



wwPDB X-ray Structure Validation Summary Report

Sep 17, 2014 – 02:52 PM EDT

PDB ID : 4LEL
Title : Crystal Structure of Frameshift Suppressor tRNA SufA6 Bound to Codon CCG-G on the Ribosome
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-06-25
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>

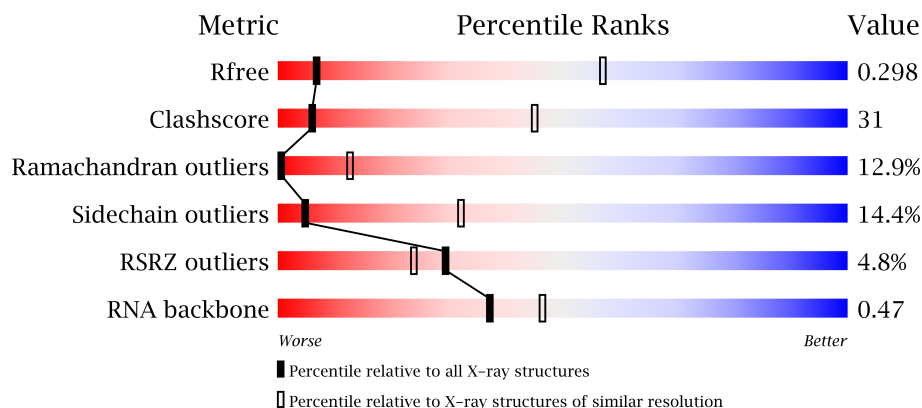
The following versions of software and data (see [references](#)) were used in the production of this report:

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	QV	77	
22	XV	77	
23	QX	25	
23	XX	25	
24	QY	18	
24	XY	18	
25	RA	2916	
25	YA	2916	
26	RB	122	
26	YB	122	
27	RD	276	

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Mol	Chain	Length	Quality of chain
27	YD	276	
28	RE	206	
28	YE	206	
29	RF	210	
29	YF	210	
30	RG	182	
30	YG	182	
31	RH	180	
31	YH	180	
32	RI	148	
32	YI	148	
33	RN	140	
33	YN	140	
34	RO	122	
34	YO	122	
35	RP	150	
35	YP	150	
36	RQ	141	
36	YQ	141	
37	RR	118	
37	YR	118	
38	RS	112	
38	YS	112	
39	RT	146	
39	YT	146	
40	RU	118	
40	YU	118	
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	

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Mol	Chain	Length	Quality of chain
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	71	
51	R5	60	
51	Y5	60	
52	R6	54	
52	Y6	54	
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	
56	Z6	3	
56	Z8	3	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291958 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 P-site tRNA fMet.

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

- Molecule 23 is a RNA chain called A-site ASL SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	8	Total	C	N	O	P	0	0	0
			173	77	33	55	8			
23	XX	8	Total	C	N	O	P	0	0	0
			173	77	33	55	8			

- Molecule 24 is a RNA chain called messenger RNA.

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

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

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

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

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

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

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

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

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

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

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

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

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

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

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

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

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

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

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

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

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

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

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

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

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

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

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

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

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
51	Y5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

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

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

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

- Molecule 54 is a protein called 50S ribosomal protein L35.

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

- Molecule 55 is a protein called 50S ribosomal protein L36.

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

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

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

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

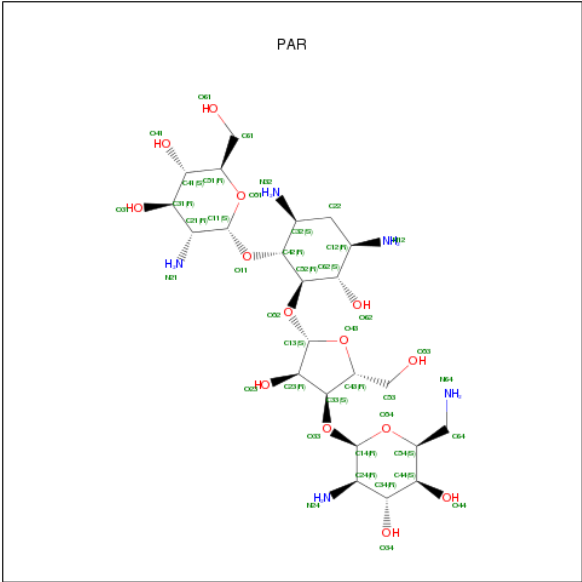
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	65	Total	Mg	0	0
			65	65		
57	RP	2	Total	Mg	0	0
			2	2		
57	YA	267	Total	Mg	0	0
			267	267		
57	QM	1	Total	Mg	0	0
			1	1		
57	YD	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	XX	1	Total 1	Mg 1	0	0
57	QV	1	Total 1	Mg 1	0	0
57	XA	70	Total 70	Mg 70	0	0
57	R0	1	Total 1	Mg 1	0	0
57	Y0	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	RD	1	Total 1	Mg 1	0	0
57	XB	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	242	Total 242	Mg 242	0	0
57	YP	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	1	Total 1	Mg 1	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
57	YE	1	Total 1	Mg 1	0	0

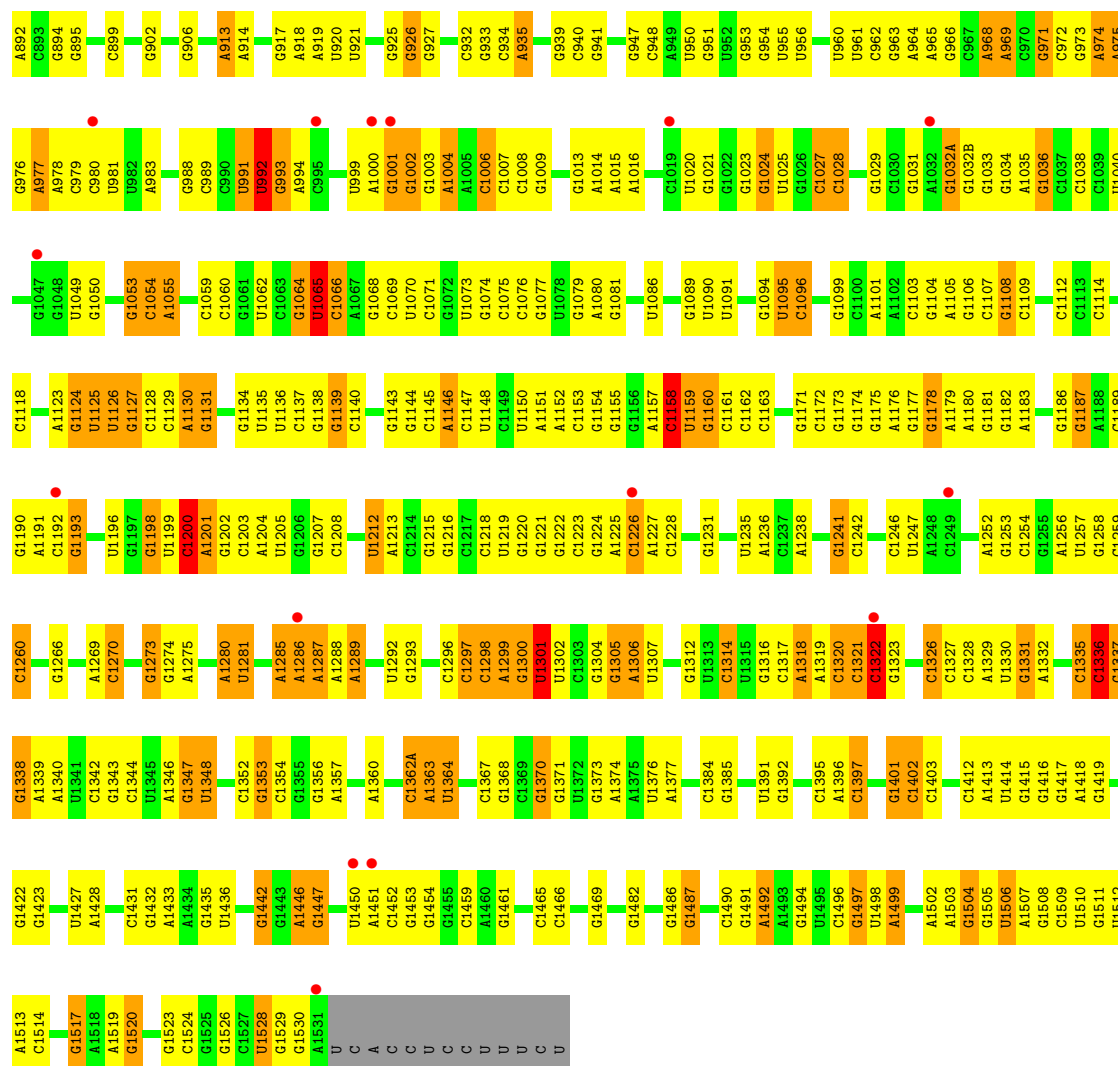
- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



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

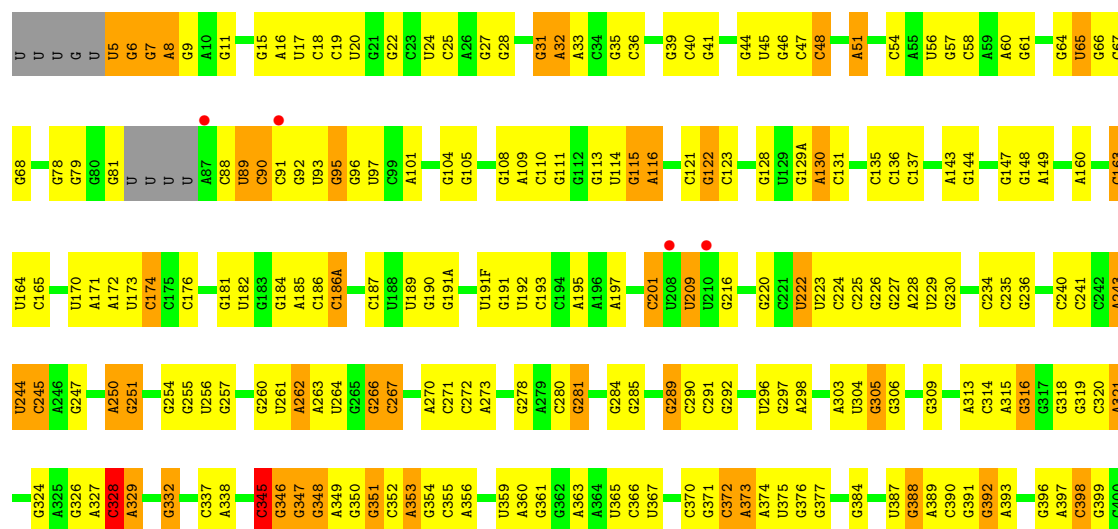
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

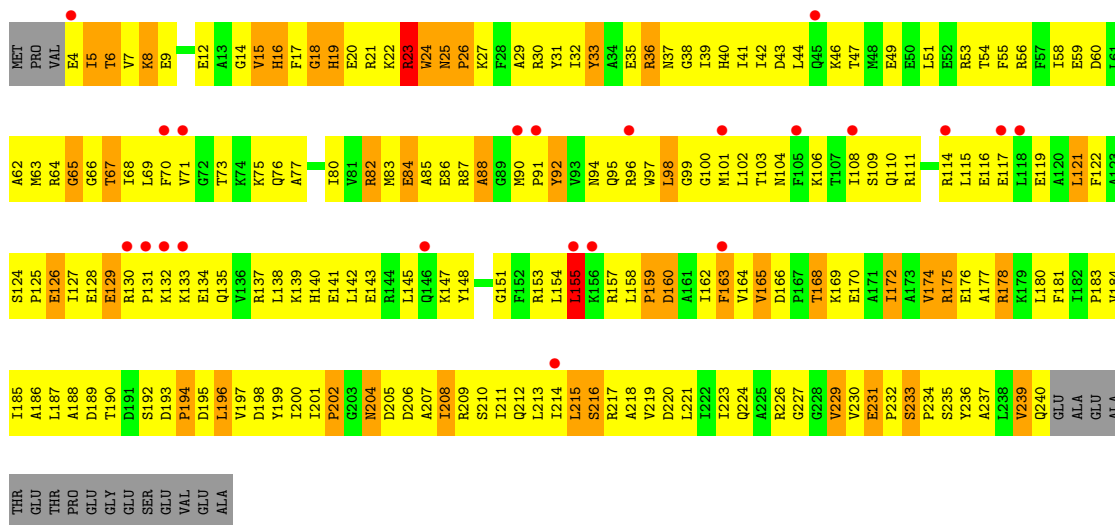


• Molecule 1: 16S rRNA

Chain XA:

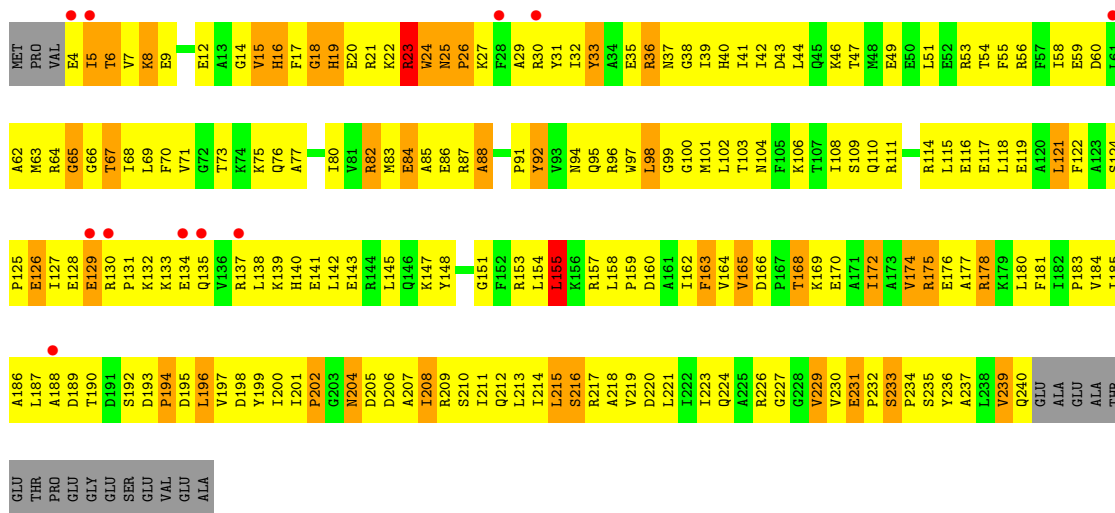






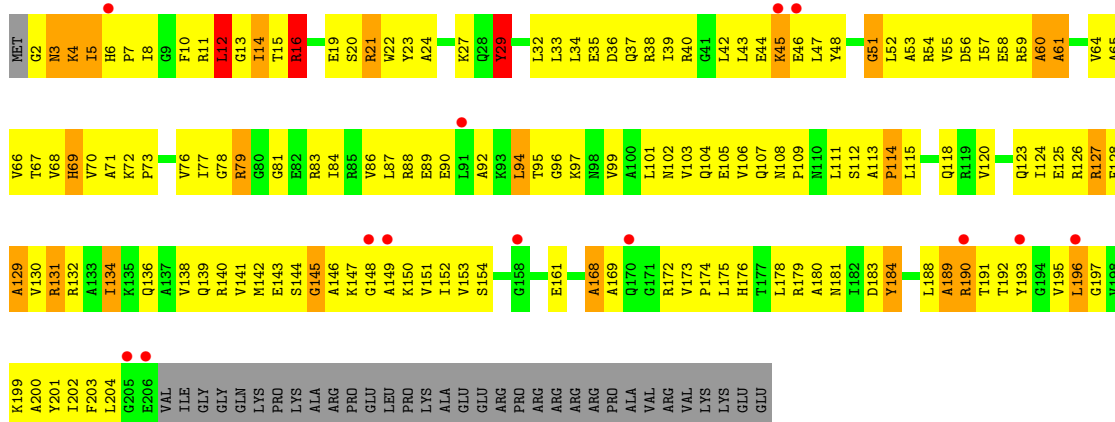
• Molecule 2: 30S ribosomal protein S2

Chain XB:



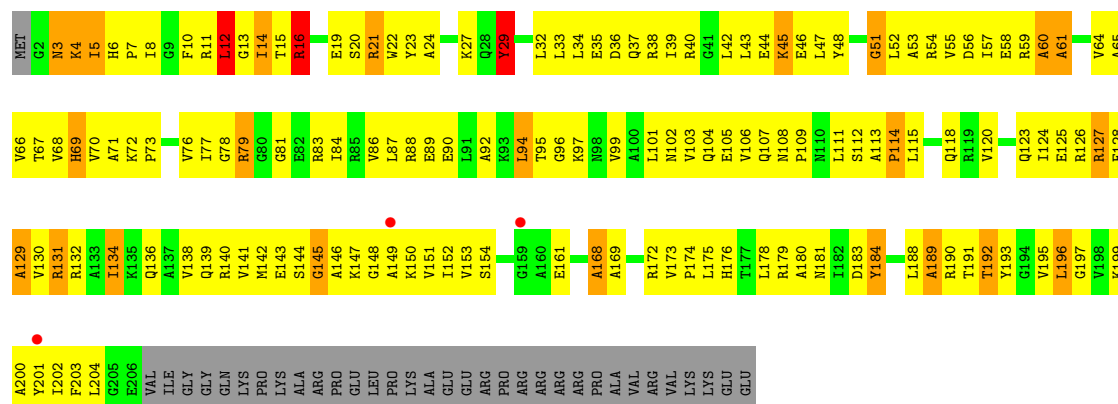
• Molecule 3: 30S ribosomal protein S3

Chain QC:



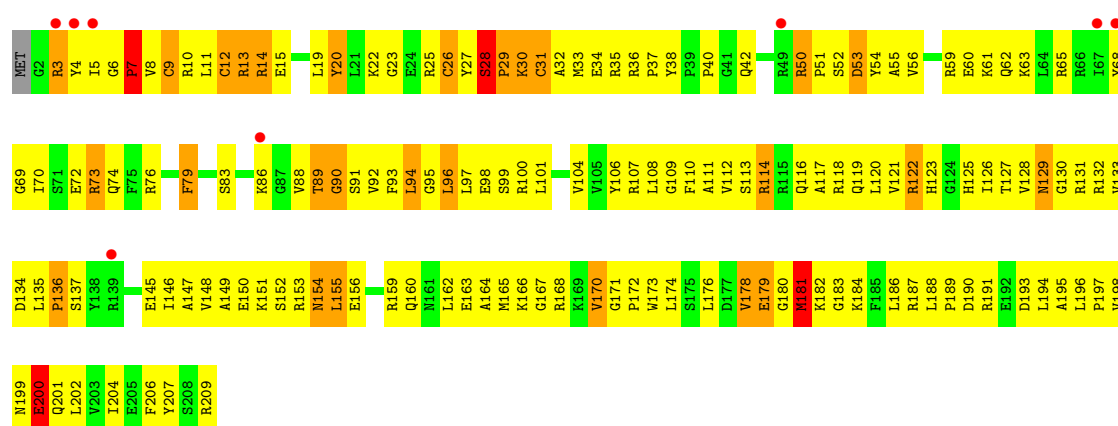
- Molecule 3: 30S ribosomal protein S3

Chain XC:



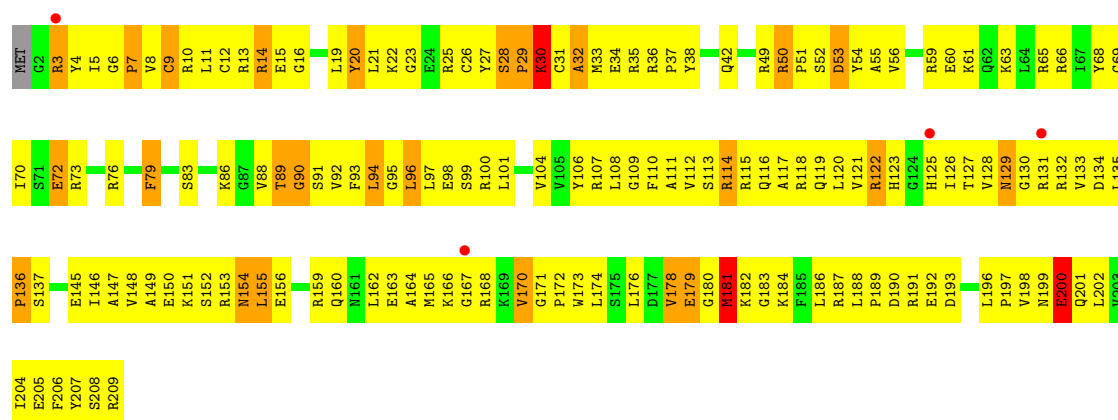
- Molecule 4: 30S ribosomal protein S4

Chain QD:



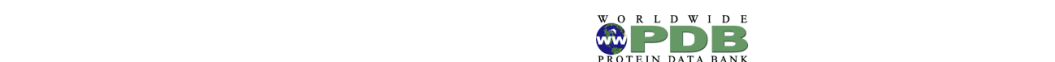
- Molecule 4: 30S ribosomal protein S4

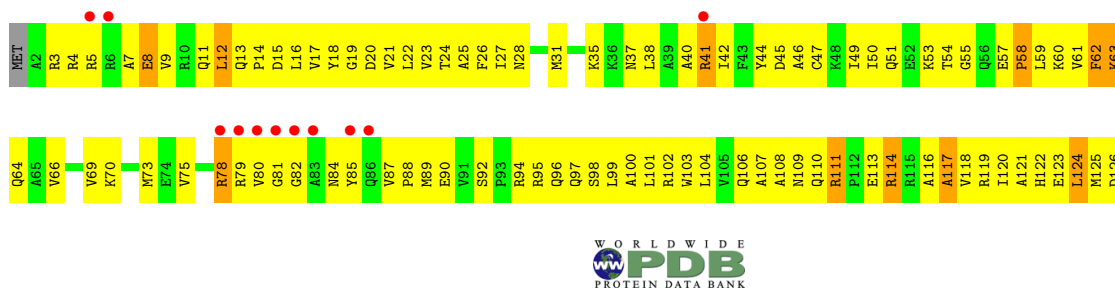
Chain XD:



- Molecule 5: 30S ribosomal protein S5

Chain QE:

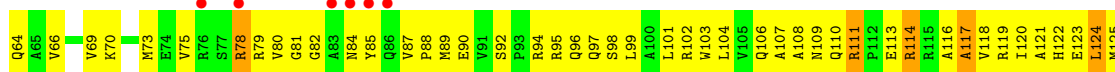






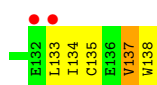
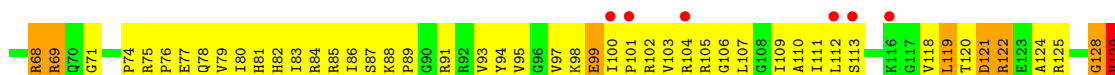
- Molecule 7: 30S ribosomal protein S7

Chain XG:



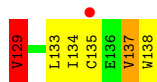
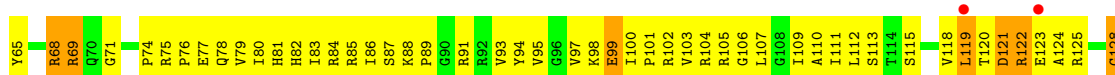
- Molecule 8: 30S ribosomal protein S8

Chain QH:



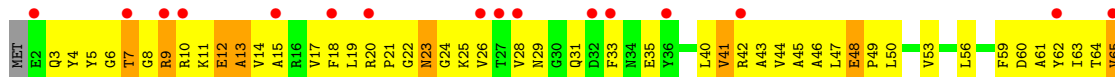
- Molecule 8: 30S ribosomal protein S8

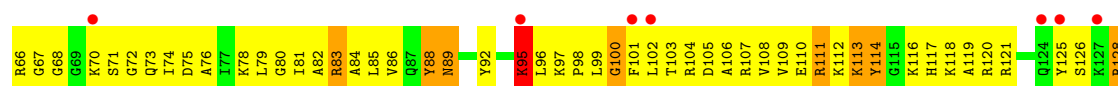
Chain XH:



- Molecule 9: 30S ribosomal protein S9

Chain QI:





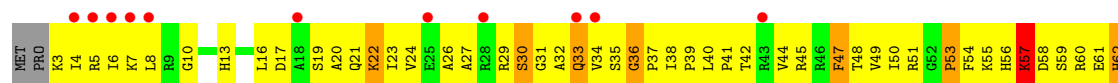
• Molecule 9: 30S ribosomal protein S9

Chain XI:



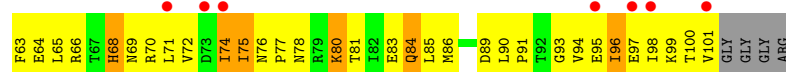
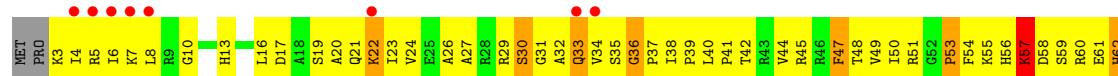
• Molecule 10: 30S ribosomal protein S10

Chain QJ:



• Molecule 10: 30S ribosomal protein S10

Chain XJ:



• Molecule 11: 30S ribosomal protein S11

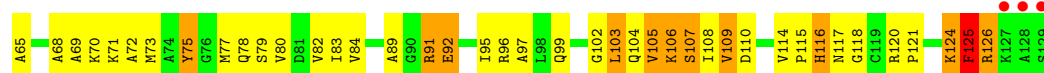
Chain QK:



• Molecule 11: 30S ribosomal protein S11

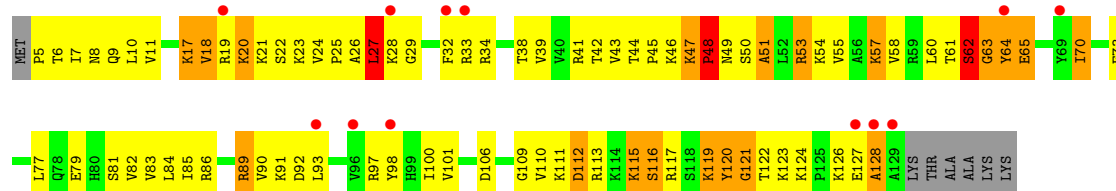
Chain XK:





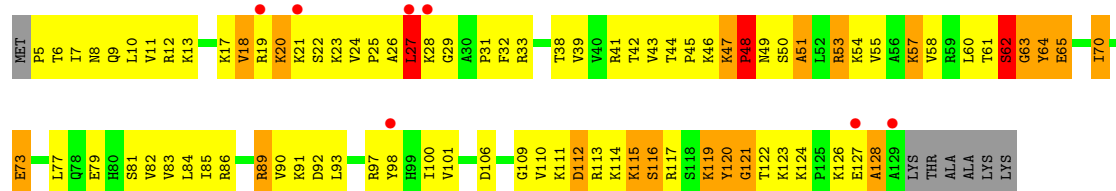
- Molecule 12: 30S ribosomal protein S12

Chain QL:



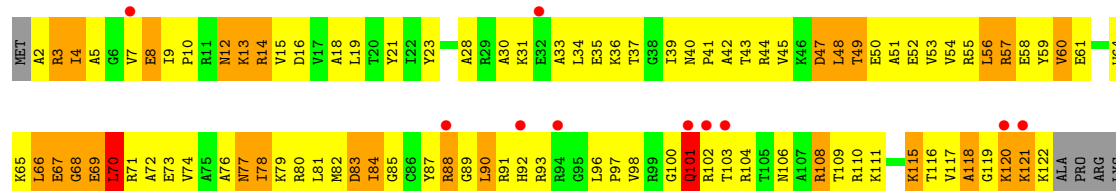
- Molecule 12: 30S ribosomal protein S12

Chain XL:



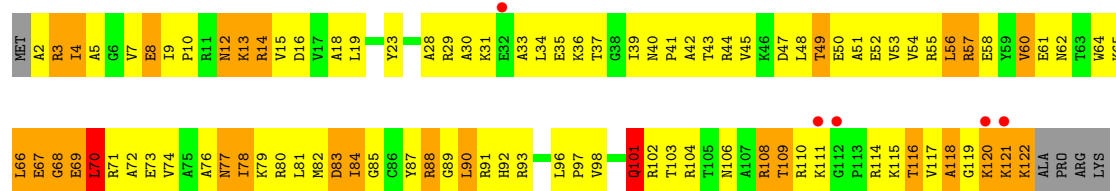
- Molecule 13: 30S ribosomal protein S13

Chain QM:



- Molecule 13: 30S ribosomal protein S13

Chain XM:



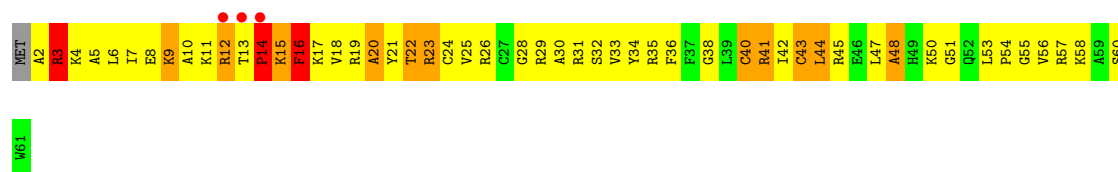
- Molecule 14: 30S ribosomal protein S14

Chain QN:



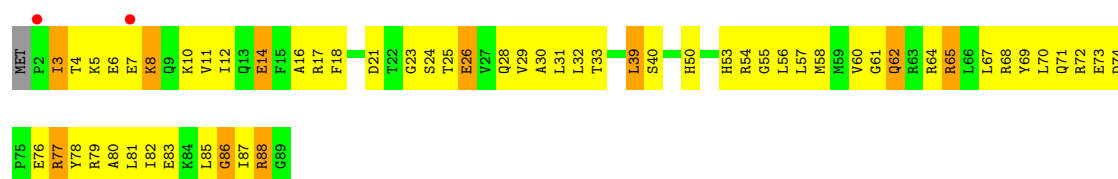
- Molecule 14: 30S ribosomal protein S14

Chain XN:



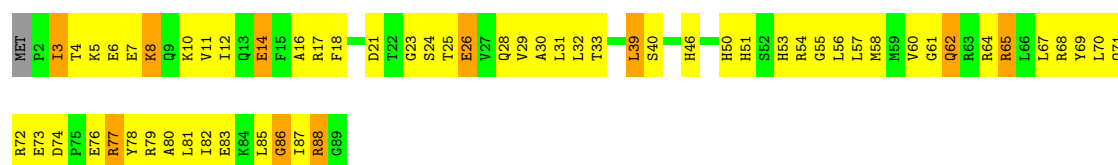
- Molecule 15: 30S ribosomal protein S15

Chain QO:



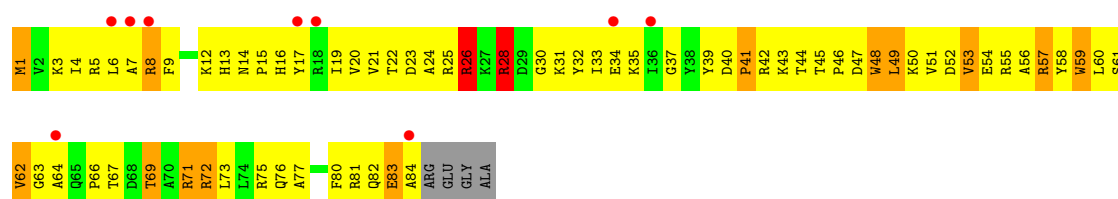
- Molecule 15: 30S ribosomal protein S15

Chain XO:



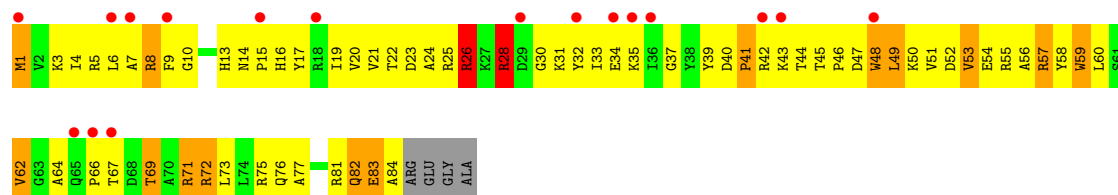
- Molecule 16: 30S ribosomal protein S16

Chain QP:



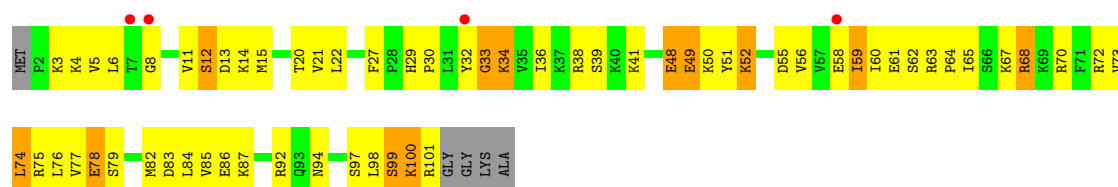
- Molecule 16: 30S ribosomal protein S16

Chain XP:



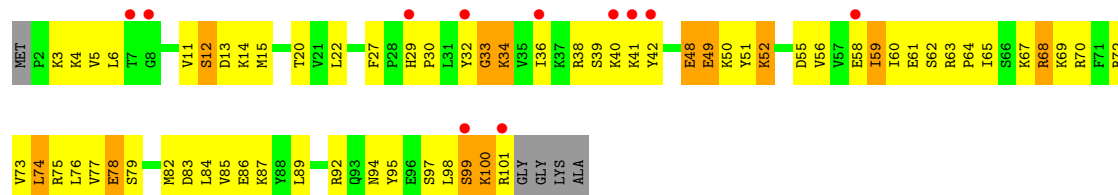
- Molecule 17: 30S ribosomal protein S17

Chain QQ:



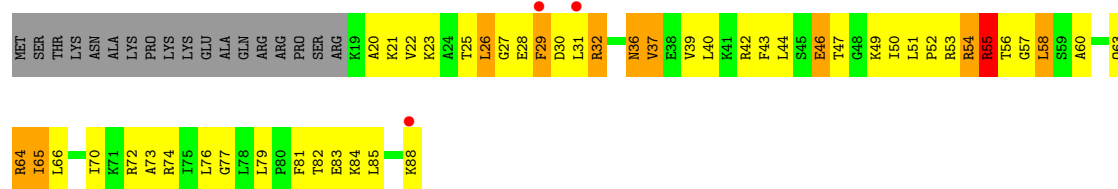
- Molecule 17: 30S ribosomal protein S17

Chain XQ:



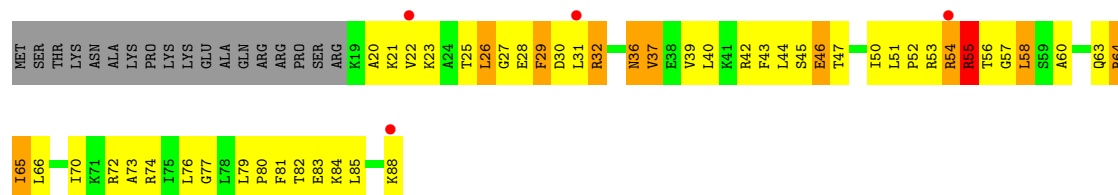
- Molecule 18: 30S ribosomal protein S18

Chain QR:



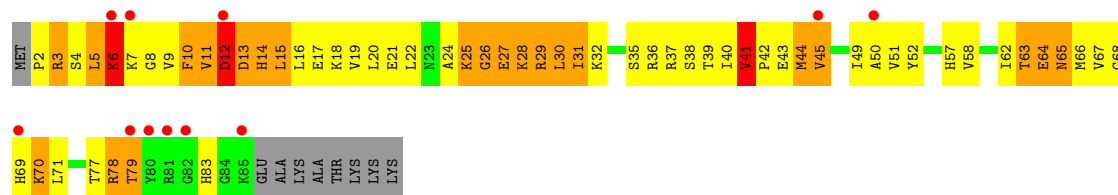
- Molecule 18: 30S ribosomal protein S18

Chain XR:



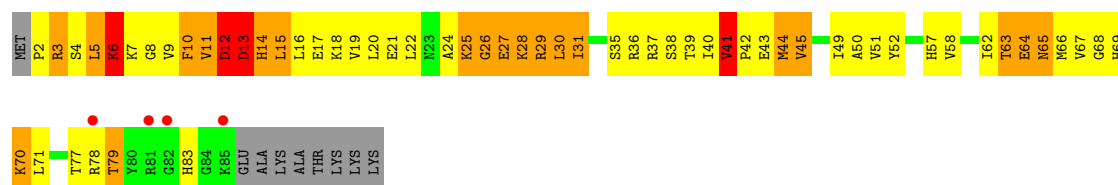
- Molecule 19: 30S ribosomal protein S19

Chain QS:



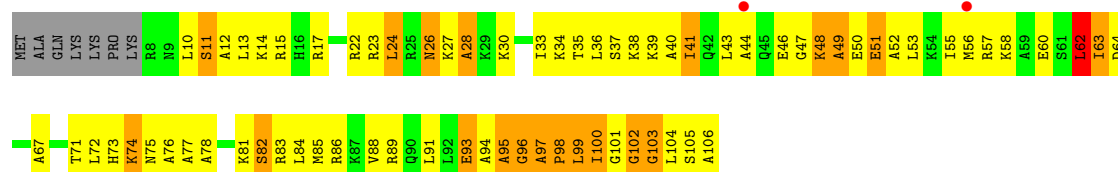
- Molecule 19: 30S ribosomal protein S19

Chain XS:



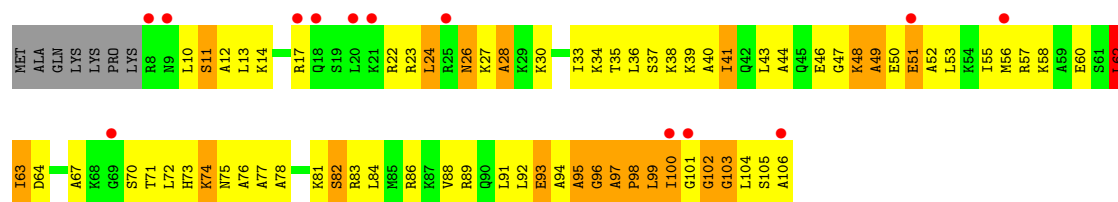
- Molecule 20: 30S ribosomal protein S20

Chain QT:



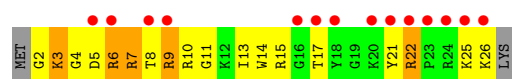
- Molecule 20: 30S ribosomal protein S20

Chain XT:



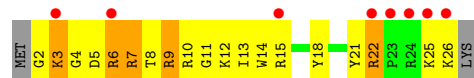
- Molecule 21: 30S ribosomal protein S21

Chain QU:



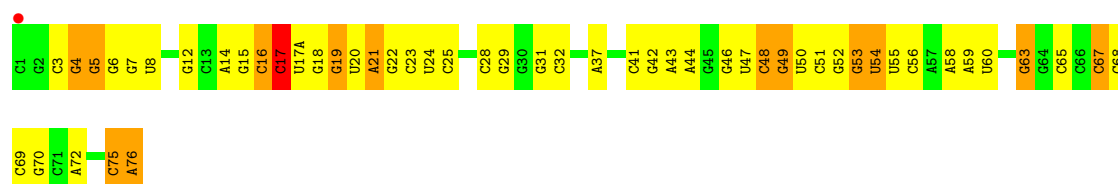
- Molecule 21: 30S ribosomal protein S21

Chain XU:



- Molecule 22: P-site tRNA fMet

Chain QV:



- Molecule 22: P-site tRNA fMet

Chain XV:



• Molecule 23: A-site ASL SufA6

Chain QX:



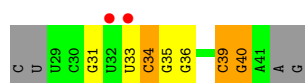
• Molecule 23: A-site ASL SufA6

Chain XX:



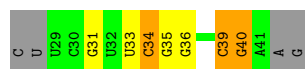
• Molecule 24: messenger RNA

Chain QY:



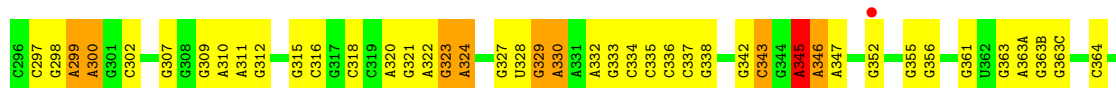
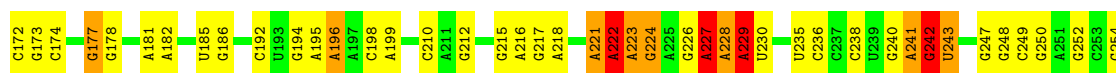
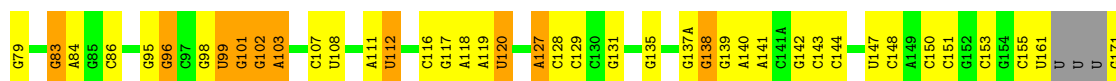
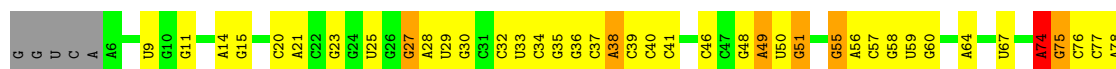
• Molecule 24: messenger RNA

Chain XY:



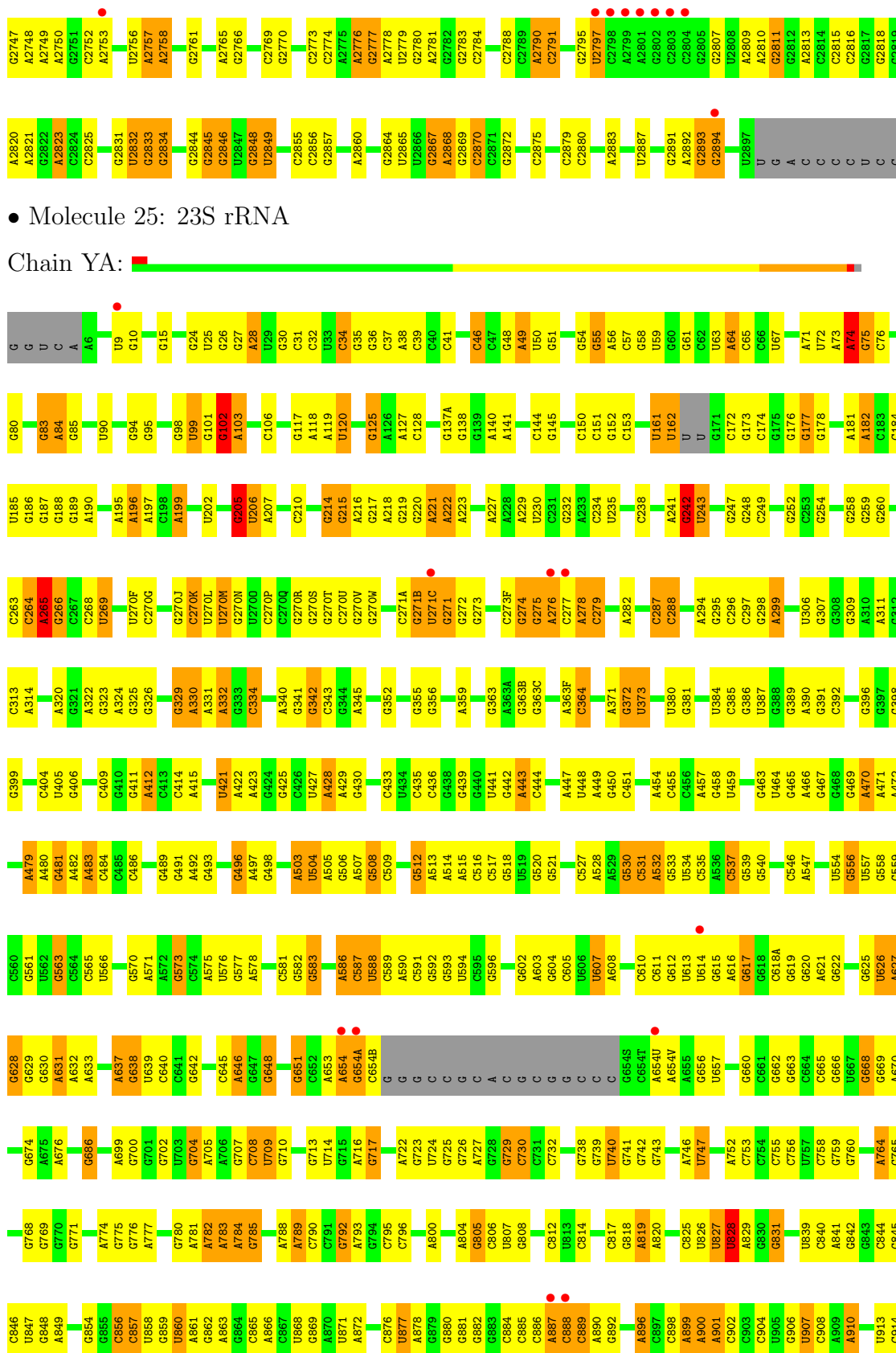
• Molecule 25: 23S rRNA

Chain RA:

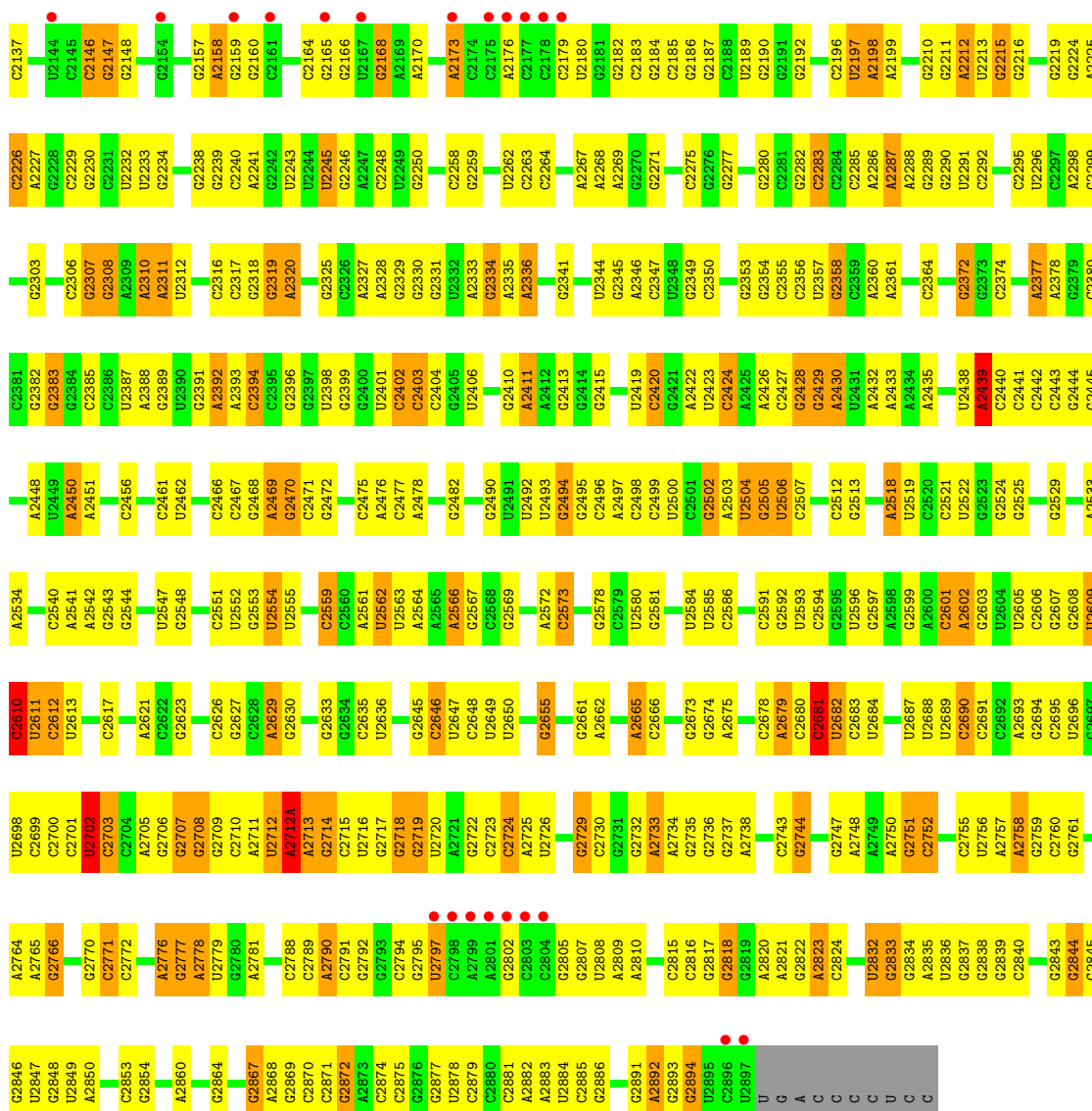


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C1417	G1339	G1264	A1182	G1100	A1029	A960	C884	A804	G728	C	G598	U524	G452	G372
G1418	G1340	G1265	G1183	U1101	G1030	C961	C885	G805	G729	C	G599	U525	G453	A373
A1419	U1341	G1266	G1184	C1102	G1031	G962	C886	G806	C730	C	G600	U526	A454	C374
U1420	U1267	G1185	C1103	U1032	U963	G963	C887	U807	A734	A	G601	C527	G455	C375
G1421	C1345	A1268	G1186	C1104	U1033	C964	C888	G808	A735	C	A602	U528	C456	C376
G1422	A1269	A1269	G1187	U1105	G1034		C889	G809	A736	C	A603	A529	A457	C377
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G1424	G1271	A1189	G1189		C1041	G972	G892	U811	C737	C	U607	G530	G459	U381
G1425	A1272	G1190	G1190	G1110	G1042	G973	C993	C812	G738	G	A608	A531	U459	G382
G1426	U1273			A1111	G1043	G974	C994	U813	G739	C	G609	A532	A460	U383
A1427	G1355	G1195	G1195	U1112	G1044	C974A	A896	C814	U740	C	G609A	U534	G463	U384
C1428	A1276			U1113	A1045	G975	C997	G741	G741	C	C610	U535	U464	C385
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C1430	U1278			G1115	G1047	G977	A899	G743	G743	C	G612	C537	G467	U387
U1431	G1279	G1203	G1203		A1048	G978	A900	A818			G613	G539	G468	G388
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G1435	G1285	A1205	A1205	C1124	A1051	A980	C902	G823	U747		U615		A470	C392
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A1444	U1292	A1210	A1210	A1129	A1056	C985	U907	U828	C753		G620	G548	G481	A401
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	U1293	U1212	U1212	G1131	G1058	G987	A910	G830	U757		A822	G550	A483	C403
G1448	U1294				U1060	G987	A911	G831	C758		G623	G551	G484	U404
A1449	C1295	G1216	G1216	C1135	U1061	C991	C915	U839	A764		G624	U554	C485	A405
G1450	G1296	C1217	C1217	G1136	G1062	C992	C916	C840	G765		G625	G556	G486	G406
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G1455	U1299	A1220	A1220	G1139	U1065	C995	G919	C843	U770		G630	U561	G489	C409
G1459	U1300	C1221	C1221	C1140	U1066	A996	G919	U847	G771		A631	G562	G491	G410
	A1301	G1224	G1224	U1141	U1067	G997	U922	G848	G772		A632	G563	A492	G411
G1461	U1308			U1142	A1068	C998	C923	A849	G773		A633	C564	G493	A412
C1462	G1309	G1228	G1228	A1143	A1070	A1000	C924		A774		A634	C565	G494	C413
	U1312				G1071	A1001		G853	G775		C635	U566	G495	C414
C1467	U1313	G1231	G1231	G1151	C1076	C1005	G928	G854	G776		G636	U567		
G1468	A1314	G1232	G1232	C1152	A1077	C1006		G855	A777		A637	A571	G498	C417
A1469	C1315	U1236	U1236	G1153	C1078	C1007	G931	C856	G780		U638	A572	U499	G418
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A1471	G1319	G1238	G1238	A1155	C1080	A1009	C935	G859	A782		C640	C574	A501	C420
	C1320	U1239	U1239	G1156	U1081	A1010	C936	U860	A783		C641	A575	A502	
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	U1322			G1163	A1084	C1013	G938	G862	G785		A643	U504	U504	A428
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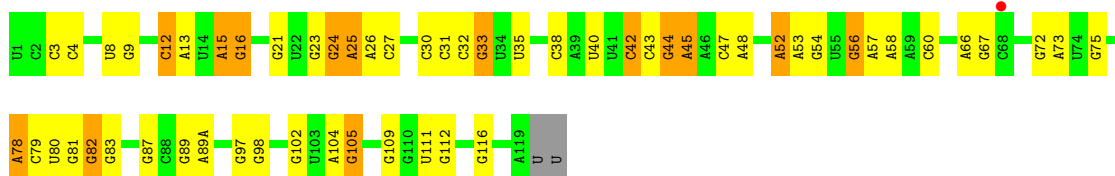


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C1404	U1405	U1406	C1407	C1408	C1411	U1415	G1416	C1417	A1418	A1419	U1420	G1421	A1427	A1428	G1429	U1430	A1431	C1432	U1433	A1434	G1440	G1441	G1442	G1443	G1444	A1444A	C1445	G1448	A1449	G1449A	U1454	G1455	C1458	G1461	C1462	C1467	A1471	A1472	G1473	C1474	G1475	C1476	A1477	G1478	G1479	G1480	U1482	G1483	G1484								
U1316	A1317	C1318	A1321	G1325	U1329	G1332	G1337	G1338	G1339	U1340	U1341	C1345	A1349	A1354	G1355	G1356	U1357	G1358	A1359	G1364	U1365	A1366	A1367	G1368	C1370	U1371	U1372	A1373	A1378	A1384	G1385	C1386	G1389	U1390	U1391	A1392	A1393	U1394	A1395	U1396	U1397	G1398	C1399	C1403													
G1226	U1229A	C1230	G1236	G1237	G1238	G1239	U1240	A1241	G1244	G1245	A1246	U1247	G1248	U1249	G1250	C1251	G1252	A1253	G1256	C1257	G1258	G1259	G1260	C1261	U1262	U1263	A1264	A1265	G1266	C1270	G1271	A1272	U1273	A1274	A1275	A1276	G1277	G1280	A1287	A1302	A1302	A1308	G1309	G1310	C1311												
G1149	C1150	C1151	C1152	C1153	G1154	A1155	A1156	C1157	C1158	C1161	C1162	U1165	C1166	G1169	G1170	G1171	C1173	A1174	U1175	G1176	A1177	C1178	C1179	C1180	G1184	C1185	G1186	G1187	A1188	A1189	G1190	G1191	G1195	G1203	A1204	G1205	G1206	C1207	A1210	U1211	G1212	G1216	C1217	C1218	G1219	A1220	C1221	C1222	G1223	G1224	C1225						
A1070	G1071	C1075	C1076	A1077	U1078	C1079	C1080	U1081	U1082	U1083	A1084	A1085	A1086	U1087	A1088	U1089	U1093	U1094	A1095	A1096	U1097	A1098	G1099	A1103	C1104	C1109	G1110	A1111	G1112	U1113	G1114	C1119	G1120	C1121	G1122	G1125	A1128	U1129	A1130	G1131	A1132	U1133	C1135	G1136	U1142	A1142A	A1143	G1144	C1145	U1066	A1067	G1068	A1069				
C915	G916	A917	A918	G919	G920	G921	U922	C923	G928	G932	A933	G934	C935	C936	U937	A941	G942	U943	G944	A945	G946	A957	U958	A959	A960	C961	G962	G966	C967	G974	C974A	G975	C976	G977	A980	A981	C982	A983	A984	C985	G989	A990	C991	C992	G993	C994	C995	A996	C997	C998	U999						



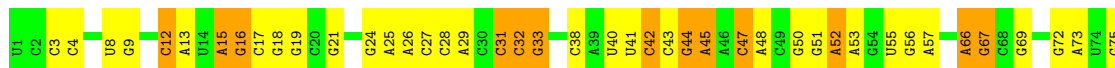
• Molecule 26: 5S rRNA

Chain RB:



• Molecule 26: 5S rRNA

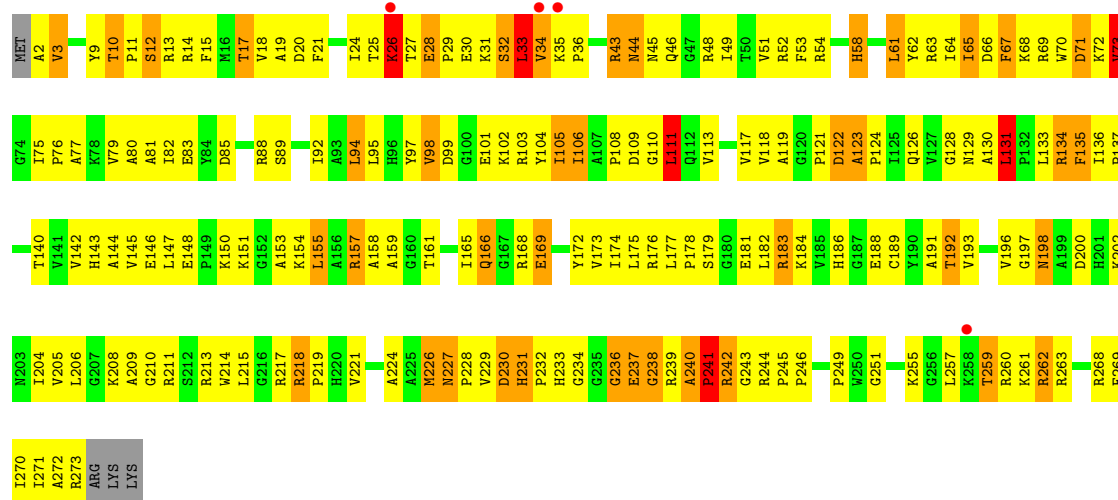
Chain YB:





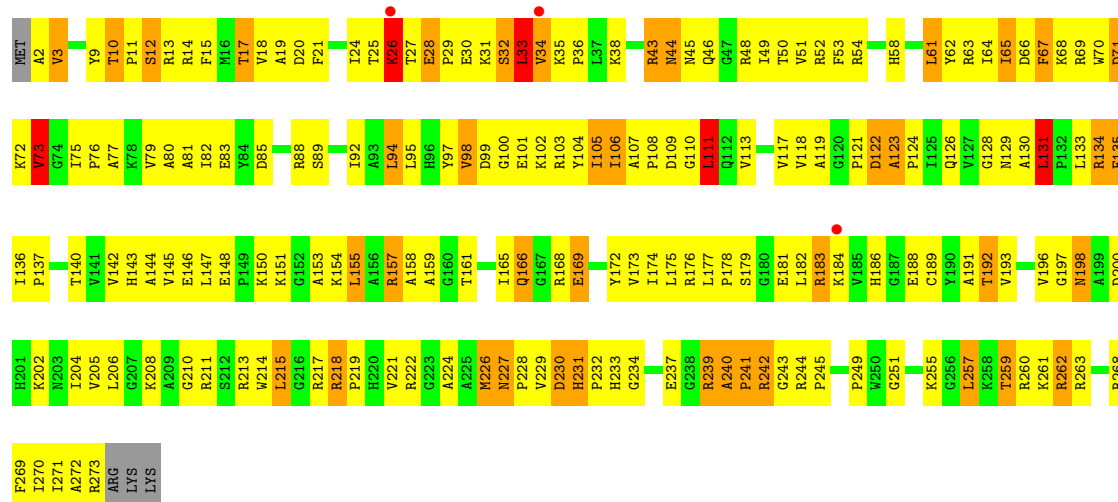
• Molecule 27: 50S ribosomal protein L2

Chain RD:



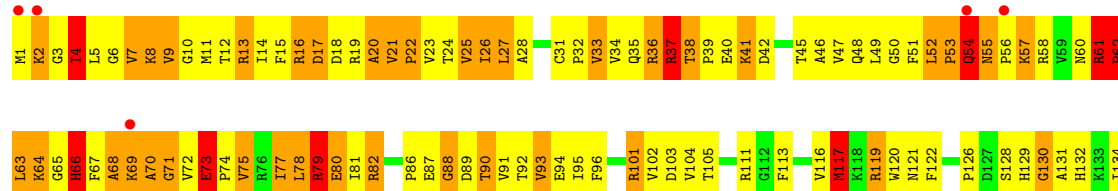
• Molecule 27: 50S ribosomal protein L2

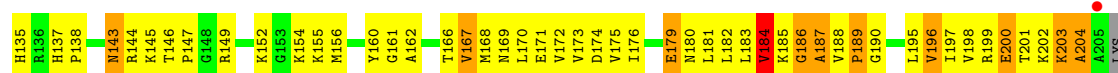
Chain YD:



• Molecule 28: 50S ribosomal protein L3

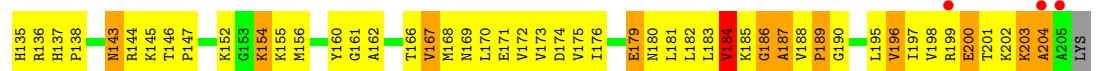
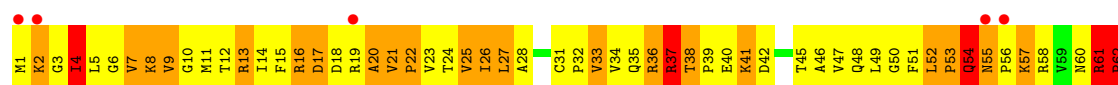
Chain RE:





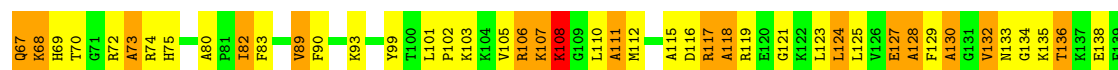
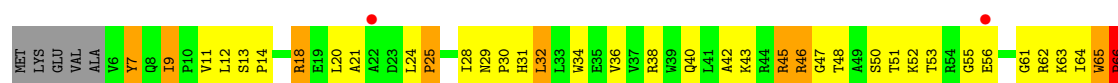
• Molecule 28: 50S ribosomal protein L3

Chain YE:



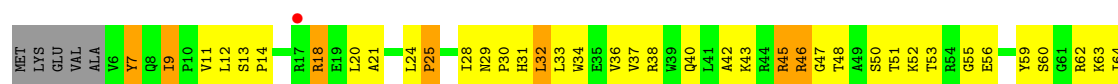
• Molecule 29: 50S ribosomal protein L4

Chain RF:



• Molecule 29: 50S ribosomal protein L4

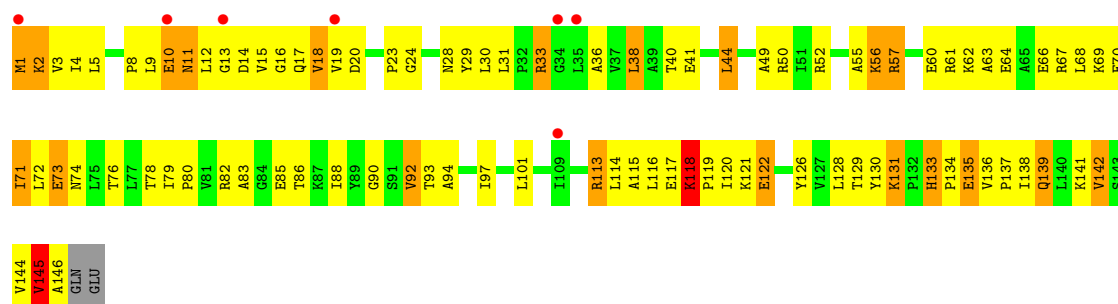
Chain YF:



• Molecule 30: 50S ribosomal protein L5

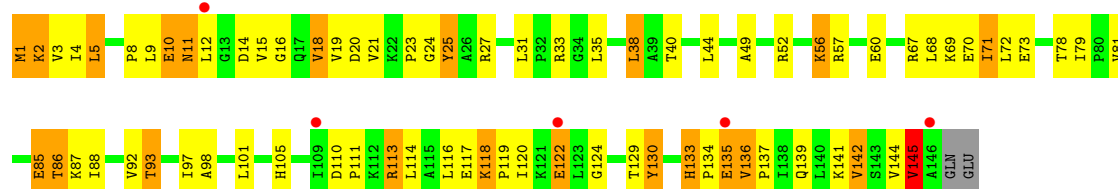
Chain RG:

Chain RI: 



- Molecule 32: 50S ribosomal protein L9

Chain YI: 



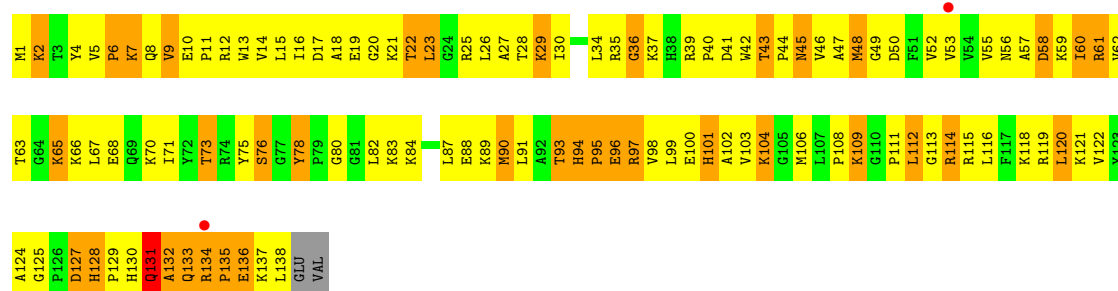
- Molecule 33: 50S ribosomal protein L13

Chain RN: 



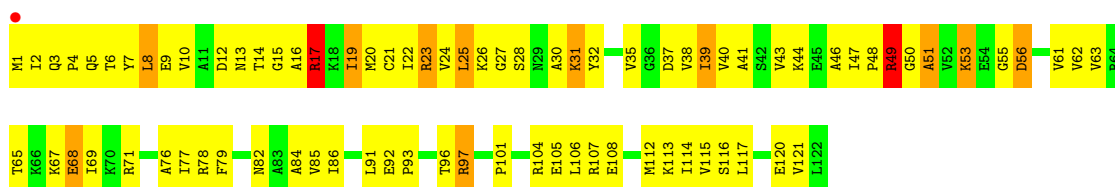
- Molecule 33: 50S ribosomal protein L13

Chain YN: 



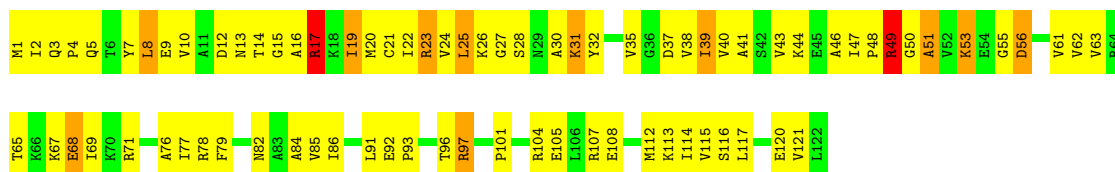
- Molecule 34: 50S ribosomal protein L14

Chain RO: 



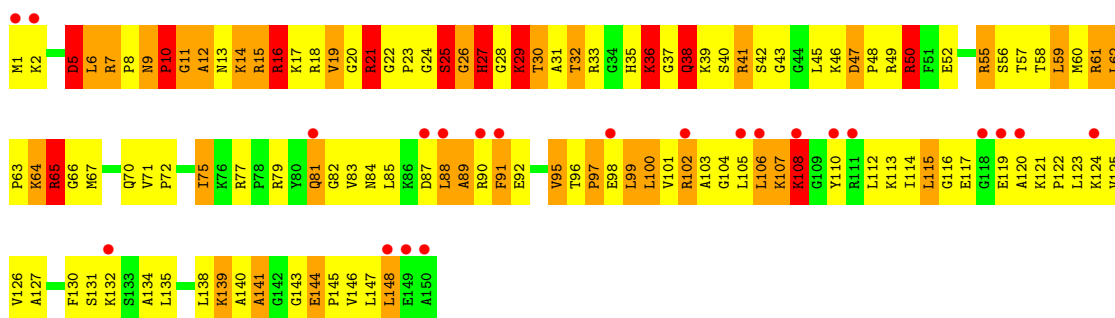
• Molecule 34: 50S ribosomal protein L14

Chain YO:



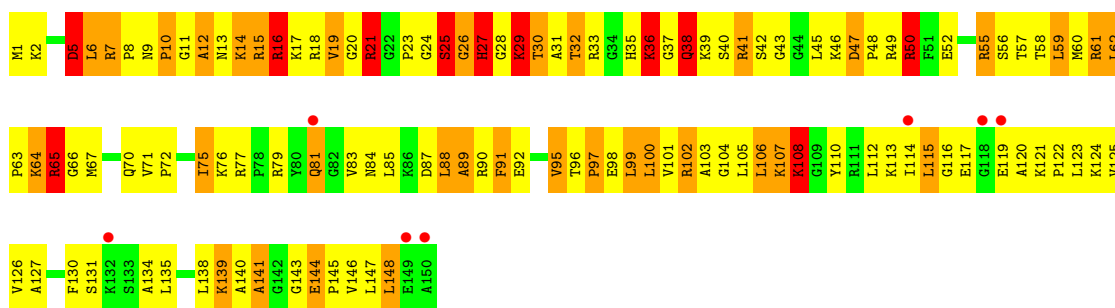
• Molecule 35: 50S ribosomal protein L15

Chain RP:



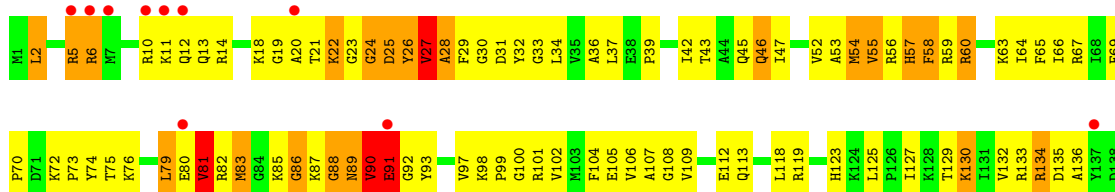
• Molecule 35: 50S ribosomal protein L15

Chain YP:



• Molecule 36: 50S ribosomal protein L16

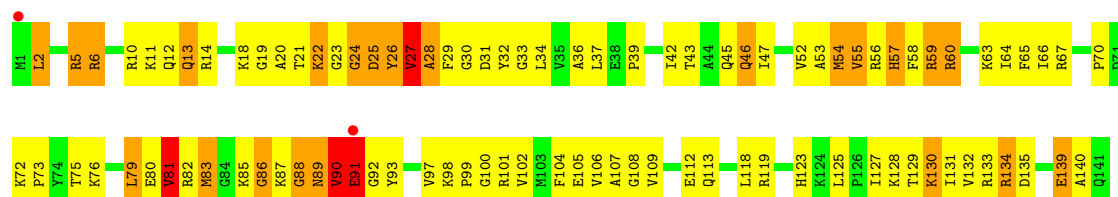
Chain RQ:





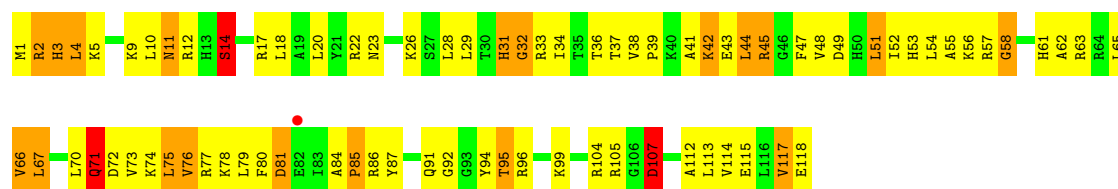
- Molecule 36: 50S ribosomal protein L16

Chain YQ:



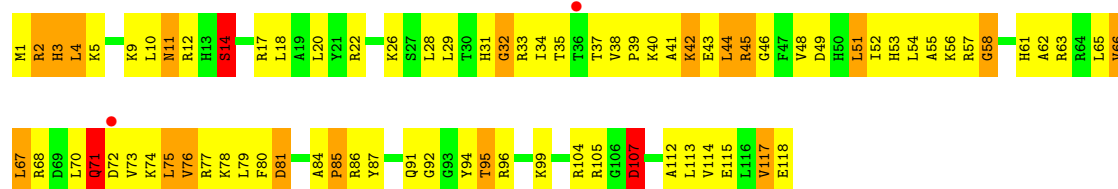
- Molecule 37: 50S ribosomal protein L17

Chain RR:



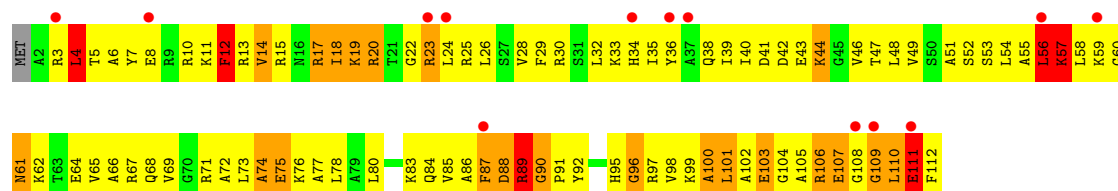
- Molecule 37: 50S ribosomal protein L17

Chain YR:



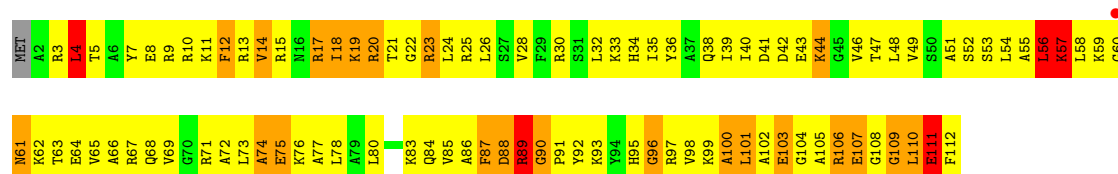
- Molecule 38: 50S ribosomal protein L18

Chain RS:

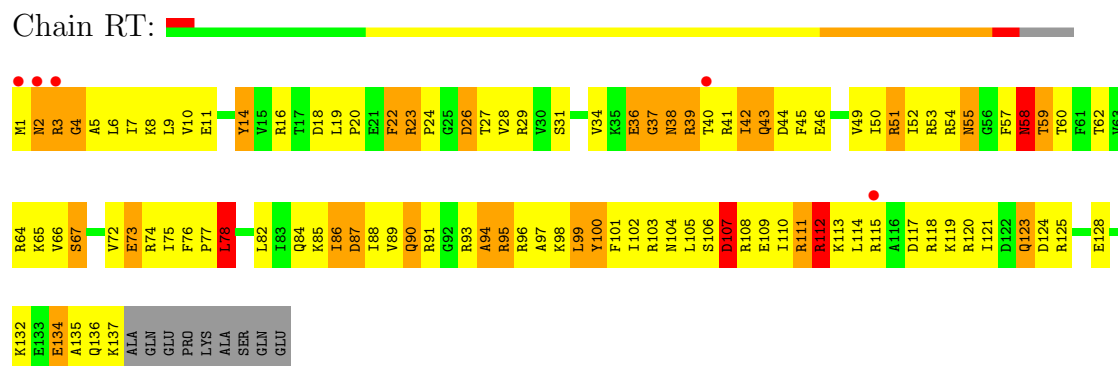


- Molecule 38: 50S ribosomal protein L18

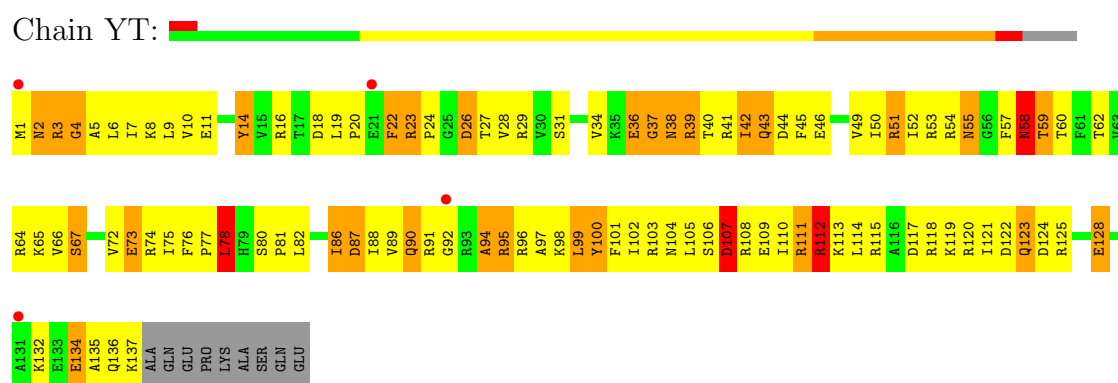
Chain YS:



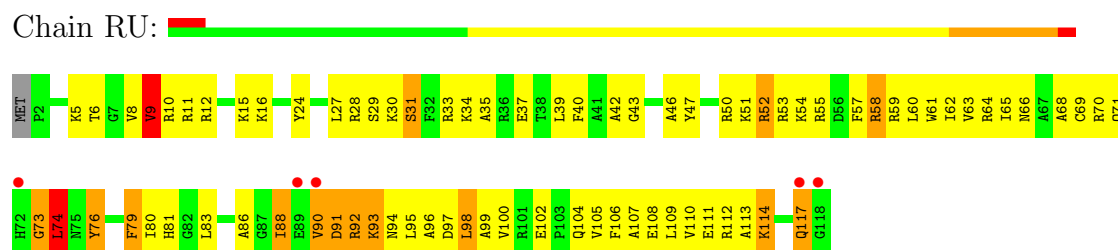
- Molecule 39: 50S ribosomal protein L19



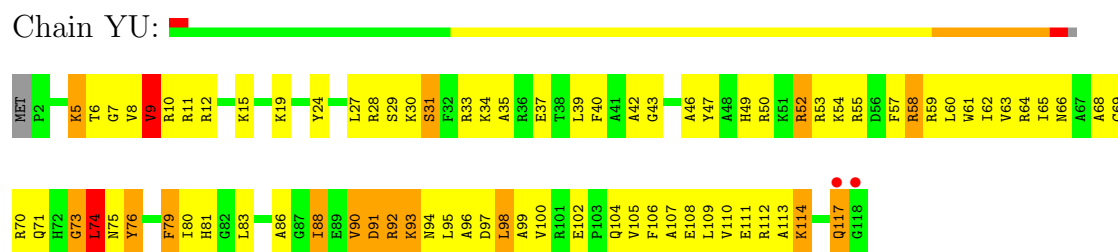
- Molecule 39: 50S ribosomal protein L19



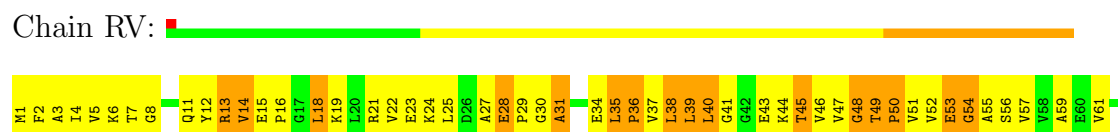
- Molecule 40: 50S ribosomal protein L20

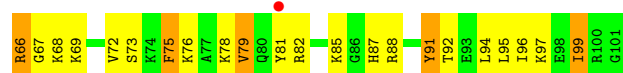


- Molecule 40: 50S ribosomal protein L20



- Molecule 41: 50S ribosomal protein L21





- Molecule 41: 50S ribosomal protein L21

Chain YV:



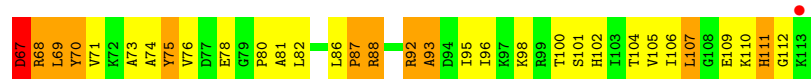
- Molecule 42: 50S ribosomal protein L22

Chain RW:



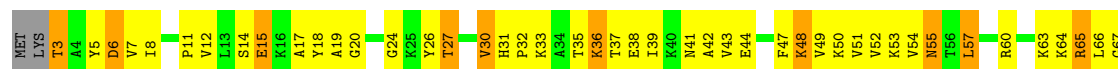
- Molecule 42: 50S ribosomal protein L22

Chain YW:



- Molecule 43: 50S ribosomal protein L23

Chain RX:



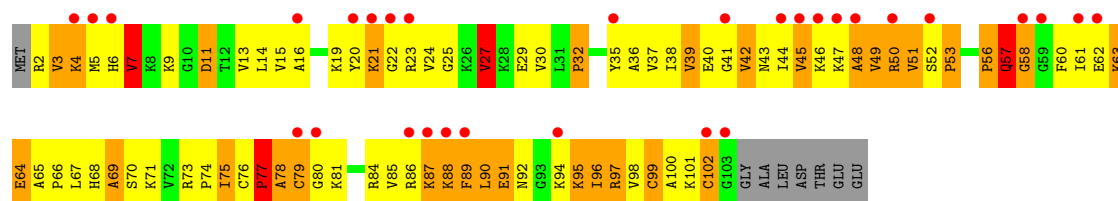
- Molecule 43: 50S ribosomal protein L23

Chain YX:



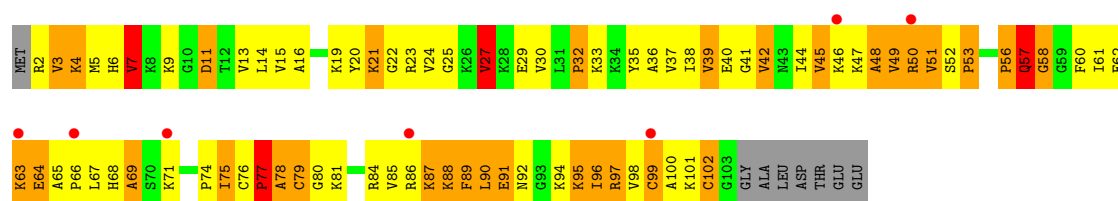
- Molecule 44: 50S ribosomal protein L24

Chain RY:



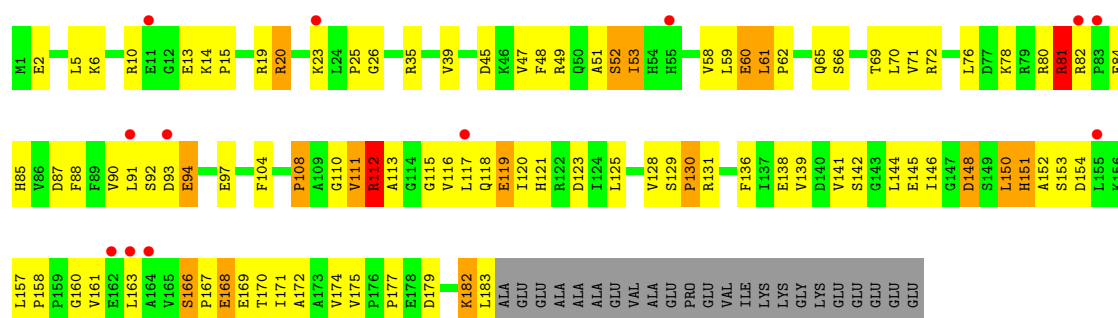
- Molecule 44: 50S ribosomal protein L24

Chain YY:



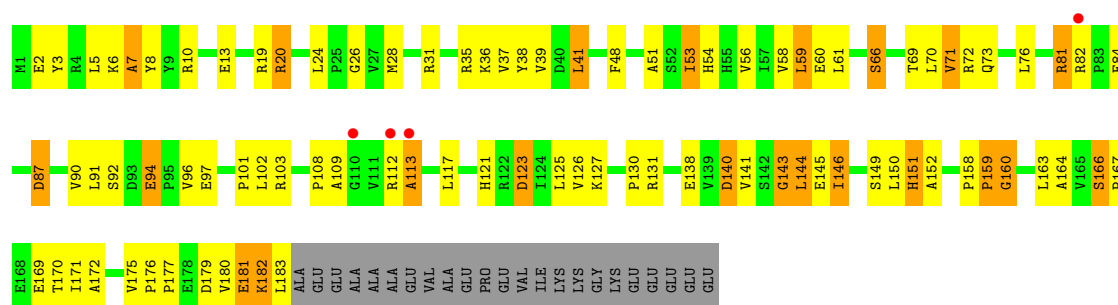
- Molecule 45: 50S ribosomal protein L25

Chain RZ:



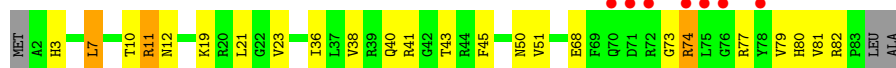
- Molecule 45: 50S ribosomal protein L25

Chain YZ:



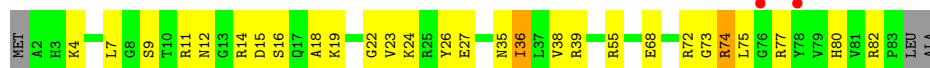
- Molecule 46: 50S ribosomal protein L27

Chain R0:



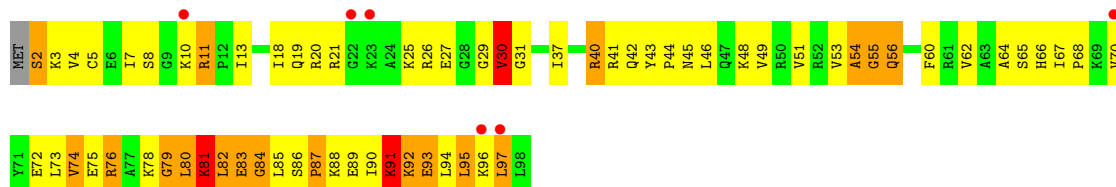
- Molecule 46: 50S ribosomal protein L27

Chain Y0:



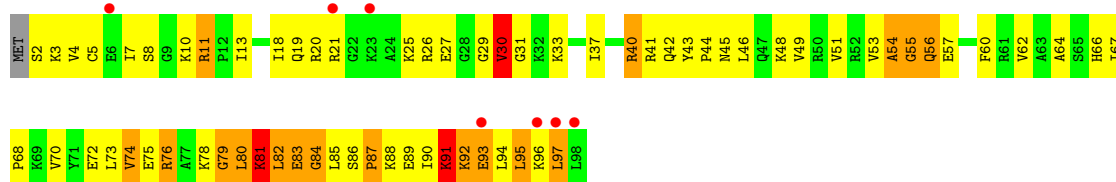
- Molecule 47: 50S ribosomal protein L28

Chain R1:



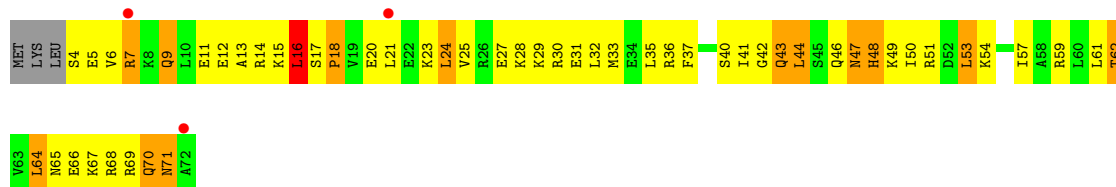
- Molecule 47: 50S ribosomal protein L28

Chain Y1:



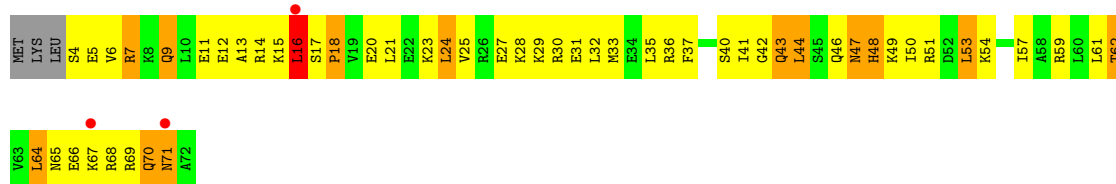
- Molecule 48: 50S ribosomal protein L29

Chain R2:



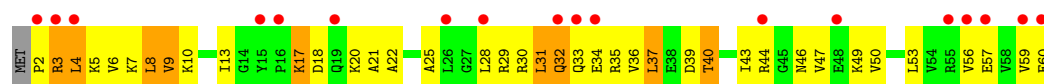
- Molecule 48: 50S ribosomal protein L29

Chain Y2:



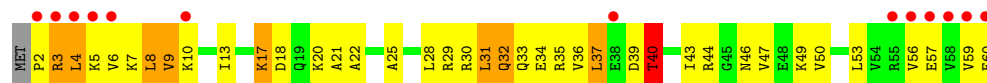
- Molecule 49: 50S ribosomal protein L30

Chain R3:



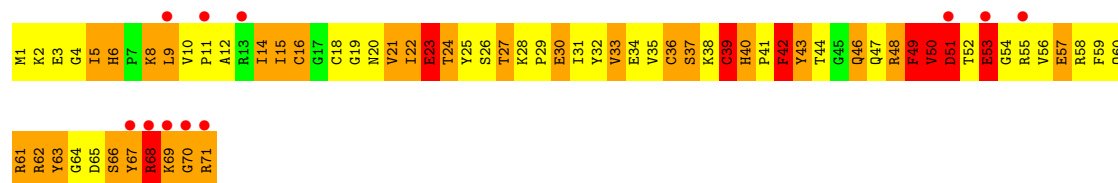
- Molecule 49: 50S ribosomal protein L30

Chain Y3:



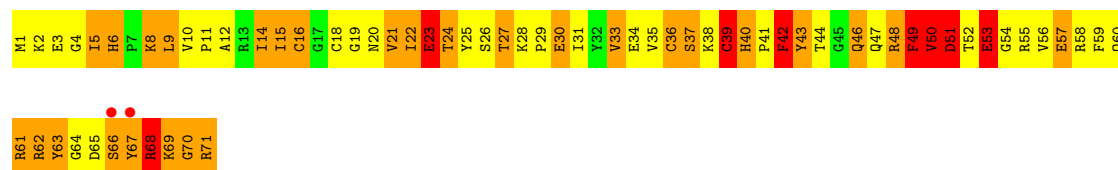
- Molecule 50: 50S ribosomal protein L31

Chain R4:



- Molecule 50: 50S ribosomal protein L31

Chain Y4:



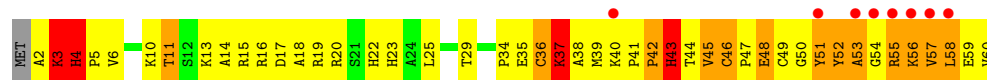
- Molecule 51: 50S ribosomal protein L32

Chain R5:



- Molecule 51: 50S ribosomal protein L32

Chain Y5:



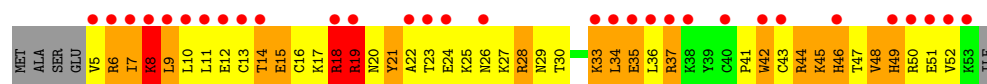
- Molecule 52: 50S ribosomal protein L33

Chain R6:



- Molecule 52: 50S ribosomal protein L33

Chain Y6:



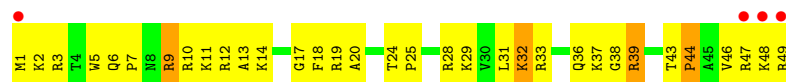
- Molecule 53: 50S ribosomal protein L34

Chain R7:



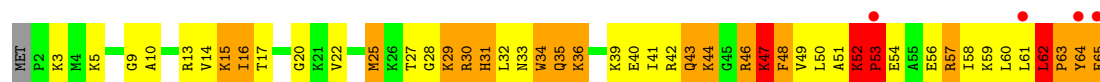
- Molecule 53: 50S ribosomal protein L34

Chain Y7:



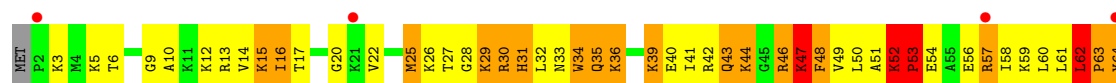
- Molecule 54: 50S ribosomal protein L35

Chain R8:



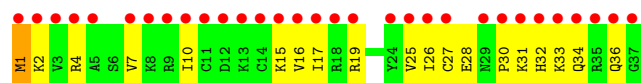
- Molecule 54: 50S ribosomal protein L35

Chain Y8:



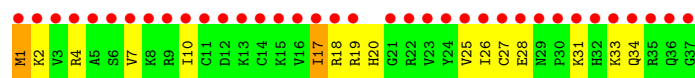
- Molecule 55: 50S ribosomal protein L36

Chain R9:



- Molecule 55: 50S ribosomal protein L36

Chain Y9:



- Molecule 56: 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	209.03Å 447.05Å 619.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.88 – 3.90 49.88 – 3.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.88-3.90) 97.9 (49.88-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.57Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.252 , 0.298 0.252 , 0.298	Depositor DCC
R_{free} test set	22759 reflections (4.44%)	DCC
Wilson B-factor (Å ²)	100.8	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 15.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 650647 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	291958	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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	0.31	0/36098	0.87	34/56341 (0.1%)
1	XA	0.33	0/36101	0.89	31/56346 (0.1%)
2	QB	0.35	0/1959	0.65	0/2642
2	XB	0.36	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	0.61	0/1709
7	XG	0.37	0/1276	0.60	0/1709
8	QH	0.40	0/1136	0.69	0/1527
8	XH	0.40	0/1136	0.69	0/1527
9	QI	0.36	0/1029	0.67	0/1379
9	XI	0.36	0/1029	0.67	0/1379
10	QJ	0.36	0/814	0.61	0/1095
10	XJ	0.36	0/814	0.61	0/1095
11	QK	0.40	0/900	0.67	0/1213
11	XK	0.40	0/900	0.67	0/1213
12	QL	0.45	0/991	1.00	4/1327 (0.3%)
12	XL	0.46	0/991	1.00	4/1327 (0.3%)
13	QM	0.34	0/974	0.66	0/1303
13	XM	0.34	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	0.67	0/992
16	QP	0.36	0/721	0.67	0/970
16	XP	0.37	0/721	0.67	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.37	0/847	0.68	0/1131
17	XQ	0.38	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	0.70	0/1007
20	XT	0.34	0/765	0.69	0/1007
21	QU	0.37	0/221	0.63	0/288
21	XU	0.37	0/221	0.63	0/288
22	QV	0.52	0/1836	1.00	6/2859 (0.2%)
22	XV	0.52	0/1836	1.00	6/2859 (0.2%)
23	QX	0.32	0/193	0.83	0/299
23	XX	0.30	0/193	0.83	0/299
24	QY	0.66	2/311 (0.6%)	0.86	0/483
24	XY	0.66	2/311 (0.6%)	0.86	0/483
25	RA	0.37	0/69521	0.92	63/108529 (0.1%)
25	YA	0.39	0/69543	0.94	68/108563 (0.1%)
26	RB	0.31	0/2878	0.86	0/4490
26	YB	0.36	0/2878	0.91	1/4490 (0.0%)
27	RD	0.60	2/2165 (0.1%)	0.90	4/2919 (0.1%)
27	YD	0.56	0/2165	0.90	4/2919 (0.1%)
28	RE	0.52	0/1601	0.91	2/2160 (0.1%)
28	YE	0.52	0/1601	0.91	2/2160 (0.1%)
29	RF	0.50	0/1620	0.76	0/2194
29	YF	0.50	0/1620	0.76	0/2194
30	RG	0.40	0/1499	0.66	0/2016
30	YG	0.40	0/1499	0.66	0/2016
31	RH	0.45	0/1332	0.85	3/1802 (0.2%)
31	YH	0.45	0/1332	0.85	4/1802 (0.2%)
32	RI	0.29	0/1151	0.55	0/1558
32	YI	0.27	0/1151	0.55	0/1558
33	RN	0.46	0/1131	0.78	1/1525 (0.1%)
33	YN	0.46	0/1131	0.78	1/1525 (0.1%)
34	RO	0.54	0/943	0.71	0/1269
34	YO	0.53	0/943	0.71	0/1269
35	RP	0.50	0/1162	0.94	3/1544 (0.2%)
35	YP	0.50	0/1162	0.95	3/1544 (0.2%)
36	RQ	0.54	0/1143	0.91	3/1527 (0.2%)
36	YQ	0.54	0/1143	0.89	3/1527 (0.2%)
37	RR	0.45	0/982	0.80	1/1312 (0.1%)
37	YR	0.45	0/982	0.80	1/1312 (0.1%)
38	RS	0.46	0/892	0.82	1/1187 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YS	0.45	0/892	0.82	1/1187 (0.1%)
39	RT	0.47	0/1155	0.73	2/1542 (0.1%)
39	YT	0.47	0/1155	0.73	2/1542 (0.1%)
40	RU	0.48	0/982	0.78	0/1306
40	YU	0.48	0/982	0.78	0/1306
41	RV	0.47	0/790	0.82	0/1057
41	YV	0.47	0/790	0.82	0/1057
42	RW	0.45	0/911	0.75	0/1220
42	YW	0.45	0/911	0.75	0/1220
43	RX	0.56	0/739	0.77	0/993
43	YX	0.56	0/739	0.78	0/993
44	RY	0.52	0/798	0.80	0/1064
44	YY	0.52	0/798	0.80	0/1064
45	RZ	0.27	0/1493	0.51	0/2026
45	YZ	0.29	0/1493	0.53	0/2026
46	R0	0.28	0/657	0.51	0/874
46	Y0	0.31	0/657	0.53	0/874
47	R1	0.49	0/770	0.85	1/1022 (0.1%)
47	Y1	0.49	0/770	0.85	1/1022 (0.1%)
48	R2	0.50	0/583	0.83	1/771 (0.1%)
48	Y2	0.51	0/583	0.83	1/771 (0.1%)
49	R3	0.47	0/474	0.72	0/635
49	Y3	0.43	0/474	0.71	0/635
50	R4	0.38	0/594	0.78	1/795 (0.1%)
50	Y4	0.38	0/594	0.78	1/795 (0.1%)
51	R5	0.50	0/473	0.74	0/639
51	Y5	0.51	0/473	0.74	0/639
52	R6	0.42	0/431	0.76	0/575
52	Y6	0.42	0/431	0.76	0/575
53	R7	0.56	0/438	0.76	0/575
53	Y7	0.56	0/438	0.76	0/575
54	R8	0.62	0/525	0.93	1/691 (0.1%)
54	Y8	0.62	0/525	0.93	1/691 (0.1%)
55	R9	0.35	0/310	0.60	0/407
55	Y9	0.37	0/310	0.61	0/407
56	Z6	0.78	0/40	1.78	1/60 (1.7%)
56	Z8	0.79	0/40	1.80	1/60 (1.7%)
All	All	0.39	6/316339 (0.0%)	0.87	274/472939 (0.1%)

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	RD	236	GLY	C-N	8.58	1.53	1.34
24	XY	34	C	C2-N3	7.54	1.41	1.35
24	QY	34	C	C2-N3	7.34	1.41	1.35
24	XY	34	C	C2-O2	6.60	1.30	1.24
24	QY	34	C	C2-O2	6.51	1.30	1.24

The worst 5 of 274 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	XL	47	LYS	C-N-CD	-20.47	75.57	120.60
12	QL	47	LYS	C-N-CD	-20.46	75.59	120.60
22	XV	17	C	C2-N1-C1'	11.76	131.74	118.80
22	QV	17	C	C2-N1-C1'	11.76	131.73	118.80
28	YE	21	VAL	C-N-CD	-10.09	98.41	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	630	0
1	XA	32249	0	16279	668	0
2	QB	1924	0	1975	286	0
2	XB	1924	0	1975	288	0
3	QC	1605	0	1668	225	0
3	XC	1605	0	1668	208	1
4	QD	1703	0	1765	276	0
4	XD	1703	0	1765	212	3
5	QE	1155	0	1213	144	0
5	XE	1155	0	1213	136	0
6	QF	843	0	857	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	XF	843	0	857	123	0
7	QG	1257	0	1296	140	0
7	XG	1257	0	1296	138	0
8	QH	1116	0	1177	148	0
8	XH	1116	0	1177	154	0
9	QI	1010	0	1037	140	0
9	XI	1010	0	1037	149	0
10	QJ	801	0	849	150	0
10	XJ	801	0	849	132	0
11	QK	885	0	904	105	1
11	XK	885	0	904	123	0
12	QL	975	0	1062	103	0
12	XL	975	0	1062	103	0
13	QM	964	0	1034	157	0
13	XM	964	0	1034	161	0
14	QN	492	0	529	100	0
14	XN	492	0	529	96	0
15	QO	734	0	771	74	0
15	XO	734	0	771	73	0
16	QP	705	0	725	110	0
16	XP	705	0	725	110	0
17	QQ	834	0	904	80	0
17	XQ	834	0	904	80	0
18	QR	574	0	644	67	0
18	XR	574	0	644	68	0
19	QS	674	0	699	106	0
19	XS	674	0	699	129	0
20	QT	763	0	860	106	0
20	XT	763	0	861	101	0
21	QU	217	0	234	26	0
21	XU	217	0	234	27	0
22	QV	1644	0	836	29	0
22	XV	1644	0	836	28	0
23	QX	173	0	88	5	0
23	XX	173	0	88	2	0
24	QY	303	0	154	4	0
24	XY	303	0	154	5	0
25	RA	62071	0	31290	1129	0
25	YA	62091	0	31295	1166	0
26	RB	2573	0	1306	46	0
26	YB	2573	0	1306	41	0
27	RD	2115	0	2195	317	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	YD	2115	0	2195	336	0
28	RE	1568	0	1634	265	0
28	YE	1568	0	1634	266	0
29	RF	1585	0	1632	178	0
29	YF	1585	0	1632	175	0
30	RG	1474	0	1535	194	0
30	YG	1474	0	1535	193	0
31	RH	1307	0	1382	224	0
31	YH	1307	0	1382	220	3
32	RI	1136	0	1223	57	0
32	YI	1136	0	1223	40	0
33	RN	1104	0	1180	194	0
33	YN	1104	0	1180	189	0
34	RO	933	0	996	124	0
34	YO	933	0	996	125	0
35	RP	1145	0	1228	243	0
35	YP	1145	0	1227	235	0
36	RQ	1122	0	1179	148	0
36	YQ	1122	0	1179	143	0
37	RR	968	0	1033	109	0
37	YR	968	0	1033	114	0
38	RS	882	0	943	153	0
38	YS	882	0	943	157	0
39	RT	1141	0	1202	156	0
39	YT	1141	0	1202	164	0
40	RU	964	0	1022	131	0
40	YU	964	0	1022	134	0
41	RV	779	0	852	130	0
41	YV	779	0	852	135	3
42	RW	900	0	964	95	0
42	YW	900	0	964	105	0
43	RX	725	0	778	68	0
43	YX	725	0	778	70	0
44	RY	785	0	878	160	0
44	YY	785	0	878	149	3
45	RZ	1461	0	1493	60	0
45	YZ	1461	0	1493	61	0
46	R0	648	0	671	19	0
46	Y0	648	0	672	23	0
47	R1	763	0	848	139	0
47	Y1	763	0	848	133	0
48	R2	581	0	629	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	Y2	581	0	629	71	0
49	R3	469	0	518	40	0
49	Y3	469	0	518	42	0
50	R4	581	0	574	154	0
50	Y4	581	0	574	169	0
51	R5	459	0	480	74	0
51	Y5	459	0	480	78	3
52	R6	424	0	450	88	0
52	Y6	424	0	450	90	0
53	R7	430	0	480	40	0
53	Y7	430	0	480	43	0
54	R8	517	0	582	97	0
54	Y8	517	0	582	105	0
55	R9	307	0	338	20	0
55	Y9	307	0	338	19	0
56	Z6	74	0	51	10	0
56	Z8	74	0	51	10	0
57	QA	65	0	0	0	0
57	QF	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	1	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	242	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	XA	70	0	0	0	0
57	XB	1	0	0	0	0
57	XM	1	0	0	0	0
57	XV	1	0	0	0	0
57	XX	1	0	0	0	0
57	Y0	1	0	0	0	0
57	YA	267	0	0	0	0
57	YB	3	0	0	0	0
57	YD	2	0	0	0	0
57	YE	1	0	0	0	0
57	YP	1	0	0	0	0
58	QA	42	0	45	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	XA	42	0	45	2	0
59	QD	1	0	0	0	0
59	QN	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
All	All	291958	0	198347	15046	10

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 31.

The worst 5 of 15046 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:YN:32:SER:CB	14:YN:41:ARG:HB3	1.23	1.55
14:YN:32:SER:HB3	14:YN:41:ARG:CB	1.28	1.54
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.36	1.52
4:QD:167:GLY:HA2	27:YD:135:PHE:CZ	1.42	1.52
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.36	1.52

The worst 5 of 10 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)
41:YV:51:VAL:N	51:Y5:60:VAL:O[4_445]	1.69	0.51
41:YV:50:PRO:CG	51:Y5:60:VAL:O[4_445]	1.99	0.21
31:YH:47:GLU:OE2	44:YY:79:CYS:CB[4_445]	2.03	0.17
41:YV:51:VAL:CB	51:Y5:60:VAL:OXT[4_445]	2.07	0.13
11:QK:99:GLN:NE2	3:XC:79:ARG:NH2[4_555]	2.08	0.12

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	102 (67%)	36 (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%)	86 (74%)	22 (19%)	9 (8%)	1	29
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	1	15
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	1	15
13	QM	119/126 (94%)	71 (60%)	28 (24%)	20 (17%)	0	6
13	XM	119/126 (94%)	72 (60%)	26 (22%)	21 (18%)	0	5
14	QN	58/61 (95%)	31 (53%)	15 (26%)	12 (21%)	0	3
14	XN	58/61 (95%)	32 (55%)	14 (24%)	12 (21%)	0	3
15	QO	86/89 (97%)	60 (70%)	20 (23%)	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
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	QR	68/88 (77%)	46 (68%)	14 (21%)	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%)	16 (70%)	3 (13%)	4 (17%)	0	6
27	RD	270/276 (98%)	203 (75%)	48 (18%)	19 (7%)	2	33
27	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	2	33
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	3
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	3
29	RF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	20
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	20
30	RG	179/182 (98%)	120 (67%)	38 (21%)	21 (12%)	1	14
30	YG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	1	14
31	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	2
31	YH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	2
32	RI	144/148 (97%)	105 (73%)	25 (17%)	14 (10%)	1	21
32	YI	144/148 (97%)	101 (70%)	29 (20%)	14 (10%)	1	21
33	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	7
33	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	7
34	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	2	30
34	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	2	30
35	RP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	3
35	YP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	3
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	1	19
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	1	19
37	RR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	1	14
37	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	1	14
38	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	YS	109/112 (97%)	63 (58%)	27 (25%)	19 (17%)	0	6
39	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	9
39	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	9
40	RU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	29
40	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	29
41	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	19
41	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	19
42	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	13
42	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	13
43	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	3	40
43	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	3	40
44	RY	100/110 (91%)	58 (58%)	16 (16%)	26 (26%)	0	2
44	YY	100/110 (91%)	57 (57%)	16 (16%)	27 (27%)	0	1
45	RZ	181/206 (88%)	131 (72%)	32 (18%)	18 (10%)	1	20
45	YZ	181/206 (88%)	129 (71%)	33 (18%)	19 (10%)	1	18
46	R0	80/85 (94%)	67 (84%)	12 (15%)	1 (1%)	18	75
46	Y0	80/85 (94%)	70 (88%)	9 (11%)	1 (1%)	18	75
47	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	1	15
47	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	1	15
48	R2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	11
48	Y2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	11
49	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	3	41
49	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	3	41
50	R4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
50	Y4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
51	R5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	2
51	Y5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	2
52	R6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	1
52	Y6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	1
53	R7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	36
53	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	R8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	5
54	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	5
55	R9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11470/12128 (95%)	7661 (67%)	2332 (20%)	1477 (13%)	0	13

5 of 1477 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%)	108 (93%)	8 (7%)	22	69
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%)	115 (91%)	11 (9%)	15	59
7	XG	126/127 (99%)	115 (91%)	11 (9%)	15	59
8	QH	119/119 (100%)	106 (89%)	13 (11%)	9	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	90 (86%)	14 (14%)	6	36
12	XL	104/109 (95%)	90 (86%)	14 (14%)	6	36
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%)	68 (90%)	8 (10%)	10	49
21	QU	20/22 (91%)	19 (95%)	1 (5%)	34	80
21	XU	20/22 (91%)	19 (95%)	1 (5%)	34	80
27	RD	214/218 (98%)	176 (82%)	38 (18%)	2	20
27	YD	214/218 (98%)	176 (82%)	38 (18%)	2	20
28	RE	165/166 (99%)	128 (78%)	37 (22%)	1	11
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	RF	161/166 (97%)	140 (87%)	21 (13%)	6	38
29	YF	161/166 (97%)	140 (87%)	21 (13%)	6	38
30	RG	155/156 (99%)	130 (84%)	25 (16%)	3	27
30	YG	155/156 (99%)	130 (84%)	25 (16%)	3	27
31	RH	142/148 (96%)	114 (80%)	28 (20%)	2	15
31	YH	142/148 (96%)	114 (80%)	28 (20%)	2	15
32	RI	122/124 (98%)	100 (82%)	22 (18%)	2	19
32	YI	122/124 (98%)	98 (80%)	24 (20%)	2	15
33	RN	117/119 (98%)	98 (84%)	19 (16%)	3	26
33	YN	117/119 (98%)	98 (84%)	19 (16%)	3	26
34	RO	100/100 (100%)	90 (90%)	10 (10%)	11	52
34	YO	100/100 (100%)	90 (90%)	10 (10%)	11	52
35	RP	116/116 (100%)	89 (77%)	27 (23%)	1	9
35	YP	116/116 (100%)	89 (77%)	27 (23%)	1	9
36	RQ	111/111 (100%)	93 (84%)	18 (16%)	3	26
36	YQ	111/111 (100%)	93 (84%)	18 (16%)	3	26
37	RR	101/101 (100%)	84 (83%)	17 (17%)	3	24
37	YR	101/101 (100%)	84 (83%)	17 (17%)	3	24
38	RS	87/88 (99%)	74 (85%)	13 (15%)	4	31
38	YS	87/88 (99%)	74 (85%)	13 (15%)	4	31
39	RT	120/127 (94%)	97 (81%)	23 (19%)	2	16
39	YT	120/127 (94%)	97 (81%)	23 (19%)	2	16
40	RU	93/94 (99%)	80 (86%)	13 (14%)	5	34
40	YU	93/94 (99%)	80 (86%)	13 (14%)	5	34
41	RV	82/82 (100%)	71 (87%)	11 (13%)	6	36
41	YV	82/82 (100%)	71 (87%)	11 (13%)	6	36
42	RW	92/92 (100%)	77 (84%)	15 (16%)	3	26
42	YW	92/92 (100%)	77 (84%)	15 (16%)	3	26
43	RX	74/78 (95%)	63 (85%)	11 (15%)	4	31
43	YX	74/78 (95%)	63 (85%)	11 (15%)	4	31
44	RY	85/91 (93%)	70 (82%)	15 (18%)	3	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	YY	85/91 (93%)	70 (82%)	15 (18%)	3	21
45	RZ	162/179 (90%)	140 (86%)	22 (14%)	5	36
45	YZ	162/179 (90%)	144 (89%)	18 (11%)	9	46
46	R0	65/67 (97%)	61 (94%)	4 (6%)	26	74
46	Y0	65/67 (97%)	61 (94%)	4 (6%)	26	74
47	R1	82/83 (99%)	67 (82%)	15 (18%)	2	18
47	Y1	82/83 (99%)	67 (82%)	15 (18%)	2	18
48	R2	64/67 (96%)	57 (89%)	7 (11%)	9	47
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	9	47
49	R3	51/52 (98%)	40 (78%)	11 (22%)	1	11
49	Y3	51/52 (98%)	40 (78%)	11 (22%)	1	11
50	R4	63/63 (100%)	44 (70%)	19 (30%)	0	5
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	5
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	9
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	9
52	R6	48/52 (92%)	38 (79%)	10 (21%)	2	13
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	2	13
53	R7	42/42 (100%)	39 (93%)	3 (7%)	21	69
53	Y7	42/42 (100%)	39 (93%)	3 (7%)	21	69
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	6
54	Y8	54/55 (98%)	39 (72%)	15 (28%)	0	6
55	R9	34/34 (100%)	32 (94%)	2 (6%)	28	75
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	28	75
All	All	9702/10066 (96%)	8303 (86%)	1399 (14%)	5	32

5 of 1399 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	R2	64	LEU
7	XG	12	LEU
45	YZ	87	ASP
50	R4	48	ARG
2	XB	33	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
48	R2	9	GLN
5	XE	72	GLN
41	YV	11	GLN
48	R2	47	ASN
2	XB	95	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	313 (20%)	45 (3%)
1	XA	1499/1522 (98%)	315 (21%)	47 (3%)
22	QV	76/77 (98%)	30 (39%)	1 (1%)
22	XV	76/77 (98%)	30 (39%)	1 (1%)
23	QX	7/25 (28%)	3 (42%)	2 (28%)
23	XX	7/25 (28%)	3 (42%)	2 (28%)
24	QY	13/18 (72%)	5 (38%)	1 (7%)
24	XY	13/18 (72%)	5 (38%)	1 (7%)
25	RA	2879/2916 (98%)	667 (23%)	61 (2%)
25	YA	2880/2916 (98%)	675 (23%)	58 (2%)
26	RB	119/122 (97%)	24 (20%)	1 (0%)
26	YB	119/122 (97%)	26 (21%)	1 (0%)
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9189/9366 (98%)	2096 (22%)	221 (2%)

5 of 2096 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	7	G
1	QA	9	G
1	QA	22	G
1	QA	32	A

5 of 221 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2439	A
1	XA	345	C
25	YA	1698	A

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Mol	Chain	Res	Type
25	RA	2566	A
1	XA	31	G

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	$\# Z > 2$
24	1MG	QY	37	24	24,26,27	2.77	5 (20%)	34,39,42	2.78	7 (20%)
24	1MG	XY	37	24	24,26,27	2.77	5 (20%)	34,39,42	2.65	8 (23%)
56	PPU	Z6	76	25,56	38,40,41	2.43	8 (21%)	54,57,60	2.62	14 (25%)
56	PPU	Z8	76	25,56	38,40,41	2.42	8 (21%)	54,57,60	2.60	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
24	1MG	QY	37	24	-	0/8/25/26	0/3/3/3
24	1MG	XY	37	24	-	0/8/25/26	0/3/3/3
56	PPU	Z6	76	25,56	-	0/26/43/44	0/4/4/4
56	PPU	Z8	76	25,56	-	0/26/43/44	0/4/4/4

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z8	76	PPU	O-C	9.20	1.41	1.23
56	Z6	76	PPU	O-C	9.19	1.41	1.23
24	XY	37	1MG	C4-N3	8.30	1.49	1.35
24	QY	37	1MG	C4-N3	8.24	1.49	1.35
24	XY	37	1MG	C2-N2	6.39	1.47	1.33

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	QY	37	1MG	C6-N1-C2	11.71	123.92	120.71
24	XY	37	1MG	C6-N1-C2	11.23	123.79	120.71
56	Z8	76	PPU	N3-C2-N1	-8.54	121.38	128.89
56	Z6	76	PPU	N3-C2-N1	-8.53	121.38	128.89
56	Z6	76	PPU	C3'-N3'-C	-8.20	110.13	123.19

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 676 ligands modelled in this entry, 674 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	1.42	9 (20%)	67,67,67	1.46	13 (19%)
58	PAR	XA	1671	-	45,45,45	1.55	9 (20%)	67,67,67	1.75	16 (23%)

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	1671	-	-	0/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	XA	1671	PAR	C31-C21	4.41	1.59	1.53
58	XA	1671	PAR	C11-C21	3.72	1.59	1.52
58	QA	1666	PAR	C64-C54	3.37	1.60	1.51
58	QA	1666	PAR	C52-C42	3.05	1.58	1.52
58	XA	1671	PAR	O54-C14	2.86	1.49	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	QA	1666	PAR	O54-C54-C64	4.54	114.61	105.97
58	XA	1671	PAR	O33-C14-C24	4.30	116.57	108.08
58	XA	1671	PAR	C32-C22-C12	-3.91	103.05	111.59
58	XA	1671	PAR	O52-C13-C23	3.90	114.46	107.50
58	XA	1671	PAR	O54-C54-C64	3.56	112.75	105.97

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%)	0.00	21 (1%) 72 56	35, 87, 182, 299	0
1	XA	1500/1522 (98%)	-0.15	10 (0%) 84 71	21, 74, 169, 271	0
2	QB	237/256 (92%)	0.73	22 (9%) 9 10	84, 154, 204, 237	0
2	XB	237/256 (92%)	0.40	11 (4%) 31 25	51, 121, 182, 226	0
3	QC	205/239 (85%)	0.44	13 (6%) 19 17	57, 135, 182, 201	0
3	XC	205/239 (85%)	0.22	3 (1%) 70 54	32, 89, 145, 177	0
4	QD	208/209 (99%)	0.53	8 (3%) 38 30	38, 99, 165, 221	0
4	XD	208/209 (99%)	0.48	4 (1%) 64 48	27, 106, 160, 186	0
5	QE	151/162 (93%)	0.53	4 (2%) 53 40	36, 111, 158, 185	0
5	XE	151/162 (93%)	0.39	5 (3%) 44 34	3, 85, 142, 170	0
6	QF	101/101 (100%)	0.46	2 (1%) 62 46	33, 99, 158, 181	0
6	XF	101/101 (100%)	0.35	1 (0%) 79 64	25, 95, 145, 243	0
7	QG	155/156 (99%)	0.71	16 (10%) 7 9	55, 123, 179, 210	0
7	XG	155/156 (99%)	0.53	11 (7%) 16 15	42, 99, 156, 197	0
8	QH	138/138 (100%)	0.79	12 (8%) 10 12	61, 120, 167, 193	0
8	XH	138/138 (100%)	0.63	4 (2%) 49 37	20, 94, 147, 198	0
9	QI	127/128 (99%)	1.18	23 (18%) 2 3	67, 134, 193, 224	0
9	XI	127/128 (99%)	0.57	3 (2%) 56 42	29, 107, 165, 195	0
10	QJ	99/105 (94%)	1.35	22 (22%) 1 3	46, 149, 202, 222	0
10	XJ	99/105 (94%)	0.92	15 (15%) 3 4	35, 115, 175, 201	0
11	QK	119/129 (92%)	0.61	8 (6%) 17 17	42, 104, 158, 202	0
11	XK	119/129 (92%)	0.61	5 (4%) 35 27	27, 87, 148, 170	0
12	QL	125/132 (94%)	0.77	12 (9%) 8 10	21, 93, 142, 192	0
12	XL	125/132 (94%)	0.43	7 (5%) 24 20	20, 66, 131, 212	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	0.72	10 (8%) 11 12	58, 122, 175, 214	0
13	XM	121/126 (96%)	0.45	5 (4%) 35 28	28, 92, 144, 180	0
14	QN	60/61 (98%)	0.98	6 (10%) 8 9	55, 129, 181, 204	0
14	XN	60/61 (98%)	0.53	3 (5%) 28 23	33, 82, 135, 170	0
15	QO	88/89 (98%)	0.43	2 (2%) 57 43	54, 105, 154, 178	0
15	XO	88/89 (98%)	0.36	0 100 100	25, 91, 141, 171	0
16	QP	84/88 (95%)	0.97	9 (10%) 6 8	42, 86, 157, 171	0
16	XP	84/88 (95%)	1.14	17 (20%) 2 3	51, 101, 152, 235	0
17	QQ	100/105 (95%)	0.71	4 (4%) 36 29	33, 91, 144, 165	0
17	XQ	100/105 (95%)	0.89	11 (11%) 6 8	37, 95, 147, 200	0
18	QR	70/88 (79%)	0.73	3 (4%) 34 27	42, 110, 160, 212	0
18	XR	70/88 (79%)	0.62	4 (5%) 23 19	34, 86, 147, 168	0
19	QS	84/93 (90%)	0.95	11 (13%) 4 5	60, 131, 184, 190	0
19	XS	84/93 (90%)	0.63	4 (4%) 29 24	45, 97, 141, 220	0
20	QT	99/106 (93%)	0.54	2 (2%) 62 46	34, 91, 154, 181	0
20	XT	99/106 (93%)	0.86	13 (13%) 4 5	50, 112, 158, 181	0
21	QU	25/27 (92%)	2.46	14 (56%) 0 1	62, 132, 185, 206	0
21	XU	25/27 (92%)	1.71	8 (32%) 1 2	45, 89, 136, 166	0
22	QV	77/77 (100%)	-0.05	1 (1%) 74 58	26, 99, 159, 205	0
22	XV	77/77 (100%)	-0.18	1 (1%) 74 58	28, 70, 121, 185	0
23	QX	8/25 (32%)	1.24	2 (25%) 1 2	70, 95, 129, 169	0
23	XX	8/25 (32%)	1.26	2 (25%) 1 2	36, 51, 102, 163	0
24	QY	14/18 (77%)	1.07	2 (14%) 3 5	100, 150, 249, 294	0
24	XY	14/18 (77%)	0.65	0 100 100	59, 106, 221, 249	0
25	RA	2882/2916 (98%)	-0.09	77 (2%) 52 39	14, 60, 203, 320	0
25	YA	2883/2916 (98%)	-0.18	59 (2%) 62 46	14, 50, 194, 329	0
26	RB	120/122 (98%)	0.09	1 (0%) 83 69	64, 113, 177, 203	0
26	YB	120/122 (98%)	-0.41	0 100 100	37, 69, 95, 158	0
27	RD	272/276 (98%)	0.34	4 (1%) 70 54	7, 56, 113, 177	0
27	YD	272/276 (98%)	0.36	3 (1%) 77 61	3, 49, 98, 152	0
28	RE	205/206 (99%)	0.51	6 (2%) 49 37	23, 73, 150, 195	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YE	205/206 (99%)	0.57	8 (3%) 37 29	15, 77, 151, 200	0
29	RF	202/210 (96%)	0.40	2 (0%) 79 64	4, 85, 151, 184	0
29	YF	202/210 (96%)	0.27	3 (1%) 70 54	8, 65, 124, 184	0
30	RG	181/182 (99%)	0.73	18 (9%) 8 10	52, 137, 205, 232	0
30	YG	181/182 (99%)	0.44	5 (2%) 50 38	25, 98, 166, 203	0
31	RH	170/180 (94%)	1.02	31 (18%) 2 3	69, 150, 202, 250	0
31	YH	170/180 (94%)	0.72	16 (9%) 9 10	32, 94, 152, 204	0
32	RI	146/148 (98%)	0.63	7 (4%) 29 24	29, 109, 161, 182	0
32	YI	146/148 (98%)	0.36	5 (3%) 43 33	18, 95, 158, 203	0
33	RN	138/140 (98%)	0.75	9 (6%) 18 17	33, 94, 152, 192	0
33	YN	138/140 (98%)	0.36	2 (1%) 72 56	19, 75, 132, 162	0
34	RO	122/122 (100%)	0.36	1 (0%) 83 69	6, 64, 120, 163	0
34	YO	122/122 (100%)	0.36	0 100 100	18, 61, 114, 144	0
35	RP	150/150 (100%)	0.85	22 (14%) 3 4	5, 87, 160, 191	0
35	YP	150/150 (100%)	0.56	7 (4%) 30 24	17, 75, 166, 203	0
36	RQ	141/141 (100%)	0.69	11 (7%) 13 13	25, 94, 140, 212	0
36	YQ	141/141 (100%)	0.44	2 (1%) 72 56	11, 61, 126, 169	0
37	RR	118/118 (100%)	0.38	1 (0%) 83 69	12, 58, 116, 154	0
37	YR	118/118 (100%)	0.58	2 (1%) 67 51	24, 68, 127, 155	0
38	RS	111/112 (99%)	0.97	13 (11%) 5 7	40, 116, 169, 194	0
38	YS	111/112 (99%)	0.43	1 (0%) 81 67	9, 79, 133, 232	0
39	RT	137/146 (93%)	0.44	5 (3%) 41 32	19, 77, 171, 214	0
39	YT	137/146 (93%)	0.38	4 (2%) 49 37	30, 84, 164, 206	0
40	RU	117/118 (99%)	0.32	5 (4%) 34 27	17, 78, 154, 194	0
40	YU	117/118 (99%)	0.21	2 (1%) 67 51	15, 65, 152, 189	0
41	RV	101/101 (100%)	0.41	1 (0%) 79 64	36, 105, 157, 216	0
41	YV	101/101 (100%)	0.49	2 (1%) 62 46	23, 84, 144, 243	0
42	RW	113/113 (100%)	0.66	6 (5%) 25 21	20, 65, 137, 216	0
42	YW	113/113 (100%)	0.32	1 (0%) 81 67	12, 56, 114, 193	0
43	RX	92/96 (95%)	0.56	3 (3%) 44 34	14, 69, 125, 158	0
43	YX	92/96 (95%)	0.51	2 (2%) 59 44	12, 56, 113, 138	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RY	102/110 (92%)	1.63	30 (29%) 1 2	36, 115, 175, 230	0
44	YY	102/110 (92%)	0.83	7 (6%) 17 16	24, 83, 156, 204	0
45	RZ	183/206 (88%)	0.61	12 (6%) 18 17	42, 122, 174, 213	0
45	YZ	183/206 (88%)	0.37	4 (2%) 59 44	23, 98, 153, 211	0
46	R0	82/85 (96%)	0.83	7 (8%) 11 12	13, 74, 111, 143	0
46	Y0	82/85 (96%)	0.62	2 (2%) 56 42	11, 54, 85, 133	0
47	R1	97/98 (98%)	0.93	6 (6%) 20 18	11, 74, 170, 241	0
47	Y1	97/98 (98%)	0.77	7 (7%) 15 15	11, 64, 144, 205	0
48	R2	69/72 (95%)	0.46	3 (4%) 34 27	26, 101, 176, 197	0
48	Y2	69/72 (95%)	0.40	3 (4%) 34 27	26, 69, 141, 177	0
49	R3	59/60 (98%)	1.62	18 (30%) 1 2	19, 95, 150, 200	0
49	Y3	59/60 (98%)	1.06	13 (22%) 1 3	9, 70, 131, 166	0
50	R4	71/71 (100%)	0.92	11 (15%) 3 4	89, 171, 218, 267	0
50	Y4	71/71 (100%)	0.42	2 (2%) 50 38	69, 145, 208, 248	0
51	R5	59/60 (98%)	0.57	3 (5%) 27 22	13, 74, 179, 222	0
51	Y5	59/60 (98%)	0.66	8 (13%) 4 5	17, 78, 189, 225	0
52	R6	49/54 (90%)	3.06	32 (65%) 0 1	101, 150, 215, 233	0
52	Y6	49/54 (90%)	2.43	31 (63%) 0 1	73, 147, 211, 217	0
53	R7	49/49 (100%)	0.44	2 (4%) 35 28	17, 47, 108, 188	0
53	Y7	49/49 (100%)	0.63	4 (8%) 12 12	6, 40, 118, 133	0
54	R8	64/65 (98%)	0.83	4 (6%) 19 17	24, 80, 155, 197	0
54	Y8	64/65 (98%)	0.62	5 (7%) 13 13	6, 54, 120, 197	0
55	R9	37/37 (100%)	4.22	31 (83%) 0 1	94, 143, 197, 202	0
55	Y9	37/37 (100%)	4.75	36 (97%) 0 1	62, 123, 202, 228	0
56	Z6	3/3 (100%)	2.52	1 (33%) 1 2	30, 30, 41, 75	0
56	Z8	3/3 (100%)	2.42	1 (33%) 1 2	30, 30, 39, 47	0
All	All	20875/21494 (97%)	0.31	1006 (4%) 29 24	3, 80, 177, 329	0

The worst 5 of 1006 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
55	R9	14	CYS	20.2
55	R9	11	CYS	11.5

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Mol	Chain	Res	Type	RSRZ
28	YE	205	ALA	9.6
55	Y9	34	GLN	9.1
25	RA	2799	A	8.8

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	Z6	76	37/38	0.26	-	41,41,41,41	0
56	PPU	Z8	76	37/38	0.28	-	38,38,38,38	0
24	1MG	XY	37	24/25	0.16	-	59,59,59,59	0
24	1MG	QY	37	24/25	0.22	-	99,99,99,99	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	QA	1603	1/1	0.99	-	27,27,27,27	0
57	MG	YA	3086	1/1	0.29	-	6,6,6,6	0
57	MG	XA	1666	1/1	0.16	-	16,16,16,16	0
57	MG	XA	1644	1/1	0.18	-	3,3,3,3	0
57	MG	RE	301	1/1	0.19	-	18,18,18,18	0
57	MG	RA	3198	1/1	0.23	-	7,7,7,7	0
59	ZN	XN	101	1/1	0.18	-	82,82,82,82	0
57	MG	RA	3179	1/1	0.35	-	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	QA	1656	1/1	0.42	-	25,25,25,25	0
57	MG	YA	3122	1/1	0.37	-	8,8,8,8	0
57	MG	QA	1626	1/1	0.23	-	10,10,10,10	0
57	MG	RA	3103	1/1	0.20	-	1,1,1,1	0
57	MG	YA	3190	1/1	0.14	-	22,22,22,22	0
57	MG	YA	3151	1/1	0.06	-	26,26,26,26	0
57	MG	YA	3087	1/1	0.40	-	8,8,8,8	0
57	MG	YA	3256	1/1	0.61	-	8,8,8,8	0
57	MG	RA	3120	1/1	0.56	-	4,4,4,4	0
57	MG	YA	3131	1/1	0.33	-	7,7,7,7	0
57	MG	RA	3052	1/1	0.28	-	3,3,3,3	0
57	MG	RA	3040	1/1	0.31	-	11,11,11,11	0
57	MG	YA	3198	1/1	0.17	-	16,16,16,16	0
57	MG	YA	3232	1/1	0.32	-	5,5,5,5	0
57	MG	XA	1652	1/1	0.16	-	1,1,1,1	0
57	MG	YA	3078	1/1	0.43	-	0,0,0,0	0
57	MG	RA	3151	1/1	0.20	-	10,10,10,10	0
57	MG	YA	3066	1/1	0.22	-	6,6,6,6	0
57	MG	RP	202	1/1	0.55	-	65,65,65,65	0
57	MG	RA	3053	1/1	0.31	-	4,4,4,4	0
57	MG	YA	3093	1/1	0.18	-	8,8,8,8	0
57	MG	YA	3243	1/1	0.29	-	0,0,0,0	0
57	MG	RA	3049	1/1	0.43	-	4,4,4,4	0
57	MG	YA	3099	1/1	0.25	-	2,2,2,2	0
57	MG	XA	1630	1/1	0.15	-	4,4,4,4	0
57	MG	XA	1618	1/1	0.26	-	26,26,26,26	0
57	MG	QA	1632	1/1	0.32	-	25,25,25,25	0
57	MG	RA	3158	1/1	0.14	-	12,12,12,12	0
57	MG	YA	3063	1/1	0.26	-	11,11,11,11	0
57	MG	RA	3009	1/1	0.53	-	84,84,84,84	0
57	MG	YA	3129	1/1	0.31	-	0,0,0,0	0
57	MG	YA	3136	1/1	0.08	-	14,14,14,14	0
57	MG	YA	3199	1/1	0.56	-	60,60,60,60	0
57	MG	YA	3138	1/1	0.20	-	1,1,1,1	0
57	MG	YA	3208	1/1	0.17	-	43,43,43,43	0
57	MG	QA	1605	1/1	0.48	-	5,5,5,5	0
57	MG	RA	3129	1/1	0.23	-	21,21,21,21	0
57	MG	RA	3219	1/1	0.10	-	4,4,4,4	0
57	MG	YA	3028	1/1	0.30	-	1,1,1,1	0
57	MG	XA	1624	1/1	0.33	-	23,23,23,23	0
57	MG	YA	3141	1/1	0.56	-	7,7,7,7	0
57	MG	RA	3102	1/1	0.11	-	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3207	1/1	0.20	-	96,96,96,96	0
57	MG	YA	3029	1/1	0.21	-	0,0,0,0	0
57	MG	YA	3187	1/1	0.17	-	55,55,55,55	0
57	MG	XM	201	1/1	0.10	-	26,26,26,26	0
57	MG	RA	3097	1/1	1.06	-	80,80,80,80	0
57	MG	QA	1613	1/1	0.26	-	36,36,36,36	0
57	MG	RA	3118	1/1	0.34	-	13,13,13,13	0
57	MG	YA	3152	1/1	0.74	-	3,3,3,3	0
57	MG	XA	1625	1/1	0.29	-	6,6,6,6	0
57	MG	RA	3161	1/1	0.59	-	75,75,75,75	0
57	MG	YA	3161	1/1	0.35	-	6,6,6,6	0
57	MG	YA	3157	1/1	0.49	-	18,18,18,18	0
57	MG	YA	3224	1/1	0.45	-	5,5,5,5	0
57	MG	YA	3266	1/1	0.38	-	1,1,1,1	0
57	MG	QA	1642	1/1	0.17	-	20,20,20,20	0
57	MG	YA	3096	1/1	0.55	-	2,2,2,2	0
57	MG	YA	3058	1/1	0.72	-	4,4,4,4	0
57	MG	QA	1615	1/1	0.23	-	74,74,74,74	0
57	MG	YA	3258	1/1	1.76	-	80,80,80,80	0
57	MG	YA	3260	1/1	0.28	-	2,2,2,2	0
59	ZN	QD	301	1/1	0.20	-	21,21,21,21	0
57	MG	RA	3078	1/1	0.10	-	5,5,5,5	0
57	MG	QA	1617	1/1	0.47	-	8,8,8,8	0
57	MG	RA	3121	1/1	0.26	-	2,2,2,2	0
57	MG	RA	3050	1/1	0.37	-	3,3,3,3	0
57	MG	RA	3063	1/1	0.71	-	0,0,0,0	0
57	MG	RA	3213	1/1	0.22	-	42,42,42,42	0
57	MG	RA	3087	1/1	0.19	-	1,1,1,1	0
57	MG	YA	3079	1/1	0.28	-	22,22,22,22	0
57	MG	XA	1648	1/1	0.49	-	28,28,28,28	0
57	MG	YA	3227	1/1	0.21	-	0,0,0,0	0
57	MG	YA	3049	1/1	0.50	-	6,6,6,6	0
57	MG	YA	3097	1/1	0.39	-	11,11,11,11	0
57	MG	YA	3001	1/1	0.50	-	0,0,0,0	0
57	MG	XA	1608	1/1	0.15	-	81,81,81,81	0
57	MG	RD	301	1/1	0.62	-	11,11,11,11	0
57	MG	RA	3156	1/1	0.41	-	19,19,19,19	0
57	MG	YA	3222	1/1	0.29	-	3,3,3,3	0
57	MG	RA	3141	1/1	0.16	-	3,3,3,3	0
57	MG	QA	1628	1/1	0.46	-	62,62,62,62	0
57	MG	YA	3041	1/1	0.39	-	10,10,10,10	0
57	MG	RA	3225	1/1	0.34	-	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3236	1/1	0.66	-	4,4,4,4	0
57	MG	YA	3068	1/1	0.22	-	3,3,3,3	0
57	MG	RA	3060	1/1	0.45	-	65,65,65,65	0
57	MG	QA	1623	1/1	0.83	-	41,41,41,41	0
57	MG	RA	3067	1/1	0.24	-	57,57,57,57	0
57	MG	YA	3239	1/1	0.21	-	19,19,19,19	0
57	MG	RA	3153	1/1	0.23	-	24,24,24,24	0
57	MG	RA	3200	1/1	0.40	-	4,4,4,4	0
57	MG	RA	3185	1/1	0.23	-	16,16,16,16	0
57	MG	XA	1643	1/1	0.50	-	34,34,34,34	0
57	MG	YA	3252	1/1	0.42	-	16,16,16,16	0
57	MG	R0	101	1/1	0.64	-	29,29,29,29	0
57	MG	YA	3221	1/1	0.34	-	42,42,42,42	0
57	MG	YA	3242	1/1	0.14	-	7,7,7,7	0
57	MG	RA	3189	1/1	0.46	-	55,55,55,55	0
57	MG	RA	3167	1/1	0.19	-	6,6,6,6	0
57	MG	RA	3089	1/1	0.49	-	2,2,2,2	0
57	MG	XA	1626	1/1	0.36	-	11,11,11,11	0
57	MG	YA	3186	1/1	0.22	-	4,4,4,4	0
57	MG	RA	3019	1/1	0.33	-	14,14,14,14	0
57	MG	RA	3122	1/1	0.09	-	5,5,5,5	0
57	MG	RA	3082	1/1	0.43	-	18,18,18,18	0
57	MG	YA	3200	1/1	0.54	-	10,10,10,10	0
57	MG	YA	3055	1/1	0.37	-	4,4,4,4	0
57	MG	Y0	101	1/1	0.25	-	3,3,3,3	0
57	MG	YA	3169	1/1	0.12	-	3,3,3,3	0
57	MG	XA	1638	1/1	0.22	-	37,37,37,37	0
57	MG	XA	1639	1/1	0.25	-	13,13,13,13	0
57	MG	YA	3173	1/1	0.50	-	0,0,0,0	0
57	MG	XA	1649	1/1	0.13	-	33,33,33,33	0
57	MG	RA	3107	1/1	0.09	-	3,3,3,3	0
57	MG	RA	3177	1/1	0.21	-	3,3,3,3	0
57	MG	RA	3028	1/1	0.24	-	2,2,2,2	0
57	MG	YA	3084	1/1	0.46	-	17,17,17,17	0
57	MG	RA	3035	1/1	0.37	-	1,1,1,1	0
57	MG	QA	1636	1/1	0.14	-	13,13,13,13	0
57	MG	YA	3140	1/1	0.25	-	8,8,8,8	0
57	MG	QA	1629	1/1	0.19	-	29,29,29,29	0
57	MG	YA	3067	1/1	0.59	-	5,5,5,5	0
57	MG	XA	1667	1/1	0.13	-	32,32,32,32	0
57	MG	RA	3119	1/1	0.29	-	18,18,18,18	0
57	MG	YA	3018	1/1	0.75	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3113	1/1	0.19	-	2,2,2,2	0
57	MG	RA	3130	1/1	0.36	-	30,30,30,30	0
57	MG	QA	1650	1/1	0.12	-	13,13,13,13	0
57	MG	QA	1649	1/1	0.13	-	2,2,2,2	0
57	MG	XA	1647	1/1	0.13	-	44,44,44,44	0
57	MG	RA	3217	1/1	0.22	-	18,18,18,18	0
57	MG	QA	1602	1/1	0.52	-	9,9,9,9	0
57	MG	YA	3235	1/1	0.39	-	8,8,8,8	0
57	MG	YA	3188	1/1	0.17	-	4,4,4,4	0
57	MG	RA	3210	1/1	0.24	-	27,27,27,27	0
57	MG	XA	1663	1/1	0.17	-	29,29,29,29	0
57	MG	XA	1641	1/1	0.25	-	2,2,2,2	0
57	MG	QM	201	1/1	0.09	-	25,25,25,25	0
57	MG	YA	3234	1/1	0.27	-	1,1,1,1	0
57	MG	QA	1609	1/1	0.06	-	9,9,9,9	0
57	MG	RA	3001	1/1	0.71	-	8,8,8,8	0
57	MG	YA	3177	1/1	0.30	-	5,5,5,5	0
57	MG	YA	3253	1/1	0.59	-	5,5,5,5	0
57	MG	XA	1633	1/1	0.48	-	33,33,33,33	0
57	MG	YA	3025	1/1	1.81	-	80,80,80,80	0
57	MG	YA	3261	1/1	0.99	-	8,8,8,8	0
57	MG	RA	3154	1/1	0.15	-	17,17,17,17	0
57	MG	RA	3206	1/1	0.27	-	40,40,40,40	0
57	MG	YA	3143	1/1	0.25	-	10,10,10,10	0
57	MG	YA	3085	1/1	0.40	-	37,37,37,37	0
57	MG	XA	1640	1/1	0.33	-	25,25,25,25	0
57	MG	RA	3066	1/1	0.57	-	8,8,8,8	0
57	MG	YA	3090	1/1	0.21	-	14,14,14,14	0
58	PAR	QA	1666	42/42	0.23	-	58,58,58,58	0
57	MG	RA	3178	1/1	0.90	-	4,4,4,4	0
57	MG	YA	3155	1/1	0.47	-	38,38,38,38	0
57	MG	YB	202	1/1	0.57	-	21,21,21,21	0
57	MG	RA	3104	1/1	0.20	-	5,5,5,5	0
57	MG	RA	3072	1/1	0.21	-	3,3,3,3	0
57	MG	XA	1664	1/1	0.28	-	8,8,8,8	0
57	MG	RE	302	1/1	0.27	-	10,10,10,10	0
57	MG	XA	1662	1/1	0.47	-	51,51,51,51	0
57	MG	YA	3139	1/1	0.16	-	19,19,19,19	0
57	MG	RA	3138	1/1	0.55	-	51,51,51,51	0
57	MG	YA	3017	1/1	0.47	-	8,8,8,8	0
57	MG	RA	3084	1/1	0.21	-	1,1,1,1	0
57	MG	YA	3037	1/1	0.37	-	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3127	1/1	0.20	-	11,11,11,11	0
57	MG	YA	3118	1/1	0.37	-	63,63,63,63	0
57	MG	RA	3016	1/1	0.12	-	1,1,1,1	0
57	MG	XA	1604	1/1	0.84	-	13,13,13,13	0
57	MG	YA	3175	1/1	0.28	-	43,43,43,43	0
57	MG	YA	3171	1/1	0.25	-	24,24,24,24	0
57	MG	QA	1638	1/1	0.51	-	27,27,27,27	0
57	MG	YA	3210	1/1	0.26	-	39,39,39,39	0
57	MG	YA	3166	1/1	0.15	-	45,45,45,45	0
57	MG	YA	3108	1/1	0.81	-	15,15,15,15	0
57	MG	YA	3075	1/1	0.23	-	3,3,3,3	0
57	MG	RA	3143	1/1	0.26	-	14,14,14,14	0
57	MG	RA	3144	1/1	0.30	-	2,2,2,2	0
57	MG	YA	3050	1/1	0.52	-	10,10,10,10	0
57	MG	RA	3047	1/1	0.34	-	1,1,1,1	0
57	MG	XA	1654	1/1	0.52	-	23,23,23,23	0
57	MG	QA	1621	1/1	0.24	-	7,7,7,7	0
57	MG	RA	3228	1/1	0.23	-	43,43,43,43	0
57	MG	QA	1631	1/1	0.33	-	15,15,15,15	0
57	MG	RA	3234	1/1	0.52	-	7,7,7,7	0
57	MG	RA	3018	1/1	0.72	-	8,8,8,8	0
57	MG	YA	3023	1/1	0.38	-	6,6,6,6	0
57	MG	XA	1634	1/1	0.78	-	23,23,23,23	0
57	MG	YA	3125	1/1	0.20	-	10,10,10,10	0
57	MG	RA	3152	1/1	0.21	-	3,3,3,3	0
57	MG	RA	3112	1/1	0.30	-	5,5,5,5	0
57	MG	YA	3104	1/1	0.10	-	3,3,3,3	0
57	MG	RA	3032	1/1	1.55	-	80,80,80,80	0
57	MG	XA	1616	1/1	0.23	-	10,10,10,10	0
57	MG	QA	1630	1/1	0.50	-	54,54,54,54	0
57	MG	RA	3056	1/1	0.29	-	21,21,21,21	0
57	MG	RA	3015	1/1	0.28	-	0,0,0,0	0
57	MG	XA	1605	1/1	0.70	-	18,18,18,18	0
57	MG	QV	101	1/1	0.70	-	80,80,80,80	0
57	MG	YA	3095	1/1	0.45	-	1,1,1,1	0
57	MG	YA	3047	1/1	0.51	-	14,14,14,14	0
57	MG	RA	3235	1/1	0.22	-	11,11,11,11	0
57	MG	RA	3030	1/1	0.36	-	2,2,2,2	0
57	MG	XA	1620	1/1	0.34	-	5,5,5,5	0
57	MG	YA	3153	1/1	0.43	-	21,21,21,21	0
57	MG	XA	1623	1/1	0.29	-	4,4,4,4	0
57	MG	YA	3168	1/1	0.26	-	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3241	1/1	0.33	-	29,29,29,29	0
57	MG	YA	3144	1/1	0.13	-	25,25,25,25	0
57	MG	QA	1608	1/1	0.08	-	11,11,11,11	0
57	MG	RA	3054	1/1	0.27	-	41,41,41,41	0
57	MG	RA	3044	1/1	0.37	-	2,2,2,2	0
57	MG	YA	3040	1/1	0.60	-	0,0,0,0	0
57	MG	XA	1631	1/1	0.35	-	0,0,0,0	0
57	MG	YA	3106	1/1	0.21	-	84,84,84,84	0
57	MG	QA	1653	1/1	0.26	-	16,16,16,16	0
57	MG	RA	3042	1/1	0.17	-	14,14,14,14	0
57	MG	RA	3202	1/1	0.19	-	9,9,9,9	0
57	MG	YA	3205	1/1	0.38	-	38,38,38,38	0
57	MG	RA	3106	1/1	0.25	-	3,3,3,3	0
57	MG	YA	3126	1/1	0.40	-	5,5,5,5	0
57	MG	RA	3175	1/1	0.30	-	20,20,20,20	0
57	MG	RA	3212	1/1	0.50	-	10,10,10,10	0
57	MG	QA	1627	1/1	0.25	-	22,22,22,22	0
57	MG	RA	3180	1/1	0.51	-	21,21,21,21	0
57	MG	RA	3083	1/1	0.29	-	12,12,12,12	0
57	MG	YA	3083	1/1	0.14	-	7,7,7,7	0
57	MG	YA	3091	1/1	0.32	-	8,8,8,8	0
57	MG	RA	3134	1/1	0.44	-	24,24,24,24	0
57	MG	YA	3044	1/1	0.17	-	75,75,75,75	0
57	MG	RA	3137	1/1	0.30	-	2,2,2,2	0
57	MG	RA	3223	1/1	0.17	-	11,11,11,11	0
57	MG	YA	3184	1/1	0.19	-	51,51,51,51	0
57	MG	QA	1664	1/1	0.17	-	24,24,24,24	0
57	MG	QA	1651	1/1	0.32	-	6,6,6,6	0
57	MG	YA	3225	1/1	0.32	-	34,34,34,34	0
57	MG	YA	3112	1/1	0.23	-	11,11,11,11	0
57	MG	YA	3094	1/1	0.24	-	0,0,0,0	0
57	MG	XX	101	1/1	0.20	-	11,11,11,11	0
57	MG	QA	1633	1/1	0.31	-	35,35,35,35	0
57	MG	YA	3032	1/1	0.50	-	8,8,8,8	0
57	MG	YA	3061	1/1	0.29	-	2,2,2,2	0
57	MG	RA	3071	1/1	0.59	-	23,23,23,23	0
57	MG	RA	3113	1/1	0.37	-	3,3,3,3	0
57	MG	RA	3094	1/1	0.61	-	3,3,3,3	0
57	MG	XA	1646	1/1	0.23	-	6,6,6,6	0
57	MG	RA	3176	1/1	0.37	-	14,14,14,14	0
57	MG	RA	3013	1/1	0.48	-	5,5,5,5	0
57	MG	YA	3098	1/1	0.16	-	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	3014	1/1	0.41	-	2,2,2,2	0
57	MG	RA	3227	1/1	0.34	-	16,16,16,16	0
57	MG	YA	3123	1/1	0.19	-	24,24,24,24	0
58	PAR	XA	1671	42/42	0.25	-	40,40,40,40	0
57	MG	YA	3150	1/1	0.21	-	11,11,11,11	0
57	MG	YA	3128	1/1	0.67	-	25,25,25,25	0
57	MG	RB	201	1/1	0.23	-	30,30,30,30	0
57	MG	XA	1617	1/1	0.29	-	2,2,2,2	0
57	MG	RA	3173	1/1	0.32	-	54,54,54,54	0
57	MG	RA	3022	1/1	0.30	-	1,1,1,1	0
57	MG	YA	3174	1/1	0.41	-	47,47,47,47	0
57	MG	RA	3162	1/1	0.17	-	22,22,22,22	0
57	MG	YA	3004	1/1	0.35	-	18,18,18,18	0
57	MG	YD	302	1/1	0.56	-	49,49,49,49	0
57	MG	YA	3130	1/1	0.07	-	7,7,7,7	0
57	MG	RA	3183	1/1	0.14	-	12,12,12,12	0
57	MG	XA	1627	1/1	0.27	-	9,9,9,9	0
57	MG	YA	3255	1/1	0.11	-	19,19,19,19	0
57	MG	RA	3240	1/1	0.39	-	2,2,2,2	0
57	MG	RA	3160	1/1	0.16	-	10,10,10,10	0
57	MG	RA	3014	1/1	0.15	-	2,2,2,2	0
57	MG	RA	3068	1/1	0.26	-	68,68,68,68	0
57	MG	YA	3181	1/1	0.23	-	4,4,4,4	0
57	MG	RA	3077	1/1	0.40	-	19,19,19,19	0
57	MG	YA	3109	1/1	1.47	-	80,80,80,80	0
57	MG	XA	1668	1/1	0.16	-	31,31,31,31	0
57	MG	YA	3203	1/1	0.33	-	21,21,21,21	0
57	MG	YA	3248	1/1	0.52	-	17,17,17,17	0
57	MG	RA	3229	1/1	0.38	-	9,9,9,9	0
57	MG	XA	1602	1/1	0.28	-	2,2,2,2	0
57	MG	YA	3201	1/1	0.40	-	2,2,2,2	0
57	MG	YA	3246	1/1	0.23	-	7,7,7,7	0
57	MG	RA	3110	1/1	0.65	-	12,12,12,12	0
57	MG	YA	3012	1/1	1.40	-	80,80,80,80	0
57	MG	YA	3114	1/1	0.16	-	29,29,29,29	0
57	MG	YA	3237	1/1	0.23	-	38,38,38,38	0
57	MG	YE	301	1/1	0.26	-	55,55,55,55	0
57	MG	XA	1660	1/1	0.58	-	21,21,21,21	0
57	MG	YA	3182	1/1	0.67	-	30,30,30,30	0
57	MG	YA	3241	1/1	0.32	-	34,34,34,34	0
57	MG	YA	3133	1/1	0.15	-	8,8,8,8	0
57	MG	RA	3045	1/1	0.16	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3244	1/1	0.10	-	0,0,0,0	0
57	MG	YA	3065	1/1	0.30	-	38,38,38,38	0
57	MG	RA	3127	1/1	0.17	-	10,10,10,10	0
57	MG	YA	3053	1/1	0.32	-	1,1,1,1	0
57	MG	RA	3007	1/1	0.76	-	26,26,26,26	0
57	MG	YA	3062	1/1	0.23	-	5,5,5,5	0
57	MG	YA	3156	1/1	0.25	-	6,6,6,6	0
57	MG	XA	1611	1/1	0.37	-	3,3,3,3	0
57	MG	RA	3006	1/1	1.51	-	80,80,80,80	0
57	MG	RA	3041	1/1	0.45	-	13,13,13,13	0
57	MG	RA	3125	1/1	0.27	-	37,37,37,37	0
57	MG	XA	1665	1/1	0.52	-	38,38,38,38	0
57	MG	RA	3114	1/1	0.21	-	2,2,2,2	0
57	MG	RA	3098	1/1	0.84	-	80,80,80,80	0
57	MG	YA	3167	1/1	0.40	-	49,49,49,49	0
57	MG	QA	1647	1/1	0.65	-	29,29,29,29	0
57	MG	YA	3045	1/1	0.35	-	20,20,20,20	0
57	MG	RA	3165	1/1	0.15	-	25,25,25,25	0
57	MG	QA	1661	1/1	0.60	-	9,9,9,9	0
57	MG	XA	1607	1/1	0.46	-	15,15,15,15	0
57	MG	YA	3046	1/1	0.43	-	0,0,0,0	0
57	MG	YA	3100	1/1	0.45	-	3,3,3,3	0
57	MG	YD	301	1/1	0.76	-	80,80,80,80	0
57	MG	QA	1665	1/1	0.34	-	27,27,27,27	0
57	MG	QA	1612	1/1	0.22	-	5,5,5,5	0
57	MG	QA	1611	1/1	0.23	-	2,2,2,2	0
57	MG	RP	201	1/1	0.40	-	10,10,10,10	0
57	MG	RA	3232	1/1	1.06	-	80,80,80,80	0
59	ZN	QN	101	1/1	0.11	-	102,102,102,102	0
57	MG	YA	3183	1/1	0.33	-	10,10,10,10	0
57	MG	RA	3131	1/1	0.21	-	0,0,0,0	0
57	MG	YA	3142	1/1	0.17	-	28,28,28,28	0
57	MG	RA	3090	1/1	0.51	-	3,3,3,3	0
57	MG	RA	3116	1/1	0.08	-	2,2,2,2	0
57	MG	YA	3223	1/1	0.37	-	27,27,27,27	0
57	MG	XA	1609	1/1	0.43	-	12,12,12,12	0
57	MG	RA	3237	1/1	0.33	-	5,5,5,5	0
57	MG	YA	3230	1/1	0.20	-	10,10,10,10	0
57	MG	QA	1622	1/1	0.40	-	44,44,44,44	0
57	MG	RA	3201	1/1	0.44	-	1,1,1,1	0
57	MG	RA	3169	1/1	0.24	-	3,3,3,3	0
57	MG	RA	3230	1/1	0.37	-	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	3015	1/1	0.11	-	4,4,4,4	0
57	MG	RA	3062	1/1	0.77	-	1,1,1,1	0
57	MG	RA	3146	1/1	0.14	-	3,3,3,3	0
57	MG	RA	3101	1/1	0.15	-	32,32,32,32	0
57	MG	RA	3012	1/1	0.49	-	7,7,7,7	0
57	MG	RA	3142	1/1	0.10	-	28,28,28,28	0
57	MG	RA	3099	1/1	0.18	-	6,6,6,6	0
57	MG	YA	3206	1/1	0.26	-	25,25,25,25	0
57	MG	YA	3250	1/1	0.52	-	6,6,6,6	0
57	MG	YA	3219	1/1	0.14	-	17,17,17,17	0
57	MG	YA	3024	1/1	0.27	-	17,17,17,17	0
57	MG	YA	3263	1/1	0.27	-	7,7,7,7	0
57	MG	RA	3123	1/1	0.28	-	24,24,24,24	0
57	MG	XA	1614	1/1	0.23	-	2,2,2,2	0
57	MG	YA	3124	1/1	0.62	-	19,19,19,19	0
57	MG	YA	3070	1/1	0.21	-	5,5,5,5	0
57	MG	RA	3132	1/1	0.19	-	4,4,4,4	0
57	MG	YA	3247	1/1	0.57	-	32,32,32,32	0
57	MG	YA	3006	1/1	0.29	-	2,2,2,2	0
57	MG	QA	1641	1/1	0.22	-	6,6,6,6	0
57	MG	QA	1601	1/1	0.30	-	12,12,12,12	0
57	MG	RA	3197	1/1	0.06	-	12,12,12,12	0
57	MG	XA	1632	1/1	0.18	-	36,36,36,36	0
57	MG	YA	3076	1/1	0.38	-	2,2,2,2	0
57	MG	YA	3204	1/1	0.17	-	23,23,23,23	0
57	MG	XA	1651	1/1	0.29	-	22,22,22,22	0
57	MG	YA	3146	1/1	0.31	-	4,4,4,4	0
57	MG	YB	201	1/1	0.40	-	48,48,48,48	0
57	MG	YA	3162	1/1	0.23	-	49,49,49,49	0
57	MG	QA	1635	1/1	0.17	-	8,8,8,8	0
57	MG	R5	101	1/1	0.18	-	33,33,33,33	0
57	MG	RA	3024	1/1	0.50	-	28,28,28,28	0
57	MG	QA	1648	1/1	0.35	-	30,30,30,30	0
57	MG	YA	3007	1/1	0.14	-	4,4,4,4	0
57	MG	YB	203	1/1	0.14	-	33,33,33,33	0
57	MG	YA	3052	1/1	0.33	-	3,3,3,3	0
57	MG	YA	3245	1/1	0.40	-	3,3,3,3	0
57	MG	RA	3147	1/1	0.22	-	0,0,0,0	0
57	MG	RA	3194	1/1	0.27	-	54,54,54,54	0
57	MG	RA	3216	1/1	0.83	-	39,39,39,39	0
57	MG	YA	3016	1/1	0.28	-	2,2,2,2	0
57	MG	RA	3075	1/1	0.20	-	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	QA	1637	1/1	0.23	-	46,46,46,46	0
57	MG	YA	3236	1/1	0.13	-	24,24,24,24	0
57	MG	RA	3034	1/1	0.47	-	2,2,2,2	0
57	MG	XA	1661	1/1	0.55	-	32,32,32,32	0
57	MG	RA	3081	1/1	0.31	-	3,3,3,3	0
57	MG	YA	3027	1/1	0.25	-	3,3,3,3	0
57	MG	RA	3166	1/1	0.26	-	20,20,20,20	0
57	MG	XA	1612	1/1	0.15	-	7,7,7,7	0
57	MG	YA	3228	1/1	0.33	-	9,9,9,9	0
57	MG	RA	3023	1/1	0.13	-	0,0,0,0	0
57	MG	RA	3182	1/1	0.39	-	23,23,23,23	0
57	MG	YA	3009	1/1	0.42	-	0,0,0,0	0
57	MG	YA	3021	1/1	0.46	-	15,15,15,15	0
57	MG	RA	3059	1/1	0.32	-	4,4,4,4	0
57	MG	YA	3265	1/1	0.66	-	1,1,1,1	0
57	MG	YA	3116	1/1	0.56	-	80,80,80,80	0
57	MG	YA	3060	1/1	0.32	-	3,3,3,3	0
57	MG	YA	3154	1/1	0.13	-	8,8,8,8	0
57	MG	RA	3043	1/1	0.19	-	6,6,6,6	0
57	MG	RA	3027	1/1	0.28	-	4,4,4,4	0
57	MG	RA	3038	1/1	0.27	-	9,9,9,9	0
57	MG	YA	3172	1/1	0.22	-	41,41,41,41	0
57	MG	RA	3174	1/1	0.40	-	17,17,17,17	0
57	MG	RA	3033	1/1	0.51	-	5,5,5,5	0
57	MG	YA	3115	1/1	0.24	-	31,31,31,31	0
57	MG	RA	3195	1/1	0.23	-	8,8,8,8	0
57	MG	XA	1610	1/1	0.12	-	6,6,6,6	0
57	MG	YA	3176	1/1	0.16	-	28,28,28,28	0
57	MG	RA	3057	1/1	0.27	-	8,8,8,8	0
57	MG	QA	1619	1/1	0.21	-	40,40,40,40	0
57	MG	XA	1621	1/1	0.10	-	23,23,23,23	0
57	MG	RA	3231	1/1	0.54	-	7,7,7,7	0
57	MG	YA	3217	1/1	0.21	-	14,14,14,14	0
57	MG	RA	3117	1/1	0.28	-	58,58,58,58	0
57	MG	YA	3213	1/1	0.26	-	17,17,17,17	0
57	MG	XA	1642	1/1	0.33	-	7,7,7,7	0
57	MG	RA	3108	1/1	0.28	-	3,3,3,3	0
57	MG	YA	3193	1/1	0.24	-	2,2,2,2	0
57	MG	XB	301	1/1	0.27	-	26,26,26,26	0
57	MG	YA	3073	1/1	0.41	-	23,23,23,23	0
57	MG	YA	3043	1/1	0.49	-	6,6,6,6	0
57	MG	YA	3107	1/1	0.30	-	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3126	1/1	0.10	-	8,8,8,8	0
57	MG	YA	3120	1/1	0.36	-	0,0,0,0	0
57	MG	QA	1625	1/1	0.15	-	25,25,25,25	0
57	MG	YA	3135	1/1	0.21	-	1,1,1,1	0
57	MG	QA	1614	1/1	0.23	-	26,26,26,26	0
57	MG	RA	3079	1/1	0.26	-	11,11,11,11	0
57	MG	YA	3035	1/1	0.84	-	80,80,80,80	0
57	MG	RA	3187	1/1	0.23	-	10,10,10,10	0
57	MG	RA	3029	1/1	0.29	-	1,1,1,1	0
57	MG	YA	3077	1/1	0.49	-	3,3,3,3	0
57	MG	RA	3069	1/1	0.53	-	2,2,2,2	0
57	MG	RA	3017	1/1	0.27	-	11,11,11,11	0
57	MG	XA	1656	1/1	0.25	-	10,10,10,10	0
57	MG	XA	1619	1/1	0.26	-	13,13,13,13	0
57	MG	YA	3071	1/1	0.12	-	40,40,40,40	0
57	MG	YA	3145	1/1	0.30	-	16,16,16,16	0
57	MG	RA	3095	1/1	0.50	-	2,2,2,2	0
57	MG	YA	3089	1/1	0.53	-	4,4,4,4	0
57	MG	YA	3034	1/1	0.39	-	4,4,4,4	0
57	MG	RA	3157	1/1	0.31	-	1,1,1,1	0
57	MG	RA	3239	1/1	0.18	-	3,3,3,3	0
57	MG	RA	3005	1/1	0.38	-	6,6,6,6	0
57	MG	RA	3171	1/1	0.20	-	15,15,15,15	0
57	MG	YA	3057	1/1	0.26	-	27,27,27,27	0
57	MG	YA	3159	1/1	0.38	-	12,12,12,12	0
57	MG	RA	3242	1/1	0.34	-	7,7,7,7	0
57	MG	YA	3209	1/1	0.43	-	69,69,69,69	0
57	MG	QA	1657	1/1	0.14	-	65,65,65,65	0
57	MG	YA	3216	1/1	0.17	-	38,38,38,38	0
57	MG	YA	3051	1/1	0.26	-	3,3,3,3	0
57	MG	YA	3026	1/1	0.48	-	32,32,32,32	0
57	MG	RA	3003	1/1	0.44	-	4,4,4,4	0
57	MG	YA	3148	1/1	0.15	-	42,42,42,42	0
57	MG	RA	3048	1/1	0.26	-	20,20,20,20	0
57	MG	YA	3231	1/1	0.14	-	2,2,2,2	0
57	MG	XA	1658	1/1	0.17	-	0,0,0,0	0
57	MG	QA	1606	1/1	0.12	-	5,5,5,5	0
57	MG	YA	3042	1/1	0.23	-	2,2,2,2	0
57	MG	XA	1615	1/1	0.43	-	2,2,2,2	0
57	MG	R8	101	1/1	0.28	-	19,19,19,19	0
57	MG	QA	1607	1/1	0.15	-	5,5,5,5	0
57	MG	YA	3022	1/1	0.24	-	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	3121	1/1	0.38	-	9,9,9,9	0
57	MG	RA	3192	1/1	0.23	-	0,0,0,0	0
57	MG	RA	3100	1/1	0.55	-	36,36,36,36	0
57	MG	QA	1654	1/1	0.11	-	55,55,55,55	0
57	MG	YA	3189	1/1	0.36	-	0,0,0,0	0
57	MG	YA	3170	1/1	0.24	-	26,26,26,26	0
57	MG	RA	3186	1/1	0.15	-	71,71,71,71	0
57	MG	RA	3026	1/1	1.10	-	80,80,80,80	0
57	MG	YA	3102	1/1	0.47	-	3,3,3,3	0
57	MG	RA	3039	1/1	0.21	-	2,2,2,2	0
57	MG	YA	3249	1/1	0.39	-	3,3,3,3	0
57	MG	RA	3025	1/1	0.15	-	66,66,66,66	0
57	MG	RA	3080	1/1	0.30	-	2,2,2,2	0
57	MG	QA	1658	1/1	0.26	-	90,90,90,90	0
57	MG	RA	3205	1/1	0.28	-	7,7,7,7	0
57	MG	RA	3149	1/1	0.17	-	15,15,15,15	0
57	MG	RA	3164	1/1	0.24	-	34,34,34,34	0
57	MG	YA	3033	1/1	0.59	-	5,5,5,5	0
57	MG	YA	3267	1/1	0.46	-	19,19,19,19	0
57	MG	RA	3203	1/1	0.48	-	30,30,30,30	0
57	MG	XA	1628	1/1	0.11	-	28,28,28,28	0
57	MG	RA	3073	1/1	0.29	-	37,37,37,37	0
57	MG	RA	3208	1/1	0.40	-	29,29,29,29	0
57	MG	RA	3008	1/1	0.42	-	3,3,3,3	0
57	MG	YA	3240	1/1	0.33	-	23,23,23,23	0
57	MG	RA	3140	1/1	0.30	-	17,17,17,17	0
57	MG	YA	3038	1/1	0.22	-	5,5,5,5	0
57	MG	RA	3172	1/1	0.17	-	4,4,4,4	0
57	MG	YA	3005	1/1	0.25	-	68,68,68,68	0
57	MG	RA	3002	1/1	0.55	-	4,4,4,4	0
57	MG	RA	3010	1/1	0.53	-	4,4,4,4	0
57	MG	YA	3002	1/1	0.96	-	80,80,80,80	0
57	MG	YA	3030	1/1	0.40	-	6,6,6,6	0
57	MG	RA	3096	1/1	0.44	-	2,2,2,2	0
57	MG	YA	3207	1/1	0.31	-	20,20,20,20	0
57	MG	YA	3048	1/1	0.24	-	21,21,21,21	0
57	MG	RA	3124	1/1	0.54	-	35,35,35,35	0
57	MG	QA	1652	1/1	0.16	-	0,0,0,0	0
57	MG	RA	3188	1/1	0.14	-	11,11,11,11	0
57	MG	YA	3164	1/1	0.27	-	8,8,8,8	0
57	MG	YA	3259	1/1	0.37	-	0,0,0,0	0
57	MG	QA	1646	1/1	0.18	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3202	1/1	0.32	-	4,4,4,4	0
57	MG	RA	3218	1/1	0.15	-	4,4,4,4	0
57	MG	YA	3158	1/1	0.30	-	23,23,23,23	0
57	MG	RA	3085	1/1	0.30	-	4,4,4,4	0
57	MG	YA	3257	1/1	0.50	-	5,5,5,5	0
57	MG	XA	1606	1/1	0.44	-	29,29,29,29	0
57	MG	RA	3058	1/1	0.37	-	9,9,9,9	0
57	MG	RA	3220	1/1	0.51	-	1,1,1,1	0
57	MG	YA	3134	1/1	0.23	-	11,11,11,11	0
57	MG	RA	3214	1/1	0.22	-	12,12,12,12	0
57	MG	RA	3190	1/1	0.40	-	8,8,8,8	0
57	MG	QA	1663	1/1	0.06	-	33,33,33,33	0
57	MG	RA	3150	1/1	0.19	-	25,25,25,25	0
57	MG	XA	1659	1/1	0.14	-	54,54,54,54	0
57	MG	QA	1639	1/1	0.17	-	18,18,18,18	0
57	MG	YA	3110	1/1	0.46	-	18,18,18,18	0
57	MG	YA	3011	1/1	0.28	-	2,2,2,2	0
57	MG	RA	3093	1/1	0.18	-	1,1,1,1	0
57	MG	RB	202	1/1	0.18	-	2,2,2,2	0
57	MG	RA	3051	1/1	0.47	-	3,3,3,3	0
57	MG	XA	1629	1/1	0.24	-	3,3,3,3	0
57	MG	QA	1660	1/1	0.26	-	26,26,26,26	0
57	MG	RA	3211	1/1	0.09	-	6,6,6,6	0
57	MG	YA	3192	1/1	0.11	-	6,6,6,6	0
57	MG	QA	1662	1/1	0.11	-	30,30,30,30	0
57	MG	RA	3036	1/1	0.48	-	2,2,2,2	0
57	MG	XA	1650	1/1	0.08	-	27,27,27,27	0
57	MG	YA	3064	1/1	0.24	-	4,4,4,4	0
57	MG	RA	3199	1/1	0.68	-	60,60,60,60	0
57	MG	QA	1616	1/1	0.15	-	10,10,10,10	0
57	MG	YA	3195	1/1	0.08	-	0,0,0,0	0
57	MG	RA	3004	1/1	0.55	-	13,13,13,13	0
57	MG	YA	3013	1/1	0.40	-	1,1,1,1	0
57	MG	YA	3165	1/1	0.29	-	7,7,7,7	0
57	MG	YA	3081	1/1	0.62	-	0,0,0,0	0
57	MG	QA	1645	1/1	0.14	-	5,5,5,5	0
57	MG	XA	1669	1/1	0.46	-	13,13,13,13	0
57	MG	YA	3069	1/1	0.34	-	10,10,10,10	0
57	MG	RA	3011	1/1	0.16	-	5,5,5,5	0
57	MG	QA	1620	1/1	0.14	-	22,22,22,22	0
57	MG	RA	3070	1/1	0.35	-	6,6,6,6	0
57	MG	YA	3072	1/1	0.17	-	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3191	1/1	0.18	-	23,23,23,23	0
57	MG	YA	3178	1/1	0.31	-	2,2,2,2	0
57	MG	YA	3238	1/1	0.22	-	11,11,11,11	0
57	MG	RA	3105	1/1	0.17	-	6,6,6,6	0
57	MG	QA	1643	1/1	0.10	-	1,1,1,1	0
57	MG	QA	1659	1/1	0.20	-	11,11,11,11	0
57	MG	YA	3088	1/1	1.18	-	80,80,80,80	0
57	MG	XA	1653	1/1	0.32	-	13,13,13,13	0
57	MG	RA	3238	1/1	0.44	-	7,7,7,7	0
57	MG	YA	3218	1/1	0.24	-	2,2,2,2	0
57	MG	RA	3145	1/1	0.22	-	5,5,5,5	0
57	MG	YA	3020	1/1	0.33	-	12,12,12,12	0
57	MG	RA	3204	1/1	0.15	-	33,33,33,33	0
57	MG	RA	3076	1/1	0.49	-	13,13,13,13	0
57	MG	YA	3056	1/1	0.28	-	0,0,0,0	0
57	MG	RA	3111	1/1	0.13	-	1,1,1,1	0
57	MG	RA	3136	1/1	0.20	-	7,7,7,7	0
57	MG	YA	3117	1/1	0.31	-	11,11,11,11	0
57	MG	YA	3220	1/1	0.27	-	2,2,2,2	0
57	MG	RA	3074	1/1	0.18	-	10,10,10,10	0
57	MG	YA	3211	1/1	0.17	-	1,1,1,1	0
57	MG	RA	3221	1/1	0.92	-	15,15,15,15	0
57	MG	YA	3254	1/1	0.57	-	1,1,1,1	0
57	MG	XA	1636	1/1	0.22	-	5,5,5,5	0
57	MG	XA	1645	1/1	0.34	-	2,2,2,2	0
57	MG	RA	3115	1/1	0.11	-	11,11,11,11	0
57	MG	RA	3233	1/1	0.23	-	17,17,17,17	0
57	MG	YA	3251	1/1	0.54	-	6,6,6,6	0
57	MG	YA	3019	1/1	0.74	-	10,10,10,10	0
57	MG	YA	3262	1/1	0.15	-	5,5,5,5	0
57	MG	QA	1634	1/1	0.43	-	6,6,6,6	0
57	MG	RA	3193	1/1	0.18	-	17,17,17,17	0
59	ZN	XD	301	1/1	0.21	-	5,5,5,5	0
57	MG	RA	3184	1/1	0.46	-	13,13,13,13	0
57	MG	YA	3163	1/1	0.23	-	41,41,41,41	0
57	MG	YA	3003	1/1	0.14	-	9,9,9,9	0
57	MG	RA	3065	1/1	0.56	-	80,80,80,80	0
57	MG	YA	3105	1/1	0.47	-	1,1,1,1	0
57	MG	RA	3061	1/1	0.16	-	32,32,32,32	0
57	MG	XA	1670	1/1	0.29	-	17,17,17,17	0
57	MG	YA	3197	1/1	0.37	-	1,1,1,1	0
57	MG	YA	3039	1/1	0.19	-	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	XA	1637	1/1	0.13	-	28,28,28,28	0
57	MG	YA	3212	1/1	0.15	-	17,17,17,17	0
57	MG	XA	1601	1/1	1.49	-	80,80,80,80	0
57	MG	RA	3148	1/1	0.14	-	39,39,39,39	0
57	MG	RA	3020	1/1	0.24	-	5,5,5,5	0
57	MG	QA	1655	1/1	0.18	-	6,6,6,6	0
57	MG	YA	3215	1/1	0.15	-	25,25,25,25	0
57	MG	RA	3037	1/1	0.15	-	15,15,15,15	0
57	MG	XV	101	1/1	0.17	-	3,3,3,3	0
57	MG	XA	1613	1/1	0.08	-	0,0,0,0	0
57	MG	YA	3149	1/1	0.21	-	17,17,17,17	0
57	MG	QF	201	1/1	0.38	-	1,1,1,1	0
57	MG	YA	3074	1/1	0.29	-	0,0,0,0	0
57	MG	YA	3132	1/1	0.07	-	31,31,31,31	0
57	MG	YA	3179	1/1	0.07	-	4,4,4,4	0
57	MG	YA	3082	1/1	0.46	-	0,0,0,0	0
57	MG	RA	3092	1/1	0.34	-	1,1,1,1	0
57	MG	YA	3080	1/1	0.27	-	9,9,9,9	0
57	MG	QA	1624	1/1	0.44	-	49,49,49,49	0
57	MG	XA	1655	1/1	0.72	-	40,40,40,40	0
57	MG	RA	3155	1/1	0.27	-	24,24,24,24	0
57	MG	RA	3086	1/1	0.26	-	19,19,19,19	0
57	MG	RA	3209	1/1	0.17	-	35,35,35,35	0
57	MG	YA	3119	1/1	0.26	-	2,2,2,2	0
57	MG	YA	3092	1/1	0.32	-	13,13,13,13	0
57	MG	XA	1657	1/1	0.19	-	27,27,27,27	0
57	MG	YA	3031	1/1	1.24	-	80,80,80,80	0
57	MG	RA	3222	1/1	0.37	-	45,45,45,45	0
57	MG	YA	3160	1/1	0.73	-	51,51,51,51	0
57	MG	YA	3226	1/1	0.54	-	4,4,4,4	0
57	MG	RA	3181	1/1	0.60	-	28,28,28,28	0
57	MG	QA	1604	1/1	0.20	-	17,17,17,17	0
57	MG	RA	3196	1/1	0.27	-	8,8,8,8	0
57	MG	YA	3036	1/1	0.22	-	7,7,7,7	0
57	MG	YA	3185	1/1	0.42	-	14,14,14,14	0
57	MG	RA	3055	1/1	0.51	-	1,1,1,1	0
57	MG	RA	3064	1/1	0.20	-	12,12,12,12	0
57	MG	RA	3215	1/1	0.20	-	1,1,1,1	0
57	MG	QA	1644	1/1	0.07	-	34,34,34,34	0
57	MG	RA	3091	1/1	0.24	-	1,1,1,1	0
57	MG	RF	301	1/1	0.20	-	49,49,49,49	0
57	MG	XA	1622	1/1	0.21	-	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3128	1/1	0.13	-	2,2,2,2	0
57	MG	RA	3170	1/1	0.50	-	23,23,23,23	0
57	MG	YP	201	1/1	0.14	-	8,8,8,8	0
57	MG	XA	1635	1/1	0.32	-	42,42,42,42	0
57	MG	RA	3159	1/1	0.18	-	0,0,0,0	0
57	MG	RA	3168	1/1	0.89	-	55,55,55,55	0
57	MG	RA	3021	1/1	0.27	-	5,5,5,5	0
57	MG	YA	3264	1/1	0.36	-	35,35,35,35	0
57	MG	RA	3163	1/1	0.95	-	13,13,13,13	0
57	MG	QA	1640	1/1	0.16	-	46,46,46,46	0
57	MG	YA	3111	1/1	0.23	-	19,19,19,19	0
57	MG	YA	3233	1/1	0.49	-	68,68,68,68	0
57	MG	RA	3226	1/1	0.24	-	26,26,26,26	0
57	MG	RA	3135	1/1	0.16	-	7,7,7,7	0
57	MG	YA	3137	1/1	0.11	-	2,2,2,2	0
57	MG	RA	3046	1/1	0.43	-	1,1,1,1	0
57	MG	YA	3196	1/1	0.71	-	6,6,6,6	0
57	MG	RA	3139	1/1	0.25	-	12,12,12,12	0
57	MG	YA	3059	1/1	0.23	-	3,3,3,3	0
57	MG	YA	3214	1/1	0.14	-	7,7,7,7	0
57	MG	YA	3103	1/1	1.26	-	80,80,80,80	0
57	MG	YA	3229	1/1	0.66	-	30,30,30,30	0
57	MG	RA	3133	1/1	0.18	-	33,33,33,33	0
57	MG	RA	3031	1/1	0.31	-	13,13,13,13	0
57	MG	YA	3008	1/1	0.15	-	1,1,1,1	0
57	MG	YA	3180	1/1	0.12	-	7,7,7,7	0
57	MG	QA	1610	1/1	0.24	-	3,3,3,3	0
57	MG	YA	3194	1/1	0.29	-	13,13,13,13	0
57	MG	YA	3054	1/1	0.85	-	80,80,80,80	0
57	MG	YA	3147	1/1	0.57	-	27,27,27,27	0
57	MG	RA	3088	1/1	0.49	-	5,5,5,5	0
57	MG	YA	3101	1/1	0.42	-	1,1,1,1	0
57	MG	RA	3191	1/1	0.13	-	26,26,26,26	0
57	MG	YA	3010	1/1	0.38	-	0,0,0,0	0
57	MG	RA	3224	1/1	0.22	-	19,19,19,19	0
57	MG	XA	1603	1/1	0.54	-	5,5,5,5	0
57	MG	QA	1618	1/1	0.38	-	49,49,49,49	0
57	MG	RA	3109	1/1	0.44	-	26,26,26,26	0

6.5 Other polymers ⓘ

There are no such residues in this entry.