



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 9, 2022 – 09:09 AM EDT

PDB ID : 4TUB
Title : Crystal structure of tRNA-Thr 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

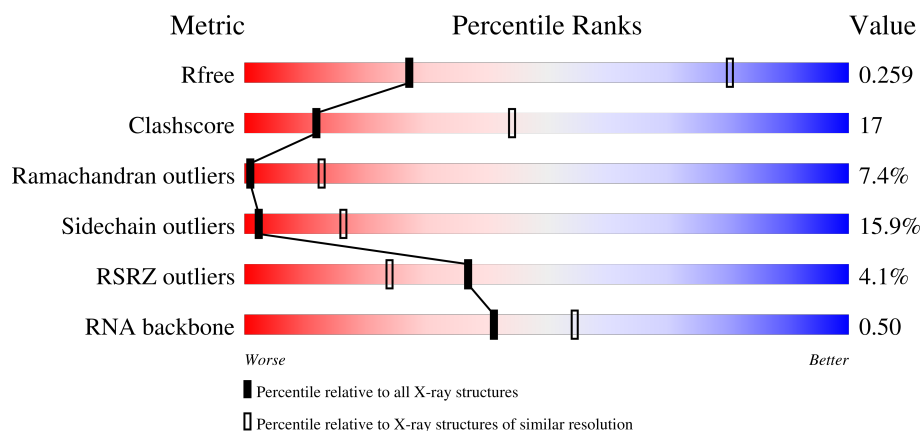
1 Overall quality at a glance

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.





















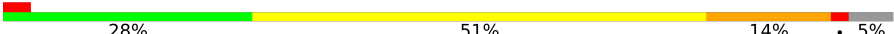






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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

Mol	Chain	Length	Quality of chain
1	QA	1522	<div> <div></div> <div>51% 38% 9% ..</div> </div>
1	XA	1522	<div> <div></div> <div>50% 38% 9% ..</div> </div>
2	QB	256	<div> <div>10%</div> <div>48% 36% 7% • 7%</div> </div>
2	XB	256	<div> <div>3%</div> <div>46% 36% 10% • 7%</div> </div>

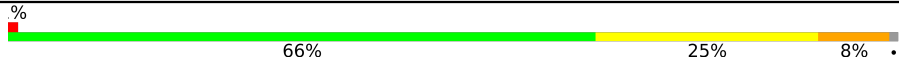

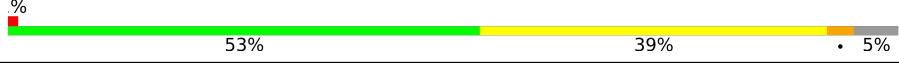

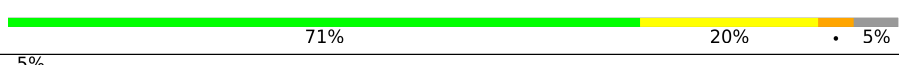
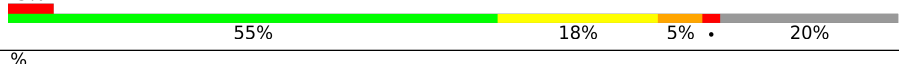
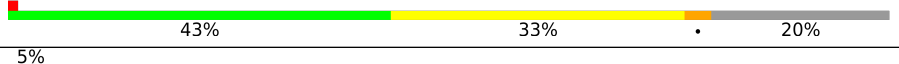
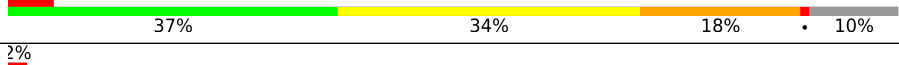
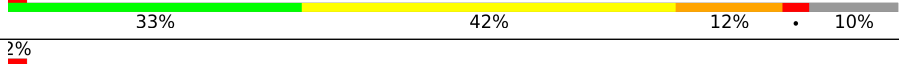


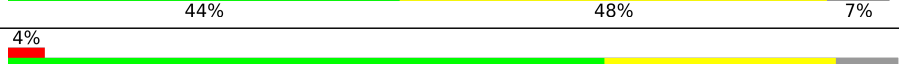

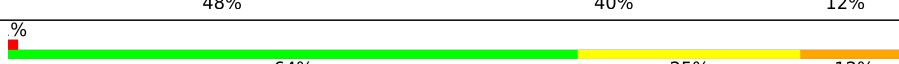
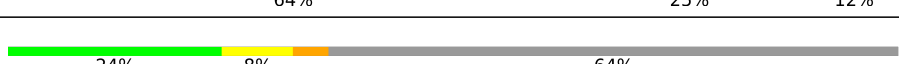

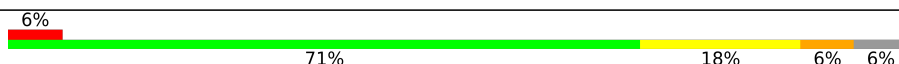

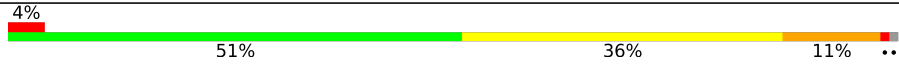


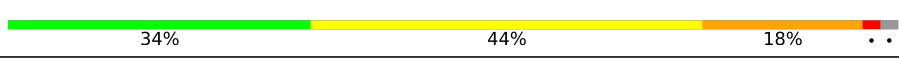

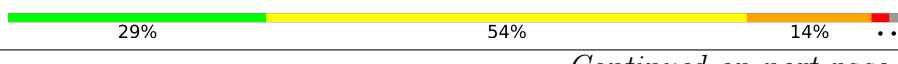

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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126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

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Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	25	
23	XX	25	
24	QY	17	
24	XY	17	
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	1603	-	-	-	X
57	MG	QA	1640	-	-	-	X
57	MG	QA	1656	-	-	-	X
57	MG	QA	1658	-	-	-	X
57	MG	QA	1661	-	-	-	X
57	MG	QA	1668	-	-	-	X
57	MG	QA	1673	-	-	-	X
57	MG	RA	3170	-	-	-	X
57	MG	RA	3197	-	-	-	X
57	MG	RA	3201	-	-	-	X
57	MG	RA	3209	-	-	-	X
57	MG	RA	3213	-	-	-	X
57	MG	RA	3251	-	-	-	X
57	MG	RA	3256	-	-	-	X
57	MG	RA	3264	-	-	-	X
57	MG	RA	3270	-	-	-	X
57	MG	RA	3271	-	-	-	X
57	MG	RA	3274	-	-	-	X
57	MG	RA	3280	-	-	-	X
57	MG	RA	3303	-	-	-	X
57	MG	RA	3308	-	-	-	X
57	MG	RA	3313	-	-	-	X
57	MG	RR	201	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	XA	1649	-	-	-	X
57	MG	XA	1662	-	-	-	X
57	MG	XA	1675	-	-	-	X
57	MG	XA	1706	-	-	-	X
57	MG	YA	3113	-	-	-	X
57	MG	YA	3117	-	-	-	X
57	MG	YA	3174	-	-	-	X
57	MG	YA	3175	-	-	-	X
57	MG	YA	3191	-	-	-	X
57	MG	YA	3194	-	-	-	X
57	MG	YA	3208	-	-	-	X
57	MG	YA	3216	-	-	-	X
57	MG	YA	3226	-	-	-	X
57	MG	YA	3227	-	-	-	X
57	MG	YA	3257	-	-	-	X
57	MG	YA	3283	-	-	-	X
57	MG	YA	3292	-	-	-	X
57	MG	YA	3295	-	-	-	X
57	MG	YA	3298	-	-	-	X
57	MG	YA	3302	-	-	-	X
57	MG	YA	3321	-	-	-	X
57	MG	YA	3333	-	-	-	X
57	MG	YA	3337	-	-	-	X
57	MG	YA	3339	-	-	-	X
57	MG	YA	3355	-	-	-	X
57	MG	YP	201	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 292320 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 f-Met.

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
			191	86	36	60	9			
23	XX	10	Total	C	N	O	P	0	0	0
			213	96	41	66	10			

- Molecule 24 is a RNA chain called A-site tRNA Thr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	16	Total	C	N	O	P	0	0	0
			344	153	62	113	16			
24	XY	16	Total	C	N	O	P	0	0	0
			344	153	62	113	16			

- 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
			647	401	137	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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	80	Total	Mg	0	0
			80	80		
57	QE	1	Total	Mg	0	0
			1	1		
57	QF	1	Total	Mg	0	0
			1	1		
57	QM	1	Total	Mg	0	0
			1	1		
57	QV	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QX	2	Total 2	Mg 2	0	0
57	QY	1	Total 1	Mg 1	0	0
57	RA	326	Total 326	Mg 326	0	0
57	RB	5	Total 5	Mg 5	0	0
57	RE	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0
57	RP	1	Total 1	Mg 1	0	0
57	RR	1	Total 1	Mg 1	0	0
57	R0	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	XA	110	Total 110	Mg 110	0	0
57	XB	1	Total 1	Mg 1	0	0
57	XD	1	Total 1	Mg 1	0	0
57	XF	1	Total 1	Mg 1	0	0
57	XV	2	Total 2	Mg 2	0	0
57	XX	1	Total 1	Mg 1	0	0
57	YA	356	Total 356	Mg 356	0	0
57	YB	4	Total 4	Mg 4	0	0
57	YD	1	Total 1	Mg 1	0	0
57	YE	2	Total 2	Mg 2	0	0
57	YP	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YQ	1	Total 1	Mg 1	0	0
57	YU	1	Total 1	Mg 1	0	0
57	YY	1	Total 1	Mg 1	0	0
57	Y0	3	Total 3	Mg 3	0	0
57	Y1	1	Total 1	Mg 1	0	0
57	Y3	1	Total 1	Mg 1	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	Y7	1	Total 1	Mg 1	0	0

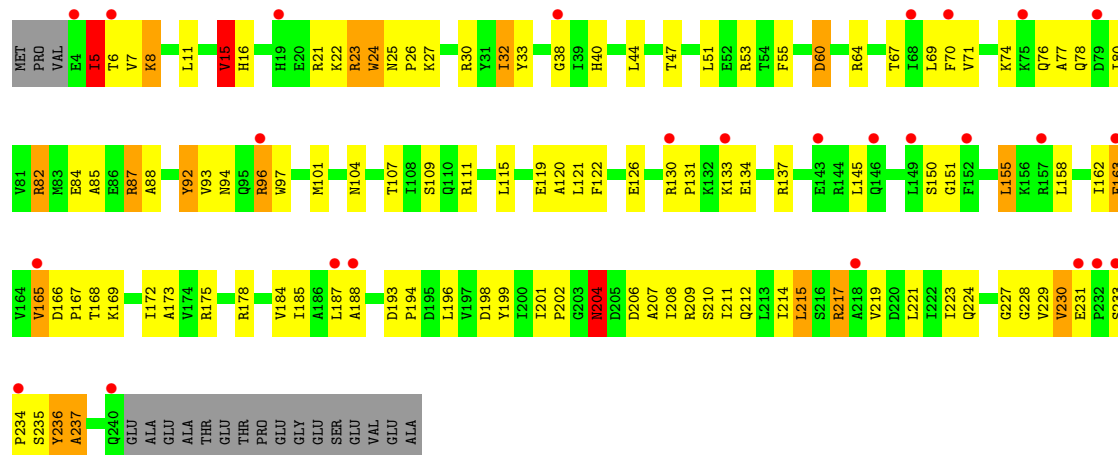
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	QA	1	Total 42	C 23	N 5	O 14	0	0
58	XA	1	Total 42	C 23	N 5	O 14	0	0

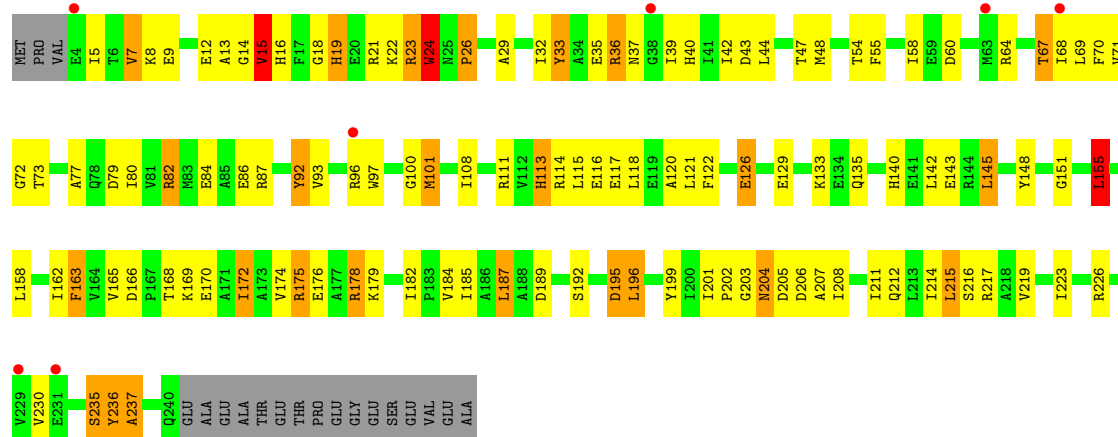
- 
- WORLD WIDE
PDB
PROTEIN DATA BANK

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

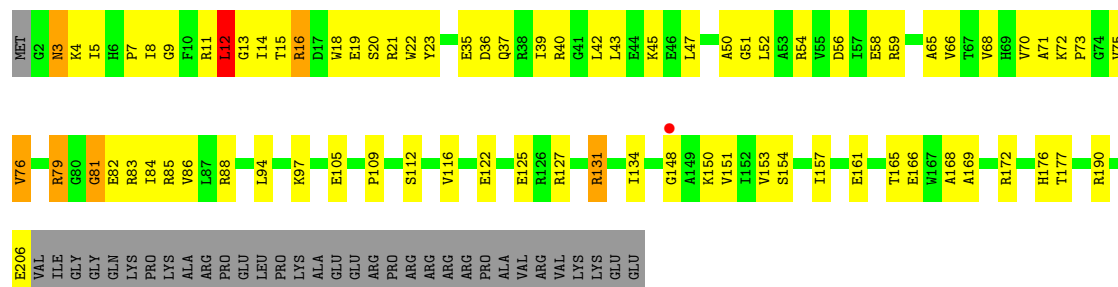




• Molecule 2: 30S ribosomal protein S2

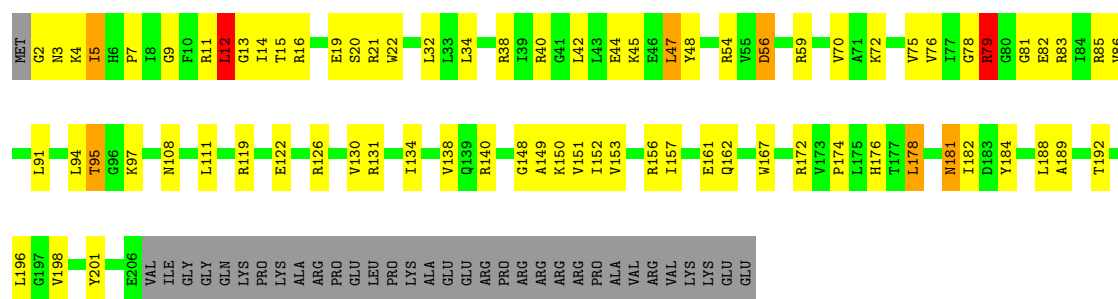


• Molecule 3: 30S ribosomal protein S3



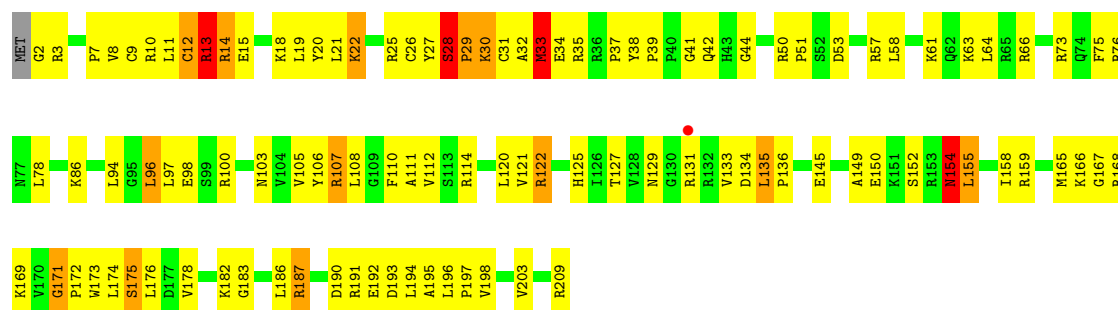
• Molecule 3: 30S ribosomal protein S3





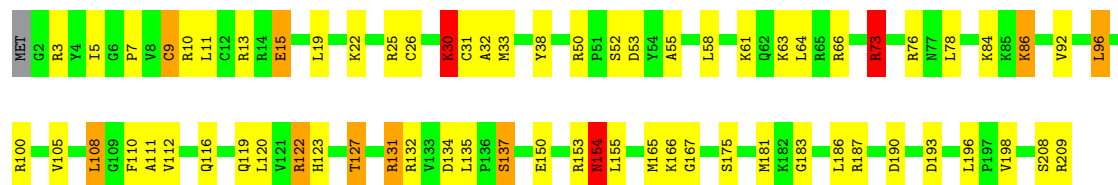
• Molecule 4: 30S ribosomal protein S4

Chain QD: 48% 43% 6%



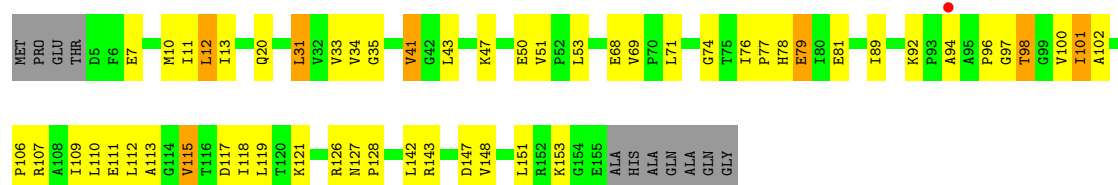
• Molecule 4: 30S ribosomal protein S4

Chain XD: 67% 27%



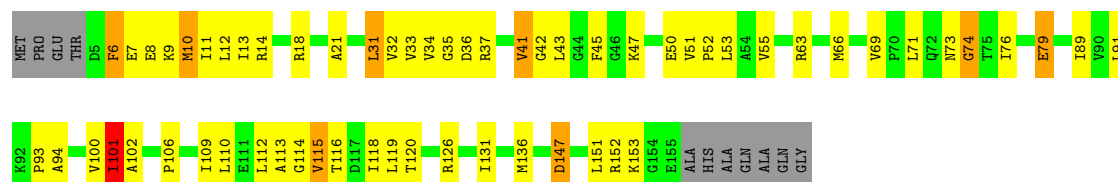
• Molecule 5: 30S ribosomal protein S5

Chain QE: 59% 30% 7%



• Molecule 5: 30S ribosomal protein S5

Chain XE: 56% 32% 5% 7%



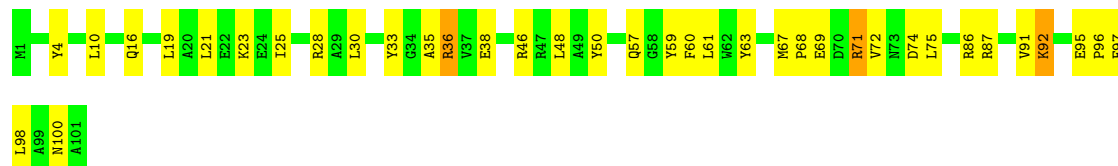
- Molecule 6: 30S ribosomal protein S6

Chain QF: 69% 27%



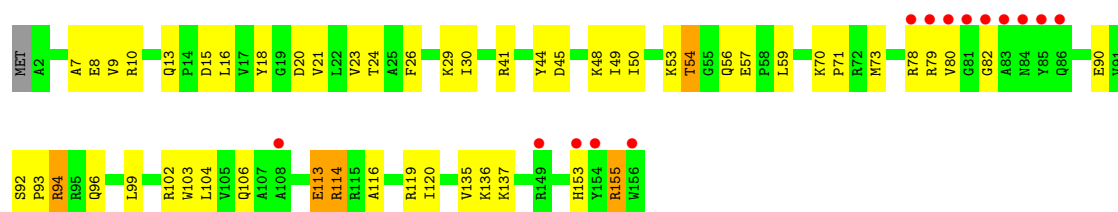
- Molecule 6: 30S ribosomal protein S6

Chain XF: 63% 34%



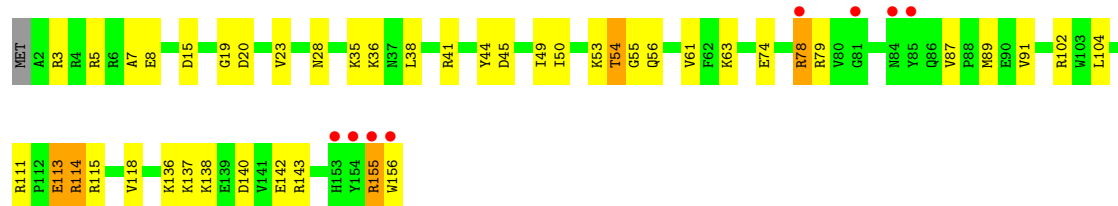
- Molecule 7: 30S ribosomal protein S7

Chain QG: 9% 65% 31%



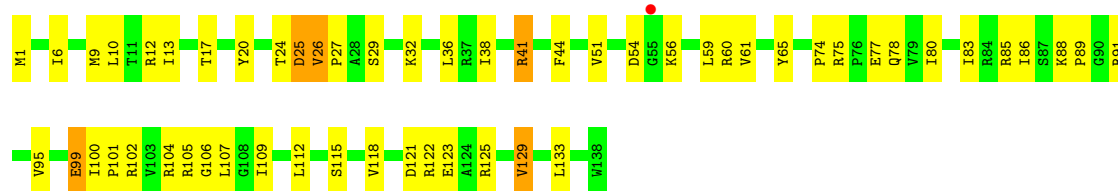
- Molecule 7: 30S ribosomal protein S7

Chain XG: 5% 71% 25%

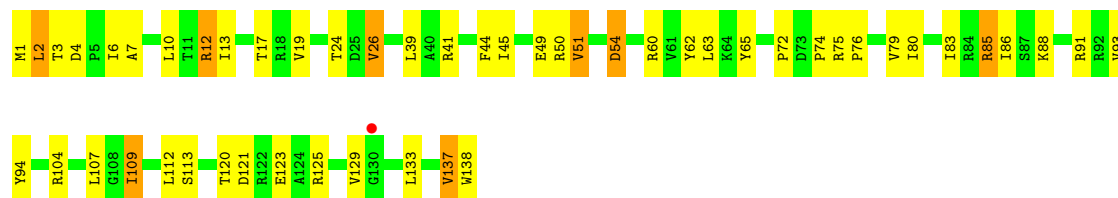


- Molecule 8: 30S ribosomal protein S8

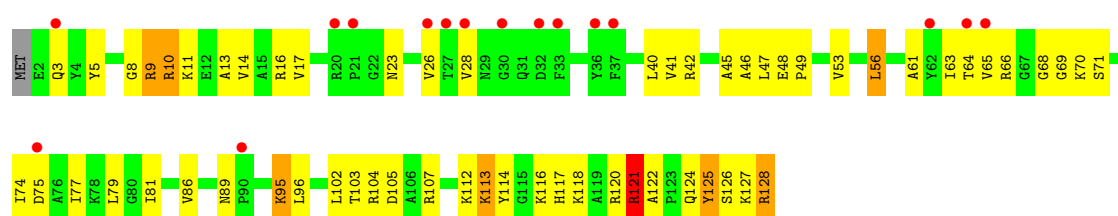
Chain QH: 60% 36%



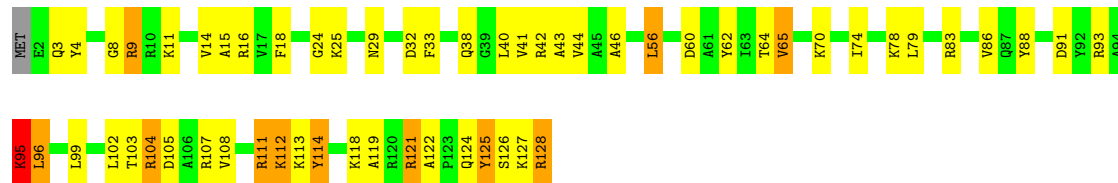
• Molecule 8: 30S ribosomal protein S8



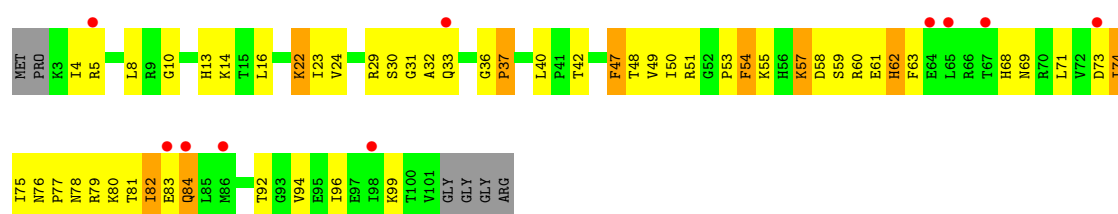
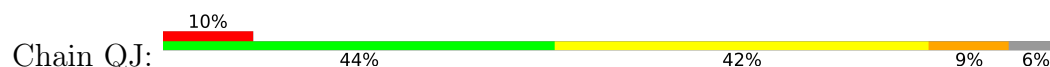
• Molecule 9: 30S ribosomal protein S9



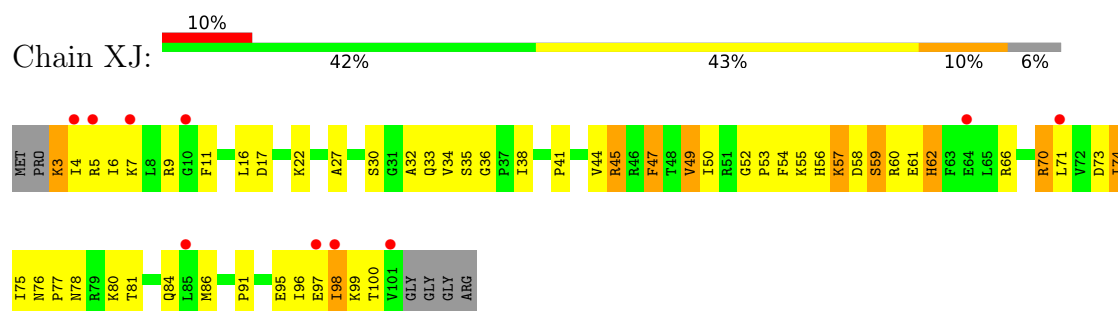
• Molecule 9: 30S ribosomal protein S9



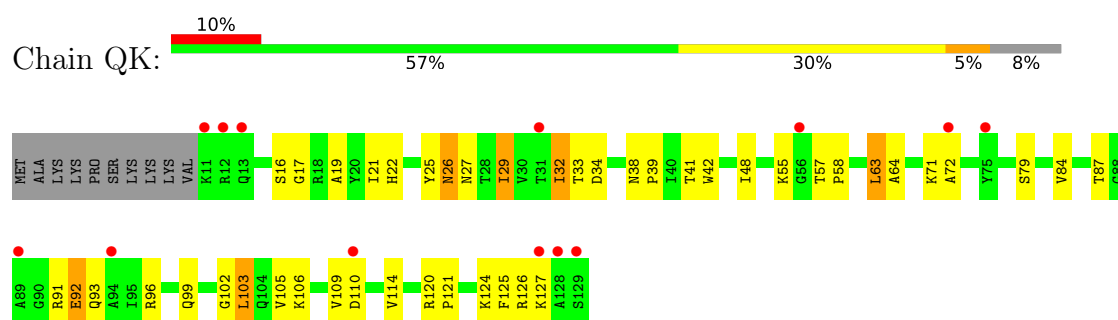
• Molecule 10: 30S ribosomal protein S10



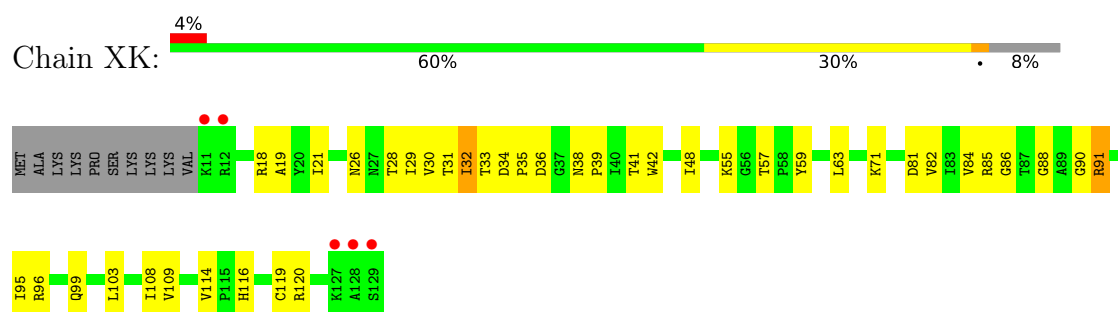
- Molecule 10: 30S ribosomal protein S10



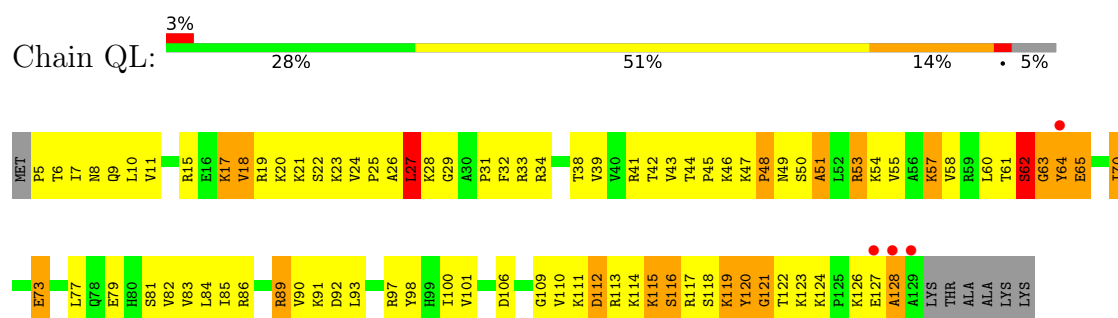
- Molecule 11: 30S ribosomal protein S11



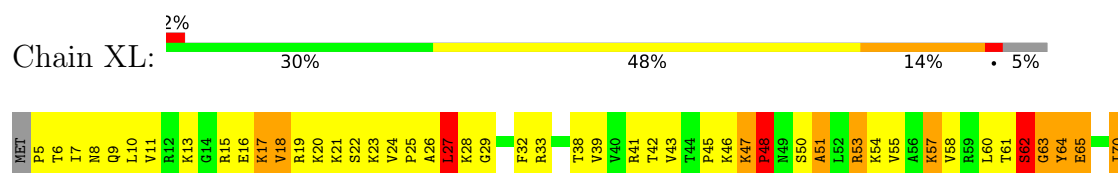
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

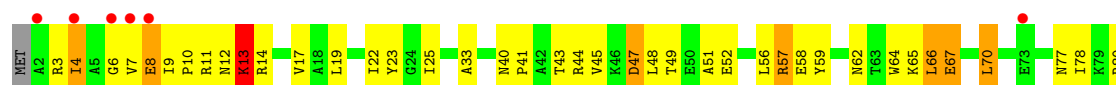


- Molecule 12: 30S ribosomal protein S12





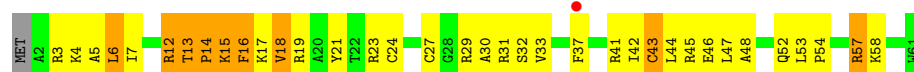
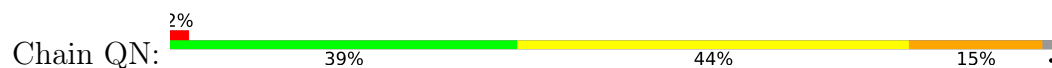
- Molecule 13: 30S ribosomal protein S13



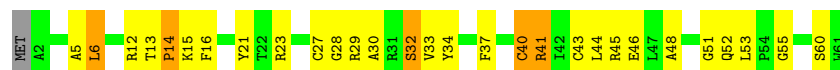
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15



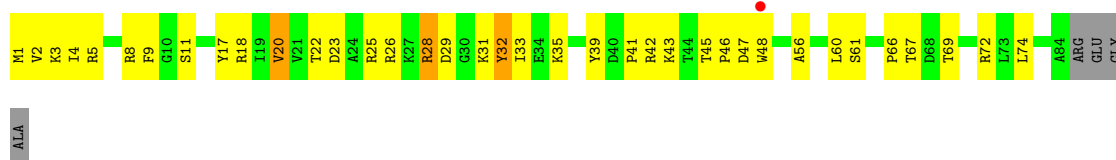
- Molecule 15: 30S ribosomal protein S15



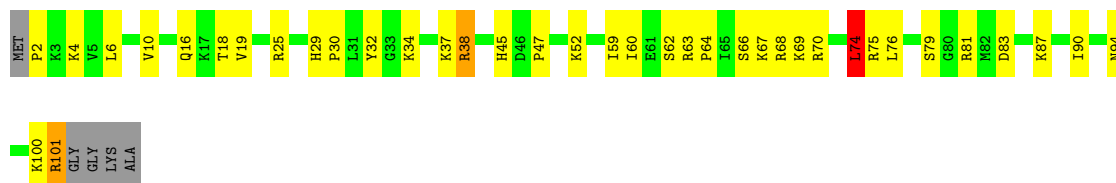
- Molecule 16: 30S ribosomal protein S16



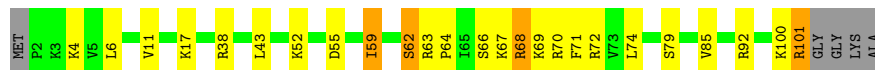
- Molecule 16: 30S ribosomal protein S16



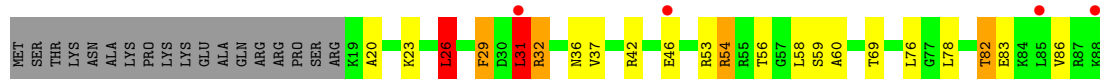
- Molecule 17: 30S ribosomal protein S17



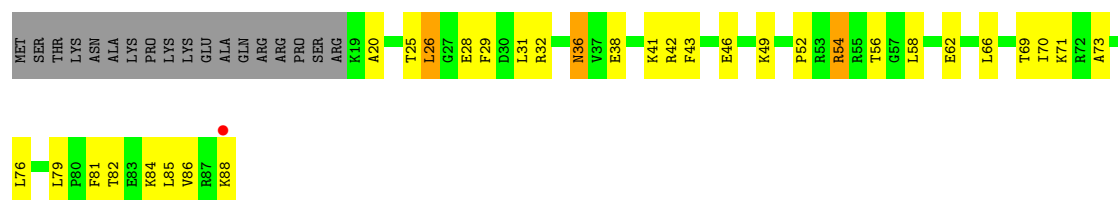
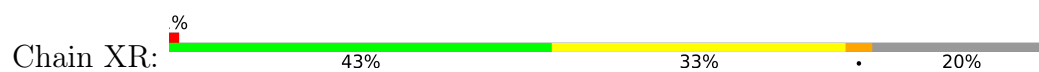
- Molecule 17: 30S ribosomal protein S17



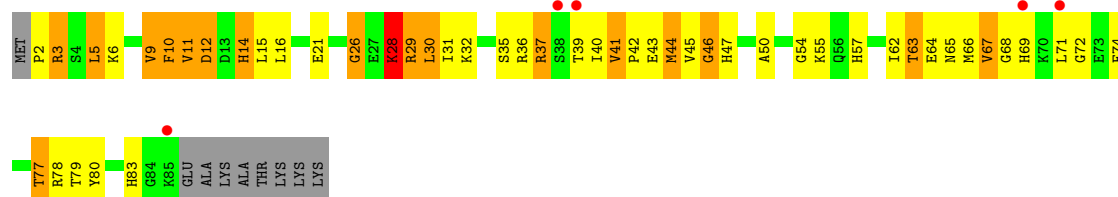
- Molecule 18: 30S ribosomal protein S18



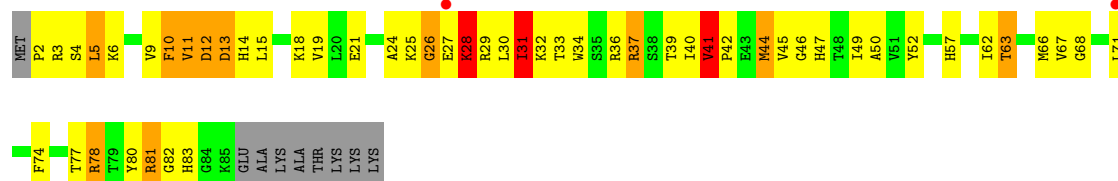
- Molecule 18: 30S ribosomal protein S18



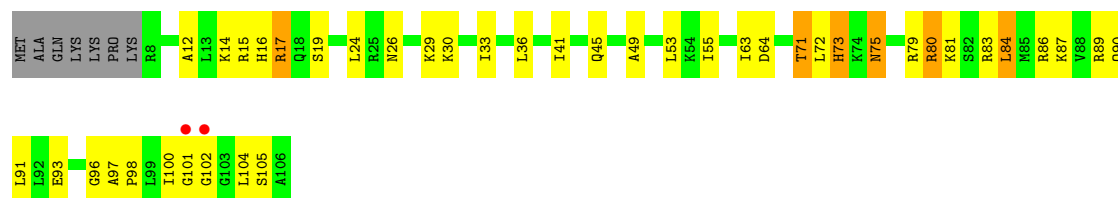
• Molecule 19: 30S ribosomal protein S19



• Molecule 19: 30S ribosomal protein S19

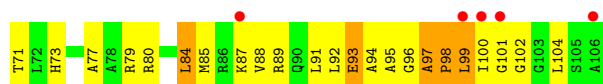


• Molecule 20: 30S ribosomal protein S20



• Molecule 20: 30S ribosomal protein S20

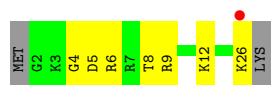




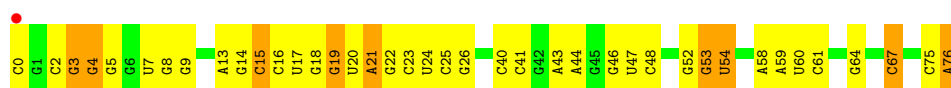
- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: P-site tRNA f-Met



- Molecule 22: P-site tRNA f-Met



- Molecule 23: messenger RNA



- Molecule 23: messenger RNA

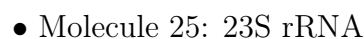


- Molecule 24: A-site tRNA Thr

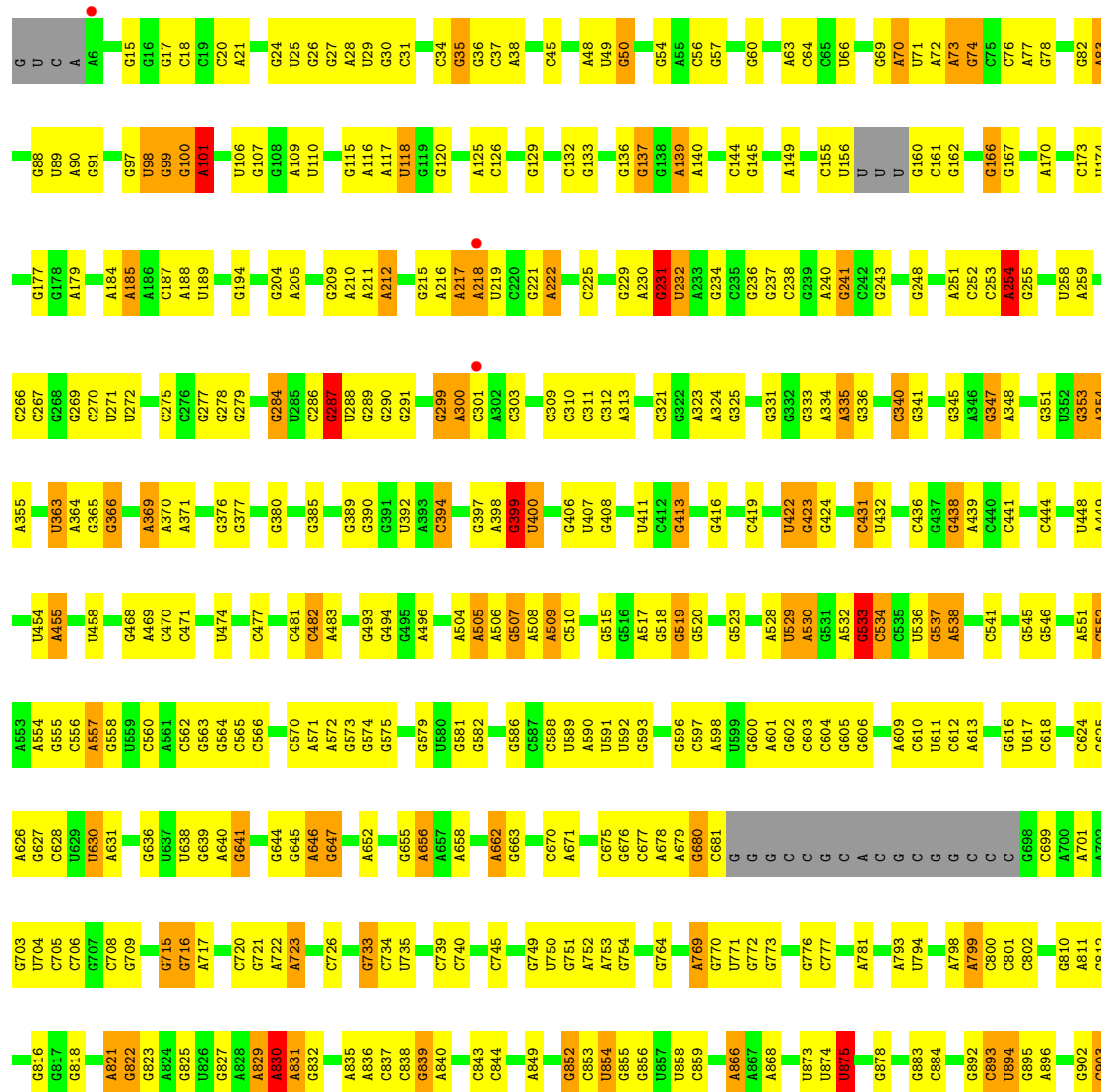
Chain QY:



Chain XY:



Chain RA:

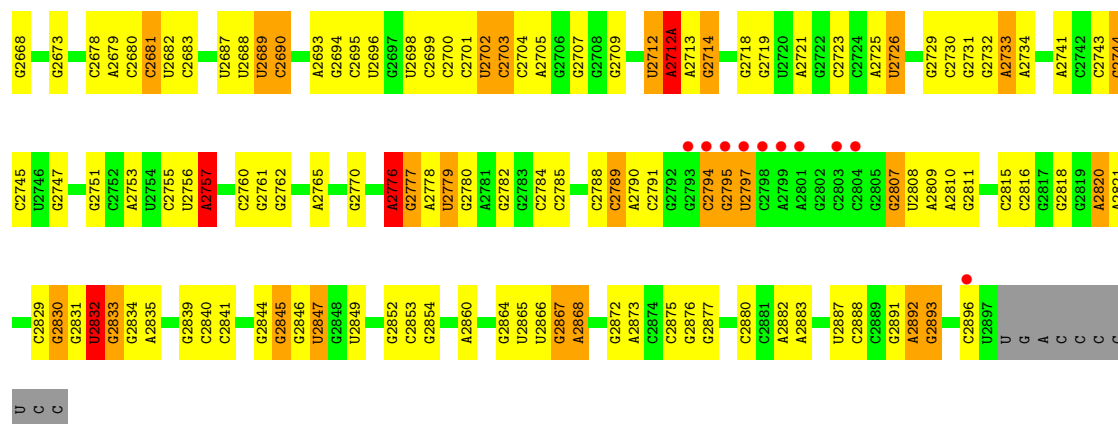


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G2002	C1904	A1818	U1745	C1658	A1554	C1474	A1382	G1294	U1212	G1133	U1069	G987	U905
A2003	A1905	C1821	A1745	G1640	A1555	C1474	G1383	A1299	G1215	G1135	G1070	G988	G906
C2004	A1906	A1822	A1745	G1641	A1557	C1479	G1384	A1299	G1215	G1136	G1071	A990	U907
G2009	C1908	G1749	G1749	C1644	C1558	U1479	U1387	G1302	G1218	G1137	A1073	G991	A908
C2010	G1909	U1825	G1750	C1644	C1559	A1480	A1388	G1305	G1219	C1138	A1074	G992	A910
G2011	G1910	C1826	G1751	C1645	U1560	A1481	G1389	G1305	A1219	G1139	A1075	G993	G916
C2012	A1911	U1827	U1752	C1646	C1561	G1482	G1390	G1305	U1220	U1140	G1076	G994	A917
U2013	U1753	U1753	U1753	C1645	U1562	G1482	C1391	C1307	G1221	A1141	G1077	G995	U918
G2014	U1829	U1753	U1753	C1645	U1563	G1487	G1394	A1308	A1222	A1142	G1078	G997	A919
U2015	G1830	A1649	U1756	C1645	C1564	G1488	A1395	U1309	G1223	U1143	G1079	G998	G920
G2021	G1831	C1653	C1757	C1653	C1565	G1489	G1394	U1309	A1222	U1143	G1080	G999	G926
C2024	G1832	A1654	C1757	A1654	U1566	G1490	A1395	A1311	C1224	U1144	U1081	A1002	G927
G2024	A1833	A1655	U1763	A1655	G1567	A1491	U1398	G1312	G1232	C1146	G1082	A1002	G928
G1928	A1834	A1656	U1765	A1656	G1568	C1492	A1399	G1315	U1233	C1148	G1083	U1003	G929
A2027	C1837	A1660	U1765	A1660	G1571	A1496	G1402	C1315	U1233	A1149	C1086	U1004	G930
C2028	G1838	C1661	U1767	C1661	A1581	G1497	A1403	C1316	A1234	A1157	C1087	A1005	G931
G2032	U1839	A1662	U1768	A1662	A1574	U1501	G1404	A1318	G1236	U1159	G1088	C1006	C932
C2034	A1840	A1664	U1770	A1664	C1579	C1505	G1405	U1319	G1240	G1156	G1089	G1011	C933
U2037	G1841	A1664	G1771	A1664	C1580	G1506	G1410	A1324	U1243	A1157	A1091	G1019	A934
G2037	A1842	G1669	C1772	G1669	A1581	G1507	A1411	G1325	U1244	G1158	A1092	C1020	C935
A2041	G1847	G1672	C1773	G1672	C1583	G1508	A1412	A1333	C1245	U1159	A1093	A937	C936
A2042	G1848	G1672	C1774	G1672	C1585	G1509	A1413	U1334	C1246	G1161	A1094	G938	C937
C2043	U1849	C1683	C1775	C1683	G1585	C1511	G1414	C1337	C1247	G1160	C1095	A1026	C939
U2044	A1850	A1684	C1776	A1684	G1588	C1514	G1415	C1338	C1248	G1161	G1097	A1029	C940
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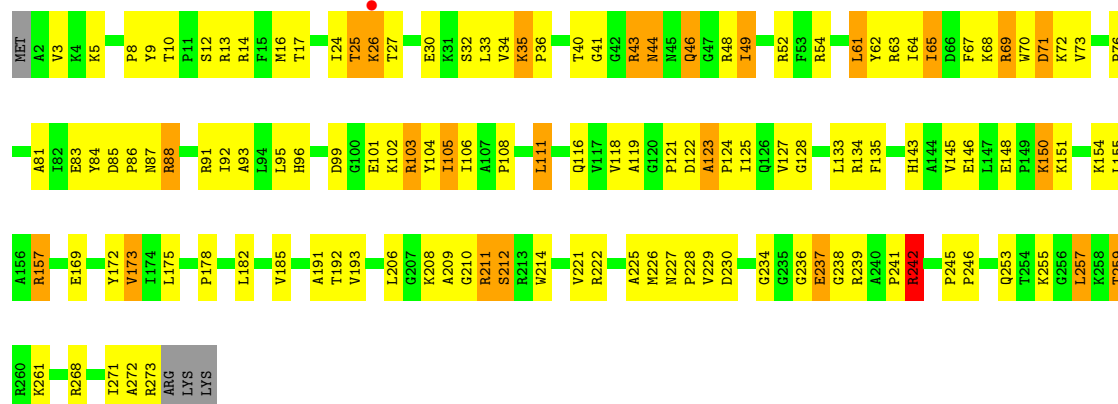
• Molecule 26: 5S rRNA



• Molecule 26: 5S rRNA

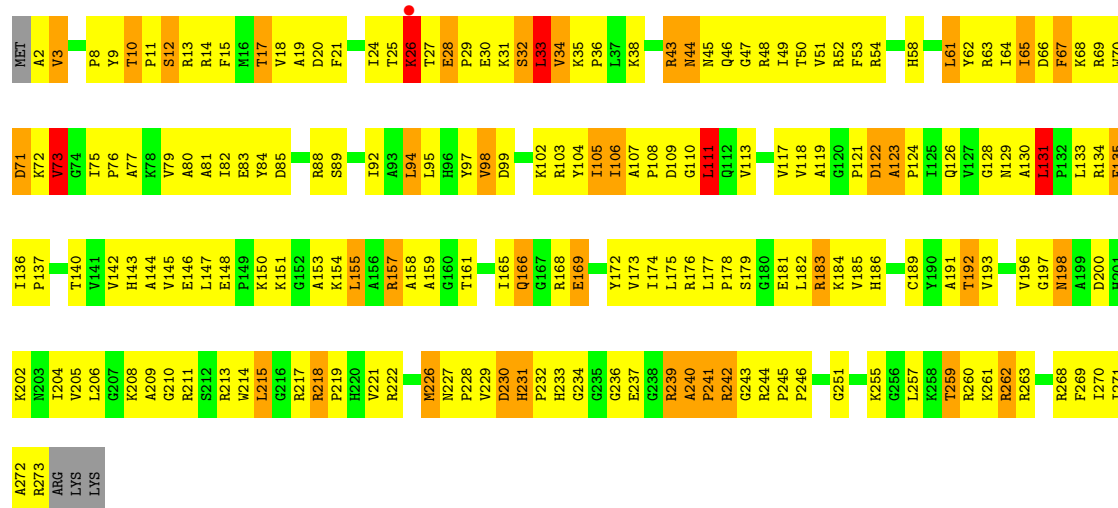


• Molecule 27: 50S ribosomal protein L2



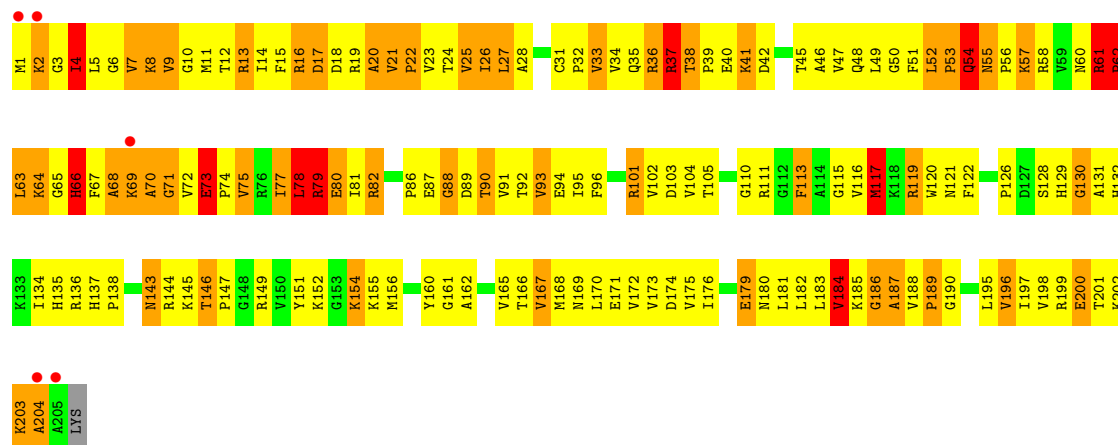
• Molecule 27: 50S ribosomal protein L2

Chain YD: 29% 54% 14% ..



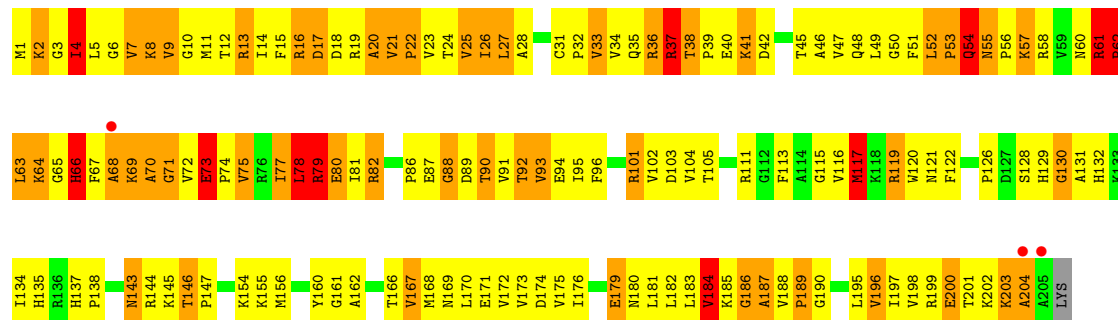
• Molecule 28: 50S ribosomal protein L3

Chain RE: 2% 21% 49% 24% 5%

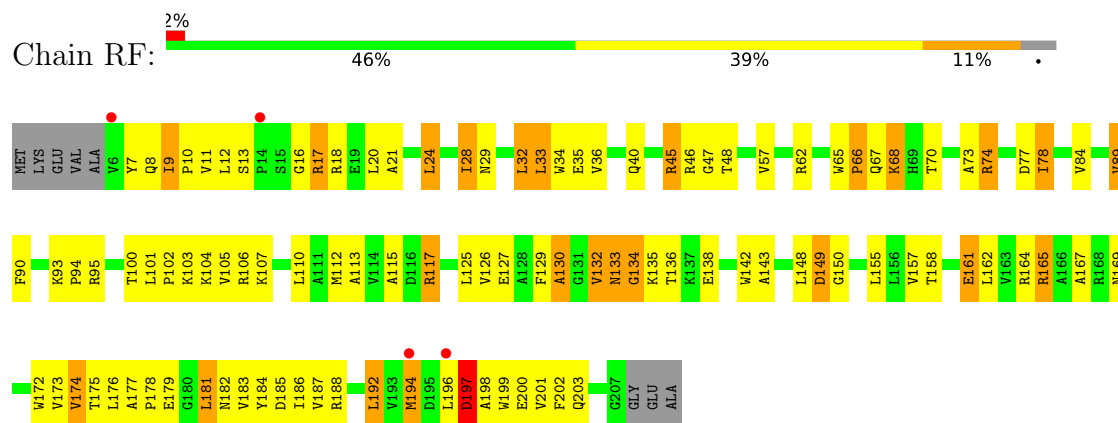


• Molecule 28: 50S ribosomal protein L3

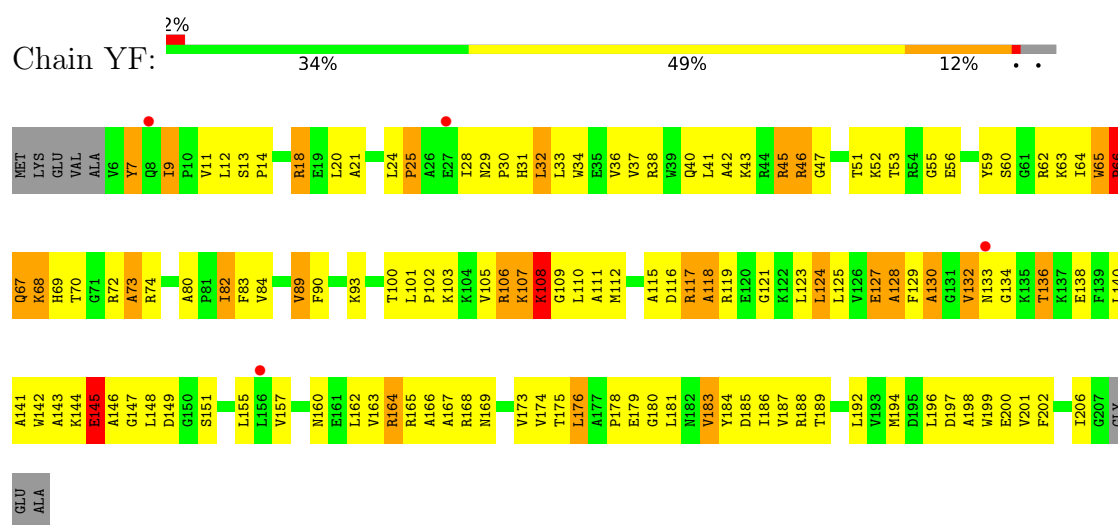
Chain YE: 24% 46% 24% 5%



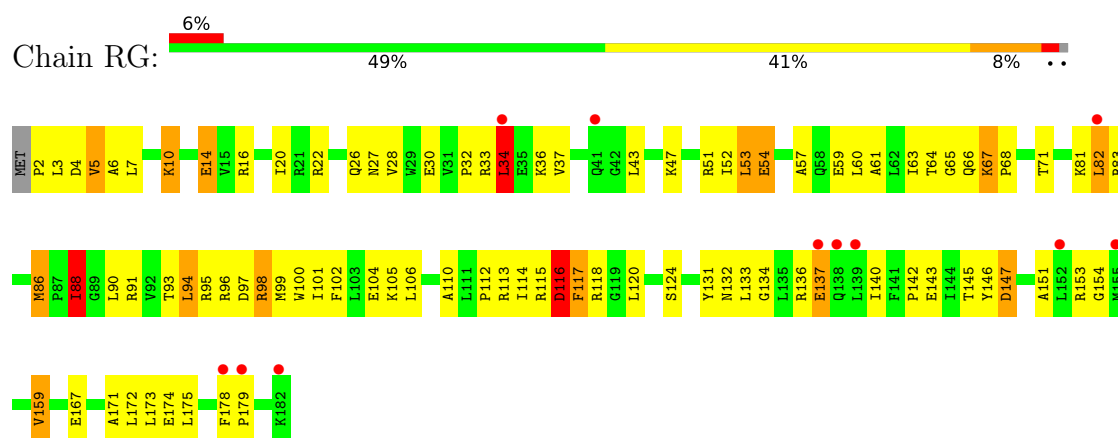
- Molecule 29: 50S ribosomal protein L4



- Molecule 29: 50S ribosomal protein L4

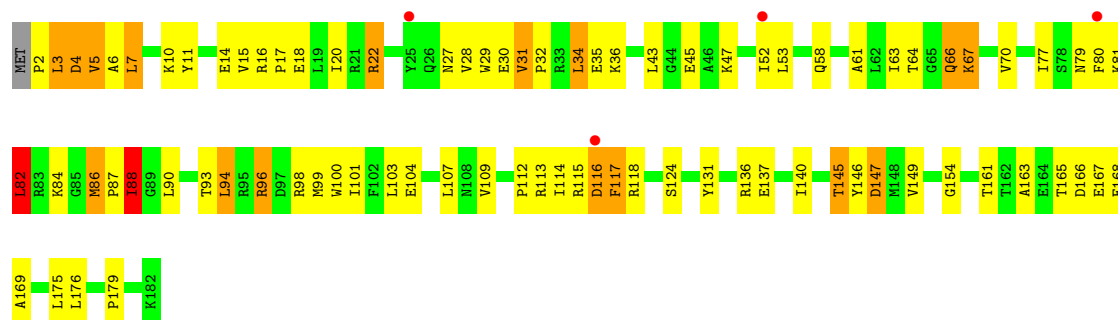


- Molecule 30: 50S ribosomal protein L5

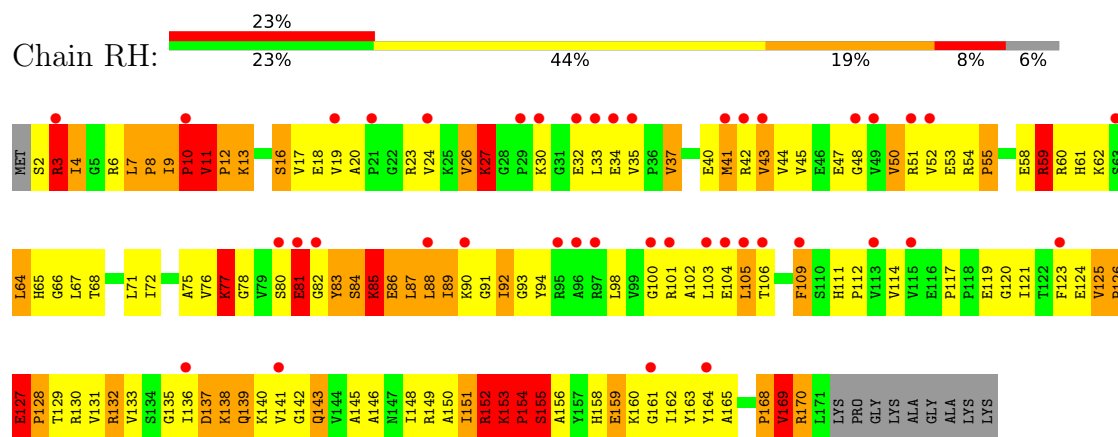


- Molecule 30: 50S ribosomal protein L5

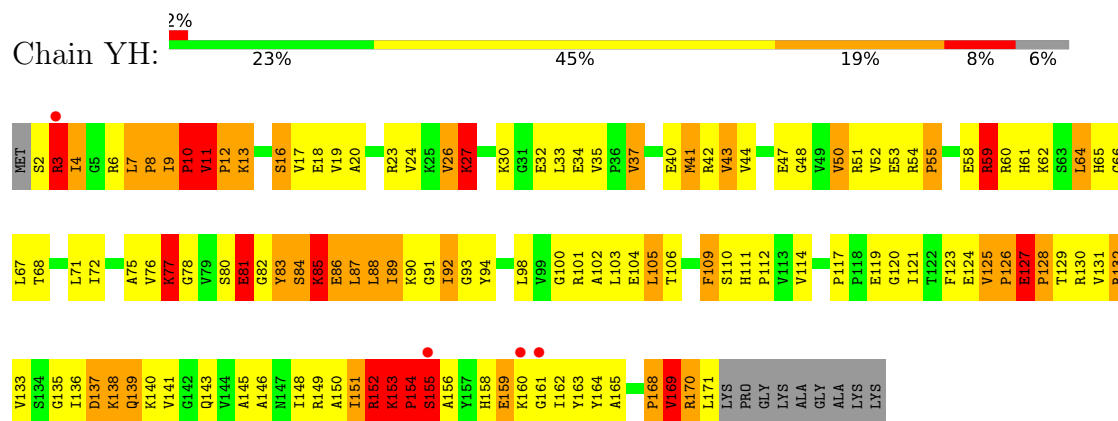




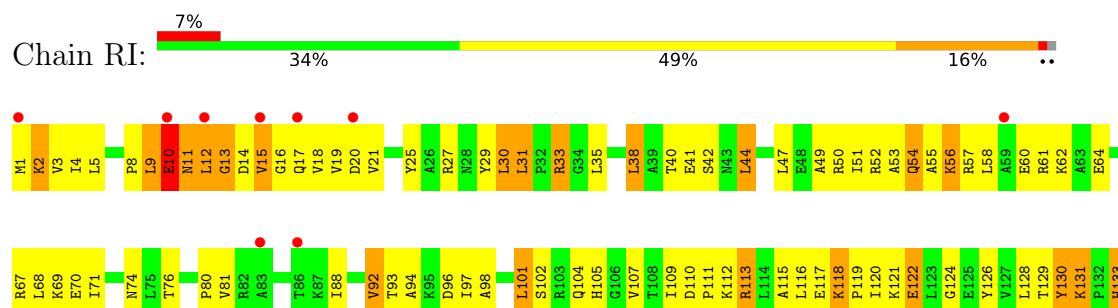
• Molecule 31: 50S ribosomal protein L6



• Molecule 31: 50S ribosomal protein L6

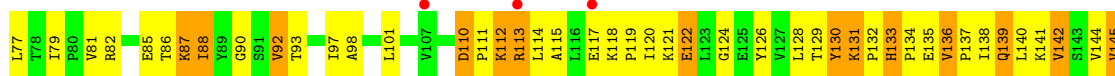
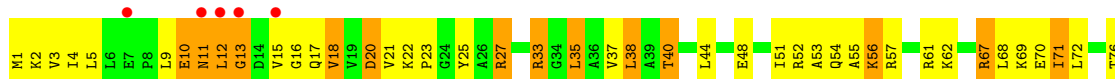


• Molecule 32: 50S ribosomal protein L9





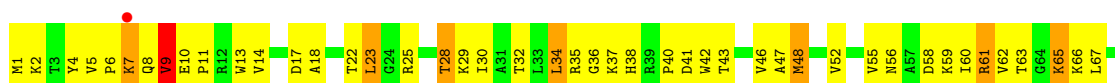
- Molecule 32: 50S ribosomal protein L9



- Molecule 33: 50S ribosomal protein L13



- Molecule 33: 50S ribosomal protein L13

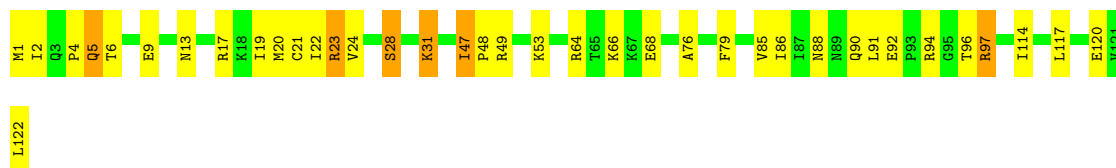


- Molecule 34: 50S ribosomal protein L14




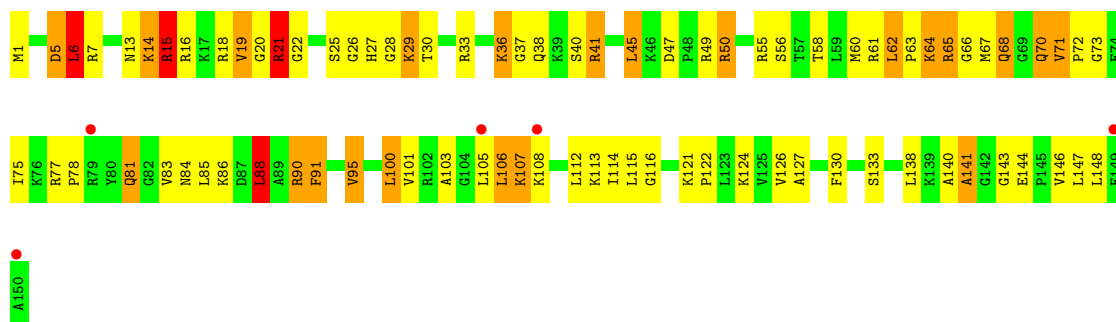
- Molecule 34: 50S ribosomal protein L14

Chain YO:  69% 26% 5%



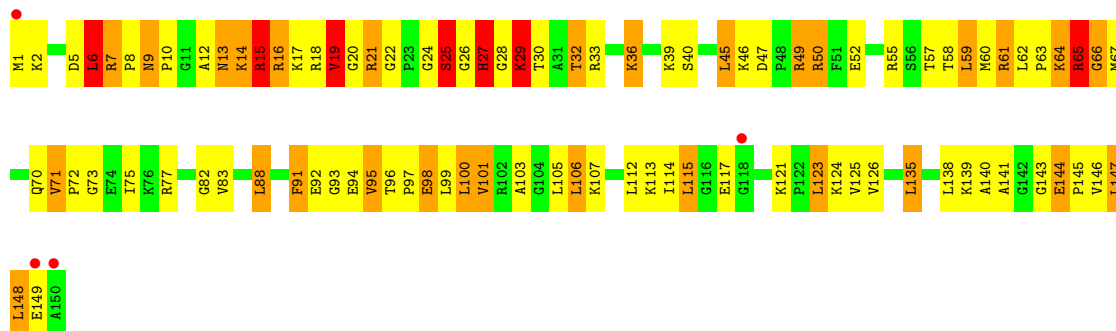
• Molecule 35: 50S ribosomal protein L15

Chain RP:  3% 44% 39% 15%



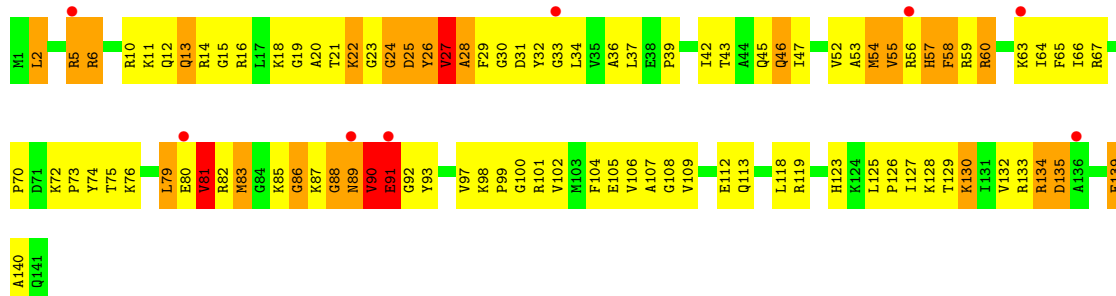
• Molecule 35: 50S ribosomal protein L15

Chain YP:  3% 37% 39% 19% 5%

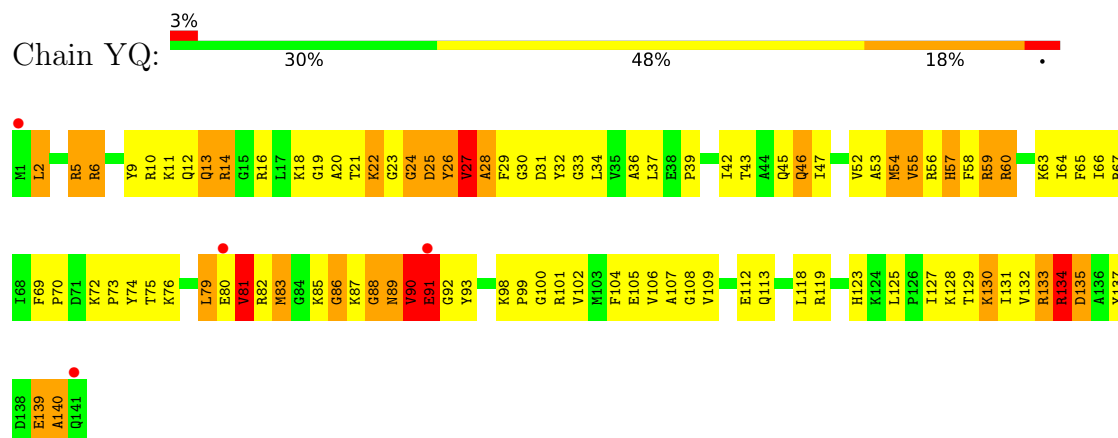


• Molecule 36: 50S ribosomal protein L16

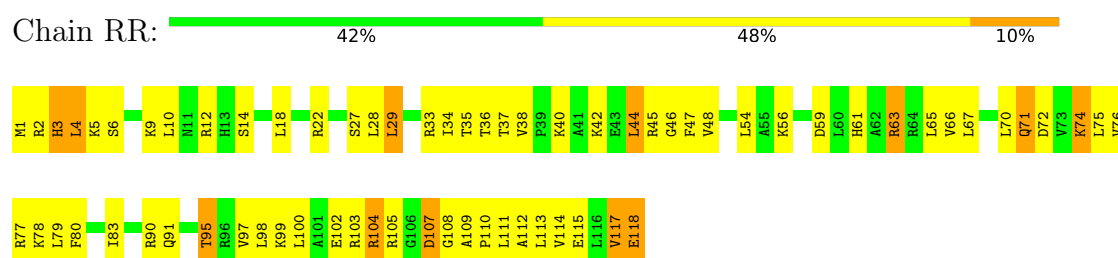
Chain RQ:  6% 30% 50% 17%



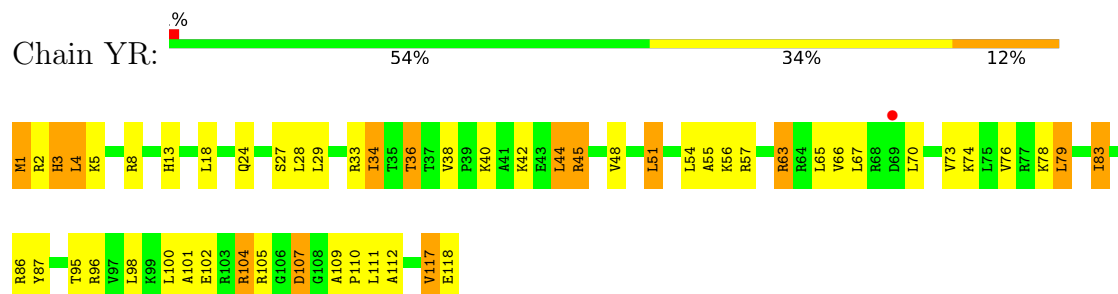
- Molecule 36: 50S ribosomal protein L16



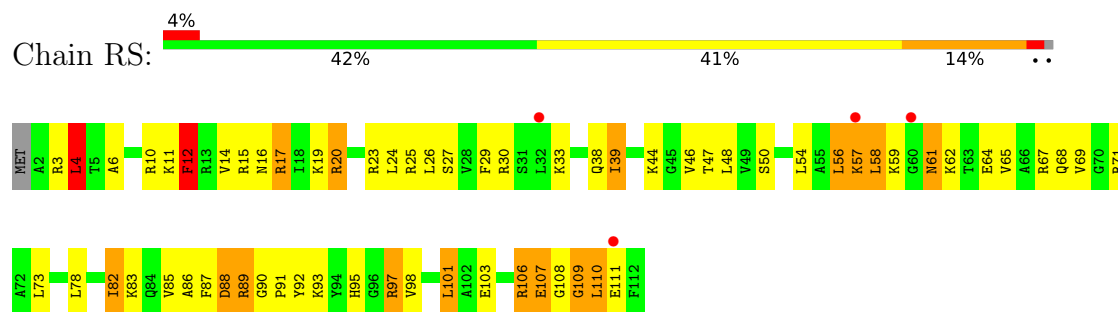
- Molecule 37: 50S ribosomal protein L17



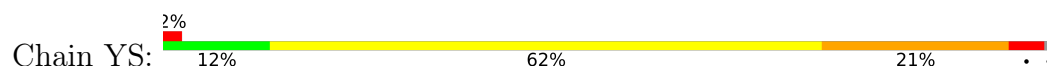
- Molecule 37: 50S ribosomal protein L17

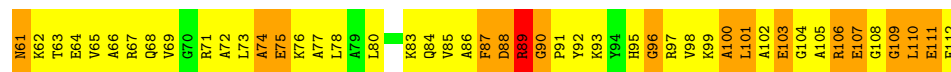
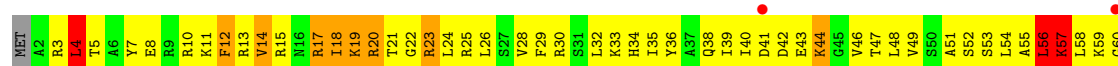


- Molecule 38: 50S ribosomal protein L18

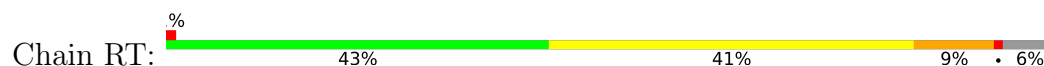


- Molecule 38: 50S ribosomal protein L18





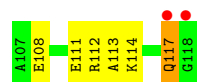
• Molecule 39: 50S ribosomal protein L19



• Molecule 39: 50S ribosomal protein L19



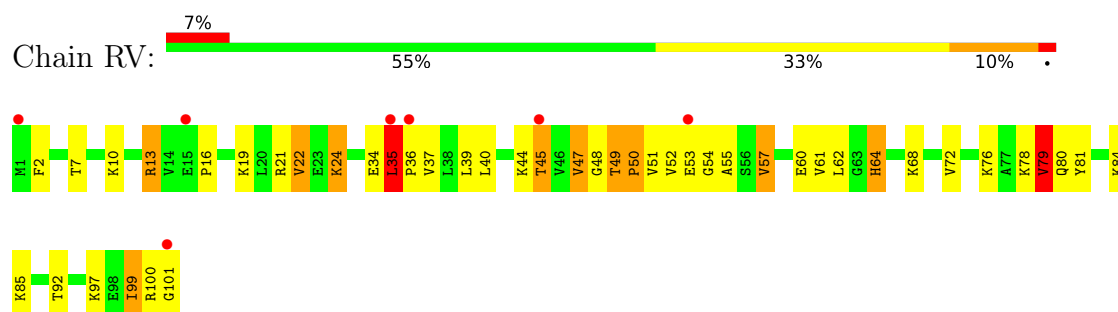
• Molecule 40: 50S ribosomal protein L20



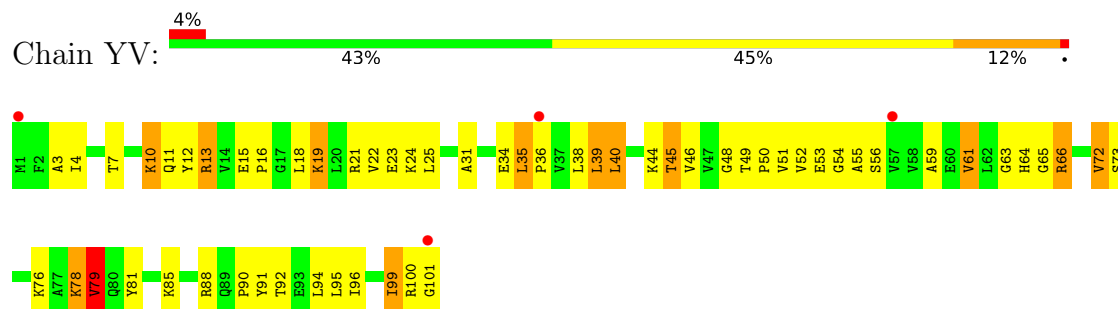
• Molecule 40: 50S ribosomal protein L20



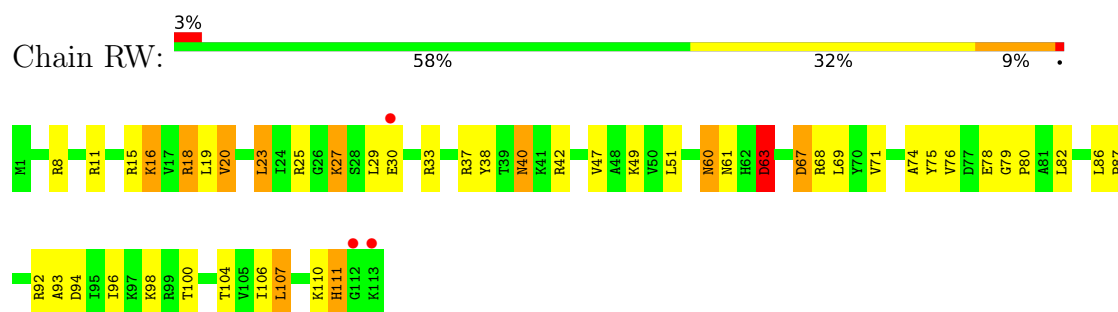
• Molecule 41: 50S ribosomal protein L21



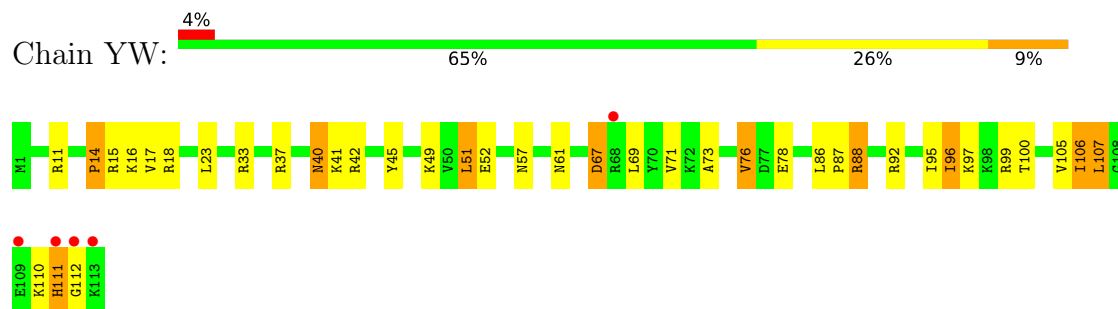
- Molecule 41: 50S ribosomal protein L21



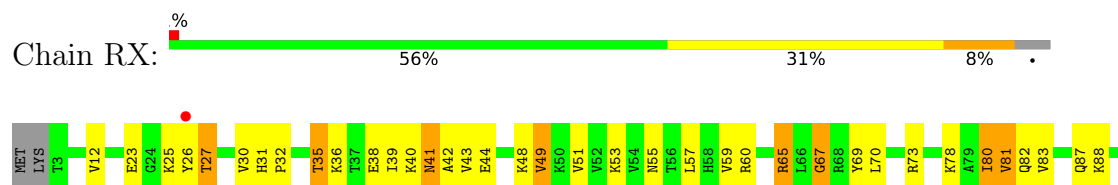
- Molecule 42: 50S ribosomal protein L22

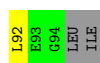


- Molecule 42: 50S ribosomal protein L22

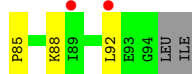
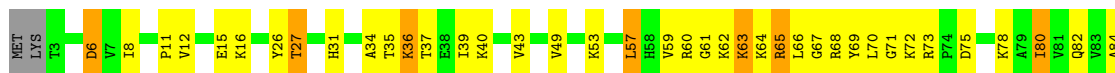


- Molecule 43: 50S ribosomal protein L23

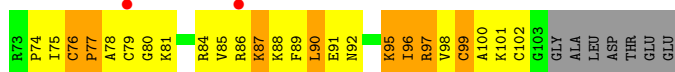
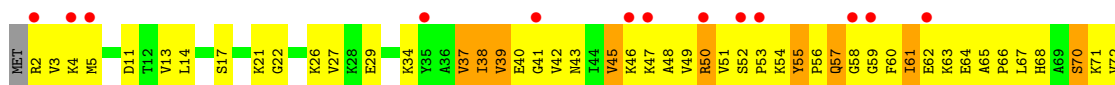




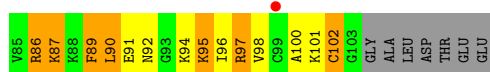
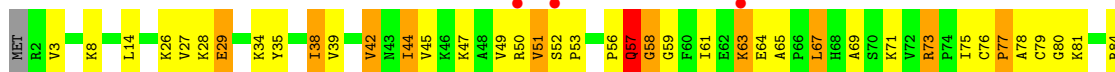
• Molecule 43: 50S ribosomal protein L23



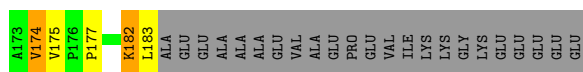
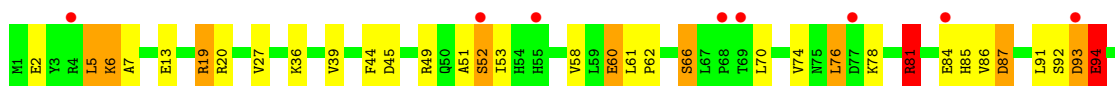
• Molecule 44: 50S ribosomal protein L24



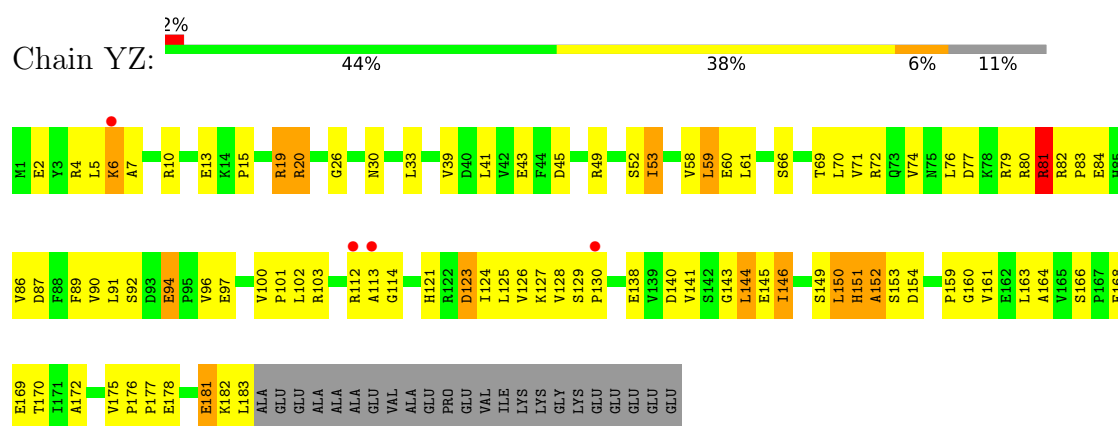
• Molecule 44: 50S ribosomal protein L24



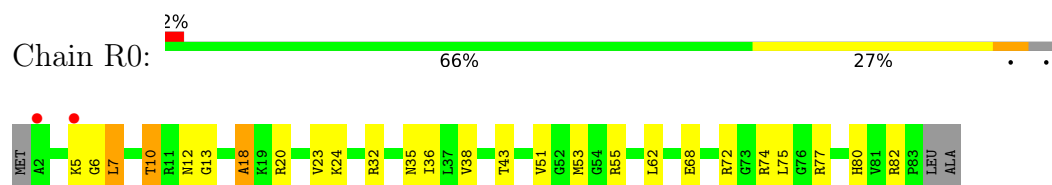
• Molecule 45: 50S ribosomal protein L25



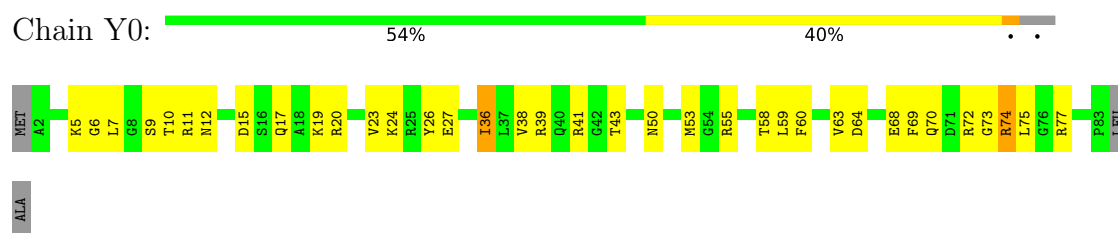
• Molecule 45: 50S ribosomal protein L25



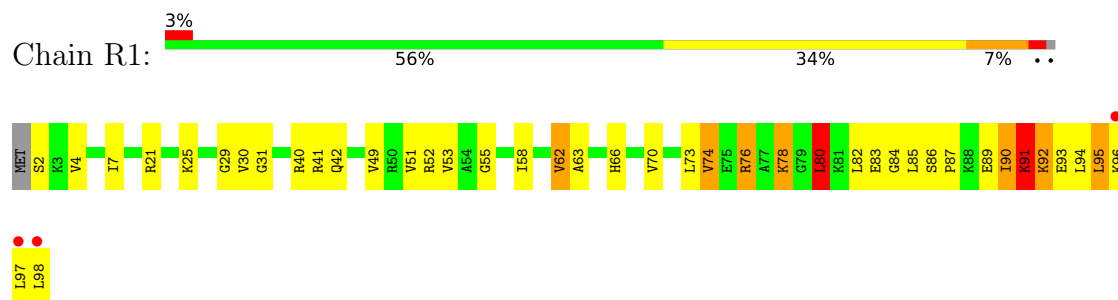
- Molecule 46: 50S ribosomal protein L27



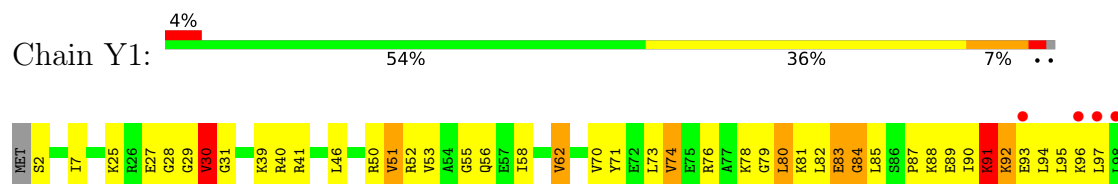
- Molecule 46: 50S ribosomal protein L27



- Molecule 47: 50S ribosomal protein L28

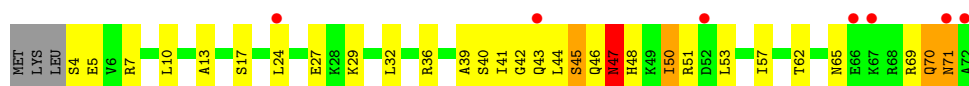


- Molecule 47: 50S ribosomal protein L28

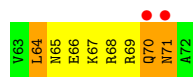
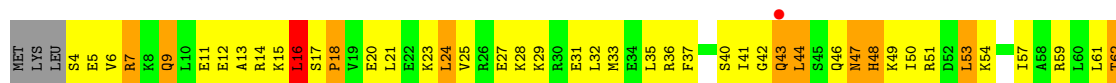


- Molecule 48: 50S ribosomal protein L29

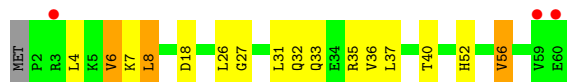
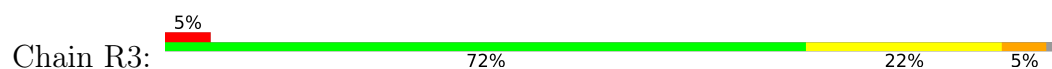




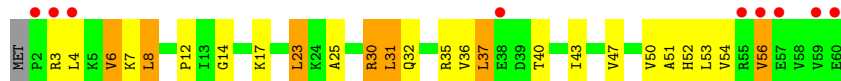
- Molecule 48: 50S ribosomal protein L29



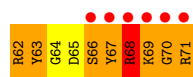
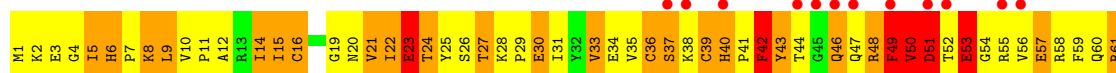
- Molecule 49: 50S ribosomal protein L30



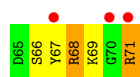
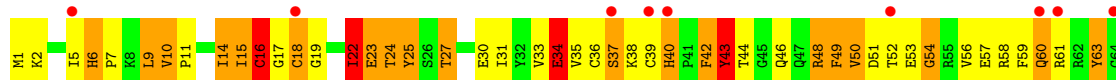
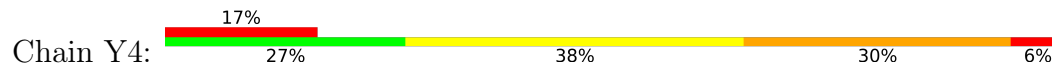
- Molecule 49: 50S ribosomal protein L30



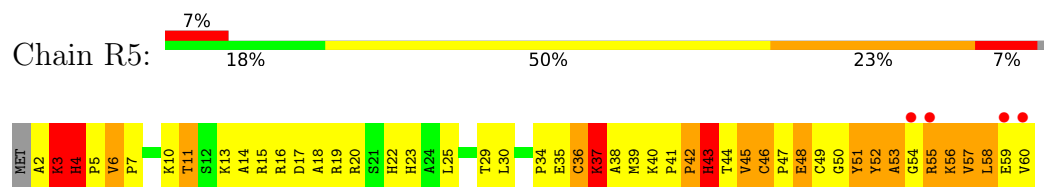
- Molecule 50: 50S ribosomal protein L31



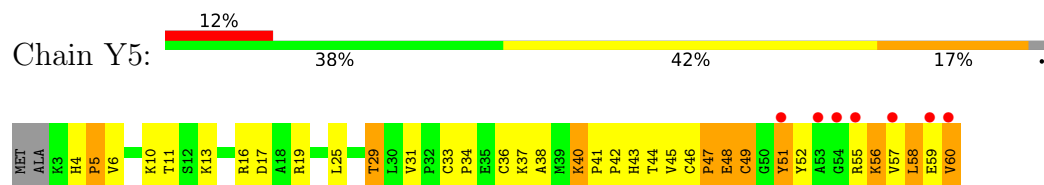
- Molecule 50: 50S ribosomal protein L31



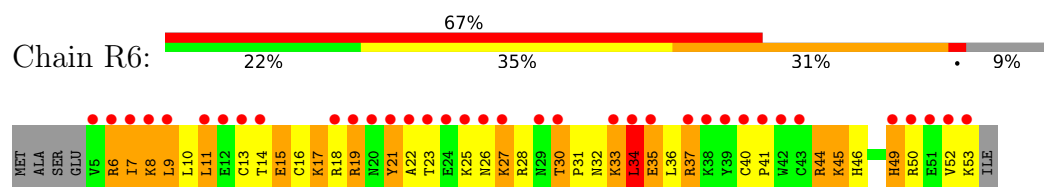
- Molecule 51: 50S ribosomal protein L32



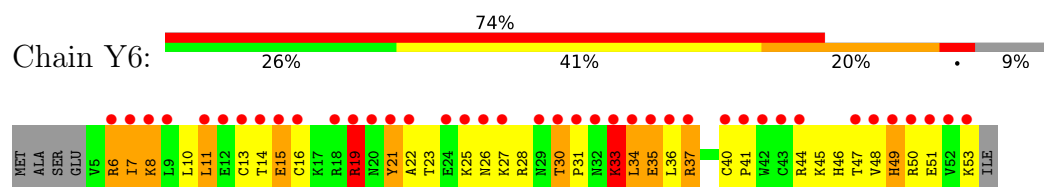
- Molecule 51: 50S ribosomal protein L32



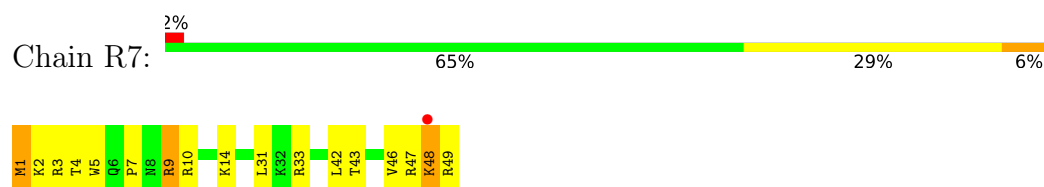
- Molecule 52: 50S ribosomal protein L33



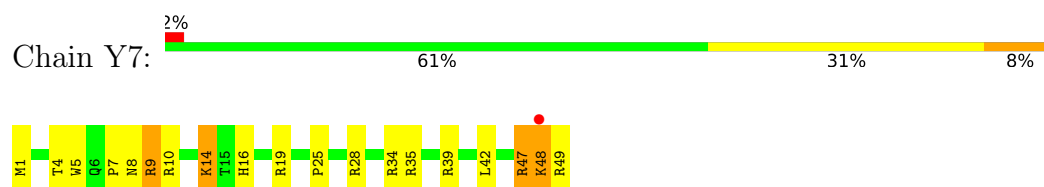
- Molecule 52: 50S ribosomal protein L33



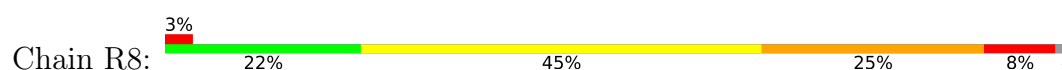
- Molecule 53: 50S ribosomal protein L34

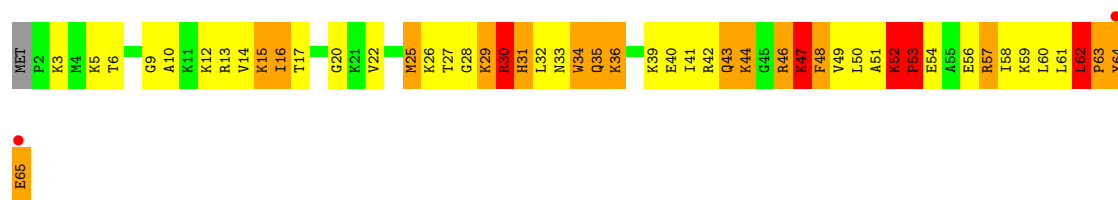


- Molecule 53: 50S ribosomal protein L34



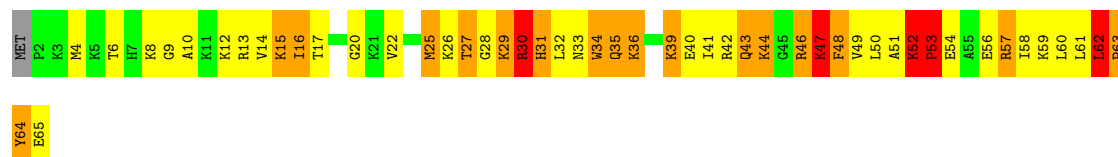
- Molecule 54: 50S ribosomal protein L35





- Molecule 54: 50S ribosomal protein L35

Chain Y8: 22% 43% 26% 8%



- Molecule 55: 50S ribosomal protein L36

Chain R9: 97% 62% 32% 5%



- Molecule 55: 50S ribosomal protein L36

Chain Y9: 97% 68% 27% 5%



- Molecule 56: CC-Puro

Chain Z5: 33% 67%



- Molecule 56: CC-Puro

Chain Z6: 33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.99Å 444.57Å 616.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.39 – 3.60 69.39 – 3.40	Depositor EDS
% Data completeness (in resolution range)	96.9 (69.39-3.60) 97.2 (69.39-3.40)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.217 , 0.259 0.217 , 0.259	Depositor DCC
R_{free} test set	34831 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	87.0	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 95.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	292320	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.32	0/36098	0.87	44/56341 (0.1%)
1	XA	0.36	0/36101	0.88	26/56346 (0.0%)
2	QB	0.32	0/1959	0.52	0/2642
2	XB	0.32	0/1959	0.54	0/2642
3	QC	0.32	0/1629	0.54	0/2195
3	XC	0.37	0/1629	0.56	0/2195
4	QD	0.41	0/1733	0.60	2/2318 (0.1%)
4	XD	0.40	0/1733	0.59	0/2318
5	QE	0.38	0/1171	0.60	0/1576
5	XE	0.43	1/1171 (0.1%)	0.63	2/1576 (0.1%)
6	QF	0.38	0/856	0.55	0/1154
6	XF	0.39	0/856	0.58	0/1154
7	QG	0.34	0/1276	0.50	0/1709
7	XG	0.34	0/1276	0.51	0/1709
8	QH	0.34	0/1136	0.55	0/1527
8	XH	0.38	0/1136	0.58	0/1527
9	QI	0.31	0/1029	0.56	0/1379
9	XI	0.34	0/1029	0.58	0/1379
10	QJ	0.33	0/814	0.54	0/1095
10	XJ	0.39	1/814 (0.1%)	0.63	1/1095 (0.1%)
11	QK	0.38	0/900	0.59	1/1213 (0.1%)
11	XK	0.39	0/900	0.59	0/1213
12	QL	0.49	1/991 (0.1%)	0.80	1/1327 (0.1%)
12	XL	0.50	0/991	0.85	3/1327 (0.2%)
13	QM	0.32	0/974	0.58	0/1303
13	XM	0.37	0/974	0.62	0/1303
14	QN	0.37	0/501	0.62	0/664
14	XN	0.43	0/501	0.66	0/664
15	QO	0.35	0/745	0.54	0/992
15	XO	0.40	0/745	0.54	0/992
16	QP	0.36	0/721	0.57	0/970
16	XP	0.35	0/721	0.57	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.35	0/847	0.54	0/1131
17	XQ	0.36	0/847	0.54	0/1131
18	QR	0.36	0/579	0.64	1/768 (0.1%)
18	XR	0.37	0/579	0.59	0/768
19	QS	0.34	0/689	0.61	0/926
19	XS	0.38	0/689	0.69	1/926 (0.1%)
20	QT	0.35	0/765	0.65	0/1007
20	XT	0.32	0/765	0.61	0/1007
21	QU	0.30	0/221	0.55	0/288
21	XU	0.31	0/221	0.62	0/288
22	QV	0.38	1/1836 (0.1%)	0.80	0/2859
22	XV	0.41	1/1836 (0.1%)	0.83	0/2859
23	QX	0.33	0/213	0.81	0/329
23	XX	0.67	0/238	0.86	0/368
24	QY	0.43	0/384	0.83	0/597
24	XY	0.36	0/384	0.85	0/597
25	RA	0.39	2/69521 (0.0%)	0.91	59/108529 (0.1%)
25	YA	0.42	1/69521 (0.0%)	0.94	81/108529 (0.1%)
26	RB	0.51	0/2878	1.17	11/4490 (0.2%)
26	YB	0.62	1/2878 (0.0%)	1.28	24/4490 (0.5%)
27	RD	0.51	0/2165	0.70	0/2919
27	YD	0.56	0/2165	0.90	4/2919 (0.1%)
28	RE	0.52	0/1601	0.91	2/2160 (0.1%)
28	YE	0.52	0/1601	0.91	2/2160 (0.1%)
29	RF	0.44	0/1620	0.70	3/2194 (0.1%)
29	YF	0.50	0/1620	0.76	0/2194
30	RG	0.32	0/1499	0.57	1/2016 (0.0%)
30	YG	0.40	0/1499	0.60	0/2016
31	RH	0.45	0/1332	0.85	3/1802 (0.2%)
31	YH	0.45	0/1332	0.85	4/1802 (0.2%)
32	RI	0.38	0/1151	0.67	0/1558
32	YI	0.38	0/1151	0.65	0/1558
33	RN	0.41	0/1131	0.62	0/1525
33	YN	0.46	0/1131	0.66	1/1525 (0.1%)
34	RO	0.41	0/943	0.63	1/1269 (0.1%)
34	YO	0.49	0/943	0.65	0/1269
35	RP	0.41	0/1162	0.79	1/1544 (0.1%)
35	YP	0.53	0/1162	0.89	2/1544 (0.1%)
36	RQ	0.54	0/1143	0.90	3/1527 (0.2%)
36	YQ	0.53	0/1143	0.87	3/1527 (0.2%)
37	RR	0.42	0/982	0.69	0/1312
37	YR	0.44	0/982	0.73	0/1312
38	RS	0.36	0/892	0.65	0/1187

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YS	0.46	0/892	0.83	1/1187 (0.1%)
39	RT	0.42	0/1155	0.63	0/1542
39	YT	0.43	0/1155	0.66	0/1542
40	RU	0.39	0/982	0.65	0/1306
40	YU	0.51	0/982	0.70	0/1306
41	RV	0.38	0/790	0.61	1/1057 (0.1%)
41	YV	0.46	0/790	0.73	1/1057 (0.1%)
42	RW	0.49	0/911	0.67	0/1220
42	YW	0.45	0/911	0.68	0/1220
43	RX	0.47	0/739	0.62	0/993
43	YX	0.48	0/739	0.65	0/993
44	RY	0.44	0/798	0.68	0/1064
44	YY	0.46	0/798	0.70	0/1064
45	RZ	0.30	0/1493	0.52	0/2026
45	YZ	0.29	0/1493	0.55	0/2026
46	R0	0.45	0/657	0.65	0/874
46	Y0	0.49	0/656	0.70	0/872
47	R1	0.44	0/770	0.66	0/1022
47	Y1	0.46	0/770	0.69	0/1022
48	R2	0.39	0/583	0.64	0/771
48	Y2	0.51	0/583	0.83	1/771 (0.1%)
49	R3	0.35	0/474	0.57	0/635
49	Y3	0.42	0/474	0.59	0/635
50	R4	0.39	0/594	0.78	1/795 (0.1%)
50	Y4	0.37	0/594	0.68	0/795
51	R5	0.51	0/473	0.74	0/639
51	Y5	0.50	0/468	0.72	0/632
52	R6	0.34	0/431	0.69	0/575
52	Y6	0.37	0/431	0.67	0/575
53	R7	0.49	0/438	0.68	0/575
53	Y7	0.56	0/438	0.71	0/575
54	R8	0.61	0/525	0.92	1/691 (0.1%)
54	Y8	0.62	0/525	0.92	1/691 (0.1%)
55	R9	0.26	0/310	0.45	0/407
55	Y9	0.33	0/310	0.48	0/407
56	Z5	0.80	0/40	1.79	1/60 (1.7%)
56	Z6	0.79	0/40	1.79	1/60 (1.7%)
All	All	0.40	9/316522 (0.0%)	0.86	296/473223 (0.1%)

The worst 5 of 9 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	0	C	OP3-P	-10.63	1.48	1.61
22	XV	0	C	OP3-P	-10.58	1.48	1.61
5	XE	101	ILE	C-N	5.68	1.47	1.34
25	RA	2299	A	N9-C4	-5.68	1.34	1.37
25	YA	1021	A	N9-C4	-5.59	1.34	1.37

The worst 5 of 296 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	YE	21	VAL	C-N-CD	-10.10	98.37	120.60
28	RE	21	VAL	C-N-CD	-10.10	98.39	120.60
1	XA	1054	C	C6-N1-C2	-9.78	116.39	120.30
1	XA	1495	U	N1-C2-O2	9.30	129.31	122.80
25	RA	2432	C	O5'-P-OP1	-9.29	97.34	105.70

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	544	0
1	XA	32249	0	16279	566	0
2	QB	1924	0	1975	64	0
2	XB	1924	0	1975	88	0
3	QC	1605	0	1668	51	0
3	XC	1605	0	1668	63	0
4	QD	1703	0	1765	106	0
4	XD	1703	0	1762	47	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	33	0
7	QG	1257	0	1296	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	27	0
8	QH	1116	0	1177	42	0
8	XH	1116	0	1177	33	0
9	QI	1010	0	1037	49	0
9	XI	1010	0	1037	51	0
10	QJ	801	0	849	52	0
10	XJ	801	0	849	63	0
11	QK	885	0	904	32	0
11	XK	885	0	904	29	0
12	QL	975	0	1062	98	0
12	XL	975	0	1062	95	0
13	QM	964	0	1034	66	0
13	XM	964	0	1034	47	0
14	QN	492	0	529	33	0
14	XN	492	0	529	20	0
15	QO	734	0	771	19	0
15	XO	734	0	771	18	0
16	QP	705	0	725	17	0
16	XP	705	0	725	24	0
17	QQ	834	0	904	25	0
17	XQ	834	0	904	17	0
18	QR	574	0	644	11	0
18	XR	574	0	644	23	0
19	QS	674	0	699	95	0
19	XS	674	0	699	43	0
20	QT	763	0	861	31	0
20	XT	763	0	861	68	0
21	QU	217	0	234	13	0
21	XU	217	0	234	5	0
22	QV	1644	0	835	20	0
22	XV	1644	0	836	18	0
23	QX	191	0	99	1	0
23	XX	213	0	110	3	0
24	QY	344	0	173	3	0
24	XY	344	0	173	14	0
25	RA	62071	0	31290	1016	0
25	YA	62071	0	31290	988	0
26	RB	2573	0	1306	57	0
26	YB	2573	0	1306	79	0
27	RD	2115	0	2195	104	0
27	YD	2115	0	2195	327	0
28	RE	1568	0	1634	282	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	YE	1568	0	1634	273	0
29	RF	1585	0	1632	78	0
29	YF	1585	0	1632	179	0
30	RG	1474	0	1535	111	0
30	YG	1474	0	1535	69	0
31	RH	1307	0	1382	228	0
31	YH	1307	0	1382	227	0
32	RI	1136	0	1223	106	0
32	YI	1136	0	1223	68	0
33	RN	1104	0	1180	45	0
33	YN	1104	0	1180	53	0
34	RO	933	0	996	26	0
34	YO	933	0	996	27	0
35	RP	1145	0	1228	117	0
35	YP	1145	0	1227	113	0
36	RQ	1122	0	1179	168	0
36	YQ	1122	0	1179	176	0
37	RR	968	0	1033	53	0
37	YR	968	0	1033	41	0
38	RS	882	0	943	54	0
38	YS	882	0	943	164	0
39	RT	1141	0	1202	72	0
39	YT	1141	0	1202	59	0
40	RU	964	0	1022	38	0
40	YU	964	0	1021	59	0
41	RV	779	0	852	26	0
41	YV	779	0	852	45	0
42	RW	900	0	964	29	0
42	YW	900	0	964	27	0
43	RX	725	0	778	31	0
43	YX	725	0	778	26	0
44	RY	785	0	878	53	0
44	YY	785	0	878	39	0
45	RZ	1461	0	1493	43	0
45	YZ	1461	0	1493	63	0
46	R0	648	0	672	26	0
46	Y0	647	0	668	41	0
47	R1	763	0	848	33	0
47	Y1	763	0	848	36	0
48	R2	581	0	629	24	0
48	Y2	581	0	629	73	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	230	0
50	Y4	581	0	577	63	0
51	R5	459	0	480	76	0
51	Y5	454	0	475	40	0
52	R6	424	0	450	41	0
52	Y6	424	0	450	38	0
53	R7	430	0	480	18	0
53	Y7	430	0	480	22	0
54	R8	517	0	582	132	0
54	Y8	517	0	582	103	0
55	R9	307	0	338	11	0
55	Y9	307	0	338	17	0
56	Z5	74	0	51	13	0
56	Z6	74	0	51	9	0
57	QA	80	0	0	0	0
57	QE	1	0	0	0	0
57	QF	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	2	0	0	0	0
57	QX	2	0	0	0	0
57	QY	1	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	RA	326	0	0	0	0
57	RB	5	0	0	0	0
57	RE	2	0	0	0	0
57	RF	1	0	0	0	0
57	RP	1	0	0	0	0
57	RR	1	0	0	0	0
57	XA	110	0	0	0	0
57	XB	1	0	0	0	0
57	XD	1	0	0	0	0
57	XF	1	0	0	0	0
57	XV	2	0	0	0	0
57	XX	1	0	0	0	0
57	Y0	3	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
57	Y7	1	0	0	0	0
57	YA	356	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	YB	4	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	YQ	1	0	0	0	0
57	YU	1	0	0	0	0
57	YY	1	0	0	0	0
58	QA	42	0	45	4	0
58	XA	42	0	45	2	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	292320	0	198405	8425	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 8425 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	1.53
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.36	1.52
32:RI:144:VAL:O	32:RI:145:VAL:HG12	1.22	1.36
4:QD:9:CYS:SG	4:QD:22:LYS:CE	2.22	1.28
32:YI:144:VAL:O	32:YI:145:VAL:HG22	1.22	1.28

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	174 (74%)	44 (19%)	17 (7%)	1	13
2	XB	235/256 (92%)	178 (76%)	42 (18%)	15 (6%)	1	17
3	QC	203/239 (85%)	163 (80%)	34 (17%)	6 (3%)	4	33
3	XC	203/239 (85%)	171 (84%)	29 (14%)	3 (2%)	10	47
4	QD	206/209 (99%)	178 (86%)	19 (9%)	9 (4%)	2	23
4	XD	206/209 (99%)	176 (85%)	25 (12%)	5 (2%)	6	37
5	QE	149/162 (92%)	136 (91%)	9 (6%)	4 (3%)	5	35
5	XE	149/162 (92%)	134 (90%)	13 (9%)	2 (1%)	12	50
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%)	136 (89%)	15 (10%)	2 (1%)	12	50
7	XG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	12	50
8	QH	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	22	61
8	XH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	4	33
9	QI	125/128 (98%)	103 (82%)	17 (14%)	5 (4%)	3	26
9	XI	125/128 (98%)	97 (78%)	24 (19%)	4 (3%)	4	31
10	QJ	97/105 (92%)	75 (77%)	19 (20%)	3 (3%)	4	32
10	XJ	97/105 (92%)	79 (81%)	13 (13%)	5 (5%)	2	20
11	QK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	9	45
11	XK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	9	45
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	6
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	6
13	QM	119/126 (94%)	95 (80%)	15 (13%)	9 (8%)	1	12
13	XM	119/126 (94%)	94 (79%)	16 (13%)	9 (8%)	1	12
14	QN	58/61 (95%)	50 (86%)	4 (7%)	4 (7%)	1	14
14	XN	58/61 (95%)	46 (79%)	6 (10%)	6 (10%)	0	7
15	QO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	13	51
15	XO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	6	38
16	QP	82/88 (93%)	73 (89%)	8 (10%)	1 (1%)	13	51
16	XP	82/88 (93%)	71 (87%)	10 (12%)	1 (1%)	13	51
17	QQ	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	7	41
17	XQ	98/105 (93%)	88 (90%)	10 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	QR	68/88 (77%)	56 (82%)	9 (13%)	3 (4%)	2	23
18	XR	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	10	47
19	QS	82/93 (88%)	55 (67%)	16 (20%)	11 (13%)	0	4
19	XS	82/93 (88%)	54 (66%)	18 (22%)	10 (12%)	0	5
20	QT	97/106 (92%)	76 (78%)	15 (16%)	6 (6%)	1	17
20	XT	97/106 (92%)	75 (77%)	17 (18%)	5 (5%)	2	20
21	QU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	2	24
21	XU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	2	24
27	RD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	2	23
27	YD	270/276 (98%)	205 (76%)	46 (17%)	19 (7%)	1	14
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%)	171 (86%)	19 (10%)	10 (5%)	2	21
29	YF	200/210 (95%)	143 (72%)	37 (18%)	20 (10%)	0	8
30	RG	179/182 (98%)	139 (78%)	26 (14%)	14 (8%)	1	11
30	YG	179/182 (98%)	143 (80%)	24 (13%)	12 (7%)	1	15
31	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
31	YH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
32	RI	144/148 (97%)	99 (69%)	31 (22%)	14 (10%)	0	8
32	YI	144/148 (97%)	106 (74%)	21 (15%)	17 (12%)	0	5
33	RN	136/140 (97%)	104 (76%)	20 (15%)	12 (9%)	1	9
33	YN	136/140 (97%)	109 (80%)	16 (12%)	11 (8%)	1	11
34	RO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	9	45
34	YO	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	9	45
35	RP	148/150 (99%)	112 (76%)	25 (17%)	11 (7%)	1	13
35	YP	148/150 (99%)	111 (75%)	22 (15%)	15 (10%)	0	7
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	0	7
36	YQ	139/141 (99%)	98 (70%)	25 (18%)	16 (12%)	0	6
37	RR	116/118 (98%)	106 (91%)	5 (4%)	5 (4%)	2	24
37	YR	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	2	20
38	RS	109/112 (97%)	76 (70%)	22 (20%)	11 (10%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	YS	109/112 (97%)	62 (57%)	29 (27%)	18 (16%)	0	3
39	RT	135/146 (92%)	107 (79%)	16 (12%)	12 (9%)	1	9
39	YT	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	1	13
40	RU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	3	30
40	YU	115/118 (98%)	101 (88%)	12 (10%)	2 (2%)	9	45
41	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	1	17
41	YV	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	11
42	RW	111/113 (98%)	99 (89%)	8 (7%)	4 (4%)	3	29
42	YW	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	8	43
43	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	6	39
43	YX	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	6	39
44	RY	100/110 (91%)	71 (71%)	13 (13%)	16 (16%)	0	3
44	YY	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	0	5
45	RZ	181/206 (88%)	128 (71%)	33 (18%)	20 (11%)	0	6
45	YZ	181/206 (88%)	135 (75%)	28 (16%)	18 (10%)	0	8
46	R0	80/85 (94%)	65 (81%)	14 (18%)	1 (1%)	12	50
46	Y0	80/85 (94%)	73 (91%)	7 (9%)	0	100	100
47	R1	95/98 (97%)	75 (79%)	11 (12%)	9 (10%)	0	8
47	Y1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	1	17
48	R2	67/72 (93%)	54 (81%)	9 (13%)	4 (6%)	1	17
48	Y2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	4
49	R3	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	3	30
49	Y3	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	8	43
50	R4	69/71 (97%)	22 (32%)	21 (30%)	26 (38%)	0	0
50	Y4	69/71 (97%)	35 (51%)	15 (22%)	19 (28%)	0	0
51	R5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	0
51	Y5	56/60 (93%)	46 (82%)	8 (14%)	2 (4%)	3	29
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%)	7	40
53	Y7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	7	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	R8	62/65 (95%)	36 (58%)	14 (23%)	12 (19%)	0	2
54	Y8	62/65 (95%)	36 (58%)	14 (23%)	12 (19%)	0	2
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%)	9009 (79%)	1610 (14%)	850 (7%)	1	13

5 of 850 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	236	TYR
3	QC	12	LEU
3	QC	190	ARG
4	QD	28	SER
4	QD	33	MET

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%)	172 (84%)	33 (16%)	2	16
2	XB	205/220 (93%)	180 (88%)	25 (12%)	5	26
3	QC	159/188 (85%)	145 (91%)	14 (9%)	10	40
3	XC	159/188 (85%)	145 (91%)	14 (9%)	10	40
4	QD	180/181 (99%)	155 (86%)	25 (14%)	3	22
4	XD	180/181 (99%)	154 (86%)	26 (14%)	3	20
5	QE	116/123 (94%)	104 (90%)	12 (10%)	7	34
5	XE	116/123 (94%)	104 (90%)	12 (10%)	7	34
6	QF	90/90 (100%)	78 (87%)	12 (13%)	4	23
6	XF	90/90 (100%)	82 (91%)	8 (9%)	9	40
7	QG	126/127 (99%)	114 (90%)	12 (10%)	8	37
7	XG	126/127 (99%)	114 (90%)	12 (10%)	8	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	QH	119/119 (100%)	109 (92%)	10 (8%)	11	42
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	32
9	QI	98/99 (99%)	80 (82%)	18 (18%)	1	10
9	XI	98/99 (99%)	79 (81%)	19 (19%)	1	9
10	QJ	89/92 (97%)	77 (86%)	12 (14%)	4	23
10	XJ	89/92 (97%)	75 (84%)	14 (16%)	2	17
11	QK	90/99 (91%)	81 (90%)	9 (10%)	7	35
11	XK	90/99 (91%)	81 (90%)	9 (10%)	7	35
12	QL	104/109 (95%)	90 (86%)	14 (14%)	4	23
12	XL	104/109 (95%)	89 (86%)	15 (14%)	3	20
13	QM	97/101 (96%)	73 (75%)	24 (25%)	0	4
13	XM	97/101 (96%)	78 (80%)	19 (20%)	1	8
14	QN	49/50 (98%)	40 (82%)	9 (18%)	1	10
14	XN	49/50 (98%)	42 (86%)	7 (14%)	3	21
15	QO	79/80 (99%)	72 (91%)	7 (9%)	9	40
15	XO	79/80 (99%)	69 (87%)	10 (13%)	4	24
16	QP	72/74 (97%)	64 (89%)	8 (11%)	6	31
16	XP	72/74 (97%)	64 (89%)	8 (11%)	6	31
17	QQ	95/97 (98%)	87 (92%)	8 (8%)	11	42
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	18	53
18	QR	61/77 (79%)	50 (82%)	11 (18%)	1	11
18	XR	61/77 (79%)	52 (85%)	9 (15%)	3	19
19	QS	73/80 (91%)	59 (81%)	14 (19%)	1	9
19	XS	73/80 (91%)	57 (78%)	16 (22%)	1	6
20	QT	76/82 (93%)	67 (88%)	9 (12%)	5	28
20	XT	76/82 (93%)	67 (88%)	9 (12%)	5	28
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	59
27	RD	214/218 (98%)	174 (81%)	40 (19%)	1	10
27	YD	214/218 (98%)	178 (83%)	36 (17%)	2	14
28	RE	165/166 (99%)	127 (77%)	38 (23%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	5
29	RF	161/166 (97%)	131 (81%)	30 (19%)	1	10
29	YF	161/166 (97%)	140 (87%)	21 (13%)	4	24
30	RG	155/156 (99%)	134 (86%)	21 (14%)	4	23
30	YG	155/156 (99%)	133 (86%)	22 (14%)	3	21
31	RH	142/148 (96%)	114 (80%)	28 (20%)	1	8
31	YH	142/148 (96%)	115 (81%)	27 (19%)	1	9
32	RI	122/124 (98%)	100 (82%)	22 (18%)	1	11
32	YI	122/124 (98%)	92 (75%)	30 (25%)	0	4
33	RN	117/119 (98%)	97 (83%)	20 (17%)	2	13
33	YN	117/119 (98%)	94 (80%)	23 (20%)	1	8
34	RO	100/100 (100%)	90 (90%)	10 (10%)	7	35
34	YO	100/100 (100%)	88 (88%)	12 (12%)	5	27
35	RP	116/116 (100%)	86 (74%)	30 (26%)	0	4
35	YP	116/116 (100%)	79 (68%)	37 (32%)	0	2
36	RQ	111/111 (100%)	93 (84%)	18 (16%)	2	15
36	YQ	111/111 (100%)	91 (82%)	20 (18%)	1	11
37	RR	101/101 (100%)	83 (82%)	18 (18%)	2	11
37	YR	101/101 (100%)	81 (80%)	20 (20%)	1	8
38	RS	87/88 (99%)	69 (79%)	18 (21%)	1	7
38	YS	87/88 (99%)	74 (85%)	13 (15%)	3	19
39	RT	120/127 (94%)	102 (85%)	18 (15%)	3	19
39	YT	120/127 (94%)	99 (82%)	21 (18%)	2	12
40	RU	93/94 (99%)	79 (85%)	14 (15%)	3	19
40	YU	93/94 (99%)	77 (83%)	16 (17%)	2	13
41	RV	82/82 (100%)	66 (80%)	16 (20%)	1	9
41	YV	82/82 (100%)	67 (82%)	15 (18%)	1	10
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%)	64 (86%)	10 (14%)	4	23
43	YX	74/78 (95%)	60 (81%)	14 (19%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	RY	85/91 (93%)	63 (74%)	22 (26%)	0	4
44	YY	85/91 (93%)	64 (75%)	21 (25%)	0	4
45	RZ	162/179 (90%)	138 (85%)	24 (15%)	3	19
45	YZ	162/179 (90%)	145 (90%)	17 (10%)	7	33
46	R0	65/67 (97%)	60 (92%)	5 (8%)	13	45
46	Y0	65/67 (97%)	59 (91%)	6 (9%)	9	39
47	R1	82/83 (99%)	73 (89%)	9 (11%)	6	31
47	Y1	82/83 (99%)	70 (85%)	12 (15%)	3	20
48	R2	64/67 (96%)	55 (86%)	9 (14%)	3	21
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	6	32
49	R3	51/52 (98%)	45 (88%)	6 (12%)	5	28
49	Y3	51/52 (98%)	43 (84%)	8 (16%)	2	17
50	R4	63/63 (100%)	46 (73%)	17 (27%)	0	3
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	2
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	5
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	5
52	R6	48/52 (92%)	35 (73%)	13 (27%)	0	3
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	7
53	R7	42/42 (100%)	34 (81%)	8 (19%)	1	9
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%)	32 (94%)	2 (6%)	19	55
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	19	55
All	All	9702/10066 (96%)	8159 (84%)	1543 (16%)	2	16

5 of 1543 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	XL	20	LYS
31	YH	11	VAL
13	XM	98	VAL
12	XL	17	LYS
27	YD	131	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
55	R9	29	ASN
39	YT	58	ASN
2	XB	204	ASN
27	YD	166	GLN
2	XB	19	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	279 (18%)	43 (2%)
1	XA	1498/1522 (98%)	282 (18%)	37 (2%)
22	QV	76/77 (98%)	21 (27%)	1 (1%)
22	XV	76/77 (98%)	13 (17%)	1 (1%)
23	QX	8/25 (32%)	2 (25%)	0
23	XX	9/25 (36%)	1 (11%)	0
24	QY	15/17 (88%)	2 (13%)	0
24	XY	15/17 (88%)	1 (6%)	0
25	RA	2879/2915 (98%)	606 (21%)	50 (1%)
25	YA	2879/2915 (98%)	607 (21%)	56 (1%)
26	RB	119/122 (97%)	22 (18%)	2 (1%)
26	YB	119/122 (97%)	27 (22%)	1 (0%)
56	Z5	1/3 (33%)	0	0
56	Z6	1/3 (33%)	0	0
All	All	9193/9362 (98%)	1863 (20%)	191 (2%)

5 of 1863 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	9	G
1	QA	32	A
1	QA	39	G
1	QA	47	C
1	QA	48	C

5 of 191 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	485	G
25	YA	271(B)	G
1	XA	687	A

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Mol	Chain	Res	Type
1	XA	1397	C
25	YA	637	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	25,56	32,40,41	2.55	6 (18%)	33,57,60	2.15	5 (15%)
56	PPU	Z5	101	25,56	32,40,41	2.55	6 (18%)	33,57,60	2.15	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PPU	Z6	101	25,56	-	2/21/43/44	0/4/4/4
56	PPU	Z5	101	25,56	-	2/21/43/44	0/4/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z5	101	PPU	O-C	9.30	1.41	1.23
56	Z6	101	PPU	O-C	9.27	1.41	1.23
56	Z6	101	PPU	C9-N6	-5.95	1.31	1.45
56	Z5	101	PPU	C9-N6	-5.95	1.32	1.45
56	Z5	101	PPU	C-N3'	5.72	1.46	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z5	101	PPU	C3'-N3'-C	-8.61	110.23	123.21
56	Z6	101	PPU	C3'-N3'-C	-8.59	110.26	123.21
56	Z5	101	PPU	N3-C2-N1	-4.65	121.42	128.68
56	Z6	101	PPU	N3-C2-N1	-4.62	121.45	128.68
56	Z5	101	PPU	CA-C-N3'	4.05	121.76	116.15

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 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z6	101	PPU	7	0
56	Z5	101	PPU	12	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 924 ligands modelled in this entry, 922 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	1710	-	45,45,45	1.60	7 (15%)	64,67,67	1.29	5 (7%)
58	PAR	QA	1681	-	45,45,45	1.59	8 (17%)	64,67,67	1.37	7 (10%)

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	1710	-	-	8/18/94/94	0/4/4/4
58	PAR	QA	1681	-	-	7/18/94/94	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	1710	PAR	C64-C54	5.12	1.59	1.52
58	QA	1681	PAR	C64-C54	5.00	1.58	1.52
58	QA	1681	PAR	C52-C42	3.19	1.58	1.52
58	QA	1681	PAR	O54-C14	3.13	1.49	1.41
58	XA	1710	PAR	C52-C42	3.11	1.58	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	QA	1681	PAR	C14-O54-C54	5.16	123.82	113.69
58	XA	1710	PAR	O33-C14-C24	4.62	116.17	108.22
58	XA	1710	PAR	C14-O54-C54	3.81	121.17	113.69
58	XA	1710	PAR	O52-C13-C23	3.55	115.33	107.96
58	QA	1681	PAR	O54-C54-C64	3.52	112.56	106.01

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

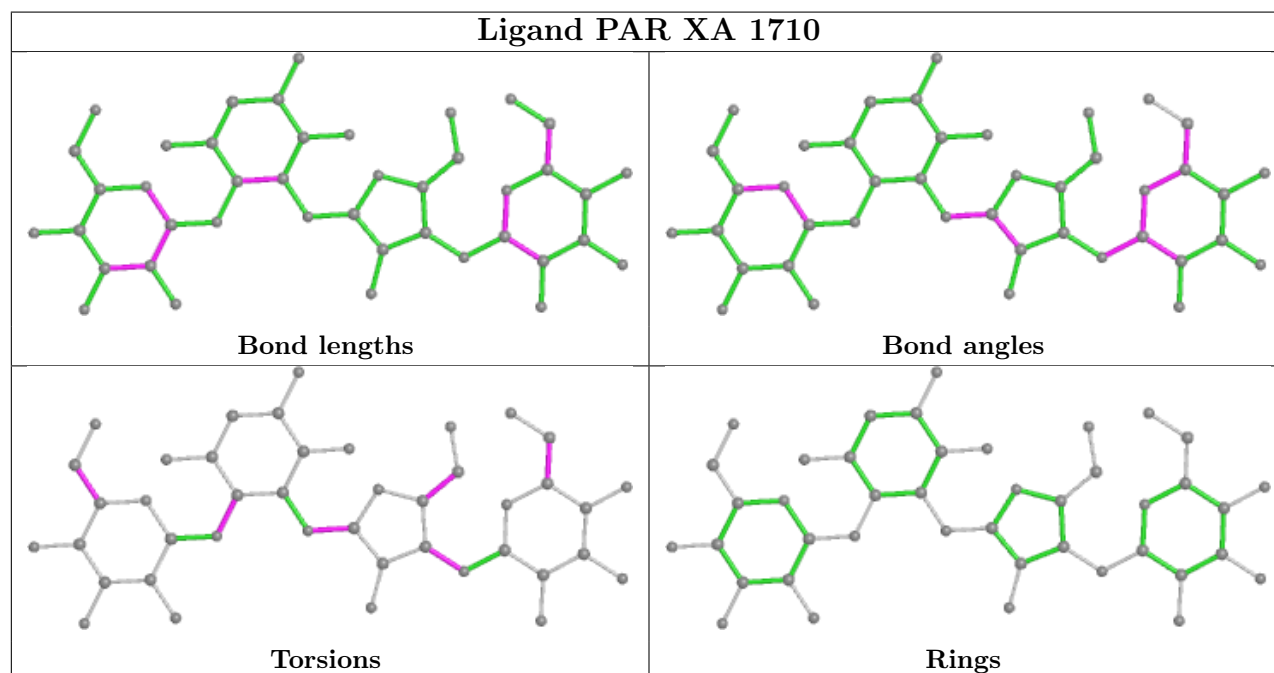
Mol	Chain	Res	Type	Atoms
58	QA	1681	PAR	C44-C54-C64-N64
58	QA	1681	PAR	O54-C54-C64-N64
58	XA	1710	PAR	C44-C54-C64-N64
58	XA	1710	PAR	O43-C43-C53-O53
58	XA	1710	PAR	C33-C43-C53-O53

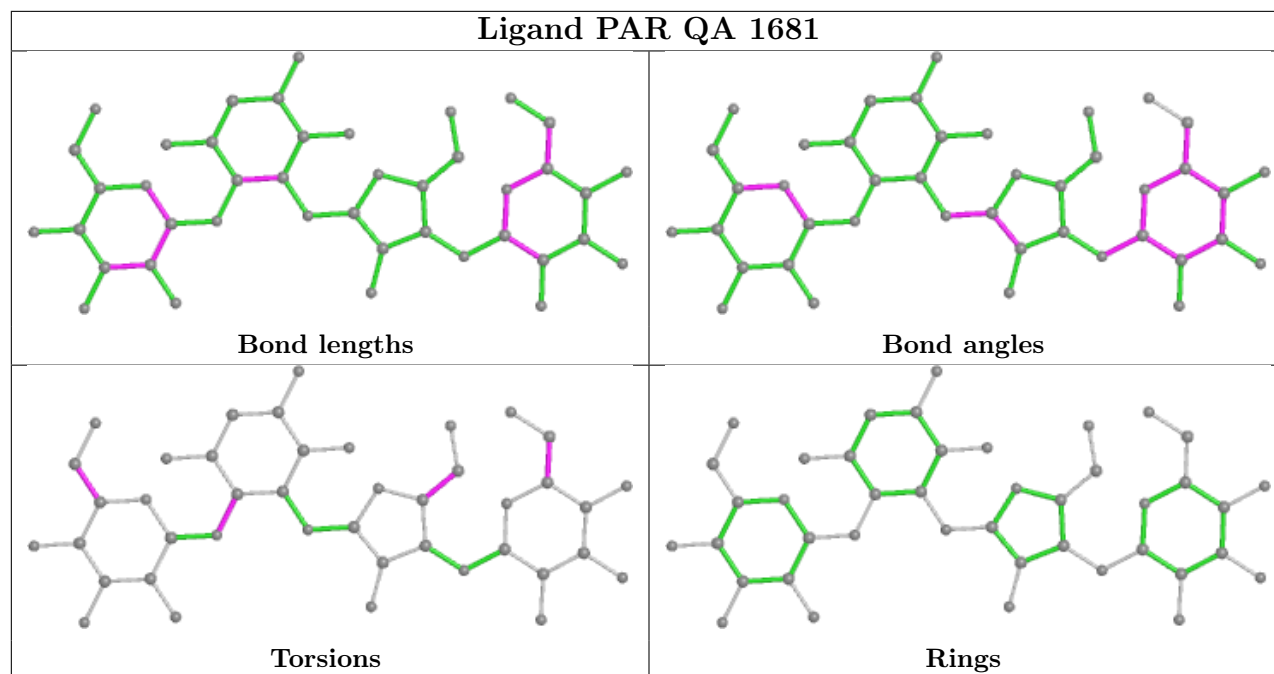
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	XA	1710	PAR	2	0
58	QA	1681	PAR	4	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%)	0.05	16 (1%) 80 68	40, 98, 191, 460	0
1	XA	1500/1522 (98%)	0.05	10 (0%) 87 78	37, 88, 192, 384	0
2	QB	237/256 (92%)	0.70	26 (10%) 5 3	91, 151, 229, 303	0
2	XB	237/256 (92%)	0.37	7 (2%) 50 34	71, 131, 209, 300	0
3	QC	205/239 (85%)	0.32	1 (0%) 91 83	79, 138, 213, 261	0
3	XC	205/239 (85%)	-0.02	0 100 100	53, 95, 150, 275	0
4	QD	208/209 (99%)	0.12	1 (0%) 91 83	59, 105, 170, 323	0
4	XD	208/209 (99%)	-0.12	0 100 100	43, 92, 156, 208	0
5	QE	151/162 (93%)	0.12	1 (0%) 87 78	66, 112, 178, 228	0
5	XE	151/162 (93%)	-0.16	0 100 100	44, 86, 140, 204	0
6	QF	101/101 (100%)	-0.14	0 100 100	48, 92, 135, 211	0
6	XF	101/101 (100%)	-0.06	0 100 100	47, 96, 150, 271	0
7	QG	155/156 (99%)	0.58	14 (9%) 9 5	86, 136, 192, 401	0
7	XG	155/156 (99%)	0.35	8 (5%) 27 17	63, 118, 165, 229	0
8	QH	138/138 (100%)	0.16	1 (0%) 87 78	66, 110, 155, 278	0
8	XH	138/138 (100%)	-0.00	1 (0%) 87 78	62, 104, 145, 170	0
9	QI	127/128 (99%)	0.84	16 (12%) 3 2	82, 153, 208, 251	0
9	XI	127/128 (99%)	0.25	0 100 100	56, 131, 179, 246	0
10	QJ	99/105 (94%)	0.81	10 (10%) 7 4	101, 158, 246, 398	0
10	XJ	99/105 (94%)	0.61	10 (10%) 7 4	60, 121, 205, 240	0
11	QK	119/129 (92%)	0.89	13 (10%) 5 3	60, 100, 188, 269	0
11	XK	119/129 (92%)	0.51	5 (4%) 36 23	37, 93, 164, 272	0
12	QL	125/132 (94%)	0.31	4 (3%) 47 32	47, 91, 145, 263	0
12	XL	125/132 (94%)	0.17	3 (2%) 59 42	42, 72, 139, 285	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	0.64	12 (9%) 7 4	91, 151, 204, 320	0
13	XM	121/126 (96%)	0.19	3 (2%) 57 41	58, 116, 178, 305	0
14	QN	60/61 (98%)	0.62	1 (1%) 70 55	88, 128, 188, 195	0
14	XN	60/61 (98%)	-0.00	0 100 100	49, 90, 129, 159	0
15	QO	88/89 (98%)	-0.00	0 100 100	41, 92, 137, 169	0
15	XO	88/89 (98%)	0.10	1 (1%) 80 68	56, 97, 143, 170	0
16	QP	84/88 (95%)	0.32	1 (1%) 79 66	62, 95, 137, 206	0
16	XP	84/88 (95%)	0.57	1 (1%) 79 66	74, 110, 158, 267	0
17	QQ	100/105 (95%)	0.26	0 100 100	57, 99, 132, 165	0
17	XQ	100/105 (95%)	0.24	0 100 100	68, 112, 143, 168	0
18	QR	70/88 (79%)	0.19	4 (5%) 23 14	64, 101, 147, 191	0
18	XR	70/88 (79%)	0.20	1 (1%) 75 61	62, 104, 164, 181	0
19	QS	84/93 (90%)	0.71	5 (5%) 21 12	100, 157, 204, 241	0
19	XS	84/93 (90%)	0.56	2 (2%) 59 42	66, 121, 190, 335	0
20	QT	99/106 (93%)	0.39	2 (2%) 65 49	55, 101, 164, 255	0
20	XT	99/106 (93%)	0.73	8 (8%) 12 7	80, 141, 215, 265	0
21	QU	25/27 (92%)	0.69	2 (8%) 12 7	95, 140, 198, 248	0
21	XU	25/27 (92%)	0.28	1 (4%) 38 25	76, 110, 159, 180	0
22	QV	77/77 (100%)	0.14	1 (1%) 77 63	38, 106, 168, 231	0
22	XV	77/77 (100%)	0.20	1 (1%) 77 63	42, 84, 137, 180	0
23	QX	9/25 (36%)	0.42	0 100 100	63, 86, 158, 171	0
23	XX	10/25 (40%)	0.50	1 (10%) 7 4	47, 69, 148, 219	0
24	QY	16/17 (94%)	0.40	1 (6%) 20 11	87, 115, 167, 175	0
24	XY	16/17 (94%)	0.18	0 100 100	68, 95, 153, 191	0
25	RA	2882/2915 (98%)	0.11	118 (4%) 37 24	27, 74, 249, 510	0
25	YA	2882/2915 (98%)	0.13	108 (3%) 41 27	27, 69, 246, 557	0
26	RB	120/122 (98%)	0.04	1 (0%) 86 75	90, 127, 170, 210	0
26	YB	120/122 (98%)	-0.17	0 100 100	61, 90, 124, 152	0
27	RD	272/276 (98%)	-0.14	1 (0%) 92 86	22, 61, 105, 222	0
27	YD	272/276 (98%)	-0.07	1 (0%) 92 86	22, 61, 105, 185	0
28	RE	205/206 (99%)	0.24	5 (2%) 59 42	39, 83, 168, 336	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YE	205/206 (99%)	0.12	3 (1%) 73 60	31, 91, 177, 273	0
29	RF	202/210 (96%)	0.27	4 (1%) 65 49	23, 99, 171, 216	0
29	YF	202/210 (96%)	0.09	4 (1%) 65 49	32, 78, 149, 227	0
30	RG	181/182 (99%)	0.67	11 (6%) 21 12	92, 150, 197, 231	0
30	YG	181/182 (99%)	0.22	4 (2%) 62 45	61, 98, 160, 244	0
31	RH	170/180 (94%)	1.43	41 (24%) 0 0	102, 193, 270, 361	0
31	YH	170/180 (94%)	0.43	4 (2%) 59 42	53, 105, 164, 210	0
32	RI	146/148 (98%)	0.53	10 (6%) 17 10	67, 125, 195, 258	0
32	YI	146/148 (98%)	0.50	8 (5%) 25 15	48, 123, 189, 271	0
33	RN	138/140 (98%)	0.19	3 (2%) 62 45	51, 93, 154, 202	0
33	YN	138/140 (98%)	0.26	2 (1%) 75 61	47, 92, 157, 220	0
34	RO	122/122 (100%)	0.15	0 100 100	48, 80, 114, 148	0
34	YO	122/122 (100%)	0.05	0 100 100	27, 64, 103, 120	0
35	RP	150/150 (100%)	0.50	5 (3%) 46 31	28, 99, 159, 288	0
35	YP	150/150 (100%)	0.20	4 (2%) 54 38	31, 90, 162, 231	0
36	RQ	141/141 (100%)	0.61	8 (5%) 23 14	54, 102, 180, 226	0
36	YQ	141/141 (100%)	0.18	4 (2%) 53 37	35, 73, 140, 222	0
37	RR	118/118 (100%)	-0.14	0 100 100	29, 70, 104, 138	0
37	YR	118/118 (100%)	0.10	1 (0%) 86 75	51, 91, 139, 190	0
38	RS	111/112 (99%)	0.50	4 (3%) 42 28	81, 120, 204, 273	0
38	YS	111/112 (99%)	0.13	2 (1%) 68 53	66, 101, 156, 201	0
39	RT	137/146 (93%)	0.07	2 (1%) 73 60	50, 91, 188, 276	0
39	YT	137/146 (93%)	0.03	0 100 100	51, 89, 212, 242	0
40	RU	117/118 (99%)	0.23	6 (5%) 28 17	35, 81, 155, 298	0
40	YU	117/118 (99%)	-0.04	1 (0%) 84 73	40, 81, 152, 243	0
41	RV	101/101 (100%)	0.73	7 (6%) 16 10	55, 114, 183, 398	0
41	YV	101/101 (100%)	0.39	4 (3%) 38 25	44, 111, 174, 335	0
42	RW	113/113 (100%)	0.10	3 (2%) 54 38	36, 63, 115, 296	0
42	YW	113/113 (100%)	0.14	5 (4%) 34 21	37, 74, 134, 258	0
43	RX	92/96 (95%)	0.34	1 (1%) 80 68	51, 77, 128, 164	0
43	YX	92/96 (95%)	0.32	2 (2%) 62 45	37, 73, 112, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RY	102/110 (92%)	0.93	15 (14%) 2 1	55, 119, 185, 325	0
44	YY	102/110 (92%)	0.20	4 (3%) 39 25	42, 92, 162, 273	0
45	RZ	183/206 (88%)	0.89	21 (11%) 4 3	104, 153, 230, 292	0
45	YZ	183/206 (88%)	0.49	4 (2%) 62 45	55, 116, 202, 300	0
46	R0	82/85 (96%)	0.44	2 (2%) 59 42	48, 88, 127, 238	0
46	Y0	82/85 (96%)	0.11	0 100 100	44, 71, 99, 142	0
47	R1	97/98 (98%)	0.43	3 (3%) 49 33	37, 80, 161, 290	0
47	Y1	97/98 (98%)	0.38	4 (4%) 37 24	39, 75, 176, 210	0
48	R2	69/72 (95%)	0.67	7 (10%) 7 4	63, 105, 160, 274	0
48	Y2	69/72 (95%)	0.17	3 (4%) 35 22	47, 80, 151, 219	0
49	R3	59/60 (98%)	0.60	3 (5%) 28 17	63, 97, 155, 205	0
49	Y3	59/60 (98%)	0.73	9 (15%) 2 1	55, 89, 162, 293	0
50	R4	71/71 (100%)	1.66	18 (25%) 0 0	150, 244, 350, 423	0
50	Y4	71/71 (100%)	0.85	12 (16%) 1 1	69, 162, 340, 411	0
51	R5	59/60 (98%)	0.24	4 (6%) 17 10	40, 77, 216, 261	0
51	Y5	58/60 (96%)	0.47	7 (12%) 4 3	44, 97, 231, 342	0
52	R6	49/54 (90%)	3.45	36 (73%) 0 0	119, 194, 264, 286	0
52	Y6	49/54 (90%)	3.18	40 (81%) 0 0	115, 171, 260, 295	0
53	R7	49/49 (100%)	-0.21	1 (2%) 65 49	27, 54, 110, 166	0
53	Y7	49/49 (100%)	-0.23	1 (2%) 65 49	32, 51, 111, 180	0
54	R8	64/65 (98%)	0.23	2 (3%) 49 33	42, 82, 134, 223	0
54	Y8	64/65 (98%)	-0.03	0 100 100	35, 68, 120, 229	0
55	R9	37/37 (100%)	5.80	36 (97%) 0 0	134, 200, 317, 510	0
55	Y9	37/37 (100%)	5.50	36 (97%) 0 0	134, 206, 322, 404	0
56	Z5	2/3 (66%)	0.18	0 100 100	50, 50, 50, 60	0
56	Z6	2/3 (66%)	0.04	0 100 100	38, 38, 38, 41	0
All	All	20878/21490 (97%)	0.25	850 (4%) 37 24	22, 92, 205, 557	0

The worst 5 of 850 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
55	R9	14	CYS	17.4
25	YA	2165	G	14.3

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Mol	Chain	Res	Type	RSRZ
25	YA	2179	C	13.2
55	Y9	34	GLN	12.6
25	RA	2138	G	11.3

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	Z6	101	37/38	0.94	0.26	36,37,38,38	0
56	PPU	Z5	101	37/38	0.95	0.27	45,47,48,48	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	3277	1/1	0.36	0.37	80,80,80,80	0
57	MG	YA	3194	1/1	0.42	0.76	60,60,60,60	0
57	MG	RA	3218	1/1	0.43	0.19	48,48,48,48	0
57	MG	QF	201	1/1	0.48	0.34	57,57,57,57	0
57	MG	QA	1656	1/1	0.50	0.40	63,63,63,63	0
57	MG	XA	1675	1/1	0.51	0.41	59,59,59,59	0
57	MG	RA	3190	1/1	0.52	0.17	69,69,69,69	0
57	MG	XA	1632	1/1	0.53	0.35	58,58,58,58	0
57	MG	YA	3153	1/1	0.54	0.27	52,52,52,52	0
57	MG	YA	3176	1/1	0.56	0.26	89,89,89,89	0
57	MG	QY	101	1/1	0.57	0.27	66,66,66,66	0
57	MG	YA	3333	1/1	0.57	0.58	69,69,69,69	0
57	MG	YA	3308	1/1	0.59	0.33	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	XA	1686	1/1	0.59	0.36	72,72,72,72	0
57	MG	QA	1658	1/1	0.60	0.73	62,62,62,62	0
57	MG	RA	3203	1/1	0.60	0.30	70,70,70,70	0
57	MG	XF	201	1/1	0.60	0.25	65,65,65,65	0
57	MG	QA	1627	1/1	0.61	0.31	69,69,69,69	0
57	MG	YA	3211	1/1	0.62	0.33	50,50,50,50	0
57	MG	YA	3174	1/1	0.62	1.17	74,74,74,74	0
57	MG	RA	3138	1/1	0.62	0.28	61,61,61,61	0
57	MG	XA	1648	1/1	0.62	0.35	59,59,59,59	0
57	MG	RA	3202	1/1	0.63	0.27	55,55,55,55	0
57	MG	YA	3295	1/1	0.64	0.53	47,47,47,47	0
57	MG	YA	3260	1/1	0.64	0.29	34,34,34,34	0
57	MG	YA	3315	1/1	0.64	0.39	50,50,50,50	0
57	MG	RA	3189	1/1	0.64	0.20	58,58,58,58	0
57	MG	RA	3059	1/1	0.65	0.20	10,10,10,10	0
57	MG	YA	3196	1/1	0.66	0.20	90,90,90,90	0
57	MG	QA	1640	1/1	0.66	0.85	63,63,63,63	0
57	MG	YA	3339	1/1	0.66	0.77	78,78,78,78	0
57	MG	YA	3355	1/1	0.66	0.63	67,67,67,67	0
57	MG	RA	3308	1/1	0.67	0.52	48,48,48,48	0
57	MG	YA	3338	1/1	0.67	0.38	89,89,89,89	0
57	MG	RA	3298	1/1	0.68	0.31	53,53,53,53	0
57	MG	QA	1629	1/1	0.68	0.31	52,52,52,52	0
57	MG	YA	3117	1/1	0.69	0.63	49,49,49,49	0
57	MG	YA	3337	1/1	0.69	0.84	57,57,57,57	0
57	MG	RA	3325	1/1	0.69	0.21	60,60,60,60	0
57	MG	XA	1705	1/1	0.69	0.30	52,52,52,52	0
57	MG	RA	3271	1/1	0.69	0.42	43,43,43,43	0
57	MG	RA	3062	1/1	0.70	0.19	61,61,61,61	0
57	MG	YA	3216	1/1	0.70	0.40	40,40,40,40	0
57	MG	YA	3302	1/1	0.71	0.66	53,53,53,53	0
57	MG	RA	3215	1/1	0.71	0.20	33,33,33,33	0
57	MG	YA	3208	1/1	0.72	0.68	49,49,49,49	0
57	MG	RA	3177	1/1	0.72	0.23	31,31,31,31	0
57	MG	YA	3283	1/1	0.72	0.56	64,64,64,64	0
57	MG	RR	201	1/1	0.72	0.60	25,25,25,25	0
57	MG	RA	3209	1/1	0.73	0.40	59,59,59,59	0
57	MG	QA	1624	1/1	0.73	0.27	77,77,77,77	0
57	MG	YA	3113	1/1	0.73	1.33	53,53,53,53	0
57	MG	QA	1661	1/1	0.73	0.45	37,37,37,37	0
57	MG	YA	3146	1/1	0.73	0.27	98,98,98,98	0
57	MG	YA	3298	1/1	0.73	0.46	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	QA	1633	1/1	0.73	0.34	52,52,52,52	0
57	MG	QA	1668	1/1	0.74	0.55	36,36,36,36	0
57	MG	RA	3176	1/1	0.74	0.32	28,28,28,28	0
57	MG	YA	3193	1/1	0.74	0.32	56,56,56,56	0
57	MG	RA	3251	1/1	0.74	0.45	46,46,46,46	0
57	MG	RA	3311	1/1	0.74	0.12	56,56,56,56	0
57	MG	RA	3264	1/1	0.74	0.47	63,63,63,63	0
57	MG	XA	1694	1/1	0.74	0.22	69,69,69,69	0
57	MG	YQ	201	1/1	0.74	0.21	61,61,61,61	0
57	MG	XA	1636	1/1	0.75	0.18	66,66,66,66	0
57	MG	RA	3213	1/1	0.75	0.80	57,57,57,57	0
57	MG	YA	3292	1/1	0.75	0.67	74,74,74,74	0
57	MG	YA	3191	1/1	0.75	0.51	62,62,62,62	0
57	MG	QA	1673	1/1	0.75	0.60	63,63,63,63	0
57	MG	YA	3227	1/1	0.75	0.66	52,52,52,52	0
57	MG	XA	1677	1/1	0.75	0.12	81,81,81,81	0
59	ZN	QD	301	1/1	0.75	0.34	77,77,77,77	0
57	MG	QA	1603	1/1	0.76	0.62	80,80,80,80	0
57	MG	YA	3181	1/1	0.76	0.12	52,52,52,52	0
57	MG	XA	1706	1/1	0.76	0.80	66,66,66,66	0
57	MG	XA	1649	1/1	0.76	0.49	39,39,39,39	0
57	MG	YP	201	1/1	0.76	0.42	66,66,66,66	0
57	MG	YA	3321	1/1	0.76	0.80	34,34,34,34	0
57	MG	YY	201	1/1	0.76	0.19	45,45,45,45	0
57	MG	XA	1623	1/1	0.76	0.28	48,48,48,48	0
57	MG	XA	1695	1/1	0.77	0.15	78,78,78,78	0
57	MG	RA	3256	1/1	0.77	1.66	78,78,78,78	0
57	MG	XA	1659	1/1	0.77	0.21	105,105,105,105	0
57	MG	XA	1662	1/1	0.77	0.52	38,38,38,38	0
57	MG	YA	3064	1/1	0.77	0.19	25,25,25,25	0
57	MG	RA	3313	1/1	0.77	0.78	68,68,68,68	0
57	MG	RA	3197	1/1	0.77	0.46	44,44,44,44	0
57	MG	XA	1643	1/1	0.77	0.40	59,59,59,59	0
57	MG	RA	3270	1/1	0.77	0.68	41,41,41,41	0
57	MG	YA	3166	1/1	0.77	0.27	51,51,51,51	0
57	MG	XA	1684	1/1	0.78	0.30	56,56,56,56	0
57	MG	YA	3275	1/1	0.78	0.31	46,46,46,46	0
57	MG	YA	3175	1/1	0.78	0.51	63,63,63,63	0
57	MG	RA	3201	1/1	0.78	0.41	65,65,65,65	0
57	MG	YA	3138	1/1	0.78	0.26	40,40,40,40	0
57	MG	RA	3280	1/1	0.79	0.48	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3226	1/1	0.79	0.48	41,41,41,41	0
57	MG	RA	3226	1/1	0.79	0.35	60,60,60,60	0
57	MG	YA	3353	1/1	0.79	0.36	66,66,66,66	0
57	MG	YA	3257	1/1	0.79	1.11	35,35,35,35	0
57	MG	RA	3303	1/1	0.79	0.65	51,51,51,51	0
57	MG	RA	3113	1/1	0.79	0.21	27,27,27,27	0
57	MG	RA	3055	1/1	0.79	0.25	15,15,15,15	0
57	MG	RA	3274	1/1	0.79	0.49	46,46,46,46	0
57	MG	YA	3297	1/1	0.80	0.53	61,61,61,61	0
57	MG	RA	3011	1/1	0.80	0.33	46,46,46,46	0
57	MG	RA	3179	1/1	0.80	0.49	47,47,47,47	0
57	MG	YA	3199	1/1	0.80	0.29	55,55,55,55	0
57	MG	RA	3134	1/1	0.80	0.16	27,27,27,27	0
57	MG	RA	3315	1/1	0.80	0.14	67,67,67,67	0
57	MG	RA	3214	1/1	0.80	0.25	46,46,46,46	0
57	MG	QA	1638	1/1	0.80	0.17	53,53,53,53	0
57	MG	R0	101	1/1	0.80	0.25	14,14,14,14	0
57	MG	R5	101	1/1	0.80	1.08	162,162,162,162	0
57	MG	RA	3149	1/1	0.80	0.16	41,41,41,41	0
57	MG	XA	1626	1/1	0.80	0.26	31,31,31,31	0
57	MG	RA	3291	1/1	0.80	0.34	45,45,45,45	0
57	MG	YA	3182	1/1	0.80	0.25	62,62,62,62	0
57	MG	RA	3170	1/1	0.80	0.42	35,35,35,35	0
57	MG	RA	3091	1/1	0.80	0.30	39,39,39,39	0
57	MG	RA	3191	1/1	0.81	0.22	49,49,49,49	0
57	MG	YA	3342	1/1	0.81	0.29	56,56,56,56	0
57	MG	RA	3044	1/1	0.81	0.41	65,65,65,65	0
57	MG	RA	3228	1/1	0.81	0.34	23,23,23,23	0
57	MG	RA	3312	1/1	0.81	0.27	55,55,55,55	0
57	MG	RA	3163	1/1	0.81	0.38	27,27,27,27	0
57	MG	YU	201	1/1	0.81	0.34	62,62,62,62	0
57	MG	XA	1646	1/1	0.81	0.17	72,72,72,72	0
57	MG	Y0	102	1/1	0.81	0.63	45,45,45,45	0
57	MG	YA	3205	1/1	0.81	0.35	73,73,73,73	0
57	MG	YA	3310	1/1	0.82	0.56	42,42,42,42	0
57	MG	RA	3233	1/1	0.82	0.40	46,46,46,46	0
57	MG	YA	3316	1/1	0.82	0.34	30,30,30,30	0
57	MG	YE	302	1/1	0.82	0.30	49,49,49,49	0
57	MG	RA	3322	1/1	0.82	0.53	40,40,40,40	0
57	MG	YP	202	1/1	0.82	0.19	52,52,52,52	0
57	MG	YA	3329	1/1	0.82	0.46	56,56,56,56	0
57	MG	RA	3200	1/1	0.82	0.46	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3220	1/1	0.82	0.45	75,75,75,75	0
57	MG	YA	3230	1/1	0.82	0.35	43,43,43,43	0
57	MG	YA	3288	1/1	0.82	0.53	58,58,58,58	0
57	MG	RA	3167	1/1	0.83	0.67	57,57,57,57	0
57	MG	YA	3336	1/1	0.83	0.23	60,60,60,60	0
57	MG	QA	1666	1/1	0.83	0.22	50,50,50,50	0
57	MG	YA	3201	1/1	0.83	0.20	63,63,63,63	0
57	MG	YA	3158	1/1	0.83	0.44	76,76,76,76	0
57	MG	YA	3207	1/1	0.83	0.28	25,25,25,25	0
57	MG	RA	3174	1/1	0.83	0.25	19,19,19,19	0
57	MG	YA	3055	1/1	0.83	0.54	52,52,52,52	0
57	MG	RA	3260	1/1	0.83	0.23	45,45,45,45	0
57	MG	YA	3303	1/1	0.83	1.31	63,63,63,63	0
57	MG	RA	3281	1/1	0.83	0.45	53,53,53,53	0
57	MG	RA	3289	1/1	0.83	0.37	26,26,26,26	0
57	MG	YA	3135	1/1	0.83	0.20	43,43,43,43	0
57	MG	YA	3136	1/1	0.83	0.55	30,30,30,30	0
57	MG	YA	3137	1/1	0.83	0.74	51,51,51,51	0
57	MG	RA	3185	1/1	0.83	0.45	60,60,60,60	0
57	MG	YA	3284	1/1	0.84	0.35	59,59,59,59	0
57	MG	YA	3080	1/1	0.84	0.23	17,17,17,17	0
57	MG	YA	3291	1/1	0.84	0.42	71,71,71,71	0
57	MG	RB	202	1/1	0.84	0.16	69,69,69,69	0
57	MG	YA	3294	1/1	0.84	0.14	62,62,62,62	0
57	MG	QA	1663	1/1	0.84	0.36	55,55,55,55	0
57	MG	YA	3349	1/1	0.84	0.41	46,46,46,46	0
57	MG	YA	3352	1/1	0.84	0.43	47,47,47,47	0
57	MG	YA	3133	1/1	0.84	0.24	71,71,71,71	0
57	MG	YA	3354	1/1	0.84	0.49	50,50,50,50	0
57	MG	RA	3262	1/1	0.84	0.29	99,99,99,99	0
57	MG	RA	3285	1/1	0.84	0.32	58,58,58,58	0
57	MG	RA	3124	1/1	0.84	0.40	33,33,33,33	0
57	MG	RA	3068	1/1	0.84	0.20	47,47,47,47	0
57	MG	XA	1664	1/1	0.84	0.51	38,38,38,38	0
57	MG	YA	3262	1/1	0.84	0.35	40,40,40,40	0
57	MG	QA	1677	1/1	0.84	0.32	29,29,29,29	0
57	MG	RA	3182	1/1	0.84	0.27	48,48,48,48	0
57	MG	YA	3072	1/1	0.84	0.18	27,27,27,27	0
57	MG	YA	3332	1/1	0.85	0.58	57,57,57,57	0
57	MG	XA	1704	1/1	0.85	0.30	44,44,44,44	0
57	MG	RA	3009	1/1	0.85	0.54	52,52,52,52	0
57	MG	RA	3267	1/1	0.85	0.23	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3140	1/1	0.85	0.29	25,25,25,25	0
57	MG	XA	1627	1/1	0.85	0.19	98,98,98,98	0
57	MG	YA	3203	1/1	0.85	0.66	51,51,51,51	0
57	MG	QA	1622	1/1	0.85	0.30	70,70,70,70	0
57	MG	YA	3162	1/1	0.85	0.14	70,70,70,70	0
57	MG	YA	3165	1/1	0.85	0.09	59,59,59,59	0
57	MG	XA	1635	1/1	0.85	0.45	58,58,58,58	0
57	MG	YA	3215	1/1	0.85	0.32	47,47,47,47	0
57	MG	YA	3073	1/1	0.85	0.60	38,38,38,38	0
57	MG	XA	1680	1/1	0.85	0.29	65,65,65,65	0
57	MG	RA	3299	1/1	0.85	0.36	53,53,53,53	0
57	MG	YA	3179	1/1	0.85	0.32	50,50,50,50	0
57	MG	YA	3234	1/1	0.85	0.56	25,25,25,25	0
57	MG	RA	3026	1/1	0.85	0.28	11,11,11,11	0
57	MG	QA	1643	1/1	0.85	0.27	23,23,23,23	0
57	MG	Y0	103	1/1	0.85	0.44	46,46,46,46	0
57	MG	RA	3192	1/1	0.85	0.27	31,31,31,31	0
57	MG	RA	3155	1/1	0.86	0.54	43,43,43,43	0
57	MG	RA	3301	1/1	0.86	0.31	48,48,48,48	0
57	MG	YA	3210	1/1	0.86	0.41	40,40,40,40	0
57	MG	RA	3100	1/1	0.86	0.29	28,28,28,28	0
57	MG	XA	1629	1/1	0.86	0.18	63,63,63,63	0
57	MG	YA	3149	1/1	0.86	0.22	27,27,27,27	0
57	MG	QA	1641	1/1	0.86	0.25	59,59,59,59	0
57	MG	RA	3114	1/1	0.86	0.39	21,21,21,21	0
57	MG	QA	1625	1/1	0.86	0.14	22,22,22,22	0
57	MG	QA	1679	1/1	0.86	0.33	52,52,52,52	0
57	MG	YA	3245	1/1	0.86	0.34	36,36,36,36	0
57	MG	YA	3031	1/1	0.86	0.51	36,36,36,36	0
57	MG	RA	3314	1/1	0.86	0.34	59,59,59,59	0
57	MG	RA	3277	1/1	0.86	0.59	59,59,59,59	0
57	MG	YA	3274	1/1	0.86	0.35	60,60,60,60	0
57	MG	QA	1670	1/1	0.86	0.35	37,37,37,37	0
57	MG	RA	3075	1/1	0.86	0.15	58,58,58,58	0
57	MG	RA	3250	1/1	0.86	0.32	57,57,57,57	0
57	MG	YA	3109	1/1	0.86	0.17	42,42,42,42	0
57	MG	RB	205	1/1	0.86	0.30	61,61,61,61	0
57	MG	RA	3142	1/1	0.86	0.34	48,48,48,48	0
57	MG	YA	3122	1/1	0.86	0.15	26,26,26,26	0
57	MG	YA	3293	1/1	0.86	0.77	60,60,60,60	0
57	MG	YA	3127	1/1	0.86	0.12	54,54,54,54	0
57	MG	YA	3128	1/1	0.86	0.11	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3131	1/1	0.86	0.21	39,39,39,39	0
57	MG	RA	3207	1/1	0.86	0.19	45,45,45,45	0
57	MG	QM	201	1/1	0.86	0.19	104,104,104,104	0
57	MG	YA	3114	1/1	0.87	0.23	39,39,39,39	0
57	MG	YA	3313	1/1	0.87	0.30	24,24,24,24	0
57	MG	QA	1634	1/1	0.87	0.28	58,58,58,58	0
57	MG	RA	3069	1/1	0.87	0.13	39,39,39,39	0
57	MG	RA	3219	1/1	0.87	0.27	58,58,58,58	0
57	MG	RA	3158	1/1	0.87	0.25	26,26,26,26	0
57	MG	YA	3129	1/1	0.87	0.27	50,50,50,50	0
57	MG	YA	3190	1/1	0.87	0.28	27,27,27,27	0
57	MG	YA	3268	1/1	0.87	0.28	52,52,52,52	0
57	MG	YA	3273	1/1	0.87	0.88	32,32,32,32	0
57	MG	RA	3159	1/1	0.87	0.35	30,30,30,30	0
57	MG	RA	3266	1/1	0.87	1.44	53,53,53,53	0
57	MG	RA	3294	1/1	0.87	0.22	39,39,39,39	0
57	MG	YA	3279	1/1	0.87	0.53	57,57,57,57	0
57	MG	RA	3178	1/1	0.87	0.36	33,33,33,33	0
57	MG	RA	3326	1/1	0.87	0.99	57,57,57,57	0
57	MG	RA	3229	1/1	0.87	0.35	37,37,37,37	0
57	MG	YA	3202	1/1	0.87	0.20	32,32,32,32	0
57	MG	YA	3356	1/1	0.87	0.54	61,61,61,61	0
57	MG	RA	3300	1/1	0.87	0.25	47,47,47,47	0
57	MG	YA	3147	1/1	0.87	0.50	34,34,34,34	0
57	MG	YA	3148	1/1	0.87	0.44	39,39,39,39	0
57	MG	QA	1680	1/1	0.87	0.58	53,53,53,53	0
57	MG	RA	3302	1/1	0.87	0.46	37,37,37,37	0
57	MG	RA	3010	1/1	0.87	0.31	39,39,39,39	0
57	MG	YA	3100	1/1	0.87	0.10	59,59,59,59	0
57	MG	XA	1618	1/1	0.87	0.22	37,37,37,37	0
57	MG	RA	3305	1/1	0.87	0.40	48,48,48,48	0
57	MG	YA	3059	1/1	0.88	0.20	12,12,12,12	0
57	MG	YA	3183	1/1	0.88	0.17	47,47,47,47	0
57	MG	RA	3273	1/1	0.88	0.58	30,30,30,30	0
57	MG	RA	3321	1/1	0.88	0.48	32,32,32,32	0
57	MG	YA	3192	1/1	0.88	0.23	48,48,48,48	0
57	MG	YA	3322	1/1	0.88	0.21	39,39,39,39	0
57	MG	YA	3326	1/1	0.88	0.40	34,34,34,34	0
57	MG	YA	3327	1/1	0.88	0.52	51,51,51,51	0
57	MG	XA	1628	1/1	0.88	0.48	36,36,36,36	0
57	MG	YA	3140	1/1	0.88	0.42	50,50,50,50	0
57	MG	YA	3270	1/1	0.88	0.51	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3335	1/1	0.88	0.36	59,59,59,59	0
57	MG	QA	1662	1/1	0.88	0.19	48,48,48,48	0
57	MG	RA	3204	1/1	0.88	0.16	47,47,47,47	0
57	MG	YA	3102	1/1	0.88	0.16	20,20,20,20	0
57	MG	RA	3181	1/1	0.88	0.33	29,29,29,29	0
57	MG	QA	1630	1/1	0.88	0.16	24,24,24,24	0
57	MG	YA	3347	1/1	0.88	0.20	57,57,57,57	0
57	MG	YA	3282	1/1	0.88	0.23	43,43,43,43	0
57	MG	XA	1638	1/1	0.88	0.32	39,39,39,39	0
57	MG	QA	1617	1/1	0.88	0.28	38,38,38,38	0
57	MG	QA	1639	1/1	0.88	0.23	67,67,67,67	0
57	MG	YA	3126	1/1	0.88	0.17	17,17,17,17	0
57	MG	RA	3290	1/1	0.88	0.35	44,44,44,44	0
57	MG	YA	3214	1/1	0.88	0.28	89,89,89,89	0
57	MG	RA	3232	1/1	0.88	0.43	36,36,36,36	0
57	MG	RA	3130	1/1	0.88	0.96	59,59,59,59	0
57	MG	YA	3219	1/1	0.88	0.52	83,83,83,83	0
57	MG	YA	3222	1/1	0.88	0.20	60,60,60,60	0
57	MG	YA	3301	1/1	0.88	0.64	48,48,48,48	0
57	MG	YA	3225	1/1	0.88	0.45	56,56,56,56	0
57	MG	YA	3045	1/1	0.88	0.30	9,9,9,9	0
57	MG	RA	3217	1/1	0.88	0.23	46,46,46,46	0
57	MG	YA	3198	1/1	0.89	0.49	62,62,62,62	0
57	MG	RA	3269	1/1	0.89	0.27	67,67,67,67	0
57	MG	XA	1676	1/1	0.89	0.22	41,41,41,41	0
57	MG	RA	3151	1/1	0.89	0.36	37,37,37,37	0
57	MG	YA	3082	1/1	0.89	0.37	51,51,51,51	0
57	MG	YA	3151	1/1	0.89	0.58	69,69,69,69	0
57	MG	QA	1660	1/1	0.89	0.41	31,31,31,31	0
57	MG	XA	1681	1/1	0.89	0.45	21,21,21,21	0
57	MG	YA	3161	1/1	0.89	0.50	51,51,51,51	0
57	MG	RA	3254	1/1	0.89	0.19	27,27,27,27	0
57	MG	QA	1604	1/1	0.89	0.60	47,47,47,47	0
57	MG	QA	1648	1/1	0.89	0.23	71,71,71,71	0
57	MG	RA	3278	1/1	0.89	0.23	34,34,34,34	0
57	MG	XA	1698	1/1	0.89	0.79	76,76,76,76	0
57	MG	RA	3160	1/1	0.89	0.23	82,82,82,82	0
57	MG	RA	3118	1/1	0.89	0.27	62,62,62,62	0
57	MG	RA	3265	1/1	0.89	0.45	58,58,58,58	0
57	MG	XA	1707	1/1	0.89	0.80	50,50,50,50	0
57	MG	XA	1612	1/1	0.89	0.15	68,68,68,68	0
57	MG	YA	3188	1/1	0.89	0.46	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	XX	101	1/1	0.89	0.47	57,57,57,57	0
57	MG	XA	1656	1/1	0.89	0.25	56,56,56,56	0
57	MG	QA	1669	1/1	0.89	0.34	59,59,59,59	0
57	MG	RA	3129	1/1	0.89	0.25	42,42,42,42	0
57	MG	YA	3319	1/1	0.89	0.38	45,45,45,45	0
57	MG	RA	3268	1/1	0.89	0.39	45,45,45,45	0
57	MG	Y7	101	1/1	0.89	0.24	33,33,33,33	0
57	MG	XA	1671	1/1	0.89	0.53	39,39,39,39	0
57	MG	RA	3297	1/1	0.90	0.57	48,48,48,48	0
57	MG	YA	3139	1/1	0.90	0.20	76,76,76,76	0
57	MG	YA	3070	1/1	0.90	0.25	29,29,29,29	0
57	MG	RA	3109	1/1	0.90	0.44	34,34,34,34	0
57	MG	RA	3320	1/1	0.90	0.43	62,62,62,62	0
57	MG	YA	3328	1/1	0.90	0.36	49,49,49,49	0
57	MG	QA	1611	1/1	0.90	0.46	21,21,21,21	0
57	MG	RA	3240	1/1	0.90	0.64	17,17,17,17	0
57	MG	RA	3164	1/1	0.90	0.25	45,45,45,45	0
57	MG	RA	3198	1/1	0.90	0.64	49,49,49,49	0
57	MG	RA	3252	1/1	0.90	0.28	47,47,47,47	0
57	MG	YA	3280	1/1	0.90	0.42	25,25,25,25	0
57	MG	RB	204	1/1	0.90	0.28	51,51,51,51	0
57	MG	XA	1700	1/1	0.90	0.57	50,50,50,50	0
57	MG	RA	3304	1/1	0.90	0.20	44,44,44,44	0
57	MG	RA	3288	1/1	0.90	0.28	49,49,49,49	0
57	MG	RA	3307	1/1	0.90	0.38	38,38,38,38	0
57	MG	RA	3186	1/1	0.90	0.25	28,28,28,28	0
57	MG	XA	1604	1/1	0.90	0.43	44,44,44,44	0
57	MG	QA	1647	1/1	0.90	0.34	35,35,35,35	0
57	MG	YA	3180	1/1	0.90	0.21	52,52,52,52	0
57	MG	YA	3224	1/1	0.90	0.34	41,41,41,41	0
57	MG	YA	3006	1/1	0.90	0.28	22,22,22,22	0
57	MG	YA	3132	1/1	0.90	0.26	37,37,37,37	0
57	MG	QA	1618	1/1	0.90	0.29	58,58,58,58	0
57	MG	YA	3228	1/1	0.90	0.91	57,57,57,57	0
57	MG	XA	1665	1/1	0.90	0.57	35,35,35,35	0
57	MG	XA	1619	1/1	0.90	0.60	40,40,40,40	0
57	MG	YA	3312	1/1	0.90	0.16	26,26,26,26	0
57	MG	YA	3238	1/1	0.90	0.40	28,28,28,28	0
57	MG	YA	3240	1/1	0.90	0.67	43,43,43,43	0
57	MG	RA	3261	1/1	0.90	0.30	56,56,56,56	0
57	MG	XA	1701	1/1	0.91	0.23	47,47,47,47	0
57	MG	RA	3084	1/1	0.91	0.41	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3152	1/1	0.91	0.12	54,54,54,54	0
57	MG	RA	3154	1/1	0.91	0.11	26,26,26,26	0
57	MG	RA	3002	1/1	0.91	0.26	47,47,47,47	0
57	MG	XA	1708	1/1	0.91	0.28	33,33,33,33	0
57	MG	RA	3003	1/1	0.91	0.56	42,42,42,42	0
57	MG	XV	101	1/1	0.91	0.25	34,34,34,34	0
57	MG	XA	1644	1/1	0.91	0.41	42,42,42,42	0
57	MG	YA	3141	1/1	0.91	0.39	48,48,48,48	0
57	MG	YA	3143	1/1	0.91	0.23	9,9,9,9	0
57	MG	RA	3102	1/1	0.91	0.14	38,38,38,38	0
57	MG	YA	3019	1/1	0.91	0.49	29,29,29,29	0
57	MG	YA	3317	1/1	0.91	0.50	38,38,38,38	0
57	MG	YA	3021	1/1	0.91	0.53	24,24,24,24	0
57	MG	RA	3132	1/1	0.91	0.13	52,52,52,52	0
57	MG	RA	3216	1/1	0.91	0.27	51,51,51,51	0
57	MG	RA	3103	1/1	0.91	0.15	25,25,25,25	0
57	MG	YA	3156	1/1	0.91	0.30	67,67,67,67	0
57	MG	YA	3229	1/1	0.91	0.40	19,19,19,19	0
57	MG	RA	3135	1/1	0.91	0.19	64,64,64,64	0
57	MG	YA	3330	1/1	0.91	0.36	45,45,45,45	0
57	MG	XA	1660	1/1	0.91	0.93	53,53,53,53	0
57	MG	RA	3042	1/1	0.91	0.33	9,9,9,9	0
57	MG	YA	3163	1/1	0.91	0.40	39,39,39,39	0
57	MG	YA	3244	1/1	0.91	0.34	33,33,33,33	0
57	MG	RA	3194	1/1	0.91	0.16	43,43,43,43	0
57	MG	RA	3225	1/1	0.91	0.55	46,46,46,46	0
57	MG	XA	1667	1/1	0.91	0.50	23,23,23,23	0
57	MG	YA	3340	1/1	0.91	0.63	55,55,55,55	0
57	MG	YA	3261	1/1	0.91	0.23	43,43,43,43	0
57	MG	QA	1659	1/1	0.91	0.51	40,40,40,40	0
57	MG	YA	3265	1/1	0.91	0.60	65,65,65,65	0
57	MG	YA	3086	1/1	0.91	0.30	51,51,51,51	0
57	MG	YA	3096	1/1	0.91	0.51	26,26,26,26	0
57	MG	XA	1606	1/1	0.91	0.40	40,40,40,40	0
57	MG	RA	3172	1/1	0.91	0.29	34,34,34,34	0
57	MG	RA	3199	1/1	0.91	0.92	44,44,44,44	0
57	MG	YB	203	1/1	0.91	0.30	37,37,37,37	0
57	MG	RA	3306	1/1	0.91	0.33	47,47,47,47	0
57	MG	QA	1626	1/1	0.91	0.20	65,65,65,65	0
57	MG	XA	1625	1/1	0.91	0.12	32,32,32,32	0
57	MG	YA	3119	1/1	0.91	0.24	42,42,42,42	0
57	MG	YA	3121	1/1	0.91	0.24	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3143	1/1	0.91	0.45	19,19,19,19	0
57	MG	RA	3234	1/1	0.91	0.48	16,16,16,16	0
57	MG	RA	3116	1/1	0.91	0.23	50,50,50,50	0
57	MG	RA	3244	1/1	0.91	0.17	47,47,47,47	0
58	PAR	QA	1681	42/42	0.91	0.27	71,71,72,72	0
57	MG	XA	1631	1/1	0.91	0.25	63,63,63,63	0
57	MG	XA	1696	1/1	0.92	0.78	65,65,65,65	0
57	MG	RA	3127	1/1	0.92	0.15	24,24,24,24	0
57	MG	RA	3153	1/1	0.92	0.25	34,34,34,34	0
57	MG	XA	1634	1/1	0.92	0.41	38,38,38,38	0
57	MG	RA	3205	1/1	0.92	0.29	59,59,59,59	0
57	MG	RA	3093	1/1	0.92	0.38	18,18,18,18	0
57	MG	YA	3300	1/1	0.92	0.17	45,45,45,45	0
57	MG	QA	1635	1/1	0.92	0.32	58,58,58,58	0
57	MG	RA	3323	1/1	0.92	0.67	39,39,39,39	0
57	MG	RA	3324	1/1	0.92	0.40	38,38,38,38	0
57	MG	YA	3305	1/1	0.92	0.49	53,53,53,53	0
57	MG	RA	3210	1/1	0.92	0.15	68,68,68,68	0
57	MG	XA	1647	1/1	0.92	0.21	82,82,82,82	0
57	MG	YA	3311	1/1	0.92	0.58	69,69,69,69	0
57	MG	RA	3183	1/1	0.92	0.13	37,37,37,37	0
57	MG	YA	3002	1/1	0.92	0.20	22,22,22,22	0
57	MG	RA	3001	1/1	0.92	0.23	27,27,27,27	0
57	MG	XA	1653	1/1	0.92	0.19	42,42,42,42	0
57	MG	YA	3020	1/1	0.92	0.43	16,16,16,16	0
57	MG	YA	3217	1/1	0.92	0.15	45,45,45,45	0
57	MG	YA	3142	1/1	0.92	0.60	58,58,58,58	0
57	MG	RB	203	1/1	0.92	0.25	47,47,47,47	0
57	MG	YA	3324	1/1	0.92	0.37	40,40,40,40	0
57	MG	YA	3025	1/1	0.92	0.41	23,23,23,23	0
57	MG	YA	3029	1/1	0.92	0.28	17,17,17,17	0
57	MG	RA	3296	1/1	0.92	0.30	45,45,45,45	0
57	MG	RA	3012	1/1	0.92	0.60	27,27,27,27	0
57	MG	YA	3049	1/1	0.92	0.32	15,15,15,15	0
57	MG	YA	3054	1/1	0.92	0.45	23,23,23,23	0
57	MG	YA	3155	1/1	0.92	0.27	37,37,37,37	0
57	MG	RA	3187	1/1	0.92	0.22	68,68,68,68	0
57	MG	RA	3263	1/1	0.92	0.47	33,33,33,33	0
57	MG	RA	3015	1/1	0.92	0.12	16,16,16,16	0
57	MG	RA	3136	1/1	0.92	0.39	15,15,15,15	0
57	MG	QE	201	1/1	0.92	0.71	59,59,59,59	0
57	MG	YA	3164	1/1	0.92	0.23	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3258	1/1	0.92	0.54	52,52,52,52	0
57	MG	YA	3343	1/1	0.92	0.27	46,46,46,46	0
57	MG	YA	3344	1/1	0.92	0.28	55,55,55,55	0
57	MG	XA	1672	1/1	0.92	0.35	36,36,36,36	0
57	MG	RA	3166	1/1	0.92	0.36	36,36,36,36	0
57	MG	YA	3170	1/1	0.92	0.24	54,54,54,54	0
57	MG	YA	3172	1/1	0.92	0.44	52,52,52,52	0
57	MG	YA	3267	1/1	0.92	0.28	42,42,42,42	0
57	MG	YA	3173	1/1	0.92	0.61	43,43,43,43	0
57	MG	RA	3139	1/1	0.92	0.30	26,26,26,26	0
57	MG	RA	3168	1/1	0.92	0.20	26,26,26,26	0
57	MG	QA	1665	1/1	0.92	0.26	55,55,55,55	0
57	MG	YA	3099	1/1	0.92	0.43	19,19,19,19	0
57	MG	RA	3078	1/1	0.92	0.25	7,7,7,7	0
57	MG	QA	1619	1/1	0.92	0.21	40,40,40,40	0
57	MG	YA	3103	1/1	0.92	0.39	36,36,36,36	0
57	MG	RA	3050	1/1	0.92	0.41	14,14,14,14	0
57	MG	XA	1690	1/1	0.92	0.61	50,50,50,50	0
57	MG	XA	1692	1/1	0.92	0.29	58,58,58,58	0
57	MG	YA	3287	1/1	0.92	0.29	44,44,44,44	0
57	MG	RA	3125	1/1	0.92	0.29	54,54,54,54	0
57	MG	RA	3239	1/1	0.92	0.30	7,7,7,7	0
57	MG	YA	3125	1/1	0.93	0.20	54,54,54,54	0
57	MG	YA	3296	1/1	0.93	0.54	48,48,48,48	0
57	MG	RA	3072	1/1	0.93	0.51	52,52,52,52	0
57	MG	RA	3258	1/1	0.93	0.40	48,48,48,48	0
57	MG	RA	3184	1/1	0.93	0.13	49,49,49,49	0
57	MG	RA	3157	1/1	0.93	0.38	42,42,42,42	0
57	MG	YA	3130	1/1	0.93	0.39	42,42,42,42	0
57	MG	XA	1652	1/1	0.93	0.34	72,72,72,72	0
57	MG	QA	1672	1/1	0.93	0.35	41,41,41,41	0
57	MG	YA	3306	1/1	0.93	0.44	50,50,50,50	0
57	MG	XA	1655	1/1	0.93	0.50	53,53,53,53	0
57	MG	RA	3027	1/1	0.93	0.41	27,27,27,27	0
57	MG	YA	3005	1/1	0.93	0.21	23,23,23,23	0
57	MG	QA	1644	1/1	0.93	0.55	54,54,54,54	0
57	MG	YA	3008	1/1	0.93	0.45	33,33,33,33	0
57	MG	YA	3016	1/1	0.93	0.30	6,6,6,6	0
57	MG	RA	3005	1/1	0.93	0.27	26,26,26,26	0
57	MG	RA	3045	1/1	0.93	0.28	5,5,5,5	0
57	MG	XA	1605	1/1	0.93	0.60	34,34,34,34	0
57	MG	YA	3223	1/1	0.93	0.22	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3165	1/1	0.93	0.06	36,36,36,36	0
57	MG	RA	3193	1/1	0.93	0.23	46,46,46,46	0
57	MG	XA	1670	1/1	0.93	0.47	37,37,37,37	0
57	MG	YA	3035	1/1	0.93	0.55	27,27,27,27	0
57	MG	RA	3008	1/1	0.93	0.55	12,12,12,12	0
57	MG	RA	3196	1/1	0.93	0.36	56,56,56,56	0
57	MG	XA	1622	1/1	0.93	0.59	33,33,33,33	0
57	MG	QA	1645	1/1	0.93	0.19	73,73,73,73	0
57	MG	RA	3309	1/1	0.93	0.51	54,54,54,54	0
57	MG	RA	3310	1/1	0.93	0.17	39,39,39,39	0
57	MG	RA	3057	1/1	0.93	0.29	48,48,48,48	0
57	MG	XA	1683	1/1	0.93	0.11	48,48,48,48	0
57	MG	RA	3108	1/1	0.93	0.17	32,32,32,32	0
57	MG	YA	3077	1/1	0.93	0.34	21,21,21,21	0
57	MG	QV	101	1/1	0.93	0.35	50,50,50,50	0
57	MG	XA	1689	1/1	0.93	0.63	51,51,51,51	0
57	MG	YA	3168	1/1	0.93	0.45	25,25,25,25	0
57	MG	QX	101	1/1	0.93	0.11	66,66,66,66	0
57	MG	YA	3171	1/1	0.93	0.66	85,85,85,85	0
57	MG	YA	3087	1/1	0.93	0.38	31,31,31,31	0
57	MG	YA	3095	1/1	0.93	0.24	42,42,42,42	0
57	MG	XA	1691	1/1	0.93	0.11	105,105,105,105	0
57	MG	QA	1642	1/1	0.93	0.21	62,62,62,62	0
57	MG	XA	1693	1/1	0.93	0.43	40,40,40,40	0
57	MG	XA	1633	1/1	0.93	0.77	47,47,47,47	0
57	MG	QA	1601	1/1	0.93	0.15	31,31,31,31	0
57	MG	RA	3070	1/1	0.93	0.35	9,9,9,9	0
57	MG	YA	3111	1/1	0.93	0.19	26,26,26,26	0
57	MG	XA	1697	1/1	0.93	0.41	47,47,47,47	0
57	MG	YP	203	1/1	0.93	0.33	32,32,32,32	0
57	MG	YA	3187	1/1	0.93	0.14	87,87,87,87	0
57	MG	YA	3286	1/1	0.93	1.02	67,67,67,67	0
57	MG	RA	3120	1/1	0.93	0.54	50,50,50,50	0
57	MG	YA	3116	1/1	0.93	0.39	40,40,40,40	0
57	MG	XA	1699	1/1	0.93	0.44	35,35,35,35	0
57	MG	RA	3122	1/1	0.93	0.16	24,24,24,24	0
57	MG	RA	3253	1/1	0.93	0.34	29,29,29,29	0
57	MG	RA	3071	1/1	0.93	0.26	32,32,32,32	0
57	MG	XA	1607	1/1	0.94	0.43	29,29,29,29	0
57	MG	YA	3017	1/1	0.94	0.09	6,6,6,6	0
57	MG	YA	3289	1/1	0.94	0.95	69,69,69,69	0
57	MG	XA	1609	1/1	0.94	0.32	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3101	1/1	0.94	0.20	32,32,32,32	0
57	MG	RA	3236	1/1	0.94	0.63	71,71,71,71	0
57	MG	RA	3206	1/1	0.94	0.15	51,51,51,51	0
57	MG	RA	3272	1/1	0.94	0.61	44,44,44,44	0
57	MG	RA	3123	1/1	0.94	0.20	74,74,74,74	0
57	MG	YA	3204	1/1	0.94	0.20	75,75,75,75	0
57	MG	QA	1646	1/1	0.94	0.32	61,61,61,61	0
57	MG	YA	3206	1/1	0.94	0.41	70,70,70,70	0
57	MG	YA	3040	1/1	0.94	0.18	8,8,8,8	0
57	MG	RA	3276	1/1	0.94	0.34	44,44,44,44	0
57	MG	YA	3209	1/1	0.94	0.63	28,28,28,28	0
57	MG	RA	3247	1/1	0.94	0.18	55,55,55,55	0
57	MG	XA	1682	1/1	0.94	0.35	60,60,60,60	0
57	MG	YA	3212	1/1	0.94	0.20	32,32,32,32	0
57	MG	RA	3249	1/1	0.94	0.41	41,41,41,41	0
57	MG	YA	3056	1/1	0.94	0.27	11,11,11,11	0
57	MG	QX	102	1/1	0.94	0.20	43,43,43,43	0
57	MG	QA	1657	1/1	0.94	0.27	29,29,29,29	0
57	MG	YA	3314	1/1	0.94	0.44	37,37,37,37	0
57	MG	YA	3218	1/1	0.94	0.28	25,25,25,25	0
57	MG	RA	3282	1/1	0.94	0.33	39,39,39,39	0
57	MG	RA	3319	1/1	0.94	0.28	32,32,32,32	0
57	MG	YA	3318	1/1	0.94	0.31	34,34,34,34	0
57	MG	RA	3283	1/1	0.94	0.46	65,65,65,65	0
57	MG	RA	3284	1/1	0.94	0.53	32,32,32,32	0
57	MG	YA	3078	1/1	0.94	0.53	15,15,15,15	0
57	MG	YA	3157	1/1	0.94	0.47	51,51,51,51	0
57	MG	YA	3325	1/1	0.94	0.50	42,42,42,42	0
57	MG	RA	3171	1/1	0.94	0.23	57,57,57,57	0
57	MG	YA	3159	1/1	0.94	0.15	44,44,44,44	0
57	MG	YA	3160	1/1	0.94	0.17	18,18,18,18	0
57	MG	XA	1637	1/1	0.94	0.13	74,74,74,74	0
57	MG	RA	3286	1/1	0.94	0.62	57,57,57,57	0
57	MG	YA	3237	1/1	0.94	0.24	26,26,26,26	0
57	MG	RA	3128	1/1	0.94	0.25	60,60,60,60	0
57	MG	QA	1628	1/1	0.94	0.20	64,64,64,64	0
57	MG	XA	1645	1/1	0.94	0.31	31,31,31,31	0
57	MG	RA	3195	1/1	0.94	0.25	15,15,15,15	0
57	MG	YA	3250	1/1	0.94	0.18	27,27,27,27	0
57	MG	YA	3252	1/1	0.94	0.49	27,27,27,27	0
57	MG	RA	3110	1/1	0.94	0.48	54,54,54,54	0
57	MG	RA	3131	1/1	0.94	0.39	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	QA	1671	1/1	0.94	0.34	23,23,23,23	0
57	MG	XA	1650	1/1	0.94	0.28	54,54,54,54	0
57	MG	RA	3224	1/1	0.94	0.19	28,28,28,28	0
57	MG	RE	302	1/1	0.94	0.32	20,20,20,20	0
57	MG	YA	3266	1/1	0.94	0.53	65,65,65,65	0
57	MG	QA	1623	1/1	0.94	0.31	54,54,54,54	0
57	MG	YA	3115	1/1	0.94	0.45	23,23,23,23	0
57	MG	XB	301	1/1	0.94	0.18	51,51,51,51	0
57	MG	YA	3272	1/1	0.94	0.41	32,32,32,32	0
57	MG	RA	3115	1/1	0.94	0.20	12,12,12,12	0
57	MG	XA	1657	1/1	0.94	0.63	49,49,49,49	0
57	MG	QA	1650	1/1	0.94	0.37	41,41,41,41	0
57	MG	YA	3276	1/1	0.94	0.68	43,43,43,43	0
57	MG	RA	3161	1/1	0.94	0.42	55,55,55,55	0
57	MG	YA	3278	1/1	0.94	0.44	50,50,50,50	0
57	MG	YA	3185	1/1	0.94	0.48	37,37,37,37	0
57	MG	YA	3123	1/1	0.94	0.70	46,46,46,46	0
57	MG	YA	3281	1/1	0.94	0.31	33,33,33,33	0
57	MG	XA	1661	1/1	0.94	0.39	44,44,44,44	0
57	MG	Y3	101	1/1	0.94	0.30	28,28,28,28	0
57	MG	RA	3029	1/1	0.94	0.30	18,18,18,18	0
57	MG	QA	1676	1/1	0.94	0.39	63,63,63,63	0
57	MG	YA	3011	1/1	0.94	0.46	30,30,30,30	0
59	ZN	QN	101	1/1	0.94	0.14	135,135,135,135	0
57	MG	QA	1620	1/1	0.95	0.20	66,66,66,66	0
57	MG	QA	1652	1/1	0.95	0.49	34,34,34,34	0
57	MG	RA	3180	1/1	0.95	0.14	28,28,28,28	0
57	MG	YA	3154	1/1	0.95	0.23	18,18,18,18	0
57	MG	XA	1702	1/1	0.95	0.31	43,43,43,43	0
57	MG	YA	3079	1/1	0.95	0.50	21,21,21,21	0
57	MG	RA	3049	1/1	0.95	0.17	7,7,7,7	0
57	MG	YA	3221	1/1	0.95	0.27	37,37,37,37	0
57	MG	YA	3304	1/1	0.95	0.54	42,42,42,42	0
57	MG	RA	3275	1/1	0.95	0.65	59,59,59,59	0
57	MG	RA	3243	1/1	0.95	0.19	84,84,84,84	0
57	MG	YA	3307	1/1	0.95	0.23	12,12,12,12	0
57	MG	RA	3077	1/1	0.95	0.27	5,5,5,5	0
57	MG	YA	3309	1/1	0.95	0.37	37,37,37,37	0
57	MG	YA	3088	1/1	0.95	0.42	56,56,56,56	0
57	MG	YA	3092	1/1	0.95	0.28	45,45,45,45	0
57	MG	XA	1663	1/1	0.95	0.28	26,26,26,26	0
57	MG	RA	3014	1/1	0.95	0.38	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3097	1/1	0.95	0.38	30,30,30,30	0
57	MG	XD	302	1/1	0.95	0.26	82,82,82,82	0
57	MG	YA	3167	1/1	0.95	0.38	43,43,43,43	0
57	MG	YA	3235	1/1	0.95	0.46	16,16,16,16	0
57	MG	RA	3279	1/1	0.95	0.90	40,40,40,40	0
57	MG	YA	3169	1/1	0.95	0.12	49,49,49,49	0
57	MG	YA	3239	1/1	0.95	0.51	31,31,31,31	0
57	MG	RA	3133	1/1	0.95	0.34	45,45,45,45	0
57	MG	YA	3241	1/1	0.95	0.20	19,19,19,19	0
57	MG	XA	1668	1/1	0.95	0.53	48,48,48,48	0
57	MG	QA	1631	1/1	0.95	0.12	69,69,69,69	0
57	MG	YA	3246	1/1	0.95	0.60	38,38,38,38	0
57	MG	YA	3247	1/1	0.95	0.34	45,45,45,45	0
57	MG	YA	3004	1/1	0.95	0.30	14,14,14,14	0
57	MG	RA	3090	1/1	0.95	0.62	31,31,31,31	0
57	MG	YA	3331	1/1	0.95	0.27	51,51,51,51	0
57	MG	RA	3316	1/1	0.95	0.74	42,42,42,42	0
57	MG	YA	3007	1/1	0.95	0.16	16,16,16,16	0
57	MG	YA	3178	1/1	0.95	0.17	56,56,56,56	0
57	MG	RA	3317	1/1	0.95	0.76	51,51,51,51	0
57	MG	RA	3117	1/1	0.95	0.13	65,65,65,65	0
57	MG	YA	3263	1/1	0.95	0.34	22,22,22,22	0
57	MG	YA	3264	1/1	0.95	0.39	30,30,30,30	0
57	MG	YA	3012	1/1	0.95	0.22	6,6,6,6	0
57	MG	RA	3137	1/1	0.95	0.47	24,24,24,24	0
57	MG	XA	1678	1/1	0.95	0.22	45,45,45,45	0
57	MG	RA	3019	1/1	0.95	0.28	18,18,18,18	0
57	MG	QA	1613	1/1	0.95	0.48	40,40,40,40	0
57	MG	RA	3097	1/1	0.95	0.46	31,31,31,31	0
57	MG	YA	3350	1/1	0.95	0.24	40,40,40,40	0
57	MG	YA	3351	1/1	0.95	0.40	39,39,39,39	0
57	MG	RA	3259	1/1	0.95	0.41	50,50,50,50	0
57	MG	QA	1678	1/1	0.95	0.45	43,43,43,43	0
57	MG	QA	1612	1/1	0.95	0.45	39,39,39,39	0
57	MG	YA	3033	1/1	0.95	0.29	11,11,11,11	0
57	MG	RA	3222	1/1	0.95	0.41	4,4,4,4	0
57	MG	YB	201	1/1	0.95	0.20	46,46,46,46	0
57	MG	RA	3169	1/1	0.95	0.28	26,26,26,26	0
57	MG	YD	301	1/1	0.95	0.32	19,19,19,19	0
57	MG	YE	301	1/1	0.95	0.25	28,28,28,28	0
57	MG	RA	3144	1/1	0.95	0.34	60,60,60,60	0
57	MG	YA	3046	1/1	0.95	0.34	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3200	1/1	0.95	0.25	45,45,45,45	0
57	MG	YA	3048	1/1	0.95	0.39	18,18,18,18	0
57	MG	RA	3145	1/1	0.95	0.41	40,40,40,40	0
57	MG	YA	3050	1/1	0.95	0.43	21,21,21,21	0
57	MG	YA	3052	1/1	0.95	0.43	22,22,22,22	0
57	MG	RA	3227	1/1	0.95	0.39	27,27,27,27	0
57	MG	RF	301	1/1	0.95	0.07	62,62,62,62	0
57	MG	RA	3146	1/1	0.95	0.17	41,41,41,41	0
57	MG	Y5	101	1/1	0.95	0.21	17,17,17,17	0
57	MG	YA	3057	1/1	0.95	0.17	13,13,13,13	0
57	MG	RA	3147	1/1	0.95	0.25	27,27,27,27	0
58	PAR	XA	1710	42/42	0.95	0.24	56,56,57,57	0
57	MG	RA	3035	1/1	0.95	0.72	49,49,49,49	0
57	MG	QA	1664	1/1	0.95	0.24	30,30,30,30	0
59	ZN	XN	101	1/1	0.95	0.16	81,81,81,81	0
57	MG	YA	3285	1/1	0.96	0.16	46,46,46,46	0
57	MG	YA	3186	1/1	0.96	0.19	22,22,22,22	0
57	MG	QA	1614	1/1	0.96	0.27	30,30,30,30	0
57	MG	RA	3092	1/1	0.96	0.30	29,29,29,29	0
57	MG	RA	3175	1/1	0.96	0.25	31,31,31,31	0
57	MG	XA	1640	1/1	0.96	0.48	41,41,41,41	0
57	MG	YA	3107	1/1	0.96	0.25	45,45,45,45	0
57	MG	YA	3108	1/1	0.96	0.16	32,32,32,32	0
57	MG	QA	1653	1/1	0.96	0.41	30,30,30,30	0
57	MG	YA	3195	1/1	0.96	0.22	39,39,39,39	0
57	MG	RA	3096	1/1	0.96	0.38	5,5,5,5	0
57	MG	YA	3197	1/1	0.96	0.08	53,53,53,53	0
57	MG	QA	1654	1/1	0.96	0.34	68,68,68,68	0
57	MG	QA	1615	1/1	0.96	0.13	57,57,57,57	0
57	MG	RA	3051	1/1	0.96	0.19	22,22,22,22	0
57	MG	RA	3318	1/1	0.96	0.35	40,40,40,40	0
57	MG	RA	3052	1/1	0.96	0.33	4,4,4,4	0
57	MG	YA	3118	1/1	0.96	0.41	58,58,58,58	0
57	MG	QV	102	1/1	0.96	0.19	27,27,27,27	0
57	MG	YA	3120	1/1	0.96	0.32	14,14,14,14	0
57	MG	RA	3104	1/1	0.96	0.20	33,33,33,33	0
57	MG	RA	3013	1/1	0.96	0.27	16,16,16,16	0
57	MG	XA	1654	1/1	0.96	0.08	78,78,78,78	0
57	MG	YA	3124	1/1	0.96	0.27	38,38,38,38	0
57	MG	RA	3058	1/1	0.96	0.43	19,19,19,19	0
57	MG	QA	1674	1/1	0.96	0.09	56,56,56,56	0
57	MG	YA	3009	1/1	0.96	0.36	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	RA	3111	1/1	0.96	0.15	33,33,33,33	0
57	MG	XA	1658	1/1	0.96	0.33	30,30,30,30	0
57	MG	YA	3015	1/1	0.96	0.51	20,20,20,20	0
57	MG	RA	3230	1/1	0.96	0.36	22,22,22,22	0
57	MG	RA	3150	1/1	0.96	0.17	37,37,37,37	0
57	MG	RA	3112	1/1	0.96	0.12	58,58,58,58	0
57	MG	YA	3134	1/1	0.96	0.31	21,21,21,21	0
57	MG	RA	3060	1/1	0.96	0.37	15,15,15,15	0
57	MG	YA	3323	1/1	0.96	0.27	49,49,49,49	0
57	MG	RA	3235	1/1	0.96	0.28	18,18,18,18	0
57	MG	YA	3024	1/1	0.96	0.41	28,28,28,28	0
57	MG	RA	3061	1/1	0.96	0.33	11,11,11,11	0
57	MG	YA	3026	1/1	0.96	0.28	15,15,15,15	0
57	MG	QA	1675	1/1	0.96	0.21	36,36,36,36	0
57	MG	XA	1666	1/1	0.96	0.28	48,48,48,48	0
57	MG	RA	3287	1/1	0.96	0.36	26,26,26,26	0
57	MG	RA	3064	1/1	0.96	0.51	9,9,9,9	0
57	MG	YA	3145	1/1	0.96	0.28	23,23,23,23	0
57	MG	RA	3156	1/1	0.96	0.47	55,55,55,55	0
57	MG	YA	3334	1/1	0.96	0.23	67,67,67,67	0
57	MG	XA	1602	1/1	0.96	0.56	19,19,19,19	0
57	MG	QA	1637	1/1	0.96	0.22	44,44,44,44	0
57	MG	RA	3021	1/1	0.96	0.31	2,2,2,2	0
57	MG	RA	3292	1/1	0.96	0.23	37,37,37,37	0
57	MG	YA	3152	1/1	0.96	0.17	41,41,41,41	0
57	MG	RA	3293	1/1	0.96	0.16	58,58,58,58	0
57	MG	RA	3024	1/1	0.96	0.16	22,22,22,22	0
57	MG	XA	1679	1/1	0.96	0.57	27,27,27,27	0
57	MG	XA	1611	1/1	0.96	0.10	20,20,20,20	0
57	MG	YA	3345	1/1	0.96	0.48	67,67,67,67	0
57	MG	YA	3346	1/1	0.96	0.20	28,28,28,28	0
57	MG	RA	3295	1/1	0.96	0.42	29,29,29,29	0
57	MG	YA	3348	1/1	0.96	0.16	49,49,49,49	0
57	MG	YA	3251	1/1	0.96	0.36	44,44,44,44	0
57	MG	XA	1615	1/1	0.96	0.26	25,25,25,25	0
57	MG	YA	3255	1/1	0.96	0.28	32,32,32,32	0
57	MG	QA	1632	1/1	0.96	0.16	28,28,28,28	0
57	MG	QA	1667	1/1	0.96	0.39	38,38,38,38	0
57	MG	YA	3259	1/1	0.96	0.20	54,54,54,54	0
57	MG	YA	3066	1/1	0.96	0.13	9,9,9,9	0
57	MG	YA	3067	1/1	0.96	0.43	22,22,22,22	0
57	MG	YA	3068	1/1	0.96	0.21	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	XA	1620	1/1	0.96	0.16	52,52,52,52	0
57	MG	YB	204	1/1	0.96	0.36	27,27,27,27	0
57	MG	XA	1688	1/1	0.96	0.61	60,60,60,60	0
57	MG	QA	1649	1/1	0.96	0.07	81,81,81,81	0
57	MG	YA	3076	1/1	0.96	0.21	22,22,22,22	0
57	MG	RA	3030	1/1	0.96	0.44	15,15,15,15	0
57	MG	RA	3033	1/1	0.96	0.38	19,19,19,19	0
57	MG	RA	3255	1/1	0.96	0.35	35,35,35,35	0
57	MG	RA	3081	1/1	0.96	0.17	24,24,24,24	0
57	MG	RA	3082	1/1	0.96	0.24	39,39,39,39	0
57	MG	YA	3084	1/1	0.96	0.34	12,12,12,12	0
57	MG	Y0	101	1/1	0.96	0.24	10,10,10,10	0
57	MG	YA	3085	1/1	0.96	0.36	7,7,7,7	0
57	MG	QA	1616	1/1	0.96	0.34	35,35,35,35	0
57	MG	XA	1630	1/1	0.96	0.45	47,47,47,47	0
57	MG	RA	3085	1/1	0.96	0.29	21,21,21,21	0
57	MG	YA	3091	1/1	0.96	0.48	17,17,17,17	0
57	MG	RA	3089	1/1	0.96	0.31	18,18,18,18	0
57	MG	YA	3093	1/1	0.96	0.24	32,32,32,32	0
57	MG	RA	3006	1/1	0.96	0.55	10,10,10,10	0
57	MG	RA	3211	1/1	0.96	0.12	62,62,62,62	0
57	MG	RA	3212	1/1	0.96	0.63	46,46,46,46	0
57	MG	RA	3076	1/1	0.97	0.22	4,4,4,4	0
57	MG	YA	3042	1/1	0.97	0.45	11,11,11,11	0
57	MG	YA	3044	1/1	0.97	0.43	15,15,15,15	0
57	MG	RA	3105	1/1	0.97	0.18	19,19,19,19	0
57	MG	RA	3242	1/1	0.97	0.24	20,20,20,20	0
57	MG	YA	3047	1/1	0.97	0.32	14,14,14,14	0
57	MG	RA	3107	1/1	0.97	0.26	21,21,21,21	0
57	MG	RA	3056	1/1	0.97	0.40	14,14,14,14	0
57	MG	YA	3213	1/1	0.97	0.22	31,31,31,31	0
57	MG	XA	1639	1/1	0.97	0.44	43,43,43,43	0
57	MG	QA	1606	1/1	0.97	0.41	20,20,20,20	0
57	MG	XA	1641	1/1	0.97	0.27	21,21,21,21	0
57	MG	RA	3248	1/1	0.97	0.43	46,46,46,46	0
57	MG	RB	201	1/1	0.97	0.13	99,99,99,99	0
57	MG	RA	3141	1/1	0.97	0.09	36,36,36,36	0
57	MG	RA	3079	1/1	0.97	0.39	53,53,53,53	0
57	MG	YA	3060	1/1	0.97	0.18	33,33,33,33	0
57	MG	YA	3144	1/1	0.97	0.29	33,33,33,33	0
57	MG	YA	3062	1/1	0.97	0.24	17,17,17,17	0
57	MG	RA	3208	1/1	0.97	0.28	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3065	1/1	0.97	0.20	55,55,55,55	0
57	MG	RA	3080	1/1	0.97	0.40	36,36,36,36	0
57	MG	RE	301	1/1	0.97	0.34	24,24,24,24	0
57	MG	RA	3023	1/1	0.97	0.34	14,14,14,14	0
57	MG	YA	3320	1/1	0.97	0.11	63,63,63,63	0
57	MG	XA	1703	1/1	0.97	0.35	46,46,46,46	0
57	MG	YA	3231	1/1	0.97	0.45	24,24,24,24	0
57	MG	YA	3071	1/1	0.97	0.34	8,8,8,8	0
57	MG	XA	1651	1/1	0.97	0.49	62,62,62,62	0
57	MG	QA	1607	1/1	0.97	0.16	35,35,35,35	0
57	MG	YA	3074	1/1	0.97	0.53	19,19,19,19	0
57	MG	YA	3075	1/1	0.97	0.28	10,10,10,10	0
57	MG	RA	3083	1/1	0.97	0.21	18,18,18,18	0
57	MG	QA	1602	1/1	0.97	0.52	22,22,22,22	0
57	MG	RA	3257	1/1	0.97	1.02	52,52,52,52	0
57	MG	XA	1709	1/1	0.97	0.23	38,38,38,38	0
57	MG	RA	3148	1/1	0.97	0.22	38,38,38,38	0
57	MG	XA	1603	1/1	0.97	0.32	16,16,16,16	0
57	MG	YA	3248	1/1	0.97	0.31	34,34,34,34	0
57	MG	YA	3083	1/1	0.97	0.38	23,23,23,23	0
57	MG	RA	3047	1/1	0.97	0.43	27,27,27,27	0
57	MG	RA	3086	1/1	0.97	0.33	9,9,9,9	0
57	MG	YA	3253	1/1	0.97	0.36	37,37,37,37	0
57	MG	YA	3254	1/1	0.97	0.21	11,11,11,11	0
57	MG	RA	3088	1/1	0.97	0.44	23,23,23,23	0
57	MG	YA	3341	1/1	0.97	0.20	39,39,39,39	0
57	MG	YA	3256	1/1	0.97	0.20	33,33,33,33	0
57	MG	YA	3001	1/1	0.97	0.24	39,39,39,39	0
57	MG	RA	3119	1/1	0.97	0.46	40,40,40,40	0
57	MG	YA	3089	1/1	0.97	0.26	51,51,51,51	0
57	MG	YA	3003	1/1	0.97	0.45	24,24,24,24	0
57	MG	XA	1608	1/1	0.97	0.13	21,21,21,21	0
57	MG	RA	3048	1/1	0.97	0.43	12,12,12,12	0
57	MG	RA	3063	1/1	0.97	0.46	3,3,3,3	0
57	MG	RA	3188	1/1	0.97	0.25	53,53,53,53	0
57	MG	RA	3223	1/1	0.97	0.33	6,6,6,6	0
57	MG	YA	3177	1/1	0.97	0.31	19,19,19,19	0
57	MG	QA	1651	1/1	0.97	0.29	29,29,29,29	0
57	MG	YA	3010	1/1	0.97	0.22	11,11,11,11	0
57	MG	YA	3269	1/1	0.97	0.37	59,59,59,59	0
57	MG	RA	3066	1/1	0.97	0.24	3,3,3,3	0
57	MG	YA	3271	1/1	0.97	0.28	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	XA	1669	1/1	0.97	0.25	21,21,21,21	0
57	MG	YA	3105	1/1	0.97	0.32	11,11,11,11	0
57	MG	YA	3014	1/1	0.97	0.45	8,8,8,8	0
57	MG	RA	3067	1/1	0.97	0.28	13,13,13,13	0
57	MG	RA	3094	1/1	0.97	0.32	45,45,45,45	0
57	MG	YA	3110	1/1	0.97	0.27	7,7,7,7	0
57	MG	QA	1605	1/1	0.97	0.47	30,30,30,30	0
57	MG	YA	3018	1/1	0.97	0.27	28,28,28,28	0
57	MG	XA	1624	1/1	0.97	0.44	41,41,41,41	0
57	MG	RA	3016	1/1	0.97	0.23	15,15,15,15	0
57	MG	RA	3098	1/1	0.97	0.35	5,5,5,5	0
57	MG	YA	3023	1/1	0.97	0.32	17,17,17,17	0
57	MG	RA	3099	1/1	0.97	0.41	14,14,14,14	0
57	MG	RA	3031	1/1	0.97	0.31	30,30,30,30	0
57	MG	Y1	101	1/1	0.97	0.10	35,35,35,35	0
57	MG	RA	3053	1/1	0.97	0.34	5,5,5,5	0
57	MG	RA	3054	1/1	0.97	0.35	10,10,10,10	0
57	MG	YA	3030	1/1	0.97	0.31	17,17,17,17	0
57	MG	QA	1621	1/1	0.97	0.52	61,61,61,61	0
57	MG	RA	3237	1/1	0.97	0.28	21,21,21,21	0
57	MG	RA	3238	1/1	0.97	0.09	57,57,57,57	0
57	MG	YA	3037	1/1	0.97	0.16	23,23,23,23	0
57	MG	YA	3039	1/1	0.97	0.26	12,12,12,12	0
57	MG	YA	3053	1/1	0.98	0.34	22,22,22,22	0
57	MG	YA	3243	1/1	0.98	0.21	45,45,45,45	0
57	MG	XA	1674	1/1	0.98	0.24	4,4,4,4	0
57	MG	RA	3106	1/1	0.98	0.17	12,12,12,12	0
57	MG	QA	1610	1/1	0.98	0.31	20,20,20,20	0
57	MG	RA	3022	1/1	0.98	0.27	4,4,4,4	0
57	MG	RA	3032	1/1	0.98	0.36	40,40,40,40	0
57	MG	YA	3249	1/1	0.98	0.41	70,70,70,70	0
57	MG	QA	1609	1/1	0.98	0.16	42,42,42,42	0
57	MG	YA	3061	1/1	0.98	0.21	2,2,2,2	0
57	MG	XA	1642	1/1	0.98	0.38	27,27,27,27	0
57	MG	YA	3184	1/1	0.98	0.18	41,41,41,41	0
57	MG	YA	3063	1/1	0.98	0.26	12,12,12,12	0
57	MG	RA	3034	1/1	0.98	0.46	16,16,16,16	0
57	MG	QA	1636	1/1	0.98	0.14	12,12,12,12	0
57	MG	RA	3036	1/1	0.98	0.12	10,10,10,10	0
57	MG	YA	3189	1/1	0.98	0.51	51,51,51,51	0
57	MG	XA	1610	1/1	0.98	0.15	21,21,21,21	0
57	MG	XA	1685	1/1	0.98	0.28	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3069	1/1	0.98	0.22	10,10,10,10	0
57	MG	RA	3073	1/1	0.98	0.30	26,26,26,26	0
57	MG	YA	3013	1/1	0.98	0.31	13,13,13,13	0
57	MG	XA	1687	1/1	0.98	0.57	33,33,33,33	0
57	MG	RA	3074	1/1	0.98	0.23	8,8,8,8	0
57	MG	XA	1613	1/1	0.98	0.36	17,17,17,17	0
57	MG	XA	1614	1/1	0.98	0.35	13,13,13,13	0
57	MG	RA	3162	1/1	0.98	0.19	18,18,18,18	0
57	MG	XA	1616	1/1	0.98	0.37	29,29,29,29	0
57	MG	XA	1617	1/1	0.98	0.22	41,41,41,41	0
57	MG	RA	3095	1/1	0.98	0.35	18,18,18,18	0
57	MG	RA	3241	1/1	0.98	0.28	35,35,35,35	0
57	MG	RA	3038	1/1	0.98	0.24	15,15,15,15	0
57	MG	XA	1621	1/1	0.98	0.29	25,25,25,25	0
57	MG	RA	3040	1/1	0.98	0.32	12,12,12,12	0
57	MG	YA	3027	1/1	0.98	0.58	39,39,39,39	0
57	MG	YA	3028	1/1	0.98	0.23	6,6,6,6	0
57	MG	RA	3025	1/1	0.98	0.23	6,6,6,6	0
57	MG	RA	3245	1/1	0.98	0.43	39,39,39,39	0
57	MG	RA	3043	1/1	0.98	0.20	12,12,12,12	0
57	MG	YA	3150	1/1	0.98	0.29	34,34,34,34	0
57	MG	RA	3121	1/1	0.98	0.18	40,40,40,40	0
57	MG	YA	3034	1/1	0.98	0.32	16,16,16,16	0
57	MG	RA	3017	1/1	0.98	0.33	15,15,15,15	0
57	MG	YA	3094	1/1	0.98	0.23	23,23,23,23	0
57	MG	YA	3036	1/1	0.98	0.27	19,19,19,19	0
57	MG	RA	3018	1/1	0.98	0.17	24,24,24,24	0
57	MG	YB	202	1/1	0.98	0.17	51,51,51,51	0
57	MG	RA	3046	1/1	0.98	0.27	13,13,13,13	0
57	MG	YA	3220	1/1	0.98	0.15	55,55,55,55	0
57	MG	YA	3098	1/1	0.98	0.44	21,21,21,21	0
57	MG	RA	3028	1/1	0.98	0.34	24,24,24,24	0
57	MG	YA	3041	1/1	0.98	0.42	12,12,12,12	0
57	MG	YA	3101	1/1	0.98	0.26	5,5,5,5	0
57	MG	RA	3173	1/1	0.98	0.33	42,42,42,42	0
57	MG	YA	3043	1/1	0.98	0.38	31,31,31,31	0
57	MG	YA	3104	1/1	0.98	0.36	16,16,16,16	0
57	MG	RP	201	1/1	0.98	0.38	31,31,31,31	0
57	MG	YA	3299	1/1	0.98	0.34	32,32,32,32	0
57	MG	YA	3106	1/1	0.98	0.15	27,27,27,27	0
57	MG	RA	3126	1/1	0.98	0.25	51,51,51,51	0
57	MG	XA	1711	1/1	0.98	0.12	27,27,27,27	0

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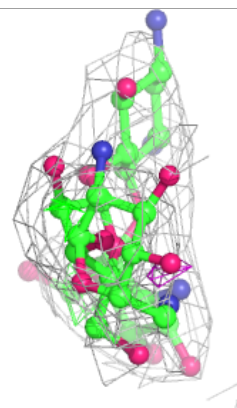
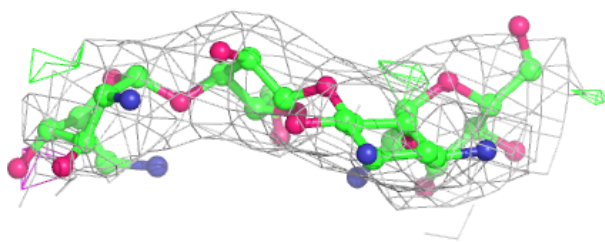
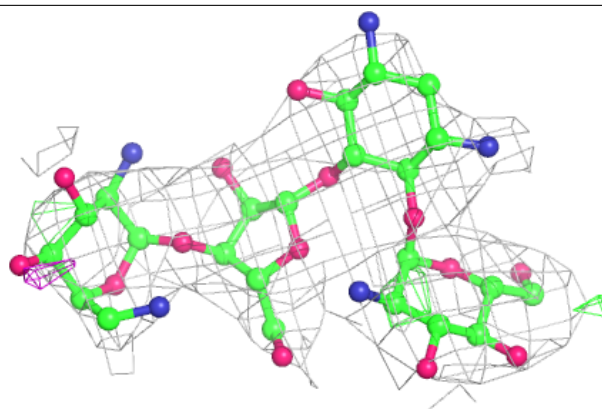
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3232	1/1	0.98	0.56	20,20,20,20	0
57	MG	YA	3233	1/1	0.98	0.38	24,24,24,24	0
57	MG	QA	1655	1/1	0.98	0.69	19,19,19,19	0
57	MG	RA	3065	1/1	0.98	0.19	13,13,13,13	0
57	MG	YA	3236	1/1	0.98	0.45	10,10,10,10	0
57	MG	XA	1601	1/1	0.98	0.89	35,35,35,35	0
57	MG	YA	3112	1/1	0.98	0.32	44,44,44,44	0
57	MG	XA	1673	1/1	0.98	0.51	21,21,21,21	0
59	ZN	XD	301	1/1	0.98	0.31	49,49,49,49	0
57	MG	XV	102	1/1	0.98	0.18	14,14,14,14	0
57	MG	YA	3022	1/1	0.99	0.39	16,16,16,16	0
57	MG	QA	1608	1/1	0.99	0.08	18,18,18,18	0
57	MG	YA	3051	1/1	0.99	0.29	8,8,8,8	0
57	MG	RA	3246	1/1	0.99	0.11	68,68,68,68	0
57	MG	YA	3038	1/1	0.99	0.25	10,10,10,10	0
57	MG	RA	3039	1/1	0.99	0.28	13,13,13,13	0
57	MG	RA	3004	1/1	0.99	0.44	11,11,11,11	0
57	MG	YA	3290	1/1	0.99	0.22	28,28,28,28	0
57	MG	RA	3041	1/1	0.99	0.31	24,24,24,24	0
57	MG	YA	3090	1/1	0.99	0.30	13,13,13,13	0
57	MG	RA	3007	1/1	0.99	0.38	7,7,7,7	0
57	MG	YA	3058	1/1	0.99	0.34	21,21,21,21	0
57	MG	RA	3221	1/1	0.99	0.34	23,23,23,23	0
57	MG	RA	3231	1/1	0.99	0.37	22,22,22,22	0
57	MG	RA	3020	1/1	0.99	0.18	9,9,9,9	0
57	MG	YA	3032	1/1	0.99	0.52	9,9,9,9	0
57	MG	RA	3037	1/1	0.99	0.24	12,12,12,12	0
57	MG	YA	3242	1/1	0.99	0.44	21,21,21,21	0
57	MG	RA	3087	1/1	0.99	0.21	30,30,30,30	0
57	MG	YA	3081	1/1	0.99	0.35	45,45,45,45	0

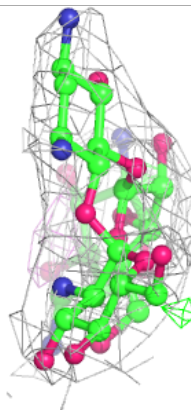
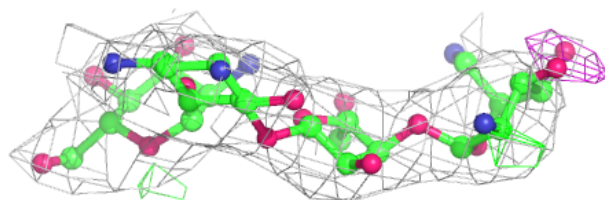
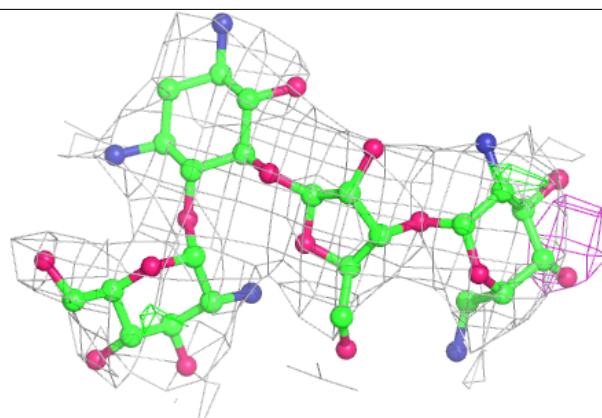
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PAR QA 1681:

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

**Electron density around PAR XA 1710:**

$2mF_o - DF_c$ (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.