



wwPDB X-ray Structure Validation Summary Report

Sep 17, 2014 – 07:04 PM EDT

PDB ID : 4L71
Title : Crystal Structure of Frameshift Suppressor tRNA SufA6 Bound to Codon CCC-A on the Ribosome
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-06-13
Resolution : 3.90 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

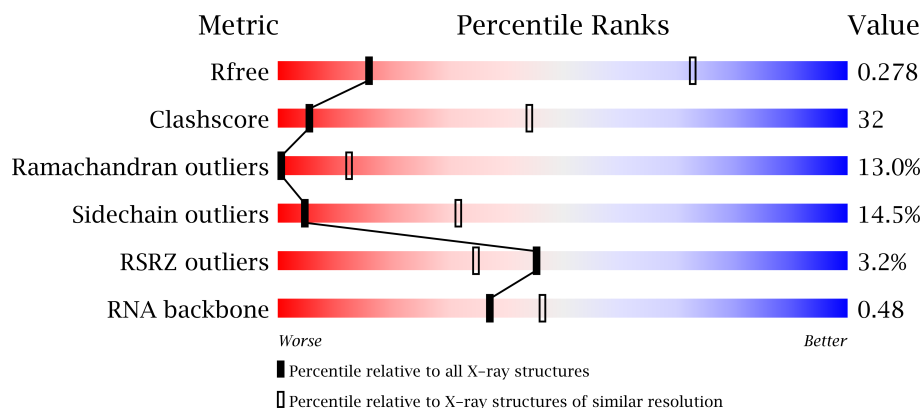
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 3.90 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}	66092	1022 (4.38-3.42)
Clashscore	79885	1173 (4.30-3.50)
Ramachandran outliers	78287	1118 (4.30-3.50)
Sidechain outliers	78261	1107 (4.30-3.50)
RSRZ outliers	66119	1000 (4.36-3.44)
RNA backbone	1838	1018 (5.00-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	QA	1522	
1	XA	1522	
2	QB	256	
2	XB	256	
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	

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Mol	Chain	Length	Quality of chain
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	
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	RA	2916	
22	YA	2916	
23	RB	122	
23	YB	122	
24	RD	276	
24	YD	276	
25	RE	206	
25	YE	206	
26	RF	210	
26	YF	210	
27	RG	182	

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Mol	Chain	Length	Quality of chain
27	YG	182	
28	RH	180	
28	YH	180	
29	RI	148	
29	YI	148	
30	RN	140	
30	YN	140	
31	RO	122	
31	YO	122	
32	RP	150	
32	YP	150	
33	RQ	141	
33	YQ	141	
34	RR	118	
34	YR	118	
35	RS	112	
35	YS	112	
36	RT	146	
36	YT	146	
37	RU	118	
37	YU	118	
38	RV	101	
38	YV	101	
39	RW	113	
39	YW	113	
40	RX	96	
40	YX	96	
41	RY	110	
41	YY	110	
42	RZ	206	
42	YZ	206	
43	R0	85	
43	Y0	85	
44	R1	98	
44	Y1	98	
45	R2	72	
45	Y2	72	
46	R3	60	
46	Y3	60	
47	R4	71	
47	Y4	71	
48	R5	60	

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Mol	Chain	Length	Quality of chain
48	Y5	60	
49	R6	54	
49	Y6	54	
50	R7	49	
50	Y7	49	
51	R8	65	
51	Y8	65	
52	R9	37	
52	Y9	37	
53	QV	77	
53	XV	77	
54	QX	25	
54	XX	25	
55	QY	18	
55	XY	18	
56	Z6	3	
56	Z8	3	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291950 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	QC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	XC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	QE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	XE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	QI	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	XI	127	Total	C	N	O		0	0	0
			1010	639	197	174				

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	XK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	121	Total	C	N	O	S	0	0	0
			964	597	199	166	2			
13	XM	121	Total	C	N	O	S	0	0	0
			964	597	199	166	2			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	XR	70	Total	C	N	O	0	0	0
			574	367	112	95			

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

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

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

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

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

- Molecule 22 is a RNA chain called 23S rRNA.

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

- Molecule 23 is a RNA chain called 5S rRNA.

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

- Molecule 24 is a protein called 50S ribosomal protein L2.

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

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

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	RF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	YF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 27 is a protein called 50S ribosomal protein L5.

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

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

- Molecule 30 is a protein called 50S ribosomal protein L13.

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

- Molecule 31 is a protein called 50S ribosomal protein L14.

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

- Molecule 32 is a protein called 50S ribosomal protein L15.

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

- Molecule 33 is a protein called 50S ribosomal protein L16.

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

- Molecule 34 is a protein called 50S ribosomal protein L17.

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

- Molecule 35 is a protein called 50S ribosomal protein L18.

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

- Molecule 36 is a protein called 50S ribosomal protein L19.

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

- Molecule 37 is a protein called 50S ribosomal protein L20.

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

- Molecule 38 is a protein called 50S ribosomal protein L21.

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

- Molecule 39 is a protein called 50S ribosomal protein L22.

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

- Molecule 40 is a protein called 50S ribosomal protein L23.

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

- Molecule 41 is a protein called 50S ribosomal protein L24.

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

- Molecule 42 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	YZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

- Molecule 43 is a protein called 50S ribosomal protein L27.

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

- Molecule 44 is a protein called 50S ribosomal protein L28.

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

- Molecule 45 is a protein called 50S ribosomal protein L29.

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

- Molecule 46 is a protein called 50S ribosomal protein L30.

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

- Molecule 47 is a protein called 50S ribosomal protein L31.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
48	Y5	58	Total	C	N	O	S	0	0	0
			451	283	89	74	5			

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	R6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			
49	Y6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

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

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	R9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
52	Y9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 53 is a RNA chain called P-site tRNA fMet.

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

- Molecule 54 is a RNA chain called A-site ASL SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	QX	8	Total	C	N	O	P	0	0	0
			169	76	31	54	8			
54	XX	8	Total	C	N	O	P	0	0	0
			169	76	31	54	8			

- Molecule 55 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	QY	14	Total	C	N	O	P	0	0	0
			303	135	55	99	14			
55	XY	14	Total	C	N	O	P	0	0	0
			303	135	55	99	14			

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

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

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	65	Total	Mg	0	0
			65	65		
57	RP	2	Total	Mg	0	0
			2	2		
57	QX	1	Total	Mg	0	0
			1	1		
57	YA	265	Total	Mg	0	0
			265	265		
57	QM	1	Total	Mg	0	0
			1	1		

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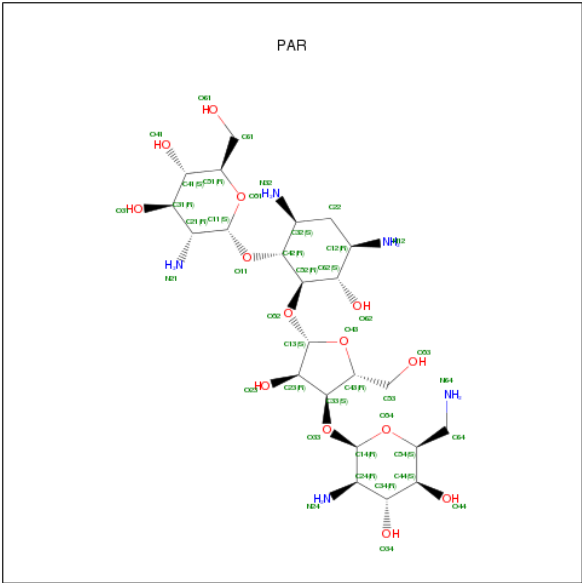
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	XX	1	Total 1	Mg 1	0	0
57	XA	72	Total 72	Mg 72	0	0
57	RU	1	Total 1	Mg 1	0	0
57	QH	1	Total 1	Mg 1	0	0
57	YQ	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	YX	1	Total 1	Mg 1	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RD	1	Total 1	Mg 1	0	0
57	Y7	1	Total 1	Mg 1	0	0
57	QF	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	RA	244	Total 244	Mg 244	0	0
57	YP	2	Total 2	Mg 2	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	RE	2	Total 2	Mg 2	0	0
57	YB	3	Total 3	Mg 3	0	0
57	XV	2	Total 2	Mg 2	0	0
57	RB	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0
57	XM	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YE	1	Total	Mg	0	0
			1	1		

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



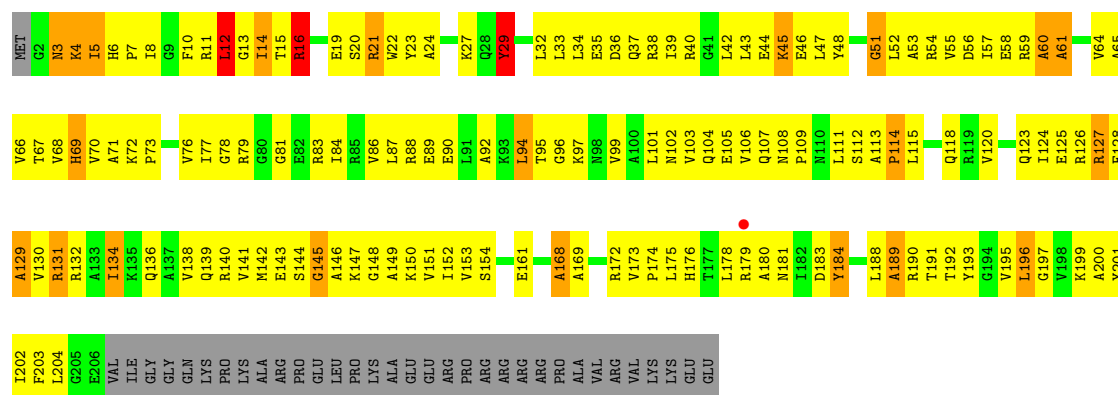
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	QA	1	Total	C	N	O	0	0
			42	23	5	14		
58	XA	1	Total	C	N	O	0	0
			42	23	5	14		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	Y9	1	Total	Zn	0	0
			1	1		
59	QN	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		
59	QD	1	Total	Zn	0	0
			1	1		
59	XD	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		

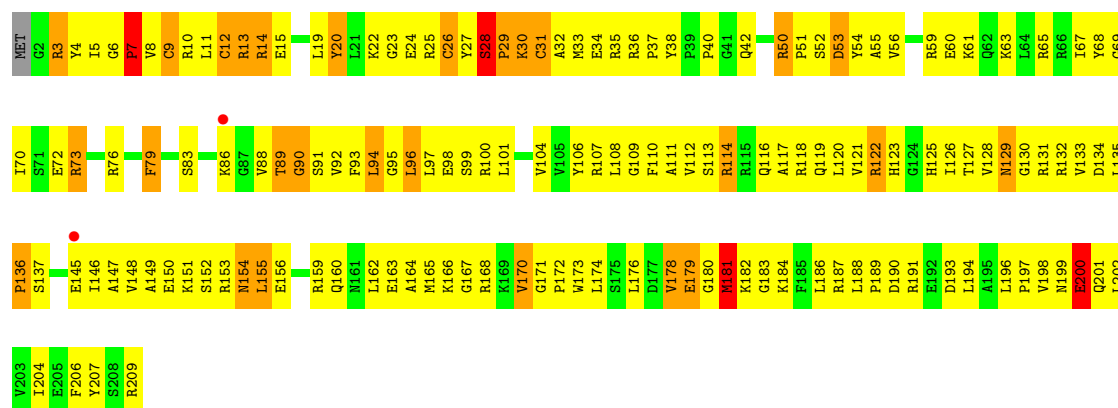






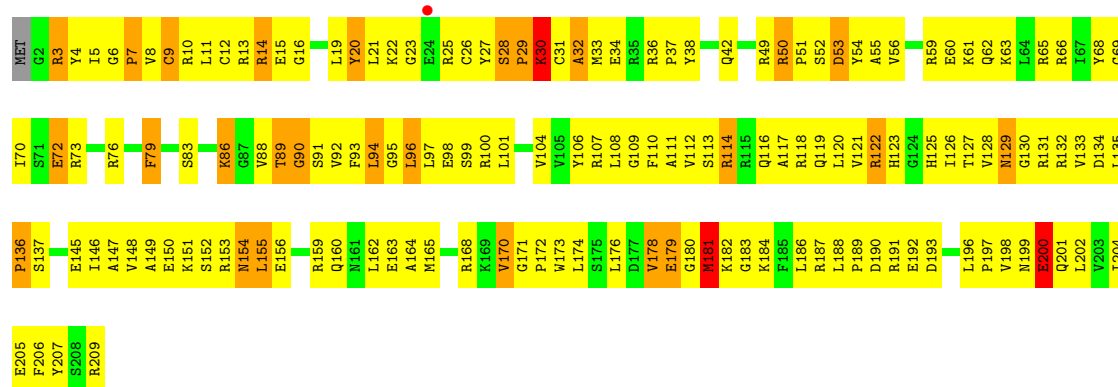
• Molecule 4: 30S ribosomal protein S4

Chain QD:



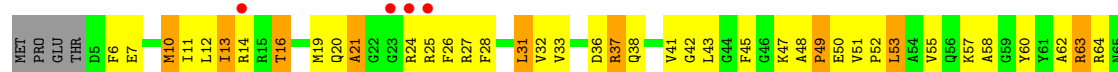
• Molecule 4: 30S ribosomal protein S4

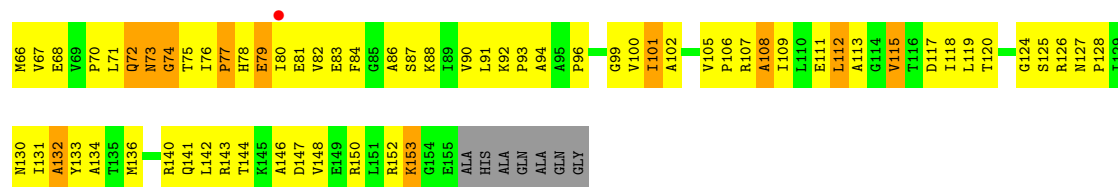
Chain XD:



• Molecule 5: 30S ribosomal protein S5

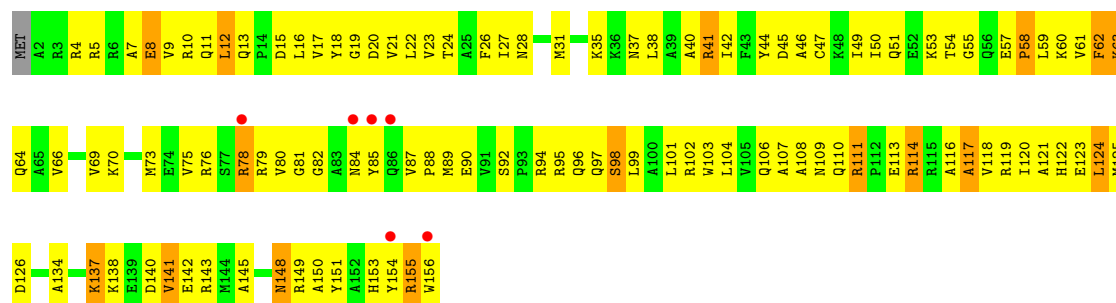
Chain QE:





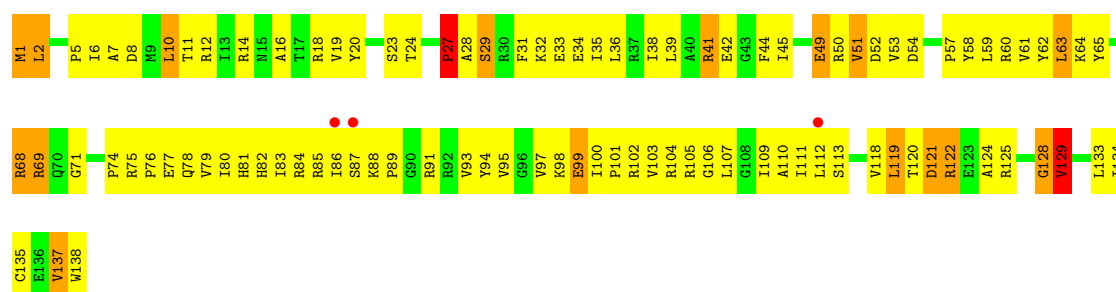
- Molecule 7: 30S ribosomal protein S7

Chain XG:



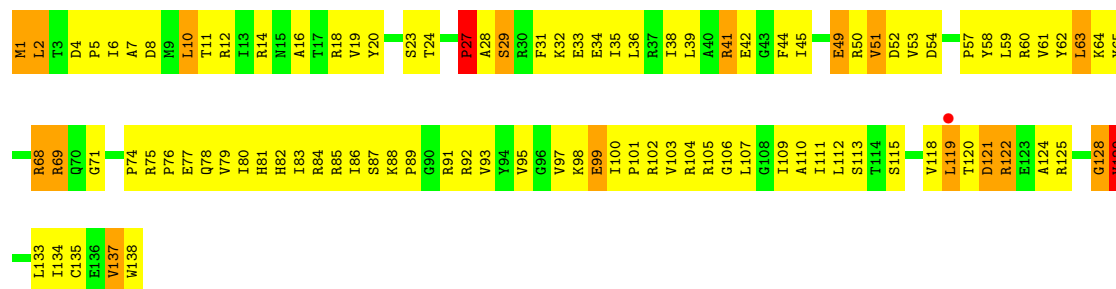
- Molecule 8: 30S ribosomal protein S8

Chain QH:



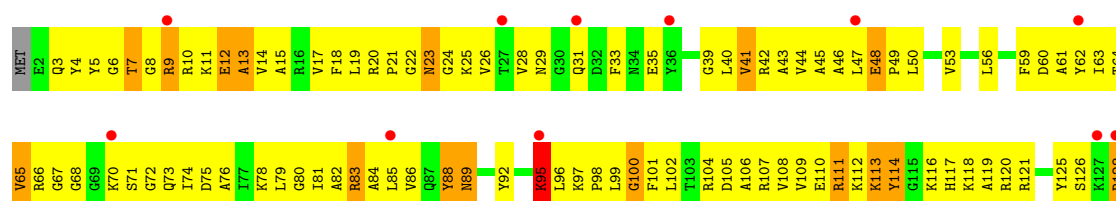
- Molecule 8: 30S ribosomal protein S8

Chain XH:



- Molecule 9: 30S ribosomal protein S9

Chain QI:



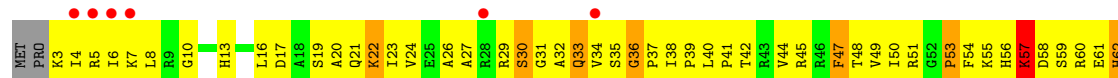
- Molecule 9: 30S ribosomal protein S9

Chain XI:



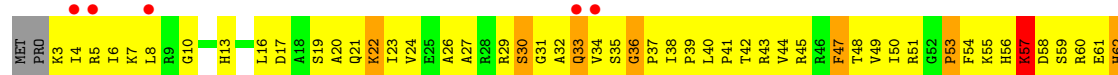
• Molecule 10: 30S ribosomal protein S10

Chain QJ:



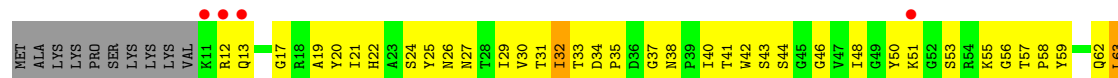
• Molecule 10: 30S ribosomal protein S10

Chain XJ:



• Molecule 11: 30S ribosomal protein S11

Chain QK:



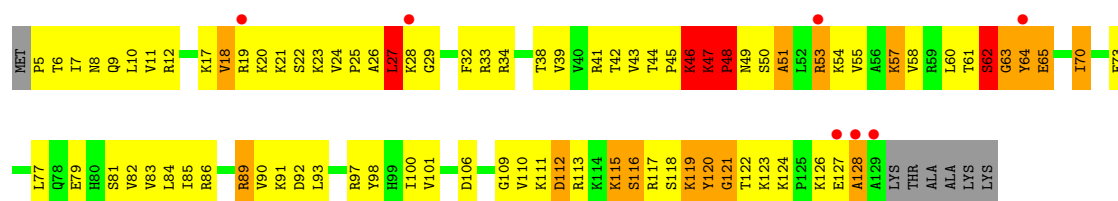
• Molecule 11: 30S ribosomal protein S11

Chain XK:



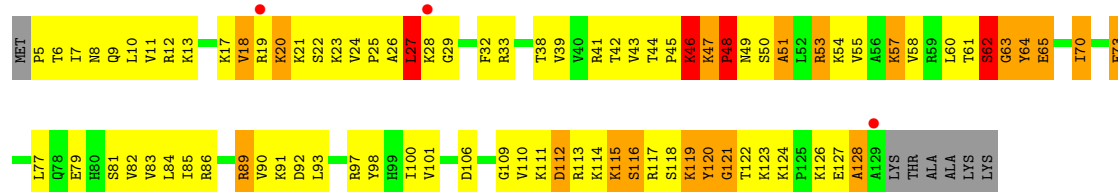
• Molecule 12: 30S ribosomal protein S12

Chain QL:



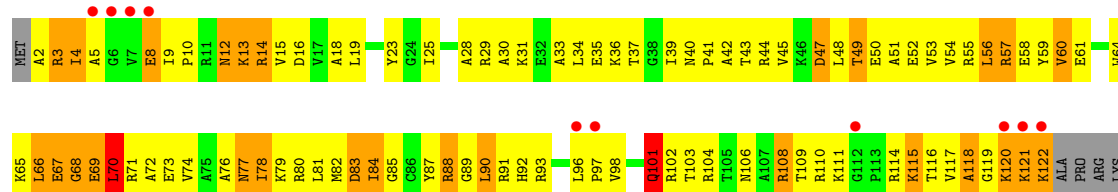
• Molecule 12: 30S ribosomal protein S12

Chain XL:



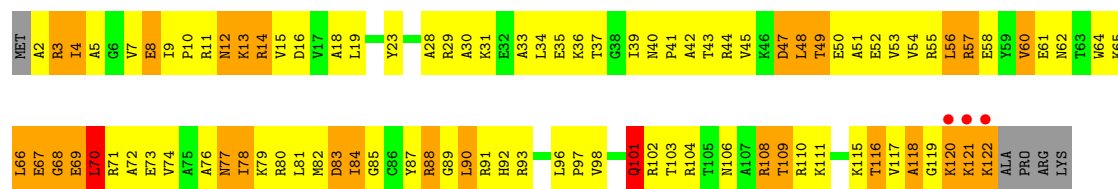
• Molecule 13: 30S ribosomal protein S13

Chain QM:



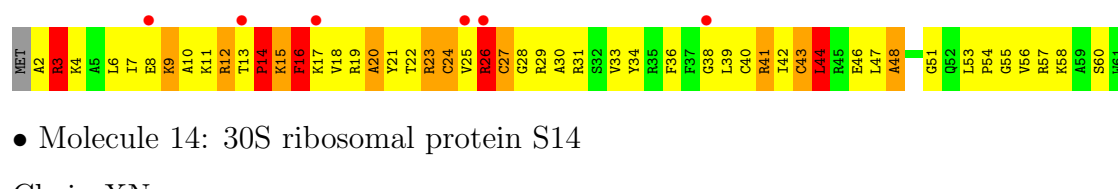
• Molecule 13: 30S ribosomal protein S13

Chain XM:



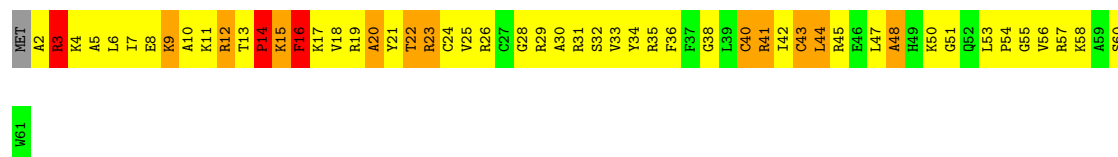
• Molecule 14: 30S ribosomal protein S14

Chain QN:



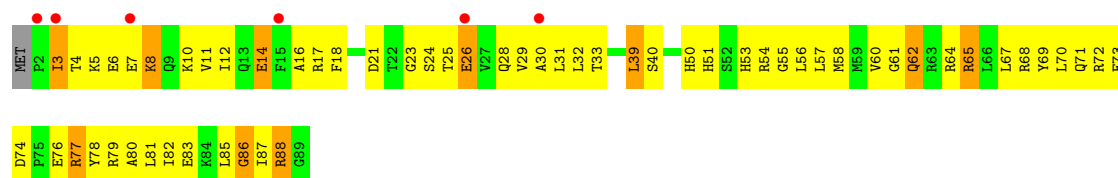
• Molecule 14: 30S ribosomal protein S14

Chain XN:



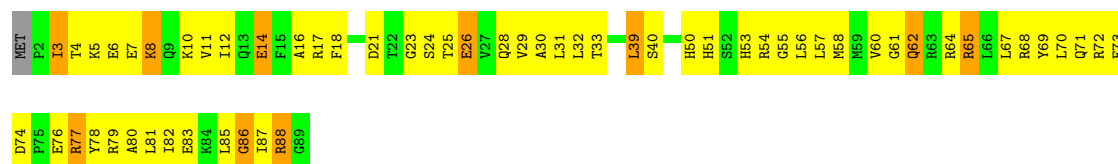
- Molecule 15: 30S ribosomal protein S15

Chain QO:



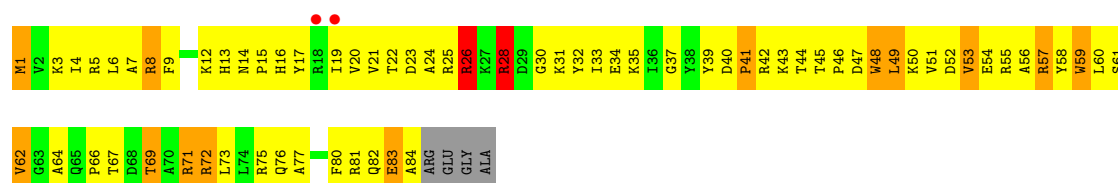
- Molecule 15: 30S ribosomal protein S15

Chain XO:



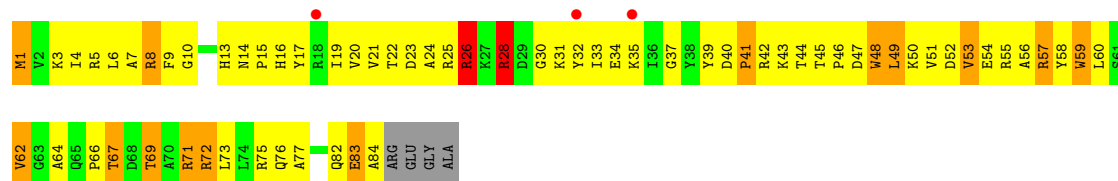
- Molecule 16: 30S ribosomal protein S16

Chain QP:



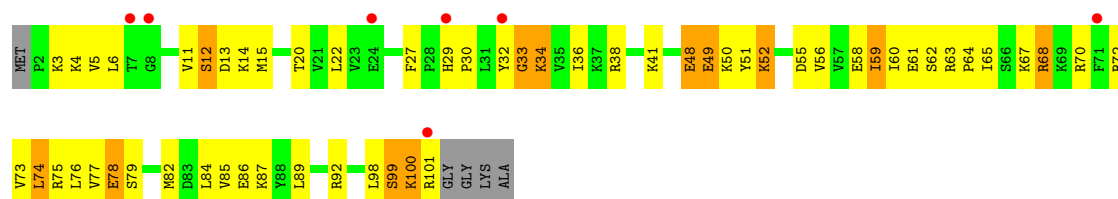
- Molecule 16: 30S ribosomal protein S16

Chain XP:



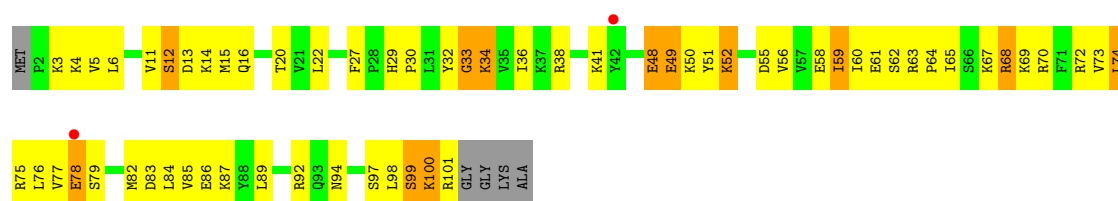
- Molecule 17: 30S ribosomal protein S17

Chain QQ:



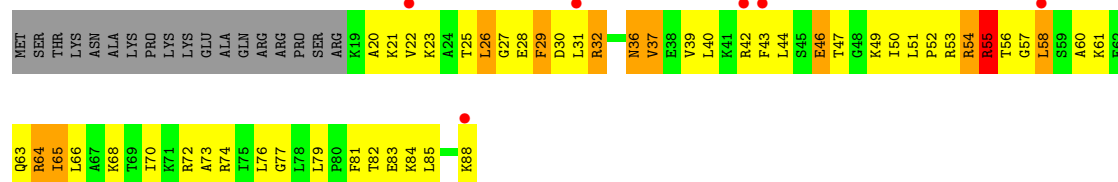
- Molecule 17: 30S ribosomal protein S17

Chain XQ:



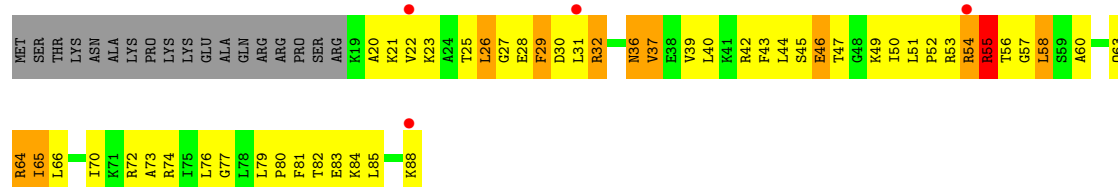
• Molecule 18: 30S ribosomal protein S18

Chain QR:



• Molecule 18: 30S ribosomal protein S18

Chain XR:



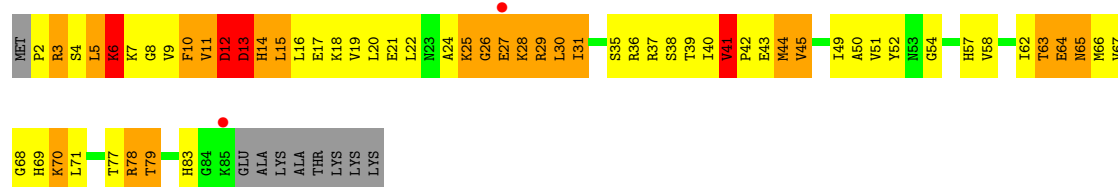
• Molecule 19: 30S ribosomal protein S19

Chain QS:



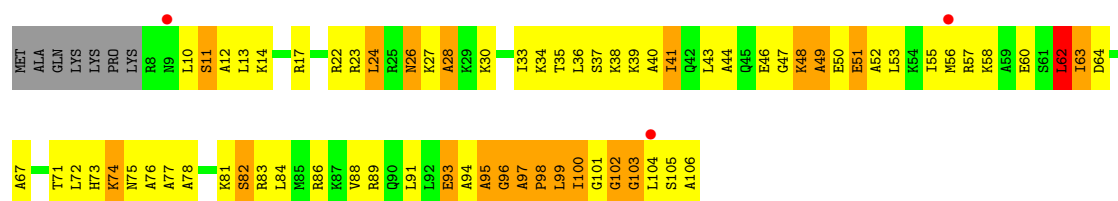
• Molecule 19: 30S ribosomal protein S19

Chain XS:



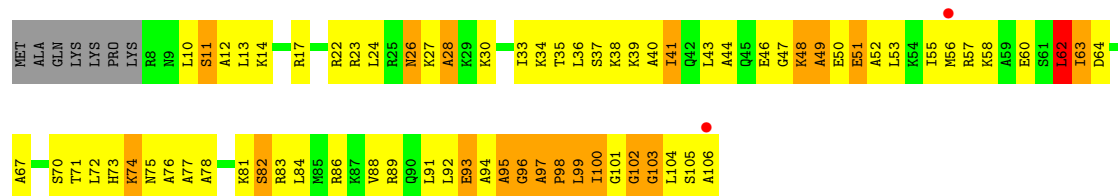
• Molecule 20: 30S ribosomal protein S20

Chain QT:



• Molecule 20: 30S ribosomal protein S20

Chain XT:



• Molecule 21: 30S ribosomal protein S21

Chain QU:



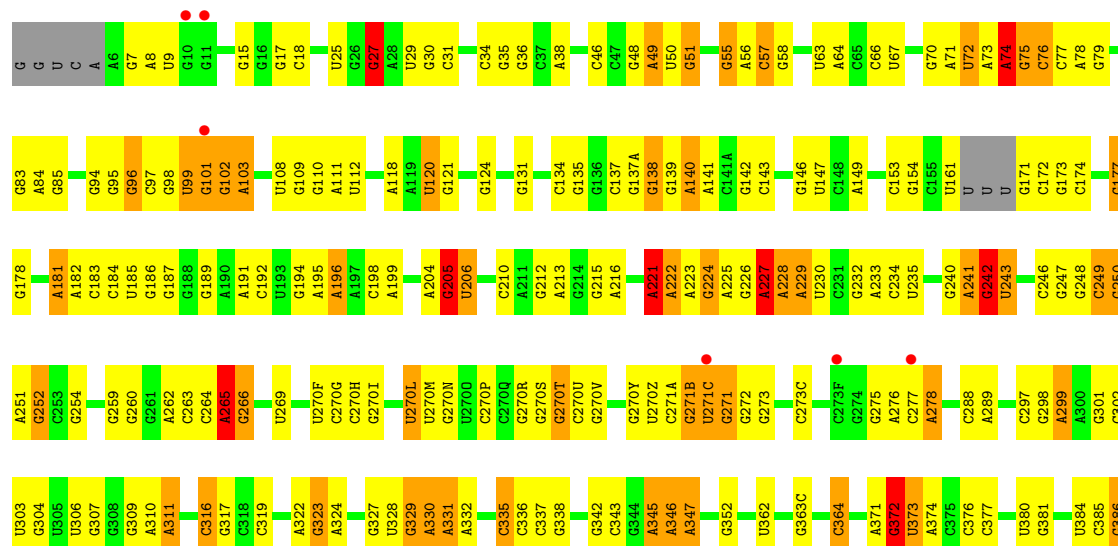
• Molecule 21: 30S ribosomal protein S21

Chain XU:



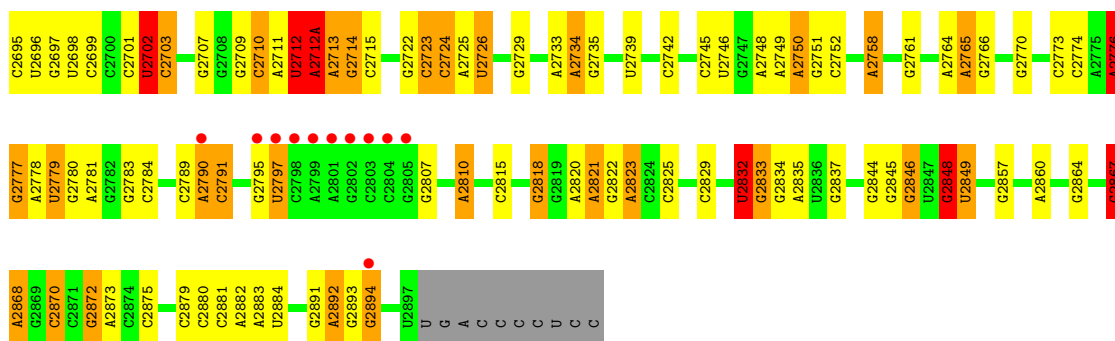
• Molecule 22: 23S rRNA

Chain RA:



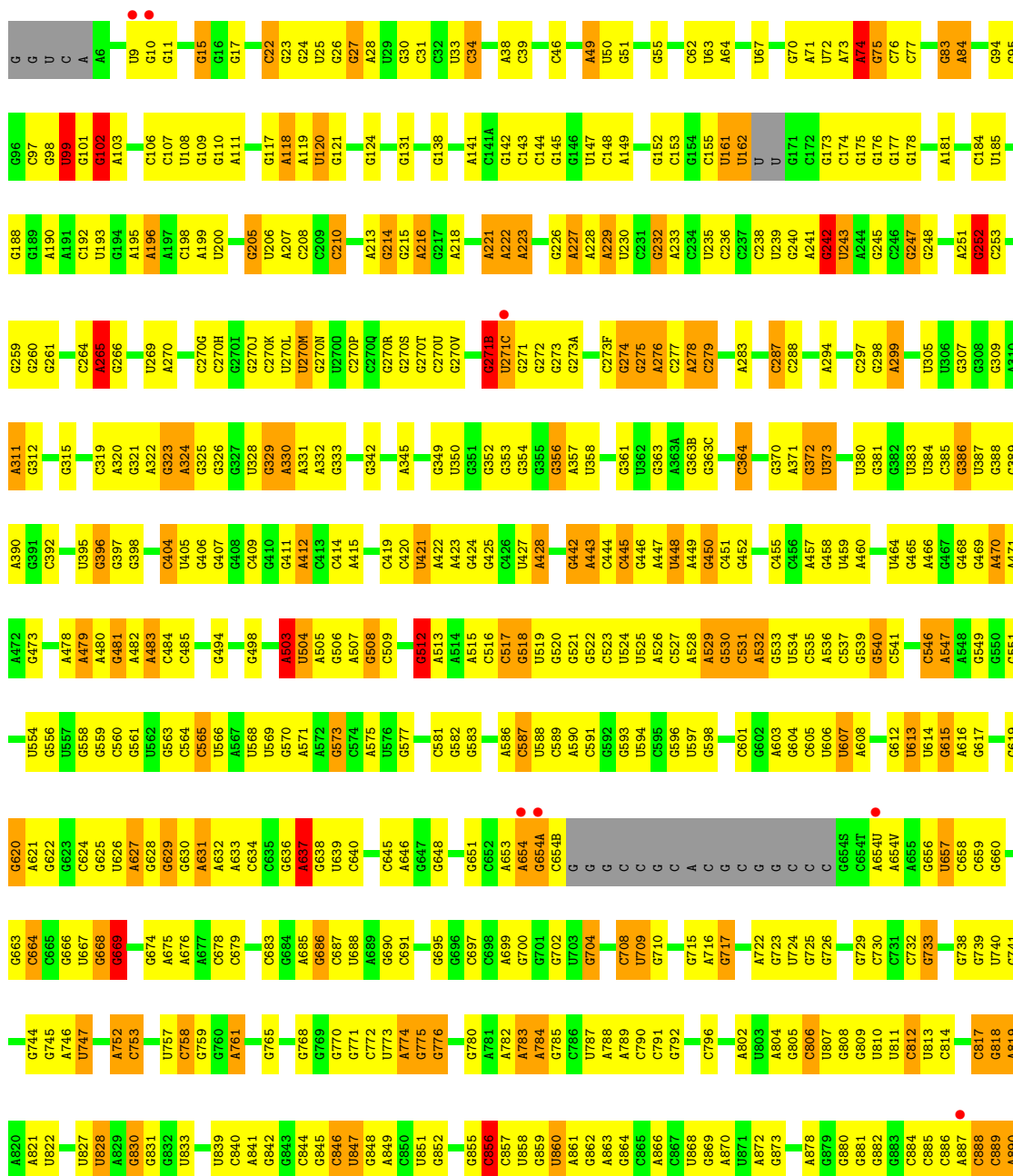
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G1418	G1337	C1180	G1099	A1027	A959	C884	G805	G737	C864	G622	U554	A471	G388
A1419	G1338	G1183	C1100	A1028	A960	C885	C806	G738	C865	G623	G556	A472	G389
U1420	G1339	G1184	C1101	A1029	C961	C886	U807	G739	C866	C624	U557	G473	A390
G1421	U1340	A1285	A1102	G1030	G962	C887	G808	G744	U677	G625	G558		G391
G1422	U1341	A1266	C1103	U1033	U963	C888	G809	G745	G668	U626		A479	C392
		U1267	C1104	U1033	C964	C889	U810	G746	A480	A627	G563	A480	C393
G1425	G1348	U1188	G1110	C1041	C965	A890	U811	U747	C870		C564	A481	C394
G1426	A1269	A1189	A1111	G1042	G966	A891	C812	G748	C871	G630	C565	A482	U395
A1427	G1270	G1190	C1112	C1043	U969	C892	C917	G749	C872	A631	U566	A483	G396
G1428	C1351	G1191	G1113	G1044	C970	A896	G818	A750	C873	A632		A484	G397
G1429	U1352	G1192	U1113	A1045	C971	C897	A819	A751	G674	G633	G570		A401
C1430	U1353	G1193	G1114	A1046	C972	C898		A752	A676	C634	A571		
U1431	A1194	G1115	C1116	A1047	A973	A899	U822	G753	A677	C635	A572		
C1432	G1355	G1122	U1048	A1048	G974	A900	G823	C754	C878	G636	G573		
U1433	U1357	G1123	A1049	C974A	C975	A901	A824	C755	C879	A637	C574		
A1434	G1358	A1050	U1049	C975	C933	C902	G825	G759	G680	U639	A575		
G1435	A1359	A1054	U1054	A980	C904	C903	U826	G760	G681	C640	G577		
		G1055	G1055	A983	C905	U905	U828	A761	C882	G641	A503		
	A1365	U1130	A1057	A984	A983	G906	G831	G764	C883	G642	U504		
A1444A	A1367	G1131	G1058	C985	U907	C907	G832	A764	A685	A643	A505		
C1445	G1368	G1135	U1059	C986	A910	C912	U833	G765	G686	A644	A507		
	U1211	G1136	U1060	C987	A911	C912		G766	C687	C645	G508		
G1449	C1370	G1137	U1061	A988	C912	C912		G767	U688	G647	C509		
G1449A	U1371	G1138	G1062	G989	C915	C915	U839	G768	A689	G648	C510		
C1450	A1372	G1139	U1063	A990	C916	C916	G843	G770	G690	G649	U511		
A1451	G1374	C1221	G1064	C991	A917	C917	G844	G771	C593	C650	A513		
A1454	U1453	C1222	U1065	C992	A917	C917	G845	A774	U694	G651	A514		
G1455	A1378	G1224	U1066	C993	C946	C946	G846	G775	G695	G652	A515		
	A1379	A1227	A1067	C994	U847	U847	G846	G776	G696	A653	C517		
C1458	G1380	A1143	G1068	C995	G848	G848	G848	G777	C597	A654	G518		
A1460	A1301	G1144	U1069	A996	A849	A849	G855	G778	G701	C654B	U519		
G1461	A1384	G1149	G1071	C997	G855	G855		U779	G702	G	G520		
C1462	G1385	C1150	C1076	A1000	C856	C856		G780	U703	G	G521		
	C1386	G1151	A1077	G1001	C857	C857		A781	G704	G	U524		
C1467	C1387	C1152	U1078	G1002	U930	U930		A782	A705	C	U525		
A1468	U1394	G1153	C1079	G1003	G859	G859		A783	C601	C	A526		
A1469	U1395	G1154	C1080	G1005	U860	U860		A784	G709	C	C527		
G1470	U1396	A1155	U1081	C1006	A861	A861		G785	G710	A	A603		
A1471	U1397	A1156	U1082	C1007	G862	G862		C786	C	C	A528		
A1472	C1473	G1162	U1083	U1083	A863	A863		U787	G717	C	A604		
C1473	U1398	C1161	A1084	U1084	G864	G864		A788	C719	C	C605		
G1474	C1403	U1165	A1085	U1085	C965	C965		C790	U607	C	U606		
G1475	C1404	C1166	G1086	U1086	A866	A866		C791	A608	C	A609		
	U1405	G1169	A1087	U1087	G1011	G1011		G792	A722	C	A609		
G1478	U1406	G1170	U1088	A1088	U1012	U1012		A793	G723	C	G612		
C1479	C1407	G1171	U1089	G1089	C1013	C1013		G794	U724	C	U613		
G1480	C1408	G1172	U1090	G1090	G1015	G1015		C795	G726	C654T	U614		
G1482	C1409	G1173	U1091	G1091	U1019	U1019		C796	A727	C	G615		
G1484	C1411	G1174	U1092	G1092	U1020	U1020		C797	G728	C	C546		
G1485	A1412	U1175	U1094	G1094	A1021	A1021		A800	G729	C	A547		
	G1413	G1176	U1095	G1095	G1022	G1022		G801	C730	C	A548		
U1488	U1415	A1177	A1096	U1096	G880	G880		A802	G734	C	A549		
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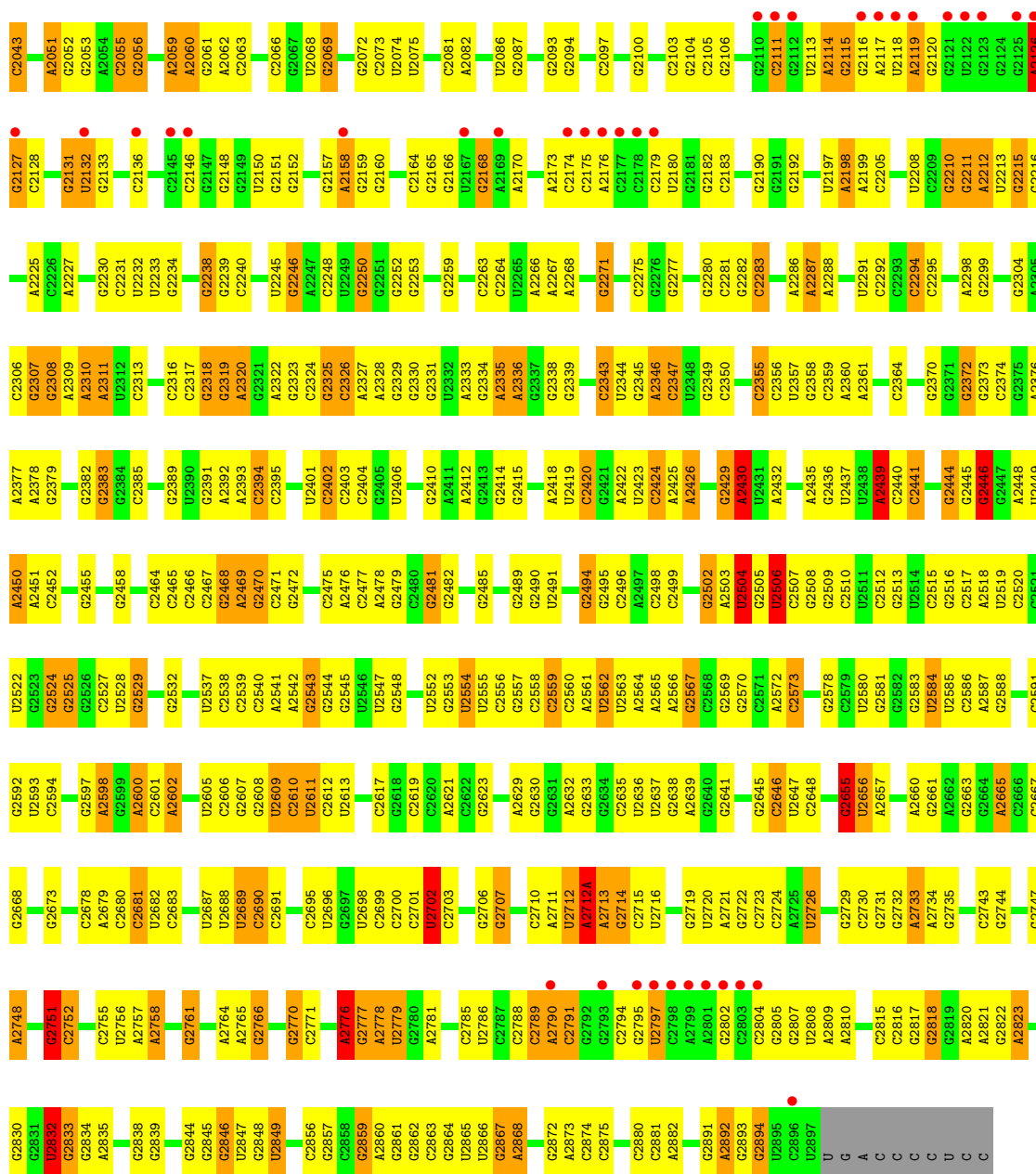


• Molecule 22: 23S rRNA

Chain YA:

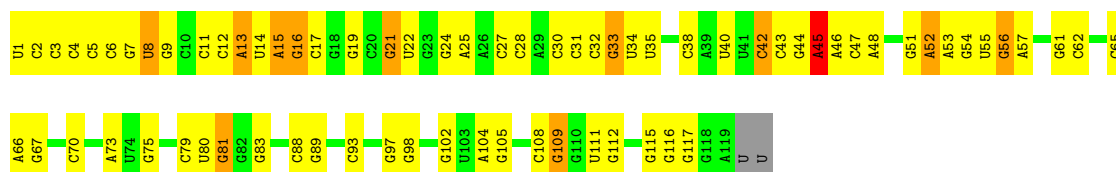


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C1965	C1893	C1804	A1729	C1636	A1543	A1471	C1403	C1333	C1258	G1190	A1111	C1043	C965	A896
C1967	C1894	G1805	G1730	A1637	A1544	A1472	C1404	C1334	G1259	G1191	G1112	G1044	C971	C897
G1968	G1895	A1812	G1732	C1638	C1547	G1475	C1406	U1335	C1261	A1194	G1114	A1045	G973	C898
A1969	G1896	G1813	G1733	U1639	C1548	G1476	C1408	U1336	A1262	G1195	G1120	A1046	A972	C899
A1970	G1897	G1814	C1734	A1640	C1549	C1476	C1409	G1337	U1263	C1196	G1121	G1047	G974	A900
A1971	G1898	A1815	C1742	A1641	C1550	G1479	C1411	G1338	A1265	U1198	G1122	A1048	C974A	A901
A1972	G1902	G1816	G1743	G1642	C1551	G1480	A1412	U1341	U1267	U1199	C1123	A1050	G975	C902
G1973	G1903	G1817	G1750	C1646	A1558	G1482	G1416	G1344	A1268	C1201	C1053	G978	G978	C903
C1974	G1904	U1818	C1751	C1647	A1559	G1483	C1417	A1349	A1269	G1202	G1054	G979	A980	C904
G1975	G1905	A1819	G1752	C1648	C1564	G1485	C1418	A1350	C1270	G1203	G1055	A981	A980	U907
U1976	G1906	U1820	C1753	G1651	C1565	G1488	G1419	A1351	G1271	A1204	G1056	A982	A980	C908
A1977	C1907	G1822	G1754	G1652	C1566	G1489	C1420	A1352	A1272	U1205	G1057	A983	A980	A909
G1978	C1908	G1823	C1755	G1653	A1566	U1489	G1421	U1353	U1273	G1206	G1058	A984	A980	A910
A1979	A1913	G1824	G1756	A1654	A1567	A1490	G1422	C1354	A1274	C1207	U1060	U1059	C974A	A911
A1980	A1914	G1825	U1757	A1655	G1568	C1493	G1423	A1355	A1275	C1208	U1061	U1060	C974A	A912
C1982	U1917	G1826	G1758	C1656	A1569	A1494	G1424	A1354	A1276	G1209	G1062	U1062	G975	U913
U1991	A1918	G1828	G1759	C1657	A1570	A1495	G1425	U1357	G1277	A1210	G1063	G989	G978	C914
G1992	A1919	A1496	A1496	A1496	A1571	A1495	G1426	G1358	A1278	U1211	U1066	A990	G979	C915
U1993	C1920	G1573	U1497	U1497	G1573	U1497	A1428	A1359	G1279	A1213	U1067	C992	C992	A917
A2001	U1923	U1833	G1763	C1662	C1573	U1503	G1429	A1360	U1282	G1217	G1151	A1000	C1007	A918
G2002	C1924	G1834	C1764	G1666	U1576	U1504	G1430	G1364	A1286	C1217	G1152	A1000	C1008	G919
C2006	A1927	G1835	C1765	G1667	U1577	C1504	G1431	A1365	A1287	A1220	G1153	A1000	C1009	U922
G2009	G1928	C1836	G1769	A1667	U1578	C1505	U1431	A1366	U1288	C1221	G1154	A1000	C1010	C923
G2010	G1929	G1837	C1770	A1668	U1579	C1506	G1432	G1368	U1291	C1222	G1155	A1000	C1011	C924
U2011	U1930	G1838	C1771	A1669	A1580	A1507	G1433	G1370	U1292	C1223	G1156	A1000	C1012	A926
G2012	U1931	C1843	G1772	U1672	C1585	A1508	G1434	G1371	C1293	G1228	G1157	A1000	C1013	G928
A2013	A1932	C1844	C1774	U1673	A1586	A1510	G1435	G1372	U1300	A1227	G1158	A1000	C1014	G929
A2014	C1933	G1845	U1775	C1675	C1592	A1511	G1436	G1373	U1301	G1228	G1159	A1000	C1015	U930
A2015	G1934	G1846	G1776	A1676	C1593	G1512	U1438	A1374	U1302	G1229	G1160	A1000	C1016	G931
A2015	G1935	A1847	U1777	A1677	G1594	G1513	G1439	G1375	A1301	C1230	G1161	A1000	C1017	G932
A2015	A1936	A1848	U1778	A1677	G1595	U1514	G1440	G1376	C1304	G1231	G1162	A1000	C1018	U937
A2020	A1937	G1849	U1779	G1681	G1596	C1515	G1441	G1377	C1305	G1232	G1163	A1000	C1019	G938
C2021	A1938	G1850	A1780	G1682	A1596	U1516	G1442	G1378	U1306	G1233	G1164	A1000	C1020	G939
U2022	U1939	A1853	C1781	G1683	A1597	C1517	G1443	A1379	A1308	C1233	G1165	A1000	C1021	A941
G2023	U1940	A1854	C1782	A1689	C1598	C1518	G1444	A1380	G1309	U1234	G1166	A1000	C1022	A942
G2024	G1941	A1855	G1783	A1689	C1599	G1519	A1444A	G1381	G1310	G1235	G1167	A1000	C1023	U943
C2025	A1942	G1857	A1784	A1690	C1600	U1520	G1445	G1382	G1311	G1236	G1168	A1000	C1024	G944
C2026	U1944	G1858	A1785	U1693	A1603	G1521	A1449	C1383	U1312	A1237	G1169	A1000	C1025	G945
G2027	G1945	A1859	A1786	C1694	A1604	G1522	G1449A	A1384	U1313	G1238	G1170	A1000	C1026	A946
U2028	U1946	U1864	C1787	G1695	C1607	A1528	U1454	A1385	C1314	G1239	G1171	A1000	C1027	G947
G2029	G1949	G1869	C1788	G1696	A1608	A1529	U1455	C1386	C1315	U1240	G1172	A1000	C1028	U948
A2030	A2031	C1870	C1789	A1698	A1609	G1530	G1455	C1387	U1316	A1241	G1173	A1000	C1029	A951
G2032	G1950	A1871	A1791	G1699	A1700	C1531	G1456	G1388	A1317	G1244	G1174	A1000	C1030	G952
A2033	U1952	A1872	A1792	A1700	A1614	C1532	C1458	G1389	G1318	G1245	G1175	A1000	C1031	G953
U2034	U1953	G1882	C1795	G1705	C1615	C1533	G1459	U1390	G1319	G1246	G1176	A1000	C1032	G954
G2035	U1954	C1883	U1796	U1706	A1616	G1534	A1460	U1391	C1320	U1249	G1177	A1000	C1033	G955
G2036	C1957	G1884	C1797	G1707	C1617	U1535	G1461	A1392	A1321	G1250	G1178	A1000	C1034	A957
G2037	C1958	A1885	U1798	C1708	A1618	A1536	G1462	U1393	A1322	C1251	G1179	A1000	C1035	U958
C2038	C1959	A1886	G1799	G1537	A1537	A1537	G1463	U1394	U1323	G1252	G1180	A1000	C1036	A959
C2039	U1960	A1887	G1799	G1538	G1465	A1538	G1466	U1395	U1324	A1253	G1181	A1000	C1037	A960
U2040	A1961	C1888	G1725	G1623	G1466	U1539	G1467	U1396	G1324	A1254	G1182	A1000	C1038	C961
C2041	U1962	A1889	G1726	G1624	C1468	U1540	C1469	U1397	G1328	U1255	G1183	A1000	C1039	G962
A2042	U1963	A1890	U1727	C1625	G1469	U1541	A1469	U1398	U1329	G1256	G1184	A1000	C1040	U963



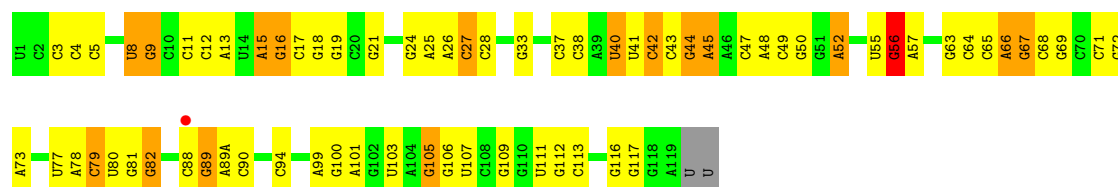
• Molecule 23: 5S rRNA

Chain RB:



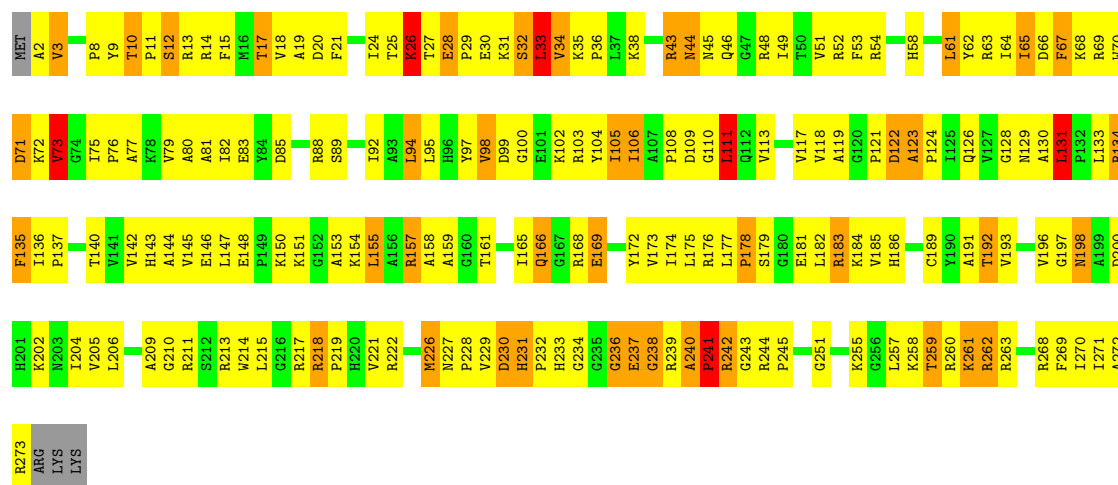
• Molecule 23: 5S rRNA

Chain YB:



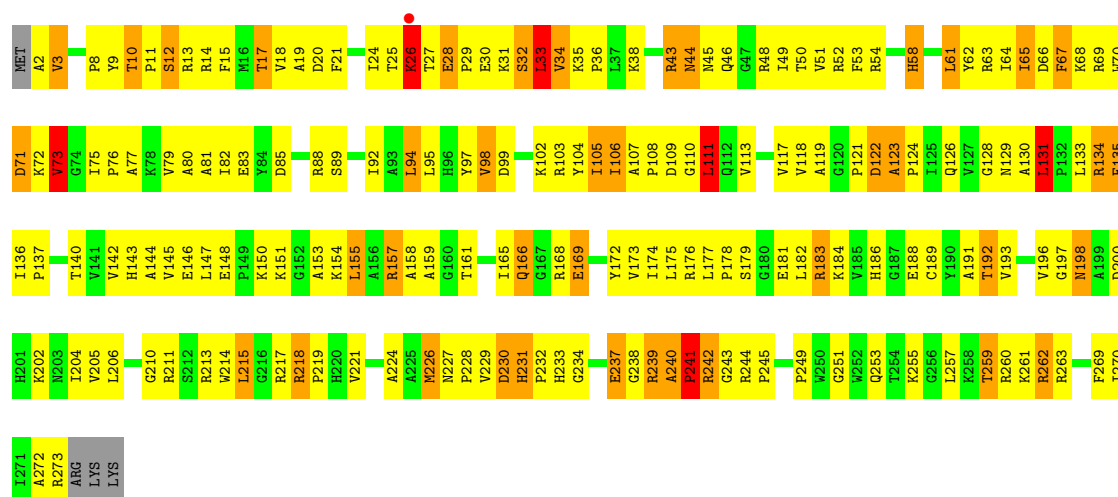
• Molecule 24: 50S ribosomal protein L2

Chain RD:



• Molecule 24: 50S ribosomal protein L2

Chain YD:



• Molecule 25: 50S ribosomal protein L3

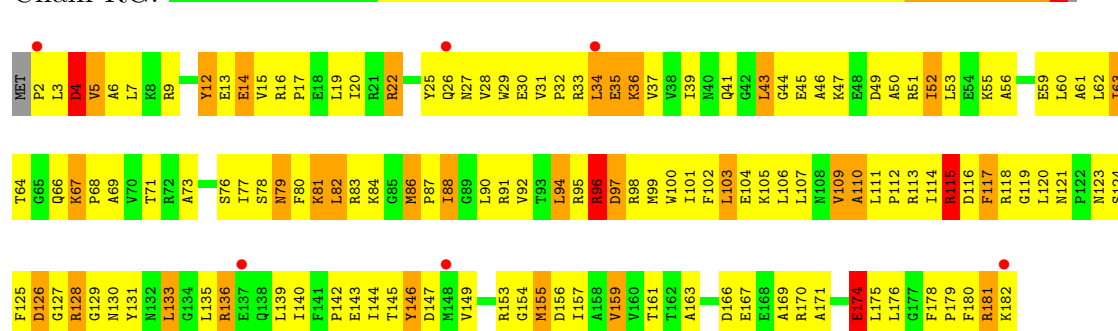
Chain RE:



ALA

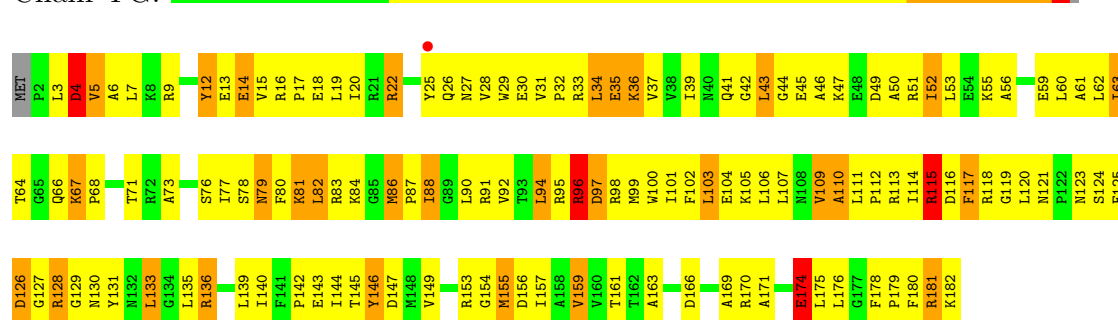
- Molecule 27: 50S ribosomal protein L5

Chain RG:



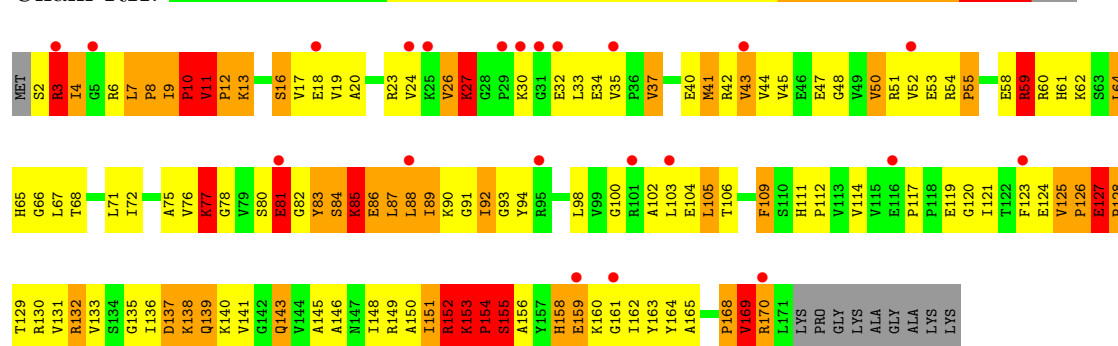
- Molecule 27: 50S ribosomal protein L5

Chain YG:



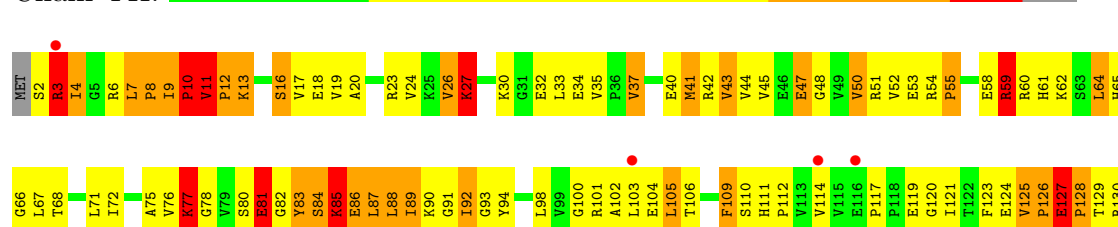
- Molecule 28: 50S ribosomal protein L6

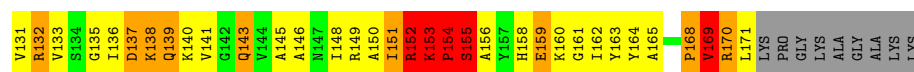
Chain RH:



- Molecule 28: 50S ribosomal protein L6

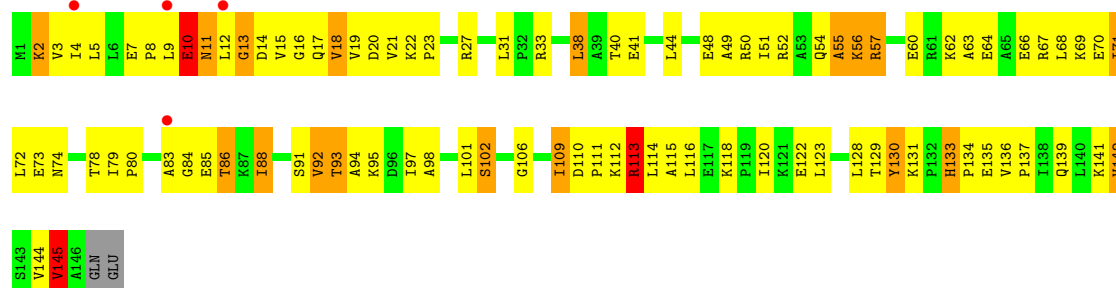
Chain YH:





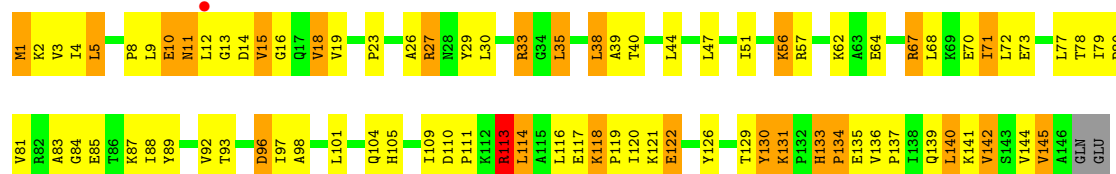
• Molecule 29: 50S ribosomal protein L9

Chain RI:



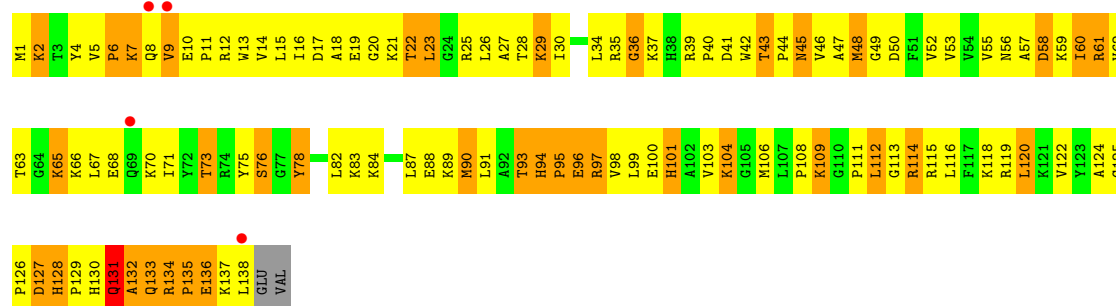
• Molecule 29: 50S ribosomal protein L9

Chain YI:



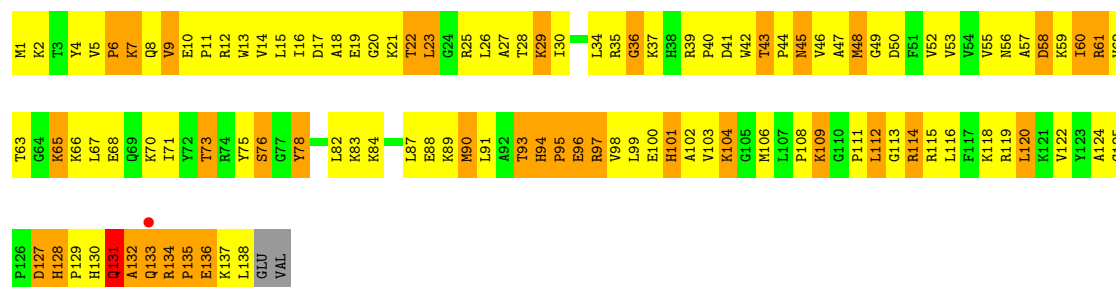
• Molecule 30: 50S ribosomal protein L13

Chain RN:



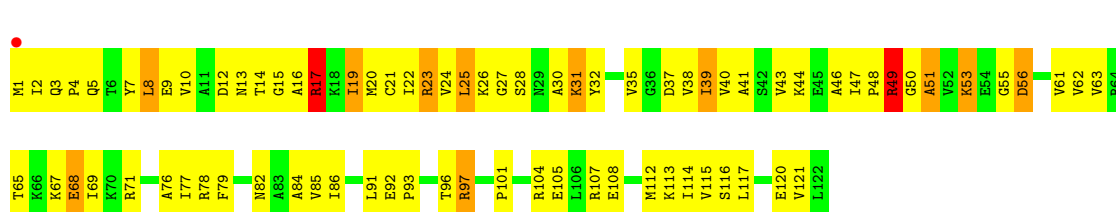
• Molecule 30: 50S ribosomal protein L13

Chain YN:



- Molecule 31: 50S ribosomal protein L14

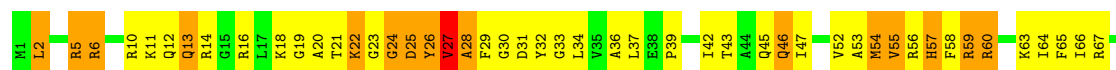
Chain RO:





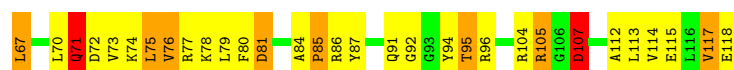
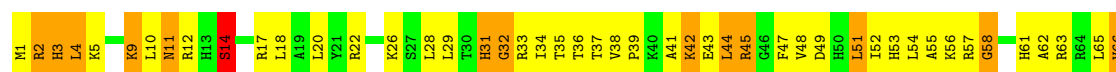
- Molecule 33: 50S ribosomal protein L16

Chain YQ:



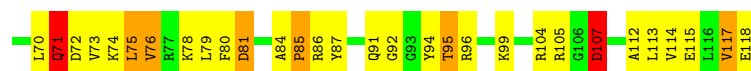
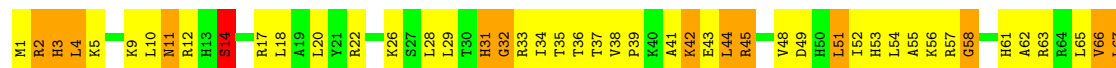
- Molecule 34: 50S ribosomal protein L17

Chain RR:



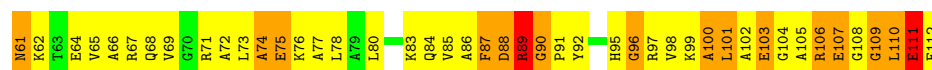
- Molecule 34: 50S ribosomal protein L17

Chain YR:



- Molecule 35: 50S ribosomal protein L18

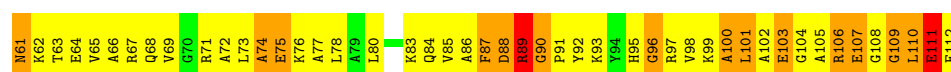
Chain RS:



- Molecule 35: 50S ribosomal protein L18

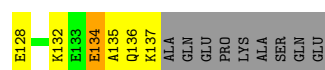
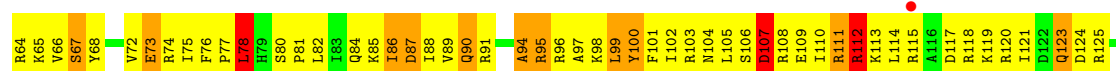
Chain YS:





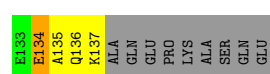
- Molecule 36: 50S ribosomal protein L19

Chain RT:



- Molecule 36: 50S ribosomal protein L19

Chain YT:



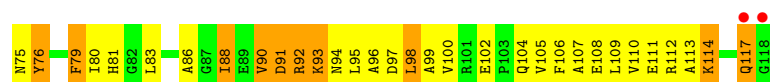
- Molecule 37: 50S ribosomal protein L20

Chain RU:



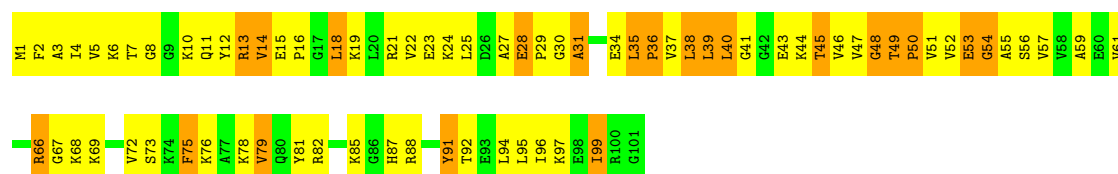
- Molecule 37: 50S ribosomal protein L20

Chain YU:



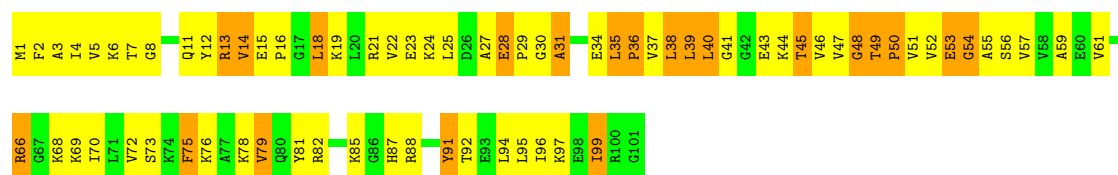
- Molecule 38: 50S ribosomal protein L21

Chain RV:



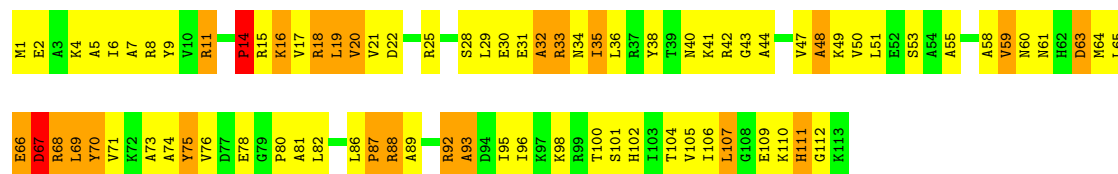
• Molecule 38: 50S ribosomal protein L21

Chain YV:



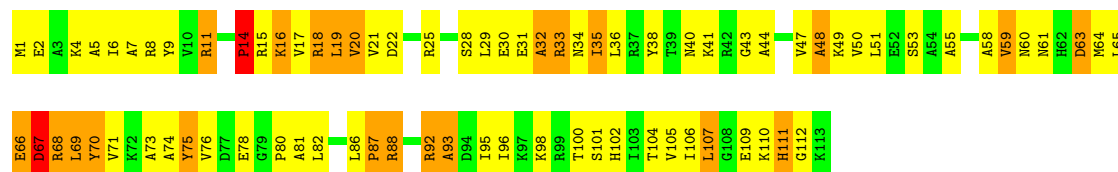
• Molecule 39: 50S ribosomal protein L22

Chain RW:



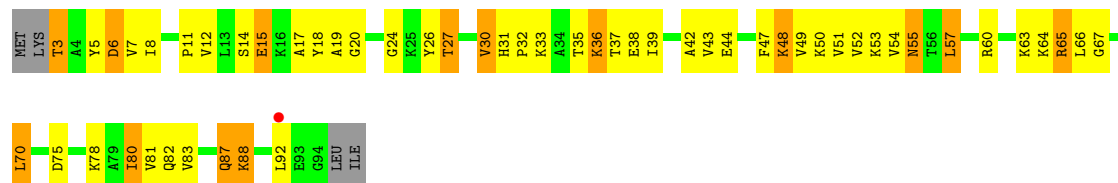
• Molecule 39: 50S ribosomal protein L22

Chain YW:



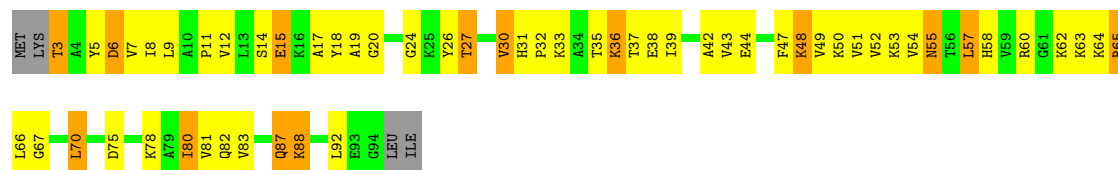
• Molecule 40: 50S ribosomal protein L23

Chain RX:



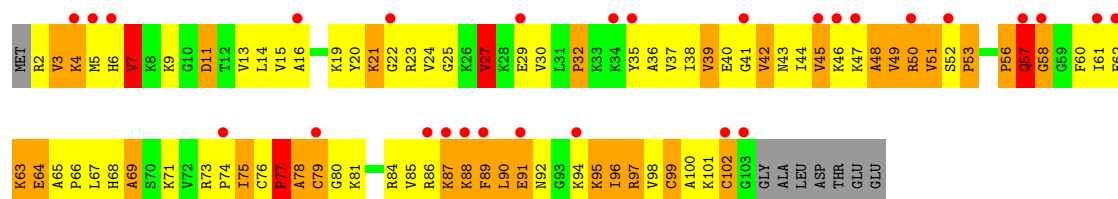
• Molecule 40: 50S ribosomal protein L23

Chain YX:



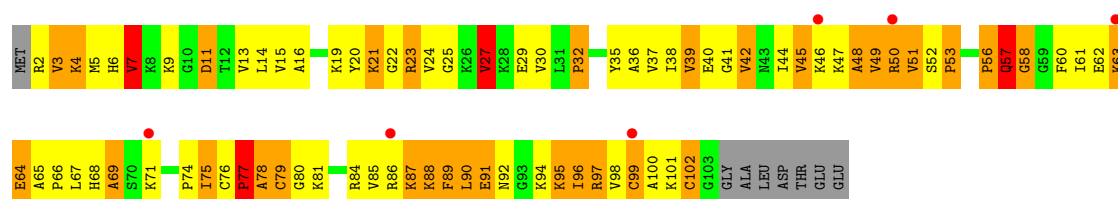
- Molecule 41: 50S ribosomal protein L24

Chain RY:



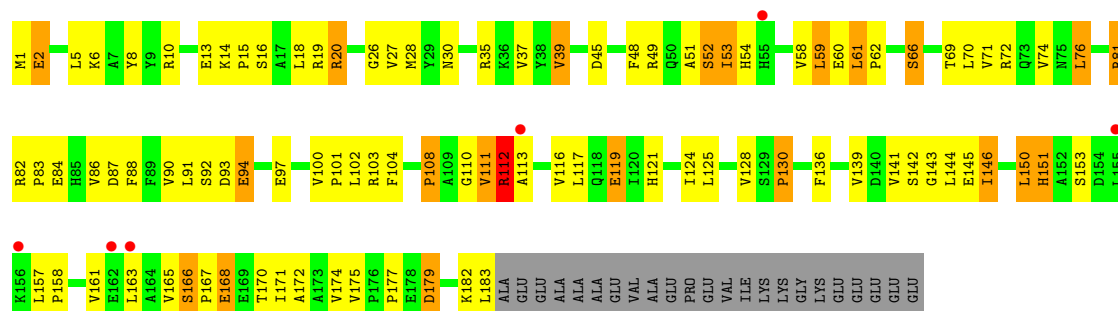
- Molecule 41: 50S ribosomal protein L24

Chain YY:



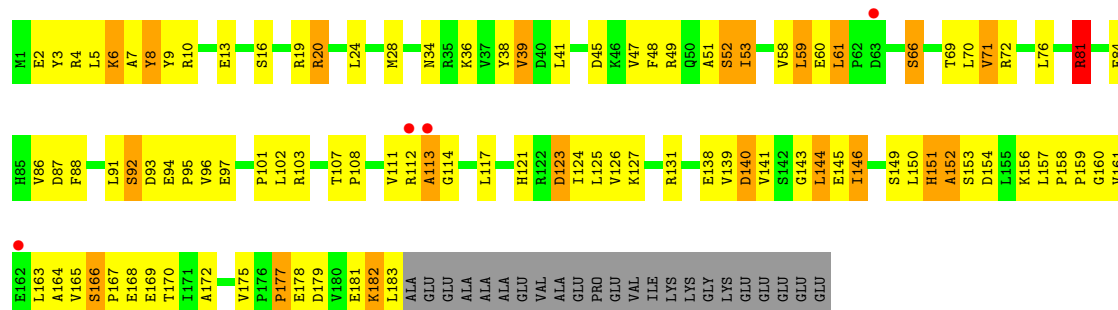
- Molecule 42: 50S ribosomal protein L25

Chain RZ:



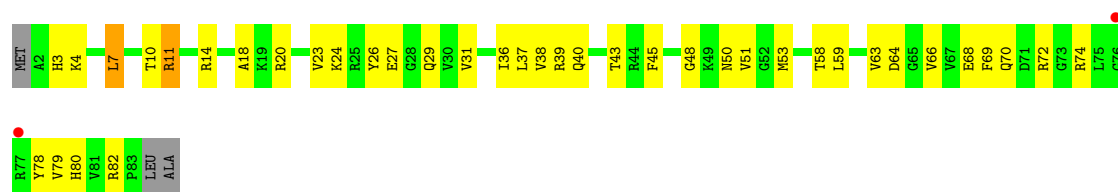
- Molecule 42: 50S ribosomal protein L25

Chain YZ:



- Molecule 43: 50S ribosomal protein L27

Chain R0:



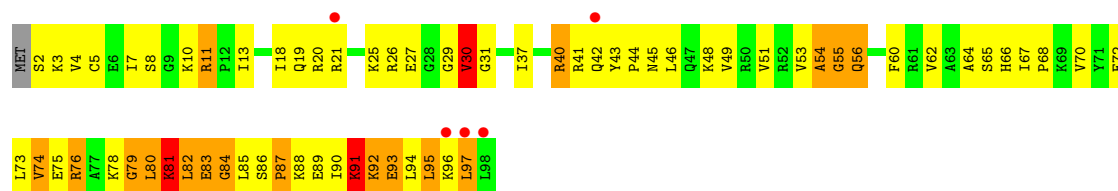
- Molecule 43: 50S ribosomal protein L27

Chain Y0:



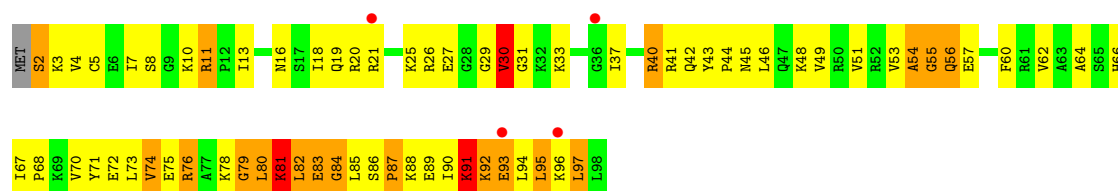
- Molecule 44: 50S ribosomal protein L28

Chain R1:



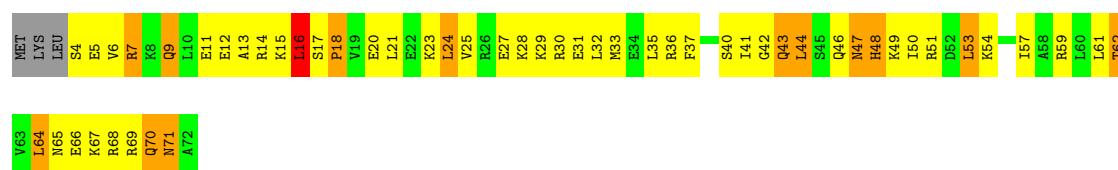
- Molecule 44: 50S ribosomal protein L28

Chain Y1:



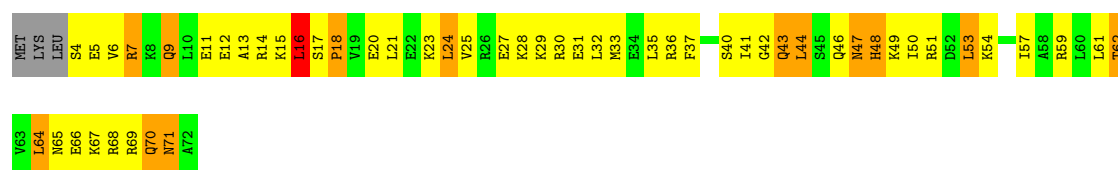
- Molecule 45: 50S ribosomal protein L29

Chain R2:



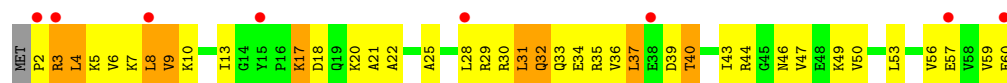
- Molecule 45: 50S ribosomal protein L29

Chain Y2:



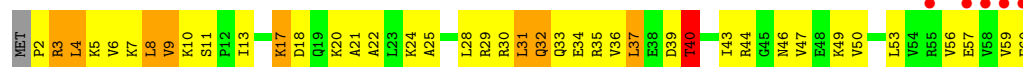
- Molecule 46: 50S ribosomal protein L30

Chain R3:



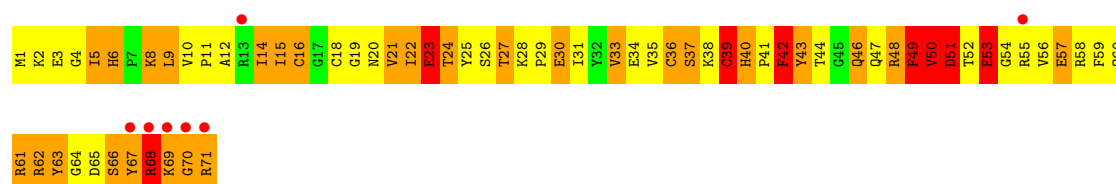
- Molecule 46: 50S ribosomal protein L30

Chain Y3:



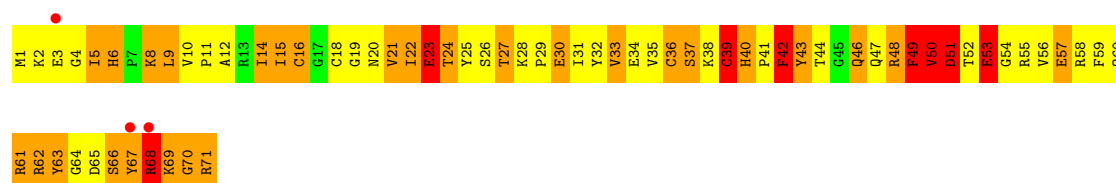
- Molecule 47: 50S ribosomal protein L31

Chain R4:



- Molecule 47: 50S ribosomal protein L31

Chain Y4:



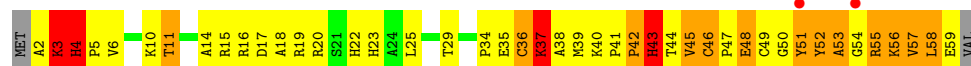
- Molecule 48: 50S ribosomal protein L32

Chain R5:



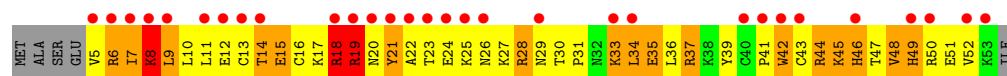
- Molecule 48: 50S ribosomal protein L32

Chain Y5:



- Molecule 49: 50S ribosomal protein L33

Chain R6:



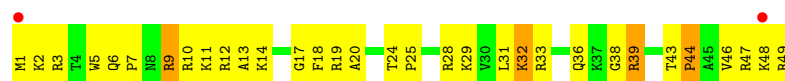
- Molecule 49: 50S ribosomal protein L33

Chain Y6: 



- Molecule 50: 50S ribosomal protein L34

Chain R7: 



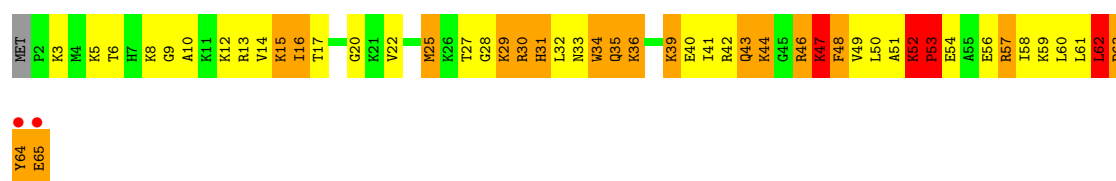
- Molecule 50: 50S ribosomal protein L34

Chain Y7: 



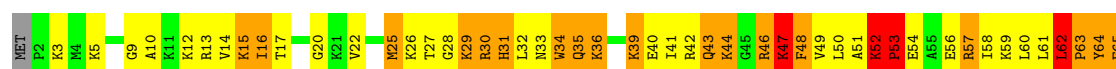
- Molecule 51: 50S ribosomal protein L35

Chain R8: 



- Molecule 51: 50S ribosomal protein L35

Chain Y8: 



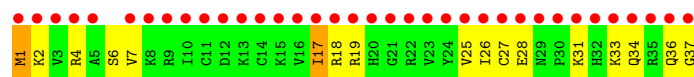
- Molecule 52: 50S ribosomal protein L36

Chain R9: 



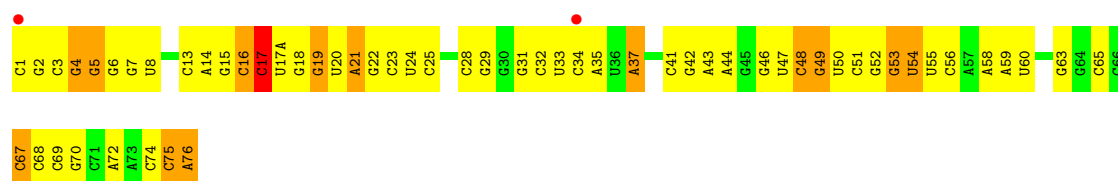
- Molecule 52: 50S ribosomal protein L36

Chain Y9: 



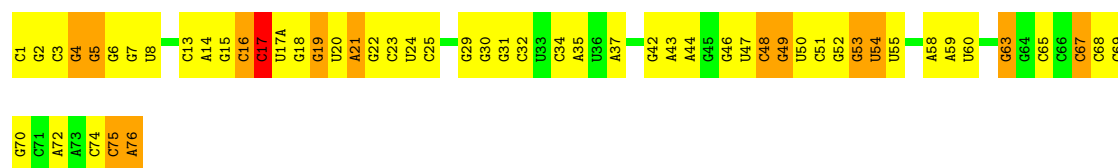
- Molecule 53: P-site tRNA fMet

Chain QV: 



- Molecule 53: P-site tRNA fMet

Chain XV:



- Molecule 54: A-site ASL SufA6

Chain QX:



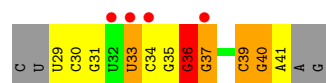
- Molecule 54: A-site ASL SufA6

Chain XX:



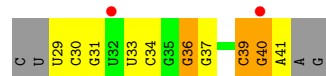
- Molecule 55: messenger RNA

Chain QY:



- Molecule 55: messenger RNA

Chain XY:



- Molecule 56: tRNA acceptor end mimic

Chain Z6:



- Molecule 56: tRNA acceptor end mimic

Chain Z8:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.24Å 446.10Å 623.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.68 – 3.90 49.68 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.68-3.90) 99.1 (49.68-3.70)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.67Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.235 , 0.278 0.235 , 0.278	Depositor DCC
R_{free} test set	23244 reflections (4.44%)	DCC
Wilson B-factor (Å ²)	88.0	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , -0.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 612965 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	291950	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PAR, 1MG, PPU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	QA	0.43	0/36098	0.95	64/56341 (0.1%)
1	XA	0.48	0/36101	1.01	70/56346 (0.1%)
2	QB	0.35	0/1959	0.65	0/2642
2	XB	0.35	0/1959	0.65	0/2642
3	QC	0.36	0/1629	0.60	0/2195
3	XC	0.37	0/1629	0.60	0/2195
4	QD	0.41	0/1733	0.68	1/2318 (0.0%)
4	XD	0.44	0/1733	0.68	1/2318 (0.0%)
5	QE	0.38	0/1171	0.66	0/1576
5	XE	0.38	0/1171	0.66	0/1576
6	QF	0.43	0/856	0.68	0/1154
6	XF	0.43	0/856	0.68	0/1154
7	QG	0.37	0/1276	0.60	0/1709
7	XG	0.36	0/1276	0.60	0/1709
8	QH	0.40	0/1136	0.69	0/1527
8	XH	0.40	0/1136	0.69	0/1527
9	QI	0.36	0/1029	0.67	0/1379
9	XI	0.36	0/1029	0.67	0/1379
10	QJ	0.35	0/814	0.61	0/1095
10	XJ	0.36	0/814	0.61	0/1095
11	QK	0.40	0/900	0.67	0/1213
11	XK	0.40	0/900	0.67	0/1213
12	QL	0.48	1/991 (0.1%)	0.79	2/1327 (0.2%)
12	XL	0.48	1/991 (0.1%)	0.79	2/1327 (0.2%)
13	QM	0.34	0/974	0.66	0/1303
13	XM	0.34	0/974	0.66	0/1303
14	QN	0.42	0/501	0.68	0/664
14	XN	0.52	0/501	0.67	0/664
15	QO	0.39	0/745	0.67	0/992
15	XO	0.39	0/745	0.66	0/992
16	QP	0.36	0/721	0.67	0/970
16	XP	0.37	0/721	0.67	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.37	0/847	0.68	0/1131
17	XQ	0.38	0/847	0.68	0/1131
18	QR	0.39	0/579	0.72	0/768
18	XR	0.39	0/579	0.72	0/768
19	QS	0.36	0/689	0.84	2/926 (0.2%)
19	XS	0.36	0/689	0.84	2/926 (0.2%)
20	QT	0.33	0/765	0.69	0/1007
20	XT	0.34	0/765	0.69	0/1007
21	QU	0.37	0/221	0.63	0/288
21	XU	0.37	0/221	0.63	0/288
22	RA	0.53	2/69521 (0.0%)	1.06	133/108529 (0.1%)
22	YA	0.59	2/69543 (0.0%)	1.12	219/108563 (0.2%)
23	RB	0.41	0/2878	0.95	4/4490 (0.1%)
23	YB	0.49	0/2878	1.04	4/4490 (0.1%)
24	RD	0.59	2/2165 (0.1%)	0.90	4/2919 (0.1%)
24	YD	0.56	1/2165 (0.0%)	0.90	4/2919 (0.1%)
25	RE	0.52	0/1601	0.91	2/2160 (0.1%)
25	YE	0.52	0/1601	0.91	2/2160 (0.1%)
26	RF	0.50	0/1620	0.76	0/2194
26	YF	0.50	0/1620	0.76	0/2194
27	RG	0.40	0/1499	0.66	0/2016
27	YG	0.40	0/1499	0.66	0/2016
28	RH	0.45	0/1332	0.85	3/1802 (0.2%)
28	YH	0.45	0/1332	0.85	4/1802 (0.2%)
29	RI	0.54	2/1151 (0.2%)	0.68	1/1558 (0.1%)
29	YI	0.34	0/1151	0.61	0/1558
30	RN	0.46	0/1131	0.78	1/1525 (0.1%)
30	YN	0.46	0/1131	0.78	1/1525 (0.1%)
31	RO	0.54	0/943	0.71	0/1269
31	YO	0.53	0/943	0.71	0/1269
32	RP	0.50	0/1162	0.94	3/1544 (0.2%)
32	YP	0.50	0/1162	0.95	3/1544 (0.2%)
33	RQ	0.54	0/1143	0.91	3/1527 (0.2%)
33	YQ	0.54	0/1143	0.89	3/1527 (0.2%)
34	RR	0.45	0/982	0.80	1/1312 (0.1%)
34	YR	0.45	0/982	0.80	1/1312 (0.1%)
35	RS	0.46	0/892	0.82	1/1187 (0.1%)
35	YS	0.45	0/892	0.83	1/1187 (0.1%)
36	RT	0.47	0/1155	0.73	2/1542 (0.1%)
36	YT	0.46	0/1155	0.73	2/1542 (0.1%)
37	RU	0.48	0/982	0.78	0/1306
37	YU	0.48	0/982	0.78	0/1306
38	RV	0.47	0/790	0.82	0/1057

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YV	0.47	0/790	0.82	0/1057
39	RW	0.45	0/911	0.75	0/1220
39	YW	0.45	0/911	0.75	0/1220
40	RX	0.56	0/739	0.77	0/993
40	YX	0.56	0/739	0.77	0/993
41	RY	0.52	0/798	0.80	0/1064
41	YY	0.52	0/798	0.80	0/1064
42	RZ	0.36	0/1493	0.58	0/2026
42	YZ	0.36	0/1493	0.62	0/2026
43	R0	0.42	0/657	0.63	0/874
43	Y0	0.42	0/657	0.65	0/874
44	R1	0.49	0/770	0.85	1/1022 (0.1%)
44	Y1	0.49	0/770	0.85	1/1022 (0.1%)
45	R2	0.50	0/583	0.84	1/771 (0.1%)
45	Y2	0.51	0/583	0.84	1/771 (0.1%)
46	R3	0.47	0/474	0.72	0/635
46	Y3	0.43	0/474	0.71	0/635
47	R4	0.38	0/594	0.78	1/795 (0.1%)
47	Y4	0.38	0/594	0.78	1/795 (0.1%)
48	R5	0.51	0/473	0.74	0/639
48	Y5	0.50	0/465	0.74	0/629
49	R6	0.42	0/431	0.76	0/575
49	Y6	0.43	0/431	0.76	0/575
50	R7	0.56	0/438	0.76	0/575
50	Y7	0.56	0/438	0.76	0/575
51	R8	0.62	0/525	0.93	1/691 (0.1%)
51	Y8	0.62	0/525	0.93	1/691 (0.1%)
52	R9	0.35	0/310	0.60	0/407
52	Y9	0.37	0/310	0.61	0/407
53	QV	0.51	0/1836	0.99	6/2859 (0.2%)
53	XV	0.51	0/1836	0.99	6/2859 (0.2%)
54	QX	0.74	0/188	0.84	0/290
54	XX	0.48	0/188	0.74	0/290
55	QY	0.78	1/311 (0.3%)	0.88	0/483
55	XY	0.51	0/311	0.88	0/483
56	Z6	0.79	0/40	1.79	1/60 (1.7%)
56	Z8	0.79	0/40	1.83	1/60 (1.7%)
All	All	0.50	12/316321 (0.0%)	0.98	568/472911 (0.1%)

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	RD	236	GLY	C-N	8.53	1.53	1.34
29	RI	54	GLN	C-O	-7.01	1.10	1.23
55	QY	36	G	C2-N2	-6.93	1.27	1.34
22	YA	1142(A)	A	N9-C4	-6.45	1.33	1.37
29	RI	55	ALA	C-O	6.04	1.34	1.23

The worst 5 of 568 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	XV	17	C	C2-N1-C1'	11.79	131.77	118.80
53	QV	17	C	C2-N1-C1'	11.74	131.72	118.80
22	YA	761	A	N1-C6-N6	11.29	125.37	118.60
1	XA	328	C	C6-N1-C2	-10.26	116.19	120.30
25	YE	21	VAL	C-N-CD	-10.09	98.39	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	672	0
1	XA	32249	0	16278	742	1
2	QB	1924	0	1975	283	0
2	XB	1924	0	1975	290	0
3	QC	1605	0	1668	210	0
3	XC	1605	0	1668	210	0
4	QD	1703	0	1764	247	0
4	XD	1703	0	1765	215	1
5	QE	1155	0	1213	159	0
5	XE	1155	0	1213	133	0
6	QF	843	0	857	92	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	XF	843	0	857	96	0
7	QG	1257	0	1296	146	0
7	XG	1257	0	1294	147	0
8	QH	1116	0	1175	151	0
8	XH	1116	0	1177	149	0
9	QI	1010	0	1037	140	0
9	XI	1010	0	1037	153	0
10	QJ	801	0	849	149	0
10	XJ	801	0	849	135	0
11	QK	885	0	904	103	0
11	XK	885	0	904	110	0
12	QL	975	0	1062	111	0
12	XL	975	0	1062	116	0
13	QM	964	0	1034	152	0
13	XM	964	0	1034	216	0
14	QN	492	0	529	103	0
14	XN	492	0	529	95	0
15	QO	734	0	771	78	0
15	XO	734	0	771	72	0
16	QP	705	0	725	115	0
16	XP	705	0	725	105	0
17	QQ	834	0	904	77	0
17	XQ	834	0	904	71	0
18	QR	574	0	644	69	0
18	XR	574	0	644	68	0
19	QS	674	0	699	117	0
19	XS	674	0	699	150	0
20	QT	763	0	860	109	0
20	XT	763	0	861	102	0
21	QU	217	0	234	25	0
21	XU	217	0	234	26	0
22	RA	62071	0	31286	1243	0
22	YA	62091	0	31295	1282	0
23	RB	2573	0	1306	68	0
23	YB	2573	0	1306	57	0
24	RD	2115	0	2195	320	0
24	YD	2115	0	2195	323	0
25	RE	1568	0	1634	268	0
25	YE	1568	0	1634	272	0
26	RF	1585	0	1632	178	0
26	YF	1585	0	1632	179	0
27	RG	1474	0	1535	202	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	YG	1474	0	1535	204	0
28	RH	1307	0	1382	220	0
28	YH	1307	0	1382	227	3
29	RI	1136	0	1223	61	1
29	YI	1136	0	1223	57	0
30	RN	1104	0	1180	190	0
30	YN	1104	0	1180	186	0
31	RO	933	0	996	124	0
31	YO	933	0	996	131	0
32	RP	1145	0	1227	247	0
32	YP	1145	0	1228	239	0
33	RQ	1122	0	1179	150	0
33	YQ	1122	0	1178	149	0
34	RR	968	0	1033	110	0
34	YR	968	0	1033	114	0
35	RS	882	0	943	156	0
35	YS	882	0	943	159	0
36	RT	1141	0	1202	156	0
36	YT	1141	0	1202	152	0
37	RU	964	0	1022	128	0
37	YU	964	0	1022	134	0
38	RV	779	0	852	130	0
38	YV	779	0	852	128	0
39	RW	900	0	964	101	0
39	YW	900	0	964	102	0
40	RX	725	0	778	67	0
40	YX	725	0	778	67	0
41	RY	785	0	878	166	0
41	YY	785	0	878	154	3
42	RZ	1461	0	1493	63	0
42	YZ	1461	0	1493	70	0
43	R0	648	0	672	28	0
43	Y0	648	0	672	44	0
44	R1	763	0	848	143	0
44	Y1	763	0	848	140	0
45	R2	581	0	629	80	0
45	Y2	581	0	629	79	0
46	R3	469	0	518	41	0
46	Y3	469	0	518	44	0
47	R4	581	0	574	156	0
47	Y4	581	0	574	225	0
48	R5	459	0	480	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	Y5	451	0	471	68	0
49	R6	424	0	450	93	0
49	Y6	424	0	450	90	0
50	R7	430	0	480	42	0
50	Y7	430	0	480	44	0
51	R8	517	0	582	102	0
51	Y8	517	0	582	102	0
52	R9	307	0	335	16	0
52	Y9	307	0	336	20	0
53	QV	1644	0	836	63	0
53	XV	1644	0	836	56	0
54	QX	169	0	88	55	0
54	XX	169	0	88	17	0
55	QY	303	0	152	22	0
55	XY	303	0	154	30	0
56	Z6	74	0	51	24	0
56	Z8	74	0	51	14	0
57	QA	65	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QM	1	0	0	0	0
57	QX	1	0	0	0	0
57	R5	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	244	0	0	0	0
57	RB	2	0	0	0	0
57	RD	1	0	0	0	0
57	RE	2	0	0	0	0
57	RF	1	0	0	0	0
57	RP	2	0	0	0	0
57	RR	1	0	0	0	0
57	RU	1	0	0	0	0
57	XA	72	0	0	0	0
57	XM	1	0	0	0	0
57	XV	2	0	0	0	0
57	XX	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y7	1	0	0	0	0
57	YA	265	0	0	0	0
57	YB	3	0	0	0	0
57	YE	1	0	0	0	0
57	YP	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	YQ	1	0	0	0	0
57	YX	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	R9	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y9	1	0	0	0	0
All	All	291950	0	198321	15633	5

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 32.

The worst 5 of 15633 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:XA:1400:C:N4	53:XV:34:C:C6	1.71	1.55
14:XN:32:SER:CB	14:XN:41:ARG:HB3	1.23	1.55
14:XN:32:SER:HB3	14:XN:41:ARG:CB	1.27	1.54
28:RH:127:GLU:CG	28:RH:128:PRO:HD3	1.35	1.53
28:YH:127:GLU:CG	28:YH:128:PRO:HD3	1.35	1.52

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
28:YH:45:VAL:O	41:YY:24:VAL:N[4_445]	1.97	0.23
29:RI:91:SER:OG	1:XA:368:U:OP1[4_555]	2.05	0.15
28:YH:44:VAL:CG2	41:YY:23:ARG:CD[4_445]	2.08	0.12
6:QF:15:ASP:OD2	4:XD:27:TYR:OH[4_555]	2.14	0.06
28:YH:47:GLU:OE2	41:YY:79:CYS:CB[4_445]	2.18	0.02

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%)	153 (65%)	52 (22%)	30 (13%)	0	13
2	XB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	13
3	QC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	1	23
3	XC	203/239 (85%)	129 (64%)	55 (27%)	19 (9%)	1	23
4	QD	206/209 (99%)	136 (66%)	50 (24%)	20 (10%)	1	21
4	XD	206/209 (99%)	135 (66%)	48 (23%)	23 (11%)	1	16
5	QE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	1	19
5	XE	149/162 (92%)	103 (69%)	30 (20%)	16 (11%)	1	17
6	QF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	24
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	24
7	QG	153/156 (98%)	101 (66%)	37 (24%)	15 (10%)	1	21
7	XG	153/156 (98%)	103 (67%)	36 (24%)	14 (9%)	1	24
8	QH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	1	16
8	XH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	1	16
9	QI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	13
9	XI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	13
10	QJ	97/105 (92%)	68 (70%)	20 (21%)	9 (9%)	1	23
10	XJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	1	19
11	QK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	2	34
11	XK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	2	34
12	QL	123/132 (93%)	84 (68%)	23 (19%)	16 (13%)	0	12
12	XL	123/132 (93%)	84 (68%)	24 (20%)	15 (12%)	1	14
13	QM	119/126 (94%)	71 (60%)	29 (24%)	19 (16%)	0	7
13	XM	119/126 (94%)	71 (60%)	27 (23%)	21 (18%)	0	5
14	QN	58/61 (95%)	31 (53%)	15 (26%)	12 (21%)	0	3
14	XN	58/61 (95%)	33 (57%)	13 (22%)	12 (21%)	0	3
15	QO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	2	33
15	XO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	2	33
16	QP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	11
16	XP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	11
17	QQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	27
18	QR	68/88 (77%)	45 (66%)	15 (22%)	8 (12%)	1	14
18	XR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	1	14
19	QS	82/93 (88%)	47 (57%)	17 (21%)	18 (22%)	0	2
19	XS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	2
20	QT	97/106 (92%)	63 (65%)	16 (16%)	18 (19%)	0	4
20	XT	97/106 (92%)	63 (65%)	15 (16%)	19 (20%)	0	4
21	QU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	6
21	XU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	6
24	RD	270/276 (98%)	203 (75%)	48 (18%)	19 (7%)	2	33
24	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	2	33
25	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	3
25	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	3
26	RF	200/210 (95%)	143 (72%)	37 (18%)	20 (10%)	1	20
26	YF	200/210 (95%)	143 (72%)	37 (18%)	20 (10%)	1	20
27	RG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	1	14
27	YG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	1	14
28	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	2
28	YH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	2
29	RI	144/148 (97%)	106 (74%)	21 (15%)	17 (12%)	1	14
29	YI	144/148 (97%)	100 (69%)	27 (19%)	17 (12%)	1	14
30	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	7
30	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	7
31	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	2	30
31	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	2	30
32	RP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	3
32	YP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	3
33	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	1	19
33	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	1	19
34	RR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	1	14
34	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	6
35	YS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	6
36	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	9
36	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	9
37	RU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	29
37	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	29
38	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	19
38	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	19
39	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	13
39	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	13
40	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	3	40
40	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	3	40
41	RY	100/110 (91%)	58 (58%)	16 (16%)	26 (26%)	0	2
41	YY	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0	2
42	RZ	181/206 (88%)	131 (72%)	28 (16%)	22 (12%)	1	14
42	YZ	181/206 (88%)	128 (71%)	35 (19%)	18 (10%)	1	20
43	R0	80/85 (94%)	67 (84%)	12 (15%)	1 (1%)	18	75
43	Y0	80/85 (94%)	67 (84%)	11 (14%)	2 (2%)	9	62
44	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	1	15
44	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	1	15
45	R2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	11
45	Y2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	11
46	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	3	41
46	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	3	41
47	R4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
47	Y4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
48	R5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	2
48	Y5	56/60 (93%)	32 (57%)	9 (16%)	15 (27%)	0	1
49	R6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	1
49	Y6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	1
50	R7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	36
51	R8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	5
51	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	5
52	R9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
52	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11469/12128 (95%)	7649 (67%)	2333 (20%)	1487 (13%)	0	12

5 of 1487 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	181 (88%)	24 (12%)	8	43
2	XB	205/220 (93%)	181 (88%)	24 (12%)	8	43
3	QC	159/188 (85%)	143 (90%)	16 (10%)	11	51
3	XC	159/188 (85%)	143 (90%)	16 (10%)	11	51
4	QD	180/181 (99%)	160 (89%)	20 (11%)	9	46
4	XD	180/181 (99%)	165 (92%)	15 (8%)	16	62
5	QE	116/123 (94%)	107 (92%)	9 (8%)	18	64
5	XE	116/123 (94%)	107 (92%)	9 (8%)	18	64
6	QF	90/90 (100%)	76 (84%)	14 (16%)	4	28
6	XF	90/90 (100%)	76 (84%)	14 (16%)	4	28
7	QG	126/127 (99%)	114 (90%)	12 (10%)	12	54
7	XG	126/127 (99%)	115 (91%)	11 (9%)	15	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	QH	119/119 (100%)	106 (89%)	13 (11%)	9	47
8	XH	119/119 (100%)	106 (89%)	13 (11%)	9	47
9	QI	98/99 (99%)	87 (89%)	11 (11%)	9	45
9	XI	98/99 (99%)	87 (89%)	11 (11%)	9	45
10	QJ	89/92 (97%)	81 (91%)	8 (9%)	14	58
10	XJ	89/92 (97%)	81 (91%)	8 (9%)	14	58
11	QK	90/99 (91%)	81 (90%)	9 (10%)	11	52
11	XK	90/99 (91%)	81 (90%)	9 (10%)	11	52
12	QL	104/109 (95%)	88 (85%)	16 (15%)	4	29
12	XL	104/109 (95%)	89 (86%)	15 (14%)	5	32
13	QM	97/101 (96%)	81 (84%)	16 (16%)	3	25
13	XM	97/101 (96%)	81 (84%)	16 (16%)	3	25
14	QN	49/50 (98%)	40 (82%)	9 (18%)	2	18
14	XN	49/50 (98%)	44 (90%)	5 (10%)	11	51
15	QO	79/80 (99%)	73 (92%)	6 (8%)	19	66
15	XO	79/80 (99%)	73 (92%)	6 (8%)	19	66
16	QP	72/74 (97%)	63 (88%)	9 (12%)	7	40
16	XP	72/74 (97%)	63 (88%)	9 (12%)	7	40
17	QQ	95/97 (98%)	89 (94%)	6 (6%)	25	73
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	25	73
18	QR	61/77 (79%)	54 (88%)	7 (12%)	8	44
18	XR	61/77 (79%)	54 (88%)	7 (12%)	8	44
19	QS	73/80 (91%)	62 (85%)	11 (15%)	4	30
19	XS	73/80 (91%)	62 (85%)	11 (15%)	4	30
20	QT	76/82 (93%)	68 (90%)	8 (10%)	10	49
20	XT	76/82 (93%)	69 (91%)	7 (9%)	13	56
21	QU	20/22 (91%)	19 (95%)	1 (5%)	34	80
21	XU	20/22 (91%)	19 (95%)	1 (5%)	34	80
24	RD	214/218 (98%)	177 (83%)	37 (17%)	3	22
24	YD	214/218 (98%)	178 (83%)	36 (17%)	3	24
25	RE	165/166 (99%)	127 (77%)	38 (23%)	1	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	YE	165/166 (99%)	127 (77%)	38 (23%)	1	10
26	RF	161/166 (97%)	140 (87%)	21 (13%)	6	38
26	YF	161/166 (97%)	140 (87%)	21 (13%)	6	38
27	RG	155/156 (99%)	130 (84%)	25 (16%)	3	27
27	YG	155/156 (99%)	131 (84%)	24 (16%)	4	28
28	RH	142/148 (96%)	114 (80%)	28 (20%)	2	15
28	YH	142/148 (96%)	114 (80%)	28 (20%)	2	15
29	RI	122/124 (98%)	100 (82%)	22 (18%)	2	19
29	YI	122/124 (98%)	101 (83%)	21 (17%)	3	22
30	RN	117/119 (98%)	98 (84%)	19 (16%)	3	26
30	YN	117/119 (98%)	98 (84%)	19 (16%)	3	26
31	RO	100/100 (100%)	90 (90%)	10 (10%)	11	52
31	YO	100/100 (100%)	90 (90%)	10 (10%)	11	52
32	RP	116/116 (100%)	89 (77%)	27 (23%)	1	9
32	YP	116/116 (100%)	89 (77%)	27 (23%)	1	9
33	RQ	111/111 (100%)	93 (84%)	18 (16%)	3	26
33	YQ	111/111 (100%)	93 (84%)	18 (16%)	3	26
34	RR	101/101 (100%)	84 (83%)	17 (17%)	3	24
34	YR	101/101 (100%)	84 (83%)	17 (17%)	3	24
35	RS	87/88 (99%)	74 (85%)	13 (15%)	4	31
35	YS	87/88 (99%)	74 (85%)	13 (15%)	4	31
36	RT	120/127 (94%)	97 (81%)	23 (19%)	2	16
36	YT	120/127 (94%)	97 (81%)	23 (19%)	2	16
37	RU	93/94 (99%)	80 (86%)	13 (14%)	5	34
37	YU	93/94 (99%)	80 (86%)	13 (14%)	5	34
38	RV	82/82 (100%)	71 (87%)	11 (13%)	6	36
38	YV	82/82 (100%)	71 (87%)	11 (13%)	6	36
39	RW	92/92 (100%)	77 (84%)	15 (16%)	3	26
39	YW	92/92 (100%)	77 (84%)	15 (16%)	3	26
40	RX	74/78 (95%)	63 (85%)	11 (15%)	4	31
40	YX	74/78 (95%)	63 (85%)	11 (15%)	4	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	RY	85/91 (93%)	70 (82%)	15 (18%)	3	21
41	YY	85/91 (93%)	70 (82%)	15 (18%)	3	21
42	RZ	162/179 (90%)	141 (87%)	21 (13%)	6	38
42	YZ	162/179 (90%)	139 (86%)	23 (14%)	5	34
43	R0	65/67 (97%)	57 (88%)	8 (12%)	7	41
43	Y0	65/67 (97%)	60 (92%)	5 (8%)	18	65
44	R1	82/83 (99%)	67 (82%)	15 (18%)	2	18
44	Y1	82/83 (99%)	67 (82%)	15 (18%)	2	18
45	R2	64/67 (96%)	57 (89%)	7 (11%)	9	47
45	Y2	64/67 (96%)	57 (89%)	7 (11%)	9	47
46	R3	51/52 (98%)	40 (78%)	11 (22%)	1	11
46	Y3	51/52 (98%)	40 (78%)	11 (22%)	1	11
47	R4	63/63 (100%)	44 (70%)	19 (30%)	0	5
47	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	5
48	R5	51/52 (98%)	39 (76%)	12 (24%)	1	9
48	Y5	50/52 (96%)	38 (76%)	12 (24%)	1	8
49	R6	48/52 (92%)	38 (79%)	10 (21%)	2	13
49	Y6	48/52 (92%)	38 (79%)	10 (21%)	2	13
50	R7	42/42 (100%)	39 (93%)	3 (7%)	21	69
50	Y7	42/42 (100%)	39 (93%)	3 (7%)	21	69
51	R8	54/55 (98%)	39 (72%)	15 (28%)	0	6
51	Y8	54/55 (98%)	39 (72%)	15 (28%)	0	6
52	R9	34/34 (100%)	32 (94%)	2 (6%)	28	75
52	Y9	34/34 (100%)	32 (94%)	2 (6%)	28	75
All	All	9701/10066 (96%)	8295 (86%)	1406 (14%)	5	32

5 of 1406 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	R2	53	LEU
6	XF	97	PHE
42	YZ	139	VAL
47	R4	23	GLU
2	XB	23	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 112 such sidechains are listed below:

Mol	Chain	Res	Type
45	R2	47	ASN
6	XF	64	GLN
42	YZ	32	HIS
46	R3	32	GLN
2	XB	204	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	281 (18%)	47 (3%)
1	XA	1498/1522 (98%)	299 (19%)	52 (3%)
22	RA	2879/2916 (98%)	658 (22%)	65 (2%)
22	YA	2880/2916 (98%)	639 (22%)	65 (2%)
23	RB	119/122 (97%)	20 (16%)	2 (1%)
23	YB	119/122 (97%)	25 (21%)	1 (0%)
53	QV	76/77 (98%)	30 (39%)	1 (1%)
53	XV	76/77 (98%)	30 (39%)	1 (1%)
54	QX	7/25 (28%)	5 (71%)	2 (28%)
54	XX	7/25 (28%)	4 (57%)	1 (14%)
55	QY	13/18 (72%)	6 (46%)	2 (15%)
55	XY	13/18 (72%)	5 (38%)	1 (7%)
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9188/9366 (98%)	2002 (21%)	240 (2%)

5 of 2002 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	22	G
1	QA	32	A
1	QA	39	G

5 of 240 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	RA	2776	A
1	XA	530	G
22	YA	2566	A

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Mol	Chain	Res	Type
22	RA	2867	G
1	XA	243	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
55	1MG	QY	37	55	24,26,27	1.53	5 (20%)	34,39,42	7.99	7 (20%)
55	1MG	XY	37	55	24,26,27	3.00	6 (25%)	34,39,42	3.70	12 (35%)
56	PPU	Z6	76	56,22	38,40,41	2.43	9 (23%)	54,57,60	2.61	14 (25%)
56	PPU	Z8	76	56,22	38,40,41	2.42	9 (23%)	54,57,60	2.61	14 (25%)

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
55	1MG	QY	37	55	-	0/8/25/26	0/3/3/3
55	1MG	XY	37	55	-	0/8/25/26	0/3/3/3
56	PPU	Z6	76	56,22	-	0/26/43/44	0/4/4/4
56	PPU	Z8	76	56,22	-	0/26/43/44	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z6	76	PPU	O-C	9.24	1.41	1.23
56	Z8	76	PPU	O-C	9.22	1.41	1.23
55	XY	37	1MG	C4-N3	8.14	1.49	1.35
55	XY	37	1MG	C2-N1	7.35	1.47	1.37
55	XY	37	1MG	C2-N2	6.72	1.48	1.33

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	QY	37	1MG	C6-C5-N7	-44.70	131.86	134.24
55	XY	37	1MG	C6-C5-N7	-14.92	133.44	134.24
55	XY	37	1MG	C6-N1-C2	11.94	123.98	120.71
55	QY	37	1MG	CM1-N1-C2	10.04	125.48	119.51
56	Z8	76	PPU	N3-C2-N1	-8.58	121.34	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 684 ligands modelled in this entry, 682 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	PAR	QA	1666	-	45,45,45	1.31	7 (15%)	67,67,67	1.40	8 (11%)
58	PAR	XA	1673	-	45,45,45	1.36	6 (13%)	67,67,67	1.33	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	QA	1666	-	-	0/18/94/94	0/4/4/4
58	PAR	XA	1673	-	-	0/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	QA	1666	PAR	C52-C42	3.18	1.58	1.52
58	XA	1673	PAR	C52-C42	3.06	1.58	1.52
58	XA	1673	PAR	O54-C14	2.92	1.49	1.41
58	QA	1666	PAR	C64-C54	2.91	1.59	1.51
58	QA	1666	PAR	O54-C14	2.88	1.49	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	QA	1666	PAR	O52-C13-C23	4.74	115.96	107.50
58	XA	1673	PAR	C14-O54-C54	4.35	122.15	113.73
58	XA	1673	PAR	O52-C13-C23	4.26	115.10	107.50
58	XA	1673	PAR	O33-C14-C24	4.19	116.36	108.08
58	QA	1666	PAR	C14-O54-C54	3.87	121.21	113.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1500/1522 (98%)	-0.14	17 (1%) 77 61	22, 75, 152, 231	0
1	XA	1500/1522 (98%)	-0.30	9 (0%) 86 74	7, 55, 142, 232	0
2	QB	237/256 (92%)	0.56	12 (5%) 27 22	47, 109, 145, 182	0
2	XB	237/256 (92%)	0.33	8 (3%) 43 33	38, 88, 133, 159	0
3	QC	205/239 (85%)	0.29	3 (1%) 70 54	39, 98, 133, 150	0
3	XC	205/239 (85%)	0.03	1 (0%) 88 77	20, 67, 110, 138	0
4	QD	208/209 (99%)	0.35	2 (0%) 79 64	29, 79, 128, 167	0
4	XD	208/209 (99%)	0.29	1 (0%) 88 77	10, 72, 110, 139	0
5	QE	151/162 (93%)	0.42	5 (3%) 44 34	25, 85, 122, 159	0
5	XE	151/162 (93%)	0.18	2 (1%) 74 58	1, 62, 104, 134	0
6	QF	101/101 (100%)	0.29	1 (0%) 79 64	16, 74, 116, 131	0
6	XF	101/101 (100%)	0.18	0 100 100	16, 65, 110, 133	0
7	QG	155/156 (99%)	0.53	12 (7%) 13 13	30, 84, 125, 149	0
7	XG	155/156 (99%)	0.36	6 (3%) 37 29	20, 71, 109, 131	0
8	QH	138/138 (100%)	0.50	3 (2%) 59 44	45, 88, 124, 156	0
8	XH	138/138 (100%)	0.36	1 (0%) 84 71	19, 70, 102, 125	0
9	QI	127/128 (99%)	0.89	11 (8%) 10 12	46, 97, 137, 144	0
9	XI	127/128 (99%)	0.44	3 (2%) 56 42	16, 79, 119, 129	0
10	QJ	99/105 (94%)	1.03	13 (13%) 4 5	44, 108, 142, 161	0
10	XJ	99/105 (94%)	0.69	10 (10%) 7 9	9, 83, 129, 147	0
11	QK	119/129 (92%)	0.43	8 (6%) 17 17	18, 71, 123, 149	0
11	XK	119/129 (92%)	0.41	5 (4%) 35 27	15, 63, 110, 147	0
12	QL	125/132 (94%)	0.66	7 (5%) 24 20	20, 72, 108, 139	0
12	XL	125/132 (94%)	0.23	3 (2%) 56 42	0, 48, 91, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	0.73	10 (8%) 11 12	39, 96, 131, 170	0
13	XM	121/126 (96%)	0.30	3 (2%) 54 41	4, 68, 125, 149	0
14	QN	60/61 (98%)	0.80	6 (10%) 8 9	52, 98, 137, 146	0
14	XN	60/61 (98%)	0.19	0 100 100	4, 60, 100, 120	0
15	QO	88/89 (98%)	0.37	6 (6%) 17 16	30, 79, 120, 136	0
15	XO	88/89 (98%)	0.18	0 100 100	10, 64, 93, 107	0
16	QP	84/88 (95%)	0.55	2 (2%) 56 42	12, 68, 103, 138	0
16	XP	84/88 (95%)	0.72	3 (3%) 41 32	30, 70, 106, 135	0
17	QQ	100/105 (95%)	0.74	7 (7%) 16 15	33, 82, 115, 141	0
17	XQ	100/105 (95%)	0.53	2 (2%) 62 46	14, 64, 102, 124	0
18	QR	70/88 (79%)	0.64	6 (8%) 11 12	18, 78, 119, 147	0
18	XR	70/88 (79%)	0.48	4 (5%) 23 19	22, 67, 109, 135	0
19	QS	84/93 (90%)	0.77	8 (9%) 8 10	60, 102, 132, 147	0
19	XS	84/93 (90%)	0.37	2 (2%) 56 42	15, 73, 112, 164	0
20	QT	99/106 (93%)	0.42	3 (3%) 48 36	3, 77, 111, 131	0
20	XT	99/106 (93%)	0.55	2 (2%) 62 46	19, 77, 117, 126	0
21	QU	25/27 (92%)	1.98	11 (44%) 1 1	37, 85, 131, 145	0
21	XU	25/27 (92%)	1.21	3 (12%) 5 7	30, 75, 103, 134	0
22	RA	2882/2916 (98%)	-0.23	81 (2%) 50 38	2, 45, 174, 236	0
22	YA	2883/2916 (98%)	-0.31	56 (1%) 64 48	1, 35, 165, 227	0
23	RB	120/122 (98%)	-0.20	0 100 100	46, 89, 131, 153	0
23	YB	120/122 (98%)	-0.45	1 (0%) 83 69	18, 58, 93, 139	0
24	RD	272/276 (98%)	0.15	0 100 100	4, 41, 81, 123	0
24	YD	272/276 (98%)	0.18	1 (0%) 90 81	1, 33, 74, 140	0
25	RE	205/206 (99%)	0.28	4 (1%) 62 46	7, 62, 112, 141	0
25	YE	205/206 (99%)	0.28	2 (0%) 79 64	6, 56, 103, 125	0
26	RF	202/210 (96%)	0.19	1 (0%) 88 77	1, 64, 110, 129	0
26	YF	202/210 (96%)	0.16	2 (0%) 79 64	1, 47, 95, 112	0
27	RG	181/182 (99%)	0.51	6 (3%) 44 34	34, 99, 142, 166	0
27	YG	181/182 (99%)	0.15	1 (0%) 86 74	9, 66, 115, 163	0
28	RH	170/180 (94%)	1.01	22 (12%) 4 6	32, 108, 152, 170	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YH	170/180 (94%)	0.37	4 (2%) 56 42	14, 68, 110, 133	0
29	RI	146/148 (98%)	0.48	4 (2%) 52 39	16, 78, 122, 154	0
29	YI	146/148 (98%)	0.36	1 (0%) 84 71	8, 72, 119, 159	0
30	RN	138/140 (98%)	0.46	4 (2%) 49 37	14, 70, 110, 124	0
30	YN	138/140 (98%)	0.25	1 (0%) 84 71	8, 55, 103, 128	0
31	RO	122/122 (100%)	0.33	1 (0%) 83 69	5, 56, 97, 126	0
31	YO	122/122 (100%)	0.19	0 100 100	0, 42, 79, 94	0
32	RP	150/150 (100%)	0.63	11 (7%) 15 14	6, 65, 126, 159	0
32	YP	150/150 (100%)	0.29	0 100 100	5, 53, 105, 154	0
33	RQ	141/141 (100%)	0.39	4 (2%) 50 38	2, 62, 106, 142	0
33	YQ	141/141 (100%)	0.14	1 (0%) 84 71	3, 42, 94, 132	0
34	RR	118/118 (100%)	0.26	0 100 100	8, 50, 92, 118	0
34	YR	118/118 (100%)	0.24	0 100 100	7, 43, 89, 109	0
35	RS	111/112 (99%)	0.58	4 (3%) 41 32	35, 78, 114, 141	0
35	YS	111/112 (99%)	0.19	0 100 100	7, 61, 94, 111	0
36	RT	137/146 (93%)	0.32	3 (2%) 59 44	13, 64, 125, 165	0
36	YT	137/146 (93%)	0.17	1 (0%) 84 71	10, 58, 111, 158	0
37	RU	117/118 (99%)	0.15	2 (1%) 67 51	10, 61, 104, 147	0
37	YU	117/118 (99%)	0.11	2 (1%) 67 51	0, 44, 108, 129	0
38	RV	101/101 (100%)	0.25	0 100 100	20, 75, 116, 144	0
38	YV	101/101 (100%)	0.29	0 100 100	11, 65, 104, 156	0
39	RW	113/113 (100%)	0.31	0 100 100	3, 43, 93, 149	0
39	YW	113/113 (100%)	0.08	0 100 100	2, 42, 91, 144	0
40	RX	92/96 (95%)	0.30	1 (1%) 77 61	15, 52, 96, 125	0
40	YX	92/96 (95%)	0.21	0 100 100	3, 37, 76, 96	0
41	RY	102/110 (92%)	1.35	28 (27%) 1 2	26, 88, 132, 159	0
41	YY	102/110 (92%)	0.53	6 (5%) 22 19	9, 63, 120, 140	0
42	RZ	183/206 (88%)	0.57	6 (3%) 44 34	21, 88, 133, 152	0
42	YZ	183/206 (88%)	0.33	4 (2%) 59 44	20, 70, 123, 155	0
43	R0	82/85 (96%)	0.51	2 (2%) 56 42	14, 48, 79, 112	0
43	Y0	82/85 (96%)	0.35	0 100 100	3, 36, 66, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	R1	97/98 (98%)	0.64	5 (5%) 26 22	5, 53, 126, 159	0
44	Y1	97/98 (98%)	0.50	4 (4%) 35 28	5, 43, 104, 139	0
45	R2	69/72 (95%)	0.24	0 100 100	13, 72, 111, 129	0
45	Y2	69/72 (95%)	0.05	0 100 100	5, 50, 104, 121	0
46	R3	59/60 (98%)	1.14	8 (13%) 4 5	12, 63, 111, 139	0
46	Y3	59/60 (98%)	0.76	5 (8%) 11 12	2, 44, 101, 174	0
47	R4	71/71 (100%)	0.79	7 (9%) 8 10	75, 131, 170, 189	0
47	Y4	71/71 (100%)	0.44	3 (4%) 35 27	46, 102, 154, 161	0
48	R5	59/60 (98%)	0.37	3 (5%) 27 22	6, 55, 133, 141	0
48	Y5	58/60 (96%)	0.35	2 (3%) 43 33	10, 59, 143, 162	0
49	R6	49/54 (90%)	2.87	30 (61%) 0 1	83, 118, 150, 157	0
49	Y6	49/54 (90%)	2.17	23 (46%) 1 1	51, 109, 141, 149	0
50	R7	49/49 (100%)	0.24	2 (4%) 35 28	8, 35, 87, 146	0
50	Y7	49/49 (100%)	0.40	2 (4%) 35 28	1, 29, 71, 121	0
51	R8	64/65 (98%)	0.47	2 (3%) 47 36	1, 52, 96, 158	0
51	Y8	64/65 (98%)	0.31	0 100 100	5, 40, 81, 149	0
52	R9	37/37 (100%)	3.98	31 (83%) 0 1	66, 110, 156, 168	0
52	Y9	37/37 (100%)	4.20	36 (97%) 0 1	78, 107, 132, 166	0
53	QV	77/77 (100%)	0.06	2 (2%) 53 40	46, 99, 145, 169	0
53	XV	77/77 (100%)	-0.03	0 100 100	28, 72, 119, 180	0
54	QX	8/25 (32%)	2.96	6 (75%) 0 1	103, 130, 144, 183	0
54	XX	8/25 (32%)	1.57	2 (25%) 1 2	56, 75, 115, 190	0
55	QY	14/18 (77%)	1.56	4 (28%) 1 2	112, 161, 199, 206	0
55	XY	14/18 (77%)	1.07	2 (14%) 3 5	65, 116, 180, 193	0
56	Z6	3/3 (100%)	2.99	1 (33%) 1 2	51, 51, 52, 57	0
56	Z8	3/3 (100%)	3.13	1 (33%) 1 2	46, 46, 46, 48	0
All	All	20874/21494 (97%)	0.14	669 (3%) 45 35	0, 61, 135, 236	0

The worst 5 of 669 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
52	R9	11	CYS	13.3
52	R9	14	CYS	12.1

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Mol	Chain	Res	Type	RSRZ
56	Z8	76	PPU	8.3
22	RA	1095	A	8.2
56	Z6	76	PPU	8.2

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	PPU	Z8	76	37/38	0.31	-	48,48,48,48	0
56	PPU	Z6	76	37/38	0.30	-	51,51,51,51	0
55	1MG	QY	37	24/25	0.31	-	125,125,125,125	0
55	1MG	XY	37	24/25	0.20	-	64,64,64,64	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
57	MG	YA	3256	1/1	0.12	-	9,9,9,9	0
57	MG	RA	3233	1/1	1.53	-	50,50,50,50	0
57	MG	RA	3227	1/1	0.13	-	39,39,39,39	0
57	MG	YA	3060	1/1	0.15	-	9,9,9,9	0
57	MG	XA	1609	1/1	0.59	-	8,8,8,8	0
57	MG	YA	3018	1/1	0.84	-	50,50,50,50	0
57	MG	YA	3048	1/1	0.49	-	50,50,50,50	0
57	MG	YA	3200	1/1	0.13	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	XA	1648	1/1	0.20	-	10,10,10,10	0
57	MG	RA	3202	1/1	0.37	-	2,2,2,2	0
57	MG	YA	3239	1/1	0.15	-	13,13,13,13	0
57	MG	RA	3095	1/1	0.43	-	24,24,24,24	0
57	MG	RA	3058	1/1	0.28	-	0,0,0,0	0
57	MG	YA	3067	1/1	0.43	-	7,7,7,7	0
57	MG	XA	1657	1/1	0.29	-	4,4,4,4	0
57	MG	RA	3157	1/1	0.27	-	39,39,39,39	0
57	MG	YA	3214	1/1	0.23	-	23,23,23,23	0
57	MG	YA	3223	1/1	1.00	-	11,11,11,11	0
57	MG	RA	3147	1/1	0.21	-	6,6,6,6	0
57	MG	QA	1628	1/1	0.42	-	21,21,21,21	0
57	MG	RA	3105	1/1	0.28	-	1,1,1,1	0
57	MG	YA	3190	1/1	0.52	-	17,17,17,17	0
57	MG	YA	3119	1/1	0.45	-	66,66,66,66	0
57	MG	R8	101	1/1	0.36	-	6,6,6,6	0
57	MG	RA	3029	1/1	0.26	-	5,5,5,5	0
57	MG	XA	1642	1/1	0.23	-	11,11,11,11	0
57	MG	RA	3037	1/1	0.45	-	0,0,0,0	0
57	MG	YA	3090	1/1	0.23	-	17,17,17,17	0
57	MG	XA	1601	1/1	1.08	-	50,50,50,50	0
57	MG	RA	3108	1/1	0.23	-	5,5,5,5	0
57	MG	YA	3077	1/1	0.19	-	0,0,0,0	0
57	MG	YA	3184	1/1	0.44	-	50,50,50,50	0
57	MG	RA	3199	1/1	0.17	-	1,1,1,1	0
57	MG	YA	3199	1/1	0.15	-	11,11,11,11	0
57	MG	YA	3131	1/1	0.56	-	17,17,17,17	0
57	MG	YA	3112	1/1	0.21	-	19,19,19,19	0
57	MG	YA	3115	1/1	0.29	-	15,15,15,15	0
57	MG	RA	3063	1/1	0.12	-	19,19,19,19	0
57	MG	RA	3032	1/1	0.65	-	50,50,50,50	0
57	MG	YA	3021	1/1	0.52	-	50,50,50,50	0
57	MG	RA	3215	1/1	0.29	-	14,14,14,14	0
57	MG	RA	3132	1/1	0.39	-	7,7,7,7	0
57	MG	YA	3087	1/1	0.38	-	6,6,6,6	0
57	MG	YA	3026	1/1	1.36	-	50,50,50,50	0
57	MG	XA	1653	1/1	0.16	-	29,29,29,29	0
57	MG	RA	3079	1/1	0.39	-	0,0,0,0	0
57	MG	YA	3253	1/1	1.87	-	50,50,50,50	0
57	MG	QA	1608	1/1	0.20	-	63,63,63,63	0
57	MG	XA	1655	1/1	0.22	-	7,7,7,7	0
57	MG	YA	3263	1/1	0.33	-	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3078	1/1	0.89	-	50,50,50,50	0
57	MG	YA	3094	1/1	0.41	-	8,8,8,8	0
57	MG	RA	3232	1/1	0.30	-	5,5,5,5	0
57	MG	XA	1615	1/1	0.50	-	50,50,50,50	0
57	MG	QA	1633	1/1	0.39	-	1,1,1,1	0
57	MG	RA	3042	1/1	0.59	-	50,50,50,50	0
57	MG	YA	3022	1/1	0.77	-	50,50,50,50	0
57	MG	RA	3131	1/1	0.16	-	25,25,25,25	0
57	MG	QA	1627	1/1	0.15	-	1,1,1,1	0
57	MG	YA	3106	1/1	0.43	-	50,50,50,50	0
57	MG	YA	3232	1/1	0.24	-	15,15,15,15	0
57	MG	YE	301	1/1	0.21	-	1,1,1,1	0
57	MG	RA	3151	1/1	0.34	-	37,37,37,37	0
57	MG	YA	3202	1/1	0.42	-	13,13,13,13	0
57	MG	RA	3122	1/1	0.33	-	19,19,19,19	0
57	MG	RA	3044	1/1	0.23	-	8,8,8,8	0
57	MG	QA	1651	1/1	0.43	-	16,16,16,16	0
57	MG	RA	3096	1/1	0.47	-	11,11,11,11	0
57	MG	YA	3011	1/1	0.40	-	3,3,3,3	0
57	MG	RA	3114	1/1	0.17	-	3,3,3,3	0
57	MG	YA	3110	1/1	0.15	-	5,5,5,5	0
57	MG	QA	1614	1/1	0.27	-	21,21,21,21	0
57	MG	YA	3189	1/1	0.43	-	7,7,7,7	0
57	MG	YA	3104	1/1	0.14	-	11,11,11,11	0
57	MG	YA	3221	1/1	0.24	-	7,7,7,7	0
57	MG	RA	3046	1/1	0.45	-	0,0,0,0	0
57	MG	RA	3178	1/1	0.34	-	5,5,5,5	0
57	MG	RA	3145	1/1	0.40	-	3,3,3,3	0
57	MG	RA	3158	1/1	0.25	-	15,15,15,15	0
57	MG	QA	1649	1/1	0.10	-	19,19,19,19	0
57	MG	RA	3087	1/1	0.47	-	0,0,0,0	0
57	MG	RA	3028	1/1	0.22	-	23,23,23,23	0
57	MG	YA	3031	1/1	1.06	-	50,50,50,50	0
57	MG	YA	3234	1/1	0.09	-	2,2,2,2	0
57	MG	RA	3111	1/1	0.40	-	4,4,4,4	0
57	MG	YA	3178	1/1	0.52	-	32,32,32,32	0
57	MG	RA	3010	1/1	0.36	-	56,56,56,56	0
57	MG	RA	3224	1/1	0.16	-	16,16,16,16	0
57	MG	XA	1645	1/1	0.47	-	8,8,8,8	0
57	MG	RA	3099	1/1	0.40	-	20,20,20,20	0
57	MG	RA	3054	1/1	0.32	-	4,4,4,4	0
57	MG	RA	3119	1/1	0.24	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3180	1/1	0.29	-	1,1,1,1	0
57	MG	RA	3039	1/1	0.64	-	50,50,50,50	0
57	MG	YA	3024	1/1	0.50	-	50,50,50,50	0
57	MG	RA	3107	1/1	0.29	-	9,9,9,9	0
57	MG	YA	3229	1/1	0.13	-	5,5,5,5	0
57	MG	XA	1659	1/1	0.17	-	15,15,15,15	0
57	MG	RA	3229	1/1	0.34	-	50,50,50,50	0
57	MG	RA	3214	1/1	0.17	-	43,43,43,43	0
57	MG	RA	3068	1/1	0.50	-	4,4,4,4	0
57	MG	YA	3176	1/1	0.34	-	11,11,11,11	0
57	MG	YA	3219	1/1	0.11	-	22,22,22,22	0
57	MG	YA	3014	1/1	0.38	-	1,1,1,1	0
57	MG	RA	3137	1/1	0.09	-	3,3,3,3	0
57	MG	QA	1647	1/1	0.16	-	55,55,55,55	0
57	MG	RA	3192	1/1	0.16	-	27,27,27,27	0
57	MG	YA	3109	1/1	0.21	-	9,9,9,9	0
57	MG	XA	1611	1/1	0.32	-	1,1,1,1	0
57	MG	YA	3152	1/1	0.34	-	7,7,7,7	0
57	MG	YA	3167	1/1	0.22	-	39,39,39,39	0
57	MG	YA	3244	1/1	0.48	-	6,6,6,6	0
57	MG	YA	3122	1/1	0.56	-	50,50,50,50	0
57	MG	YA	3030	1/1	0.94	-	50,50,50,50	0
57	MG	QA	1662	1/1	0.09	-	39,39,39,39	0
57	MG	XA	1628	1/1	0.13	-	2,2,2,2	0
57	MG	XA	1635	1/1	1.66	-	50,50,50,50	0
57	MG	YA	3074	1/1	0.65	-	4,4,4,4	0
57	MG	YA	3017	1/1	0.29	-	7,7,7,7	0
57	MG	RA	3142	1/1	0.46	-	8,8,8,8	0
57	MG	RA	3036	1/1	0.46	-	0,0,0,0	0
57	MG	RA	3162	1/1	0.25	-	18,18,18,18	0
57	MG	YA	3065	1/1	0.72	-	8,8,8,8	0
59	ZN	QD	301	1/1	0.17	-	12,12,12,12	0
57	MG	YA	3237	1/1	0.20	-	38,38,38,38	0
57	MG	QA	1638	1/1	0.19	-	8,8,8,8	0
57	MG	RA	3160	1/1	0.36	-	2,2,2,2	0
57	MG	RA	3228	1/1	0.16	-	7,7,7,7	0
57	MG	YA	3174	1/1	0.38	-	3,3,3,3	0
57	MG	YA	3038	1/1	0.25	-	5,5,5,5	0
57	MG	QA	1603	1/1	0.55	-	10,10,10,10	0
57	MG	RE	301	1/1	0.12	-	2,2,2,2	0
57	MG	YA	3117	1/1	0.81	-	50,50,50,50	0
57	MG	YA	3059	1/1	0.29	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3002	1/1	0.75	-	50,50,50,50	0
57	MG	QA	1642	1/1	0.14	-	9,9,9,9	0
57	MG	RA	3074	1/1	0.23	-	20,20,20,20	0
57	MG	YA	3025	1/1	0.29	-	3,3,3,3	0
57	MG	YA	3209	1/1	0.19	-	9,9,9,9	0
57	MG	XA	1647	1/1	0.36	-	11,11,11,11	0
57	MG	YA	3186	1/1	0.19	-	10,10,10,10	0
57	MG	QA	1640	1/1	0.26	-	6,6,6,6	0
57	MG	YA	3262	1/1	0.32	-	9,9,9,9	0
57	MG	RA	3091	1/1	0.49	-	2,2,2,2	0
57	MG	QA	1621	1/1	0.18	-	35,35,35,35	0
57	MG	YA	3039	1/1	0.24	-	0,0,0,0	0
57	MG	YA	3062	1/1	0.22	-	0,0,0,0	0
57	MG	YA	3096	1/1	0.23	-	17,17,17,17	0
57	MG	XA	1627	1/1	0.39	-	9,9,9,9	0
57	MG	RA	3212	1/1	0.27	-	33,33,33,33	0
57	MG	QA	1661	1/1	0.08	-	44,44,44,44	0
57	MG	YA	3071	1/1	0.32	-	6,6,6,6	0
57	MG	XA	1624	1/1	0.62	-	8,8,8,8	0
57	MG	XA	1663	1/1	0.19	-	3,3,3,3	0
57	MG	QA	1658	1/1	0.43	-	46,46,46,46	0
57	MG	RA	3197	1/1	0.16	-	9,9,9,9	0
57	MG	Y7	101	1/1	0.25	-	14,14,14,14	0
57	MG	YA	3210	1/1	0.32	-	30,30,30,30	0
57	MG	YA	3027	1/1	0.18	-	1,1,1,1	0
57	MG	RA	3168	1/1	0.20	-	10,10,10,10	0
57	MG	RA	3006	1/1	1.07	-	50,50,50,50	0
57	MG	QA	1653	1/1	0.11	-	6,6,6,6	0
57	MG	YA	3016	1/1	0.21	-	8,8,8,8	0
57	MG	YA	3154	1/1	0.30	-	5,5,5,5	0
57	MG	RA	3066	1/1	0.26	-	23,23,23,23	0
57	MG	QA	1605	1/1	0.52	-	4,4,4,4	0
57	MG	XA	1652	1/1	0.27	-	50,50,50,50	0
57	MG	YA	3029	1/1	0.36	-	6,6,6,6	0
57	MG	YA	3185	1/1	0.15	-	74,74,74,74	0
57	MG	YA	3207	1/1	0.26	-	0,0,0,0	0
57	MG	XA	1632	1/1	0.41	-	2,2,2,2	0
57	MG	YA	3169	1/1	0.86	-	7,7,7,7	0
57	MG	RA	3154	1/1	0.46	-	6,6,6,6	0
57	MG	YA	3098	1/1	0.87	-	50,50,50,50	0
57	MG	YA	3164	1/1	0.84	-	97,97,97,97	0
57	MG	QA	1616	1/1	0.28	-	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	QA	1625	1/1	0.07	-	74,74,74,74	0
57	MG	YA	3251	1/1	1.34	-	50,50,50,50	0
57	MG	RA	3117	1/1	0.34	-	4,4,4,4	0
57	MG	RA	3222	1/1	0.38	-	4,4,4,4	0
57	MG	YA	3081	1/1	0.33	-	7,7,7,7	0
57	MG	RA	3024	1/1	0.36	-	15,15,15,15	0
57	MG	QA	1622	1/1	0.47	-	52,52,52,52	0
57	MG	RA	3056	1/1	0.20	-	0,0,0,0	0
57	MG	YA	3243	1/1	0.83	-	50,50,50,50	0
57	MG	XA	1613	1/1	0.09	-	16,16,16,16	0
57	MG	YA	3023	1/1	0.42	-	5,5,5,5	0
57	MG	YA	3064	1/1	0.17	-	4,4,4,4	0
57	MG	RA	3051	1/1	0.88	-	50,50,50,50	0
57	MG	YA	3197	1/1	1.44	-	50,50,50,50	0
57	MG	RA	3218	1/1	0.34	-	10,10,10,10	0
57	MG	YA	3127	1/1	0.09	-	12,12,12,12	0
57	MG	QA	1609	1/1	0.15	-	10,10,10,10	0
57	MG	YA	3129	1/1	0.14	-	1,1,1,1	0
57	MG	RA	3206	1/1	0.23	-	11,11,11,11	0
57	MG	RA	3238	1/1	0.73	-	3,3,3,3	0
57	MG	RA	3191	1/1	0.26	-	38,38,38,38	0
57	MG	RA	3072	1/1	0.33	-	0,0,0,0	0
57	MG	YA	3054	1/1	0.63	-	50,50,50,50	0
57	MG	RA	3097	1/1	0.60	-	11,11,11,11	0
57	MG	YA	3224	1/1	0.73	-	50,50,50,50	0
57	MG	RA	3069	1/1	0.27	-	9,9,9,9	0
57	MG	XA	1666	1/1	0.25	-	34,34,34,34	0
57	MG	YA	3037	1/1	0.34	-	3,3,3,3	0
57	MG	YA	3236	1/1	0.21	-	12,12,12,12	0
57	MG	RA	3183	1/1	0.52	-	11,11,11,11	0
57	MG	XA	1604	1/1	1.12	-	50,50,50,50	0
57	MG	RA	3146	1/1	0.42	-	7,7,7,7	0
57	MG	RA	3172	1/1	0.32	-	17,17,17,17	0
57	MG	YA	3161	1/1	0.32	-	14,14,14,14	0
57	MG	YA	3212	1/1	0.24	-	8,8,8,8	0
57	MG	YA	3084	1/1	0.28	-	2,2,2,2	0
57	MG	RA	3242	1/1	0.63	-	8,8,8,8	0
57	MG	RA	3082	1/1	0.15	-	5,5,5,5	0
57	MG	RA	3141	1/1	0.44	-	5,5,5,5	0
57	MG	XA	1634	1/1	0.21	-	11,11,11,11	0
57	MG	YA	3141	1/1	0.09	-	18,18,18,18	0
57	MG	XA	1670	1/1	0.20	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3208	1/1	0.15	-	50,50,50,50	0
57	MG	QA	1613	1/1	0.41	-	1,1,1,1	0
57	MG	RA	3121	1/1	0.17	-	0,0,0,0	0
57	MG	YA	3257	1/1	0.82	-	50,50,50,50	0
57	MG	YA	3194	1/1	0.19	-	15,15,15,15	0
59	ZN	QN	101	1/1	0.12	-	56,56,56,56	0
57	MG	RA	3118	1/1	0.22	-	1,1,1,1	0
57	MG	XA	1671	1/1	0.18	-	28,28,28,28	0
57	MG	YA	3192	1/1	0.15	-	15,15,15,15	0
57	MG	YA	3245	1/1	0.58	-	3,3,3,3	0
57	MG	QA	1663	1/1	0.09	-	19,19,19,19	0
57	MG	YA	3076	1/1	0.40	-	1,1,1,1	0
57	MG	YA	3173	1/1	0.17	-	14,14,14,14	0
57	MG	YA	3153	1/1	0.27	-	16,16,16,16	0
57	MG	YA	3242	1/1	0.20	-	5,5,5,5	0
57	MG	RA	3164	1/1	0.55	-	15,15,15,15	0
57	MG	RA	3167	1/1	0.10	-	26,26,26,26	0
57	MG	RA	3092	1/1	0.23	-	59,59,59,59	0
57	MG	QA	1606	1/1	0.07	-	23,23,23,23	0
57	MG	RA	3207	1/1	0.25	-	5,5,5,5	0
57	MG	YA	3088	1/1	0.26	-	3,3,3,3	0
57	MG	RA	3030	1/1	0.77	-	50,50,50,50	0
57	MG	QA	1630	1/1	0.14	-	14,14,14,14	0
57	MG	XA	1629	1/1	0.14	-	32,32,32,32	0
57	MG	YA	3036	1/1	0.18	-	3,3,3,3	0
57	MG	RA	3005	1/1	0.85	-	50,50,50,50	0
57	MG	RA	3059	1/1	0.56	-	50,50,50,50	0
57	MG	XA	1650	1/1	0.29	-	22,22,22,22	0
57	MG	RF	301	1/1	0.28	-	10,10,10,10	0
57	MG	YA	3004	1/1	0.45	-	5,5,5,5	0
57	MG	XA	1619	1/1	0.42	-	8,8,8,8	0
57	MG	YA	3068	1/1	0.24	-	1,1,1,1	0
57	MG	RA	3015	1/1	0.34	-	15,15,15,15	0
57	MG	YA	3235	1/1	0.40	-	34,34,34,34	0
57	MG	XA	1616	1/1	0.88	-	50,50,50,50	0
57	MG	RA	3130	1/1	0.16	-	19,19,19,19	0
57	MG	RA	3126	1/1	0.25	-	14,14,14,14	0
57	MG	YA	3144	1/1	0.53	-	6,6,6,6	0
57	MG	RA	3098	1/1	0.40	-	4,4,4,4	0
57	MG	YB	202	1/1	0.45	-	5,5,5,5	0
57	MG	YA	3052	1/1	0.35	-	5,5,5,5	0
57	MG	YA	3120	1/1	0.13	-	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3153	1/1	0.48	-	36,36,36,36	0
57	MG	RA	3102	1/1	0.12	-	10,10,10,10	0
57	MG	XA	1621	1/1	0.57	-	6,6,6,6	0
57	MG	YA	3138	1/1	0.52	-	4,4,4,4	0
57	MG	RA	3112	1/1	0.38	-	2,2,2,2	0
57	MG	RA	3094	1/1	0.35	-	3,3,3,3	0
57	MG	XA	1672	1/1	0.26	-	5,5,5,5	0
57	MG	YQ	201	1/1	0.23	-	79,79,79,79	0
57	MG	YA	3160	1/1	0.36	-	4,4,4,4	0
57	MG	RA	3204	1/1	0.49	-	15,15,15,15	0
57	MG	RA	3149	1/1	0.58	-	17,17,17,17	0
57	MG	YA	3264	1/1	0.46	-	14,14,14,14	0
57	MG	QA	1652	1/1	0.20	-	24,24,24,24	0
57	MG	RA	3003	1/1	1.16	-	50,50,50,50	0
57	MG	YA	3083	1/1	0.22	-	16,16,16,16	0
57	MG	RA	3221	1/1	0.69	-	79,79,79,79	0
57	MG	RA	3196	1/1	0.30	-	22,22,22,22	0
57	MG	RA	3080	1/1	0.14	-	5,5,5,5	0
57	MG	RA	3216	1/1	0.29	-	1,1,1,1	0
57	MG	RA	3209	1/1	0.13	-	44,44,44,44	0
57	MG	YA	3102	1/1	0.80	-	6,6,6,6	0
57	MG	YA	3195	1/1	0.17	-	21,21,21,21	0
57	MG	YA	3008	1/1	0.20	-	1,1,1,1	0
57	MG	QF	201	1/1	0.34	-	40,40,40,40	0
57	MG	RA	3181	1/1	0.32	-	9,9,9,9	0
57	MG	QA	1643	1/1	0.16	-	20,20,20,20	0
57	MG	RA	3034	1/1	1.56	-	50,50,50,50	0
57	MG	XA	1633	1/1	0.18	-	13,13,13,13	0
57	MG	RA	3129	1/1	0.11	-	19,19,19,19	0
57	MG	RA	3089	1/1	0.37	-	0,0,0,0	0
57	MG	RA	3033	1/1	0.58	-	16,16,16,16	0
57	MG	RA	3170	1/1	0.33	-	2,2,2,2	0
57	MG	XA	1638	1/1	0.19	-	27,27,27,27	0
57	MG	YA	3191	1/1	0.41	-	14,14,14,14	0
57	MG	YA	3126	1/1	0.36	-	50,50,50,50	0
57	MG	YA	3058	1/1	0.20	-	13,13,13,13	0
57	MG	XA	1669	1/1	0.10	-	15,15,15,15	0
57	MG	QA	1623	1/1	0.53	-	13,13,13,13	0
57	MG	YA	3231	1/1	0.47	-	11,11,11,11	0
57	MG	YA	3139	1/1	0.23	-	13,13,13,13	0
57	MG	RA	3135	1/1	0.12	-	28,28,28,28	0
57	MG	RA	3120	1/1	0.23	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3057	1/1	0.50	-	8,8,8,8	0
57	MG	XA	1665	1/1	0.24	-	18,18,18,18	0
57	MG	RA	3198	1/1	0.05	-	35,35,35,35	0
57	MG	RA	3086	1/1	0.32	-	50,50,50,50	0
57	MG	YA	3082	1/1	0.59	-	50,50,50,50	0
57	MG	RA	3043	1/1	0.73	-	50,50,50,50	0
57	MG	YA	3179	1/1	0.27	-	20,20,20,20	0
57	MG	RA	3193	1/1	0.14	-	17,17,17,17	0
57	MG	RA	3040	1/1	0.21	-	11,11,11,11	0
57	MG	RA	3237	1/1	0.25	-	4,4,4,4	0
57	MG	RA	3171	1/1	0.48	-	15,15,15,15	0
57	MG	RA	3081	1/1	0.31	-	10,10,10,10	0
57	MG	YA	3142	1/1	0.28	-	9,9,9,9	0
57	MG	YA	3187	1/1	0.19	-	47,47,47,47	0
57	MG	YA	3182	1/1	0.56	-	14,14,14,14	0
57	MG	RA	3161	1/1	0.16	-	8,8,8,8	0
57	MG	YA	3168	1/1	0.17	-	13,13,13,13	0
57	MG	QM	201	1/1	0.10	-	34,34,34,34	0
57	MG	RA	3235	1/1	0.12	-	2,2,2,2	0
57	MG	QA	1634	1/1	0.11	-	44,44,44,44	0
57	MG	RA	3014	1/1	1.01	-	50,50,50,50	0
57	MG	YA	3124	1/1	0.31	-	13,13,13,13	0
57	MG	RA	3115	1/1	0.18	-	8,8,8,8	0
57	MG	YA	3085	1/1	0.79	-	50,50,50,50	0
57	MG	QA	1615	1/1	0.21	-	54,54,54,54	0
59	ZN	Y9	101	1/1	0.65	-	158,158,158,158	0
57	MG	RA	3004	1/1	0.49	-	9,9,9,9	0
57	MG	RA	3159	1/1	0.17	-	18,18,18,18	0
57	MG	RA	3053	1/1	0.64	-	50,50,50,50	0
57	MG	QA	1664	1/1	0.36	-	10,10,10,10	0
57	MG	RA	3057	1/1	0.77	-	50,50,50,50	0
57	MG	XA	1656	1/1	0.95	-	12,12,12,12	0
57	MG	YA	3107	1/1	0.43	-	2,2,2,2	0
57	MG	YA	3137	1/1	0.28	-	22,22,22,22	0
57	MG	QA	1657	1/1	0.10	-	19,19,19,19	0
57	MG	RA	3075	1/1	0.36	-	37,37,37,37	0
57	MG	YA	3156	1/1	0.24	-	8,8,8,8	0
57	MG	QA	1612	1/1	0.36	-	4,4,4,4	0
57	MG	QA	1624	1/1	0.26	-	16,16,16,16	0
57	MG	YA	3201	1/1	0.19	-	10,10,10,10	0
57	MG	XA	1614	1/1	0.25	-	25,25,25,25	0
57	MG	RA	3021	1/1	1.06	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3111	1/1	0.23	-	7,7,7,7	0
57	MG	RA	3009	1/1	0.55	-	7,7,7,7	0
57	MG	XA	1649	1/1	0.43	-	16,16,16,16	0
57	MG	QA	1626	1/1	0.17	-	17,17,17,17	0
57	MG	RA	3017	1/1	0.29	-	0,0,0,0	0
57	MG	YA	3047	1/1	1.04	-	50,50,50,50	0
57	MG	RA	3027	1/1	0.85	-	50,50,50,50	0
57	MG	RA	3103	1/1	0.22	-	8,8,8,8	0
57	MG	QA	1604	1/1	0.42	-	7,7,7,7	0
57	MG	RA	3211	1/1	0.24	-	11,11,11,11	0
57	MG	RA	3240	1/1	0.64	-	12,12,12,12	0
57	MG	YA	3177	1/1	0.06	-	92,92,92,92	0
57	MG	YA	3208	1/1	0.14	-	0,0,0,0	0
57	MG	YA	3007	1/1	0.20	-	1,1,1,1	0
57	MG	RA	3236	1/1	0.45	-	2,2,2,2	0
57	MG	XA	1608	1/1	0.17	-	50,50,50,50	0
57	MG	RA	3070	1/1	0.17	-	21,21,21,21	0
57	MG	RA	3016	1/1	0.66	-	50,50,50,50	0
57	MG	RA	3093	1/1	0.70	-	50,50,50,50	0
57	MG	RA	3213	1/1	0.31	-	10,10,10,10	0
57	MG	YA	3220	1/1	0.14	-	26,26,26,26	0
57	MG	RU	201	1/1	0.16	-	86,86,86,86	0
57	MG	RA	3128	1/1	0.23	-	10,10,10,10	0
57	MG	YA	3227	1/1	0.15	-	15,15,15,15	0
57	MG	RA	3052	1/1	0.49	-	50,50,50,50	0
57	MG	YA	3132	1/1	0.35	-	26,26,26,26	0
57	MG	XA	1639	1/1	0.08	-	11,11,11,11	0
57	MG	YA	3044	1/1	0.54	-	16,16,16,16	0
57	MG	YA	3146	1/1	0.20	-	6,6,6,6	0
57	MG	RP	201	1/1	0.46	-	85,85,85,85	0
57	MG	RA	3007	1/1	1.23	-	50,50,50,50	0
57	MG	XA	1623	1/1	0.23	-	23,23,23,23	0
57	MG	YA	3050	1/1	0.51	-	50,50,50,50	0
57	MG	YA	3205	1/1	0.19	-	40,40,40,40	0
57	MG	RA	3174	1/1	0.15	-	40,40,40,40	0
57	MG	R5	101	1/1	0.17	-	14,14,14,14	0
57	MG	YA	3121	1/1	0.21	-	8,8,8,8	0
57	MG	YA	3203	1/1	0.37	-	29,29,29,29	0
57	MG	YA	3151	1/1	0.54	-	50,50,50,50	0
57	MG	RA	3076	1/1	0.17	-	3,3,3,3	0
57	MG	RA	3136	1/1	0.24	-	14,14,14,14	0
59	ZN	XN	101	1/1	0.17	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3156	1/1	0.16	-	7,7,7,7	0
57	MG	YA	3165	1/1	0.23	-	42,42,42,42	0
57	MG	YA	3093	1/1	0.47	-	4,4,4,4	0
57	MG	RA	3018	1/1	0.32	-	3,3,3,3	0
57	MG	YA	3238	1/1	0.08	-	33,33,33,33	0
57	MG	RA	3179	1/1	0.31	-	10,10,10,10	0
57	MG	XA	1664	1/1	0.42	-	27,27,27,27	0
57	MG	RA	3124	1/1	0.29	-	19,19,19,19	0
57	MG	RB	201	1/1	0.10	-	38,38,38,38	0
57	MG	QX	101	1/1	0.15	-	6,6,6,6	0
57	MG	RA	3031	1/1	0.75	-	50,50,50,50	0
57	MG	YA	3079	1/1	1.28	-	50,50,50,50	0
57	MG	RA	3194	1/1	0.15	-	82,82,82,82	0
57	MG	XA	1612	1/1	0.24	-	23,23,23,23	0
57	MG	YP	202	1/1	0.33	-	5,5,5,5	0
57	MG	XA	1654	1/1	0.42	-	17,17,17,17	0
57	MG	YA	3193	1/1	0.71	-	7,7,7,7	0
57	MG	XV	101	1/1	0.40	-	1,1,1,1	0
57	MG	YA	3134	1/1	0.62	-	50,50,50,50	0
57	MG	YA	3188	1/1	0.15	-	36,36,36,36	0
57	MG	XV	102	1/1	0.16	-	16,16,16,16	0
57	MG	RA	3226	1/1	0.28	-	29,29,29,29	0
57	MG	YA	3222	1/1	0.10	-	2,2,2,2	0
57	MG	YA	3061	1/1	0.50	-	9,9,9,9	0
57	MG	YA	3113	1/1	0.47	-	50,50,50,50	0
57	MG	RA	3140	1/1	0.25	-	61,61,61,61	0
57	MG	YA	3265	1/1	0.66	-	11,11,11,11	0
57	MG	QA	1619	1/1	0.17	-	29,29,29,29	0
57	MG	YA	3170	1/1	0.26	-	8,8,8,8	0
57	MG	RA	3189	1/1	0.16	-	16,16,16,16	0
57	MG	XA	1662	1/1	0.78	-	50,50,50,50	0
57	MG	YA	3045	1/1	0.55	-	0,0,0,0	0
57	MG	RA	3230	1/1	0.48	-	45,45,45,45	0
57	MG	YA	3181	1/1	0.60	-	5,5,5,5	0
57	MG	RA	3223	1/1	0.30	-	16,16,16,16	0
57	MG	RA	3219	1/1	0.60	-	40,40,40,40	0
57	MG	RA	3187	1/1	0.12	-	10,10,10,10	0
57	MG	RA	3116	1/1	0.33	-	0,0,0,0	0
57	MG	XA	1605	1/1	0.59	-	16,16,16,16	0
57	MG	YA	3175	1/1	0.14	-	2,2,2,2	0
57	MG	YA	3140	1/1	0.21	-	19,19,19,19	0
57	MG	RA	3048	1/1	1.20	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3163	1/1	0.36	-	9,9,9,9	0
57	MG	RA	3239	1/1	0.82	-	10,10,10,10	0
57	MG	YP	201	1/1	0.06	-	83,83,83,83	0
57	MG	QA	1629	1/1	0.10	-	38,38,38,38	0
57	MG	XA	1618	1/1	0.30	-	4,4,4,4	0
57	MG	XA	1668	1/1	0.31	-	6,6,6,6	0
57	MG	YA	3147	1/1	0.19	-	0,0,0,0	0
57	MG	QA	1645	1/1	0.27	-	37,37,37,37	0
57	MG	YA	3217	1/1	0.56	-	52,52,52,52	0
57	MG	XX	101	1/1	0.17	-	88,88,88,88	0
57	MG	YA	3258	1/1	0.51	-	4,4,4,4	0
57	MG	RA	3045	1/1	0.30	-	0,0,0,0	0
57	MG	RA	3064	1/1	1.69	-	50,50,50,50	0
57	MG	YA	3056	1/1	0.90	-	50,50,50,50	0
57	MG	YA	3215	1/1	0.28	-	2,2,2,2	0
57	MG	RA	3026	1/1	0.16	-	13,13,13,13	0
57	MG	YA	3095	1/1	0.33	-	8,8,8,8	0
57	MG	YA	3162	1/1	0.28	-	30,30,30,30	0
57	MG	RA	3152	1/1	0.21	-	26,26,26,26	0
57	MG	YA	3260	1/1	0.55	-	50,50,50,50	0
57	MG	YA	3063	1/1	0.30	-	15,15,15,15	0
57	MG	RA	3020	1/1	0.71	-	50,50,50,50	0
57	MG	QA	1631	1/1	0.20	-	63,63,63,63	0
57	MG	YA	3033	1/1	0.71	-	50,50,50,50	0
57	MG	RA	3148	1/1	0.12	-	0,0,0,0	0
57	MG	YA	3250	1/1	1.17	-	50,50,50,50	0
57	MG	RA	3065	1/1	1.32	-	50,50,50,50	0
57	MG	YA	3247	1/1	0.56	-	16,16,16,16	0
57	MG	XA	1644	1/1	0.34	-	11,11,11,11	0
57	MG	YA	3089	1/1	0.27	-	13,13,13,13	0
57	MG	YA	3019	1/1	0.81	-	50,50,50,50	0
57	MG	Y5	101	1/1	0.14	-	2,2,2,2	0
57	MG	YA	3010	1/1	0.60	-	50,50,50,50	0
57	MG	RA	3241	1/1	0.38	-	0,0,0,0	0
57	MG	RA	3077	1/1	0.41	-	50,50,50,50	0
57	MG	RA	3182	1/1	0.42	-	10,10,10,10	0
57	MG	QA	1610	1/1	0.62	-	50,50,50,50	0
58	PAR	QA	1666	42/42	0.39	-	104,104,104,104	0
57	MG	XA	1661	1/1	0.09	-	14,14,14,14	0
57	MG	YA	3005	1/1	0.21	-	2,2,2,2	0
57	MG	RR	201	1/1	0.25	-	9,9,9,9	0
57	MG	YA	3198	1/1	0.27	-	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3249	1/1	0.74	-	5,5,5,5	0
57	MG	XA	1602	1/1	0.92	-	50,50,50,50	0
57	MG	RA	3201	1/1	0.32	-	41,41,41,41	0
57	MG	QA	1654	1/1	0.12	-	17,17,17,17	0
57	MG	YA	3055	1/1	0.18	-	24,24,24,24	0
57	MG	YA	3145	1/1	0.21	-	25,25,25,25	0
57	MG	YB	203	1/1	0.18	-	17,17,17,17	0
57	MG	YA	3225	1/1	0.40	-	23,23,23,23	0
57	MG	RA	3073	1/1	0.28	-	36,36,36,36	0
57	MG	RA	3203	1/1	0.21	-	34,34,34,34	0
57	MG	XA	1631	1/1	0.19	-	10,10,10,10	0
57	MG	YA	3157	1/1	0.27	-	8,8,8,8	0
57	MG	YA	3042	1/1	0.46	-	50,50,50,50	0
57	MG	RA	3100	1/1	1.02	-	50,50,50,50	0
57	MG	RA	3185	1/1	0.21	-	3,3,3,3	0
57	MG	QA	1665	1/1	0.42	-	37,37,37,37	0
57	MG	YA	3246	1/1	0.49	-	2,2,2,2	0
57	MG	QH	201	1/1	0.27	-	27,27,27,27	0
57	MG	YA	3150	1/1	0.60	-	16,16,16,16	0
57	MG	YA	3133	1/1	0.08	-	12,12,12,12	0
57	MG	XA	1658	1/1	0.23	-	17,17,17,17	0
57	MG	RA	3134	1/1	0.08	-	23,23,23,23	0
57	MG	YA	3216	1/1	0.28	-	30,30,30,30	0
57	MG	YA	3073	1/1	0.28	-	4,4,4,4	0
57	MG	YA	3099	1/1	0.80	-	50,50,50,50	0
57	MG	RA	3011	1/1	0.41	-	7,7,7,7	0
57	MG	YA	3015	1/1	0.81	-	50,50,50,50	0
57	MG	XA	1625	1/1	0.53	-	50,50,50,50	0
57	MG	YA	3091	1/1	0.54	-	12,12,12,12	0
57	MG	YB	201	1/1	0.28	-	14,14,14,14	0
57	MG	RA	3055	1/1	0.24	-	12,12,12,12	0
57	MG	XA	1641	1/1	0.36	-	14,14,14,14	0
57	MG	YA	3204	1/1	0.17	-	11,11,11,11	0
57	MG	XA	1651	1/1	0.17	-	84,84,84,84	0
57	MG	RE	302	1/1	0.19	-	15,15,15,15	0
57	MG	RA	3139	1/1	0.47	-	18,18,18,18	0
57	MG	XA	1617	1/1	0.26	-	2,2,2,2	0
57	MG	RA	3085	1/1	0.21	-	27,27,27,27	0
57	MG	RA	3127	1/1	0.48	-	15,15,15,15	0
59	ZN	R9	101	1/1	0.90	-	177,177,177,177	0
57	MG	RA	3013	1/1	0.38	-	0,0,0,0	0
57	MG	RA	3061	1/1	0.84	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	QA	1632	1/1	0.09	-	71,71,71,71	0
57	MG	RA	3088	1/1	0.25	-	10,10,10,10	0
57	MG	YA	3123	1/1	0.18	-	0,0,0,0	0
57	MG	YA	3180	1/1	0.71	-	5,5,5,5	0
57	MG	RA	3225	1/1	0.29	-	47,47,47,47	0
57	MG	RA	3231	1/1	0.34	-	3,3,3,3	0
57	MG	RA	3110	1/1	0.09	-	15,15,15,15	0
57	MG	RA	3184	1/1	0.34	-	40,40,40,40	0
57	MG	YA	3103	1/1	0.14	-	31,31,31,31	0
57	MG	YA	3034	1/1	0.36	-	7,7,7,7	0
57	MG	RA	3150	1/1	0.26	-	4,4,4,4	0
57	MG	QA	1611	1/1	0.29	-	4,4,4,4	0
57	MG	YA	3255	1/1	1.33	-	50,50,50,50	0
57	MG	YA	3240	1/1	0.14	-	15,15,15,15	0
57	MG	QA	1641	1/1	0.09	-	3,3,3,3	0
57	MG	RA	3205	1/1	0.51	-	33,33,33,33	0
57	MG	YA	3101	1/1	0.16	-	11,11,11,11	0
57	MG	RA	3106	1/1	0.28	-	3,3,3,3	0
57	MG	YA	3078	1/1	0.25	-	10,10,10,10	0
57	MG	YA	3155	1/1	0.23	-	8,8,8,8	0
57	MG	YA	3259	1/1	0.63	-	2,2,2,2	0
57	MG	YA	3108	1/1	0.14	-	10,10,10,10	0
57	MG	YA	3135	1/1	0.42	-	9,9,9,9	0
57	MG	XA	1630	1/1	0.35	-	1,1,1,1	0
57	MG	YA	3116	1/1	0.41	-	11,11,11,11	0
57	MG	YA	3230	1/1	0.15	-	19,19,19,19	0
57	MG	YA	3086	1/1	0.39	-	19,19,19,19	0
57	MG	YA	3080	1/1	0.85	-	50,50,50,50	0
57	MG	YA	3040	1/1	0.68	-	50,50,50,50	0
57	MG	XA	1660	1/1	0.10	-	19,19,19,19	0
57	MG	XA	1643	1/1	0.63	-	50,50,50,50	0
57	MG	YA	3171	1/1	0.20	-	7,7,7,7	0
57	MG	QA	1620	1/1	0.13	-	21,21,21,21	0
57	MG	RA	3143	1/1	0.07	-	12,12,12,12	0
57	MG	QA	1637	1/1	0.25	-	3,3,3,3	0
57	MG	YA	3148	1/1	0.22	-	38,38,38,38	0
57	MG	RA	3144	1/1	0.24	-	29,29,29,29	0
57	MG	RA	3084	1/1	0.37	-	6,6,6,6	0
57	MG	QA	1655	1/1	0.39	-	66,66,66,66	0
57	MG	RA	3195	1/1	0.15	-	23,23,23,23	0
57	MG	RA	3101	1/1	0.27	-	9,9,9,9	0
57	MG	RA	3035	1/1	0.80	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3183	1/1	0.19	-	17,17,17,17	0
57	MG	YA	3049	1/1	1.09	-	50,50,50,50	0
57	MG	RA	3047	1/1	0.15	-	2,2,2,2	0
57	MG	RA	3217	1/1	0.88	-	16,16,16,16	0
57	MG	RA	3002	1/1	0.20	-	8,8,8,8	0
57	MG	YA	3172	1/1	0.14	-	19,19,19,19	0
57	MG	YA	3066	1/1	0.20	-	9,9,9,9	0
57	MG	YA	3125	1/1	0.43	-	15,15,15,15	0
57	MG	YA	3012	1/1	1.41	-	50,50,50,50	0
57	MG	RA	3038	1/1	0.84	-	50,50,50,50	0
57	MG	YA	3218	1/1	0.26	-	5,5,5,5	0
57	MG	RA	3176	1/1	0.30	-	30,30,30,30	0
57	MG	XA	1626	1/1	0.24	-	1,1,1,1	0
57	MG	RA	3023	1/1	0.47	-	50,50,50,50	0
57	MG	YA	3051	1/1	0.23	-	5,5,5,5	0
57	MG	YA	3233	1/1	0.11	-	3,3,3,3	0
57	MG	QA	1660	1/1	0.37	-	16,16,16,16	0
57	MG	QA	1659	1/1	0.21	-	4,4,4,4	0
57	MG	YA	3032	1/1	0.51	-	50,50,50,50	0
57	MG	YA	3053	1/1	1.02	-	50,50,50,50	0
57	MG	QA	1602	1/1	1.00	-	11,11,11,11	0
57	MG	YA	3261	1/1	0.95	-	50,50,50,50	0
57	MG	RA	3050	1/1	0.14	-	8,8,8,8	0
57	MG	YA	3035	1/1	0.80	-	50,50,50,50	0
57	MG	RA	3071	1/1	0.86	-	50,50,50,50	0
57	MG	YA	3128	1/1	0.24	-	0,0,0,0	0
57	MG	XA	1620	1/1	0.14	-	0,0,0,0	0
57	MG	XA	1603	1/1	1.02	-	50,50,50,50	0
57	MG	YA	3072	1/1	0.46	-	50,50,50,50	0
57	MG	YA	3028	1/1	0.24	-	8,8,8,8	0
57	MG	YA	3130	1/1	0.10	-	3,3,3,3	0
57	MG	YA	3149	1/1	0.76	-	7,7,7,7	0
57	MG	RA	3166	1/1	1.00	-	9,9,9,9	0
57	MG	RA	3210	1/1	0.17	-	11,11,11,11	0
57	MG	XA	1622	1/1	0.10	-	6,6,6,6	0
57	MG	RB	202	1/1	0.23	-	15,15,15,15	0
57	MG	YA	3166	1/1	0.13	-	14,14,14,14	0
57	MG	YA	3248	1/1	0.75	-	15,15,15,15	0
57	MG	YA	3241	1/1	0.28	-	13,13,13,13	0
57	MG	YA	3100	1/1	0.74	-	0,0,0,0	0
57	MG	RA	3175	1/1	0.26	-	12,12,12,12	0
57	MG	RA	3008	1/1	0.27	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3143	1/1	0.22	-	11,11,11,11	0
57	MG	YA	3003	1/1	0.45	-	50,50,50,50	0
57	MG	YA	3206	1/1	0.26	-	20,20,20,20	0
57	MG	YA	3043	1/1	1.13	-	50,50,50,50	0
57	MG	YA	3211	1/1	0.15	-	3,3,3,3	0
57	MG	RA	3012	1/1	0.29	-	1,1,1,1	0
57	MG	QA	1639	1/1	0.24	-	27,27,27,27	0
57	MG	XA	1640	1/1	0.14	-	119,119,119,119	0
57	MG	YA	3020	1/1	0.58	-	6,6,6,6	0
57	MG	RA	3190	1/1	0.16	-	4,4,4,4	0
57	MG	RA	3155	1/1	0.20	-	9,9,9,9	0
57	MG	YA	3092	1/1	0.42	-	2,2,2,2	0
57	MG	RA	3083	1/1	0.38	-	3,3,3,3	0
59	ZN	XD	301	1/1	0.39	-	50,50,50,50	0
57	MG	RA	3200	1/1	0.26	-	31,31,31,31	0
57	MG	YA	3226	1/1	0.29	-	10,10,10,10	0
57	MG	YA	3252	1/1	0.17	-	4,4,4,4	0
57	MG	XA	1610	1/1	0.24	-	1,1,1,1	0
57	MG	RA	3025	1/1	0.27	-	7,7,7,7	0
57	MG	RA	3220	1/1	0.17	-	25,25,25,25	0
57	MG	YA	3136	1/1	0.10	-	1,1,1,1	0
57	MG	QA	1607	1/1	0.08	-	30,30,30,30	0
57	MG	YA	3069	1/1	0.11	-	8,8,8,8	0
57	MG	YA	3228	1/1	0.15	-	67,67,67,67	0
57	MG	YA	3070	1/1	0.26	-	33,33,33,33	0
57	MG	RA	3177	1/1	0.26	-	30,30,30,30	0
57	MG	QA	1636	1/1	0.18	-	11,11,11,11	0
57	MG	YA	3013	1/1	0.36	-	1,1,1,1	0
57	MG	RA	3104	1/1	0.11	-	5,5,5,5	0
57	MG	XA	1646	1/1	0.17	-	8,8,8,8	0
57	MG	RA	3234	1/1	0.86	-	50,50,50,50	0
57	MG	YA	3213	1/1	0.33	-	15,15,15,15	0
57	MG	QA	1648	1/1	0.23	-	16,16,16,16	0
57	MG	RA	3188	1/1	0.12	-	16,16,16,16	0
57	MG	RA	3060	1/1	0.72	-	13,13,13,13	0
57	MG	RA	3090	1/1	0.47	-	4,4,4,4	0
57	MG	YX	101	1/1	0.41	-	50,50,50,50	0
57	MG	XA	1606	1/1	0.61	-	13,13,13,13	0
57	MG	RA	3113	1/1	0.32	-	1,1,1,1	0
57	MG	YA	3046	1/1	0.27	-	12,12,12,12	0
57	MG	QA	1650	1/1	0.26	-	8,8,8,8	0
57	MG	RA	3067	1/1	0.17	-	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	XM	201	1/1	0.18	-	78,78,78,78	0
57	MG	XA	1607	1/1	0.34	-	17,17,17,17	0
57	MG	QA	1656	1/1	0.10	-	63,63,63,63	0
57	MG	RP	202	1/1	0.31	-	75,75,75,75	0
57	MG	QA	1635	1/1	0.20	-	11,11,11,11	0
57	MG	RA	3022	1/1	0.26	-	5,5,5,5	0
57	MG	YA	3006	1/1	0.81	-	50,50,50,50	0
57	MG	YA	3105	1/1	0.76	-	8,8,8,8	0
57	MG	RA	3062	1/1	0.51	-	2,2,2,2	0
57	MG	RA	3173	1/1	0.32	-	3,3,3,3	0
57	MG	RA	3243	1/1	0.37	-	18,18,18,18	0
57	MG	RA	3138	1/1	0.34	-	8,8,8,8	0
57	MG	QA	1617	1/1	0.44	-	2,2,2,2	0
57	MG	XA	1637	1/1	0.31	-	13,13,13,13	0
57	MG	YA	3158	1/1	0.25	-	6,6,6,6	0
57	MG	RA	3244	1/1	0.17	-	9,9,9,9	0
57	MG	QA	1644	1/1	0.28	-	24,24,24,24	0
57	MG	YA	3118	1/1	0.45	-	12,12,12,12	0
57	MG	XA	1636	1/1	0.21	-	9,9,9,9	0
57	MG	RA	3133	1/1	0.16	-	4,4,4,4	0
57	MG	YA	3254	1/1	0.41	-	0,0,0,0	0
57	MG	RA	3186	1/1	0.87	-	51,51,51,51	0
57	MG	RA	3165	1/1	0.27	-	3,3,3,3	0
57	MG	YA	3001	1/1	1.15	-	50,50,50,50	0
57	MG	XA	1667	1/1	0.17	-	4,4,4,4	0
57	MG	YA	3196	1/1	0.22	-	76,76,76,76	0
57	MG	YA	3097	1/1	0.71	-	50,50,50,50	0
58	PAR	XA	1673	42/42	0.30	-	132,132,132,132	0
57	MG	RA	3169	1/1	0.16	-	19,19,19,19	0
57	MG	YA	3159	1/1	0.20	-	22,22,22,22	0
57	MG	RA	3123	1/1	0.96	-	50,50,50,50	0
57	MG	QA	1601	1/1	0.43	-	21,21,21,21	0
57	MG	QA	1618	1/1	0.35	-	8,8,8,8	0
57	MG	RA	3163	1/1	0.19	-	38,38,38,38	0
57	MG	RA	3001	1/1	0.75	-	1,1,1,1	0
57	MG	RA	3019	1/1	1.20	-	50,50,50,50	0
57	MG	RA	3125	1/1	0.08	-	14,14,14,14	0
57	MG	YA	3075	1/1	1.17	-	50,50,50,50	0
57	MG	RA	3109	1/1	0.25	-	11,11,11,11	0
57	MG	YA	3114	1/1	0.33	-	16,16,16,16	0
57	MG	RA	3041	1/1	0.63	-	50,50,50,50	0
57	MG	QA	1646	1/1	0.66	-	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3041	1/1	0.84	-	50,50,50,50	0
57	MG	RD	301	1/1	0.30	-	15,15,15,15	0
57	MG	YA	3009	1/1	0.76	-	50,50,50,50	0
57	MG	RA	3049	1/1	0.31	-	1,1,1,1	0

6.5 Other polymers ⓘ

There are no such residues in this entry.