0.68	0.24	66,66,66,66	0
57	MG	QA	1638	1/1	0.68	0.35	74,74,74,74	0
57	MG	YA	3119	1/1	0.69	0.29	46,46,46,46	0
57	MG	RA	3191	1/1	0.69	0.19	57,57,57,57	0
57	MG	YA	3192	1/1	0.70	0.25	66,66,66,66	0
57	MG	YA	3112	1/1	0.71	0.27	62,62,62,62	0
57	MG	YA	3065	1/1	0.72	0.24	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3184	1/1	0.72	0.15	102,102,102,102	0
57	MG	XA	1634	1/1	0.72	0.22	92,92,92,92	0
57	MG	RQ	201	1/1	0.72	0.33	91,91,91,91	0
57	MG	YA	3206	1/1	0.73	0.18	33,33,33,33	0
57	MG	XA	1632	1/1	0.73	0.35	65,65,65,65	0
57	MG	RA	3189	1/1	0.73	0.12	75,75,75,75	0
57	MG	YA	3268	1/1	0.73	0.37	103,103,103,103	0
57	MG	YA	3007	1/1	0.74	0.32	62,62,62,62	0
57	MG	QA	1644	1/1	0.74	0.33	62,62,62,62	0
57	MG	YA	3116	1/1	0.74	0.27	43,43,43,43	0
57	MG	RF	301	1/1	0.74	0.20	86,86,86,86	0
57	MG	RA	3109	1/1	0.75	0.31	48,48,48,48	0
57	MG	YA	3267	1/1	0.75	0.31	66,66,66,66	0
57	MG	R5	101	1/1	0.75	0.17	49,49,49,49	0
57	MG	YA	3064	1/1	0.75	0.12	42,42,42,42	0
57	MG	XA	1680	1/1	0.75	0.32	61,61,61,61	0
57	MG	YD	301	1/1	0.75	0.22	52,52,52,52	0
57	MG	XA	1682	1/1	0.75	0.28	68,68,68,68	0
57	MG	RA	3224	1/1	0.75	0.23	57,57,57,57	0
57	MG	RA	3180	1/1	0.76	0.36	75,75,75,75	0
57	MG	RA	3061	1/1	0.76	0.11	81,81,81,81	0
57	MG	RA	3194	1/1	0.76	0.14	45,45,45,45	0
57	MG	XA	1654	1/1	0.76	0.10	84,84,84,84	0
57	MG	RA	3207	1/1	0.76	0.15	70,70,70,70	0
57	MG	YA	3161	1/1	0.76	0.24	69,69,69,69	0
57	MG	YA	3266	1/1	0.76	0.19	62,62,62,62	0
57	MG	XA	1675	1/1	0.76	0.29	56,56,56,56	0
57	MG	RA	3120	1/1	0.76	0.17	69,69,69,69	0
57	MG	YA	3175	1/1	0.76	0.28	56,56,56,56	0
57	MG	RA	3239	1/1	0.76	0.21	54,54,54,54	0
57	MG	XA	1686	1/1	0.76	0.14	69,69,69,69	0
57	MG	YA	3191	1/1	0.76	0.32	38,38,38,38	0
57	MG	XX	101	1/1	0.76	0.17	68,68,68,68	0
57	MG	YA	3205	1/1	0.77	0.22	84,84,84,84	0
57	MG	YA	3176	1/1	0.77	0.31	57,57,57,57	0
57	MG	YA	3178	1/1	0.77	0.09	55,55,55,55	0
57	MG	YA	3137	1/1	0.77	0.14	64,64,64,64	0
57	MG	RA	3234	1/1	0.77	0.32	63,63,63,63	0
57	MG	QA	1690	1/1	0.77	0.31	79,79,79,79	0
57	MG	RA	3273	1/1	0.77	0.25	63,63,63,63	0
57	MG	RD	301	1/1	0.77	0.19	66,66,66,66	0
57	MG	RA	3082	1/1	0.77	0.17	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3199	1/1	0.77	0.28	83,83,83,83	0
57	MG	YA	3200	1/1	0.77	0.11	93,93,93,93	0
57	MG	XA	1661	1/1	0.77	0.18	58,58,58,58	0
57	MG	QA	1620	1/1	0.78	0.17	62,62,62,62	0
57	MG	XA	1701	1/1	0.78	0.13	67,67,67,67	0
57	MG	YA	3123	1/1	0.78	0.18	34,34,34,34	0
57	MG	XA	1626	1/1	0.78	0.18	38,38,38,38	0
57	MG	QA	1604	1/1	0.78	0.35	64,64,64,64	0
57	MG	XA	1702	1/1	0.79	0.35	75,75,75,75	0
57	MG	RA	3001	1/1	0.79	0.22	35,35,35,35	0
57	MG	YA	3208	1/1	0.79	0.10	48,48,48,48	0
57	MG	YA	3214	1/1	0.79	0.33	77,77,77,77	0
57	MG	XA	1649	1/1	0.79	0.26	77,77,77,77	0
57	MG	YA	3255	1/1	0.79	0.27	67,67,67,67	0
57	MG	RA	3183	1/1	0.79	0.33	68,68,68,68	0
57	MG	RA	3233	1/1	0.79	0.27	77,77,77,77	0
57	MG	QA	1640	1/1	0.79	0.25	51,51,51,51	0
57	MG	XA	1619	1/1	0.79	0.33	43,43,43,43	0
57	MG	QA	1619	1/1	0.79	0.23	58,58,58,58	0
57	MG	QA	1661	1/1	0.79	0.36	65,65,65,65	0
57	MG	YB	202	1/1	0.79	0.18	83,83,83,83	0
57	MG	YA	3166	1/1	0.79	0.13	90,90,90,90	0
57	MG	RA	3167	1/1	0.79	0.17	40,40,40,40	0
57	MG	RA	3170	1/1	0.79	0.14	40,40,40,40	0
57	MG	QA	1689	1/1	0.80	0.25	80,80,80,80	0
57	MG	RA	3193	1/1	0.80	0.13	35,35,35,35	0
57	MG	YA	3162	1/1	0.80	0.23	64,64,64,64	0
57	MG	QA	1676	1/1	0.80	0.18	66,66,66,66	0
57	MG	RA	3196	1/1	0.80	0.13	43,43,43,43	0
57	MG	RA	3199	1/1	0.80	0.24	64,64,64,64	0
57	MG	YA	3111	1/1	0.80	0.22	45,45,45,45	0
57	MG	XA	1636	1/1	0.80	0.12	82,82,82,82	0
57	MG	QT	201	1/1	0.80	0.18	70,70,70,70	0
57	MG	XD	302	1/1	0.80	0.17	90,90,90,90	0
57	MG	XV	102	1/1	0.80	0.30	47,47,47,47	0
57	MG	YA	3127	1/1	0.80	0.29	58,58,58,58	0
57	MG	XA	1648	1/1	0.80	0.26	92,92,92,92	0
57	MG	RA	3223	1/1	0.80	0.24	46,46,46,46	0
57	MG	QV	101	1/1	0.80	0.27	55,55,55,55	0
57	MG	YA	3142	1/1	0.80	0.20	56,56,56,56	0
57	MG	RA	3123	1/1	0.80	0.21	52,52,52,52	0
57	MG	XA	1618	1/1	0.81	0.23	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3188	1/1	0.81	0.40	57,57,57,57	0
57	MG	YA	3235	1/1	0.81	0.44	52,52,52,52	0
57	MG	XA	1650	1/1	0.81	0.37	67,67,67,67	0
57	MG	RA	3261	1/1	0.81	0.31	80,80,80,80	0
57	MG	XA	1658	1/1	0.81	0.29	72,72,72,72	0
57	MG	RA	3118	1/1	0.81	0.30	47,47,47,47	0
57	MG	RA	3213	1/1	0.81	0.28	66,66,66,66	0
57	MG	QA	1613	1/1	0.81	0.37	40,40,40,40	0
57	MG	YA	3201	1/1	0.81	0.17	79,79,79,79	0
57	MG	RA	3157	1/1	0.81	0.34	41,41,41,41	0
57	MG	RA	3195	1/1	0.81	0.11	48,48,48,48	0
57	MG	YE	302	1/1	0.81	0.15	30,30,30,30	0
57	MG	QA	1664	1/1	0.81	0.32	52,52,52,52	0
57	MG	RA	3176	1/1	0.81	0.15	58,58,58,58	0
57	MG	XV	101	1/1	0.82	0.27	53,53,53,53	0
57	MG	RA	3252	1/1	0.82	0.23	66,66,66,66	0
57	MG	RA	3013	1/1	0.82	0.29	22,22,22,22	0
57	MG	QA	1656	1/1	0.82	0.16	64,64,64,64	0
57	MG	YA	3012	1/1	0.82	0.24	22,22,22,22	0
57	MG	RA	3278	1/1	0.82	0.47	69,69,69,69	0
57	MG	QA	1665	1/1	0.82	0.41	55,55,55,55	0
57	MG	RA	3137	1/1	0.82	0.20	45,45,45,45	0
57	MG	QA	1685	1/1	0.82	0.41	60,60,60,60	0
57	MG	RA	3007	1/1	0.82	0.23	20,20,20,20	0
57	MG	XA	1688	1/1	0.82	0.12	57,57,57,57	0
57	MG	RA	3240	1/1	0.82	0.43	77,77,77,77	0
57	MG	RA	3248	1/1	0.82	0.22	52,52,52,52	0
57	MG	YA	3168	1/1	0.82	0.26	52,52,52,52	0
57	MG	XA	1616	1/1	0.82	0.30	47,47,47,47	0
57	MG	YA	3114	1/1	0.82	0.18	45,45,45,45	0
57	MG	YA	3103	1/1	0.83	0.13	23,23,23,23	0
57	MG	YA	3282	1/1	0.83	0.24	66,66,66,66	0
57	MG	YA	3189	1/1	0.83	0.23	39,39,39,39	0
57	MG	YA	3030	1/1	0.83	0.25	21,21,21,21	0
57	MG	YA	3177	1/1	0.83	0.20	54,54,54,54	0
57	MG	XA	1656	1/1	0.83	0.19	67,67,67,67	0
57	MG	XA	1697	1/1	0.83	0.21	68,68,68,68	0
57	MG	YA	3025	1/1	0.83	0.32	22,22,22,22	0
57	MG	YA	3102	1/1	0.84	0.17	25,25,25,25	0
57	MG	RA	3018	1/1	0.84	0.24	27,27,27,27	0
57	MG	XA	1660	1/1	0.84	0.14	46,46,46,46	0
57	MG	QA	1687	1/1	0.84	0.10	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3104	1/1	0.84	0.16	49,49,49,49	0
57	MG	QA	1679	1/1	0.84	0.15	54,54,54,54	0
57	MG	YA	3018	1/1	0.84	0.25	42,42,42,42	0
57	MG	YA	3020	1/1	0.84	0.29	30,30,30,30	0
57	MG	RA	3110	1/1	0.84	0.20	54,54,54,54	0
57	MG	YA	3184	1/1	0.84	0.26	55,55,55,55	0
57	MG	QA	1653	1/1	0.84	0.21	69,69,69,69	0
57	MG	XA	1687	1/1	0.84	0.11	120,120,120,120	0
57	MG	RA	3243	1/1	0.84	0.27	53,53,53,53	0
57	MG	YA	3140	1/1	0.84	0.13	52,52,52,52	0
57	MG	XA	1696	1/1	0.84	0.23	37,37,37,37	0
57	MG	RA	3012	1/1	0.84	0.29	24,24,24,24	0
57	MG	QA	1663	1/1	0.84	0.27	68,68,68,68	0
57	MG	YA	3160	1/1	0.84	0.24	48,48,48,48	0
57	MG	RA	3154	1/1	0.84	0.38	60,60,60,60	0
57	MG	RA	3156	1/1	0.84	0.20	50,50,50,50	0
57	MG	YA	3094	1/1	0.85	0.34	43,43,43,43	0
57	MG	YA	3237	1/1	0.85	0.45	76,76,76,76	0
57	MG	YA	3193	1/1	0.85	0.10	44,44,44,44	0
57	MG	QA	1678	1/1	0.85	0.21	53,53,53,53	0
57	MG	QA	1605	1/1	0.85	0.28	30,30,30,30	0
57	MG	XA	1685	1/1	0.85	0.20	60,60,60,60	0
57	MG	QA	1650	1/1	0.85	0.10	72,72,72,72	0
57	MG	YA	3276	1/1	0.85	0.17	65,65,65,65	0
57	MG	RA	3200	1/1	0.85	0.28	74,74,74,74	0
57	MG	XA	1641	1/1	0.85	0.25	68,68,68,68	0
57	MG	QA	1675	1/1	0.85	0.21	75,75,75,75	0
57	MG	YA	3286	1/1	0.85	0.44	61,61,61,61	0
57	MG	YA	3287	1/1	0.85	0.45	81,81,81,81	0
57	MG	YA	3288	1/1	0.85	0.31	54,54,54,54	0
57	MG	YB	201	1/1	0.85	0.35	71,71,71,71	0
57	MG	QY	101	1/1	0.85	0.16	61,61,61,61	0
57	MG	QA	1658	1/1	0.85	0.16	50,50,50,50	0
57	MG	YA	3084	1/1	0.85	0.24	32,32,32,32	0
57	MG	YA	3222	1/1	0.85	0.23	54,54,54,54	0
57	MG	YA	3169	1/1	0.85	0.30	39,39,39,39	0
57	MG	YA	3202	1/1	0.86	0.29	56,56,56,56	0
57	MG	YA	3159	1/1	0.86	0.13	47,47,47,47	0
57	MG	QA	1683	1/1	0.86	0.14	96,96,96,96	0
57	MG	RB	203	1/1	0.86	0.27	46,46,46,46	0
57	MG	RA	3043	1/1	0.86	0.20	43,43,43,43	0
57	MG	YA	3213	1/1	0.86	0.37	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1645	1/1	0.86	0.15	59,59,59,59	0
57	MG	YA	3216	1/1	0.86	0.48	77,77,77,77	0
57	MG	XA	1698	1/1	0.86	0.24	77,77,77,77	0
57	MG	YA	3098	1/1	0.86	0.35	45,45,45,45	0
57	MG	XA	1647	1/1	0.86	0.35	74,74,74,74	0
57	MG	RA	3058	1/1	0.86	0.21	21,21,21,21	0
57	MG	YA	3105	1/1	0.86	0.23	41,41,41,41	0
57	MG	RA	3130	1/1	0.86	0.30	68,68,68,68	0
57	MG	RA	3015	1/1	0.86	0.26	17,17,17,17	0
57	MG	R3	101	1/1	0.86	0.28	49,49,49,49	0
57	MG	QA	1646	1/1	0.86	0.17	80,80,80,80	0
57	MG	RA	3068	1/1	0.86	0.18	35,35,35,35	0
57	MG	YA	3279	1/1	0.86	0.53	65,65,65,65	0
57	MG	XA	1612	1/1	0.86	0.22	54,54,54,54	0
57	MG	RA	3169	1/1	0.86	0.23	53,53,53,53	0
57	MG	RA	3070	1/1	0.86	0.30	43,43,43,43	0
57	MG	YA	3285	1/1	0.86	0.31	66,66,66,66	0
57	MG	YA	3132	1/1	0.86	0.27	51,51,51,51	0
57	MG	XA	1664	1/1	0.86	0.27	50,50,50,50	0
57	MG	RA	3173	1/1	0.86	0.30	84,84,84,84	0
57	MG	RA	3254	1/1	0.86	0.19	53,53,53,53	0
57	MG	RA	3146	1/1	0.86	0.21	50,50,50,50	0
57	MG	YA	3198	1/1	0.86	0.23	72,72,72,72	0
57	MG	QA	1645	1/1	0.86	0.21	52,52,52,52	0
57	MG	YA	3156	1/1	0.86	0.21	51,51,51,51	0
57	MG	RA	3277	1/1	0.86	0.21	51,51,51,51	0
57	MG	Y7	101	1/1	0.86	0.12	52,52,52,52	0
57	MG	RA	3128	1/1	0.87	0.21	30,30,30,30	0
57	MG	XA	1605	1/1	0.87	0.39	55,55,55,55	0
57	MG	XA	1606	1/1	0.87	0.18	42,42,42,42	0
57	MG	YA	3113	1/1	0.87	0.26	35,35,35,35	0
57	MG	QA	1682	1/1	0.87	0.30	67,67,67,67	0
57	MG	RA	3201	1/1	0.87	0.29	69,69,69,69	0
57	MG	YA	3239	1/1	0.87	0.23	48,48,48,48	0
57	MG	RA	3259	1/1	0.87	0.32	52,52,52,52	0
57	MG	QA	1670	1/1	0.87	0.16	45,45,45,45	0
57	MG	XA	1669	1/1	0.87	0.17	55,55,55,55	0
57	MG	RA	3265	1/1	0.87	0.30	60,60,60,60	0
57	MG	YA	3130	1/1	0.87	0.08	57,57,57,57	0
57	MG	YA	3272	1/1	0.87	0.42	43,43,43,43	0
57	MG	XA	1677	1/1	0.87	0.11	62,62,62,62	0
57	MG	YA	3031	1/1	0.87	0.17	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3134	1/1	0.87	0.25	31,31,31,31	0
57	MG	QA	1673	1/1	0.87	0.10	55,55,55,55	0
57	MG	QA	1633	1/1	0.87	0.23	35,35,35,35	0
57	MG	RA	3084	1/1	0.87	0.30	28,28,28,28	0
57	MG	RA	3230	1/1	0.87	0.27	94,94,94,94	0
57	MG	RA	3168	1/1	0.87	0.10	40,40,40,40	0
57	MG	RE	302	1/1	0.87	0.17	41,41,41,41	0
57	MG	YA	3158	1/1	0.87	0.29	50,50,50,50	0
57	MG	QA	1639	1/1	0.87	0.22	62,62,62,62	0
57	MG	QA	1666	1/1	0.87	0.24	71,71,71,71	0
57	MG	RA	3172	1/1	0.87	0.31	57,57,57,57	0
57	MG	QA	1649	1/1	0.87	0.15	77,77,77,77	0
57	MG	RA	3244	1/1	0.87	0.22	41,41,41,41	0
57	MG	XA	1704	1/1	0.87	0.27	68,68,68,68	0
57	MG	YA	3125	1/1	0.88	0.40	60,60,60,60	0
57	MG	YA	3040	1/1	0.88	0.11	30,30,30,30	0
57	MG	QA	1614	1/1	0.88	0.20	43,43,43,43	0
57	MG	XA	1657	1/1	0.88	0.24	47,47,47,47	0
57	MG	RA	3242	1/1	0.88	0.10	58,58,58,58	0
57	MG	YA	3180	1/1	0.88	0.11	62,62,62,62	0
57	MG	RA	3074	1/1	0.88	0.22	39,39,39,39	0
57	MG	RA	3203	1/1	0.88	0.17	60,60,60,60	0
57	MG	YA	3082	1/1	0.88	0.26	47,47,47,47	0
57	MG	YA	3138	1/1	0.88	0.31	50,50,50,50	0
57	MG	RA	3206	1/1	0.88	0.08	69,69,69,69	0
57	MG	XA	1662	1/1	0.88	0.15	29,29,29,29	0
57	MG	YA	3146	1/1	0.88	0.14	41,41,41,41	0
57	MG	YA	3151	1/1	0.88	0.12	44,44,44,44	0
57	MG	RA	3136	1/1	0.88	0.29	42,42,42,42	0
57	MG	YA	3195	1/1	0.88	0.33	44,44,44,44	0
57	MG	RA	3108	1/1	0.88	0.25	39,39,39,39	0
57	MG	RA	3125	1/1	0.88	0.24	51,51,51,51	0
57	MG	QA	1659	1/1	0.88	0.26	50,50,50,50	0
57	MG	XA	1679	1/1	0.88	0.18	41,41,41,41	0
57	MG	RA	3127	1/1	0.88	0.41	65,65,65,65	0
57	MG	RA	3269	1/1	0.88	0.51	70,70,70,70	0
57	MG	RA	3031	1/1	0.88	0.29	50,50,50,50	0
57	MG	YA	3028	1/1	0.88	0.21	22,22,22,22	0
57	MG	RA	3089	1/1	0.88	0.19	70,70,70,70	0
57	MG	XA	1652	1/1	0.88	0.16	70,70,70,70	0
57	MG	YA	3170	1/1	0.88	0.07	63,63,63,63	0
57	MG	QA	1601	1/1	0.88	0.26	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3236	1/1	0.89	0.39	64,64,64,64	0
57	MG	YA	3045	1/1	0.89	0.23	14,14,14,14	0
57	MG	RA	3117	1/1	0.89	0.32	64,64,64,64	0
57	MG	YA	3062	1/1	0.89	0.30	31,31,31,31	0
57	MG	QA	1630	1/1	0.89	0.20	64,64,64,64	0
57	MG	RA	3038	1/1	0.89	0.20	33,33,33,33	0
57	MG	YA	3148	1/1	0.89	0.15	68,68,68,68	0
57	MG	YA	3149	1/1	0.89	0.27	36,36,36,36	0
57	MG	XA	1690	1/1	0.89	0.26	57,57,57,57	0
57	MG	YA	3153	1/1	0.89	0.28	79,79,79,79	0
57	MG	YA	3069	1/1	0.89	0.29	36,36,36,36	0
57	MG	XA	1695	1/1	0.89	0.11	57,57,57,57	0
57	MG	YA	3074	1/1	0.89	0.39	44,44,44,44	0
57	MG	RR	201	1/1	0.89	0.16	50,50,50,50	0
57	MG	QA	1615	1/1	0.89	0.18	58,58,58,58	0
57	MG	YA	3233	1/1	0.89	0.21	47,47,47,47	0
57	MG	RA	3175	1/1	0.89	0.36	61,61,61,61	0
57	MG	RA	3245	1/1	0.89	0.28	55,55,55,55	0
57	MG	YA	3238	1/1	0.89	0.25	15,15,15,15	0
57	MG	YA	3095	1/1	0.89	0.22	28,28,28,28	0
57	MG	YA	3250	1/1	0.89	0.24	53,53,53,53	0
57	MG	YA	3252	1/1	0.89	0.21	51,51,51,51	0
57	MG	YA	3164	1/1	0.89	0.24	47,47,47,47	0
57	MG	RA	3247	1/1	0.89	0.39	59,59,59,59	0
57	MG	YA	3261	1/1	0.89	0.24	59,59,59,59	0
57	MG	YA	3100	1/1	0.89	0.35	48,48,48,48	0
57	MG	YA	3101	1/1	0.89	0.13	55,55,55,55	0
57	MG	RA	3044	1/1	0.89	0.21	29,29,29,29	0
57	MG	RA	3204	1/1	0.89	0.36	76,76,76,76	0
57	MG	YA	3274	1/1	0.89	0.28	44,44,44,44	0
57	MG	RA	3155	1/1	0.89	0.20	46,46,46,46	0
57	MG	YA	3109	1/1	0.89	0.20	44,44,44,44	0
57	MG	RA	3052	1/1	0.89	0.34	29,29,29,29	0
57	MG	RA	3260	1/1	0.89	0.18	63,63,63,63	0
57	MG	YA	3004	1/1	0.89	0.20	17,17,17,17	0
57	MG	RA	3211	1/1	0.89	0.09	60,60,60,60	0
57	MG	XA	1622	1/1	0.89	0.20	53,53,53,53	0
57	MG	XA	1668	1/1	0.89	0.30	51,51,51,51	0
57	MG	QA	1647	1/1	0.89	0.15	39,39,39,39	0
57	MG	YA	3024	1/1	0.89	0.25	31,31,31,31	0
57	MG	YA	3126	1/1	0.89	0.21	26,26,26,26	0
57	MG	QA	1624	1/1	0.89	0.31	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1668	1/1	0.89	0.29	75,75,75,75	0
57	MG	QA	1616	1/1	0.89	0.15	97,97,97,97	0
57	MG	QV	102	1/1	0.89	0.22	43,43,43,43	0
57	MG	QA	1651	1/1	0.89	0.18	85,85,85,85	0
57	MG	RA	3231	1/1	0.90	0.21	58,58,58,58	0
57	MG	RA	3040	1/1	0.90	0.21	29,29,29,29	0
57	MG	XA	1670	1/1	0.90	0.37	57,57,57,57	0
57	MG	RA	3162	1/1	0.90	0.16	62,62,62,62	0
57	MG	XA	1631	1/1	0.90	0.25	49,49,49,49	0
57	MG	RA	3041	1/1	0.90	0.24	40,40,40,40	0
57	MG	XA	1633	1/1	0.90	0.32	47,47,47,47	0
57	MG	YA	3033	1/1	0.90	0.23	18,18,18,18	0
57	MG	YA	3121	1/1	0.90	0.18	37,37,37,37	0
57	MG	YA	3173	1/1	0.90	0.32	46,46,46,46	0
57	MG	YA	3247	1/1	0.90	0.23	56,56,56,56	0
57	MG	YA	3035	1/1	0.90	0.26	20,20,20,20	0
57	MG	QF	201	1/1	0.90	0.06	70,70,70,70	0
57	MG	YA	3253	1/1	0.90	0.22	87,87,87,87	0
57	MG	QM	201	1/1	0.90	0.10	87,87,87,87	0
57	MG	RA	3048	1/1	0.90	0.12	30,30,30,30	0
57	MG	RA	3049	1/1	0.90	0.23	47,47,47,47	0
57	MG	QA	1654	1/1	0.90	0.07	87,87,87,87	0
57	MG	YA	3183	1/1	0.90	0.12	58,58,58,58	0
57	MG	QA	1625	1/1	0.90	0.22	68,68,68,68	0
57	MG	QA	1635	1/1	0.90	0.15	51,51,51,51	0
57	MG	YA	3273	1/1	0.90	0.32	57,57,57,57	0
57	MG	QA	1621	1/1	0.90	0.20	62,62,62,62	0
57	MG	YA	3275	1/1	0.90	0.30	82,82,82,82	0
57	MG	RA	3113	1/1	0.90	0.13	34,34,34,34	0
57	MG	RA	3253	1/1	0.90	0.16	49,49,49,49	0
57	MG	XA	1601	1/1	0.90	0.23	43,43,43,43	0
57	MG	QA	1609	1/1	0.90	0.17	55,55,55,55	0
57	MG	XA	1703	1/1	0.90	0.36	58,58,58,58	0
57	MG	QA	1631	1/1	0.90	0.07	68,68,68,68	0
57	MG	YA	3092	1/1	0.90	0.31	32,32,32,32	0
57	MG	YA	3150	1/1	0.90	0.10	69,69,69,69	0
57	MG	XA	1610	1/1	0.90	0.14	30,30,30,30	0
57	MG	RA	3073	1/1	0.90	0.10	61,61,61,61	0
57	MG	RA	3039	1/1	0.90	0.28	39,39,39,39	0
57	MG	YB	203	1/1	0.90	0.30	61,61,61,61	0
57	MG	RA	3078	1/1	0.90	0.26	30,30,30,30	0
57	MG	RA	3268	1/1	0.90	0.26	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1621	1/1	0.90	0.14	39,39,39,39	0
57	MG	XA	1667	1/1	0.90	0.27	56,56,56,56	0
57	MG	YA	3104	1/1	0.90	0.20	47,47,47,47	0
57	MG	RA	3270	1/1	0.91	0.30	62,62,62,62	0
57	MG	YA	3218	1/1	0.91	0.10	50,50,50,50	0
57	MG	YA	3019	1/1	0.91	0.27	34,34,34,34	0
57	MG	YA	3165	1/1	0.91	0.32	38,38,38,38	0
57	MG	YA	3107	1/1	0.91	0.30	24,24,24,24	0
57	MG	RA	3272	1/1	0.91	0.32	61,61,61,61	0
57	MG	XA	1630	1/1	0.91	0.23	46,46,46,46	0
57	MG	XA	1676	1/1	0.91	0.30	58,58,58,58	0
57	MG	RA	3138	1/1	0.91	0.12	59,59,59,59	0
57	MG	YA	3243	1/1	0.91	0.16	47,47,47,47	0
57	MG	RA	3140	1/1	0.91	0.20	32,32,32,32	0
57	MG	RA	3235	1/1	0.91	0.14	36,36,36,36	0
57	MG	RA	3279	1/1	0.91	0.25	48,48,48,48	0
57	MG	XA	1683	1/1	0.91	0.09	74,74,74,74	0
57	MG	RA	3124	1/1	0.91	0.25	39,39,39,39	0
57	MG	YA	3259	1/1	0.91	0.29	71,71,71,71	0
57	MG	QA	1628	1/1	0.91	0.19	55,55,55,55	0
57	MG	YA	3042	1/1	0.91	0.21	9,9,9,9	0
57	MG	YA	3043	1/1	0.91	0.25	42,42,42,42	0
57	MG	RA	3023	1/1	0.91	0.12	34,34,34,34	0
57	MG	QA	1688	1/1	0.91	0.18	54,54,54,54	0
57	MG	YA	3270	1/1	0.91	0.38	68,68,68,68	0
57	MG	YA	3050	1/1	0.91	0.31	23,23,23,23	0
57	MG	YA	3051	1/1	0.91	0.29	24,24,24,24	0
57	MG	RA	3088	1/1	0.91	0.19	49,49,49,49	0
57	MG	RA	3179	1/1	0.91	0.23	61,61,61,61	0
57	MG	RA	3004	1/1	0.91	0.14	17,17,17,17	0
57	MG	RA	3205	1/1	0.91	0.18	51,51,51,51	0
57	MG	RA	3095	1/1	0.91	0.17	31,31,31,31	0
57	MG	XA	1700	1/1	0.91	0.26	61,61,61,61	0
57	MG	RA	3034	1/1	0.91	0.25	31,31,31,31	0
57	MG	RA	3208	1/1	0.91	0.16	25,25,25,25	0
57	MG	RA	3100	1/1	0.91	0.32	45,45,45,45	0
57	MG	RA	3186	1/1	0.91	0.10	38,38,38,38	0
57	MG	RA	3187	1/1	0.91	0.07	79,79,79,79	0
57	MG	YA	3291	1/1	0.91	0.15	57,57,57,57	0
57	MG	QA	1680	1/1	0.91	0.24	54,54,54,54	0
57	MG	RA	3263	1/1	0.91	0.10	70,70,70,70	0
57	MG	RA	3225	1/1	0.91	0.13	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3266	1/1	0.91	0.23	48,48,48,48	0
57	MG	YE	301	1/1	0.91	0.21	37,37,37,37	0
57	MG	RA	3020	1/1	0.91	0.24	17,17,17,17	0
57	MG	YA	3212	1/1	0.91	0.23	49,49,49,49	0
57	MG	YA	3010	1/1	0.91	0.32	40,40,40,40	0
57	MG	Y3	101	1/1	0.91	0.24	35,35,35,35	0
57	MG	RA	3192	1/1	0.91	0.24	45,45,45,45	0
57	MG	RA	3030	1/1	0.92	0.17	41,41,41,41	0
57	MG	YA	3223	1/1	0.92	0.26	39,39,39,39	0
57	MG	YA	3224	1/1	0.92	0.16	56,56,56,56	0
57	MG	YA	3163	1/1	0.92	0.12	59,59,59,59	0
57	MG	QA	1655	1/1	0.92	0.06	120,120,120,120	0
57	MG	RA	3246	1/1	0.92	0.24	64,64,64,64	0
57	MG	XA	1643	1/1	0.92	0.19	42,42,42,42	0
57	MG	RA	3163	1/1	0.92	0.16	39,39,39,39	0
57	MG	QA	1603	1/1	0.92	0.43	83,83,83,83	0
57	MG	YA	3242	1/1	0.92	0.18	27,27,27,27	0
57	MG	XA	1646	1/1	0.92	0.10	49,49,49,49	0
57	MG	YA	3246	1/1	0.92	0.23	32,32,32,32	0
57	MG	YA	3037	1/1	0.92	0.17	30,30,30,30	0
57	MG	RA	3250	1/1	0.92	0.25	47,47,47,47	0
57	MG	RA	3165	1/1	0.92	0.05	37,37,37,37	0
57	MG	XA	1693	1/1	0.92	0.19	62,62,62,62	0
57	MG	RA	3021	1/1	0.92	0.18	23,23,23,23	0
57	MG	YA	3258	1/1	0.92	0.28	52,52,52,52	0
57	MG	YA	3122	1/1	0.92	0.26	26,26,26,26	0
57	MG	RA	3216	1/1	0.92	0.22	41,41,41,41	0
57	MG	YA	3124	1/1	0.92	0.08	32,32,32,32	0
57	MG	XA	1651	1/1	0.92	0.18	38,38,38,38	0
57	MG	YA	3047	1/1	0.92	0.16	23,23,23,23	0
57	MG	RA	3256	1/1	0.92	0.31	37,37,37,37	0
57	MG	QA	1632	1/1	0.92	0.06	50,50,50,50	0
57	MG	YA	3054	1/1	0.92	0.23	24,24,24,24	0
57	MG	YA	3055	1/1	0.92	0.17	63,63,63,63	0
57	MG	RA	3054	1/1	0.92	0.16	51,51,51,51	0
57	MG	RA	3142	1/1	0.92	0.12	58,58,58,58	0
57	MG	YA	3135	1/1	0.92	0.15	40,40,40,40	0
57	MG	RA	3228	1/1	0.92	0.12	46,46,46,46	0
57	MG	QK	201	1/1	0.92	0.10	64,64,64,64	0
57	MG	RA	3059	1/1	0.92	0.24	14,14,14,14	0
57	MG	QA	1672	1/1	0.92	0.12	61,61,61,61	0
57	MG	RA	3197	1/1	0.92	0.15	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3065	1/1	0.92	0.27	17,17,17,17	0
57	MG	XY	101	1/1	0.92	0.08	54,54,54,54	0
57	MG	RA	3094	1/1	0.92	0.22	30,30,30,30	0
57	MG	YA	3203	1/1	0.92	0.12	76,76,76,76	0
57	MG	YA	3086	1/1	0.92	0.15	23,23,23,23	0
57	MG	XA	1627	1/1	0.92	0.10	36,36,36,36	0
57	MG	YA	3093	1/1	0.92	0.18	40,40,40,40	0
57	MG	RA	3178	1/1	0.92	0.06	60,60,60,60	0
57	MG	RA	3202	1/1	0.92	0.16	46,46,46,46	0
57	MG	YA	3013	1/1	0.92	0.22	13,13,13,13	0
57	MG	RA	3241	1/1	0.92	0.19	49,49,49,49	0
57	MG	RA	3133	1/1	0.92	0.24	21,21,21,21	0
57	MG	Y1	101	1/1	0.92	0.12	37,37,37,37	0
57	MG	YA	3217	1/1	0.92	0.16	34,34,34,34	0
57	MG	RA	3158	1/1	0.92	0.06	47,47,47,47	0
58	PAR	QA	1691	42/42	0.92	0.14	82,82,83,83	0
57	MG	YA	3081	1/1	0.93	0.16	47,47,47,47	0
57	MG	RA	3174	1/1	0.93	0.08	44,44,44,44	0
57	MG	RA	3066	1/1	0.93	0.17	29,29,29,29	0
57	MG	RA	3087	1/1	0.93	0.17	30,30,30,30	0
57	MG	YA	3001	1/1	0.93	0.08	23,23,23,23	0
57	MG	YA	3089	1/1	0.93	0.26	54,54,54,54	0
57	MG	YA	3002	1/1	0.93	0.20	22,22,22,22	0
57	MG	YA	3225	1/1	0.93	0.22	42,42,42,42	0
57	MG	RA	3276	1/1	0.93	0.30	68,68,68,68	0
57	MG	RA	3177	1/1	0.93	0.14	40,40,40,40	0
57	MG	XA	1628	1/1	0.93	0.07	47,47,47,47	0
57	MG	RA	3129	1/1	0.93	0.15	69,69,69,69	0
57	MG	XA	1671	1/1	0.93	0.23	54,54,54,54	0
57	MG	YA	3014	1/1	0.93	0.22	18,18,18,18	0
57	MG	XA	1674	1/1	0.93	0.22	39,39,39,39	0
57	MG	QA	1671	1/1	0.93	0.19	48,48,48,48	0
57	MG	QA	1662	1/1	0.93	0.27	34,34,34,34	0
57	MG	RA	3181	1/1	0.93	0.17	57,57,57,57	0
57	MG	YA	3248	1/1	0.93	0.12	31,31,31,31	0
57	MG	XA	1678	1/1	0.93	0.19	82,82,82,82	0
57	MG	RE	301	1/1	0.93	0.14	26,26,26,26	0
57	MG	RA	3159	1/1	0.93	0.16	45,45,45,45	0
57	MG	RA	3093	1/1	0.93	0.30	39,39,39,39	0
57	MG	YA	3032	1/1	0.93	0.23	11,11,11,11	0
57	MG	YA	3174	1/1	0.93	0.18	53,53,53,53	0
57	MG	RA	3056	1/1	0.93	0.19	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3115	1/1	0.93	0.25	70,70,70,70	0
57	MG	RA	3046	1/1	0.93	0.21	25,25,25,25	0
57	MG	YA	3117	1/1	0.93	0.25	23,23,23,23	0
57	MG	YA	3179	1/1	0.93	0.24	22,22,22,22	0
57	MG	RA	3220	1/1	0.93	0.32	44,44,44,44	0
57	MG	YA	3120	1/1	0.93	0.19	36,36,36,36	0
57	MG	RA	3047	1/1	0.93	0.17	22,22,22,22	0
57	MG	RA	3121	1/1	0.93	0.15	45,45,45,45	0
57	MG	RA	3122	1/1	0.93	0.19	33,33,33,33	0
57	MG	YA	3186	1/1	0.93	0.23	52,52,52,52	0
57	MG	YA	3277	1/1	0.93	0.22	51,51,51,51	0
57	MG	XA	1692	1/1	0.93	0.30	68,68,68,68	0
57	MG	RA	3076	1/1	0.93	0.16	34,34,34,34	0
57	MG	XA	1694	1/1	0.93	0.10	117,117,117,117	0
57	MG	XA	1602	1/1	0.93	0.15	19,19,19,19	0
57	MG	XA	1604	1/1	0.93	0.30	53,53,53,53	0
57	MG	QA	1623	1/1	0.93	0.23	64,64,64,64	0
57	MG	YA	3131	1/1	0.93	0.14	65,65,65,65	0
57	MG	RA	3143	1/1	0.93	0.28	55,55,55,55	0
57	MG	XA	1699	1/1	0.93	0.25	64,64,64,64	0
57	MG	XA	1653	1/1	0.93	0.09	48,48,48,48	0
57	MG	RA	3081	1/1	0.93	0.27	44,44,44,44	0
57	MG	RA	3171	1/1	0.93	0.11	50,50,50,50	0
57	MG	XA	1615	1/1	0.93	0.13	33,33,33,33	0
57	MG	YA	3139	1/1	0.93	0.10	40,40,40,40	0
57	MG	RA	3019	1/1	0.93	0.23	22,22,22,22	0
57	MG	XA	1617	1/1	0.93	0.21	21,21,21,21	0
57	MG	YR	201	1/1	0.93	0.23	54,54,54,54	0
57	MG	YA	3144	1/1	0.93	0.25	45,45,45,45	0
57	MG	YA	3145	1/1	0.93	0.12	14,14,14,14	0
57	MG	YA	3209	1/1	0.93	0.07	64,64,64,64	0
57	MG	RA	3150	1/1	0.93	0.23	47,47,47,47	0
57	MG	YA	3078	1/1	0.93	0.14	40,40,40,40	0
58	PAR	XA	1705	42/42	0.93	0.12	68,68,69,69	0
57	MG	RA	3281	1/1	0.94	0.05	145,145,145,145	0
57	MG	RB	201	1/1	0.94	0.09	71,71,71,71	0
57	MG	RA	3218	1/1	0.94	0.22	32,32,32,32	0
57	MG	RA	3249	1/1	0.94	0.31	62,62,62,62	0
57	MG	RA	3098	1/1	0.94	0.27	52,52,52,52	0
57	MG	RA	3147	1/1	0.94	0.07	57,57,57,57	0
57	MG	RA	3002	1/1	0.94	0.15	41,41,41,41	0
57	MG	RA	3075	1/1	0.94	0.17	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3249	1/1	0.94	0.27	52,52,52,52	0
57	MG	QA	1669	1/1	0.94	0.12	41,41,41,41	0
57	MG	RA	3057	1/1	0.94	0.28	32,32,32,32	0
57	MG	R0	102	1/1	0.94	0.32	64,64,64,64	0
57	MG	YA	3070	1/1	0.94	0.14	19,19,19,19	0
57	MG	XA	1672	1/1	0.94	0.19	57,57,57,57	0
57	MG	XA	1673	1/1	0.94	0.35	54,54,54,54	0
57	MG	YA	3077	1/1	0.94	0.19	24,24,24,24	0
57	MG	RA	3107	1/1	0.94	0.17	37,37,37,37	0
57	MG	YA	3190	1/1	0.94	0.10	70,70,70,70	0
57	MG	YA	3080	1/1	0.94	0.13	25,25,25,25	0
57	MG	RA	3005	1/1	0.94	0.21	20,20,20,20	0
57	MG	XA	1637	1/1	0.94	0.39	55,55,55,55	0
57	MG	YA	3011	1/1	0.94	0.16	21,21,21,21	0
57	MG	XA	1638	1/1	0.94	0.22	62,62,62,62	0
57	MG	YA	3143	1/1	0.94	0.31	61,61,61,61	0
57	MG	RA	3042	1/1	0.94	0.14	34,34,34,34	0
57	MG	YA	3088	1/1	0.94	0.19	21,21,21,21	0
57	MG	XA	1642	1/1	0.94	0.11	40,40,40,40	0
57	MG	YA	3016	1/1	0.94	0.27	28,28,28,28	0
57	MG	YA	3280	1/1	0.94	0.34	64,64,64,64	0
57	MG	QA	1634	1/1	0.94	0.11	68,68,68,68	0
57	MG	QA	1643	1/1	0.94	0.06	50,50,50,50	0
57	MG	RA	3112	1/1	0.94	0.24	42,42,42,42	0
57	MG	YA	3097	1/1	0.94	0.23	36,36,36,36	0
57	MG	YA	3022	1/1	0.94	0.18	15,15,15,15	0
57	MG	XA	1684	1/1	0.94	0.15	52,52,52,52	0
57	MG	QA	1648	1/1	0.94	0.11	42,42,42,42	0
57	MG	QA	1681	1/1	0.94	0.19	50,50,50,50	0
57	MG	XA	1607	1/1	0.94	0.19	36,36,36,36	0
57	MG	RA	3091	1/1	0.94	0.21	27,27,27,27	0
57	MG	YA	3215	1/1	0.94	0.16	36,36,36,36	0
57	MG	XA	1689	1/1	0.94	0.21	55,55,55,55	0
57	MG	RA	3033	1/1	0.94	0.43	48,48,48,48	0
57	MG	XA	1613	1/1	0.94	0.22	26,26,26,26	0
57	MG	XA	1614	1/1	0.94	0.16	25,25,25,25	0
57	MG	QA	1610	1/1	0.94	0.07	31,31,31,31	0
57	MG	YR	202	1/1	0.94	0.18	46,46,46,46	0
57	MG	YY	201	1/1	0.94	0.12	67,67,67,67	0
57	MG	YA	3039	1/1	0.94	0.16	28,28,28,28	0
57	MG	QA	1606	1/1	0.94	0.29	39,39,39,39	0
57	MG	XA	1655	1/1	0.94	0.18	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3215	1/1	0.94	0.27	41,41,41,41	0
57	MG	RA	3096	1/1	0.94	0.30	33,33,33,33	0
57	MG	YA	3236	1/1	0.94	0.31	29,29,29,29	0
59	ZN	XD	301	1/1	0.94	0.22	65,65,65,65	0
57	MG	RA	3011	1/1	0.95	0.12	22,22,22,22	0
57	MG	XA	1665	1/1	0.95	0.15	51,51,51,51	0
57	MG	RA	3026	1/1	0.95	0.31	16,16,16,16	0
57	MG	RA	3153	1/1	0.95	0.21	59,59,59,59	0
57	MG	RB	202	1/1	0.95	0.06	63,63,63,63	0
57	MG	RA	3102	1/1	0.95	0.12	27,27,27,27	0
57	MG	YA	3067	1/1	0.95	0.32	34,34,34,34	0
57	MG	YA	3068	1/1	0.95	0.11	46,46,46,46	0
57	MG	RA	3083	1/1	0.95	0.19	23,23,23,23	0
57	MG	QA	1641	1/1	0.95	0.11	45,45,45,45	0
57	MG	RA	3085	1/1	0.95	0.14	53,53,53,53	0
57	MG	YA	3256	1/1	0.95	0.26	46,46,46,46	0
57	MG	YA	3257	1/1	0.95	0.17	38,38,38,38	0
57	MG	YA	3187	1/1	0.95	0.08	60,60,60,60	0
57	MG	RA	3086	1/1	0.95	0.25	37,37,37,37	0
57	MG	YA	3008	1/1	0.95	0.12	17,17,17,17	0
57	MG	XA	1635	1/1	0.95	0.07	36,36,36,36	0
57	MG	YA	3262	1/1	0.95	0.34	63,63,63,63	0
57	MG	YA	3265	1/1	0.95	0.31	44,44,44,44	0
57	MG	QA	1642	1/1	0.95	0.13	35,35,35,35	0
57	MG	QA	1617	1/1	0.95	0.11	39,39,39,39	0
57	MG	RA	3132	1/1	0.95	0.15	43,43,43,43	0
57	MG	XA	1640	1/1	0.95	0.13	60,60,60,60	0
57	MG	QA	1611	1/1	0.95	0.21	29,29,29,29	0
57	MG	YA	3085	1/1	0.95	0.26	39,39,39,39	0
57	MG	XA	1681	1/1	0.95	0.07	58,58,58,58	0
57	MG	RA	3255	1/1	0.95	0.32	64,64,64,64	0
57	MG	QA	1612	1/1	0.95	0.21	23,23,23,23	0
57	MG	RA	3257	1/1	0.95	0.25	59,59,59,59	0
57	MG	RA	3114	1/1	0.95	0.14	55,55,55,55	0
57	MG	RA	3226	1/1	0.95	0.16	25,25,25,25	0
57	MG	RA	3115	1/1	0.95	0.08	58,58,58,58	0
57	MG	YA	3096	1/1	0.95	0.12	44,44,44,44	0
57	MG	YA	3154	1/1	0.95	0.22	52,52,52,52	0
57	MG	YA	3207	1/1	0.95	0.15	16,16,16,16	0
57	MG	RA	3262	1/1	0.95	0.28	57,57,57,57	0
57	MG	RA	3229	1/1	0.95	0.14	38,38,38,38	0
57	MG	YA	3211	1/1	0.95	0.22	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3072	1/1	0.95	0.11	26,26,26,26	0
57	MG	XA	1691	1/1	0.95	0.15	66,66,66,66	0
57	MG	YA	3034	1/1	0.95	0.23	20,20,20,20	0
57	MG	QA	1684	1/1	0.95	0.10	76,76,76,76	0
57	MG	YA	3036	1/1	0.95	0.20	16,16,16,16	0
57	MG	RA	3055	1/1	0.95	0.27	29,29,29,29	0
57	MG	RA	3119	1/1	0.95	0.16	40,40,40,40	0
57	MG	QA	1652	1/1	0.95	0.12	44,44,44,44	0
57	MG	YP	202	1/1	0.95	0.14	48,48,48,48	0
57	MG	RA	3144	1/1	0.95	0.27	70,70,70,70	0
57	MG	RA	3237	1/1	0.95	0.15	72,72,72,72	0
57	MG	RA	3274	1/1	0.95	0.35	57,57,57,57	0
57	MG	YA	3229	1/1	0.95	0.12	26,26,26,26	0
57	MG	RA	3275	1/1	0.95	0.09	58,58,58,58	0
57	MG	QA	1627	1/1	0.95	0.05	44,44,44,44	0
57	MG	Y5	101	1/1	0.95	0.10	28,28,28,28	0
57	MG	XA	1620	1/1	0.95	0.10	56,56,56,56	0
57	MG	YA	3048	1/1	0.95	0.32	23,23,23,23	0
57	MG	RA	3008	1/1	0.95	0.23	44,44,44,44	0
57	MG	RA	3148	1/1	0.95	0.26	37,37,37,37	0
57	MG	RA	3221	1/1	0.96	0.22	20,20,20,20	0
57	MG	YA	3009	1/1	0.96	0.17	21,21,21,21	0
57	MG	RA	3222	1/1	0.96	0.19	23,23,23,23	0
57	MG	YA	3129	1/1	0.96	0.07	58,58,58,58	0
57	MG	XA	1639	1/1	0.96	0.07	54,54,54,54	0
57	MG	RA	3097	1/1	0.96	0.15	24,24,24,24	0
57	MG	YA	3075	1/1	0.96	0.21	21,21,21,21	0
57	MG	RA	3258	1/1	0.96	0.51	60,60,60,60	0
57	MG	RA	3188	1/1	0.96	0.17	34,34,34,34	0
57	MG	RA	3032	1/1	0.96	0.26	16,16,16,16	0
57	MG	YA	3136	1/1	0.96	0.15	17,17,17,17	0
57	MG	RA	3139	1/1	0.96	0.24	23,23,23,23	0
57	MG	XA	1603	1/1	0.96	0.18	31,31,31,31	0
57	MG	RA	3079	1/1	0.96	0.17	42,42,42,42	0
57	MG	RA	3141	1/1	0.96	0.14	44,44,44,44	0
57	MG	YA	3263	1/1	0.96	0.34	53,53,53,53	0
57	MG	YA	3264	1/1	0.96	0.25	34,34,34,34	0
57	MG	YA	3141	1/1	0.96	0.35	217,217,217,217	0
57	MG	QA	1622	1/1	0.96	0.17	80,80,80,80	0
57	MG	YA	3197	1/1	0.96	0.10	30,30,30,30	0
57	MG	QA	1607	1/1	0.96	0.14	37,37,37,37	0
57	MG	YA	3269	1/1	0.96	0.20	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1609	1/1	0.96	0.17	39,39,39,39	0
57	MG	RA	3267	1/1	0.96	0.28	54,54,54,54	0
57	MG	RA	3232	1/1	0.96	0.34	59,59,59,59	0
57	MG	YA	3147	1/1	0.96	0.09	65,65,65,65	0
57	MG	RA	3036	1/1	0.96	0.14	32,32,32,32	0
57	MG	RA	3145	1/1	0.96	0.07	34,34,34,34	0
57	MG	RA	3198	1/1	0.96	0.13	21,21,21,21	0
57	MG	RA	3103	1/1	0.96	0.11	28,28,28,28	0
57	MG	RA	3024	1/1	0.96	0.16	27,27,27,27	0
57	MG	RA	3050	1/1	0.96	0.12	22,22,22,22	0
57	MG	RA	3051	1/1	0.96	0.16	14,14,14,14	0
57	MG	RA	3069	1/1	0.96	0.23	27,27,27,27	0
57	MG	RA	3151	1/1	0.96	0.16	36,36,36,36	0
57	MG	RA	3152	1/1	0.96	0.17	32,32,32,32	0
57	MG	QA	1660	1/1	0.96	0.19	30,30,30,30	0
57	MG	RA	3071	1/1	0.96	0.08	29,29,29,29	0
57	MG	XA	1666	1/1	0.96	0.12	71,71,71,71	0
57	MG	RA	3090	1/1	0.96	0.11	33,33,33,33	0
57	MG	RA	3053	1/1	0.96	0.11	17,17,17,17	0
57	MG	YA	3221	1/1	0.96	0.21	41,41,41,41	0
57	MG	RA	3182	1/1	0.96	0.10	53,53,53,53	0
57	MG	XV	103	1/1	0.96	0.24	36,36,36,36	0
57	MG	YA	3052	1/1	0.96	0.15	28,28,28,28	0
57	MG	YA	3053	1/1	0.96	0.08	23,23,23,23	0
57	MG	YA	3226	1/1	0.96	0.18	40,40,40,40	0
57	MG	YP	203	1/1	0.96	0.19	53,53,53,53	0
57	MG	RA	3214	1/1	0.96	0.32	64,64,64,64	0
57	MG	RA	3009	1/1	0.96	0.06	45,45,45,45	0
57	MG	YA	3118	1/1	0.96	0.14	66,66,66,66	0
57	MG	YA	3056	1/1	0.96	0.14	29,29,29,29	0
57	MG	YA	3058	1/1	0.96	0.21	19,19,19,19	0
57	MG	RA	3027	1/1	0.96	0.14	26,26,26,26	0
57	MG	QA	1657	1/1	0.96	0.22	64,64,64,64	0
57	MG	QA	1674	1/1	0.96	0.19	55,55,55,55	0
57	MG	YA	3005	1/1	0.96	0.13	14,14,14,14	0
57	MG	RR	202	1/1	0.96	0.13	30,30,30,30	0
57	MG	YA	3245	1/1	0.96	0.19	26,26,26,26	0
57	MG	YA	3254	1/1	0.97	0.07	53,53,53,53	0
57	MG	XA	1624	1/1	0.97	0.05	45,45,45,45	0
57	MG	YA	3006	1/1	0.97	0.09	18,18,18,18	0
57	MG	RA	3238	1/1	0.97	0.27	55,55,55,55	0
57	MG	RA	3029	1/1	0.97	0.16	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1677	1/1	0.97	0.23	45,45,45,45	0
57	MG	RA	3280	1/1	0.97	0.08	60,60,60,60	0
57	MG	YA	3041	1/1	0.97	0.12	8,8,8,8	0
57	MG	RA	3092	1/1	0.97	0.12	27,27,27,27	0
57	MG	RA	3080	1/1	0.97	0.15	34,34,34,34	0
57	MG	YA	3167	1/1	0.97	0.06	41,41,41,41	0
57	MG	YA	3210	1/1	0.97	0.11	53,53,53,53	0
57	MG	RA	3161	1/1	0.97	0.16	38,38,38,38	0
57	MG	RA	3190	1/1	0.97	0.24	45,45,45,45	0
57	MG	YA	3087	1/1	0.97	0.20	24,24,24,24	0
57	MG	YA	3015	1/1	0.97	0.19	12,12,12,12	0
57	MG	RA	3016	1/1	0.97	0.12	30,30,30,30	0
57	MG	YA	3090	1/1	0.97	0.10	54,54,54,54	0
57	MG	YA	3091	1/1	0.97	0.15	33,33,33,33	0
57	MG	YA	3049	1/1	0.97	0.19	18,18,18,18	0
57	MG	YA	3219	1/1	0.97	0.13	48,48,48,48	0
57	MG	YA	3220	1/1	0.97	0.23	45,45,45,45	0
57	MG	XA	1611	1/1	0.97	0.07	32,32,32,32	0
57	MG	RA	3010	1/1	0.97	0.38	48,48,48,48	0
57	MG	RA	3006	1/1	0.97	0.27	29,29,29,29	0
57	MG	YA	3021	1/1	0.97	0.33	25,25,25,25	0
57	MG	QA	1629	1/1	0.97	0.32	64,64,64,64	0
57	MG	YA	3181	1/1	0.97	0.20	26,26,26,26	0
57	MG	YA	3227	1/1	0.97	0.27	20,20,20,20	0
57	MG	YA	3228	1/1	0.97	0.32	17,17,17,17	0
57	MG	YA	3023	1/1	0.97	0.25	20,20,20,20	0
57	MG	YA	3230	1/1	0.97	0.24	23,23,23,23	0
57	MG	YA	3231	1/1	0.97	0.13	18,18,18,18	0
57	MG	YA	3099	1/1	0.97	0.15	13,13,13,13	0
57	MG	RA	3212	1/1	0.97	0.29	56,56,56,56	0
57	MG	YA	3234	1/1	0.97	0.24	39,39,39,39	0
57	MG	RA	3063	1/1	0.97	0.41	19,19,19,19	0
57	MG	YA	3059	1/1	0.97	0.09	20,20,20,20	0
57	MG	YA	3026	1/1	0.97	0.19	17,17,17,17	0
57	MG	YA	3063	1/1	0.97	0.09	16,16,16,16	0
57	MG	YA	3027	1/1	0.97	0.50	31,31,31,31	0
57	MG	RA	3271	1/1	0.97	0.16	47,47,47,47	0
57	MG	YA	3108	1/1	0.97	0.06	23,23,23,23	0
57	MG	YA	3244	1/1	0.97	0.08	35,35,35,35	0
57	MG	YA	3029	1/1	0.97	0.11	18,18,18,18	0
57	MG	YA	3110	1/1	0.97	0.09	49,49,49,49	0
57	MG	RA	3064	1/1	0.97	0.12	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3035	1/1	0.97	0.10	21,21,21,21	0
57	MG	QA	1602	1/1	0.97	0.32	37,37,37,37	0
57	MG	RA	3217	1/1	0.97	0.20	48,48,48,48	0
57	MG	YA	3251	1/1	0.97	0.20	25,25,25,25	0
57	MG	RA	3077	1/1	0.97	0.10	39,39,39,39	0
57	MG	YA	3073	1/1	0.97	0.06	38,38,38,38	0
57	MG	XA	1608	1/1	0.98	0.08	23,23,23,23	0
57	MG	XA	1623	1/1	0.98	0.04	54,54,54,54	0
57	MG	RA	3045	1/1	0.98	0.10	17,17,17,17	0
57	MG	YA	3072	1/1	0.98	0.20	21,21,21,21	0
57	MG	YA	3284	1/1	0.98	0.30	47,47,47,47	0
57	MG	XA	1625	1/1	0.98	0.21	38,38,38,38	0
57	MG	RA	3219	1/1	0.98	0.13	34,34,34,34	0
57	MG	RA	3210	1/1	0.98	0.17	12,12,12,12	0
57	MG	YA	3076	1/1	0.98	0.19	21,21,21,21	0
57	MG	YA	3289	1/1	0.98	0.34	63,63,63,63	0
57	MG	YA	3290	1/1	0.98	0.28	52,52,52,52	0
57	MG	YA	3152	1/1	0.98	0.14	40,40,40,40	0
57	MG	RA	3062	1/1	0.98	0.28	12,12,12,12	0
57	MG	YA	3017	1/1	0.98	0.07	27,27,27,27	0
57	MG	RA	3106	1/1	0.98	0.11	24,24,24,24	0
57	MG	RA	3037	1/1	0.98	0.12	18,18,18,18	0
57	MG	YA	3106	1/1	0.98	0.13	13,13,13,13	0
57	MG	YA	3057	1/1	0.98	0.06	19,19,19,19	0
57	MG	RA	3028	1/1	0.98	0.21	20,20,20,20	0
57	MG	YA	3003	1/1	0.98	0.24	26,26,26,26	0
57	MG	YA	3060	1/1	0.98	0.06	59,59,59,59	0
57	MG	YA	3240	1/1	0.98	0.40	39,39,39,39	0
57	MG	YA	3241	1/1	0.98	0.11	37,37,37,37	0
57	MG	YA	3061	1/1	0.98	0.12	24,24,24,24	0
57	MG	RA	3003	1/1	0.98	0.26	27,27,27,27	0
57	MG	RA	3017	1/1	0.98	0.09	27,27,27,27	0
57	MG	RA	3227	1/1	0.98	0.28	41,41,41,41	0
57	MG	RA	3060	1/1	0.98	0.10	17,17,17,17	0
57	MG	YA	3044	1/1	0.98	0.21	13,13,13,13	0
57	MG	RA	3251	1/1	0.98	0.31	65,65,65,65	0
57	MG	YA	3278	1/1	0.98	0.21	58,58,58,58	0
59	ZN	QD	301	1/1	0.98	0.19	74,74,74,74	0
57	MG	RA	3264	1/1	0.98	0.23	43,43,43,43	0
57	MG	YA	3271	1/1	0.99	0.24	63,63,63,63	0
57	MG	YA	3079	1/1	0.99	0.29	21,21,21,21	0
57	MG	RA	3105	1/1	0.99	0.03	24,24,24,24	0

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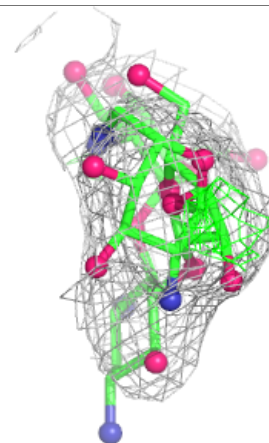
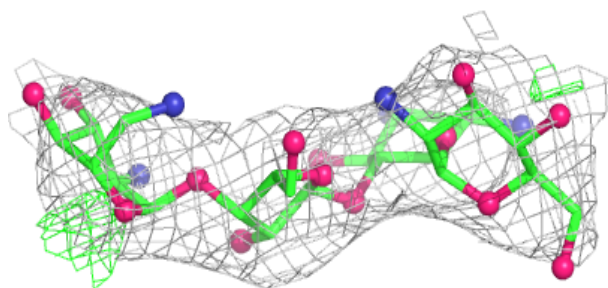
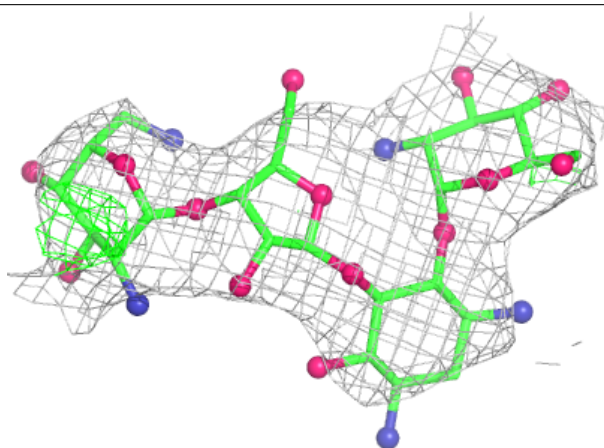
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1608	1/1	0.99	0.03	28,28,28,28	0
57	MG	RA	3209	1/1	0.99	0.23	22,22,22,22	0
57	MG	RA	3014	1/1	0.99	0.08	20,20,20,20	0
59	ZN	QN	101	1/1	0.99	0.03	104,104,104,104	0
57	MG	XA	1663	1/1	0.99	0.08	35,35,35,35	0
59	ZN	XN	101	1/1	0.99	0.04	122,122,122,122	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.

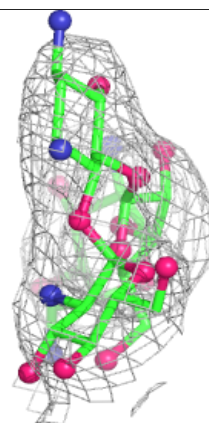
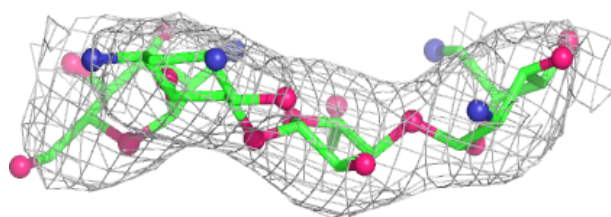
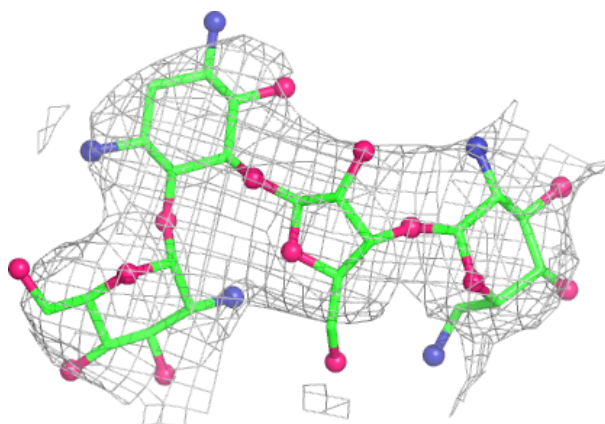
Electron density around PAR QA 1691:

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 1705:

$2mF_o - DF_c$ (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.