



wwPDB X-ray Structure Validation Summary Report i

Sep 25, 2014 – 01:41 AM EDT

PDB ID : 4P6F
Title : Crystal structure of the peptolide 12C bound to bacterial ribosome
Authors : Fagan, C.E.; Dunham, C.M.
Deposited on : 2014-03-24
Resolution : 3.60 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>

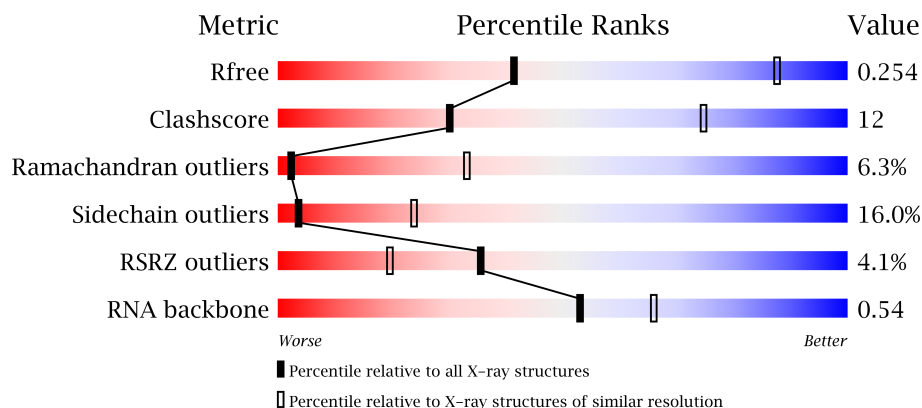
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1020 (3.86-3.34)
Clashscore	79885	1155 (3.80-3.40)
Ramachandran outliers	78287	1109 (3.80-3.40)
Sidechain outliers	78261	1108 (3.80-3.40)
RSRZ outliers	66119	1000 (3.84-3.36)
RNA backbone	1838	1012 (4.40-2.76)

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	QW	76	
23	QY	76	
23	XW	76	
23	XY	76	
24	QX	24	
24	XX	24	
25	RA	2915	
25	YA	2915	
26	RB	122	

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Mol	Chain	Length	Quality of chain
26	YB	122	
27	RD	276	
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	

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Mol	Chain	Length	Quality of chain
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	71	
51	R5	60	
51	Y5	60	
52	R6	54	
52	Y6	54	
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	
56	Z7	12	
56	Z8	12	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 295487 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 ribosomal RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called 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 E-Site tRNA-Phe or A-Site tRNA-Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
23	QY	17	Total	C	N	O	P	0	0	0
			364	163	68	116	17			
23	XW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
23	XY	17	Total	C	N	O	P	0	0	0
			364	163	68	116	17			

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QX	10	Total	C	N	O	P	0	0	0
			210	96	39	66	9			
24	XX	10	Total	C	N	O	P	0	0	0
			210	96	39	66	9			

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

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 ribosomal RNA.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	0	0	0
			882	556	176	150			
38	YS	111	Total	C	N	O	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			
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	S	0	0	0
			725	471	131	123				
43	YX	92	Total	C	N	O	S	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	57	Total	C	N	O	S	0	0	0
			442	278	88	71	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 protein called T17-GLY-GLY-PRO-LYS-LYS-LYS-LYS-LYS-VAL-GLY-GLY.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	Z7	9	Total	C	N	O	0	0	0
			116	78	18	20			
56	Z8	9	Total	C	N	O	0	0	0
			116	78	18	20			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	67	Total	Mg	0	0
			67	67		
57	RP	4	Total	Mg	0	0
			4	4		
57	YA	278	Total	Mg	0	0
			278	278		
57	Y5	1	Total	Mg	0	0
			1	1		

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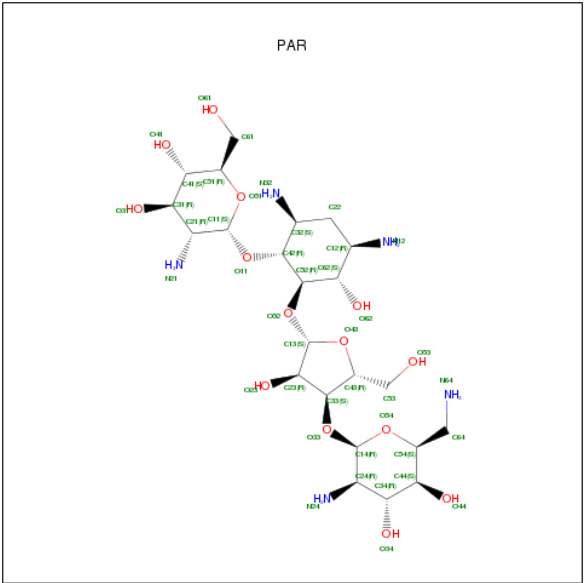
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YD	1	Total 1	Mg 1	0	0
57	XX	1	Total 1	Mg 1	0	0
57	QV	2	Total 2	Mg 2	0	0
57	XA	71	Total 71	Mg 71	0	0
57	R0	1	Total 1	Mg 1	0	0
57	QH	1	Total 1	Mg 1	0	0
57	XY	1	Total 1	Mg 1	0	0
57	YX	1	Total 1	Mg 1	0	0
57	RD	1	Total 1	Mg 1	0	0
57	Y7	1	Total 1	Mg 1	0	0
57	XB	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	246	Total 246	Mg 246	0	0
57	YP	1	Total 1	Mg 1	0	0
57	RE	1	Total 1	Mg 1	0	0
57	YB	5	Total 5	Mg 5	0	0
57	QY	1	Total 1	Mg 1	0	0
57	XV	3	Total 3	Mg 3	0	0
57	RB	2	Total 2	Mg 2	0	0
57	XM	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YE	2	Total	Mg	0	0
			2	2		

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



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

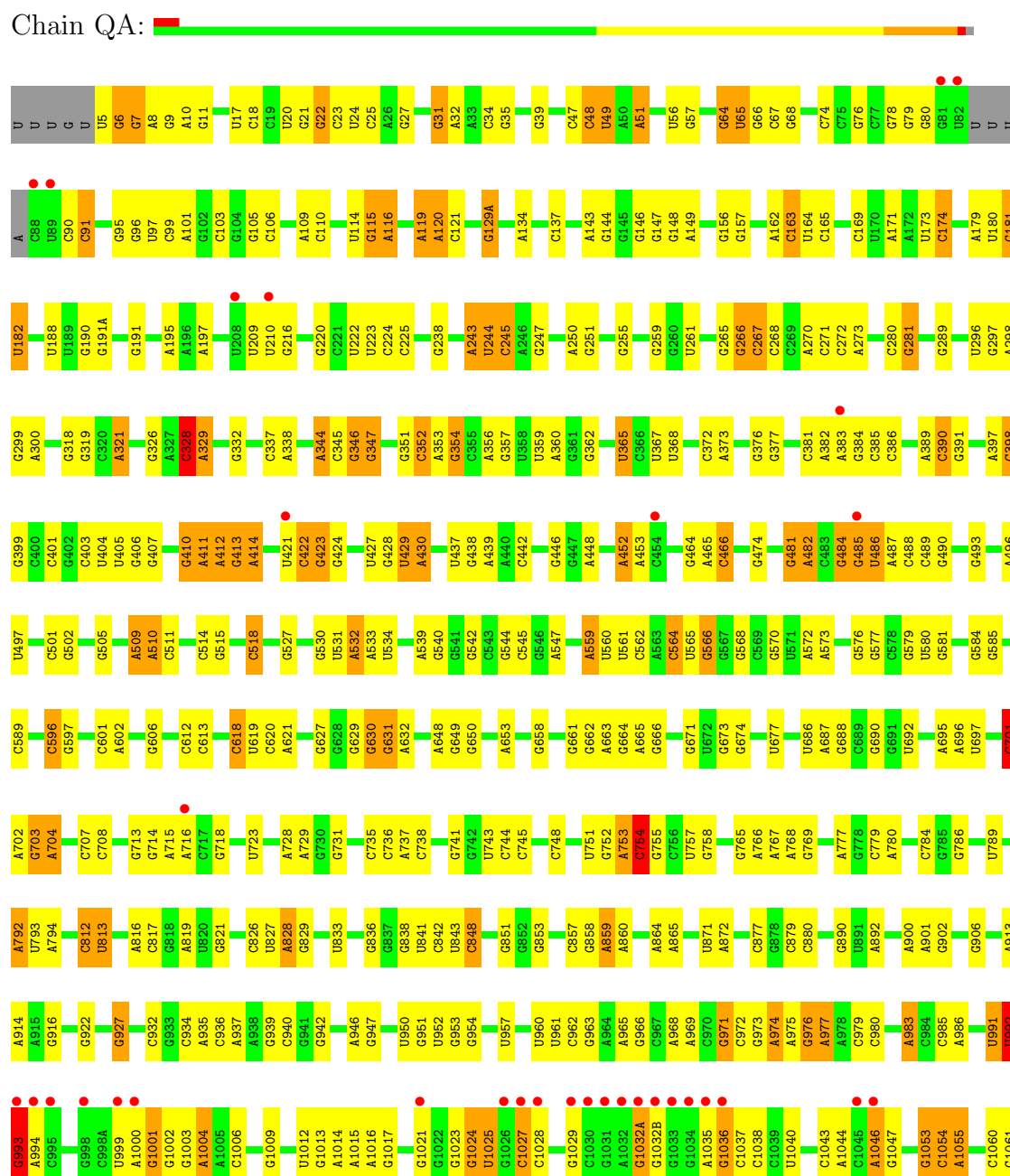
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

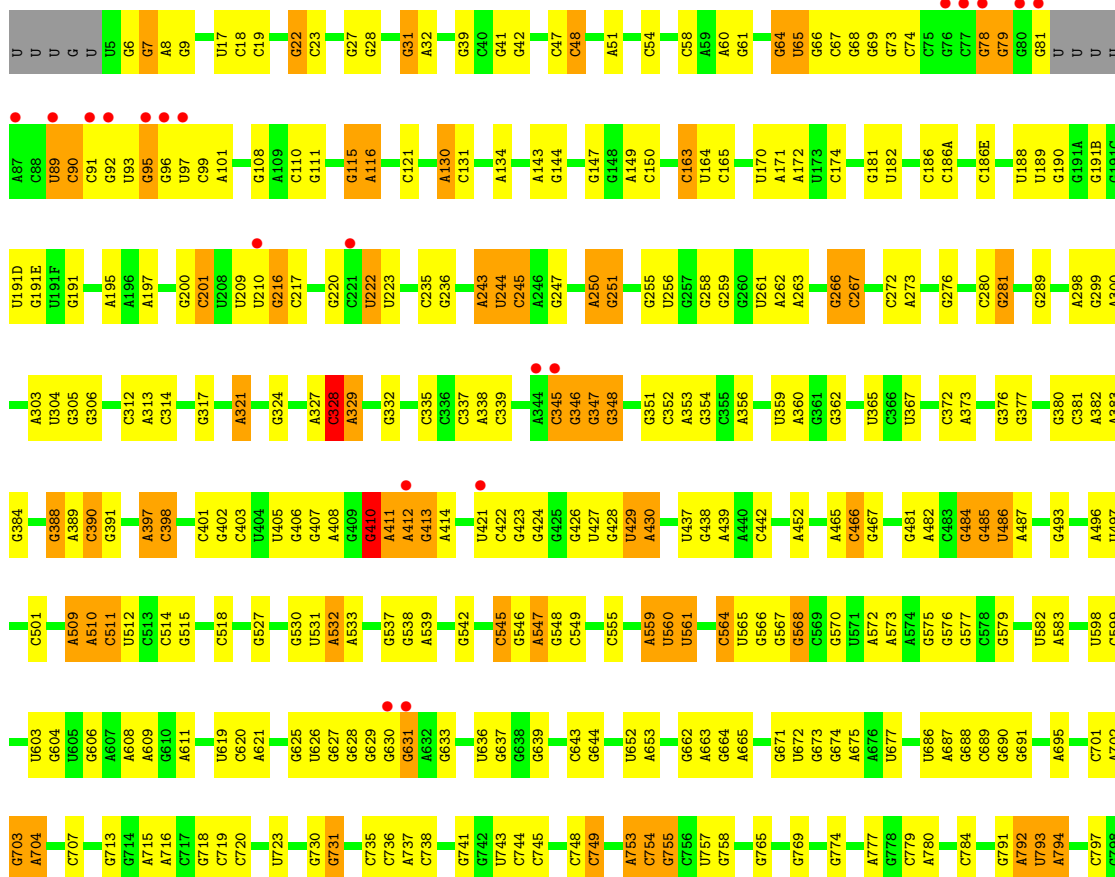
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	Y9	1	Total	Zn	0	0
			1	1		
59	QN	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		
59	R5	1	Total	Zn	0	0
			1	1		
59	QD	1	Total	Zn	0	0
			1	1		
59	XD	1	Total	Zn	0	0
			1	1		

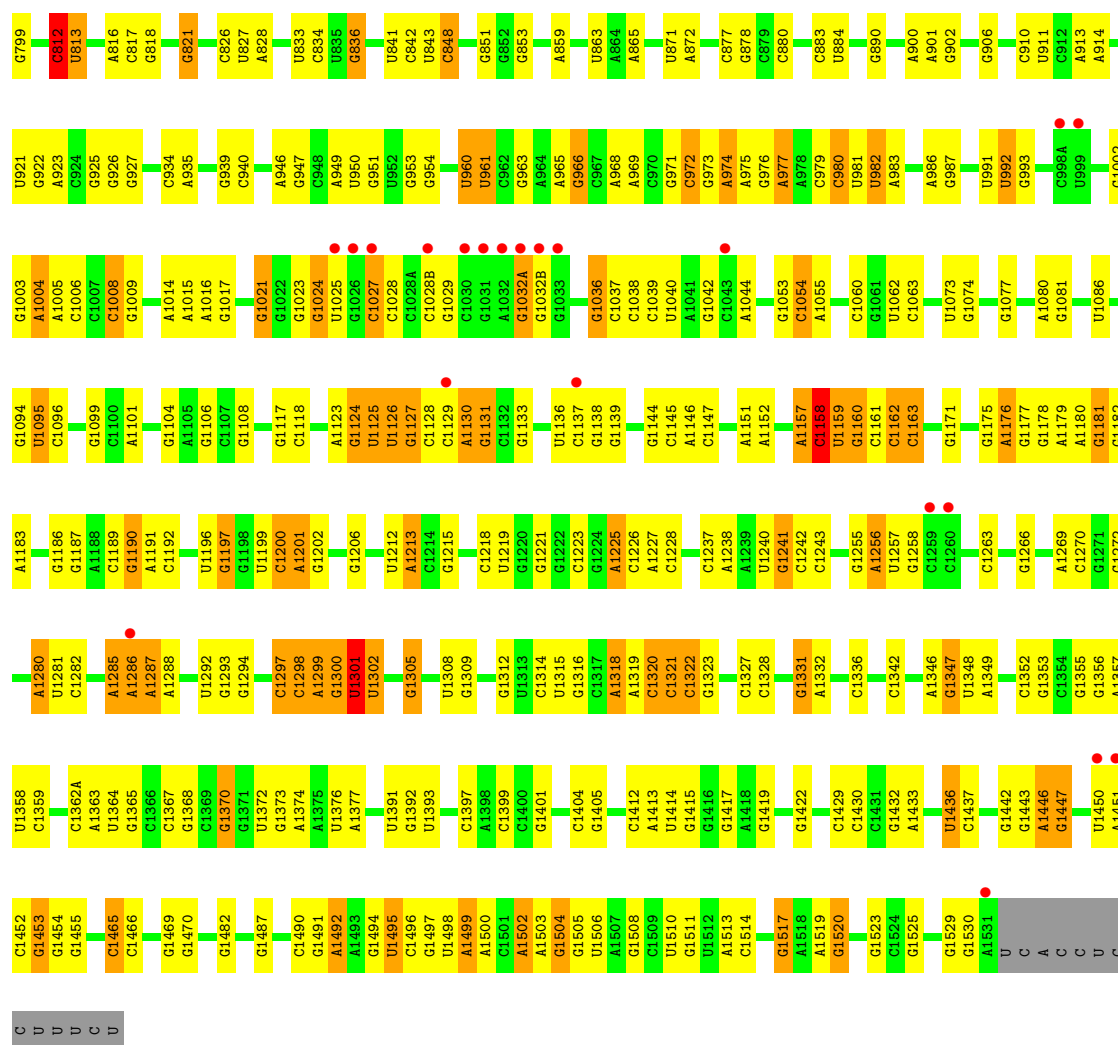
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 16S ribosomal RNA

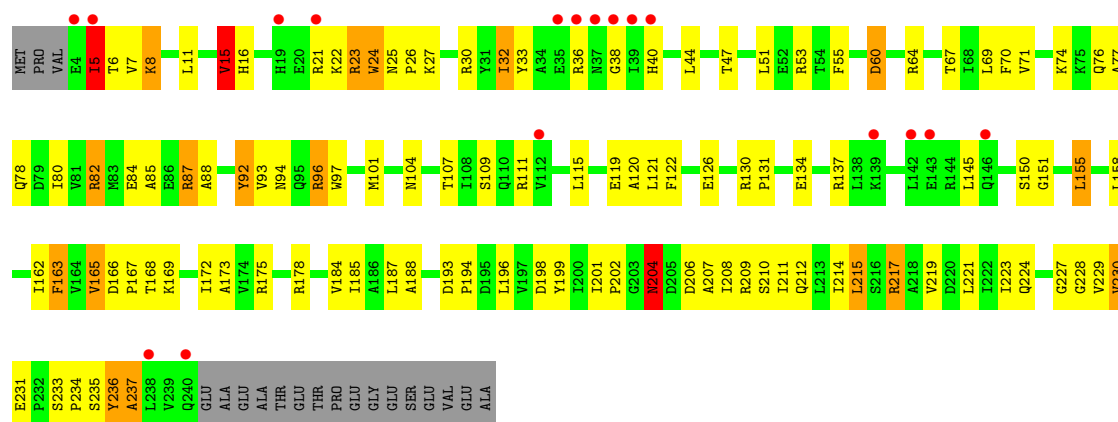






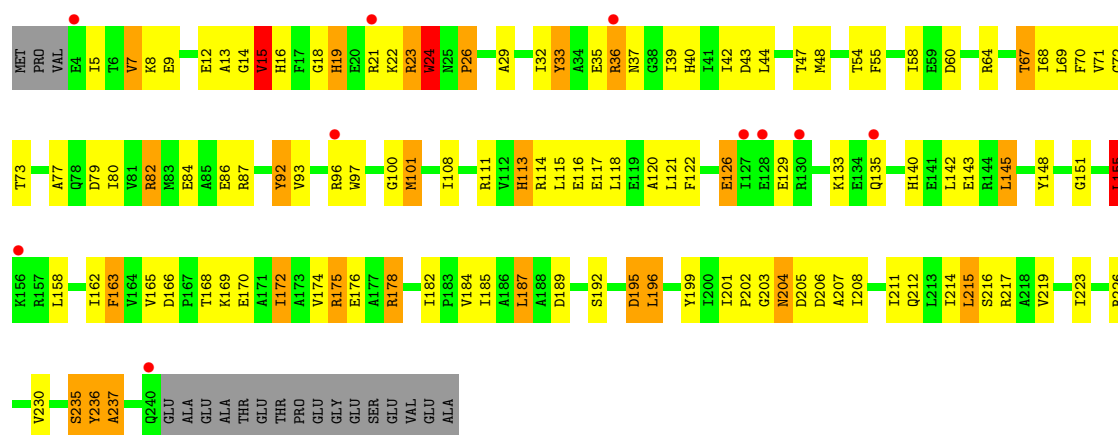
• Molecule 2: 30S ribosomal protein S2

Chain QB:



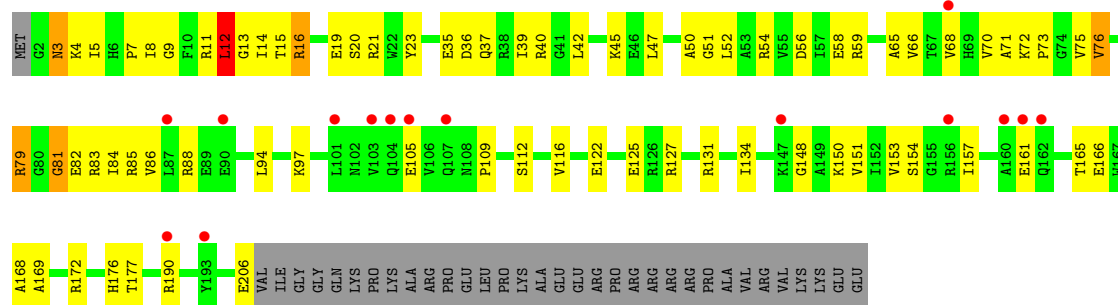
• Molecule 2: 30S ribosomal protein S2

Chain XB:



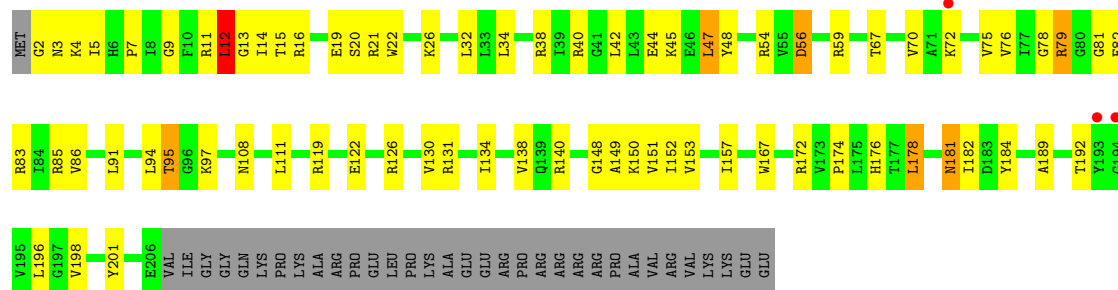
• Molecule 3: 30S ribosomal protein S3

Chain QC:



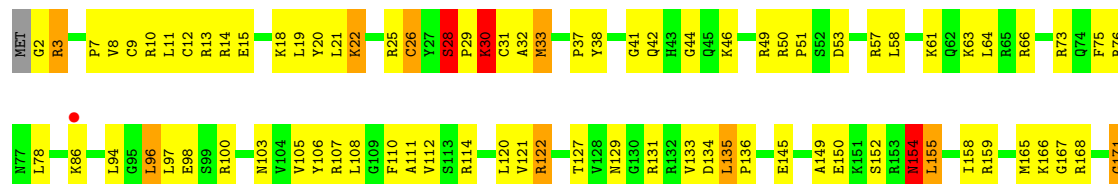
• Molecule 3: 30S ribosomal protein S3

Chain XC:



• Molecule 4: 30S ribosomal protein S4

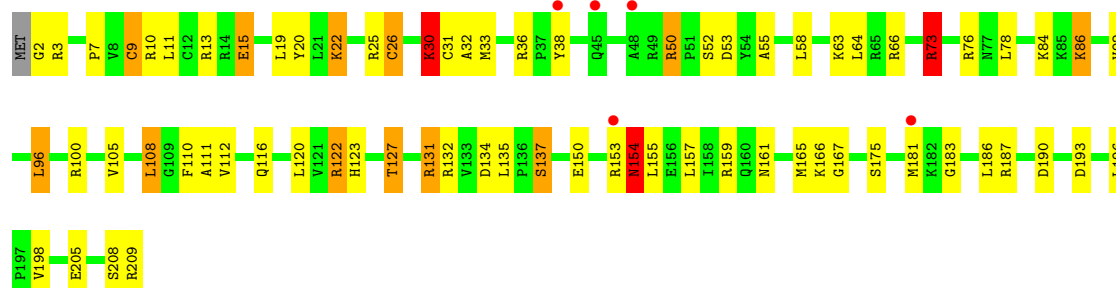
Chain QD:





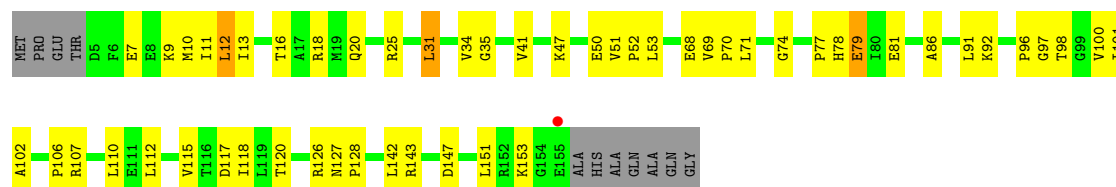
• Molecule 4: 30S ribosomal protein S4

Chain XD:



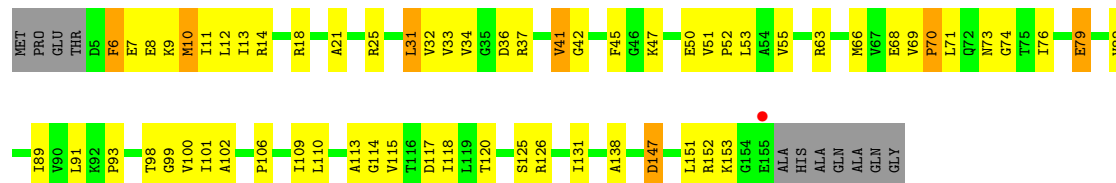
• Molecule 5: 30S ribosomal protein S5

Chain QE:



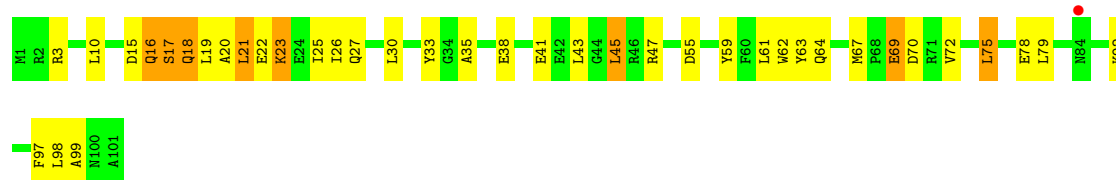
• Molecule 5: 30S ribosomal protein S5

Chain XE:



• Molecule 6: 30S ribosomal protein S6

Chain QF:



• Molecule 6: 30S ribosomal protein S6

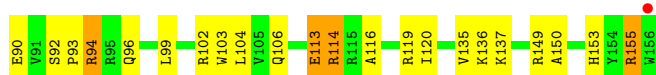
Chain XF:





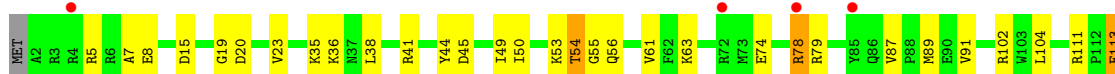
- Molecule 7: 30S ribosomal protein S7

Chain QG:



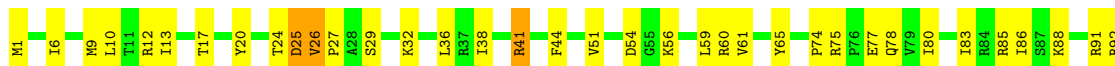
- Molecule 7: 30S ribosomal protein S7

Chain XG:



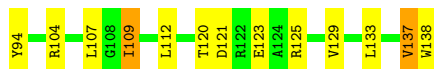
- Molecule 8: 30S ribosomal protein S8

Chain QH:



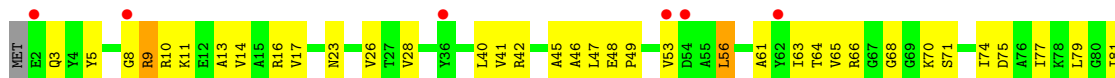
- Molecule 8: 30S ribosomal protein S8

Chain XH:



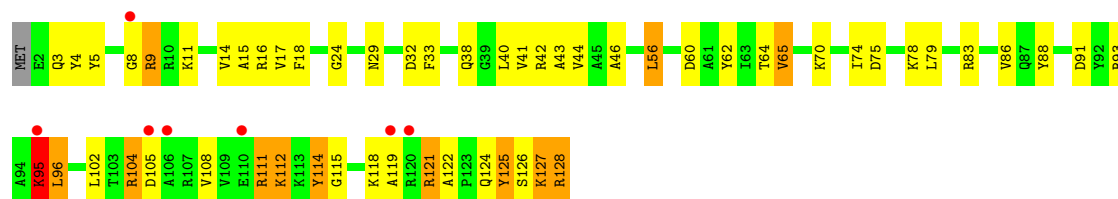
- Molecule 9: 30S ribosomal protein S9

Chain QI:



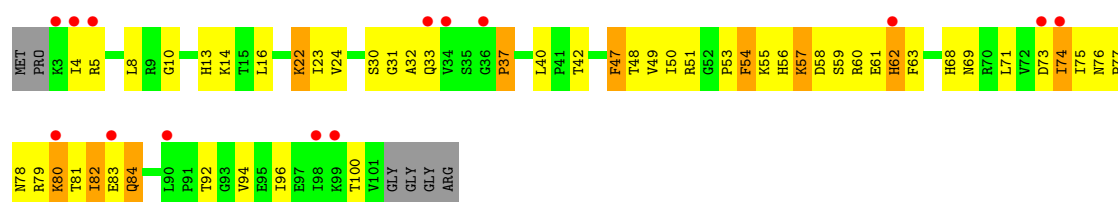
- Molecule 9: 30S ribosomal protein S9

Chain XI:



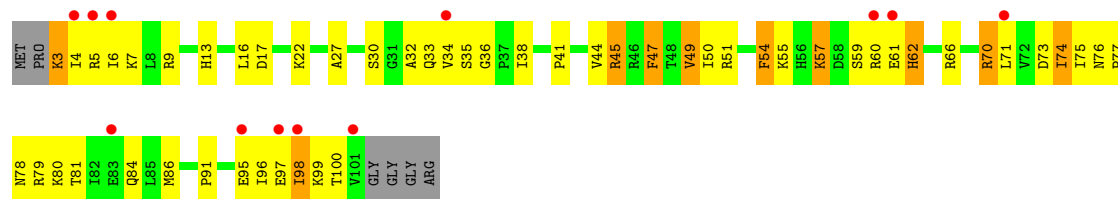
- Molecule 10: 30S ribosomal protein S10

Chain QJ:



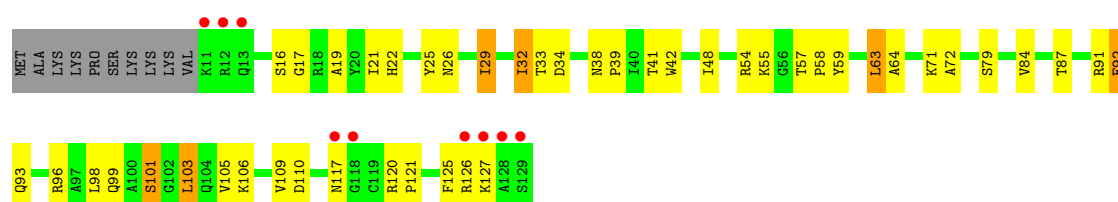
- Molecule 10: 30S ribosomal protein S10

Chain XJ:



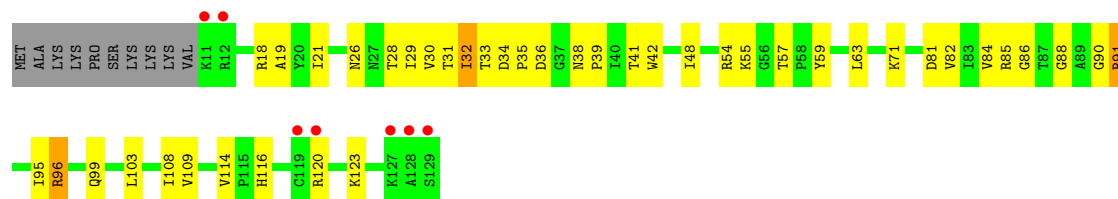
- Molecule 11: 30S ribosomal protein S11

Chain QK:



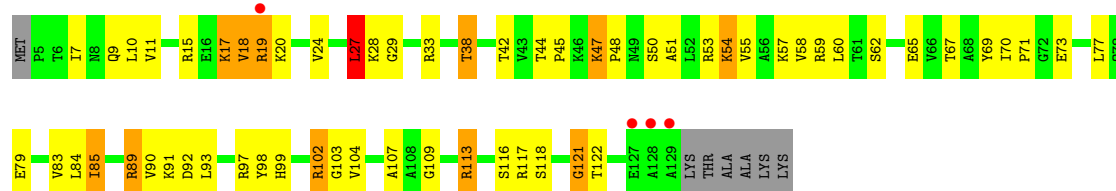
- Molecule 11: 30S ribosomal protein S11

Chain XK:



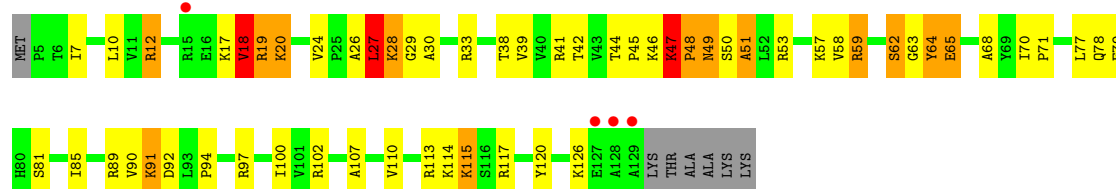
- Molecule 12: 30S ribosomal protein S12

Chain QL:



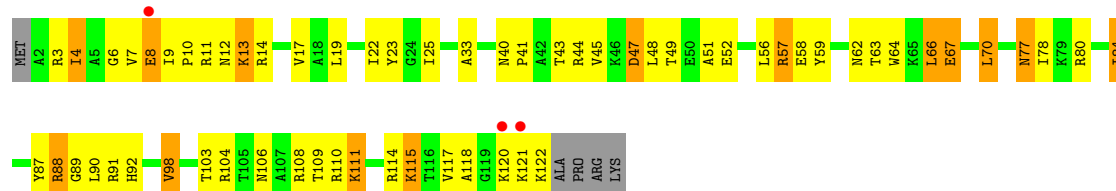
- Molecule 12: 30S ribosomal protein S12

Chain XL:



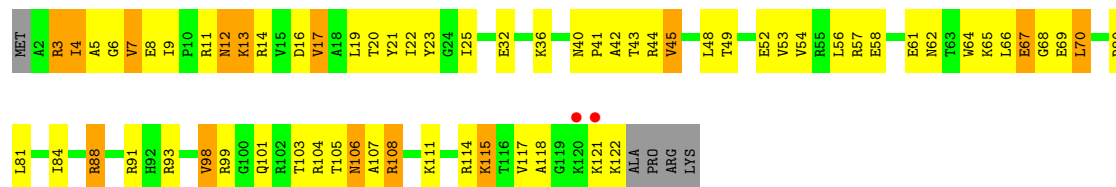
- Molecule 13: 30S ribosomal protein S13

Chain QM:



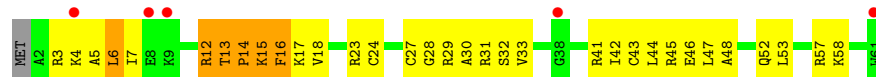
- Molecule 13: 30S ribosomal protein S13

Chain XM:



- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:



- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:



- Molecule 15: 30S ribosomal protein S15

Chain QO:



- Molecule 15: 30S ribosomal protein S15

Chain XO:



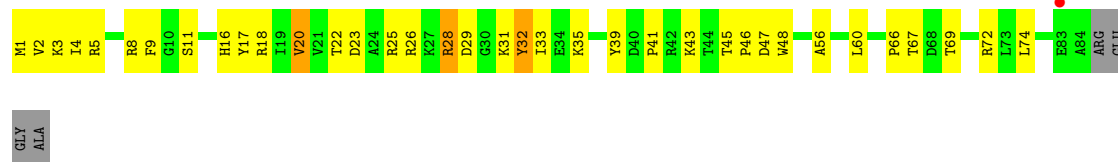
- Molecule 16: 30S ribosomal protein S16

Chain QP:



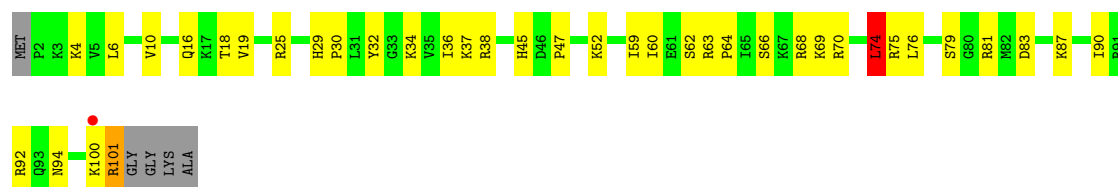
- Molecule 16: 30S ribosomal protein S16

Chain XP:



- Molecule 17: 30S ribosomal protein S17

Chain QQ:



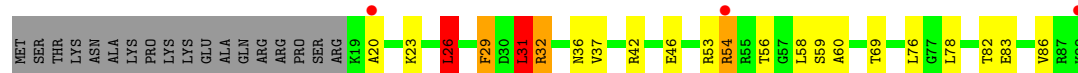
- Molecule 17: 30S ribosomal protein S17

Chain XQ:



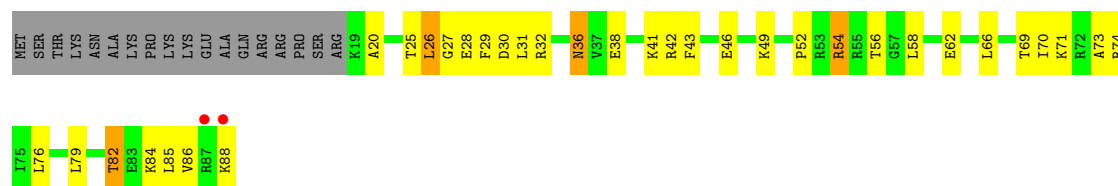
- Molecule 18: 30S ribosomal protein S18

Chain QR:



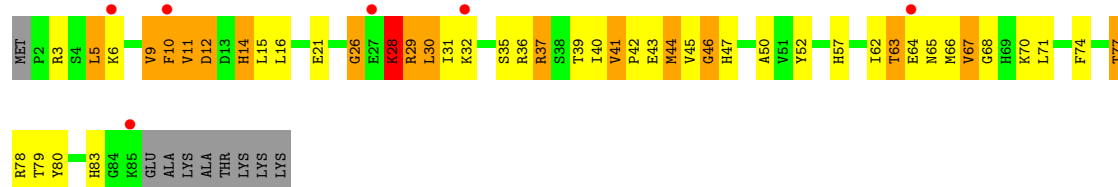
- Molecule 18: 30S ribosomal protein S18

Chain XR:



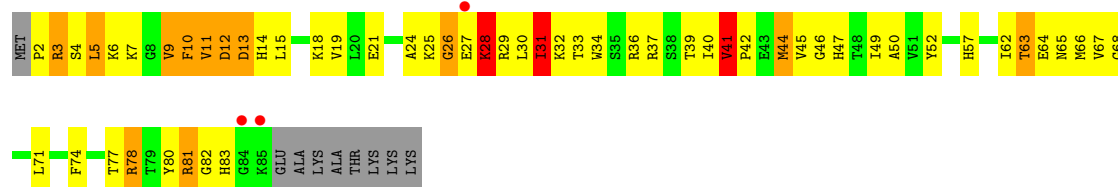
- Molecule 19: 30S ribosomal protein S19

Chain QS:



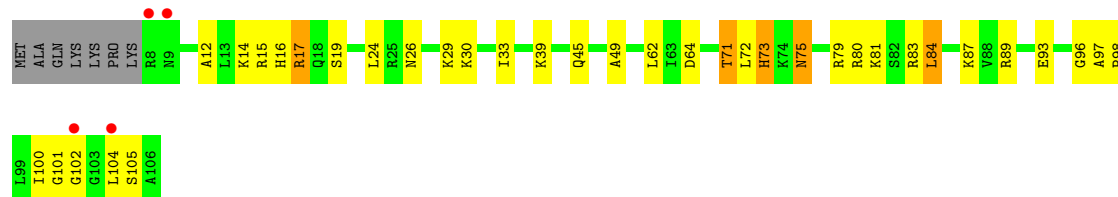
- Molecule 19: 30S ribosomal protein S19

Chain XS:



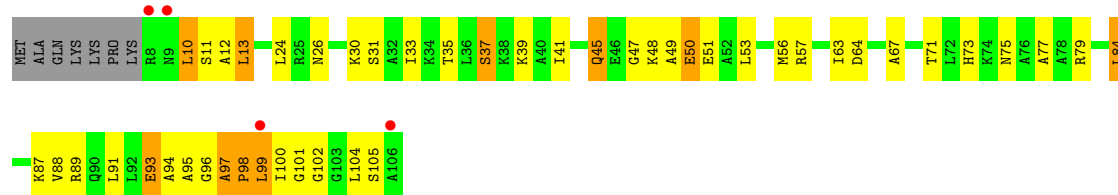
- Molecule 20: 30S ribosomal protein S20

Chain QT:



- Molecule 20: 30S ribosomal protein S20

Chain XT:



- Molecule 21: 30S ribosomal protein Thx

Chain QU:



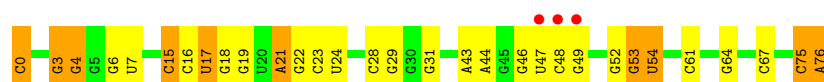
- Molecule 21: 30S ribosomal protein Thx

Chain XU:



- Molecule 22: tRNA-fMet

Chain QV:



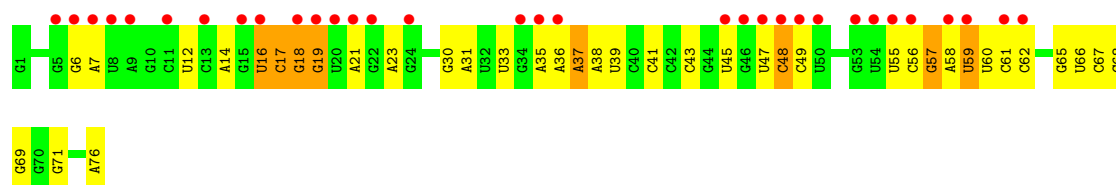
- Molecule 22: tRNA-fMet

Chain XV:



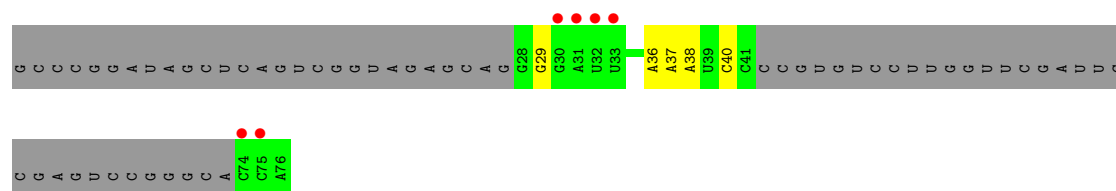
- Molecule 23: E-Site tRNA-Phe or A-Site tRNA-Phe

Chain QW:



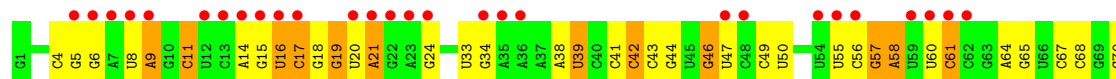
- Molecule 23: E-Site tRNA-Phe or A-Site tRNA-Phe

Chain QY:



- Molecule 23: E-Site tRNA-Phe or A-Site tRNA-Phe

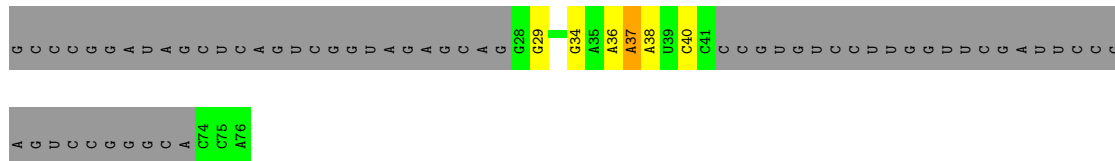
Chain XW:





- Molecule 23: E-Site tRNA-Phe or A-Site tRNA-Phe

Chain XY:



- Molecule 24: mRNA

Chain QX:



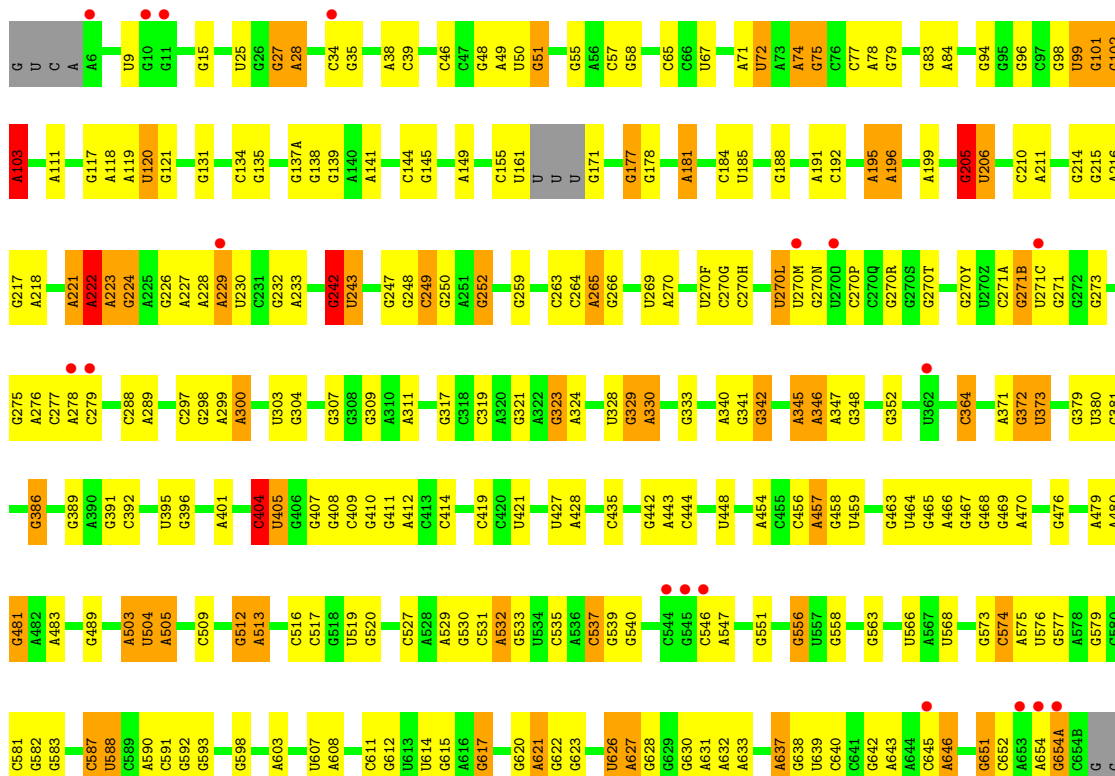
- Molecule 24: mRNA

Chain XX:



- Molecule 25: 23S ribosomal RNA

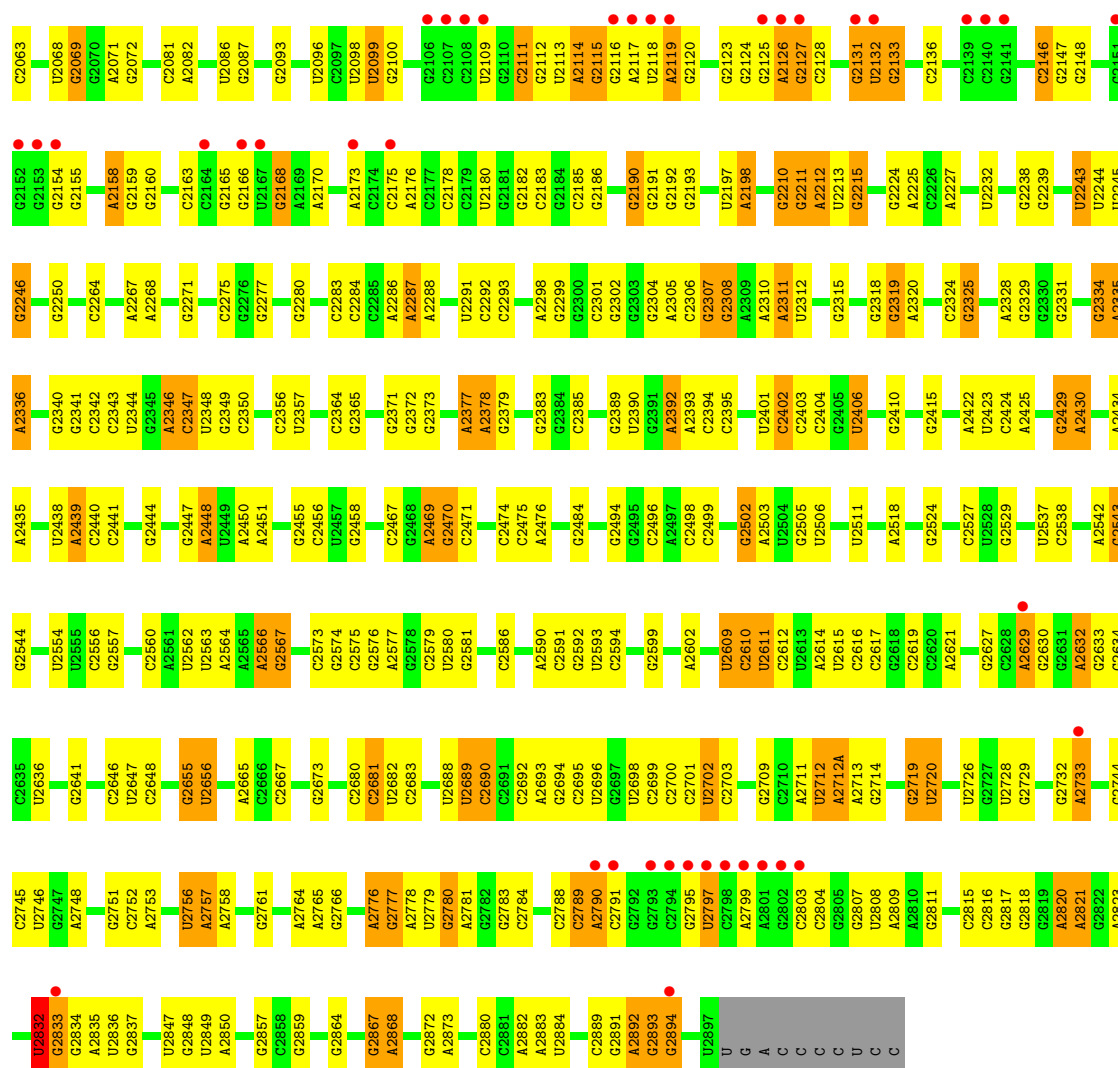
Chain RA:



A2054	C2055	U1955	A1698	C1585	A1471	C1370	A1272	C1178	G1092	G1022	A933	A849	G748	G
C2056	U1962	C1962	G1725	A1586	G1479	G1371	U1273	C1179	G1093	U1023	A941	C856	C755	C
A2057	U1963	G1828	G1726	G1591	G1480	A1372	A1278	C1180	A1094	G1024	G942	C857	C756	C
A2058	A1829	U1492	G1728	G1592	U1482	A1373	G1278	G1183	A1095	G1025	G943	U858		C
A2059	G1835	G1729	U1730	G1593	G1483	A1378	A1287	G1184	A1096	U1026	G944	G859	G760	A
A2060	C1836	U1731	G1485	G1594	G1484	A1379	U1288	G1187	A1097	A1027	G945	U860	A761	C
A2062	G1837	G1732	G1486	G1595	G1485	G1380	C1291	U1188	A1098	A1028	G946	A861		G
U2068	A1847	G1733	G1487	C1598	G1490	A1384	U1292	A1189	A1099	A1029	G947	G862	A764	C
G2069	A1848	G1734	G1488	A1603	G1491	A1385	C1293	G1190	C1100	U1033	G948	A863		G
G2070	G1492	C1386	G1489	G1493	G1492	C1386	G1296	G1191	A1103	G1043	C955	A866	G768	G
A2071	G1743	U1394	A1494	C1297	A1494	U1394	C1297	G1195	C1104	C1044	C956	C867	A774	C
U2086	G1752	A1608	A1495	C1298	A1495	C1403	G1298	G1201	G1107	A1045	U988	U868	G775	C
G2087	G1753	A1609	A1496	G1299	A1496	C1403	G1299	G1202	U1108	A1046	A959	A870	G776	G654S
G2093	C1754	A1610	U1497	U1300	U1497	G1407	U1301	G1203	C1109	G1047	C961	U871	A782	C854T
U2099	A1755	A1614	C1498	A1301	C1498	C1408	A1301	G1204	G1110	A1050	G974	A872	A783	G662
G2100	U1757	C1615	C1505	A1308	C1505	C1411	A1308	U1205	G1111	G1051	C974A	A878	G785	G663
G2101	G1758	A1616	C1506	G1309	C1506	A1412	G1309	U1206	U1112	C1052	G975	G879	G786	G664
C1994	A1871	C1617	A1507	G1310	A1507	G1413	G1310	G1209	G1113	C1053	G978	G880	U787	C665
U1995	G1872	A1618	A1508	G1311	A1508	G1413	U1312	G1210	G1114	G1054	G979	G881	A788	G668
C1996	G1878	C1509	C1509	U1312	C1509	G1416	U1312	A1210	G1122	G1055	A980	G882	A789	G669
C2107	G1622	A1510	A1510	C1314	A1510	C1417	C1314	U1211	G1125	A1056		G883	C790	A670
C2110	C1636	U1514	U1514	G1315	U1514	G1418	C1315	A1220	A1126	A1057	A983	C884	A793	C672
G2111	A1637	A1515	A1515	G1316	A1515	A1419	G1316	C1221	G1137	G1058	A984	C885	C673	C671
G2112	C1638	G1519	G1519	A1317	G1519	U1420	A1317	G1226	U1138	U1060	C993	C886	G674	C675
U2011	U1639	U1421	G1421	G1421	U1421	A1427	G1421	G1227	G1139	A1067	C995	C887	C797	A675
G2012	G1640	G1522	G1522	A1321	G1522	C1428	A1321	G1228	U1141	G1062	A986	C888	A802	A676
A2015	A1641	G1527	G1527	A1322	G1527	G1429	A1322	G1231	C1136	C1063	A988	C889		G686
U2016	C1642	G1533	G1533	C1329	G1533	C1430	C1329	G1232	G1137	U1065	G993	G892	G805	C693
U2017	G1646	U1534	U1534	U1330	U1534	G1431	G1330	G1233	U1142	U1066	C994	C893	C806	
G2018	G1647	A1535	A1535	A1331	A1535	U1431	A1331	G1236	G1140	A1067	C995	C894	U807	
A2019	G1648	G1536	G1536	G1332	G1536	G1441	G1332	A1237	U1141	G1068	A996	H895	G808	G700
C2021	G1649	G1537	G1537	A1336	G1537	G1442	A1336	G1238	U1142	A1069	C997	A896	G701	G702
U2022	G1653	G1538	G1538	G1337	G1538	G1443	G1337	G1244	A1142A	G1070	A1000	C897	U811	
G2023	A1654	G1542	G1542	G1338	G1542	G1444	G1338	G1245	G1149	C1072	G1003	C898	U812	A705
A2030	A1664	G1543	G1543	U1341	G1543	C1445	U1341	G1252	G1150	A1073	G1004	A899	U813	A706
A2031	G1667	A1544	A1544	U1341	A1544	G1449	U1341	A1253	G1151	G1074	C1005	A901	C814	G707
G2032	G1674	C1547	C1547	G1348	C1547	G1449A	G1348	G1254	C1152	C1075	G1006	C904	G818	C708
A2033	C1675	C1548	C1548	A1349	C1548	U1454	A1349	U1255	G1153	A1077	C1007	A819	U709	G710
G2037	A1676	A1558	A1558	A1353	A1558	G1455	A1353	G1256	G1154	U1078	A1009	U907	A820	
G2038	A1677	G1559	G1559	U1357	G1559	G1455	U1357	G1259	A1155	C1079	A1010	U827	G717	G717
C2043	G1678	U1569	U1569	A1358	U1569	C1458	A1358	G1260	U1165	U1081	G1011	A910	U828	C721
G2046	U1688	A1569	A1569	A1359	A1569	G1459	A1359	G1264	C1166	U1082	G1012	A917	U833	A722
C2050	A1690	C1577	C1577	C1363	C1577	A1460	C1363	G1265	G1169	U1083	C1013	A918	G723	A722
U2051	G1693	U1578	U1578	G1461	U1578	G1461	G1364	G1266	G1171	A1084	U1014	A918	U724	G725
G2140	U1698	A1579	A1579	G1467	A1579	C1467	A1365	U1267	G1173	A1086	G1015	G921	U839	G725
C2143	C1694	G1581	G1581	C1468	G1581	G1468	A1366	A1268	A1174	G1087	G1016	U922	C840	
	G1695	U1580	U1580	G1469	U1580	G1469	A1367	C1270	U1175	A1088	G1017	C923	A841	C730
				G1470		G1470	G1368	G1271	G1176	G1089	U1019	G929	C846	U740
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												G932	G848	

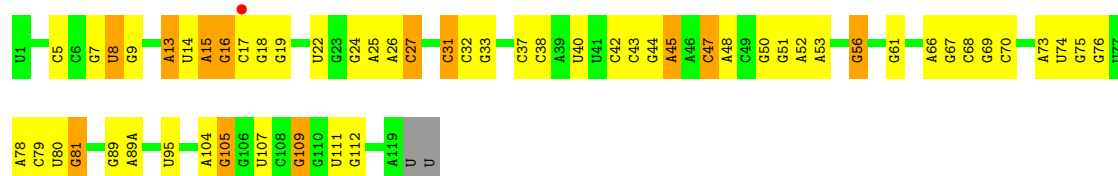


G1968	G1850	G1756	C1646	A1536	C1428	A1342	G1231	C1135	U1061	A980	A887	A802	G686	G622
A1969	G1850	A1759	G1647	C1537	A1434	G1343	C1232	G1136	G1062	A981	C888	A802	G686	G622
A1970	G1858	A1762	C1648	G1538	A1434	G1344	C1233	G1137	C889	C982	C889	A805	G690	G625
A1972	G1864	G1763	G1649	U1541	A1444A	G1348	U1234	G1138	U1066	A983	G592	G806	C691	A627
G1973	G1869	G1764	G1650	G1542	C1445	A1349	G1236	C1140	A1067	G887	C893	U807	G704	G628
G1980	C1870	A1652	A1543	G1543	A1449	U1352	G1238	U1141	G1068	A990	C894	G808	G715	G629
A1981	G1653	C1544	G1653	C1544	A1449A	A1353	U1239	U1142	A1069	C990	U895	C812	A716	A630
C1982	A1654	A1545	A1654	A1545	G1449A	A1354	U1240	A1142A	G1071	C991	C897	U813	C991	A631
G1983	G1657	U1775	C1657	C1547	U1454	U1357	G1248	G1149	G1072	G983	C898	C814	G717	A632
A1984	C1658	G1776	C1658	U1547	G1455	U1357	G1248	G1149	C1073	C994	C899	C814	A722	A633
G1985	U1659	A1554	C1659	A1554	G1455	G1358	U1248	C1153	A1074	C995	A900	C817	A722	G636
G1989	C1660	A1558	C1660	A1558	C1458	A1359	A1253	G1154	C1075	A996	A901	C818	G723	G636
U1990	A1664	G1559	A1664	G1559	A1460	A1360	U1254	U1165	C1076	A996	U907	A819	U724	A637
U1991	A1668	G1567	A1668	G1567	G1461	G1364	G1256	C1166	A1077	A1000	G906	U826	G726	U639
C1992	G1674	A1570	G1674	A1570	G1461	A1365	U1266	G1166	U1078	A1000	U907	U826	G726	C640
C1996	G1678	A1578	G1678	A1578	C1464	A1366	G1264	G1169	C1079	G1003	U910	U827	G729	C645
G2010	U1679	A1578	U1679	A1578	G1472	A1367	A1266	G1170	U1080	C1004	A910	U828	C730	A646
G2012	U1680	A1580	U1680	A1580	G1473	G1368	G1266	G1171	U1082	C1005	A911	G831	C731	G651
A2015	U1688	C1585	U1688	C1585	G1479	G1369	C1270	G1173	U1083	C1006	C914	G832	C732	G652
A2019	A1689	C1586	A1689	C1586	U1480	C1370	U1271	A1174	A1084	C1007	C915	U833	C733	A734
C2021	C1694	A1587	C1694	A1587	G1482	G1371	G1271	U1175	A1085	G1011	G918	U833	A734	A652
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G2023	A1697	C1589	G1697	C1589	G1473	A1373	U1273	G1177	A1087	A917	A918	C840	G741	A654
A1919	A1802	C1592	A1698	C1592	G1479	G1374	A1278	C1178	A1088	U1014	U922	G842	A746	G654A
C2025	G1699	A1803	G1699	G1595	U1497	U1391	G1296	U1188	A1096	G1024	G938	C848	C755	A
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C2042	A1937	G1826	U1730	A1610	A1510	U1406	U1313	A1204	U1105	U1035	G946	G862	G780	G654S
A1938	G1731	G1826	G1731	A1611	A1511	C1407	U1316	G1206	G1106	G1036	G954	C863	G780	U657
U1939	A1732	A1614	C1409	A1614	U1514	C1408	A1317	G1206	C1109	A1045	G957	C863	A782	C658
G1939	G1733	C1615	C1409	C1615	U1514	C1409	A1317	G1206	G1110	A1046	U957	C863	A782	C659
U1950	C1742	A1616	C1411	C1617	U1520	C1411	A1321	A1210	A1111	A1046	U958	C874	A784	G661
G2052	U1834	G1743	G1522	A1618	G1522	G1416	U1329	G1212	G1113	G1047	C961	G875	C786	C661
A2054	G1835	G1746	G1522	A1618	G1522	C1417	A1330	G1212	G1114	A1050	C961	G875	C786	C661
C2055	C1836	G1622	A1528	G1622	A1528	G1417	G1332	A1220	G1114	C1053	G968	A878	A789	G669
U1955	G1837	G1747	A1528	G1622	A1528	C1418	G1332	A1220	G1122	G1055	U969	C881	C790	A670
G2056	C1838	G1748	G1530	U1639	A1529	U1419	A1336	G1223	G1125	A1056	G974	C882	C792	C671
U1963	U1839	A1749	G1530	U1639	A1529	U1419	A1336	G1223	G1125	G1056	G974	C882	C792	C672
A2059	G1750	C1640	G1533	A1641	C1533	G1421	G1337	G1225	U1130	A1057	C974A	C883	A793	G674
G1964	C1843	G1642	C1533	A1641	C1533	G1421	G1338	G1226	U1130	G1058	G975	C884	A793	G674
A2060	A1937	A1755	U1535	G1642	U1535	A1426	U1341	A1227	G1131	U1059	C979	C885	A676	A676
C2062	C1967	A1937	U1535	G1642	U1535	A1426	U1341	A1227	G1131	U1059	C979	C885	A676	A676



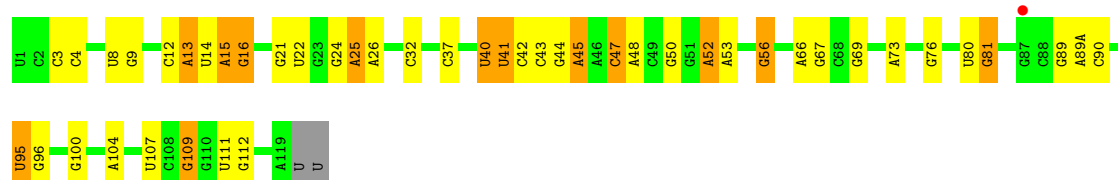
• Molecule 26: 5S ribosomal RNA

Chain RB:



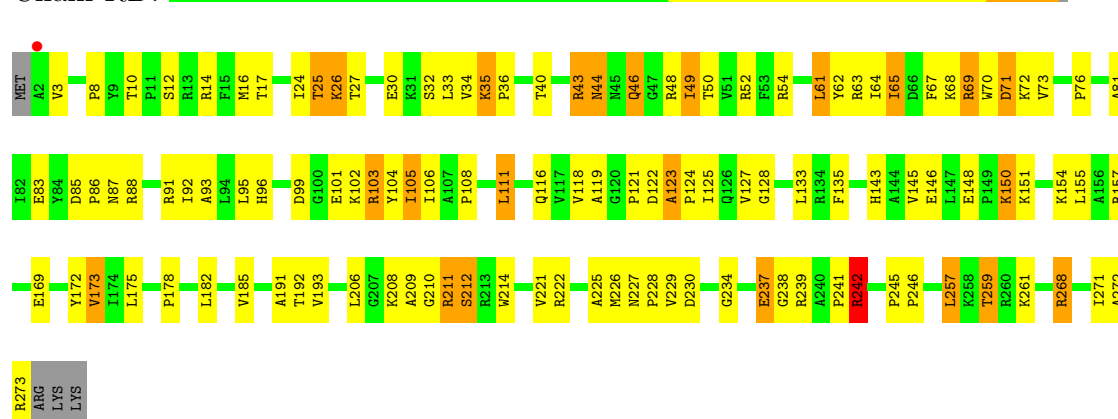
• Molecule 26: 5S ribosomal RNA

Chain YB:



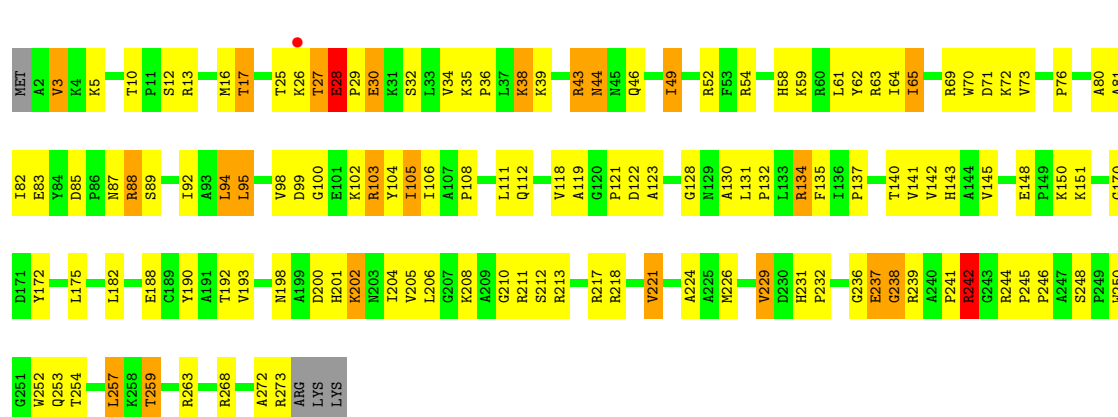
- Molecule 27: 50S ribosomal protein L2

Chain RD:



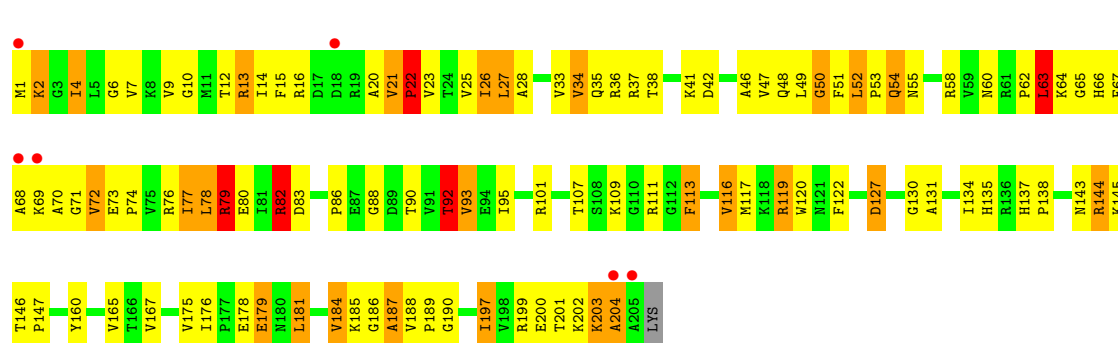
- Molecule 27: 50S ribosomal protein L2

Chain YD:



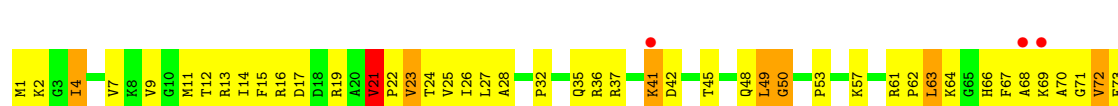
- Molecule 28: 50S ribosomal protein L3

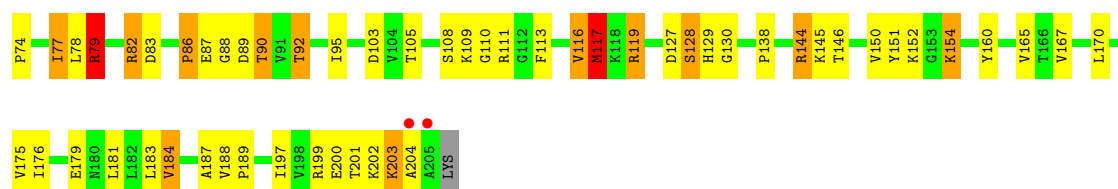
Chain RE:



- Molecule 28: 50S ribosomal protein L3

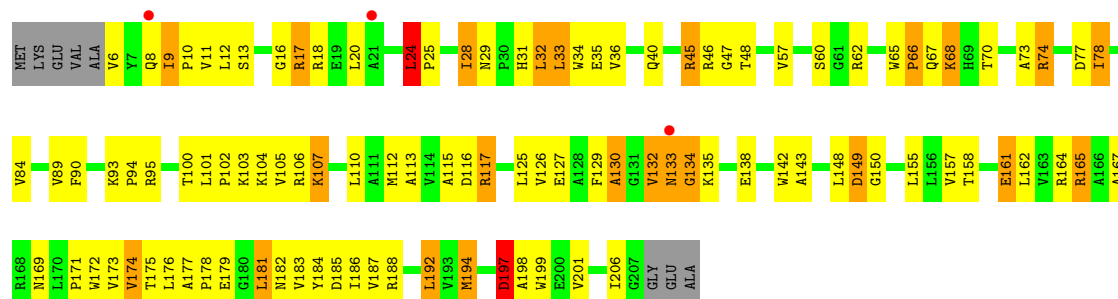
Chain YE:





- Molecule 29: 50S ribosomal protein L4

Chain RF:



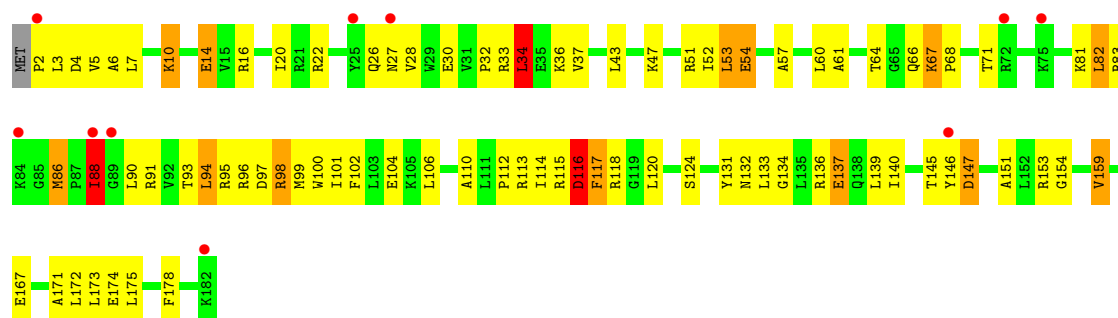
- Molecule 29: 50S ribosomal protein L4

Chain YF:



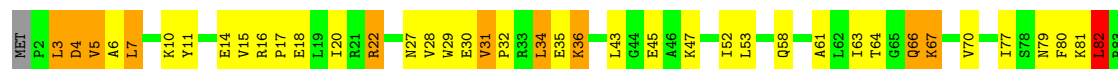
- Molecule 30: 50S ribosomal protein L5

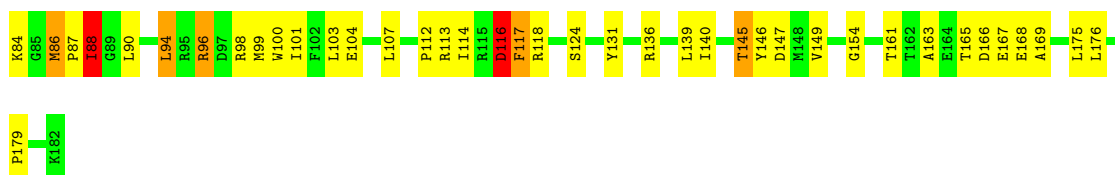
Chain RG:



- Molecule 30: 50S ribosomal protein L5

Chain YG:





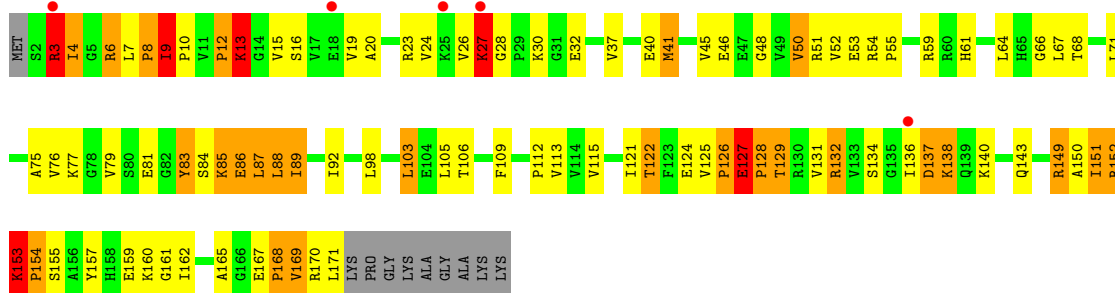
- Molecule 31: 50S ribosomal protein L6

Chain RH:



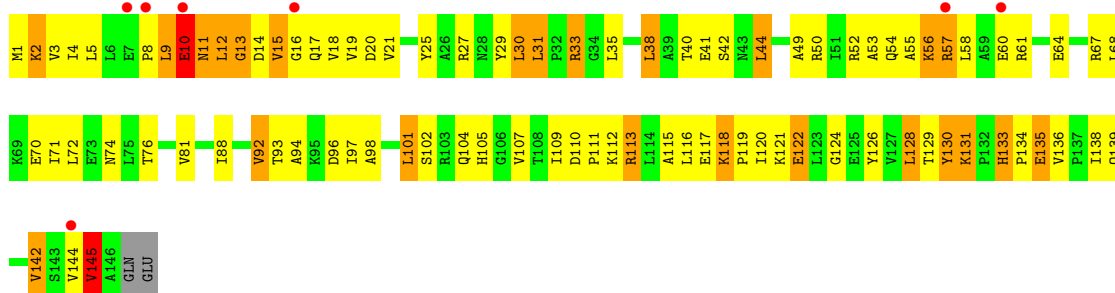
- Molecule 31: 50S ribosomal protein L6

Chain YH:



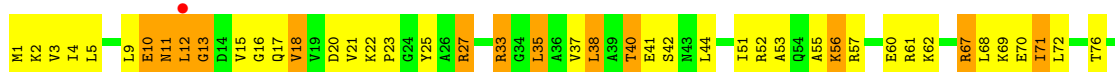
- Molecule 32: 50S ribosomal protein L9

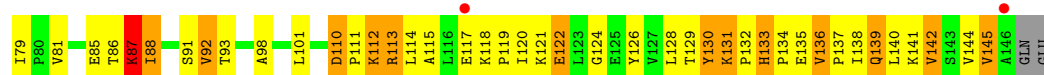
Chain RI:



- Molecule 32: 50S ribosomal protein L9

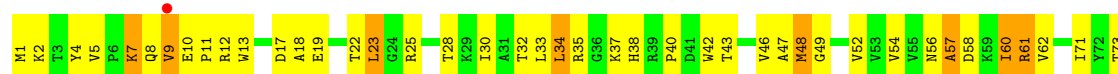
Chain YI:





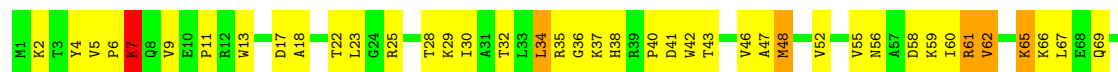
• Molecule 33: 50S ribosomal protein L13

Chain RN:



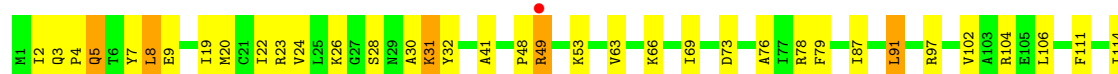
• Molecule 33: 50S ribosomal protein L13

Chain YN:



• Molecule 34: 50S ribosomal protein L14

Chain RO:



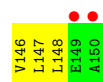
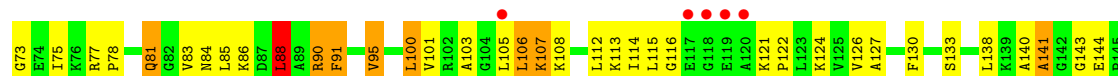
• Molecule 34: 50S ribosomal protein L14

Chain YO:



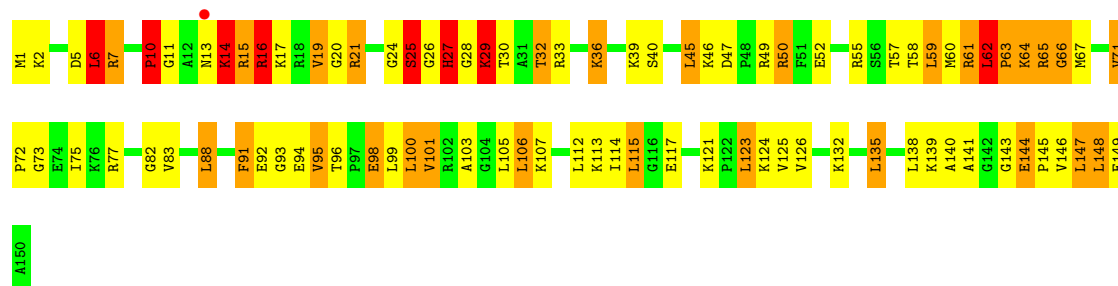
• Molecule 35: 50S ribosomal protein L15

Chain RP:



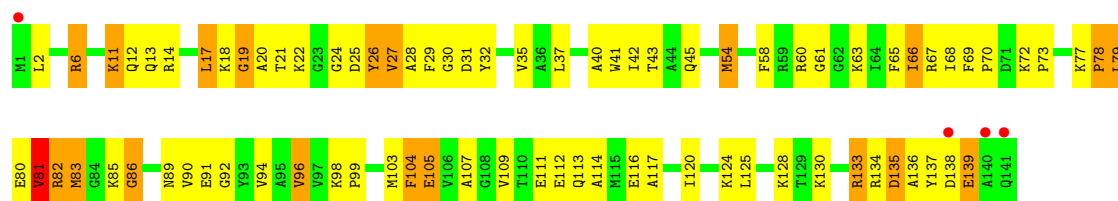
- Molecule 35: 50S ribosomal protein L15

Chain YP:



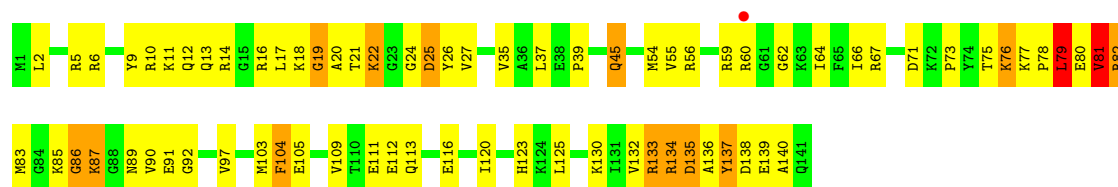
- Molecule 36: 50S ribosomal protein L16

Chain RQ:



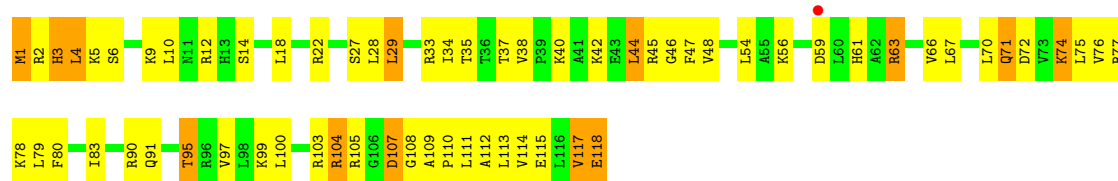
- Molecule 36: 50S ribosomal protein L16

Chain YQ:



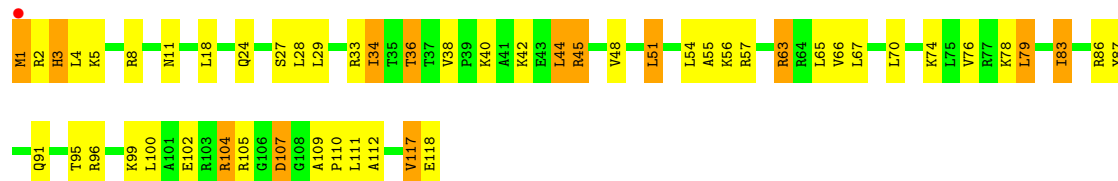
- Molecule 37: 50S ribosomal protein L17

Chain RR:



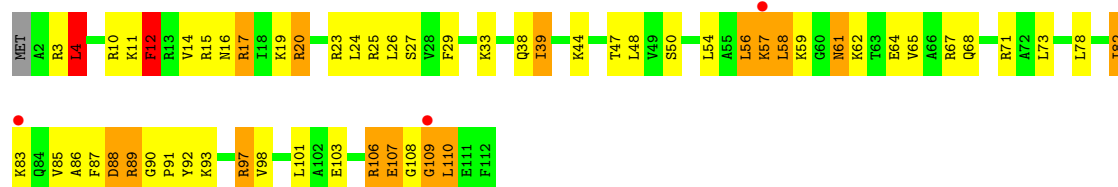
- Molecule 37: 50S ribosomal protein L17

Chain YR:



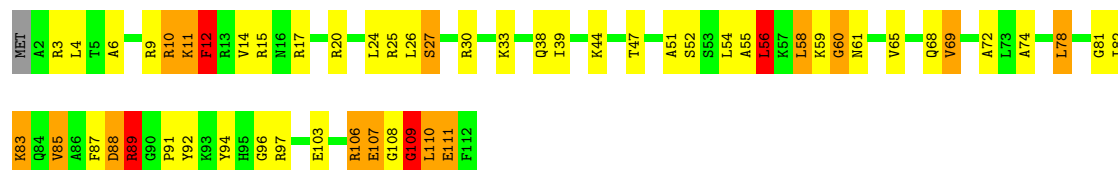
- Molecule 38: 50S ribosomal protein L18

Chain RS:



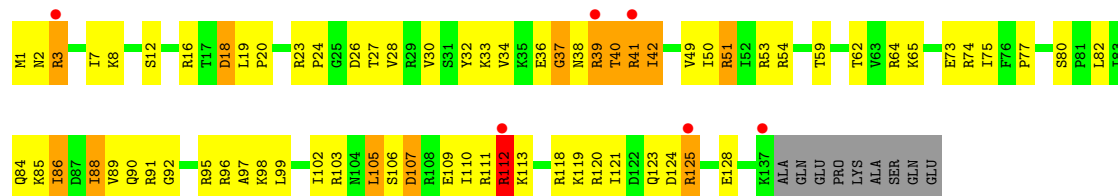
- Molecule 38: 50S ribosomal protein L18

Chain YS:



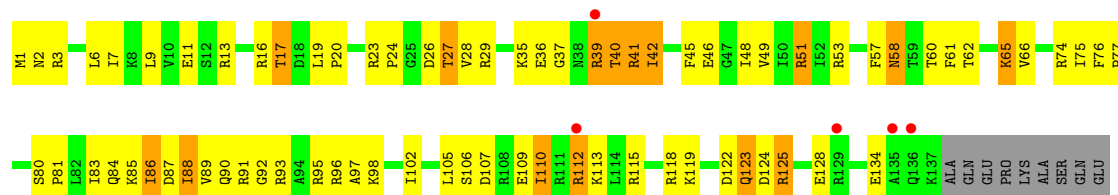
- Molecule 39: 50S ribosomal protein L19

Chain RT:



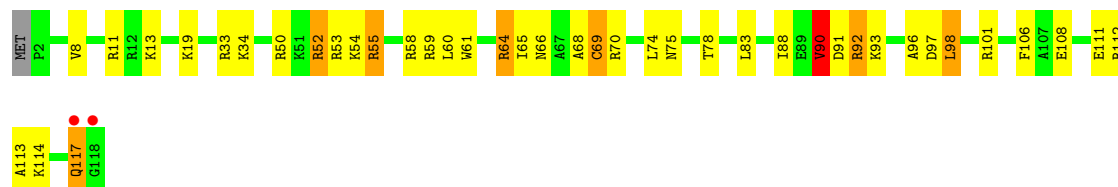
- Molecule 39: 50S ribosomal protein L19

Chain YT:



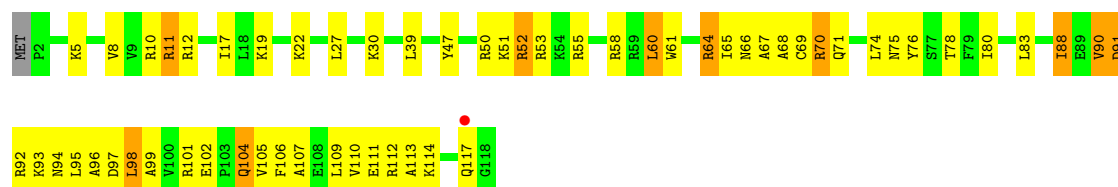
- Molecule 40: 50S ribosomal protein L20

Chain RU:



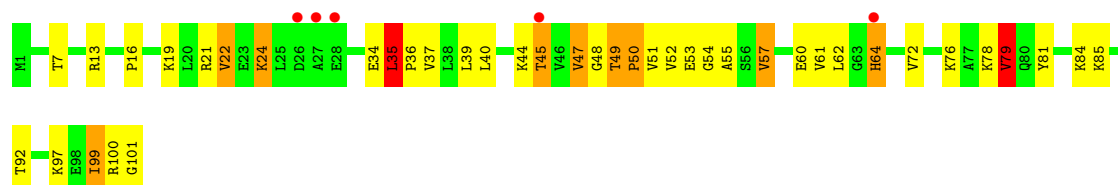
- Molecule 40: 50S ribosomal protein L20

Chain YU:



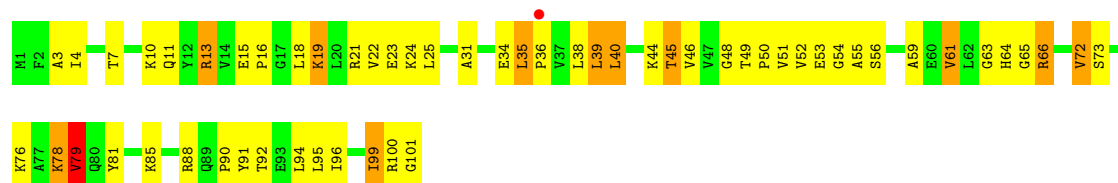
• Molecule 41: 50S ribosomal protein L21

Chain RV:



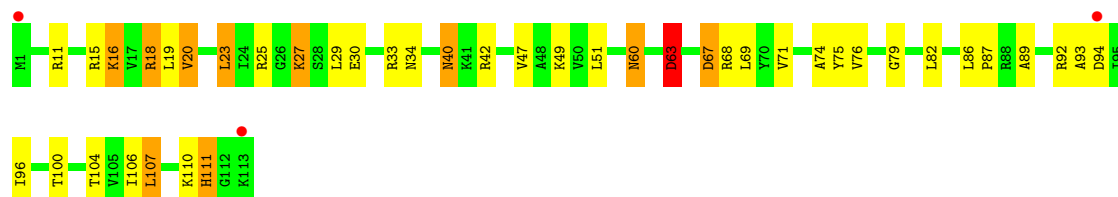
• Molecule 41: 50S ribosomal protein L21

Chain YV:



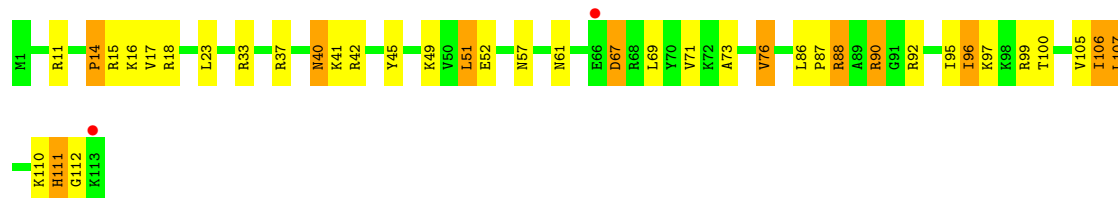
• Molecule 42: 50S ribosomal protein L22

Chain RW:



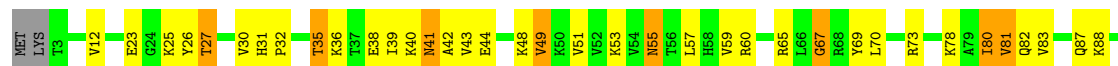
• Molecule 42: 50S ribosomal protein L22

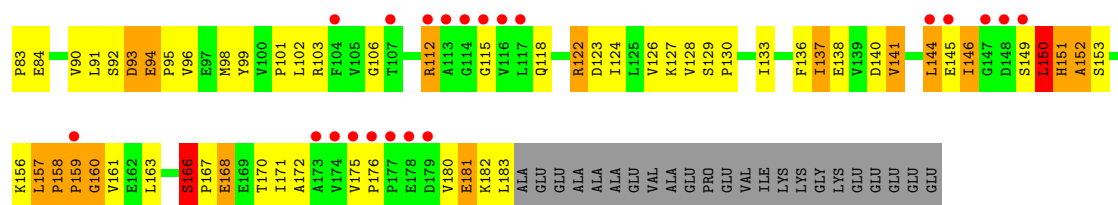
Chain YW:



• Molecule 43: 50S ribosomal protein L23

Chain RX:





- Molecule 46: 50S ribosomal protein L27

Chain R0:



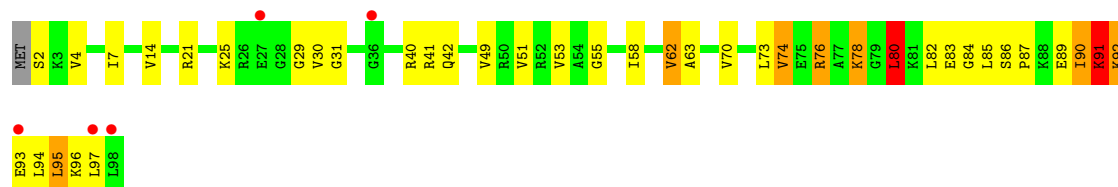
- Molecule 46: 50S ribosomal protein L27

Chain Y0:



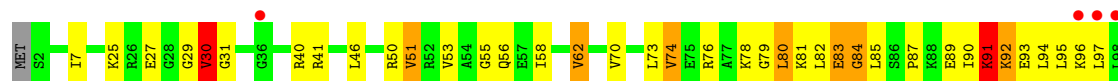
- Molecule 47: 50S ribosomal protein L28

Chain R1:



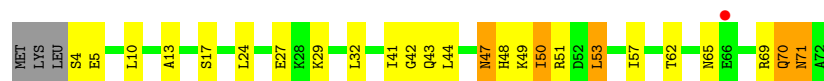
- Molecule 47: 50S ribosomal protein L28

Chain Y1:



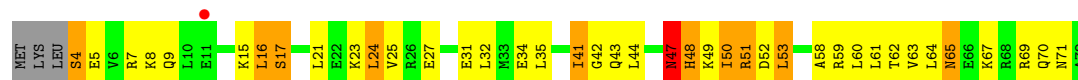
- Molecule 48: 50S ribosomal protein L29

Chain R2:



- Molecule 48: 50S ribosomal protein L29

Chain Y2:



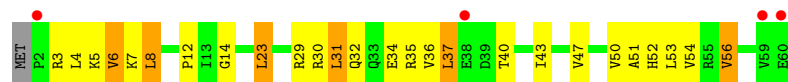
- Molecule 49: 50S ribosomal protein L30

Chain R3:



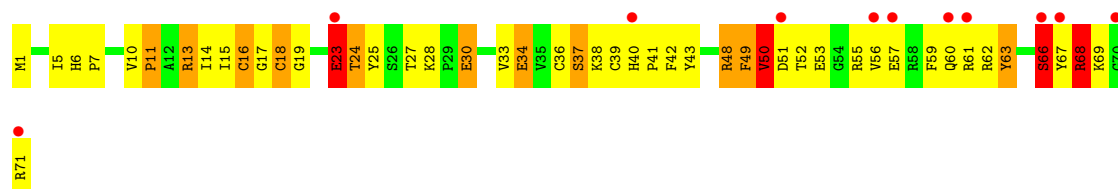
- Molecule 49: 50S ribosomal protein L30

Chain Y3:



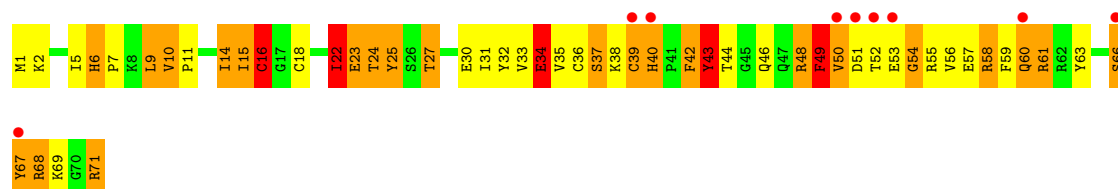
- Molecule 50: 50S ribosomal protein L31

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: 



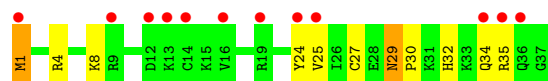
- Molecule 54: 50S ribosomal protein L35

Chain Y8: 



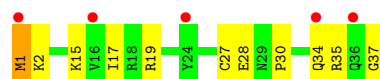
- Molecule 55: 50S ribosomal protein L36

Chain R9: 



- Molecule 55: 50S ribosomal protein L36

Chain Y9: 



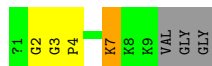
- Molecule 56: T17-GLY-GLY-PRO-LYS-LYS-LYS-LYS-LYS-VAL-GLY-GLY

Chain Z7: 



- Molecule 56: T17-GLY-GLY-PRO-LYS-LYS-LYS-LYS-LYS-VAL-GLY-GLY

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	209.24Å 443.46Å 618.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 3.60 34.94 – 3.61	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.79-3.60) 98.0 (34.94-3.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 3.66Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.222 , 0.254 0.223 , 0.254	Depositor DCC
R_{free} test set	28964 reflections (4.54%)	DCC
Wilson B-factor (Å ²)	104.1	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 56.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	0 of 638335 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	295487	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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, T17, PAR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	QA	0.23	0/36098	0.81	32/56341 (0.1%)
1	XA	0.24	0/36101	0.81	18/56346 (0.0%)
2	QB	0.31	0/1959	0.52	0/2642
2	XB	0.32	0/1959	0.54	0/2642
3	QC	0.32	0/1629	0.53	0/2195
3	XC	0.37	0/1629	0.56	0/2195
4	QD	0.45	0/1733	0.62	1/2318 (0.0%)
4	XD	0.39	0/1733	0.60	0/2318
5	QE	0.35	0/1171	0.56	0/1576
5	XE	0.39	0/1171	0.59	0/1576
6	QF	0.39	0/856	0.57	0/1154
6	XF	0.39	0/856	0.61	0/1154
7	QG	0.33	0/1276	0.50	0/1709
7	XG	0.34	0/1276	0.51	0/1709
8	QH	0.33	0/1136	0.55	0/1527
8	XH	0.38	0/1136	0.58	0/1527
9	QI	0.31	0/1029	0.55	0/1379
9	XI	0.34	0/1029	0.58	0/1379
10	QJ	0.33	0/814	0.54	0/1095
10	XJ	0.35	0/814	0.60	0/1095
11	QK	0.37	0/900	0.57	0/1213
11	XK	0.39	0/900	0.58	0/1213
12	QL	0.37	0/991	0.61	0/1327
12	XL	0.50	1/991 (0.1%)	0.77	2/1327 (0.2%)
13	QM	0.32	0/974	0.59	0/1303
13	XM	0.36	0/974	0.63	0/1303
14	QN	0.40	0/501	0.60	0/664
14	XN	0.42	0/501	0.66	0/664
15	QO	0.35	0/745	0.53	0/992
15	XO	0.39	0/745	0.54	0/992
16	QP	0.36	0/721	0.57	0/970
16	XP	0.35	0/721	0.57	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.35	0/847	0.53	0/1131
17	XQ	0.35	0/847	0.54	0/1131
18	QR	0.35	0/579	0.64	1/768 (0.1%)
18	XR	0.37	0/579	0.60	0/768
19	QS	0.33	0/689	0.60	0/926
19	XS	0.38	0/689	0.69	1/926 (0.1%)
20	QT	0.36	0/765	0.64	0/1007
20	XT	0.31	0/765	0.60	0/1007
21	QU	0.31	0/221	0.53	0/288
21	XU	0.32	0/221	0.61	0/288
22	QV	0.32	1/1836 (0.1%)	0.80	0/2859
22	XV	0.33	1/1836 (0.1%)	0.81	1/2859 (0.0%)
23	QW	0.19	0/1809	0.79	0/2819
23	QY	0.17	0/406	0.73	0/628
23	XW	0.20	0/1809	0.80	0/2819
23	XY	0.20	0/406	0.74	0/628
24	QX	0.19	0/235	0.71	0/364
24	XX	0.18	0/235	0.65	0/364
25	RA	0.26	0/69521	0.81	28/108529 (0.0%)
25	YA	0.29	0/69543	0.83	41/108563 (0.0%)
26	RB	0.26	0/2878	0.88	7/4490 (0.2%)
26	YB	0.29	0/2878	0.91	11/4490 (0.2%)
27	RD	0.51	0/2165	0.70	0/2919
27	YD	0.57	0/2165	0.77	1/2919 (0.0%)
28	RE	0.46	1/1601 (0.1%)	0.73	3/2160 (0.1%)
28	YE	0.48	1/1601 (0.1%)	0.74	2/2160 (0.1%)
29	RF	0.45	1/1620 (0.1%)	0.64	1/2194 (0.0%)
29	YF	0.48	0/1620	0.71	1/2194 (0.0%)
30	RG	0.31	0/1499	0.57	1/2016 (0.0%)
30	YG	0.40	0/1499	0.60	0/2016
31	RH	0.33	1/1332 (0.1%)	0.73	2/1802 (0.1%)
31	YH	0.50	1/1332 (0.1%)	0.76	2/1802 (0.1%)
32	RI	0.40	0/1151	0.75	1/1558 (0.1%)
32	YI	0.38	0/1151	0.66	0/1558
33	RN	0.41	0/1131	0.62	0/1525
33	YN	0.43	0/1131	0.64	0/1525
34	RO	0.41	0/943	0.62	1/1269 (0.1%)
34	YO	0.50	0/943	0.65	0/1269
35	RP	0.48	1/1162 (0.1%)	0.83	1/1544 (0.1%)
35	YP	0.55	2/1162 (0.2%)	0.93	4/1544 (0.3%)
36	RQ	0.44	0/1143	0.71	1/1527 (0.1%)
36	YQ	0.56	0/1143	0.78	0/1527
37	RR	0.42	0/982	0.69	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	YR	0.45	0/982	0.73	0/1312
38	RS	0.36	0/892	0.64	0/1187
38	YS	0.39	0/892	0.71	0/1187
39	RT	0.41	0/1155	0.63	0/1542
39	YT	0.44	0/1155	0.67	0/1542
40	RU	0.40	0/982	0.65	0/1306
40	YU	0.50	0/982	0.69	0/1306
41	RV	0.38	0/790	0.61	1/1057 (0.1%)
41	YV	0.46	0/790	0.73	1/1057 (0.1%)
42	RW	0.50	0/911	0.67	0/1220
42	YW	0.45	0/911	0.68	0/1220
43	RX	0.47	0/739	0.62	0/993
43	YX	0.50	0/739	0.66	0/993
44	RY	0.44	0/798	0.68	0/1064
44	YY	0.45	0/798	0.69	0/1064
45	RZ	0.34	0/1493	0.60	0/2026
45	YZ	0.45	2/1493 (0.1%)	0.68	4/2026 (0.2%)
46	R0	0.45	0/657	0.65	0/874
46	Y0	0.48	0/657	0.69	0/874
47	R1	0.44	0/770	0.66	0/1022
47	Y1	0.46	0/770	0.69	0/1022
48	R2	0.39	0/583	0.65	0/771
48	Y2	0.52	0/583	0.73	0/771
49	R3	0.35	0/474	0.57	0/635
49	Y3	0.41	0/474	0.59	0/635
50	R4	0.33	0/594	0.68	0/795
50	Y4	0.37	0/594	0.69	0/795
51	R5	0.43	0/473	0.78	0/639
51	Y5	0.68	3/456 (0.7%)	0.89	3/617 (0.5%)
52	R6	0.35	0/431	0.69	0/575
52	Y6	0.37	0/431	0.68	0/575
53	R7	0.49	0/438	0.68	0/575
53	Y7	0.57	0/438	0.71	0/575
54	R8	0.55	0/525	0.79	0/691
54	Y8	0.58	0/525	0.82	0/691
55	R9	0.26	0/310	0.45	0/407
55	Y9	0.32	0/310	0.48	0/407
56	Z7	0.22	0/56	0.45	0/70
56	Z8	0.25	0/56	0.45	0/70
All	All	0.32	16/320246 (0.0%)	0.78	173/478995 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is

detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
12	QL	0	1
12	XL	0	1
29	YF	0	1
31	RH	0	1
31	YH	0	1
38	YS	0	1
45	YZ	0	1
48	Y2	0	1
50	R4	0	1
54	R8	0	2
54	Y8	0	2
All	All	0	13

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	0	C	OP3-P	-10.61	1.48	1.61
22	XV	0	C	OP3-P	-10.59	1.48	1.61
35	YP	63	PRO	N-CD	6.16	1.56	1.47
45	YZ	159	PRO	N-CD	5.60	1.55	1.47
35	RP	10	PRO	N-CD	5.58	1.55	1.47

The worst 5 of 173 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	RH	125	VAL	C-N-CD	-17.76	81.53	120.60
25	YA	771	G	C2-N3-C4	-10.26	106.77	111.90
36	RQ	77	LYS	C-N-CD	-8.42	102.08	120.60
25	YA	771	G	N9-C4-C5	-8.13	102.15	105.40
25	YA	673	C	C2-N3-C4	-7.98	115.91	119.90

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	QL	47	LYS	Peptide
50	R4	38	LYS	Peptide
54	R8	30	ARG	Peptide
54	R8	35	GLN	Peptide
31	RH	153	LYS	Peptide

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	479	0
1	XA	32249	0	16279	433	0
2	QB	1924	0	1975	62	0
2	XB	1924	0	1975	83	0
3	QC	1605	0	1668	49	0
3	XC	1605	0	1668	57	0
4	QD	1703	0	1763	93	0
4	XD	1703	0	1765	50	1
5	QE	1155	0	1213	28	0
5	XE	1155	0	1213	42	0
6	QF	843	0	857	29	0
6	XF	843	0	857	40	0
7	QG	1257	0	1296	46	0
7	XG	1257	0	1296	24	0
8	QH	1116	0	1175	38	0
8	XH	1116	0	1177	28	0
9	QI	1010	0	1037	37	0
9	XI	1010	0	1037	49	0
10	QJ	801	0	849	51	0
10	XJ	801	0	849	42	0
11	QK	885	0	904	36	0
11	XK	885	0	904	37	0
12	QL	975	0	1062	39	0
12	XL	975	0	1062	50	0
13	QM	964	0	1034	64	0
13	XM	964	0	1034	61	0
14	QN	492	0	529	27	0
14	XN	492	0	529	18	0
15	QO	734	0	771	20	0
15	XO	734	0	771	18	0
16	QP	705	0	725	16	0
16	XP	705	0	725	25	0
17	QQ	834	0	904	23	0
17	XQ	834	0	904	14	0
18	QR	574	0	644	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	XR	574	0	644	25	0
19	QS	674	0	699	74	0
19	XS	674	0	699	74	0
20	QT	763	0	861	20	0
20	XT	763	0	861	35	0
21	QU	217	0	234	11	0
21	XU	217	0	234	2	0
22	QV	1644	0	835	17	0
22	XV	1644	0	836	18	0
23	QW	1619	0	822	25	0
23	QY	364	0	186	2	0
23	XW	1619	0	822	30	0
23	XY	364	0	186	2	0
24	QX	210	0	109	0	0
24	XX	210	0	109	1	0
25	RA	62071	0	31284	756	1
25	YA	62091	0	31294	730	0
26	RB	2573	0	1306	41	0
26	YB	2573	0	1306	34	0
27	RD	2115	0	2195	95	0
27	YD	2115	0	2195	139	0
28	RE	1568	0	1634	92	0
28	YE	1568	0	1634	72	0
29	RF	1585	0	1632	85	0
29	YF	1585	0	1632	62	0
30	RG	1474	0	1535	65	0
30	YG	1474	0	1535	62	0
31	RH	1307	0	1382	74	0
31	YH	1307	0	1382	89	0
32	RI	1136	0	1223	75	0
32	YI	1136	0	1223	52	0
33	RN	1104	0	1180	41	0
33	YN	1104	0	1180	50	0
34	RO	933	0	996	23	0
34	YO	933	0	996	21	0
35	RP	1145	0	1226	82	0
35	YP	1145	0	1228	88	0
36	RQ	1122	0	1179	57	0
36	YQ	1122	0	1178	50	0
37	RR	968	0	1033	49	0
37	YR	968	0	1033	35	0
38	RS	882	0	943	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	YS	882	0	943	45	0
39	RT	1141	0	1202	63	0
39	YT	1141	0	1202	53	0
40	RU	964	0	1022	31	0
40	YU	964	0	1022	52	0
41	RV	779	0	852	20	0
41	YV	779	0	852	43	0
42	RW	900	0	964	24	0
42	YW	900	0	964	27	0
43	RX	725	0	778	29	0
43	YX	725	0	778	23	0
44	RY	785	0	878	48	0
44	YY	785	0	878	40	0
45	RZ	1461	0	1493	64	0
45	YZ	1461	0	1493	80	0
46	R0	648	0	672	21	0
46	Y0	648	0	672	31	0
47	R1	763	0	848	29	0
47	Y1	763	0	848	28	0
48	R2	581	0	629	15	0
48	Y2	581	0	629	23	0
49	R3	469	0	518	6	0
49	Y3	469	0	518	15	0
50	R4	581	0	574	77	0
50	Y4	581	0	574	98	0
51	R5	459	0	476	67	0
51	Y5	442	0	465	35	0
52	R6	424	0	450	26	0
52	Y6	424	0	450	32	0
53	R7	430	0	480	20	0
53	Y7	430	0	480	15	0
54	R8	517	0	582	30	0
54	Y8	517	0	582	40	0
55	R9	307	0	338	8	0
55	Y9	307	0	336	8	0
56	Z7	116	0	67	6	0
56	Z8	116	0	67	2	0
57	QA	67	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QV	2	0	0	0	0
57	QY	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	RA	246	0	0	0	0
57	RB	2	0	0	0	0
57	RD	1	0	0	0	0
57	RE	1	0	0	0	0
57	RP	4	0	0	0	0
57	XA	71	0	0	0	0
57	XB	1	0	0	0	0
57	XM	1	0	0	0	0
57	XV	3	0	0	0	0
57	XX	1	0	0	0	0
57	XY	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y7	1	0	0	0	0
57	YA	278	0	0	0	0
57	YB	5	0	0	0	0
57	YD	1	0	0	0	0
57	YE	2	0	0	0	0
57	YP	1	0	0	0	0
57	YX	1	0	0	0	0
58	QA	42	0	45	1	0
58	XA	42	0	45	4	0
59	QD	1	0	0	0	0
59	QN	1	0	0	0	0
59	R5	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y9	1	0	0	0	0
All	All	295487	0	200096	5879	1

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 12.

The worst 5 of 5879 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:YQ:134:ARG:CZ	45:YZ:122:ARG:HH21	1.34	1.39
28:YE:14:ILE:HG22	28:YE:21:VAL:CG2	1.56	1.35
27:YD:121:PRO:HB3	27:YD:135:PHE:CE2	1.64	1.31
28:YE:14:ILE:CG2	28:YE:21:VAL:HG23	1.62	1.29
31:RH:125:VAL:HG12	31:RH:126:PRO:CD	1.64	1.25

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:RA:2197:U:OP1	4:XD:159:ARG:NH2[4.555]	2.05	0.15

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%)	173 (74%)	45 (19%)	17 (7%)	2	29
2	XB	235/256 (92%)	177 (75%)	43 (18%)	15 (6%)	2	33
3	QC	203/239 (85%)	163 (80%)	34 (17%)	6 (3%)	7	57
3	XC	203/239 (85%)	171 (84%)	29 (14%)	3 (2%)	15	72
4	QD	206/209 (99%)	177 (86%)	22 (11%)	7 (3%)	6	54
4	XD	206/209 (99%)	178 (86%)	23 (11%)	5 (2%)	9	62
5	QE	149/162 (92%)	136 (91%)	8 (5%)	5 (3%)	6	54
5	XE	149/162 (92%)	133 (89%)	13 (9%)	3 (2%)	11	66
6	QF	99/101 (98%)	93 (94%)	3 (3%)	3 (3%)	7	57
6	XF	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	QG	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	18	75
7	XG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	18	75
8	QH	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	30	84
8	XH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	7	58
9	QI	125/128 (98%)	103 (82%)	17 (14%)	5 (4%)	5	48
9	XI	125/128 (98%)	97 (78%)	24 (19%)	4 (3%)	6	55
10	QJ	97/105 (92%)	75 (77%)	19 (20%)	3 (3%)	7	57
10	XJ	97/105 (92%)	78 (80%)	14 (14%)	5 (5%)	3	39
11	QK	117/129 (91%)	100 (86%)	14 (12%)	3 (3%)	8	60
11	XK	117/129 (91%)	100 (86%)	15 (13%)	2 (2%)	14	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	QL	123/132 (93%)	98 (80%)	18 (15%)	7 (6%)	3	36
12	XL	123/132 (93%)	97 (79%)	14 (11%)	12 (10%)	1	18
13	QM	119/126 (94%)	95 (80%)	15 (13%)	9 (8%)	2	26
13	XM	119/126 (94%)	94 (79%)	15 (13%)	10 (8%)	1	23
14	QN	58/61 (95%)	49 (84%)	5 (9%)	4 (7%)	2	30
14	XN	58/61 (95%)	46 (79%)	6 (10%)	6 (10%)	1	16
15	QO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	19	77
15	XO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	10	63
16	QP	82/88 (93%)	73 (89%)	8 (10%)	1 (1%)	19	77
16	XP	82/88 (93%)	71 (87%)	10 (12%)	1 (1%)	19	77
17	QQ	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	11	66
17	XQ	98/105 (93%)	88 (90%)	10 (10%)	0	100	100
18	QR	68/88 (77%)	56 (82%)	9 (13%)	3 (4%)	4	45
18	XR	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	15	72
19	QS	82/93 (88%)	55 (67%)	16 (20%)	11 (13%)	0	10
19	XS	82/93 (88%)	54 (66%)	17 (21%)	11 (13%)	0	10
20	QT	97/106 (92%)	76 (78%)	15 (16%)	6 (6%)	2	34
20	XT	97/106 (92%)	75 (77%)	16 (16%)	6 (6%)	2	34
21	QU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	4	46
21	XU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	4	46
27	RD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	4	45
27	YD	270/276 (98%)	228 (84%)	33 (12%)	9 (3%)	6	55
28	RE	203/206 (98%)	148 (73%)	35 (17%)	20 (10%)	1	18
28	YE	203/206 (98%)	144 (71%)	42 (21%)	17 (8%)	1	23
29	RF	200/210 (95%)	170 (85%)	18 (9%)	12 (6%)	2	34
29	YF	200/210 (95%)	168 (84%)	24 (12%)	8 (4%)	5	48
30	RG	179/182 (98%)	139 (78%)	26 (14%)	14 (8%)	1	25
30	YG	179/182 (98%)	142 (79%)	25 (14%)	12 (7%)	2	31
31	RH	168/180 (93%)	116 (69%)	33 (20%)	19 (11%)	1	14
31	YH	168/180 (93%)	124 (74%)	23 (14%)	21 (12%)	1	12
32	RI	144/148 (97%)	104 (72%)	27 (19%)	13 (9%)	1	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	YI	144/148 (97%)	107 (74%)	20 (14%)	17 (12%)	1	13
33	RN	136/140 (97%)	104 (76%)	20 (15%)	12 (9%)	1	22
33	YN	136/140 (97%)	105 (77%)	17 (12%)	14 (10%)	1	16
34	RO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	14	70
34	YO	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	14	70
35	RP	148/150 (99%)	106 (72%)	28 (19%)	14 (10%)	1	19
35	YP	148/150 (99%)	108 (73%)	22 (15%)	18 (12%)	1	12
36	RQ	139/141 (99%)	99 (71%)	22 (16%)	18 (13%)	0	11
36	YQ	139/141 (99%)	98 (70%)	22 (16%)	19 (14%)	0	9
37	RR	116/118 (98%)	106 (91%)	5 (4%)	5 (4%)	4	46
37	YR	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	3	39
38	RS	109/112 (97%)	76 (70%)	22 (20%)	11 (10%)	1	17
38	YS	109/112 (97%)	79 (72%)	17 (16%)	13 (12%)	1	12
39	RT	135/146 (92%)	107 (79%)	16 (12%)	12 (9%)	1	21
39	YT	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	2	28
40	RU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	6	53
40	YU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	6	53
41	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	2	34
41	YV	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	24
42	RW	111/113 (98%)	99 (89%)	8 (7%)	4 (4%)	5	52
42	YW	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	13	68
43	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	10	64
43	YX	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	10	64
44	RY	100/110 (91%)	71 (71%)	13 (13%)	16 (16%)	0	6
44	YY	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	1	12
45	RZ	181/206 (88%)	126 (70%)	34 (19%)	21 (12%)	1	13
45	YZ	181/206 (88%)	125 (69%)	38 (21%)	18 (10%)	1	18
46	R0	80/85 (94%)	65 (81%)	14 (18%)	1 (1%)	18	75
46	Y0	80/85 (94%)	73 (91%)	7 (9%)	0	100	100
47	R1	95/98 (97%)	76 (80%)	10 (10%)	9 (10%)	1	19
47	Y1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	2	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	R2	67/72 (93%)	53 (79%)	9 (13%)	5 (8%)	2	27
48	Y2	67/72 (93%)	55 (82%)	6 (9%)	6 (9%)	1	21
49	R3	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	6	53
49	Y3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	13	68
50	R4	69/71 (97%)	35 (51%)	18 (26%)	16 (23%)	0	2
50	Y4	69/71 (97%)	35 (51%)	15 (22%)	19 (28%)	0	1
51	R5	57/60 (95%)	47 (82%)	7 (12%)	3 (5%)	3	38
51	Y5	55/60 (92%)	45 (82%)	9 (16%)	1 (2%)	13	68
52	R6	47/54 (87%)	23 (49%)	13 (28%)	11 (23%)	0	1
52	Y6	47/54 (87%)	22 (47%)	17 (36%)	8 (17%)	0	5
53	R7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	11	65
53	Y7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	11	65
54	R8	62/65 (95%)	51 (82%)	6 (10%)	5 (8%)	1	24
54	Y8	62/65 (95%)	48 (77%)	10 (16%)	4 (6%)	2	32
55	R9	35/37 (95%)	35 (100%)	0	0	100	100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
56	Z7	7/12 (58%)	5 (71%)	2 (29%)	0	100	100
56	Z8	7/12 (58%)	3 (43%)	3 (43%)	1 (14%)	0	8
All	All	11482/12152 (94%)	9247 (80%)	1516 (13%)	719 (6%)	2	33

5 of 719 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	236	TYR
3	QC	12	LEU
3	QC	190	ARG
4	QD	28	SER
6	QF	16	GLN

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%)	171 (83%)	34 (17%)	3	21
2	XB	205/220 (93%)	180 (88%)	25 (12%)	7	37
3	QC	159/188 (85%)	145 (91%)	14 (9%)	14	58
3	XC	159/188 (85%)	146 (92%)	13 (8%)	17	62
4	QD	180/181 (99%)	157 (87%)	23 (13%)	6	35
4	XD	180/181 (99%)	152 (84%)	28 (16%)	4	25
5	QE	116/123 (94%)	104 (90%)	12 (10%)	10	48
5	XE	116/123 (94%)	104 (90%)	12 (10%)	10	48
6	QF	90/90 (100%)	78 (87%)	12 (13%)	6	33
6	XF	90/90 (100%)	81 (90%)	9 (10%)	11	50
7	QG	126/127 (99%)	114 (90%)	12 (10%)	12	52
7	XG	126/127 (99%)	114 (90%)	12 (10%)	12	52
8	QH	119/119 (100%)	109 (92%)	10 (8%)	16	61
8	XH	119/119 (100%)	106 (89%)	13 (11%)	9	45
9	QI	98/99 (99%)	81 (83%)	17 (17%)	3	19
9	XI	98/99 (99%)	80 (82%)	18 (18%)	2	15
10	QJ	89/92 (97%)	77 (86%)	12 (14%)	6	32
10	XJ	89/92 (97%)	74 (83%)	15 (17%)	3	20
11	QK	90/99 (91%)	81 (90%)	9 (10%)	11	50
11	XK	90/99 (91%)	81 (90%)	9 (10%)	11	50
12	QL	104/109 (95%)	87 (84%)	17 (16%)	3	22
12	XL	104/109 (95%)	92 (88%)	12 (12%)	8	40
13	QM	97/101 (96%)	73 (75%)	24 (25%)	1	7
13	XM	97/101 (96%)	78 (80%)	19 (20%)	2	13
14	QN	49/50 (98%)	40 (82%)	9 (18%)	2	15
14	XN	49/50 (98%)	42 (86%)	7 (14%)	5	29
15	QO	79/80 (99%)	72 (91%)	7 (9%)	14	58
15	XO	79/80 (99%)	69 (87%)	10 (13%)	6	35
16	QP	72/74 (97%)	63 (88%)	9 (12%)	7	36
16	XP	72/74 (97%)	64 (89%)	8 (11%)	9	43
17	QQ	95/97 (98%)	87 (92%)	8 (8%)	16	61
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	25	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	QR	61/77 (79%)	50 (82%)	11 (18%)	2	16
18	XR	61/77 (79%)	52 (85%)	9 (15%)	4	27
19	QS	73/80 (91%)	59 (81%)	14 (19%)	2	13
19	XS	73/80 (91%)	57 (78%)	16 (22%)	1	9
20	QT	76/82 (93%)	67 (88%)	9 (12%)	8	39
20	XT	76/82 (93%)	66 (87%)	10 (13%)	6	33
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	34	80
27	RD	214/218 (98%)	176 (82%)	38 (18%)	2	17
27	YD	214/218 (98%)	180 (84%)	34 (16%)	4	24
28	RE	165/166 (99%)	126 (76%)	39 (24%)	1	8
28	YE	165/166 (99%)	135 (82%)	30 (18%)	2	16
29	RF	161/166 (97%)	132 (82%)	29 (18%)	2	16
29	YF	161/166 (97%)	137 (85%)	24 (15%)	4	27
30	RG	155/156 (99%)	134 (86%)	21 (14%)	6	32
30	YG	155/156 (99%)	134 (86%)	21 (14%)	6	32
31	RH	142/148 (96%)	120 (84%)	22 (16%)	4	25
31	YH	142/148 (96%)	116 (82%)	26 (18%)	2	16
32	RI	122/124 (98%)	98 (80%)	24 (20%)	2	12
32	YI	122/124 (98%)	92 (75%)	30 (25%)	1	7
33	RN	117/119 (98%)	97 (83%)	20 (17%)	3	20
33	YN	117/119 (98%)	96 (82%)	21 (18%)	2	17
34	RO	100/100 (100%)	90 (90%)	10 (10%)	11	50
34	YO	100/100 (100%)	89 (89%)	11 (11%)	9	44
35	RP	116/116 (100%)	86 (74%)	30 (26%)	1	6
35	YP	116/116 (100%)	81 (70%)	35 (30%)	0	4
36	RQ	111/111 (100%)	94 (85%)	17 (15%)	4	26
36	YQ	111/111 (100%)	92 (83%)	19 (17%)	3	20
37	RR	101/101 (100%)	83 (82%)	18 (18%)	2	17
37	YR	101/101 (100%)	80 (79%)	21 (21%)	2	11
38	RS	87/88 (99%)	69 (79%)	18 (21%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	YS	87/88 (99%)	68 (78%)	19 (22%)	1	9
39	RT	120/127 (94%)	102 (85%)	18 (15%)	4	27
39	YT	120/127 (94%)	98 (82%)	22 (18%)	2	16
40	RU	93/94 (99%)	79 (85%)	14 (15%)	4	27
40	YU	93/94 (99%)	77 (83%)	16 (17%)	3	19
41	RV	82/82 (100%)	66 (80%)	16 (20%)	2	13
41	YV	82/82 (100%)	67 (82%)	15 (18%)	2	16
42	RW	92/92 (100%)	73 (79%)	19 (21%)	2	11
42	YW	92/92 (100%)	75 (82%)	17 (18%)	2	15
43	RX	74/78 (95%)	63 (85%)	11 (15%)	4	27
43	YX	74/78 (95%)	60 (81%)	14 (19%)	2	14
44	RY	85/91 (93%)	63 (74%)	22 (26%)	1	6
44	YY	85/91 (93%)	64 (75%)	21 (25%)	1	7
45	RZ	162/179 (90%)	132 (82%)	30 (18%)	2	15
45	YZ	162/179 (90%)	133 (82%)	29 (18%)	2	17
46	R0	65/67 (97%)	60 (92%)	5 (8%)	18	65
46	Y0	65/67 (97%)	59 (91%)	6 (9%)	13	55
47	R1	82/83 (99%)	73 (89%)	9 (11%)	9	44
47	Y1	82/83 (99%)	70 (85%)	12 (15%)	5	28
48	R2	64/67 (96%)	57 (89%)	7 (11%)	9	45
48	Y2	64/67 (96%)	47 (73%)	17 (27%)	1	6
49	R3	51/52 (98%)	45 (88%)	6 (12%)	8	39
49	Y3	51/52 (98%)	43 (84%)	8 (16%)	4	25
50	R4	63/63 (100%)	45 (71%)	18 (29%)	0	4
50	Y4	63/63 (100%)	43 (68%)	20 (32%)	0	3
51	R5	51/52 (98%)	36 (71%)	15 (29%)	0	4
51	Y5	49/52 (94%)	36 (74%)	13 (26%)	1	6
52	R6	48/52 (92%)	35 (73%)	13 (27%)	1	5
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	2	11
53	R7	42/42 (100%)	34 (81%)	8 (19%)	2	14
53	Y7	42/42 (100%)	35 (83%)	7 (17%)	3	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	R8	54/55 (98%)	44 (82%)	10 (18%)	2	15
54	Y8	54/55 (98%)	41 (76%)	13 (24%)	1	7
55	R9	34/34 (100%)	32 (94%)	2 (6%)	28	76
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	28	76
56	Z7	5/7 (71%)	5 (100%)	0	100	100
56	Z8	5/7 (71%)	4 (80%)	1 (20%)	2	12
All	All	9710/10080 (96%)	8152 (84%)	1558 (16%)	3	24

5 of 1558 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	R3	40	THR
8	XH	12	ARG
45	YZ	140	ASP
51	R5	6	VAL
2	XB	187	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
19	QS	47	HIS
38	RS	34	HIS
2	XB	19	HIS
13	QM	92	HIS
2	XB	204	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	267 (17%)	43 (2%)
1	XA	1498/1522 (98%)	277 (18%)	38 (2%)
22	QV	76/77 (98%)	19 (25%)	1 (1%)
22	XV	76/77 (98%)	17 (22%)	1 (1%)
23	QW	75/76 (98%)	16 (21%)	0
23	QY	15/76 (19%)	3 (20%)	0
23	XW	75/76 (98%)	19 (25%)	0
23	XY	15/76 (19%)	4 (26%)	0
24	QX	9/24 (37%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	XX	9/24 (37%)	0	0
25	RA	2879/2915 (98%)	567 (19%)	57 (1%)
25	YA	2880/2915 (98%)	563 (19%)	57 (1%)
26	RB	119/122 (97%)	21 (17%)	1 (0%)
26	YB	119/122 (97%)	21 (17%)	1 (0%)
All	All	9344/9624 (97%)	1794 (19%)	199 (2%)

5 of 1794 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	7	G
1	QA	22	G
1	QA	32	A
1	QA	39	G

5 of 199 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2405	G
1	XA	250	A
25	YA	1955	U
25	RA	2481	G
26	RB	66	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 704 ligands modelled in this entry, 702 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	1667	-	45,45,45	1.40	7 (15%)	67,67,67	1.19	5 (7%)
58	PAR	XA	1672	-	45,45,45	1.38	6 (13%)	67,67,67	1.28	6 (8%)

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	1667	-	-	0/18/94/94	0/4/4/4
58	PAR	XA	1672	-	-	0/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	QA	1667	PAR	C52-C42	3.24	1.58	1.52
58	XA	1672	PAR	C52-C42	3.16	1.58	1.52
58	XA	1672	PAR	O54-C14	3.01	1.49	1.41
58	QA	1667	PAR	O54-C14	2.93	1.49	1.41
58	QA	1667	PAR	C64-C54	2.87	1.59	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	QA	1667	PAR	O52-C13-C23	4.40	115.35	107.50
58	XA	1672	PAR	C14-O54-C54	4.13	121.73	113.73
58	QA	1667	PAR	C14-O54-C54	4.08	121.62	113.73
58	XA	1672	PAR	O52-C13-C23	3.79	114.27	107.50
58	XA	1672	PAR	O54-C54-C64	3.32	112.29	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%)	0.07	44 (2%)	49	28	68, 102, 211, 576	0
1	XA	1500/1522 (98%)	0.05	41 (2%)	52	29	57, 88, 196, 440	0
2	QB	237/256 (92%)	0.52	17 (7%)	15	9	106, 186, 344, 418	0
2	XB	237/256 (92%)	0.35	10 (4%)	35	19	88, 156, 283, 529	0
3	QC	205/239 (85%)	0.57	15 (7%)	15	9	103, 172, 294, 429	0
3	XC	205/239 (85%)	0.30	3 (1%)	70	43	80, 124, 195, 316	0
4	QD	208/209 (99%)	0.20	1 (0%)	88	71	85, 114, 192, 458	0
4	XD	208/209 (99%)	0.26	5 (2%)	56	32	71, 109, 190, 368	0
5	QE	151/162 (93%)	0.26	1 (0%)	84	63	90, 128, 201, 260	0
5	XE	151/162 (93%)	0.15	1 (0%)	84	63	72, 101, 185, 236	0
6	QF	101/101 (100%)	0.18	1 (0%)	79	53	80, 109, 175, 310	0
6	XF	101/101 (100%)	0.26	3 (2%)	48	27	73, 107, 161, 559	0
7	QG	155/156 (99%)	0.41	11 (7%)	16	9	83, 150, 262, 534	0
7	XG	155/156 (99%)	0.21	5 (3%)	45	25	76, 129, 209, 334	0
8	QH	138/138 (100%)	0.18	0	100	100	92, 133, 195, 285	0
8	XH	138/138 (100%)	0.12	0	100	100	80, 113, 165, 331	0
9	QI	127/128 (99%)	0.63	13 (10%)	7	6	96, 189, 303, 476	0
9	XI	127/128 (99%)	0.52	7 (5%)	24	13	76, 153, 232, 396	0
10	QJ	99/105 (94%)	0.86	14 (14%)	3	3	107, 196, 431, 583	0
10	XJ	99/105 (94%)	0.77	12 (12%)	5	5	85, 164, 316, 369	0
11	QK	119/129 (92%)	0.53	9 (7%)	14	8	77, 112, 201, 335	0
11	XK	119/129 (92%)	0.33	7 (5%)	22	12	67, 105, 181, 251	0
12	QL	125/132 (94%)	0.35	4 (3%)	45	25	79, 101, 176, 309	0
12	XL	125/132 (94%)	0.29	4 (3%)	45	25	55, 78, 146, 341	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	0.33	3 (2%) 54 31	101, 160, 265, 447	0
13	XM	121/126 (96%)	0.24	2 (1%) 67 40	78, 126, 200, 488	0
14	QN	60/61 (98%)	0.66	5 (8%) 11 8	117, 157, 211, 250	0
14	XN	60/61 (98%)	0.32	2 (3%) 44 25	89, 106, 151, 194	0
15	QO	88/89 (98%)	0.36	1 (1%) 77 50	77, 113, 167, 241	0
15	XO	88/89 (98%)	0.32	0 100 100	69, 101, 153, 171	0
16	QP	84/88 (95%)	0.25	2 (2%) 56 32	85, 102, 164, 241	0
16	XP	84/88 (95%)	0.26	1 (1%) 75 49	87, 111, 187, 400	0
17	QQ	100/105 (95%)	0.30	1 (1%) 79 53	82, 107, 157, 336	0
17	XQ	100/105 (95%)	0.26	0 100 100	71, 105, 171, 330	0
18	QR	70/88 (79%)	0.35	3 (4%) 34 19	83, 114, 185, 205	0
18	XR	70/88 (79%)	0.34	2 (2%) 49 28	77, 112, 187, 227	0
19	QS	84/93 (90%)	0.58	6 (7%) 16 9	109, 181, 257, 381	0
19	XS	84/93 (90%)	0.29	3 (3%) 41 23	80, 133, 207, 286	0
20	QT	99/106 (93%)	0.39	4 (4%) 36 20	87, 122, 208, 237	0
20	XT	99/106 (93%)	0.50	4 (4%) 36 20	87, 136, 211, 236	0
21	QU	25/27 (92%)	1.76	7 (28%) 1 2	112, 155, 238, 264	0
21	XU	25/27 (92%)	1.06	4 (16%) 3 3	102, 128, 202, 210	0
22	QV	77/77 (100%)	0.24	3 (3%) 37 21	91, 114, 175, 228	0
22	XV	77/77 (100%)	0.02	3 (3%) 37 21	70, 91, 164, 210	0
23	QW	76/76 (100%)	1.87	32 (42%) 1 1	91, 205, 292, 361	0
23	QY	17/76 (22%)	1.46	6 (35%) 1 1	120, 132, 201, 212	0
23	XW	76/76 (100%)	1.82	28 (36%) 1 1	88, 196, 373, 402	0
23	XY	17/76 (22%)	0.42	0 100 100	94, 101, 177, 187	0
24	QX	10/24 (41%)	2.06	3 (30%) 1 1	102, 106, 257, 377	0
24	XX	10/24 (41%)	2.38	5 (50%) 0 1	94, 99, 237, 284	0
25	RA	2882/2915 (98%)	0.17	147 (5%) 27 15	53, 82, 254, 563	0
25	YA	2883/2915 (98%)	0.04	96 (3%) 44 25	39, 64, 217, 437	0
26	RB	120/122 (98%)	0.35	1 (0%) 83 60	119, 162, 204, 242	0
26	YB	120/122 (98%)	0.05	1 (0%) 83 60	71, 106, 119, 200	0
27	RD	272/276 (98%)	0.04	1 (0%) 90 76	54, 74, 127, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	YD	272/276 (98%)	-0.00	1 (0%) 90 76	40, 66, 120, 213	0
28	RE	205/206 (99%)	0.22	6 (2%) 49 28	55, 94, 188, 447	0
28	YE	205/206 (99%)	0.22	5 (2%) 56 32	43, 78, 167, 453	0
29	RF	202/210 (96%)	0.15	3 (1%) 70 43	54, 110, 191, 469	0
29	YF	202/210 (96%)	0.01	0 100 100	39, 71, 138, 248	0
30	RG	181/182 (99%)	0.67	10 (5%) 24 13	122, 192, 303, 490	0
30	YG	181/182 (99%)	0.24	0 100 100	82, 117, 183, 391	0
31	RH	170/180 (94%)	0.84	18 (10%) 7 6	113, 199, 359, 517	0
31	YH	170/180 (94%)	0.36	5 (2%) 49 28	65, 114, 180, 363	0
32	RI	146/148 (98%)	0.33	7 (4%) 29 16	73, 155, 265, 529	0
32	YI	146/148 (98%)	0.32	3 (2%) 60 35	62, 143, 271, 559	0
33	RN	138/140 (98%)	0.27	5 (3%) 41 23	64, 111, 186, 302	0
33	YN	138/140 (98%)	0.03	2 (1%) 72 45	49, 78, 167, 266	0
34	RO	122/122 (100%)	0.06	1 (0%) 83 60	63, 94, 139, 155	0
34	YO	122/122 (100%)	-0.01	0 100 100	51, 68, 115, 146	0
35	RP	150/150 (100%)	0.33	8 (5%) 25 14	61, 122, 202, 369	0
35	YP	150/150 (100%)	0.11	1 (0%) 84 63	42, 81, 157, 361	0
36	RQ	141/141 (100%)	0.38	4 (2%) 50 29	80, 122, 205, 332	0
36	YQ	141/141 (100%)	0.07	1 (0%) 84 63	56, 73, 148, 430	0
37	RR	118/118 (100%)	0.12	1 (0%) 83 60	61, 86, 134, 160	0
37	YR	118/118 (100%)	0.10	1 (0%) 83 60	51, 71, 120, 207	0
38	RS	111/112 (99%)	0.49	3 (2%) 52 29	109, 160, 253, 420	0
38	YS	111/112 (99%)	0.17	0 100 100	73, 102, 175, 285	0
39	RT	137/146 (93%)	0.20	6 (4%) 33 18	70, 107, 263, 350	0
39	YT	137/146 (93%)	0.22	5 (3%) 41 23	60, 84, 192, 451	0
40	RU	117/118 (99%)	0.21	2 (1%) 67 40	62, 106, 174, 287	0
40	YU	117/118 (99%)	0.04	1 (0%) 81 57	47, 71, 134, 425	0
41	RV	101/101 (100%)	0.43	5 (4%) 28 15	64, 129, 225, 419	0
41	YV	101/101 (100%)	0.16	1 (0%) 79 53	46, 89, 172, 424	0
42	RW	113/113 (100%)	0.16	3 (2%) 52 29	55, 75, 154, 298	0
42	YW	113/113 (100%)	0.23	2 (1%) 65 39	42, 67, 139, 206	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	RX	92/96 (95%)	0.25	0 100 100	67, 95, 161, 200	0
43	YX	92/96 (95%)	0.21	2 (2%) 59 34	50, 72, 129, 260	0
44	RY	102/110 (92%)	0.57	9 (8%) 10 7	79, 132, 238, 489	0
44	YY	102/110 (92%)	0.19	2 (1%) 62 36	63, 103, 175, 385	0
45	RZ	183/206 (88%)	1.00	29 (15%) 3 3	123, 195, 338, 497	0
45	YZ	183/206 (88%)	0.86	23 (12%) 4 4	76, 148, 434, 554	0
46	R0	82/85 (96%)	0.39	4 (4%) 28 15	69, 114, 152, 188	0
46	Y0	82/85 (96%)	0.19	2 (2%) 56 32	47, 70, 126, 171	0
47	R1	97/98 (98%)	0.61	5 (5%) 26 14	58, 95, 208, 261	0
47	Y1	97/98 (98%)	0.42	4 (4%) 35 20	45, 72, 181, 340	0
48	R2	69/72 (95%)	0.14	1 (1%) 72 45	80, 129, 215, 245	0
48	Y2	69/72 (95%)	0.26	1 (1%) 72 45	60, 88, 176, 274	0
49	R3	59/60 (98%)	0.49	2 (3%) 43 24	82, 121, 199, 517	0
49	Y3	59/60 (98%)	0.39	4 (6%) 17 10	55, 76, 140, 319	0
50	R4	71/71 (100%)	0.90	11 (15%) 3 3	132, 253, 520, 577	0
50	Y4	71/71 (100%)	0.74	9 (12%) 4 4	103, 196, 455, 567	0
51	R5	59/60 (98%)	0.55	7 (11%) 5 5	46, 95, 288, 394	0
51	Y5	57/60 (95%)	0.34	1 (1%) 65 39	23, 73, 267, 342	0
52	R6	49/54 (90%)	0.75	3 (6%) 21 11	88, 156, 225, 300	0
52	Y6	49/54 (90%)	0.66	2 (4%) 35 20	53, 118, 199, 327	0
53	R7	49/49 (100%)	0.18	1 (2%) 62 36	38, 65, 157, 188	0
53	Y7	49/49 (100%)	0.11	1 (2%) 62 36	26, 48, 108, 212	0
54	R8	64/65 (98%)	0.27	1 (1%) 68 41	53, 93, 152, 285	0
54	Y8	64/65 (98%)	0.16	1 (1%) 68 41	29, 61, 107, 272	0
55	R9	37/37 (100%)	1.68	12 (32%) 1 1	92, 141, 227, 400	0
55	Y9	37/37 (100%)	1.23	5 (13%) 4 4	45, 101, 162, 378	0
56	Z7	8/12 (66%)	1.38	0 100 100	115, 174, 254, 280	0
56	Z8	8/12 (66%)	1.09	0 100 100	124, 137, 204, 234	0
All	All	21045/21776 (96%)	0.24	856 (4%) 35 20	23, 99, 241, 583	0

The worst 5 of 856 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
28	YE	205	ALA	20.2
25	RA	1096	A	18.7
25	RA	1068	G	14.6
1	QA	1032	A	13.5
23	XW	20	U	13.4

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

There are no non-standard protein/DNA/RNA residues in this entry.

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	RA	3222	1/1	0.34	-	49,49,49,49	0
57	MG	XA	1632	1/1	0.43	-	41,41,41,41	0
57	MG	YA	3113	1/1	0.34	-	50,50,50,50	0
57	MG	RA	3232	1/1	0.34	-	40,40,40,40	0
57	MG	RA	3158	1/1	0.26	-	56,56,56,56	0
57	MG	RA	3229	1/1	0.39	-	88,88,88,88	0
57	MG	YA	3176	1/1	0.26	-	106,106,106,106	0
57	MG	YA	3261	1/1	0.61	-	70,70,70,70	0
57	MG	RA	3217	1/1	1.09	-	133,133,133,133	0
57	MG	YA	3251	1/1	1.04	-	52,52,52,52	0
57	MG	YA	3213	1/1	0.13	-	54,54,54,54	0
57	MG	YA	3249	1/1	0.36	-	27,27,27,27	0
57	MG	YA	3124	1/1	0.31	-	84,84,84,84	0
57	MG	RA	3036	1/1	0.48	-	29,29,29,29	0
57	MG	YA	3040	1/1	0.60	-	28,28,28,28	0
57	MG	RA	3133	1/1	0.36	-	118,118,118,118	0
57	MG	YA	3047	1/1	0.58	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3272	1/1	0.26	-	78,78,78,78	0
57	MG	RA	3001	1/1	0.89	-	44,44,44,44	0
57	MG	RA	3198	1/1	0.19	-	49,49,49,49	0
57	MG	YA	3017	1/1	0.33	-	31,31,31,31	0
57	MG	RA	3028	1/1	0.38	-	39,39,39,39	0
57	MG	RA	3184	1/1	0.16	-	48,48,48,48	0
57	MG	RA	3008	1/1	0.88	-	62,62,62,62	0
58	PAR	QA	1667	42/42	0.21	-	72,72,72,72	0
57	MG	YA	3037	1/1	0.36	-	50,50,50,50	0
57	MG	RA	3194	1/1	0.51	-	51,51,51,51	0
57	MG	RA	3002	1/1	1.15	-	70,70,70,70	0
57	MG	RA	3062	1/1	0.88	-	28,28,28,28	0
57	MG	RA	3087	1/1	0.43	-	54,54,54,54	0
57	MG	YA	3049	1/1	0.40	-	27,27,27,27	0
57	MG	QA	1654	1/1	0.20	-	45,45,45,45	0
57	MG	XA	1656	1/1	0.59	-	89,89,89,89	0
57	MG	XA	1666	1/1	0.32	-	55,55,55,55	0
57	MG	RA	3119	1/1	0.48	-	76,76,76,76	0
57	MG	RB	201	1/1	0.12	-	79,79,79,79	0
57	MG	YA	3170	1/1	0.62	-	38,38,38,38	0
57	MG	Y7	101	1/1	0.23	-	40,40,40,40	0
57	MG	RA	3021	1/1	0.30	-	29,29,29,29	0
57	MG	YP	201	1/1	0.53	-	380,380,380,380	0
59	ZN	QD	301	1/1	0.23	-	59,59,59,59	0
57	MG	RA	3195	1/1	0.25	-	102,102,102,102	0
57	MG	YA	3259	1/1	0.65	-	40,40,40,40	0
57	MG	QA	1647	1/1	0.50	-	67,67,67,67	0
57	MG	RA	3126	1/1	0.27	-	58,58,58,58	0
57	MG	XA	1633	1/1	0.29	-	47,47,47,47	0
57	MG	RA	3121	1/1	0.33	-	69,69,69,69	0
57	MG	YA	3134	1/1	0.28	-	39,39,39,39	0
57	MG	YA	3123	1/1	0.36	-	51,51,51,51	0
57	MG	YA	3065	1/1	0.33	-	53,53,53,53	0
57	MG	QH	201	1/1	0.32	-	105,105,105,105	0
57	MG	YA	3030	1/1	0.74	-	36,36,36,36	0
57	MG	YA	3104	1/1	0.19	-	39,39,39,39	0
57	MG	YA	3262	1/1	0.65	-	63,63,63,63	0
57	MG	QA	1638	1/1	0.47	-	63,63,63,63	0
57	MG	YA	3026	1/1	0.88	-	30,30,30,30	0
57	MG	YA	3235	1/1	0.34	-	63,63,63,63	0
57	MG	RA	3070	1/1	0.45	-	58,58,58,58	0
57	MG	YA	3148	1/1	0.72	-	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3021	1/1	0.36	-	24,24,24,24	0
57	MG	RA	3227	1/1	1.26	-	40,40,40,40	0
57	MG	YA	3227	1/1	0.54	-	121,121,121,121	0
57	MG	RA	3041	1/1	0.34	-	32,32,32,32	0
57	MG	YA	3149	1/1	1.88	-	106,106,106,106	0
57	MG	YA	3271	1/1	0.98	-	84,84,84,84	0
57	MG	YA	3109	1/1	0.20	-	30,30,30,30	0
57	MG	YA	3101	1/1	0.36	-	30,30,30,30	0
57	MG	XA	1623	1/1	0.15	-	42,42,42,42	0
57	MG	RA	3205	1/1	0.17	-	40,40,40,40	0
57	MG	YA	3066	1/1	0.73	-	42,42,42,42	0
57	MG	RA	3240	1/1	0.57	-	70,70,70,70	0
57	MG	YA	3277	1/1	0.34	-	42,42,42,42	0
57	MG	YA	3011	1/1	0.44	-	29,29,29,29	0
57	MG	QA	1610	1/1	0.26	-	34,34,34,34	0
57	MG	XA	1621	1/1	0.55	-	46,46,46,46	0
57	MG	XA	1668	1/1	0.37	-	136,136,136,136	0
57	MG	QF	201	1/1	0.58	-	166,166,166,166	0
57	MG	YA	3196	1/1	0.31	-	34,34,34,34	0
57	MG	RA	3207	1/1	0.27	-	156,156,156,156	0
57	MG	RA	3182	1/1	0.34	-	92,92,92,92	0
57	MG	YA	3083	1/1	0.44	-	50,50,50,50	0
57	MG	RA	3176	1/1	0.26	-	25,25,25,25	0
59	ZN	XN	101	1/1	0.15	-	76,76,76,76	0
57	MG	YA	3188	1/1	0.40	-	39,39,39,39	0
57	MG	YA	3118	1/1	0.54	-	35,35,35,35	0
57	MG	RA	3067	1/1	0.32	-	85,85,85,85	0
57	MG	RA	3124	1/1	0.19	-	61,61,61,61	0
57	MG	YA	3094	1/1	0.60	-	60,60,60,60	0
57	MG	RA	3242	1/1	0.69	-	67,67,67,67	0
57	MG	RA	3196	1/1	0.38	-	108,108,108,108	0
57	MG	YA	3164	1/1	0.33	-	72,72,72,72	0
57	MG	XA	1657	1/1	0.42	-	65,65,65,65	0
57	MG	XA	1619	1/1	0.48	-	46,46,46,46	0
57	MG	YA	3192	1/1	0.19	-	57,57,57,57	0
57	MG	QA	1613	1/1	0.61	-	57,57,57,57	0
57	MG	R5	101	1/1	1.55	-	291,291,291,291	0
57	MG	XA	1617	1/1	0.14	-	40,40,40,40	0
57	MG	YA	3168	1/1	0.14	-	69,69,69,69	0
57	MG	QA	1616	1/1	0.23	-	81,81,81,81	0
57	MG	YA	3205	1/1	0.26	-	78,78,78,78	0
57	MG	RA	3153	1/1	0.45	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3198	1/1	0.12	-	86,86,86,86	0
57	MG	RD	301	1/1	1.05	-	91,91,91,91	0
57	MG	YA	3080	1/1	0.93	-	53,53,53,53	0
57	MG	RA	3188	1/1	0.56	-	103,103,103,103	0
57	MG	RA	3026	1/1	0.74	-	33,33,33,33	0
57	MG	YE	301	1/1	0.38	-	47,47,47,47	0
57	MG	RA	3031	1/1	0.42	-	52,52,52,52	0
57	MG	YA	3160	1/1	0.20	-	89,89,89,89	0
57	MG	QA	1605	1/1	1.08	-	44,44,44,44	0
57	MG	XA	1634	1/1	0.48	-	98,98,98,98	0
57	MG	YA	3220	1/1	0.68	-	45,45,45,45	0
57	MG	RA	3075	1/1	0.79	-	46,46,46,46	0
57	MG	XA	1645	1/1	0.20	-	25,25,25,25	0
57	MG	RA	3016	1/1	0.45	-	39,39,39,39	0
57	MG	RA	3235	1/1	0.19	-	59,59,59,59	0
57	MG	YA	3244	1/1	0.45	-	75,75,75,75	0
57	MG	YA	3232	1/1	0.16	-	28,28,28,28	0
57	MG	YA	3254	1/1	0.65	-	61,61,61,61	0
57	MG	RA	3061	1/1	0.17	-	64,64,64,64	0
57	MG	YA	3060	1/1	0.50	-	35,35,35,35	0
57	MG	RA	3141	1/1	0.25	-	45,45,45,45	0
57	MG	YA	3076	1/1	0.70	-	25,25,25,25	0
57	MG	YA	3035	1/1	0.49	-	42,42,42,42	0
57	MG	QA	1630	1/1	0.14	-	101,101,101,101	0
57	MG	RA	3163	1/1	0.26	-	38,38,38,38	0
57	MG	YB	203	1/1	0.21	-	91,91,91,91	0
57	MG	RA	3102	1/1	0.51	-	30,30,30,30	0
57	MG	RA	3116	1/1	0.29	-	30,30,30,30	0
57	MG	XA	1654	1/1	0.45	-	39,39,39,39	0
57	MG	YA	3127	1/1	0.14	-	39,39,39,39	0
57	MG	RA	3218	1/1	0.74	-	132,132,132,132	0
57	MG	YA	3019	1/1	0.53	-	25,25,25,25	0
57	MG	YA	3020	1/1	0.93	-	34,34,34,34	0
57	MG	QA	1658	1/1	0.32	-	71,71,71,71	0
57	MG	YA	3270	1/1	0.85	-	57,57,57,57	0
57	MG	XA	1612	1/1	0.21	-	37,37,37,37	0
57	MG	RA	3038	1/1	0.29	-	29,29,29,29	0
57	MG	RA	3231	1/1	0.63	-	29,29,29,29	0
57	MG	RA	3135	1/1	0.58	-	53,53,53,53	0
57	MG	RA	3080	1/1	0.86	-	75,75,75,75	0
57	MG	QA	1609	1/1	0.11	-	154,154,154,154	0
57	MG	RA	3166	1/1	0.78	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3237	1/1	0.42	-	29,29,29,29	0
57	MG	QA	1608	1/1	0.13	-	36,36,36,36	0
57	MG	RA	3123	1/1	0.31	-	55,55,55,55	0
57	MG	XV	103	1/1	1.09	-	54,54,54,54	0
57	MG	YA	3274	1/1	0.62	-	57,57,57,57	0
57	MG	XA	1650	1/1	0.67	-	60,60,60,60	0
57	MG	RB	202	1/1	0.07	-	100,100,100,100	0
57	MG	XA	1615	1/1	0.46	-	29,29,29,29	0
57	MG	YA	3212	1/1	0.20	-	38,38,38,38	0
57	MG	YA	3145	1/1	0.23	-	35,35,35,35	0
57	MG	RA	3089	1/1	0.36	-	114,114,114,114	0
57	MG	RA	3206	1/1	0.63	-	140,140,140,140	0
57	MG	YA	3138	1/1	0.47	-	34,34,34,34	0
57	MG	YA	3258	1/1	1.06	-	68,68,68,68	0
57	MG	YA	3226	1/1	0.16	-	74,74,74,74	0
57	MG	YA	3023	1/1	0.29	-	39,39,39,39	0
57	MG	YA	3189	1/1	0.34	-	49,49,49,49	0
57	MG	QA	1657	1/1	0.29	-	112,112,112,112	0
57	MG	YA	3117	1/1	0.18	-	39,39,39,39	0
57	MG	RA	3236	1/1	0.95	-	46,46,46,46	0
57	MG	YA	3161	1/1	0.66	-	43,43,43,43	0
57	MG	YA	3055	1/1	0.61	-	43,43,43,43	0
57	MG	YA	3013	1/1	0.89	-	28,28,28,28	0
57	MG	YA	3056	1/1	0.22	-	33,33,33,33	0
57	MG	YA	3111	1/1	0.21	-	63,63,63,63	0
57	MG	XA	1603	1/1	0.43	-	43,43,43,43	0
57	MG	YA	3038	1/1	0.21	-	50,50,50,50	0
57	MG	RA	3081	1/1	0.41	-	28,28,28,28	0
57	MG	RA	3073	1/1	0.24	-	70,70,70,70	0
57	MG	YA	3075	1/1	0.26	-	42,42,42,42	0
57	MG	YA	3151	1/1	0.29	-	28,28,28,28	0
57	MG	RA	3219	1/1	0.74	-	138,138,138,138	0
57	MG	YA	3131	1/1	0.71	-	55,55,55,55	0
57	MG	RA	3164	1/1	0.52	-	82,82,82,82	0
57	MG	XA	1652	1/1	0.47	-	104,104,104,104	0
57	MG	RA	3024	1/1	0.32	-	28,28,28,28	0
57	MG	YA	3253	1/1	0.92	-	55,55,55,55	0
57	MG	RA	3187	1/1	0.27	-	49,49,49,49	0
57	MG	YA	3096	1/1	0.78	-	53,53,53,53	0
57	MG	RA	3225	1/1	0.59	-	161,161,161,161	0
57	MG	QA	1620	1/1	0.33	-	80,80,80,80	0
57	MG	YA	3045	1/1	0.50	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3041	1/1	0.38	-	35,35,35,35	0
57	MG	XA	1614	1/1	0.29	-	153,153,153,153	0
57	MG	RA	3211	1/1	0.43	-	67,67,67,67	0
57	MG	RA	3032	1/1	0.46	-	29,29,29,29	0
57	MG	RA	3105	1/1	0.21	-	43,43,43,43	0
57	MG	QA	1649	1/1	0.65	-	104,104,104,104	0
57	MG	RA	3113	1/1	0.58	-	34,34,34,34	0
57	MG	RA	3040	1/1	0.21	-	35,35,35,35	0
57	MG	QA	1665	1/1	0.51	-	82,82,82,82	0
57	MG	YA	3048	1/1	0.36	-	58,58,58,58	0
57	MG	YA	3208	1/1	0.26	-	51,51,51,51	0
57	MG	YA	3218	1/1	0.20	-	58,58,58,58	0
57	MG	RA	3142	1/1	0.24	-	38,38,38,38	0
57	MG	YA	3034	1/1	0.44	-	27,27,27,27	0
57	MG	YA	3143	1/1	0.50	-	60,60,60,60	0
57	MG	RA	3042	1/1	0.30	-	53,53,53,53	0
57	MG	RA	3071	1/1	0.25	-	51,51,51,51	0
57	MG	YA	3230	1/1	0.24	-	45,45,45,45	0
57	MG	RA	3049	1/1	0.56	-	49,49,49,49	0
57	MG	YA	3245	1/1	0.60	-	25,25,25,25	0
57	MG	RA	3238	1/1	0.39	-	51,51,51,51	0
57	MG	YA	3106	1/1	0.74	-	42,42,42,42	0
57	MG	RA	3039	1/1	0.49	-	36,36,36,36	0
57	MG	RA	3150	1/1	0.15	-	42,42,42,42	0
57	MG	RA	3190	1/1	0.38	-	107,107,107,107	0
57	MG	YA	3039	1/1	0.30	-	59,59,59,59	0
57	MG	RA	3146	1/1	0.17	-	137,137,137,137	0
57	MG	QA	1636	1/1	0.19	-	44,44,44,44	0
57	MG	YA	3265	1/1	0.44	-	41,41,41,41	0
57	MG	QV	102	1/1	0.23	-	69,69,69,69	0
57	MG	YA	3219	1/1	0.35	-	105,105,105,105	0
57	MG	RA	3066	1/1	0.32	-	37,37,37,37	0
57	MG	RP	204	1/1	0.46	-	183,183,183,183	0
57	MG	YA	3179	1/1	0.32	-	44,44,44,44	0
57	MG	RP	203	1/1	0.19	-	381,381,381,381	0
57	MG	YA	3103	1/1	0.58	-	31,31,31,31	0
57	MG	YA	3044	1/1	0.77	-	33,33,33,33	0
57	MG	YA	3024	1/1	0.38	-	33,33,33,33	0
57	MG	YA	3162	1/1	0.17	-	35,35,35,35	0
57	MG	RA	3077	1/1	0.28	-	52,52,52,52	0
57	MG	QA	1619	1/1	0.18	-	68,68,68,68	0
57	MG	RA	3192	1/1	0.32	-	250,250,250,250	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	QA	1661	1/1	0.12	-	126,126,126,126	0
57	MG	QA	1641	1/1	0.25	-	76,76,76,76	0
57	MG	YA	3093	1/1	0.51	-	24,24,24,24	0
57	MG	XA	1625	1/1	0.21	-	53,53,53,53	0
57	MG	RA	3223	1/1	0.15	-	113,113,113,113	0
57	MG	QA	1603	1/1	2.06	-	66,66,66,66	0
57	MG	XA	1661	1/1	0.95	-	75,75,75,75	0
57	MG	RA	3058	1/1	0.32	-	49,49,49,49	0
57	MG	YA	3278	1/1	0.27	-	85,85,85,85	0
57	MG	RA	3159	1/1	0.68	-	72,72,72,72	0
57	MG	YA	3081	1/1	0.92	-	31,31,31,31	0
57	MG	YA	3217	1/1	0.38	-	76,76,76,76	0
57	MG	QA	1656	1/1	0.30	-	87,87,87,87	0
57	MG	YA	3222	1/1	0.17	-	71,71,71,71	0
57	MG	RA	3103	1/1	0.43	-	41,41,41,41	0
57	MG	QA	1635	1/1	0.32	-	58,58,58,58	0
57	MG	YA	3058	1/1	0.41	-	31,31,31,31	0
57	MG	RA	3170	1/1	0.24	-	55,55,55,55	0
57	MG	RA	3068	1/1	0.74	-	45,45,45,45	0
57	MG	RA	3104	1/1	0.43	-	42,42,42,42	0
57	MG	YA	3276	1/1	0.44	-	37,37,37,37	0
57	MG	YA	3158	1/1	0.32	-	69,69,69,69	0
57	MG	YA	3116	1/1	1.20	-	89,89,89,89	0
57	MG	RA	3143	1/1	0.29	-	69,69,69,69	0
57	MG	RA	3201	1/1	1.28	-	128,128,128,128	0
57	MG	XX	101	1/1	0.32	-	64,64,64,64	0
57	MG	YA	3203	1/1	0.26	-	139,139,139,139	0
57	MG	YA	3120	1/1	0.27	-	54,54,54,54	0
57	MG	RA	3228	1/1	0.79	-	25,25,25,25	0
57	MG	RA	3136	1/1	0.37	-	105,105,105,105	0
57	MG	YA	3268	1/1	0.23	-	66,66,66,66	0
57	MG	QA	1611	1/1	0.24	-	28,28,28,28	0
57	MG	YA	3002	1/1	0.47	-	37,37,37,37	0
57	MG	YA	3184	1/1	0.17	-	37,37,37,37	0
57	MG	XA	1630	1/1	0.56	-	33,33,33,33	0
57	MG	RA	3230	1/1	1.07	-	92,92,92,92	0
57	MG	QA	1650	1/1	0.49	-	91,91,91,91	0
57	MG	RA	3239	1/1	0.99	-	90,90,90,90	0
57	MG	YA	3152	1/1	0.49	-	57,57,57,57	0
57	MG	YA	3125	1/1	0.61	-	60,60,60,60	0
57	MG	YA	3207	1/1	0.22	-	116,116,116,116	0
57	MG	YA	3194	1/1	0.84	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3016	1/1	0.19	-	31,31,31,31	0
57	MG	YA	3250	1/1	0.59	-	52,52,52,52	0
57	MG	RA	3178	1/1	0.26	-	99,99,99,99	0
57	MG	XA	1653	1/1	0.39	-	83,83,83,83	0
57	MG	YA	3108	1/1	0.44	-	33,33,33,33	0
57	MG	YA	3036	1/1	0.28	-	38,38,38,38	0
57	MG	XA	1643	1/1	0.23	-	56,56,56,56	0
57	MG	RA	3209	1/1	0.13	-	57,57,57,57	0
57	MG	RA	3076	1/1	0.51	-	28,28,28,28	0
57	MG	YA	3067	1/1	0.27	-	37,37,37,37	0
57	MG	RA	3144	1/1	0.51	-	70,70,70,70	0
57	MG	RA	3044	1/1	1.44	-	75,75,75,75	0
57	MG	RP	202	1/1	0.40	-	64,64,64,64	0
57	MG	RA	3114	1/1	0.24	-	37,37,37,37	0
57	MG	RA	3180	1/1	0.14	-	86,86,86,86	0
57	MG	YA	3053	1/1	0.65	-	51,51,51,51	0
57	MG	RA	3091	1/1	0.68	-	73,73,73,73	0
57	MG	YA	3084	1/1	0.22	-	71,71,71,71	0
57	MG	RA	3165	1/1	0.48	-	82,82,82,82	0
57	MG	YA	3191	1/1	0.20	-	39,39,39,39	0
57	MG	QA	1633	1/1	0.12	-	143,143,143,143	0
57	MG	RA	3204	1/1	0.18	-	167,167,167,167	0
57	MG	RA	3005	1/1	0.61	-	31,31,31,31	0
57	MG	YA	3078	1/1	0.41	-	51,51,51,51	0
59	ZN	XD	301	1/1	0.31	-	52,52,52,52	0
57	MG	YA	3209	1/1	0.30	-	52,52,52,52	0
57	MG	XA	1618	1/1	0.31	-	37,37,37,37	0
57	MG	XA	1667	1/1	0.62	-	75,75,75,75	0
57	MG	QA	1631	1/1	0.45	-	72,72,72,72	0
57	MG	RA	3090	1/1	0.48	-	40,40,40,40	0
57	MG	YA	3105	1/1	0.33	-	31,31,31,31	0
57	MG	YA	3154	1/1	0.24	-	40,40,40,40	0
57	MG	RA	3099	1/1	0.29	-	48,48,48,48	0
57	MG	YA	3004	1/1	0.39	-	50,50,50,50	0
57	MG	RA	3082	1/1	0.70	-	61,61,61,61	0
57	MG	XA	1602	1/1	0.28	-	36,36,36,36	0
57	MG	RA	3174	1/1	0.41	-	36,36,36,36	0
57	MG	RA	3244	1/1	0.26	-	35,35,35,35	0
57	MG	YA	3193	1/1	0.41	-	230,230,230,230	0
57	MG	YA	3107	1/1	0.54	-	26,26,26,26	0
57	MG	XA	1639	1/1	0.11	-	71,71,71,71	0
57	MG	RA	3172	1/1	0.31	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	QA	1653	1/1	0.17	-	79,79,79,79	0
57	MG	RA	3152	1/1	0.25	-	50,50,50,50	0
57	MG	RA	3034	1/1	0.91	-	42,42,42,42	0
57	MG	RA	3179	1/1	0.16	-	113,113,113,113	0
57	MG	RA	3074	1/1	0.21	-	51,51,51,51	0
57	MG	YA	3010	1/1	0.48	-	33,33,33,33	0
57	MG	RP	201	1/1	0.20	-	166,166,166,166	0
57	MG	RA	3112	1/1	0.31	-	78,78,78,78	0
57	MG	XA	1616	1/1	0.30	-	25,25,25,25	0
57	MG	YA	3246	1/1	0.60	-	32,32,32,32	0
57	MG	RA	3160	1/1	0.27	-	39,39,39,39	0
57	MG	RA	3213	1/1	0.29	-	62,62,62,62	0
57	MG	YA	3085	1/1	0.43	-	44,44,44,44	0
57	MG	YA	3062	1/1	0.43	-	51,51,51,51	0
57	MG	YA	3267	1/1	0.73	-	59,59,59,59	0
57	MG	RA	3162	1/1	0.18	-	72,72,72,72	0
57	MG	RA	3088	1/1	0.46	-	59,59,59,59	0
57	MG	XA	1607	1/1	0.28	-	53,53,53,53	0
57	MG	YA	3173	1/1	0.17	-	37,37,37,37	0
57	MG	RA	3168	1/1	0.71	-	44,44,44,44	0
57	MG	XA	1665	1/1	0.34	-	74,74,74,74	0
59	ZN	QN	101	1/1	0.11	-	127,127,127,127	0
57	MG	YA	3043	1/1	0.79	-	27,27,27,27	0
57	MG	YA	3022	1/1	0.39	-	45,45,45,45	0
57	MG	XA	1628	1/1	0.29	-	41,41,41,41	0
57	MG	RA	3023	1/1	0.14	-	32,32,32,32	0
57	MG	QA	1660	1/1	0.32	-	193,193,193,193	0
57	MG	YA	3186	1/1	0.17	-	64,64,64,64	0
57	MG	YA	3264	1/1	0.43	-	75,75,75,75	0
57	MG	QA	1617	1/1	0.29	-	48,48,48,48	0
57	MG	RA	3110	1/1	0.17	-	50,50,50,50	0
57	MG	RA	3085	1/1	0.31	-	55,55,55,55	0
57	MG	RA	3139	1/1	0.26	-	70,70,70,70	0
57	MG	YA	3221	1/1	0.25	-	40,40,40,40	0
57	MG	YA	3095	1/1	0.18	-	49,49,49,49	0
57	MG	RA	3059	1/1	0.40	-	30,30,30,30	0
57	MG	YA	3166	1/1	1.29	-	74,74,74,74	0
57	MG	RA	3094	1/1	0.88	-	28,28,28,28	0
57	MG	RA	3134	1/1	0.39	-	31,31,31,31	0
57	MG	XA	1608	1/1	0.53	-	119,119,119,119	0
57	MG	YA	3169	1/1	0.27	-	93,93,93,93	0
57	MG	YA	3153	1/1	0.80	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3165	1/1	0.32	-	77,77,77,77	0
57	MG	YA	3028	1/1	0.33	-	25,25,25,25	0
57	MG	YA	3001	1/1	0.69	-	38,38,38,38	0
57	MG	YA	3181	1/1	0.26	-	32,32,32,32	0
57	MG	YA	3003	1/1	0.29	-	42,42,42,42	0
57	MG	RA	3029	1/1	0.29	-	35,35,35,35	0
57	MG	YA	3256	1/1	0.29	-	128,128,128,128	0
57	MG	YA	3171	1/1	0.63	-	33,33,33,33	0
57	MG	RA	3241	1/1	0.37	-	46,46,46,46	0
57	MG	RA	3148	1/1	0.39	-	90,90,90,90	0
57	MG	XA	1649	1/1	0.30	-	61,61,61,61	0
57	MG	QA	1659	1/1	0.40	-	70,70,70,70	0
57	MG	QA	1629	1/1	0.34	-	85,85,85,85	0
57	MG	YA	3211	1/1	0.39	-	72,72,72,72	0
57	MG	XA	1638	1/1	0.12	-	59,59,59,59	0
57	MG	YA	3144	1/1	0.26	-	62,62,62,62	0
57	MG	RA	3173	1/1	0.14	-	38,38,38,38	0
57	MG	YA	3092	1/1	0.30	-	25,25,25,25	0
57	MG	XA	1662	1/1	0.73	-	61,61,61,61	0
57	MG	YD	301	1/1	0.44	-	42,42,42,42	0
57	MG	XA	1624	1/1	0.52	-	42,42,42,42	0
57	MG	RA	3125	1/1	0.15	-	48,48,48,48	0
57	MG	YA	3240	1/1	0.89	-	52,52,52,52	0
57	MG	XA	1626	1/1	0.43	-	59,59,59,59	0
57	MG	RA	3210	1/1	0.36	-	74,74,74,74	0
57	MG	RA	3051	1/1	0.29	-	27,27,27,27	0
57	MG	XA	1658	1/1	0.54	-	101,101,101,101	0
57	MG	QA	1634	1/1	0.84	-	53,53,53,53	0
57	MG	QA	1652	1/1	0.61	-	77,77,77,77	0
57	MG	RA	3013	1/1	0.47	-	27,27,27,27	0
57	MG	RA	3022	1/1	0.14	-	30,30,30,30	0
57	MG	YA	3177	1/1	0.64	-	51,51,51,51	0
57	MG	RA	3079	1/1	0.35	-	48,48,48,48	0
57	MG	RA	3128	1/1	0.37	-	91,91,91,91	0
57	MG	RA	3138	1/1	1.55	-	95,95,95,95	0
57	MG	XV	101	1/1	0.30	-	49,49,49,49	0
57	MG	RA	3208	1/1	0.42	-	74,74,74,74	0
57	MG	RA	3052	1/1	0.26	-	27,27,27,27	0
57	MG	YA	3247	1/1	1.00	-	29,29,29,29	0
57	MG	YA	3150	1/1	0.40	-	114,114,114,114	0
57	MG	XA	1635	1/1	0.87	-	74,74,74,74	0
57	MG	YA	3051	1/1	0.47	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3046	1/1	0.74	-	35,35,35,35	0
57	MG	RA	3083	1/1	0.18	-	50,50,50,50	0
57	MG	YA	3018	1/1	0.58	-	48,48,48,48	0
57	MG	XA	1641	1/1	0.27	-	74,74,74,74	0
57	MG	RA	3131	1/1	0.20	-	57,57,57,57	0
57	MG	YA	3210	1/1	0.47	-	135,135,135,135	0
57	MG	RA	3115	1/1	0.41	-	82,82,82,82	0
57	MG	YA	3115	1/1	0.33	-	64,64,64,64	0
57	MG	XV	102	1/1	0.31	-	61,61,61,61	0
57	MG	YA	3147	1/1	0.19	-	75,75,75,75	0
57	MG	YA	3061	1/1	0.14	-	26,26,26,26	0
57	MG	YA	3237	1/1	0.56	-	52,52,52,52	0
57	MG	QA	1643	1/1	0.35	-	67,67,67,67	0
57	MG	RA	3145	1/1	0.24	-	43,43,43,43	0
57	MG	RA	3185	1/1	0.60	-	48,48,48,48	0
57	MG	YA	3187	1/1	0.51	-	73,73,73,73	0
57	MG	XA	1642	1/1	0.44	-	41,41,41,41	0
57	MG	RA	3037	1/1	0.43	-	32,32,32,32	0
57	MG	YA	3141	1/1	0.34	-	69,69,69,69	0
57	MG	YA	3174	1/1	0.25	-	53,53,53,53	0
57	MG	YA	3006	1/1	0.69	-	59,59,59,59	0
57	MG	RA	3147	1/1	0.30	-	120,120,120,120	0
57	MG	YA	3012	1/1	0.95	-	36,36,36,36	0
57	MG	RA	3004	1/1	0.71	-	39,39,39,39	0
57	MG	YA	3046	1/1	0.63	-	38,38,38,38	0
57	MG	YA	3180	1/1	0.47	-	79,79,79,79	0
57	MG	YA	3128	1/1	0.15	-	52,52,52,52	0
57	MG	XA	1648	1/1	0.21	-	75,75,75,75	0
57	MG	YA	3014	1/1	0.40	-	29,29,29,29	0
57	MG	XA	1655	1/1	0.87	-	53,53,53,53	0
57	MG	RA	3078	1/1	0.64	-	54,54,54,54	0
57	MG	RA	3035	1/1	0.52	-	43,43,43,43	0
57	MG	YA	3059	1/1	0.21	-	45,45,45,45	0
57	MG	RA	3127	1/1	0.39	-	74,74,74,74	0
57	MG	QA	1618	1/1	0.52	-	47,47,47,47	0
57	MG	RA	3043	1/1	0.22	-	47,47,47,47	0
57	MG	YA	3007	1/1	0.21	-	40,40,40,40	0
57	MG	YA	3099	1/1	0.58	-	32,32,32,32	0
57	MG	RA	3100	1/1	0.28	-	43,43,43,43	0
57	MG	RA	3053	1/1	0.33	-	33,33,33,33	0
57	MG	XA	1640	1/1	0.85	-	43,43,43,43	0
57	MG	QA	1640	1/1	0.39	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	XA	1651	1/1	0.28	-	111,111,111,111	0
57	MG	RA	3072	1/1	0.30	-	54,54,54,54	0
57	MG	RA	3154	1/1	0.34	-	42,42,42,42	0
57	MG	QA	1662	1/1	0.18	-	100,100,100,100	0
57	MG	XY	101	1/1	0.16	-	74,74,74,74	0
57	MG	RA	3191	1/1	0.23	-	34,34,34,34	0
57	MG	YA	3087	1/1	0.54	-	29,29,29,29	0
57	MG	RA	3012	1/1	0.32	-	45,45,45,45	0
57	MG	YA	3239	1/1	0.19	-	85,85,85,85	0
57	MG	QA	1627	1/1	0.26	-	33,33,33,33	0
57	MG	YA	3088	1/1	0.35	-	26,26,26,26	0
57	MG	XA	1610	1/1	0.32	-	32,32,32,32	0
57	MG	QA	1623	1/1	0.45	-	79,79,79,79	0
57	MG	RA	3234	1/1	0.34	-	48,48,48,48	0
57	MG	XA	1660	1/1	0.22	-	77,77,77,77	0
57	MG	XM	201	1/1	0.41	-	173,173,173,173	0
57	MG	YE	302	1/1	0.33	-	31,31,31,31	0
57	MG	RA	3246	1/1	0.30	-	198,198,198,198	0
57	MG	YA	3112	1/1	0.26	-	47,47,47,47	0
57	MG	YA	3029	1/1	0.81	-	39,39,39,39	0
57	MG	RA	3018	1/1	0.58	-	32,32,32,32	0
57	MG	XA	1620	1/1	0.29	-	83,83,83,83	0
57	MG	YA	3231	1/1	0.46	-	79,79,79,79	0
57	MG	YA	3033	1/1	0.50	-	28,28,28,28	0
57	MG	YA	3133	1/1	0.14	-	50,50,50,50	0
57	MG	XA	1647	1/1	0.38	-	49,49,49,49	0
57	MG	YA	3126	1/1	0.44	-	46,46,46,46	0
57	MG	RA	3171	1/1	0.35	-	85,85,85,85	0
57	MG	YA	3199	1/1	0.27	-	54,54,54,54	0
57	MG	XA	1659	1/1	0.55	-	102,102,102,102	0
57	MG	QA	1642	1/1	0.35	-	56,56,56,56	0
57	MG	RA	3181	1/1	0.19	-	49,49,49,49	0
57	MG	RA	3199	1/1	0.73	-	56,56,56,56	0
57	MG	YA	3242	1/1	0.83	-	46,46,46,46	0
57	MG	RA	3025	1/1	0.10	-	34,34,34,34	0
57	MG	YA	3025	1/1	0.43	-	31,31,31,31	0
57	MG	YA	3079	1/1	0.25	-	26,26,26,26	0
57	MG	RA	3224	1/1	0.54	-	91,91,91,91	0
57	MG	YA	3132	1/1	0.23	-	56,56,56,56	0
57	MG	RA	3095	1/1	0.44	-	34,34,34,34	0
57	MG	RA	3101	1/1	0.31	-	56,56,56,56	0
57	MG	RA	3065	1/1	0.49	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3215	1/1	0.33	-	61,61,61,61	0
57	MG	YA	3082	1/1	0.24	-	44,44,44,44	0
57	MG	YA	3069	1/1	0.45	-	29,29,29,29	0
57	MG	YA	3255	1/1	0.73	-	34,34,34,34	0
57	MG	XA	1671	1/1	0.26	-	76,76,76,76	0
57	MG	XA	1637	1/1	0.22	-	59,59,59,59	0
57	MG	RA	3216	1/1	0.78	-	110,110,110,110	0
57	MG	RA	3092	1/1	0.43	-	71,71,71,71	0
57	MG	QA	1639	1/1	0.37	-	49,49,49,49	0
57	MG	RA	3215	1/1	0.33	-	68,68,68,68	0
57	MG	QA	1626	1/1	0.19	-	156,156,156,156	0
57	MG	YA	3146	1/1	0.24	-	48,48,48,48	0
57	MG	RA	3151	1/1	0.23	-	69,69,69,69	0
57	MG	YA	3090	1/1	0.15	-	30,30,30,30	0
57	MG	QA	1615	1/1	0.43	-	88,88,88,88	0
57	MG	YB	205	1/1	0.25	-	231,231,231,231	0
57	MG	RA	3161	1/1	1.46	-	76,76,76,76	0
57	MG	RA	3097	1/1	0.56	-	44,44,44,44	0
57	MG	QA	1646	1/1	0.09	-	65,65,65,65	0
57	MG	YA	3074	1/1	0.26	-	33,33,33,33	0
57	MG	RA	3084	1/1	0.36	-	28,28,28,28	0
57	MG	YA	3102	1/1	0.14	-	27,27,27,27	0
57	MG	RA	3109	1/1	0.16	-	51,51,51,51	0
57	MG	RA	3014	1/1	0.18	-	64,64,64,64	0
57	MG	QA	1606	1/1	0.21	-	57,57,57,57	0
57	MG	YA	3142	1/1	0.68	-	50,50,50,50	0
57	MG	XA	1605	1/1	0.67	-	45,45,45,45	0
57	MG	RA	3054	1/1	0.21	-	85,85,85,85	0
57	MG	RA	3156	1/1	0.19	-	48,48,48,48	0
57	MG	RA	3149	1/1	0.14	-	29,29,29,29	0
57	MG	QA	1655	1/1	0.64	-	74,74,74,74	0
57	MG	YA	3273	1/1	0.85	-	55,55,55,55	0
57	MG	XA	1646	1/1	0.18	-	49,49,49,49	0
57	MG	YA	3129	1/1	0.07	-	59,59,59,59	0
57	MG	YA	3015	1/1	0.60	-	29,29,29,29	0
57	MG	RA	3020	1/1	0.79	-	33,33,33,33	0
57	MG	YA	3114	1/1	0.30	-	27,27,27,27	0
58	PAR	XA	1672	42/42	0.26	-	66,66,66,66	0
57	MG	YA	3225	1/1	0.30	-	67,67,67,67	0
57	MG	RA	3108	1/1	0.34	-	43,43,43,43	0
57	MG	XA	1631	1/1	0.29	-	68,68,68,68	0
57	MG	RA	3027	1/1	0.26	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3063	1/1	0.41	-	27,27,27,27	0
57	MG	RA	3019	1/1	0.37	-	61,61,61,61	0
57	MG	YA	3216	1/1	0.18	-	72,72,72,72	0
57	MG	YA	3223	1/1	0.17	-	59,59,59,59	0
57	MG	XA	1636	1/1	0.27	-	36,36,36,36	0
57	MG	YA	3057	1/1	0.77	-	33,33,33,33	0
57	MG	YA	3266	1/1	0.59	-	64,64,64,64	0
57	MG	YA	3263	1/1	0.57	-	60,60,60,60	0
57	MG	YA	3228	1/1	0.40	-	59,59,59,59	0
57	MG	YA	3233	1/1	0.53	-	58,58,58,58	0
57	MG	RA	3177	1/1	0.79	-	72,72,72,72	0
57	MG	XB	301	1/1	0.46	-	87,87,87,87	0
57	MG	RA	3200	1/1	0.23	-	76,76,76,76	0
57	MG	YA	3121	1/1	0.26	-	32,32,32,32	0
57	MG	RA	3137	1/1	0.32	-	42,42,42,42	0
57	MG	YA	3136	1/1	0.23	-	39,39,39,39	0
57	MG	QA	1637	1/1	0.11	-	53,53,53,53	0
57	MG	RA	3117	1/1	0.34	-	84,84,84,84	0
57	MG	QA	1664	1/1	0.48	-	78,78,78,78	0
57	MG	RA	3157	1/1	0.55	-	54,54,54,54	0
57	MG	RA	3245	1/1	0.76	-	128,128,128,128	0
57	MG	RA	3060	1/1	0.30	-	44,44,44,44	0
57	MG	RA	3183	1/1	0.10	-	67,67,67,67	0
57	MG	YA	3091	1/1	0.21	-	37,37,37,37	0
57	MG	QA	1632	1/1	0.15	-	69,69,69,69	0
57	MG	RA	3130	1/1	0.11	-	64,64,64,64	0
57	MG	XA	1609	1/1	0.43	-	35,35,35,35	0
57	MG	YA	3234	1/1	0.12	-	147,147,147,147	0
57	MG	RA	3221	1/1	0.37	-	50,50,50,50	0
57	MG	Y5	101	1/1	1.30	-	162,162,162,162	0
57	MG	RA	3011	1/1	0.79	-	52,52,52,52	0
57	MG	YA	3073	1/1	0.40	-	37,37,37,37	0
57	MG	YB	202	1/1	0.84	-	70,70,70,70	0
57	MG	YA	3243	1/1	0.45	-	60,60,60,60	0
57	MG	YA	3275	1/1	0.71	-	35,35,35,35	0
57	MG	YA	3089	1/1	0.43	-	53,53,53,53	0
57	MG	RA	3122	1/1	0.89	-	45,45,45,45	0
59	ZN	Y9	300	1/1	0.08	-	101,101,101,101	0
57	MG	YA	3175	1/1	0.51	-	38,38,38,38	0
57	MG	YA	3200	1/1	0.53	-	58,58,58,58	0
57	MG	YA	3032	1/1	0.35	-	28,28,28,28	0
57	MG	XA	1629	1/1	0.36	-	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3106	1/1	0.23	-	32,32,32,32	0
57	MG	YA	3238	1/1	0.17	-	36,36,36,36	0
57	MG	RA	3056	1/1	0.45	-	38,38,38,38	0
57	MG	XA	1613	1/1	0.19	-	50,50,50,50	0
57	MG	YA	3178	1/1	0.43	-	64,64,64,64	0
57	MG	YA	3157	1/1	0.24	-	42,42,42,42	0
57	MG	YA	3072	1/1	0.29	-	30,30,30,30	0
57	MG	YA	3185	1/1	0.15	-	61,61,61,61	0
57	MG	RA	3197	1/1	0.79	-	84,84,84,84	0
57	MG	RA	3096	1/1	0.31	-	36,36,36,36	0
57	MG	YA	3190	1/1	0.75	-	51,51,51,51	0
57	MG	XA	1601	1/1	0.73	-	29,29,29,29	0
57	MG	QA	1607	1/1	0.34	-	124,124,124,124	0
57	MG	R0	101	1/1	0.61	-	78,78,78,78	0
57	MG	RA	3214	1/1	0.42	-	119,119,119,119	0
57	MG	RA	3203	1/1	0.53	-	74,74,74,74	0
57	MG	XA	1622	1/1	0.14	-	49,49,49,49	0
57	MG	YA	3068	1/1	0.46	-	42,42,42,42	0
57	MG	XA	1663	1/1	0.30	-	75,75,75,75	0
57	MG	QA	1645	1/1	0.20	-	55,55,55,55	0
57	MG	RA	3009	1/1	0.29	-	68,68,68,68	0
57	MG	RA	3111	1/1	0.24	-	48,48,48,48	0
57	MG	RA	3006	1/1	0.51	-	25,25,25,25	0
57	MG	QA	1644	1/1	0.63	-	114,114,114,114	0
57	MG	RA	3017	1/1	0.36	-	52,52,52,52	0
57	MG	YA	3183	1/1	0.49	-	67,67,67,67	0
57	MG	YA	3054	1/1	0.43	-	65,65,65,65	0
57	MG	RA	3047	1/1	0.44	-	26,26,26,26	0
57	MG	QA	1604	1/1	0.28	-	30,30,30,30	0
57	MG	YA	3110	1/1	0.27	-	45,45,45,45	0
57	MG	YA	3214	1/1	0.40	-	244,244,244,244	0
57	MG	RA	3045	1/1	0.19	-	27,27,27,27	0
57	MG	YA	3100	1/1	0.47	-	40,40,40,40	0
57	MG	QA	1628	1/1	0.27	-	103,103,103,103	0
57	MG	QA	1666	1/1	0.54	-	57,57,57,57	0
57	MG	YA	3140	1/1	0.26	-	33,33,33,33	0
57	MG	YB	201	1/1	0.35	-	57,57,57,57	0
57	MG	YA	3224	1/1	0.17	-	44,44,44,44	0
57	MG	YA	3052	1/1	0.52	-	41,41,41,41	0
57	MG	XA	1670	1/1	0.39	-	47,47,47,47	0
57	MG	RA	3063	1/1	1.07	-	43,43,43,43	0
57	MG	YA	3269	1/1	0.29	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3167	1/1	0.28	-	69,69,69,69	0
57	MG	YA	3252	1/1	0.37	-	42,42,42,42	0
57	MG	YX	101	1/1	0.18	-	196,196,196,196	0
57	MG	YA	3071	1/1	0.16	-	37,37,37,37	0
57	MG	QA	1614	1/1	0.74	-	76,76,76,76	0
57	MG	YA	3050	1/1	0.40	-	25,25,25,25	0
57	MG	QA	1601	1/1	0.43	-	36,36,36,36	0
57	MG	XA	1627	1/1	0.30	-	43,43,43,43	0
57	MG	QA	1621	1/1	0.16	-	51,51,51,51	0
57	MG	XA	1669	1/1	0.22	-	155,155,155,155	0
57	MG	YA	3201	1/1	0.36	-	61,61,61,61	0
57	MG	YA	3248	1/1	0.31	-	27,27,27,27	0
57	MG	RA	3107	1/1	0.23	-	45,45,45,45	0
57	MG	YA	3260	1/1	0.59	-	67,67,67,67	0
57	MG	RA	3233	1/1	0.34	-	33,33,33,33	0
57	MG	YA	3257	1/1	0.87	-	42,42,42,42	0
57	MG	RA	3015	1/1	0.48	-	26,26,26,26	0
57	MG	RA	3175	1/1	0.91	-	57,57,57,57	0
57	MG	YA	3122	1/1	0.63	-	30,30,30,30	0
57	MG	RA	3055	1/1	0.75	-	34,34,34,34	0
57	MG	RA	3098	1/1	0.20	-	65,65,65,65	0
57	MG	XA	1644	1/1	0.37	-	60,60,60,60	0
57	MG	YA	3042	1/1	0.38	-	45,45,45,45	0
57	MG	RA	3129	1/1	0.67	-	45,45,45,45	0
57	MG	YA	3009	1/1	0.66	-	25,25,25,25	0
57	MG	RA	3140	1/1	0.24	-	74,74,74,74	0
57	MG	RA	3189	1/1	0.19	-	96,96,96,96	0
57	MG	YA	3236	1/1	0.33	-	52,52,52,52	0
57	MG	YA	3241	1/1	0.27	-	54,54,54,54	0
57	MG	XA	1604	1/1	1.03	-	64,64,64,64	0
57	MG	QA	1622	1/1	0.28	-	103,103,103,103	0
57	MG	RA	3186	1/1	0.63	-	72,72,72,72	0
57	MG	QA	1625	1/1	0.82	-	92,92,92,92	0
57	MG	YA	3197	1/1	0.14	-	42,42,42,42	0
57	MG	YA	3195	1/1	0.24	-	88,88,88,88	0
57	MG	YA	3086	1/1	0.53	-	28,28,28,28	0
57	MG	RA	3167	1/1	0.17	-	54,54,54,54	0
57	MG	RA	3226	1/1	0.30	-	63,63,63,63	0
57	MG	XA	1664	1/1	0.24	-	51,51,51,51	0
57	MG	QA	1602	1/1	0.52	-	39,39,39,39	0
57	MG	YA	3139	1/1	0.91	-	57,57,57,57	0
57	MG	YA	3077	1/1	0.29	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3229	1/1	0.31	-	36,36,36,36	0
57	MG	QA	1668	1/1	0.08	-	101,101,101,101	0
57	MG	RA	3202	1/1	0.70	-	32,32,32,32	0
57	MG	YA	3137	1/1	0.19	-	27,27,27,27	0
57	MG	YA	3202	1/1	0.39	-	54,54,54,54	0
57	MG	YA	3070	1/1	0.25	-	50,50,50,50	0
57	MG	QA	1612	1/1	0.50	-	44,44,44,44	0
57	MG	RA	3069	1/1	0.51	-	49,49,49,49	0
57	MG	RA	3050	1/1	0.37	-	46,46,46,46	0
57	MG	YA	3119	1/1	0.28	-	52,52,52,52	0
57	MG	RA	3118	1/1	0.58	-	44,44,44,44	0
57	MG	YA	3130	1/1	0.15	-	84,84,84,84	0
57	MG	RA	3193	1/1	0.33	-	87,87,87,87	0
57	MG	RA	3033	1/1	0.47	-	49,49,49,49	0
57	MG	YA	3008	1/1	0.32	-	48,48,48,48	0
57	MG	RA	3003	1/1	0.43	-	28,28,28,28	0
57	MG	RA	3132	1/1	0.44	-	66,66,66,66	0
57	MG	YA	3027	1/1	0.19	-	38,38,38,38	0
57	MG	XA	1611	1/1	0.30	-	28,28,28,28	0
57	MG	RA	3243	1/1	0.62	-	32,32,32,32	0
57	MG	YA	3135	1/1	0.39	-	65,65,65,65	0
59	ZN	R5	102	1/1	0.07	-	306,306,306,306	0
57	MG	YA	3097	1/1	0.21	-	29,29,29,29	0
57	MG	RA	3212	1/1	0.51	-	89,89,89,89	0
57	MG	RA	3010	1/1	0.37	-	89,89,89,89	0
57	MG	YA	3064	1/1	0.23	-	29,29,29,29	0
57	MG	RA	3220	1/1	0.59	-	83,83,83,83	0
57	MG	RA	3155	1/1	0.67	-	71,71,71,71	0
57	MG	RA	3086	1/1	0.77	-	53,53,53,53	0
57	MG	YA	3206	1/1	0.43	-	88,88,88,88	0
57	MG	YA	3159	1/1	0.37	-	34,34,34,34	0
57	MG	YA	3031	1/1	0.79	-	37,37,37,37	0
57	MG	RA	3030	1/1	0.23	-	35,35,35,35	0
57	MG	QV	101	1/1	0.14	-	48,48,48,48	0
57	MG	QA	1648	1/1	0.06	-	93,93,93,93	0
57	MG	YA	3155	1/1	0.26	-	44,44,44,44	0
57	MG	RA	3007	1/1	0.54	-	59,59,59,59	0
57	MG	RA	3064	1/1	0.30	-	48,48,48,48	0
57	MG	RA	3048	1/1	0.45	-	47,47,47,47	0
57	MG	QA	1624	1/1	0.97	-	68,68,68,68	0
57	MG	YA	3098	1/1	0.57	-	29,29,29,29	0
57	MG	XA	1606	1/1	0.52	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3182	1/1	0.07	-	53,53,53,53	0
57	MG	QA	1651	1/1	0.32	-	49,49,49,49	0
57	MG	RA	3120	1/1	0.13	-	49,49,49,49	0
57	MG	YA	3163	1/1	0.19	-	48,48,48,48	0
57	MG	YA	3172	1/1	0.09	-	62,62,62,62	0
57	MG	YB	204	1/1	0.62	-	37,37,37,37	0
57	MG	YA	3005	1/1	0.22	-	26,26,26,26	0
57	MG	RA	3093	1/1	0.49	-	34,34,34,34	0
57	MG	QY	101	1/1	0.13	-	83,83,83,83	0
57	MG	RA	3057	1/1	0.52	-	133,133,133,133	0
57	MG	RA	3169	1/1	0.18	-	47,47,47,47	0
57	MG	YA	3156	1/1	0.35	-	58,58,58,58	0
57	MG	YA	3204	1/1	0.54	-	182,182,182,182	0
57	MG	RE	301	1/1	0.25	-	58,58,58,58	0
57	MG	QA	1663	1/1	0.19	-	40,40,40,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.