



wwPDB X-ray Structure Validation Summary Report

Sep 18, 2014 – 03:32 AM EDT

PDB ID : 4LT8
Title : Crystal Structure of tRNA Proline (CGG) Bound to Codon CCC-G on the Ribosome
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-07-23
Resolution : 3.14 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>

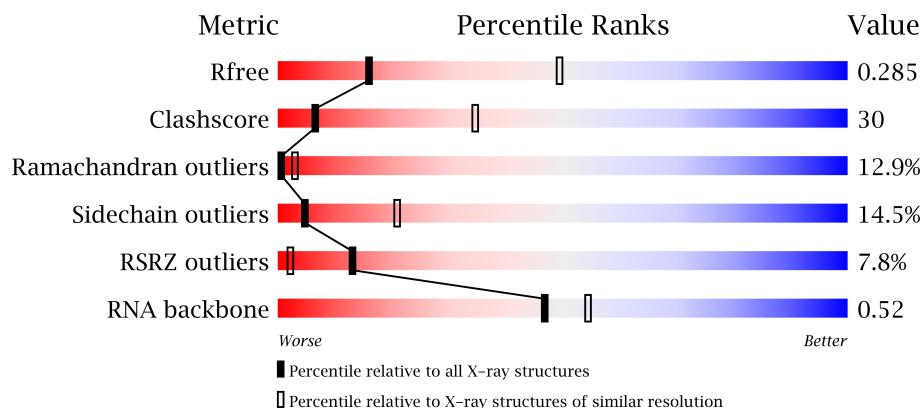
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.14 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	1337 (3.20-3.08)
Clashscore	79885	1656 (3.20-3.08)
Ramachandran outliers	78287	1614 (3.20-3.08)
Sidechain outliers	78261	1613 (3.20-3.08)
RSRZ outliers	66119	1338 (3.20-3.08)
RNA backbone	1838	1002 (3.66-2.62)

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	QY	17	
23	XY	17	
24	QX	25	
24	XX	25	
25	RA	2916	
25	YA	2916	
26	RB	122	
26	YB	122	
27	RD	276	

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

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

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291998 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QY	15	Total	C	N	O	P	0	0	0
			323	144	58	106	15			
23	XY	15	Total	C	N	O	P	0	0	0
			323	144	58	106	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QX	8	Total	C	N	O	P	0	0	0
			170	76	31	55	8			
24	XX	8	Total	C	N	O	P	0	0	0
			170	76	31	55	8			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 33 is a protein called 50S ribosomal protein L11.

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 L13.

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 L14.

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 L15.

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 L16.

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 L17.

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

- Molecule 39 is a protein called 50S ribosomal protein L18.

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 L19.

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 L20.

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 L21.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

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 L24.

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 L25.

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 L27.

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

- Molecule 48 is a protein called 50S ribosomal protein L28.

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 L29.

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 L30.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

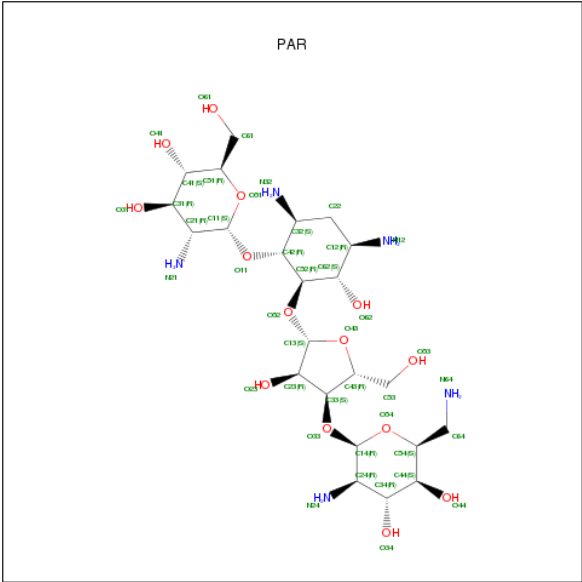
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	69	Total	Mg	0	0
			69	69		
57	RP	1	Total	Mg	0	0
			1	1		
57	YA	265	Total	Mg	0	0
			265	265		
57	QM	1	Total	Mg	0	0
			1	1		
57	XX	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QV	1	Total 1	Mg 1	0	0
57	XA	74	Total 74	Mg 74	0	0
57	R0	1	Total 1	Mg 1	0	0
57	QH	1	Total 1	Mg 1	0	0
57	YQ	1	Total 1	Mg 1	0	0
57	RR	2	Total 2	Mg 2	0	0
57	RD	1	Total 1	Mg 1	0	0
57	Y7	1	Total 1	Mg 1	0	0
57	QF	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	Y0	1	Total 1	Mg 1	0	0
57	RA	240	Total 240	Mg 240	0	0
57	YP	1	Total 1	Mg 1	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	RE	2	Total 2	Mg 2	0	0
57	YB	3	Total 3	Mg 3	0	0
57	XV	2	Total 2	Mg 2	0	0
57	RB	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0
57	YE	2	Total 2	Mg 2	0	0

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



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

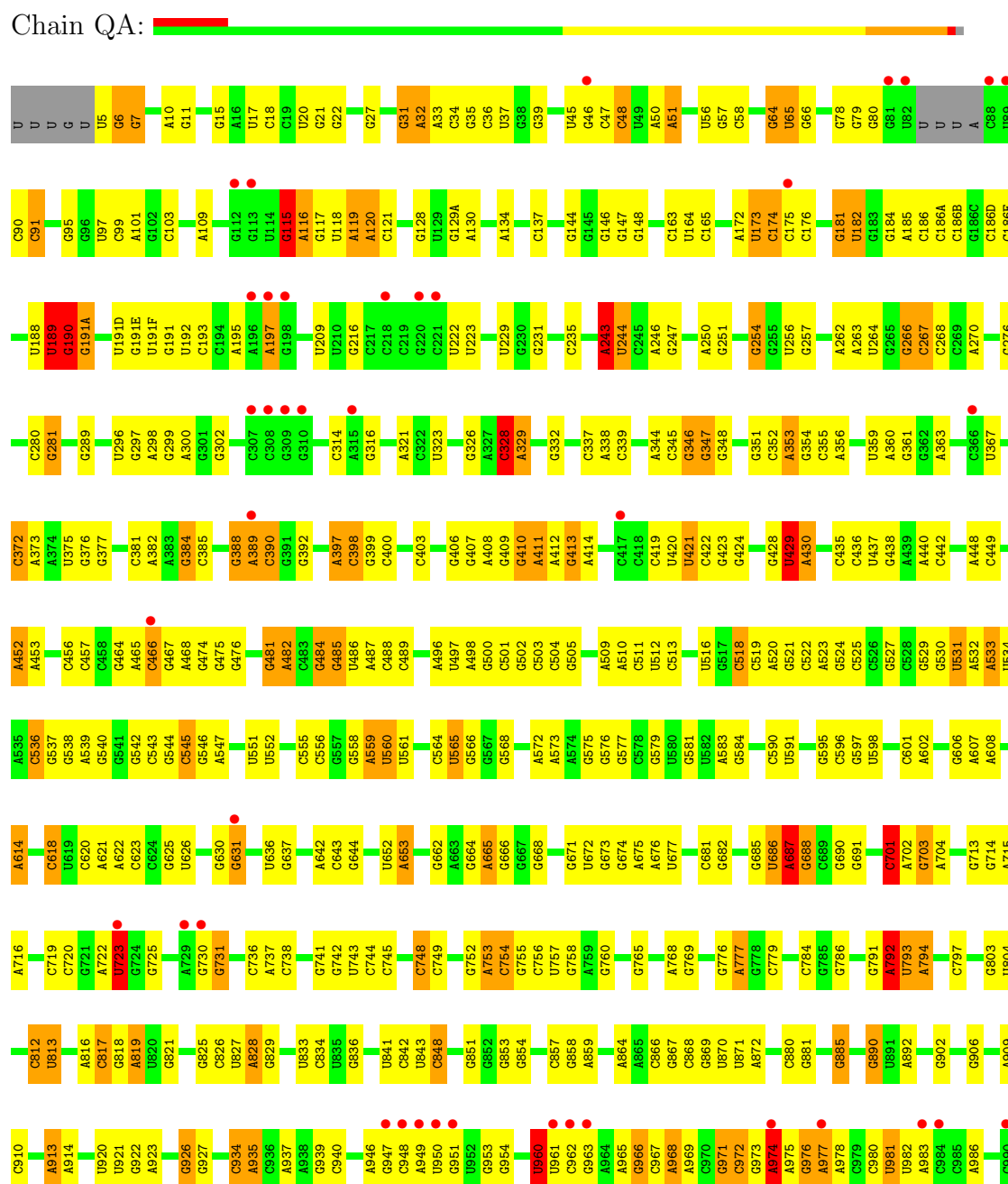
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

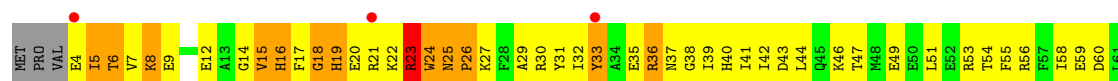
3 Residue-property plots

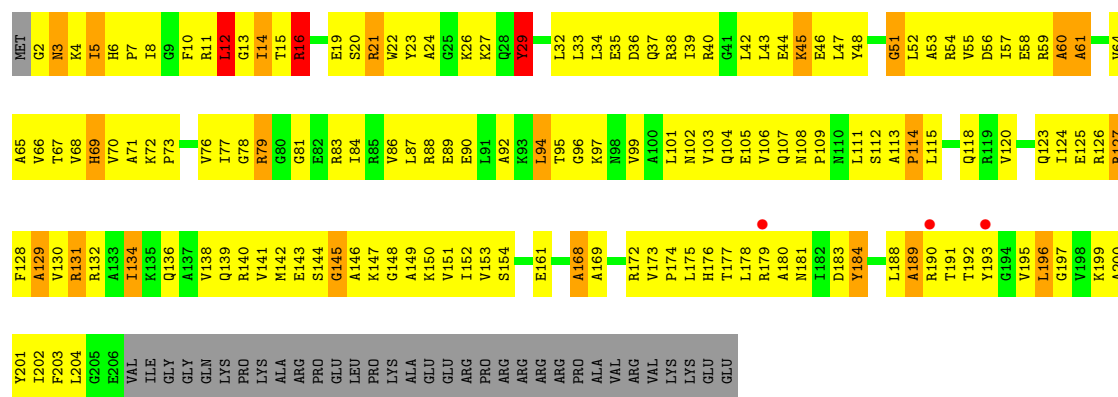
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 rRNA



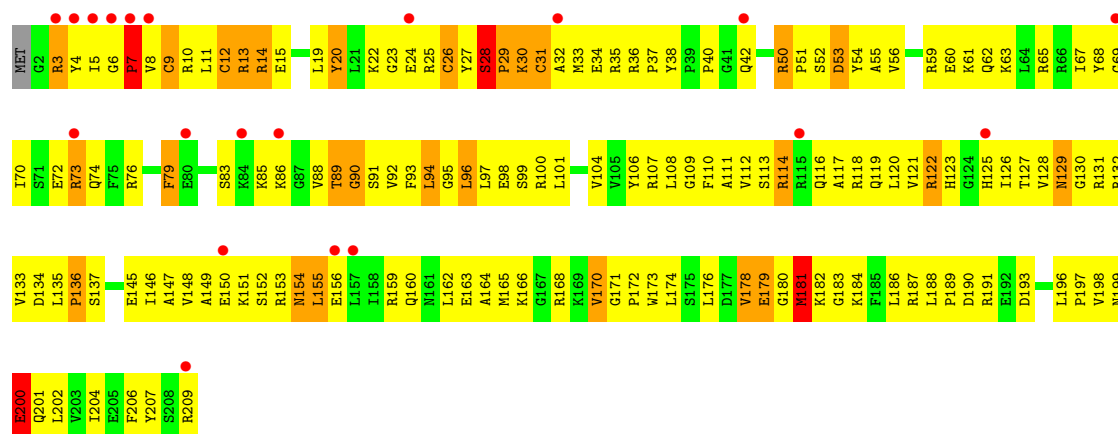






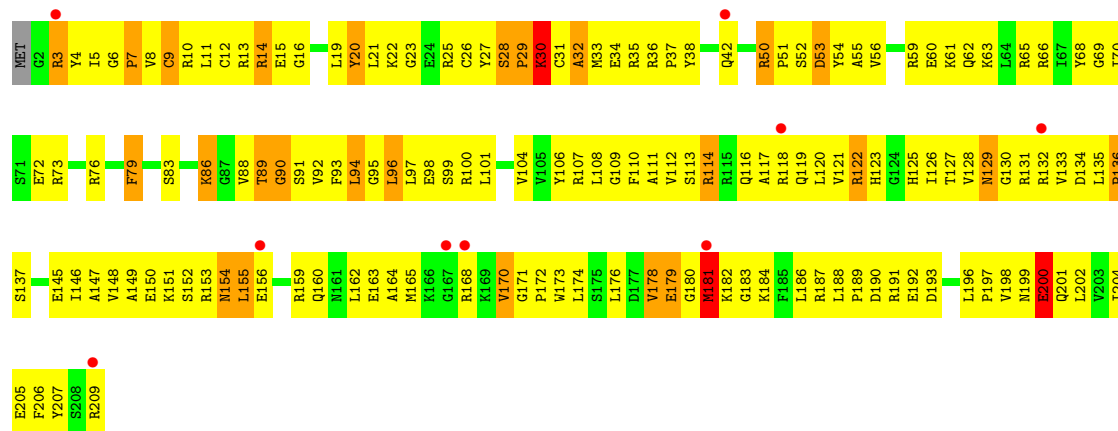
• Molecule 4: 30S ribosomal protein S4

Chain QD:



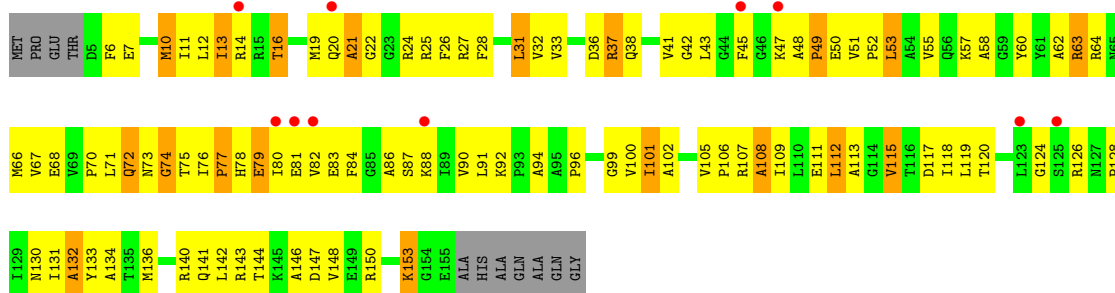
• Molecule 4: 30S ribosomal protein S4

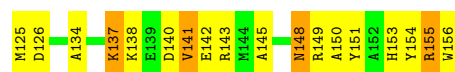
Chain XD:



• Molecule 5: 30S ribosomal protein S5

Chain QE:





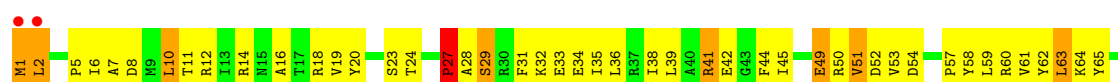
• Molecule 7: 30S ribosomal protein S7

Chain XG:



• Molecule 8: 30S ribosomal protein S8

Chain QH:



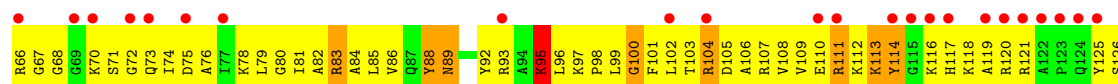
• Molecule 8: 30S ribosomal protein S8

Chain XH:



• Molecule 9: 30S ribosomal protein S9

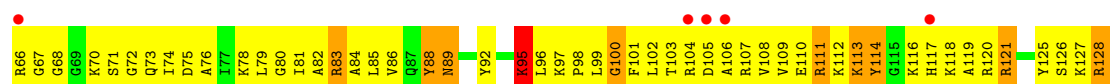
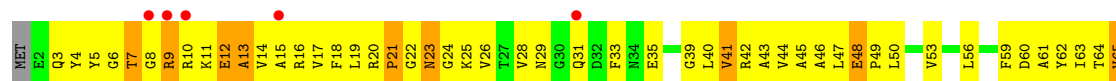
Chain QI:





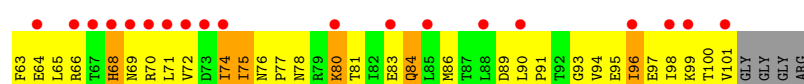
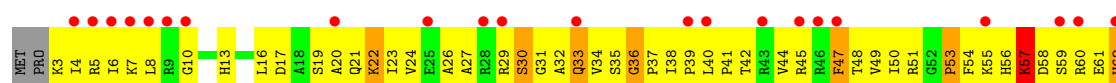
• Molecule 9: 30S ribosomal protein S9

Chain XI:



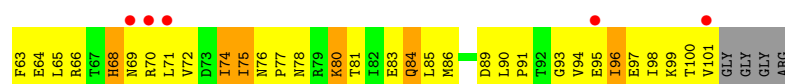
• Molecule 10: 30S ribosomal protein S10

Chain QJ:



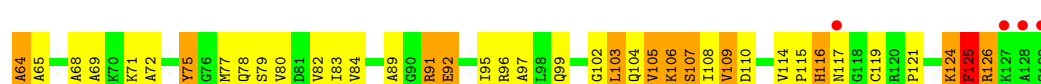
• Molecule 10: 30S ribosomal protein S10

Chain XJ:



• Molecule 11: 30S ribosomal protein S11

Chain QK:



• Molecule 11: 30S ribosomal protein S11

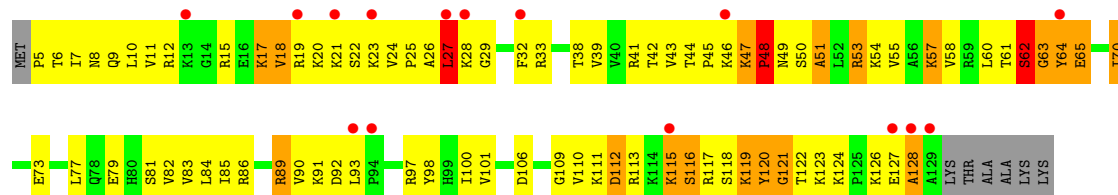
Chain XK:





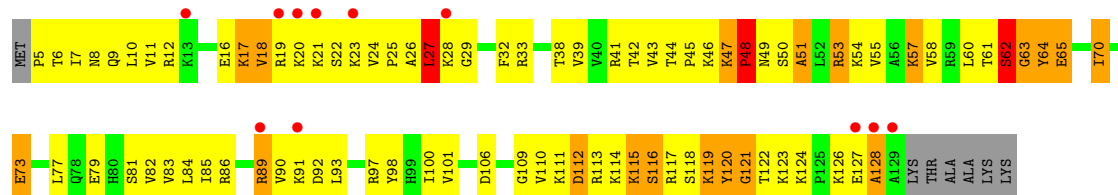
- Molecule 12: 30S ribosomal protein S12

Chain QL:



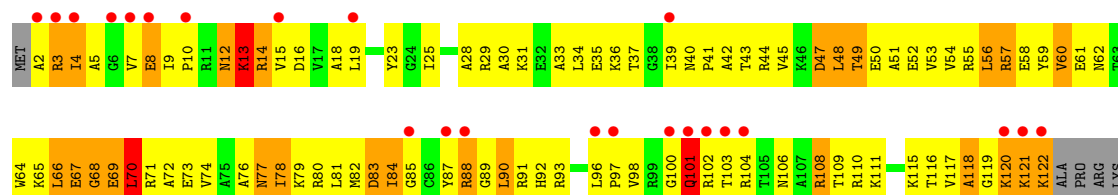
- Molecule 12: 30S ribosomal protein S12

Chain XL:



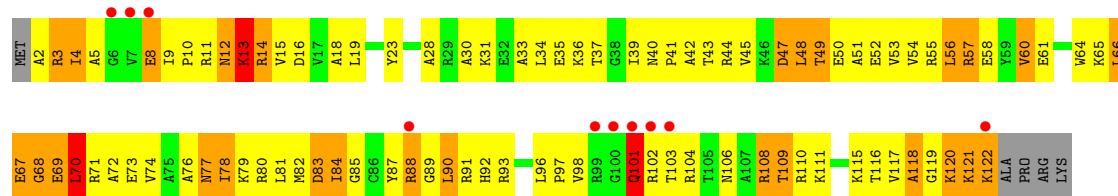
- Molecule 13: 30S ribosomal protein S13

Chain QM:



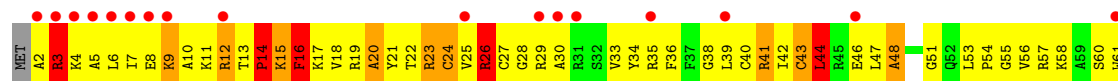
- Molecule 13: 30S ribosomal protein S13

Chain XM:



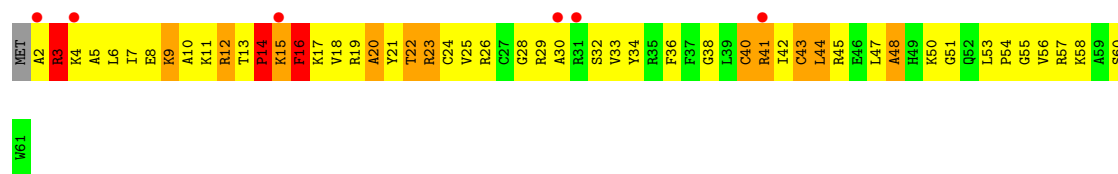
- Molecule 14: 30S ribosomal protein S14

Chain QN:



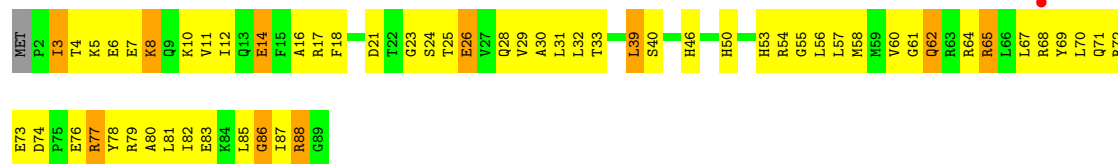
- Molecule 14: 30S ribosomal protein S14

Chain XN:



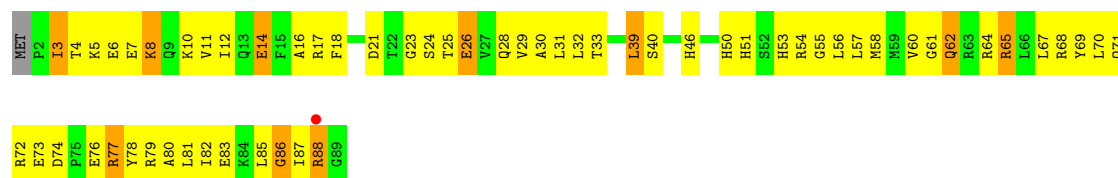
- Molecule 15: 30S ribosomal protein S15

Chain QO:



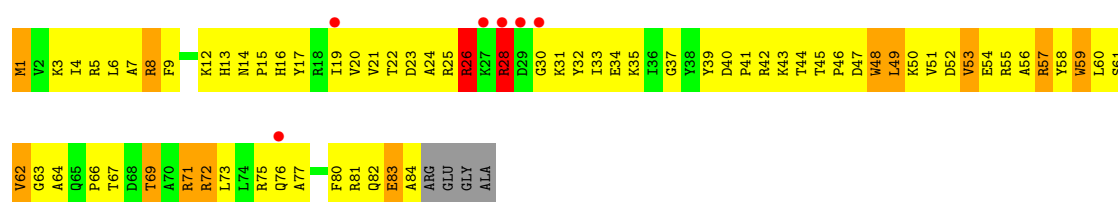
- Molecule 15: 30S ribosomal protein S15

Chain XO:



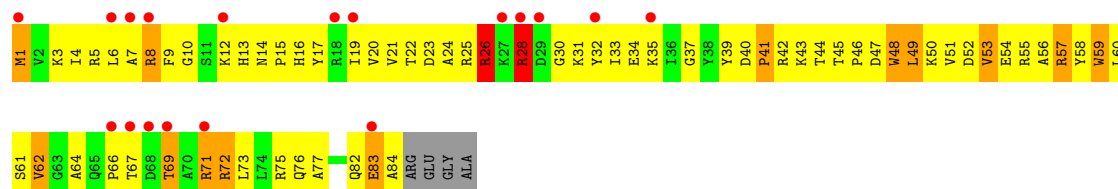
- Molecule 16: 30S ribosomal protein S16

Chain QP:



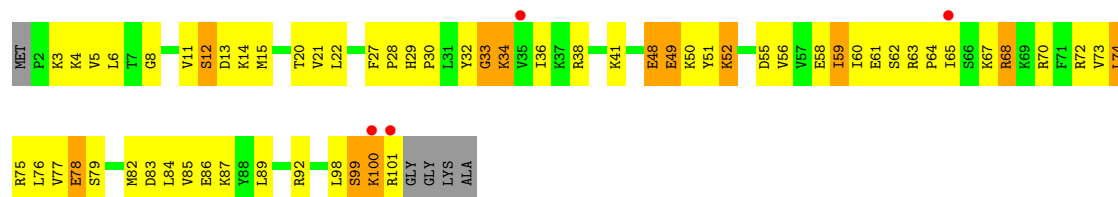
- Molecule 16: 30S ribosomal protein S16

Chain XP:



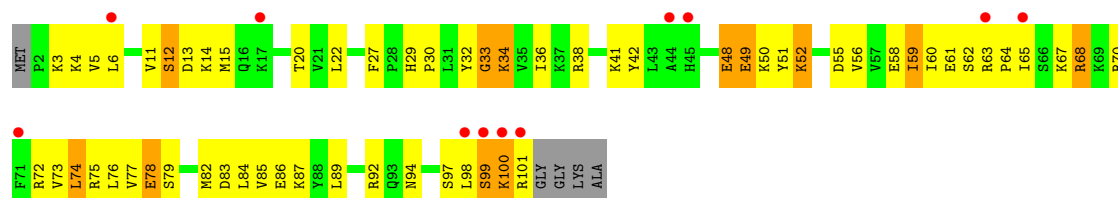
- Molecule 17: 30S ribosomal protein S17

Chain QQ:



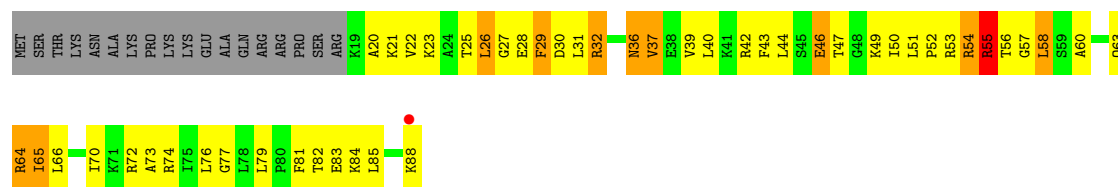
- Molecule 17: 30S ribosomal protein S17

Chain XQ:



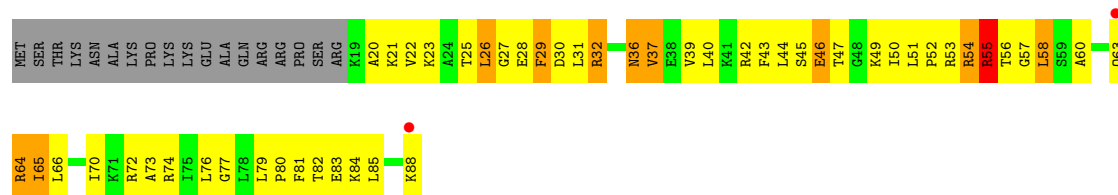
- Molecule 18: 30S ribosomal protein S18

Chain QR:



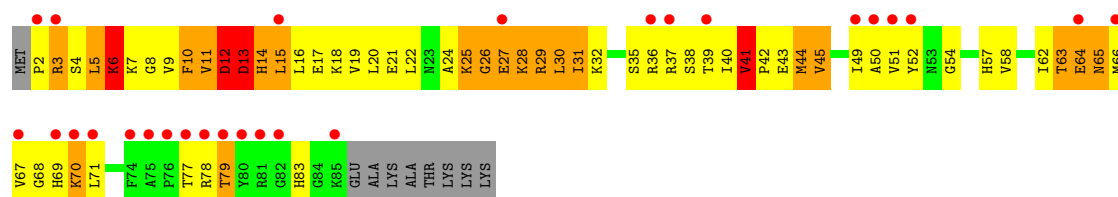
- Molecule 18: 30S ribosomal protein S18

Chain XR:



- Molecule 19: 30S ribosomal protein S19

Chain QS:



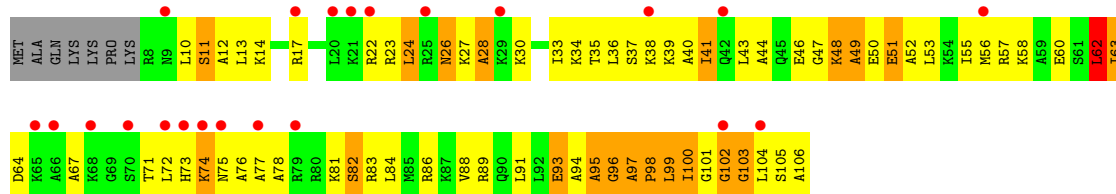
- Molecule 19: 30S ribosomal protein S19

Chain XS:



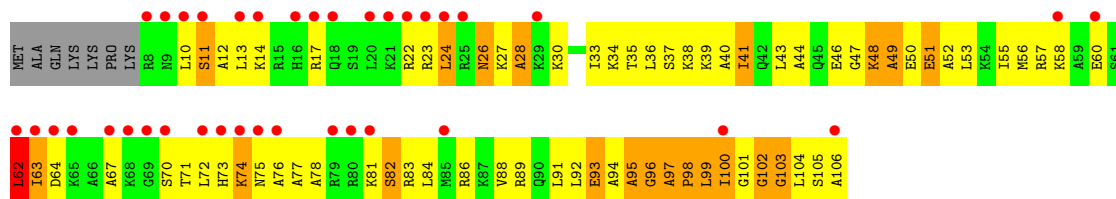
- Molecule 20: 30S ribosomal protein S20

Chain QT:



- Molecule 20: 30S ribosomal protein S20

Chain XT:



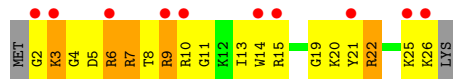
- Molecule 21: 30S ribosomal protein S21

Chain QU:



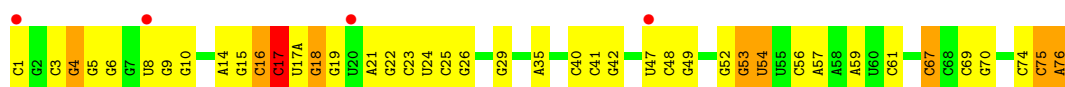
- Molecule 21: 30S ribosomal protein S21

Chain XU:



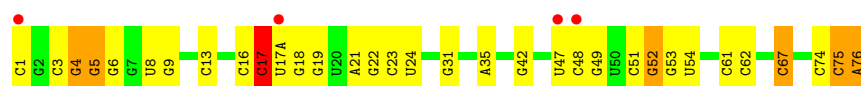
- Molecule 22: P-site tRNA fMet

Chain QV:



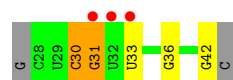
- Molecule 22: P-site tRNA fMet

Chain XV:



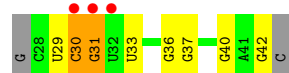
- Molecule 23: messenger RNA

Chain QY:



- Molecule 23: messenger RNA

Chain XY:



- Molecule 24: A-site ASL Pro

Chain QX:



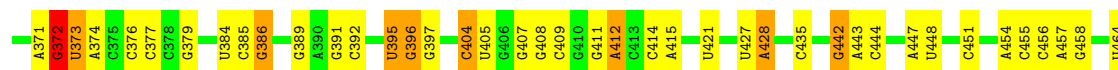
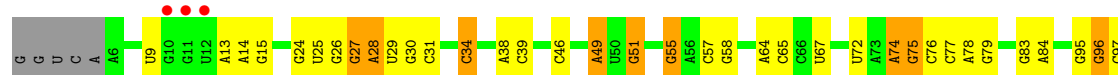
- Molecule 24: A-site ASL Pro

Chain XX:



- Molecule 25: 23S rRNA

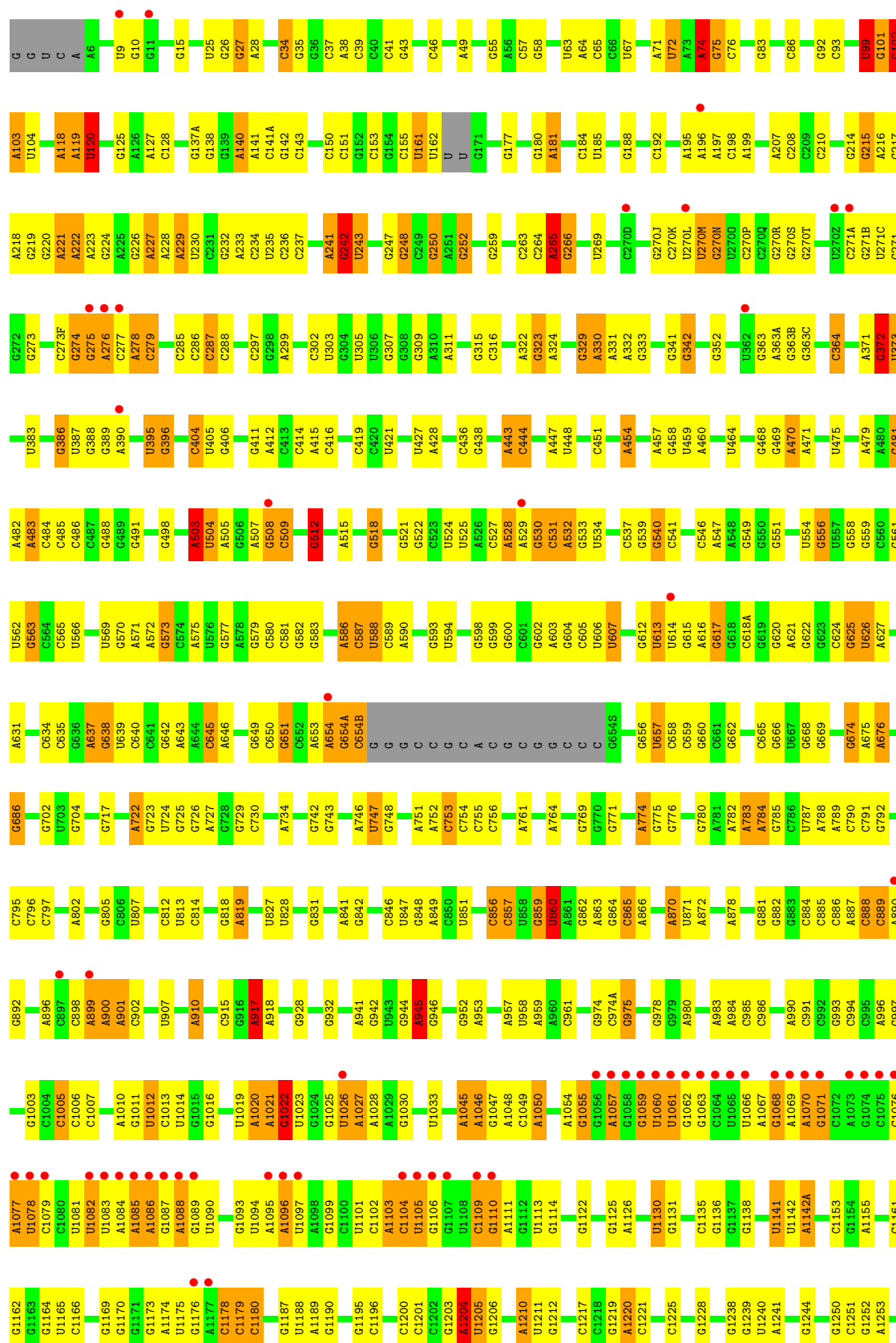
Chain RA:



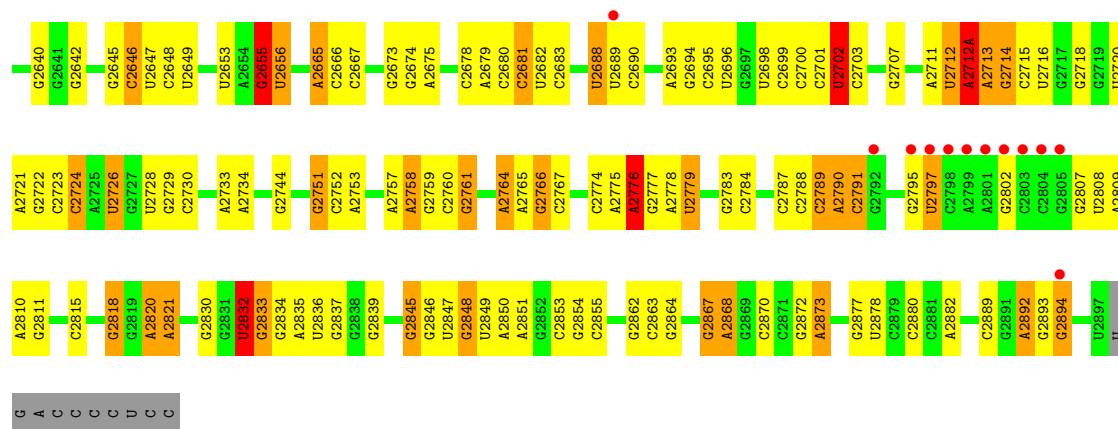


A2873	C2874	C2875	C2880	C2881	A2882	G2891	A2892	G2893	G2894	G2897	G2898	G2899	A2799	A2801	G2802	C2803	C2804	G2805	G2807	G2808	A2809	A2810	G2811	C2815	G2818	A2819	A2820	A2821	G2822	G2832	G2833	G2834	A2835	U2836	G2837	G2838	G2839	G2844	G2845	G2846	U2847	G2848	U2849	C2853	G2854	A2860	G2861	G2862	C2863	G2864	G2867	A2868	G2872												
C2709	C2710	A2711	U2712	A2713	A2714	C2715	U2716	U2720	A2721	G2722	C2723	C2724	A2725	U2726	G2729	A2733	A2734	G2735	U2739	C2742	C2745	U2746	G2747	A2748	A2749	A2750	G2751	C2752	C2755	U2756	G2757	A2758	G2759	C2760	G2761	A2764	A2765	G2770	C2771	C2774	A2775	A2776	G2777	U2778	U2779	G2780	A2781																		
C2612	U2613	A2614	G2617	G2618	G2619	G2623	G2629	A2629	G2630	C2635	U2636	U2637	G2638	A2639	G2645	U2646	U2647	U2648	U2649	U2653	A2654	A2655	C2656	G2657	C2658	G2659	A2572	C2573	C2574	C2575	G2576	A2577	C2578	C2579	U2580	G2581	G2582	G2583	U2584	U2585	C2586	C2591	G2592	A2602	G2603	U2604	U2605	C2606	U2609	C2610	U2611														
C2443	G2444	G2445	G2446	G2447	A2448	A2451	A2452	A2453	G2454	U2457	C2466	C2467	G2468	A2469	G2470	C2471	U2472	U2473	C2474	C2475	A2476	C2477	G2481	U2482	C2483	G2484	G2485	G2486	G2487	G2490	G2494	G2495	C2498	G2502	A2503	U2504	G2505	U2506	G2507	G2508	C2512	G2513	U2514	G2515	U2516	U2517	U2518	G2523																	
C2356	G2357	A2358	G2359	G2360	G2361	G2362	G2363	G2364	G2365	A2366	C2367	G2368	G2369	G2370	G2371	G2372	G2373	C2374	A2377	A2378	C2379	G2380	G2381	G2382	G2383	G2384	G2385	A2386	C2387	G2388	G2389	A2390	C2391	A2392	C2393	G2394	C2395	G2396	C2397	U2398	U2401	C2402	C2403	C2404	U2405	U2406	A2411	A2412	G2415	C2416	C2417	U2418	U2419	C2420	U2423	C2424	A2425	G2429	A2430	U2434	A2435	U2438	A2439	C2440	C2441
G2276	G2277	G2280	G2283	C2284	C2285	A2286	A2287	A2288	U2289	C2292	C2295	A2298	G2299	G2300	C2301	A2305	G2306	G2307	G2308	C2309	A2310	A2311	U2312	C2313	C2314	G2318	G2319	A2320	G2325	C2326	A2327	A2328	G2329	G2330	G2331	A2335	C2336	G2340	G2341	C2342	C2343	U2344	G2345	A2346	C2347	C2348	C2350	C2351																	
C2178	C2179	C2183	G2184	C2188	U2189	G2190	G2192	G2193	G2194	C2195	U2196	U2197	A2198	C2199	C2200	C2201	G2202	G2203	G2204	G2205	U2208	C2209	G2210	G2211	U2212	U2213	G2215	G2219	G2224	G2225	C2226	A2227	C2231	U2232	U2233	G2234	G2238	G2239	U2243	U2244	U2245	G2246	G2250	C2261	C2264	A2269	G2270	G2271	U2272	A2273	G2275	C2276													
G2116	A2117	U2118	A2119	G2120	G2121	U2122	G2123	G2124	G2125	A2126	G2127	C2128	G2129	U2130	U2131	U2132	G2133	A2134	A2135	G2136	C2137	G2138	C2139	C2140	G2141	C2145	C2146	G2147	G2148	G2149	U2150	G2151	G2152	G2153	G2154	G2155	G2156	A2157	G2158	G2159	C2160	C2161	G2162	C2163	C2164	G2165	U2166	G2167	G2168	A2169	A2170	A2171	A2172	A2173	C2174	C2175	A2176	C2177							
C2021	U2022	G2023	G2024	C2025	C2026	A2030	A2031	G2032	A2033	G2037	A2037	A2038	A2042	C2043	A2051	G2052	G2053	A2054	C2055	G2056	A2059	A2060	G2061	A2062	U2068	G2069	G2070	A2071	G2072	C2073	U2074	U2075	U2086	G2087	G2093	U2096	U2099	U2102	C2103	G2104	C2105	G2106	A2012	A2013	A2014	A2015	G2110	G2112	U2113	A2114	G2115														
G1814	A1815	G1816	C1925	U1926	A1927	A1928	G1929	U1931	A1936	A1937	A1938	U1939	G1950	U1951	A1952	U1955	C1958	U1963	G1964	C1967	G1968	A1969	A1970	A1971	A1972	G1973	C1974	G1980	A1981	C1982	G1989	C1990	U1991	G1992	U1993	G1998	C1999	G2008	G2009	G2012	A2013	A2014	A2015	G2018	C2019	A2020																			
G1725	G1728	A1729	U1730	G1731	A1732	G1733	C1742	G1743	G1750	C1751	G1752	G1753	A1754	A1755	G1756	U1757	G1759	A1762	G1763	G1764	G1769	G1770	C1771	G1772	A1773	U1778	U1779	A1780	C1781	G1782	A1783	A1784	A1785	A1786	A1791	G1792	C1793	U1794	C1795	U1796	C1797	U1798	G1799	C1800	G1801	A1802	A1803	A1810	G1811	A1812	G1813														

• Molecule 25: 23S rRNA

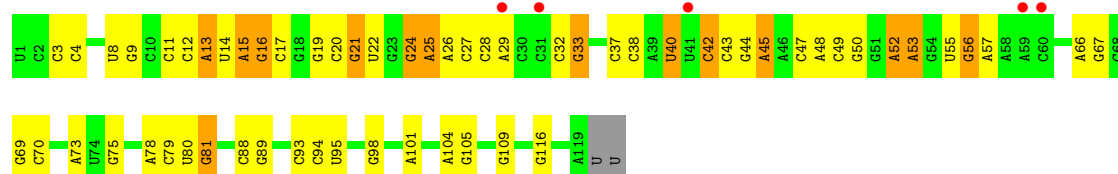
Chain YA: 

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C2558	G2445	A2369	G2277	G2165	G2104	A1928	A1819	G1731	A1610	G1522	G1441	A1354	C1257
U2562	A2448	C2283	C2283	U2167	C2105	A1929	U1820	A1732	C1617	A1528	G1442	A1355	A1262
U2563	C2284	C2285	C2285	A2169	C2021	U1931	A1821	G1733	A1618	A1529	A1444	U1263	G1264
A2564	A2450	A2286	A2286	A2170	U2022	U1932	G1824	C1734	A1637	G1530	A1444	A1265	A1266
A2565	A2451	A2287	A2287	A2171	G2023	G1933	G1825	G1742	A1637	C1531	G1448	G1363	U1267
A2566	C2452	A2288	A2288	U2172	G2024	G1933	G1826	G1743	C1640	C1532	A1449	G1364	G1268
G2567	A2376	A2377	A2377	A2173	G2025	A1936	A1829	G1750	G1647	U1535	G1454	A1269	A1270
G2568	A2378	A2378	A2378	C2174	G2026	A1937	A1830	G1751	G1648	G1536	U1454	G1369	G1271
G2569	G2379	G2379	G2379	A2175	U2030	A1938	A1831	C1752	C1648	U1537	G1455	G1370	A1272
G2570	G2382	C2293	C2293	A2176	A2031	U1939	G1835	G1753	G1653	C1537	U1454	G1371	U1273
G2571	G2383	C2294	C2294	C2177	G2032	A1940	G1836	G1754	A1654	G1538	G1458	A1372	
G2572	C2295	C2295	C2295	C2178	A2033	U1950	G1837	A1755	A1654	G1542	G1459	A1373	
G2573	C2296	C2296	C2296	C2179	U2034	U1951	G1842	G1756	C1657	A1543	G1460	G1279	
G2574	C2297	C2297	C2297	U2180	G2035	A1953	C1843	A1759	C1658	C1544	G1461	G1280	
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G2576	G2303	G2303	G2303	G2182	U2122	U1955	G1845	A1763	G1667	A1546	C1463	U1282	
G2577	C2306	C2306	C2306	C2183	U2123	U1956	G1846	G1764	A1668	C1547	C1464	A1287	
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G2579	C2308	G2308	G2308	U2189	A2126	C1958	A1848	G1766	G1674	C1551	A1471	U1292	
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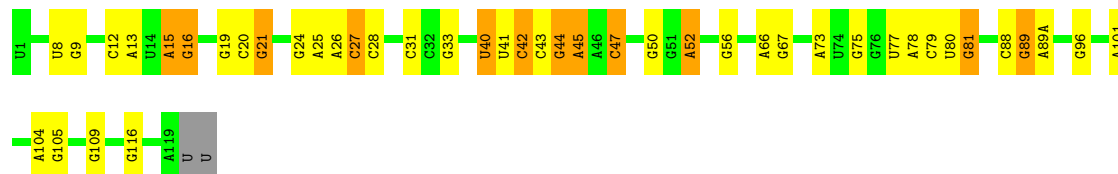
- Molecule 26: 5S rRNA

Chain RB:



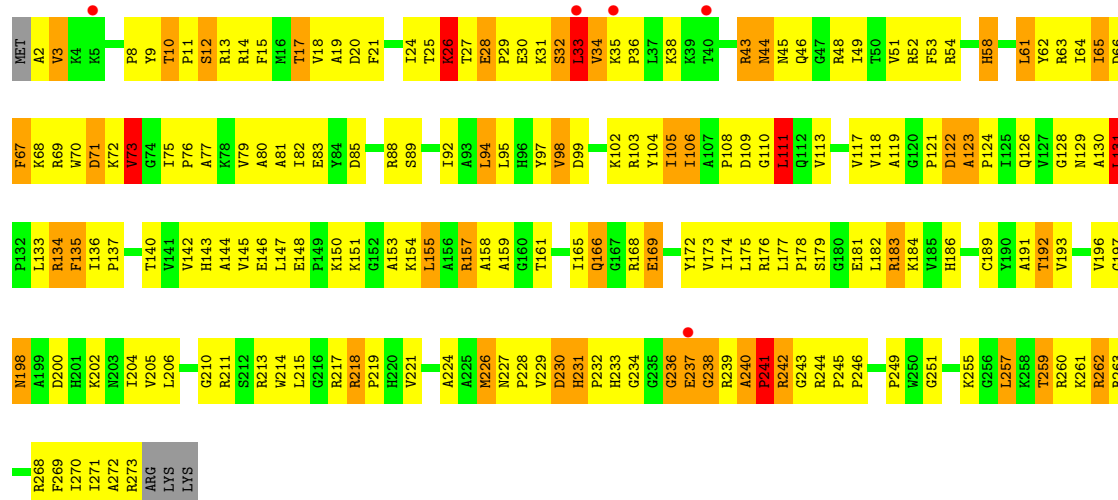
- Molecule 26: 5S rRNA

Chain YB:



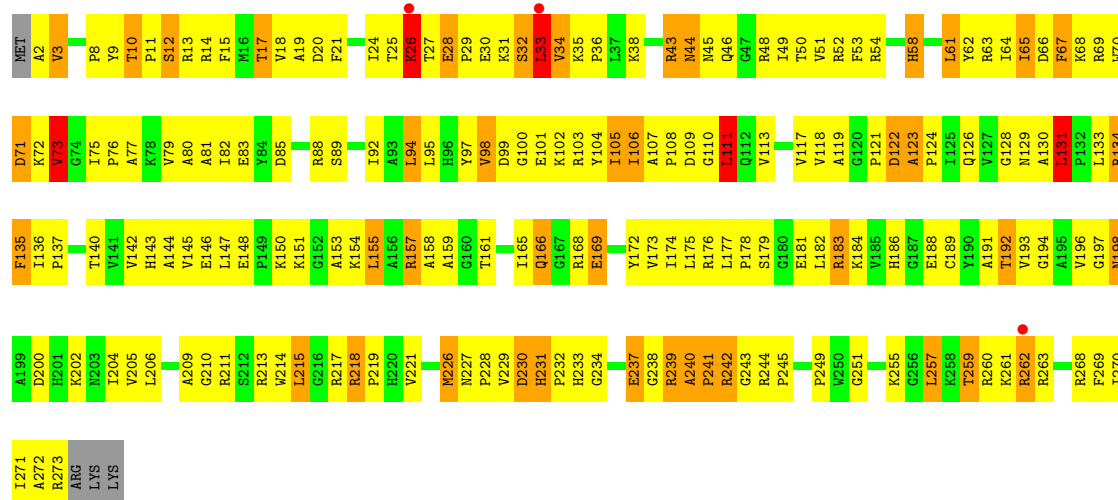
- Molecule 27: 50S ribosomal protein L2

Chain RD:



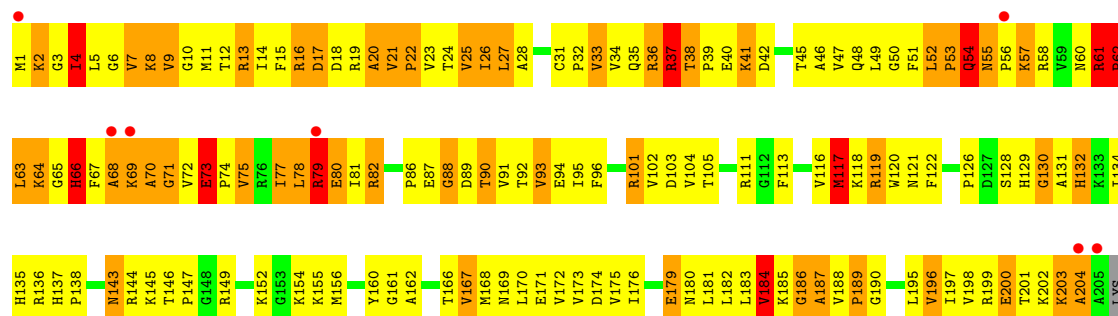
- Molecule 27: 50S ribosomal protein L2

Chain YD:



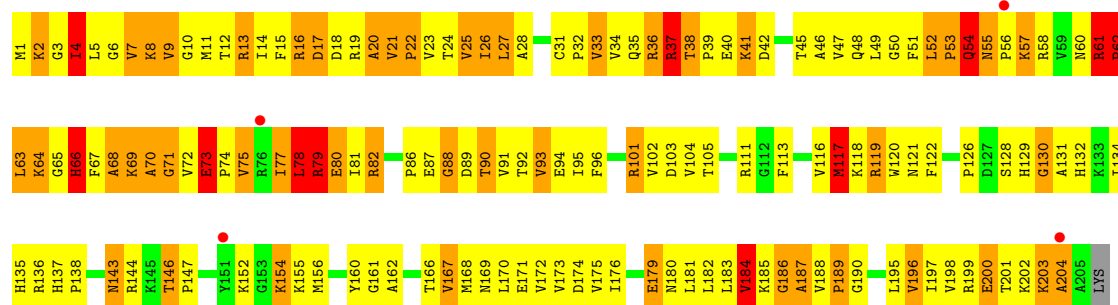
- Molecule 28: 50S ribosomal protein L3

Chain RE:



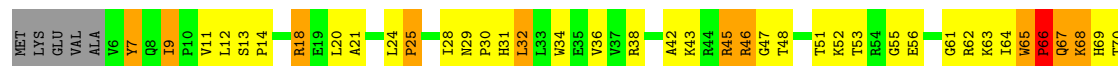
- Molecule 28: 50S ribosomal protein L3

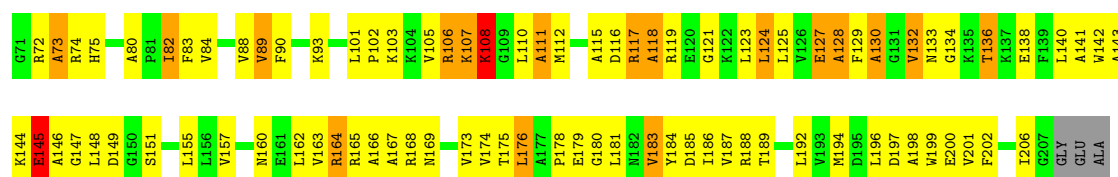
Chain YE:



- Molecule 29: 50S ribosomal protein L4

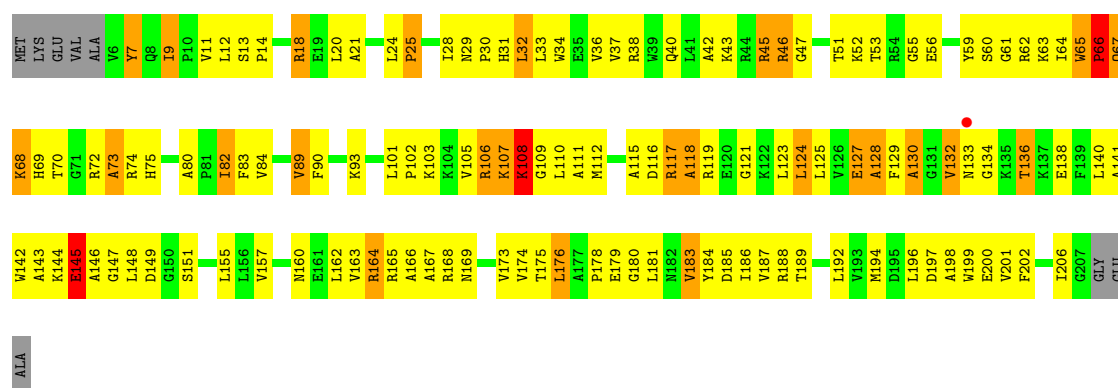
Chain RF:





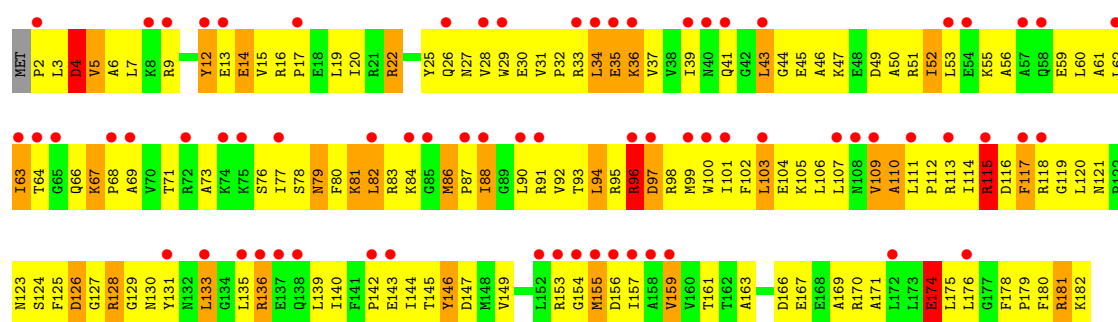
- Molecule 29: 50S ribosomal protein L4

Chain YF:



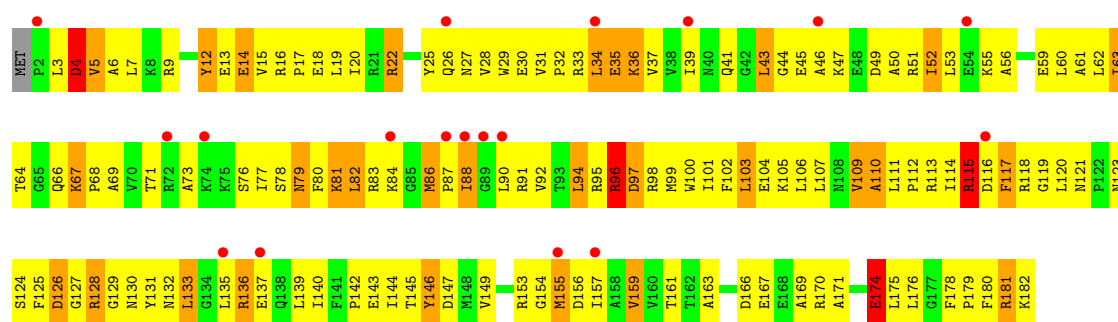
- Molecule 30: 50S ribosomal protein L5

Chain RG:



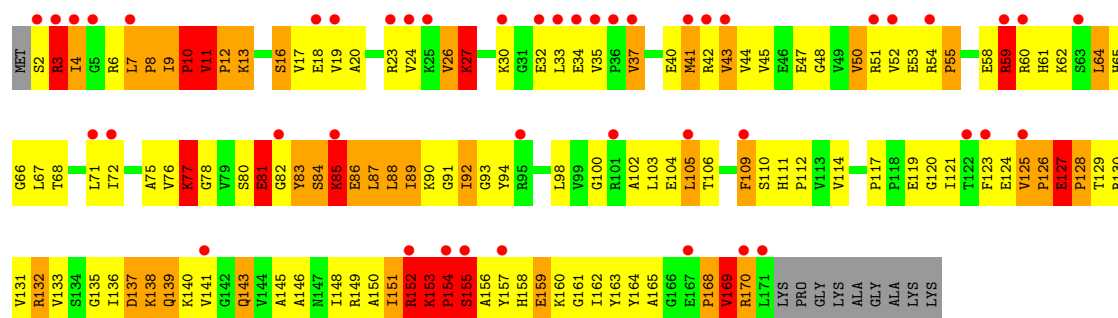
- Molecule 30: 50S ribosomal protein L5

Chain YG:



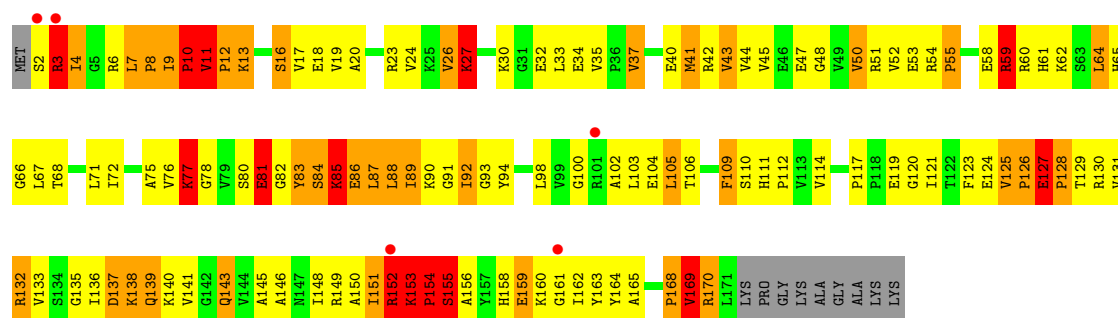
- Molecule 31: 50S ribosomal protein L6

Chain RH:



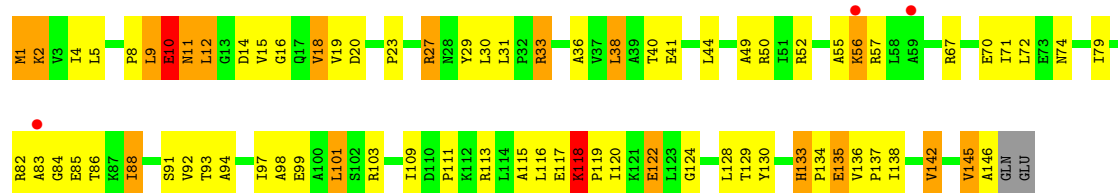
- Molecule 31: 50S ribosomal protein L6

Chain YH:



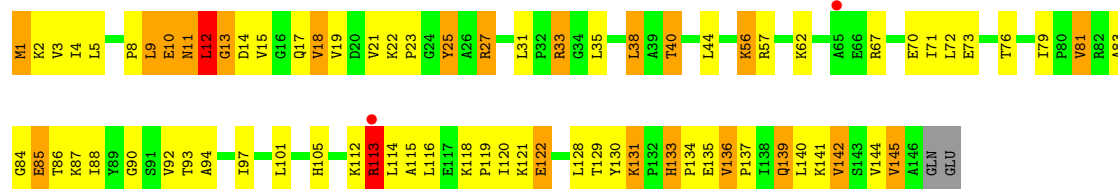
- Molecule 32: 50S ribosomal protein L9

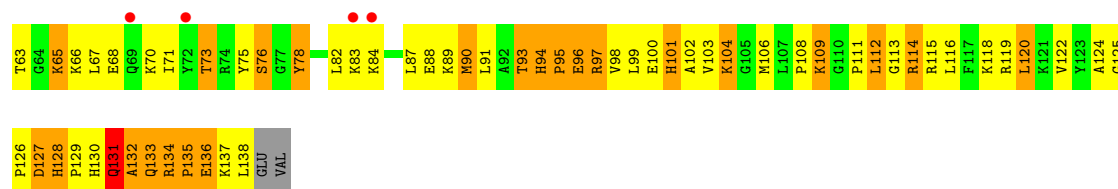
Chain RI:



- Molecule 32: 50S ribosomal protein L9

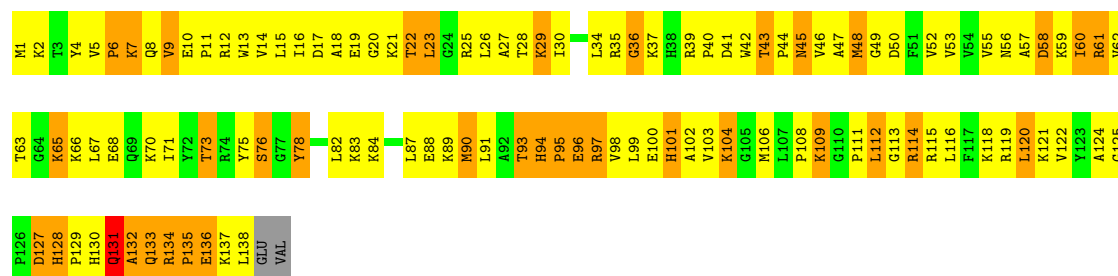
Chain YI:





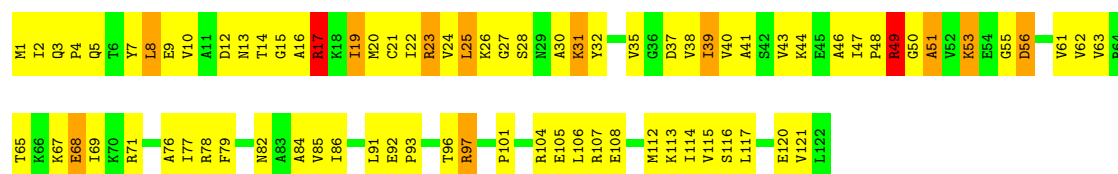
- Molecule 33: 50S ribosomal protein L11

Chain YN:



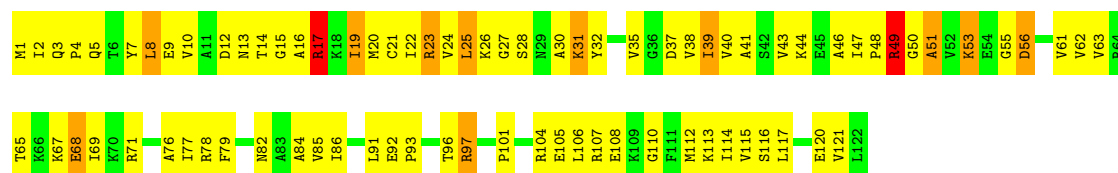
- Molecule 34: 50S ribosomal protein L13

Chain RO:



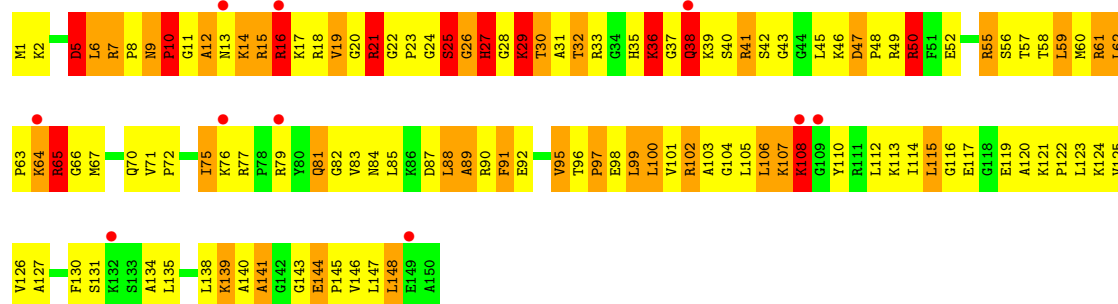
- Molecule 34: 50S ribosomal protein L13

Chain YO:

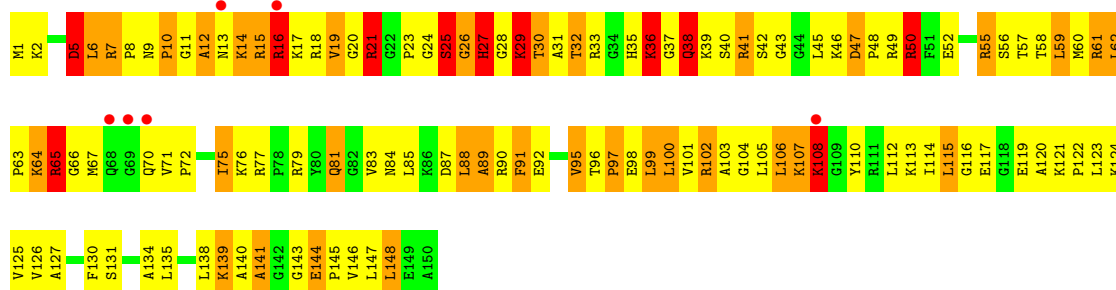


- Molecule 35: 50S ribosomal protein L14

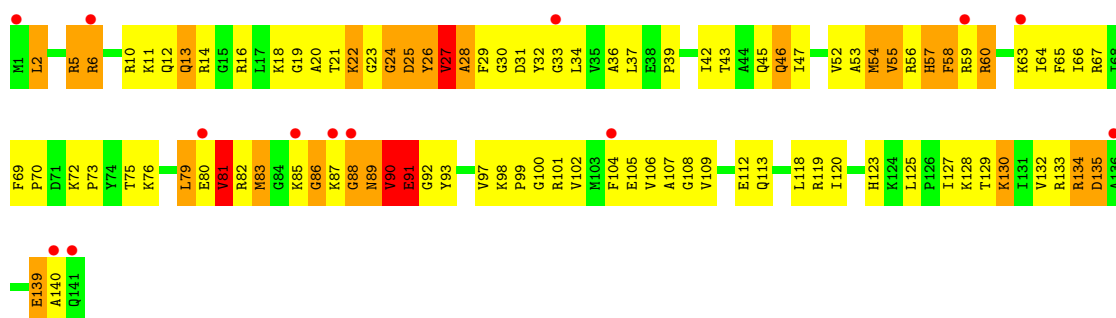
Chain RP:



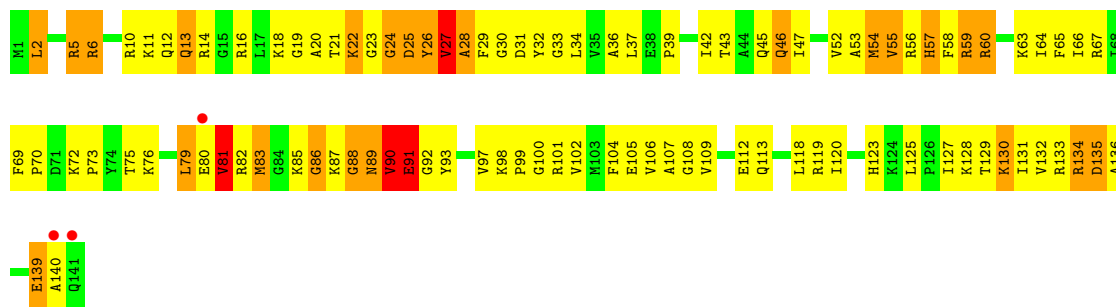
- Molecule 35: 50S ribosomal protein L14

Chain YP: 

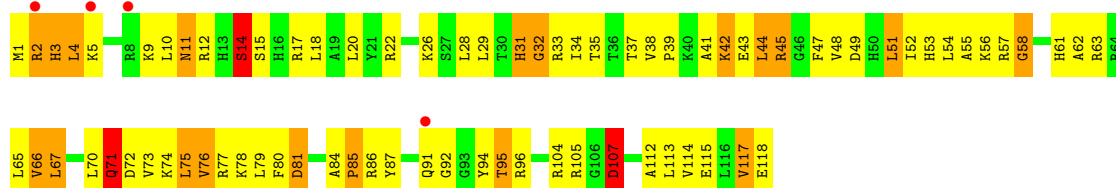
- Molecule 36: 50S ribosomal protein L15

Chain RQ: 

- Molecule 36: 50S ribosomal protein L15

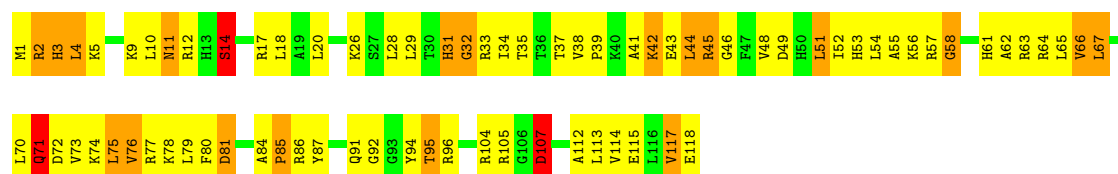
Chain YQ: 

- Molecule 37: 50S ribosomal protein L16

Chain RR: 

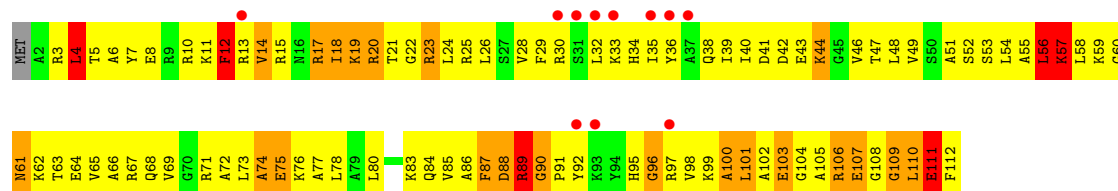
- Molecule 37: 50S ribosomal protein L16

Chain YR: 



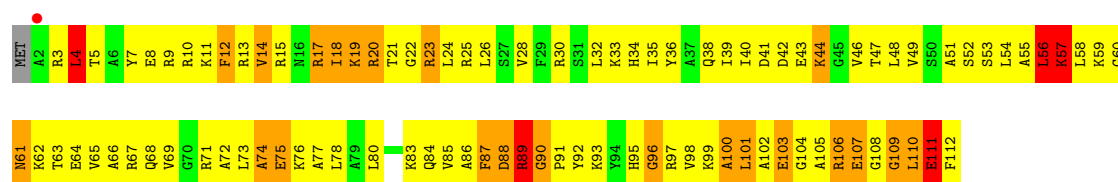
• Molecule 38: 50S ribosomal protein L17

Chain RS:



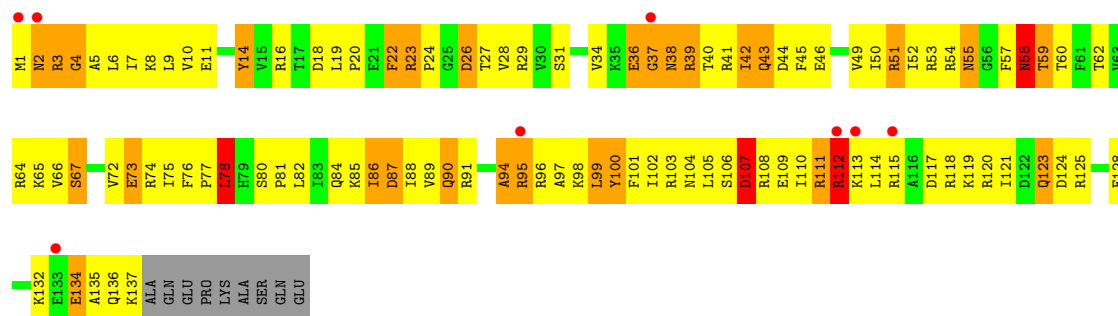
• Molecule 38: 50S ribosomal protein L17

Chain YS:



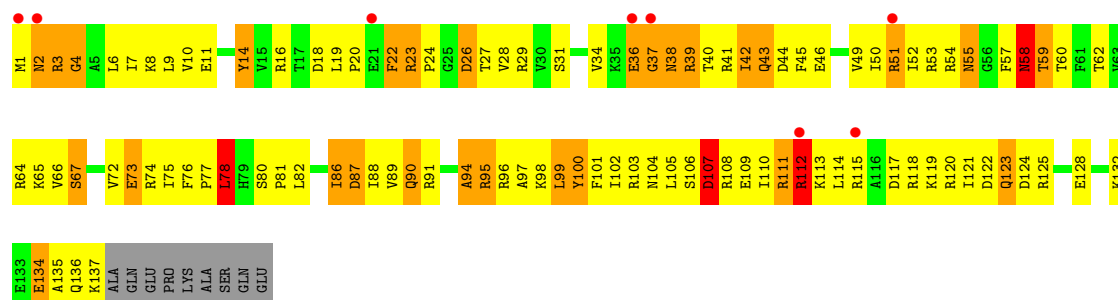
• Molecule 39: 50S ribosomal protein L18

Chain RT:

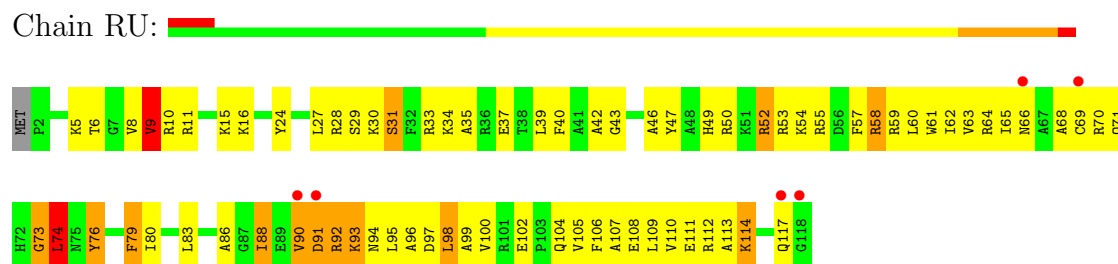


• Molecule 39: 50S ribosomal protein L18

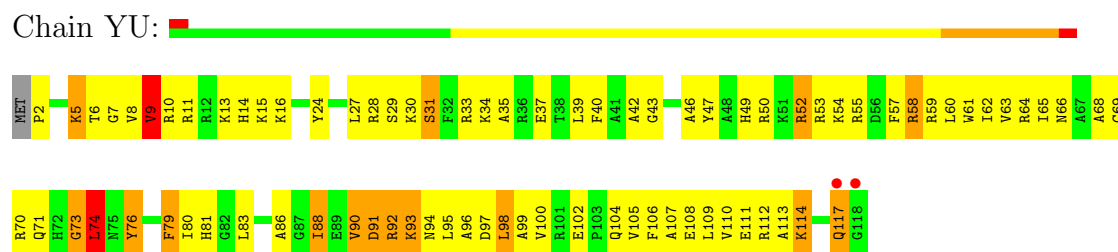
Chain YT:



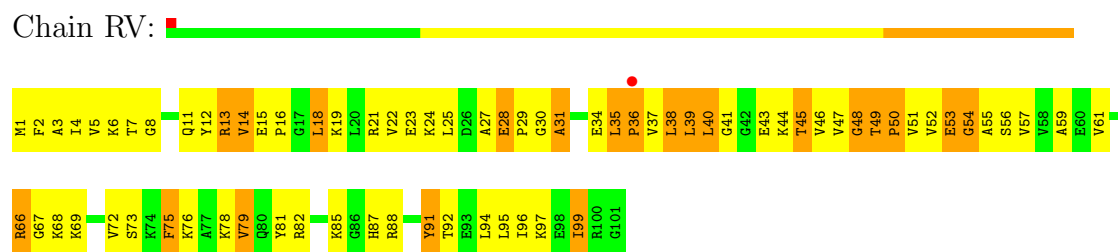
- Molecule 40: 50S ribosomal protein L19

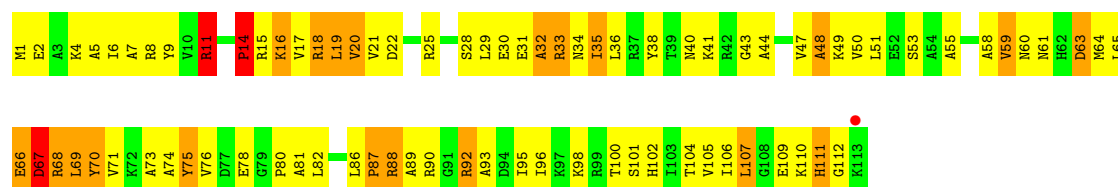


- Molecule 40: 50S ribosomal protein L19



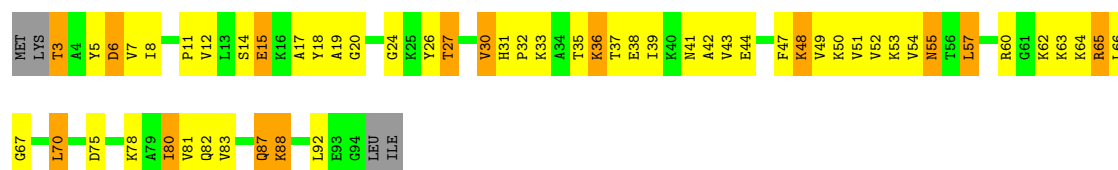
- Molecule 41: 50S ribosomal protein L20





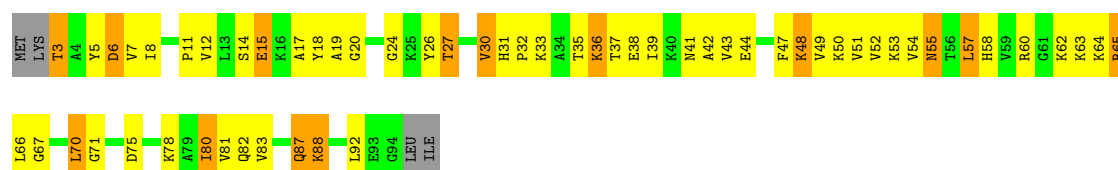
• Molecule 43: 50S ribosomal protein L22

Chain RX:



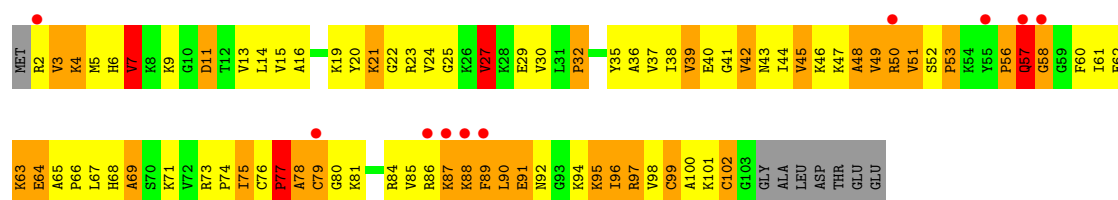
• Molecule 43: 50S ribosomal protein L22

Chain YX:



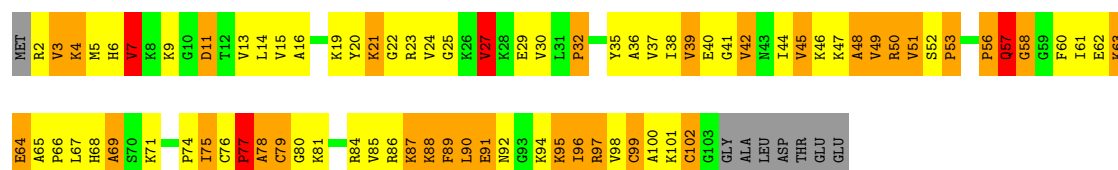
• Molecule 44: 50S ribosomal protein L23

Chain RY:



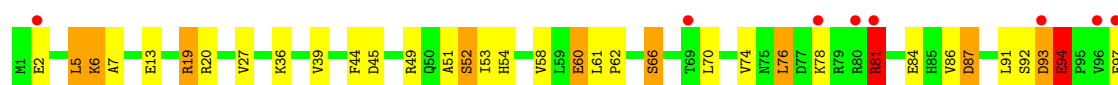
• Molecule 44: 50S ribosomal protein L23

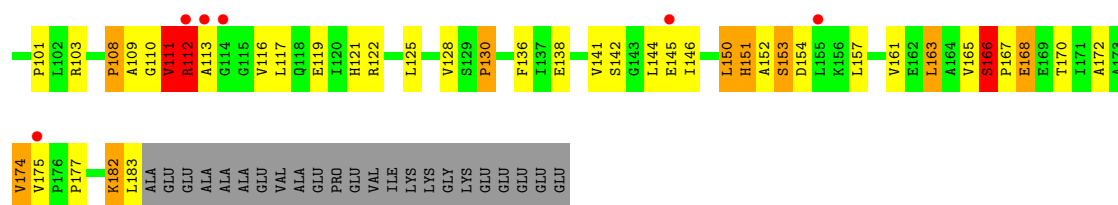
Chain YY:



• Molecule 45: 50S ribosomal protein L24

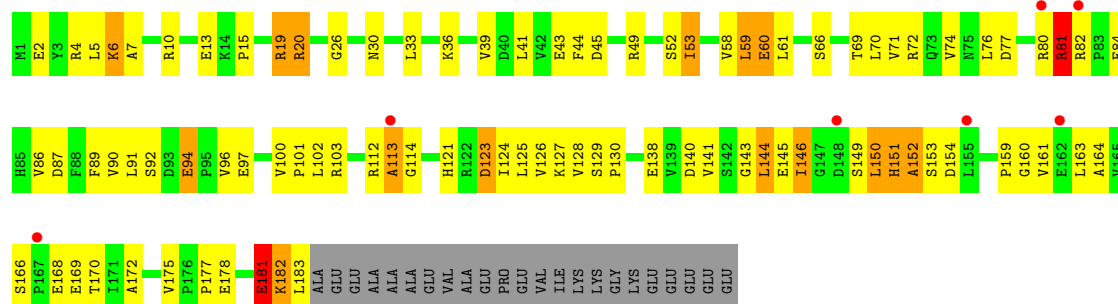
Chain RZ:





- Molecule 45: 50S ribosomal protein L24

Chain YZ:



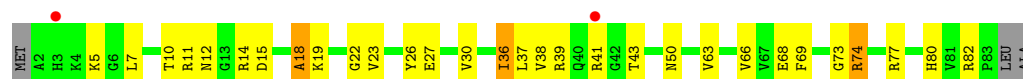
- Molecule 46: 50S ribosomal protein L25

Chain R0:



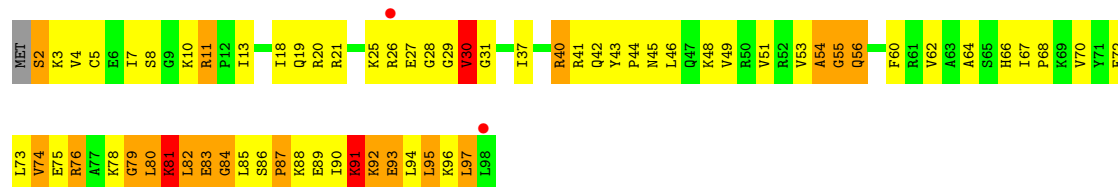
- Molecule 46: 50S ribosomal protein L25

Chain Y0:



- Molecule 47: 50S ribosomal protein L27

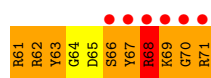
Chain R1:



- Molecule 47: 50S ribosomal protein L27

Chain Y1:





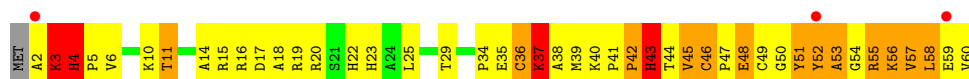
- Molecule 51: 50S ribosomal protein L32

Chain R5:



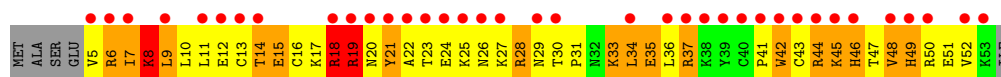
- Molecule 51: 50S ribosomal protein L32

Chain Y5:



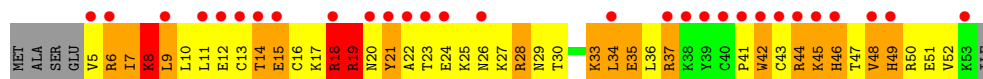
- Molecule 52: 50S ribosomal protein L33

Chain R6:



- Molecule 52: 50S ribosomal protein L33

Chain Y6:



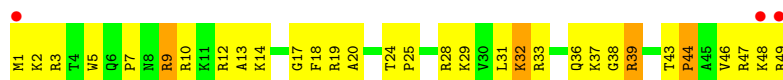
- Molecule 53: 50S ribosomal protein L34

Chain R7:



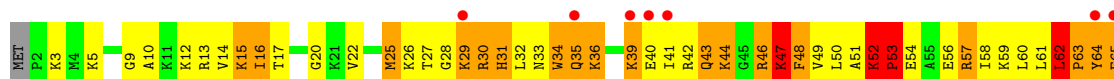
- Molecule 53: 50S ribosomal protein L34

Chain Y7:



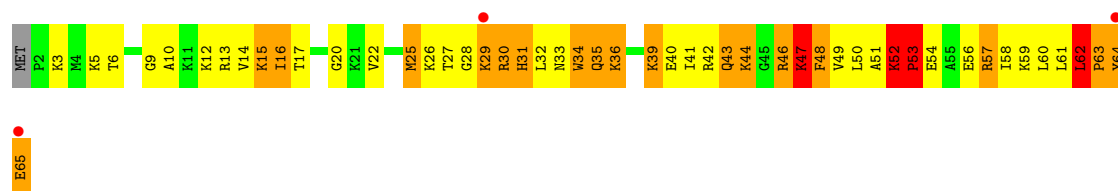
- Molecule 54: 50S ribosomal protein L35

Chain R8:



- Molecule 54: 50S ribosomal protein L35

Chain Y8: 



- Molecule 55: 50S ribosomal protein L36

Chain R9: 



- Molecule 55: 50S ribosomal protein L36

Chain Y9: 



- Molecule 56: tRNA acceptor end mimic

Chain Z6: 



- Molecule 56: tRNA acceptor end mimic

Chain Z8: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.21Å 448.45Å 619.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	189.60 – 3.14 189.60 – 3.09	Depositor EDS
% Data completeness (in resolution range)	99.6 (189.60-3.14) 99.5 (189.60-3.09)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.230 , 0.262 0.258 , 0.285	Depositor DCC
R_{free} test set	49008 reflections (4.91%)	DCC
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 28.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 1047220 reflections	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	291998	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	QA	0.37	0/36098	0.89	48/56341 (0.1%)
1	XA	0.37	0/36101	0.89	50/56346 (0.1%)
2	QB	0.35	0/1959	0.65	0/2642
2	XB	0.35	0/1959	0.65	0/2642
3	QC	0.36	0/1629	0.60	0/2195
3	XC	0.36	0/1629	0.60	0/2195
4	QD	0.41	0/1733	0.68	1/2318 (0.0%)
4	XD	0.44	0/1733	0.68	1/2318 (0.0%)
5	QE	0.38	0/1171	0.66	0/1576
5	XE	0.38	0/1171	0.66	0/1576
6	QF	0.43	0/856	0.68	0/1154
6	XF	0.43	0/856	0.68	0/1154
7	QG	0.37	0/1276	0.61	0/1709
7	XG	0.37	0/1276	0.60	0/1709
8	QH	0.40	0/1136	0.69	0/1527
8	XH	0.40	0/1136	0.69	0/1527
9	QI	0.36	0/1029	0.67	0/1379
9	XI	0.36	0/1029	0.67	0/1379
10	QJ	0.35	0/814	0.61	0/1095
10	XJ	0.36	0/814	0.61	0/1095
11	QK	0.40	0/900	0.67	0/1213
11	XK	0.40	0/900	0.67	0/1213
12	QL	0.45	0/991	1.00	4/1327 (0.3%)
12	XL	0.46	0/991	1.00	4/1327 (0.3%)
13	QM	0.34	0/974	0.66	0/1303
13	XM	0.35	0/974	0.66	0/1303
14	QN	0.42	0/501	0.68	0/664
14	XN	0.52	0/501	0.67	0/664
15	QO	0.39	0/745	0.67	0/992
15	XO	0.39	0/745	0.67	0/992
16	QP	0.36	0/721	0.67	0/970
16	XP	0.37	0/721	0.67	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.37	0/847	0.68	0/1131
17	XQ	0.37	0/847	0.68	0/1131
18	QR	0.39	0/579	0.72	0/768
18	XR	0.39	0/579	0.72	0/768
19	QS	0.36	0/689	0.84	2/926 (0.2%)
19	XS	0.36	0/689	0.84	2/926 (0.2%)
20	QT	0.33	0/765	0.70	0/1007
20	XT	0.34	0/765	0.69	0/1007
21	QU	0.37	0/221	0.63	0/288
21	XU	0.37	0/221	0.63	0/288
22	QV	0.39	1/1836 (0.1%)	0.81	3/2859 (0.1%)
22	XV	0.42	1/1836 (0.1%)	0.84	4/2859 (0.1%)
23	QY	0.24	0/333	0.81	0/517
23	XY	0.24	0/333	0.74	0/517
24	QX	0.65	0/189	1.41	5/292 (1.7%)
24	XX	0.39	0/189	1.08	2/292 (0.7%)
25	RA	0.39	0/69521	0.88	70/108529 (0.1%)
25	YA	0.43	1/69543 (0.0%)	0.92	116/108563 (0.1%)
26	RB	0.32	0/2878	0.84	0/4490
26	YB	0.36	0/2878	0.88	1/4490 (0.0%)
27	RD	0.60	2/2165 (0.1%)	0.90	4/2919 (0.1%)
27	YD	0.56	0/2165	0.90	4/2919 (0.1%)
28	RE	0.52	0/1601	0.91	2/2160 (0.1%)
28	YE	0.52	0/1601	0.91	2/2160 (0.1%)
29	RF	0.50	0/1620	0.76	0/2194
29	YF	0.50	0/1620	0.76	0/2194
30	RG	0.40	0/1499	0.66	0/2016
30	YG	0.40	0/1499	0.66	0/2016
31	RH	0.45	0/1332	0.85	3/1802 (0.2%)
31	YH	0.45	0/1332	0.85	4/1802 (0.2%)
32	RI	0.28	0/1151	0.56	0/1558
32	YI	0.27	0/1151	0.58	0/1558
33	RN	0.46	0/1131	0.78	1/1525 (0.1%)
33	YN	0.46	0/1131	0.78	1/1525 (0.1%)
34	RO	0.54	0/943	0.71	0/1269
34	YO	0.53	0/943	0.71	0/1269
35	RP	0.50	0/1162	0.95	3/1544 (0.2%)
35	YP	0.50	0/1162	0.95	3/1544 (0.2%)
36	RQ	0.54	0/1143	0.91	3/1527 (0.2%)
36	YQ	0.54	0/1143	0.89	3/1527 (0.2%)
37	RR	0.45	0/982	0.80	1/1312 (0.1%)
37	YR	0.45	0/982	0.80	1/1312 (0.1%)
38	RS	0.46	0/892	0.82	1/1187 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YS	0.45	0/892	0.83	1/1187 (0.1%)
39	RT	0.47	0/1155	0.73	2/1542 (0.1%)
39	YT	0.46	0/1155	0.73	2/1542 (0.1%)
40	RU	0.48	0/982	0.78	0/1306
40	YU	0.48	0/982	0.77	0/1306
41	RV	0.47	0/790	0.82	0/1057
41	YV	0.47	0/790	0.82	0/1057
42	RW	0.45	0/911	0.75	0/1220
42	YW	0.45	0/911	0.75	0/1220
43	RX	0.56	0/739	0.77	0/993
43	YX	0.56	0/739	0.77	0/993
44	RY	0.52	0/798	0.80	0/1064
44	YY	0.52	0/798	0.80	0/1064
45	RZ	0.27	0/1493	0.52	0/2026
45	YZ	0.28	0/1493	0.54	0/2026
46	R0	0.30	0/657	0.54	0/874
46	Y0	0.34	0/657	0.53	0/874
47	R1	0.49	0/770	0.85	1/1022 (0.1%)
47	Y1	0.49	0/770	0.85	1/1022 (0.1%)
48	R2	0.51	0/583	0.83	1/771 (0.1%)
48	Y2	0.50	0/583	0.83	1/771 (0.1%)
49	R3	0.47	0/474	0.72	0/635
49	Y3	0.43	0/474	0.71	0/635
50	R4	0.38	0/594	0.78	1/795 (0.1%)
50	Y4	0.38	0/594	0.78	1/795 (0.1%)
51	R5	0.51	0/473	0.74	0/639
51	Y5	0.51	0/473	0.74	0/639
52	R6	0.42	0/431	0.76	0/575
52	Y6	0.42	0/431	0.76	0/575
53	R7	0.56	0/438	0.76	0/575
53	Y7	0.56	0/438	0.76	0/575
54	R8	0.62	0/525	0.93	1/691 (0.1%)
54	Y8	0.62	0/525	0.93	1/691 (0.1%)
55	R9	0.35	0/310	0.59	0/407
55	Y9	0.37	0/310	0.61	0/407
56	Z6	0.79	0/40	1.81	1/60 (1.7%)
56	Z8	0.77	0/40	1.81	1/60 (1.7%)
All	All	0.41	5/316375 (0.0%)	0.86	364/472993 (0.1%)

All (5) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	1	C	OP3-P	-10.56	1.48	1.61
22	XV	1	C	OP3-P	-10.53	1.48	1.61
27	RD	236	GLY	C-N	8.57	1.53	1.34
25	YA	774	A	N9-C4	-5.56	1.34	1.37
27	RD	241	PRO	N-CD	5.19	1.55	1.47

The worst 5 of 364 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	XL	47	LYS	C-N-CD	-20.45	75.61	120.60
12	QL	47	LYS	C-N-CD	-20.44	75.62	120.60
25	YA	2506	U	N3-C2-O2	-10.56	114.81	122.20
28	YE	21	VAL	C-N-CD	-10.11	98.35	120.60
28	RE	21	VAL	C-N-CD	-10.09	98.41	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	576	0
1	XA	32249	0	16279	575	1
2	QB	1924	0	1975	287	0
2	XB	1924	0	1975	293	0
3	QC	1605	0	1668	212	0
3	XC	1605	0	1668	215	2
4	QD	1703	0	1765	261	0
4	XD	1703	0	1764	217	0
5	QE	1155	0	1213	140	0
5	XE	1155	0	1213	141	0
6	QF	843	0	857	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	XF	843	0	857	101	0
7	QG	1257	0	1296	148	0
7	XG	1257	0	1296	143	0
8	QH	1116	0	1175	148	0
8	XH	1116	0	1177	154	0
9	QI	1010	0	1037	145	0
9	XI	1010	0	1037	153	0
10	QJ	801	0	849	152	0
10	XJ	801	0	849	141	0
11	QK	885	0	904	103	2
11	XK	885	0	904	109	0
12	QL	975	0	1062	107	0
12	XL	975	0	1062	110	0
13	QM	964	0	1034	163	0
13	XM	964	0	1034	150	0
14	QN	492	0	529	100	0
14	XN	492	0	529	94	0
15	QO	734	0	771	73	0
15	XO	734	0	771	72	0
16	QP	705	0	725	115	0
16	XP	705	0	725	113	0
17	QQ	834	0	904	85	0
17	XQ	834	0	904	78	0
18	QR	574	0	644	66	0
18	XR	574	0	644	69	0
19	QS	674	0	699	103	0
19	XS	674	0	699	136	0
20	QT	763	0	860	108	0
20	XT	763	0	861	103	0
21	QU	217	0	234	27	0
21	XU	217	0	234	28	0
22	QV	1644	0	836	22	0
22	XV	1644	0	836	15	0
23	QY	323	0	165	2	0
23	XY	323	0	165	6	0
24	QX	170	0	88	2	0
24	XX	170	0	88	1	0
25	RA	62071	0	31288	992	0
25	YA	62091	0	31296	935	0
26	RB	2573	0	1306	62	0
26	YB	2573	0	1306	26	0
27	RD	2115	0	2195	319	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	YD	2115	0	2195	332	0
28	RE	1568	0	1634	270	0
28	YE	1568	0	1634	265	0
29	RF	1585	0	1632	181	0
29	YF	1585	0	1632	180	0
30	RG	1474	0	1535	211	0
30	YG	1474	0	1535	193	0
31	RH	1307	0	1382	225	0
31	YH	1307	0	1382	221	0
32	RI	1136	0	1223	42	1
32	YI	1136	0	1223	40	0
33	RN	1104	0	1180	191	0
33	YN	1104	0	1180	183	0
34	RO	933	0	996	123	0
34	YO	933	0	996	123	0
35	RP	1145	0	1228	250	0
35	YP	1145	0	1228	245	0
36	RQ	1122	0	1179	159	0
36	YQ	1122	0	1179	158	0
37	RR	968	0	1033	113	0
37	YR	968	0	1033	113	0
38	RS	882	0	943	165	0
38	YS	882	0	943	159	0
39	RT	1141	0	1202	154	0
39	YT	1141	0	1202	153	0
40	RU	964	0	1022	131	0
40	YU	964	0	1022	137	0
41	RV	779	0	852	129	0
41	YV	779	0	852	136	3
42	RW	900	0	964	99	0
42	YW	900	0	964	100	0
43	RX	725	0	778	69	0
43	YX	725	0	778	74	0
44	RY	785	0	878	163	0
44	YY	785	0	878	151	0
45	RZ	1461	0	1493	46	0
45	YZ	1461	0	1493	57	0
46	R0	648	0	672	20	0
46	Y0	648	0	672	28	0
47	R1	763	0	848	146	0
47	Y1	763	0	848	142	0
48	R2	581	0	629	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	Y2	581	0	629	77	0
49	R3	469	0	518	41	0
49	Y3	469	0	518	41	0
50	R4	581	0	574	153	0
50	Y4	581	0	574	164	0
51	R5	459	0	480	77	0
51	Y5	459	0	480	75	3
52	R6	424	0	450	92	0
52	Y6	424	0	450	89	0
53	R7	430	0	480	43	0
53	Y7	430	0	480	44	0
54	R8	517	0	582	106	0
54	Y8	517	0	582	103	0
55	R9	307	0	338	18	0
55	Y9	307	0	338	18	0
56	Z6	74	0	51	6	0
56	Z8	74	0	51	7	0
57	QA	69	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	1	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	RA	240	0	0	0	0
57	RB	2	0	0	0	0
57	RD	1	0	0	0	0
57	RE	2	0	0	0	0
57	RF	1	0	0	0	0
57	RP	1	0	0	0	0
57	RR	2	0	0	0	0
57	XA	74	0	0	0	0
57	XV	2	0	0	0	0
57	XX	1	0	0	0	0
57	Y0	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y7	1	0	0	0	0
57	YA	265	0	0	0	0
57	YB	3	0	0	0	0
57	YE	2	0	0	0	0
57	YP	1	0	0	0	0
57	YQ	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	QA	42	0	45	3	0
58	XA	42	0	45	1	0
59	QD	1	0	0	0	0
59	QN	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
All	All	291998	0	198367	14453	6

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 30.

The worst 5 of 14453 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:YN:32:SER:CB	14:YN:41:ARG:HB3	1.23	1.55
14:YN:32:SER:HB3	14:YN:41:ARG:CB	1.28	1.54
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.35	1.53
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.35	1.52
4:XD:22:LYS:CG	4:XD:26:CYS:SG	2.01	1.49

The worst 5 of 6 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)
11:QK:99:GLN:NE2	3:XC:79:ARG:NH2[4.555]	1.49	0.71
41:YV:51:VAL:N	51:Y5:60:VAL:O[4.445]	1.70	0.50
11:QK:99:GLN:OE1	3:XC:79:ARG:NE[4.555]	2.04	0.16
41:YV:50:PRO:CG	51:Y5:60:VAL:O[4.445]	2.14	0.06
32:RI:91:SER:OG	1:XA:368:U:OP1[4.555]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	3
2	XB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	3
3	QC	203/239 (85%)	129 (64%)	55 (27%)	19 (9%)	1	7
3	XC	203/239 (85%)	129 (64%)	55 (27%)	19 (9%)	1	7
4	QD	206/209 (99%)	136 (66%)	50 (24%)	20 (10%)	1	7
4	XD	206/209 (99%)	135 (66%)	49 (24%)	22 (11%)	1	5
5	QE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	1	6
5	XE	149/162 (92%)	103 (69%)	30 (20%)	16 (11%)	1	5
6	QF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	8
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	8
7	QG	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	1	7
7	XG	153/156 (98%)	103 (67%)	36 (24%)	14 (9%)	1	8
8	QH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	1	5
8	XH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	1	5
9	QI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	3
9	XI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	3
10	QJ	97/105 (92%)	68 (70%)	20 (21%)	9 (9%)	1	8
10	XJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	1	6
11	QK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	12
11	XK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	12
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	1	4
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	1	4
13	QM	119/126 (94%)	71 (60%)	27 (23%)	21 (18%)	0	0
13	XM	119/126 (94%)	71 (60%)	26 (22%)	22 (18%)	0	0
14	QN	58/61 (95%)	31 (53%)	15 (26%)	12 (21%)	0	0
14	XN	58/61 (95%)	32 (55%)	14 (24%)	12 (21%)	0	0
15	QO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	2	14
15	XO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	2	14
16	QP	82/88 (93%)	48 (58%)	24 (29%)	10 (12%)	1	4
16	XP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	2
17	QQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	10
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	QR	68/88 (77%)	45 (66%)	15 (22%)	8 (12%)	1	4
18	XR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	1	4
19	QS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	0
19	XS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	0
20	QT	97/106 (92%)	63 (65%)	16 (16%)	18 (19%)	0	0
20	XT	97/106 (92%)	63 (65%)	15 (16%)	19 (20%)	0	0
21	QU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	0
21	XU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	0
27	RD	270/276 (98%)	203 (75%)	48 (18%)	19 (7%)	2	14
27	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	2	14
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	0
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	0
29	RF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	6
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	6
30	RG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	1	4
30	YG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	1	4
31	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	0
31	YH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	0
32	RI	144/148 (97%)	102 (71%)	27 (19%)	15 (10%)	1	6
32	YI	144/148 (97%)	103 (72%)	25 (17%)	16 (11%)	1	5
33	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	1
33	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	1
34	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	2	12
34	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	2	12
35	RP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	0
35	YP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	0
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	1	6
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	1	6
37	RR	116/118 (98%)	83 (72%)	19 (16%)	14 (12%)	1	4
37	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	1	4
38	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	YS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	0
39	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	2
39	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	2
40	RU	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	11
40	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	11
41	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	6
41	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	6
42	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	3
42	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	3
43	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	3	22
43	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	3	22
44	RY	100/110 (91%)	58 (58%)	16 (16%)	26 (26%)	0	0
44	YY	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0	0
45	RZ	181/206 (88%)	126 (70%)	35 (19%)	20 (11%)	1	5
45	YZ	181/206 (88%)	135 (75%)	28 (16%)	18 (10%)	1	7
46	R0	80/85 (94%)	71 (89%)	7 (9%)	2 (2%)	9	47
46	Y0	80/85 (94%)	72 (90%)	6 (8%)	2 (2%)	9	47
47	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	1	4
47	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	1	4
48	R2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	2
48	Y2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	2
49	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	3	24
49	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	3	24
50	R4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
50	Y4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
51	R5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	0
51	Y5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	0
52	R6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
52	Y6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
53	R7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	17
53	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	R8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	0
54	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	0
55	R9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11470/12128 (95%)	7666 (67%)	2321 (20%)	1483 (13%)	0	3

5 of 1483 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	181 (88%)	24 (12%)	8	33
2	XB	205/220 (93%)	181 (88%)	24 (12%)	8	33
3	QC	159/188 (85%)	143 (90%)	16 (10%)	11	41
3	XC	159/188 (85%)	143 (90%)	16 (10%)	11	41
4	QD	180/181 (99%)	160 (89%)	20 (11%)	9	36
4	XD	180/181 (99%)	165 (92%)	15 (8%)	16	55
5	QE	116/123 (94%)	108 (93%)	8 (7%)	22	65
5	XE	116/123 (94%)	107 (92%)	9 (8%)	18	59
6	QF	90/90 (100%)	76 (84%)	14 (16%)	4	16
6	XF	90/90 (100%)	76 (84%)	14 (16%)	4	16
7	QG	126/127 (99%)	114 (90%)	12 (10%)	12	45
7	XG	126/127 (99%)	115 (91%)	11 (9%)	15	52
8	QH	119/119 (100%)	106 (89%)	13 (11%)	9	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	XH	119/119 (100%)	106 (89%)	13 (11%)	9	37
9	QI	98/99 (99%)	87 (89%)	11 (11%)	9	36
9	XI	98/99 (99%)	87 (89%)	11 (11%)	9	36
10	QJ	89/92 (97%)	81 (91%)	8 (9%)	14	49
10	XJ	89/92 (97%)	81 (91%)	8 (9%)	14	49
11	QK	90/99 (91%)	81 (90%)	9 (10%)	11	41
11	XK	90/99 (91%)	81 (90%)	9 (10%)	11	41
12	QL	104/109 (95%)	90 (86%)	14 (14%)	6	24
12	XL	104/109 (95%)	90 (86%)	14 (14%)	6	24
13	QM	97/101 (96%)	81 (84%)	16 (16%)	3	14
13	XM	97/101 (96%)	81 (84%)	16 (16%)	3	14
14	QN	49/50 (98%)	40 (82%)	9 (18%)	2	11
14	XN	49/50 (98%)	44 (90%)	5 (10%)	11	40
15	QO	79/80 (99%)	73 (92%)	6 (8%)	19	60
15	XO	79/80 (99%)	73 (92%)	6 (8%)	19	60
16	QP	72/74 (97%)	63 (88%)	9 (12%)	7	29
16	XP	72/74 (97%)	63 (88%)	9 (12%)	7	29
17	QQ	95/97 (98%)	89 (94%)	6 (6%)	25	69
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	25	69
18	QR	61/77 (79%)	54 (88%)	7 (12%)	8	34
18	XR	61/77 (79%)	54 (88%)	7 (12%)	8	34
19	QS	73/80 (91%)	62 (85%)	11 (15%)	4	18
19	XS	73/80 (91%)	62 (85%)	11 (15%)	4	18
20	QT	76/82 (93%)	68 (90%)	8 (10%)	10	39
20	XT	76/82 (93%)	68 (90%)	8 (10%)	10	39
21	QU	20/22 (91%)	19 (95%)	1 (5%)	34	78
21	XU	20/22 (91%)	19 (95%)	1 (5%)	34	78
27	RD	214/218 (98%)	177 (83%)	37 (17%)	3	13
27	YD	214/218 (98%)	177 (83%)	37 (17%)	3	13
28	RE	165/166 (99%)	128 (78%)	37 (22%)	1	6
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	RF	161/166 (97%)	140 (87%)	21 (13%)	6	26
29	YF	161/166 (97%)	140 (87%)	21 (13%)	6	26
30	RG	155/156 (99%)	130 (84%)	25 (16%)	3	15
30	YG	155/156 (99%)	130 (84%)	25 (16%)	3	15
31	RH	142/148 (96%)	114 (80%)	28 (20%)	2	9
31	YH	142/148 (96%)	114 (80%)	28 (20%)	2	9
32	RI	122/124 (98%)	100 (82%)	22 (18%)	2	12
32	YI	122/124 (98%)	98 (80%)	24 (20%)	2	9
33	RN	117/119 (98%)	98 (84%)	19 (16%)	3	15
33	YN	117/119 (98%)	98 (84%)	19 (16%)	3	15
34	RO	100/100 (100%)	90 (90%)	10 (10%)	11	41
34	YO	100/100 (100%)	90 (90%)	10 (10%)	11	41
35	RP	116/116 (100%)	89 (77%)	27 (23%)	1	5
35	YP	116/116 (100%)	89 (77%)	27 (23%)	1	5
36	RQ	111/111 (100%)	93 (84%)	18 (16%)	3	15
36	YQ	111/111 (100%)	93 (84%)	18 (16%)	3	15
37	RR	101/101 (100%)	84 (83%)	17 (17%)	3	13
37	YR	101/101 (100%)	84 (83%)	17 (17%)	3	13
38	RS	87/88 (99%)	74 (85%)	13 (15%)	4	19
38	YS	87/88 (99%)	74 (85%)	13 (15%)	4	19
39	RT	120/127 (94%)	97 (81%)	23 (19%)	2	10
39	YT	120/127 (94%)	97 (81%)	23 (19%)	2	10
40	RU	93/94 (99%)	80 (86%)	13 (14%)	5	23
40	YU	93/94 (99%)	80 (86%)	13 (14%)	5	23
41	RV	82/82 (100%)	71 (87%)	11 (13%)	6	25
41	YV	82/82 (100%)	71 (87%)	11 (13%)	6	25
42	RW	92/92 (100%)	77 (84%)	15 (16%)	3	15
42	YW	92/92 (100%)	77 (84%)	15 (16%)	3	15
43	RX	74/78 (95%)	63 (85%)	11 (15%)	4	19
43	YX	74/78 (95%)	63 (85%)	11 (15%)	4	19
44	RY	85/91 (93%)	70 (82%)	15 (18%)	3	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	YY	85/91 (93%)	70 (82%)	15 (18%)	3	12
45	RZ	162/179 (90%)	138 (85%)	24 (15%)	4	19
45	YZ	162/179 (90%)	142 (88%)	20 (12%)	7	29
46	R0	65/67 (97%)	58 (89%)	7 (11%)	9	37
46	Y0	65/67 (97%)	63 (97%)	2 (3%)	52	88
47	R1	82/83 (99%)	67 (82%)	15 (18%)	2	11
47	Y1	82/83 (99%)	67 (82%)	15 (18%)	2	11
48	R2	64/67 (96%)	57 (89%)	7 (11%)	9	37
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	9	37
49	R3	51/52 (98%)	40 (78%)	11 (22%)	1	7
49	Y3	51/52 (98%)	40 (78%)	11 (22%)	1	7
50	R4	63/63 (100%)	44 (70%)	19 (30%)	0	1
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	1
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	5
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	5
52	R6	48/52 (92%)	38 (79%)	10 (21%)	2	8
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	2	8
53	R7	42/42 (100%)	39 (93%)	3 (7%)	21	64
53	Y7	42/42 (100%)	39 (93%)	3 (7%)	21	64
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	1
54	Y8	54/55 (98%)	39 (72%)	15 (28%)	0	1
55	R9	34/34 (100%)	32 (94%)	2 (6%)	28	72
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	28	72
All	All	9702/10066 (96%)	8299 (86%)	1403 (14%)	5	21

5 of 1403 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	R2	53	LEU
6	XF	97	PHE
45	YZ	76	LEU
50	R4	39	CYS
2	XB	23	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
47	R1	56	GLN
5	XE	78	HIS
43	YX	87	GLN
48	R2	47	ASN
2	XB	95	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	293 (19%)	45 (3%)
1	XA	1498/1522 (98%)	299 (19%)	47 (3%)
22	QV	76/77 (98%)	21 (27%)	1 (1%)
22	XV	76/77 (98%)	21 (27%)	1 (1%)
23	QY	14/17 (82%)	4 (28%)	1 (7%)
23	XY	14/17 (82%)	4 (28%)	1 (7%)
24	QX	7/25 (28%)	4 (57%)	0
24	XX	7/25 (28%)	3 (42%)	2 (28%)
25	RA	2879/2916 (98%)	618 (21%)	67 (2%)
25	YA	2880/2916 (98%)	612 (21%)	64 (2%)
26	RB	119/122 (97%)	24 (20%)	2 (1%)
26	YB	119/122 (97%)	29 (24%)	1 (0%)
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9190/9364 (98%)	1932 (21%)	232 (2%)

5 of 1932 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	7	G
1	QA	32	A
1	QA	39	G
1	QA	47	C

5 of 232 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2566	A
1	XA	345	C
25	YA	1955	U

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Mol	Chain	Res	Type
25	RA	2723	C
1	XA	60	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	1MG	QY	37	23	24,26,27	2.87	5 (20%)	34,39,42	3.29	8 (23%)
23	1MG	XY	37	23	24,26,27	2.82	5 (20%)	34,39,42	3.24	7 (20%)
56	PPU	Z6	76	25,56	38,40,41	2.42	8 (21%)	54,57,60	2.62	14 (25%)
56	PPU	Z8	76	25,56	38,40,41	2.42	9 (23%)	54,57,60	2.60	14 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	1MG	QY	37	23	-	0/8/25/26	0/3/3/3
23	1MG	XY	37	23	-	0/8/25/26	0/3/3/3
56	PPU	Z6	76	25,56	-	0/26/43/44	0/4/4/4
56	PPU	Z8	76	25,56	-	0/26/43/44	0/4/4/4

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z6	76	PPU	O-C	9.24	1.41	1.23
56	Z8	76	PPU	O-C	9.16	1.41	1.23
23	QY	37	1MG	C4-N3	8.32	1.49	1.35
23	XY	37	1MG	C4-N3	8.22	1.49	1.35
23	QY	37	1MG	C2-N2	6.48	1.47	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	XY	37	1MG	C6-N1-C2	11.79	123.94	120.71
23	QY	37	1MG	C6-C5-N7	-11.67	133.62	134.24
23	QY	37	1MG	C6-N1-C2	11.37	123.83	120.71
23	XY	37	1MG	C6-C5-N7	-11.10	133.65	134.24
56	Z8	76	PPU	N3-C2-N1	-8.51	121.40	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 682 ligands modelled in this entry, 680 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	1670	-	45,45,45	1.31	6 (13%)	67,67,67	1.40	8 (11%)
58	PAR	XA	1675	-	45,45,45	1.35	6 (13%)	67,67,67	1.33	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	QA	1670	-	-	0/18/94/94	0/4/4/4
58	PAR	XA	1675	-	-	0/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	QA	1670	PAR	C52-C42	3.23	1.58	1.52
58	XA	1675	PAR	C52-C42	3.13	1.58	1.52
58	QA	1670	PAR	O54-C14	2.93	1.49	1.41
58	XA	1675	PAR	O54-C14	2.88	1.49	1.41
58	QA	1670	PAR	C64-C54	2.86	1.59	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	QA	1670	PAR	O52-C13-C23	4.72	115.92	107.50
58	XA	1675	PAR	C14-O54-C54	4.35	122.16	113.73
58	XA	1675	PAR	O52-C13-C23	4.25	115.08	107.50
58	XA	1675	PAR	O33-C14-C24	4.14	116.26	108.08
58	QA	1670	PAR	C14-O54-C54	3.84	121.16	113.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1500/1522 (98%)	0.62	141 (9%) 9 1	27, 67, 148, 352	0
1	XA	1500/1522 (98%)	0.64	125 (8%) 11 2	18, 55, 149, 326	0
2	QB	237/256 (92%)	0.54	11 (4%) 31 5	54, 126, 215, 288	0
2	XB	237/256 (92%)	0.36	11 (4%) 31 5	43, 102, 177, 293	0
3	QC	205/239 (85%)	0.56	13 (6%) 19 3	56, 108, 175, 255	0
3	XC	205/239 (85%)	0.27	3 (1%) 70 18	30, 78, 132, 181	0
4	QD	208/209 (99%)	0.72	20 (9%) 8 1	41, 79, 136, 185	0
4	XD	208/209 (99%)	0.55	9 (4%) 34 5	30, 74, 134, 231	0
5	QE	151/162 (93%)	0.56	10 (6%) 18 3	42, 85, 148, 260	0
5	XE	151/162 (93%)	0.34	2 (1%) 74 21	23, 61, 121, 196	0
6	QF	101/101 (100%)	0.15	0 100 100	30, 74, 112, 155	0
6	XF	101/101 (100%)	0.22	0 100 100	26, 69, 110, 146	0
7	QG	155/156 (99%)	0.63	13 (8%) 11 2	46, 97, 158, 302	0
7	XG	155/156 (99%)	0.37	9 (5%) 22 3	35, 82, 149, 230	0
8	QH	138/138 (100%)	0.36	2 (1%) 72 19	39, 83, 130, 174	0
8	XH	138/138 (100%)	0.41	4 (2%) 49 8	34, 68, 117, 169	0
9	QI	127/128 (99%)	1.60	42 (33%) 1 0	48, 117, 170, 243	0
9	XI	127/128 (99%)	0.74	10 (7%) 13 2	33, 91, 152, 203	0
10	QJ	99/105 (94%)	1.75	41 (41%) 1 0	53, 140, 243, 283	0
10	XJ	99/105 (94%)	1.10	18 (18%) 2 0	21, 100, 169, 213	0
11	QK	119/129 (92%)	0.60	5 (4%) 35 5	42, 77, 149, 228	0
11	XK	119/129 (92%)	0.87	15 (12%) 4 1	28, 70, 134, 196	0
12	QL	125/132 (94%)	0.93	15 (12%) 5 1	35, 69, 140, 262	0
12	XL	125/132 (94%)	0.64	11 (8%) 10 2	22, 51, 113, 282	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	1.24	23 (19%) 2 0	43, 108, 185, 410	0
13	XM	121/126 (96%)	0.68	10 (8%) 11 2	36, 86, 141, 273	0
14	QN	60/61 (98%)	1.59	17 (28%) 1 0	59, 101, 150, 166	0
14	XN	60/61 (98%)	0.86	6 (10%) 8 1	36, 67, 127, 143	0
15	QO	88/89 (98%)	0.41	1 (1%) 77 24	32, 78, 150, 180	0
15	XO	88/89 (98%)	0.42	1 (1%) 77 24	27, 62, 111, 129	0
16	QP	84/88 (95%)	0.82	6 (7%) 16 2	38, 71, 115, 186	0
16	XP	84/88 (95%)	1.20	18 (21%) 1 0	39, 73, 119, 211	0
17	QQ	100/105 (95%)	0.75	4 (4%) 36 5	44, 79, 131, 161	0
17	XQ	100/105 (95%)	1.05	11 (11%) 6 1	35, 75, 127, 166	0
18	QR	70/88 (79%)	0.33	1 (1%) 72 19	28, 73, 141, 149	0
18	XR	70/88 (79%)	0.32	2 (2%) 49 8	27, 66, 118, 171	0
19	QS	84/93 (90%)	1.65	27 (32%) 1 0	80, 119, 195, 275	0
19	XS	84/93 (90%)	0.86	5 (5%) 21 3	47, 88, 168, 219	0
20	QT	99/106 (93%)	1.16	22 (22%) 1 0	37, 82, 140, 220	0
20	XT	99/106 (93%)	1.57	37 (37%) 1 0	28, 86, 149, 177	0
21	QU	25/27 (92%)	4.68	24 (96%) 0 0	45, 98, 150, 185	0
21	XU	25/27 (92%)	2.28	10 (40%) 1 0	43, 69, 139, 153	0
22	QV	77/77 (100%)	0.35	4 (5%) 26 4	27, 73, 146, 212	0
22	XV	77/77 (100%)	0.42	4 (5%) 26 4	17, 59, 103, 207	0
23	QY	15/17 (88%)	1.32	3 (20%) 2 0	64, 98, 169, 189	0
23	XY	15/17 (88%)	1.43	3 (20%) 2 0	41, 84, 143, 157	0
24	QX	8/25 (32%)	1.37	2 (25%) 1 0	49, 58, 151, 164	0
24	XX	8/25 (32%)	1.80	2 (25%) 1 0	32, 38, 89, 104	0
25	RA	2882/2916 (98%)	0.59	203 (7%) 16 3	13, 44, 212, 472	0
25	YA	2883/2916 (98%)	0.51	161 (5%) 24 3	7, 35, 201, 461	0
26	RB	120/122 (98%)	0.36	5 (4%) 35 5	43, 69, 105, 120	0
26	YB	120/122 (98%)	-0.03	0 100 100	29, 51, 71, 110	0
27	RD	272/276 (98%)	0.30	5 (1%) 65 15	9, 42, 81, 176	0
27	YD	272/276 (98%)	0.34	3 (1%) 77 24	5, 35, 71, 188	0
28	RE	205/206 (99%)	0.47	7 (3%) 43 6	11, 56, 123, 335	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YE	205/206 (99%)	0.37	4 (1%) 62 14	2, 52, 123, 250	0
29	RF	202/210 (96%)	0.28	0 100 100	15, 62, 132, 185	0
29	YF	202/210 (96%)	0.23	1 (0%) 88 42	8, 45, 121, 194	0
30	RG	181/182 (99%)	1.85	70 (38%) 1 0	79, 156, 284, 386	0
30	YG	181/182 (99%)	0.82	18 (9%) 8 1	30, 89, 155, 309	0
31	RH	170/180 (94%)	1.55	45 (26%) 1 0	79, 145, 235, 306	0
31	YH	170/180 (94%)	0.46	5 (2%) 49 8	31, 79, 122, 167	0
32	RI	146/148 (98%)	0.30	3 (2%) 60 12	25, 87, 178, 297	0
32	YI	146/148 (98%)	0.24	2 (1%) 72 19	22, 83, 152, 183	0
33	RN	138/140 (98%)	0.32	4 (2%) 49 8	26, 64, 124, 179	0
33	YN	138/140 (98%)	0.24	0 100 100	16, 54, 108, 166	0
34	RO	122/122 (100%)	0.22	0 100 100	22, 55, 103, 142	0
34	YO	122/122 (100%)	0.32	0 100 100	16, 48, 78, 126	0
35	RP	150/150 (100%)	0.69	10 (6%) 17 3	18, 68, 154, 247	0
35	YP	150/150 (100%)	0.58	6 (4%) 36 5	9, 53, 126, 253	0
36	RQ	141/141 (100%)	0.91	13 (9%) 9 1	28, 67, 128, 178	0
36	YQ	141/141 (100%)	0.33	3 (2%) 60 12	14, 47, 124, 154	0
37	RR	118/118 (100%)	0.36	4 (3%) 43 6	18, 48, 81, 170	0
37	YR	118/118 (100%)	0.30	0 100 100	20, 46, 85, 137	0
38	RS	111/112 (99%)	0.76	11 (9%) 8 1	38, 76, 131, 184	0
38	YS	111/112 (99%)	0.32	1 (0%) 81 29	28, 58, 106, 195	0
39	RT	137/146 (93%)	0.52	8 (5%) 22 3	29, 67, 161, 259	0
39	YT	137/146 (93%)	0.51	8 (5%) 22 3	27, 61, 152, 303	0
40	RU	117/118 (99%)	0.59	6 (5%) 27 4	20, 54, 114, 221	0
40	YU	117/118 (99%)	0.34	2 (1%) 67 16	19, 39, 97, 221	0
41	RV	101/101 (100%)	0.32	1 (0%) 79 26	21, 77, 140, 320	0
41	YV	101/101 (100%)	0.25	3 (2%) 48 8	13, 63, 124, 304	0
42	RW	113/113 (100%)	0.15	0 100 100	19, 41, 99, 220	0
42	YW	113/113 (100%)	0.04	1 (0%) 81 29	15, 41, 95, 193	0
43	RX	92/96 (95%)	0.28	0 100 100	26, 53, 87, 135	0
43	YX	92/96 (95%)	0.25	0 100 100	12, 39, 76, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RY	102/110 (92%)	0.89	10 (9%) 8 1	40, 99, 177, 285	0
44	YY	102/110 (92%)	0.49	0 100 100	31, 73, 155, 210	0
45	RZ	183/206 (88%)	0.62	14 (7%) 13 2	41, 93, 178, 292	0
45	YZ	183/206 (88%)	0.30	7 (3%) 38 6	32, 71, 179, 271	0
46	R0	82/85 (96%)	0.50	5 (6%) 21 3	18, 49, 71, 179	0
46	Y0	82/85 (96%)	0.35	2 (2%) 56 10	11, 34, 60, 87	0
47	R1	97/98 (98%)	0.59	2 (2%) 60 12	21, 51, 160, 335	0
47	Y1	97/98 (98%)	0.61	5 (5%) 26 4	16, 49, 139, 210	0
48	R2	69/72 (95%)	0.16	0 100 100	28, 69, 143, 169	0
48	Y2	69/72 (95%)	0.32	1 (1%) 72 19	19, 59, 119, 177	0
49	R3	59/60 (98%)	0.54	0 100 100	31, 71, 112, 169	0
49	Y3	59/60 (98%)	0.19	1 (1%) 67 16	22, 49, 91, 198	0
50	R4	71/71 (100%)	1.64	22 (30%) 1 0	107, 211, 311, 396	0
50	Y4	71/71 (100%)	1.32	13 (18%) 2 0	66, 156, 274, 384	0
51	R5	59/60 (98%)	0.60	4 (6%) 17 3	8, 49, 223, 238	0
51	Y5	59/60 (98%)	0.43	3 (5%) 27 4	11, 49, 223, 335	0
52	R6	49/54 (90%)	3.92	37 (75%) 0 0	86, 175, 268, 291	0
52	Y6	49/54 (90%)	2.98	29 (59%) 0 0	76, 163, 229, 312	0
53	R7	49/49 (100%)	0.63	3 (6%) 21 3	16, 29, 87, 168	0
53	Y7	49/49 (100%)	0.48	3 (6%) 21 3	8, 23, 87, 176	0
54	R8	64/65 (98%)	1.10	7 (10%) 6 1	20, 53, 102, 208	0
54	Y8	64/65 (98%)	0.81	3 (4%) 30 5	16, 44, 97, 214	0
55	R9	37/37 (100%)	5.74	37 (100%) 0 0	82, 138, 203, 344	0
55	Y9	37/37 (100%)	4.44	35 (94%) 0 0	57, 119, 223, 246	0
56	Z6	3/3 (100%)	5.46	1 (33%) 1 0	33, 33, 41, 47	0
56	Z8	3/3 (100%)	5.35	1 (33%) 1 0	24, 24, 36, 38	0
All	All	20877/21492 (97%)	0.62	1631 (7%) 13 2	2, 61, 174, 472	0

The worst 5 of 1631 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	YA	2117	A	22.4
25	YA	1060	U	16.8

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Mol	Chain	Res	Type	RSRZ
25	YA	2112	G	15.1
25	YA	2116	G	15.0
25	RA	1088	A	14.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	PPU	Z8	76	37/38	0.42	-	37,37,37,37	0
56	PPU	Z6	76	37/38	0.44	-	41,41,41,41	0
23	1MG	QY	37	24/25	0.22	-	63,63,63,63	0
23	1MG	XY	37	24/25	0.21	-	45,45,45,45	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
57	MG	RA	3098	1/1	0.22	-	10,10,10,10	0
57	MG	RA	3080	1/1	0.22	-	19,19,19,19	0
57	MG	YA	3019	1/1	0.24	-	1,1,1,1	0
57	MG	YA	3201	1/1	0.13	-	14,14,14,14	0
57	MG	QA	1617	1/1	0.20	-	19,19,19,19	0
57	MG	RA	3020	1/1	0.20	-	1,1,1,1	0
57	MG	QA	1604	1/1	0.19	-	12,12,12,12	0
57	MG	YE	302	1/1	0.17	-	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YP	201	1/1	0.13	-	23,23,23,23	0
57	MG	YA	3061	1/1	0.16	-	15,15,15,15	0
57	MG	XA	1659	1/1	0.15	-	34,34,34,34	0
57	MG	YA	3039	1/1	0.09	-	19,19,19,19	0
57	MG	RA	3053	1/1	0.33	-	16,16,16,16	0
57	MG	RA	3167	1/1	0.25	-	29,29,29,29	0
57	MG	RA	3128	1/1	0.31	-	31,31,31,31	0
57	MG	YA	3226	1/1	0.15	-	3,3,3,3	0
57	MG	YA	3257	1/1	0.20	-	3,3,3,3	0
57	MG	YA	3178	1/1	0.22	-	35,35,35,35	0
57	MG	RA	3065	1/1	0.10	-	16,16,16,16	0
57	MG	RA	3150	1/1	0.14	-	25,25,25,25	0
57	MG	XA	1654	1/1	0.35	-	53,53,53,53	0
57	MG	RA	3145	1/1	0.15	-	27,27,27,27	0
57	MG	YA	3255	1/1	0.25	-	13,13,13,13	0
57	MG	YA	3129	1/1	0.18	-	27,27,27,27	0
57	MG	YA	3234	1/1	0.11	-	21,21,21,21	0
57	MG	RA	3067	1/1	0.13	-	9,9,9,9	0
57	MG	RA	3168	1/1	0.28	-	22,22,22,22	0
57	MG	YA	3214	1/1	0.15	-	35,35,35,35	0
57	MG	YA	3209	1/1	0.21	-	27,27,27,27	0
57	MG	YA	3161	1/1	0.13	-	25,25,25,25	0
57	MG	YA	3151	1/1	0.13	-	25,25,25,25	0
57	MG	RA	3182	1/1	0.17	-	10,10,10,10	0
57	MG	YA	3077	1/1	0.19	-	16,16,16,16	0
57	MG	YA	3265	1/1	0.34	-	27,27,27,27	0
57	MG	RA	3159	1/1	0.16	-	30,30,30,30	0
57	MG	YA	3249	1/1	0.19	-	26,26,26,26	0
57	MG	YA	3171	1/1	0.35	-	32,32,32,32	0
57	MG	XA	1646	1/1	0.32	-	45,45,45,45	0
57	MG	YA	3159	1/1	0.20	-	18,18,18,18	0
57	MG	QA	1667	1/1	0.11	-	32,32,32,32	0
57	MG	RE	302	1/1	0.25	-	23,23,23,23	0
57	MG	RA	3025	1/1	0.13	-	15,15,15,15	0
57	MG	YA	3225	1/1	0.18	-	9,9,9,9	0
57	MG	YA	3063	1/1	0.12	-	13,13,13,13	0
57	MG	YA	3162	1/1	0.13	-	20,20,20,20	0
57	MG	YA	3050	1/1	0.32	-	9,9,9,9	0
57	MG	XA	1658	1/1	0.27	-	46,46,46,46	0
57	MG	RA	3074	1/1	0.17	-	4,4,4,4	0
57	MG	RA	3125	1/1	0.26	-	28,28,28,28	0
57	MG	RA	3005	1/1	0.30	-	13,13,13,13	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	0.23	-	26,26,26,26	0
57	MG	XA	1637	1/1	0.35	-	24,24,24,24	0
57	MG	RA	3154	1/1	0.16	-	22,22,22,22	0
57	MG	YA	3187	1/1	0.08	-	29,29,29,29	0
57	MG	YA	3094	1/1	0.17	-	2,2,2,2	0
57	MG	YA	3147	1/1	0.23	-	8,8,8,8	0
57	MG	YA	3026	1/1	0.29	-	8,8,8,8	0
57	MG	RA	3152	1/1	0.12	-	14,14,14,14	0
57	MG	RA	3200	1/1	0.23	-	38,38,38,38	0
57	MG	RA	3174	1/1	0.16	-	38,38,38,38	0
57	MG	XA	1674	1/1	0.10	-	25,25,25,25	0
57	MG	YA	3139	1/1	0.26	-	70,70,70,70	0
57	MG	YA	3240	1/1	0.23	-	43,43,43,43	0
57	MG	RA	3036	1/1	0.14	-	4,4,4,4	0
57	MG	YA	3053	1/1	0.25	-	5,5,5,5	0
57	MG	QA	1628	1/1	0.20	-	25,25,25,25	0
57	MG	YA	3146	1/1	0.29	-	57,57,57,57	0
57	MG	YA	3126	1/1	0.16	-	22,22,22,22	0
57	MG	XA	1672	1/1	0.21	-	40,40,40,40	0
57	MG	RA	3055	1/1	0.15	-	7,7,7,7	0
57	MG	RA	3196	1/1	0.24	-	15,15,15,15	0
57	MG	RA	3034	1/1	0.38	-	30,30,30,30	0
57	MG	RA	3110	1/1	0.15	-	9,9,9,9	0
57	MG	RA	3178	1/1	0.16	-	22,22,22,22	0
57	MG	QA	1659	1/1	0.10	-	39,39,39,39	0
57	MG	YA	3111	1/1	0.14	-	34,34,34,34	0
57	MG	RA	3052	1/1	0.23	-	4,4,4,4	0
57	MG	YA	3004	1/1	0.22	-	5,5,5,5	0
57	MG	YA	3194	1/1	0.24	-	41,41,41,41	0
57	MG	RA	3229	1/1	0.26	-	5,5,5,5	0
57	MG	YA	3098	1/1	0.21	-	16,16,16,16	0
57	MG	YA	3211	1/1	0.14	-	14,14,14,14	0
57	MG	QA	1633	1/1	0.28	-	44,44,44,44	0
57	MG	YA	3224	1/1	0.07	-	24,24,24,24	0
57	MG	XA	1606	1/1	0.20	-	17,17,17,17	0
57	MG	YA	3069	1/1	0.28	-	15,15,15,15	0
57	MG	YA	3015	1/1	0.30	-	8,8,8,8	0
57	MG	RA	3183	1/1	0.16	-	19,19,19,19	0
57	MG	YA	3008	1/1	0.21	-	9,9,9,9	0
57	MG	YA	3158	1/1	0.20	-	24,24,24,24	0
57	MG	XA	1615	1/1	0.06	-	15,15,15,15	0
57	MG	RR	202	1/1	0.23	-	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3082	1/1	0.11	-	8,8,8,8	0
57	MG	QV	101	1/1	0.12	-	26,26,26,26	0
57	MG	YA	3130	1/1	0.25	-	17,17,17,17	0
57	MG	RA	3226	1/1	0.24	-	48,48,48,48	0
57	MG	XA	1647	1/1	0.17	-	49,49,49,49	0
57	MG	YA	3215	1/1	0.19	-	25,25,25,25	0
57	MG	YA	3055	1/1	0.23	-	10,10,10,10	0
57	MG	RA	3113	1/1	0.14	-	32,32,32,32	0
57	MG	XA	1627	1/1	0.08	-	7,7,7,7	0
57	MG	YA	3041	1/1	0.21	-	5,5,5,5	0
57	MG	QA	1654	1/1	0.12	-	79,79,79,79	0
57	MG	RA	3096	1/1	0.25	-	23,23,23,23	0
57	MG	RA	3148	1/1	0.33	-	36,36,36,36	0
57	MG	QA	1610	1/1	0.11	-	11,11,11,11	0
57	MG	XA	1650	1/1	0.10	-	26,26,26,26	0
57	MG	XA	1630	1/1	0.15	-	16,16,16,16	0
57	MG	YA	3070	1/1	0.16	-	8,8,8,8	0
57	MG	QA	1636	1/1	0.10	-	16,16,16,16	0
57	MG	YA	3180	1/1	0.16	-	49,49,49,49	0
57	MG	YB	202	1/1	0.26	-	20,20,20,20	0
57	MG	YA	3217	1/1	0.14	-	29,29,29,29	0
57	MG	YA	3145	1/1	0.21	-	11,11,11,11	0
57	MG	RA	3024	1/1	0.18	-	5,5,5,5	0
57	MG	RA	3175	1/1	0.17	-	21,21,21,21	0
57	MG	YA	3132	1/1	0.11	-	18,18,18,18	0
57	MG	YA	3237	1/1	0.15	-	44,44,44,44	0
57	MG	YA	3035	1/1	0.18	-	5,5,5,5	0
57	MG	RA	3004	1/1	0.37	-	15,15,15,15	0
57	MG	YA	3078	1/1	0.15	-	19,19,19,19	0
57	MG	RA	3180	1/1	0.15	-	34,34,34,34	0
57	MG	YA	3009	1/1	0.26	-	12,12,12,12	0
57	MG	RA	3223	1/1	0.14	-	23,23,23,23	0
57	MG	QH	201	1/1	0.08	-	58,58,58,58	0
57	MG	RA	3238	1/1	0.35	-	32,32,32,32	0
57	MG	QA	1635	1/1	0.07	-	33,33,33,33	0
57	MG	RA	3127	1/1	0.20	-	23,23,23,23	0
57	MG	XA	1604	1/1	0.12	-	15,15,15,15	0
57	MG	YA	3007	1/1	0.18	-	9,9,9,9	0
57	MG	XV	102	1/1	0.17	-	0,0,0,0	0
57	MG	RA	3042	1/1	0.21	-	3,3,3,3	0
59	ZN	QN	101	1/1	0.10	-	80,80,80,80	0
57	MG	RA	3027	1/1	0.18	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3131	1/1	0.35	-	41,41,41,41	0
57	MG	YA	3102	1/1	0.29	-	12,12,12,12	0
57	MG	QA	1614	1/1	0.12	-	26,26,26,26	0
57	MG	YA	3189	1/1	0.24	-	23,23,23,23	0
57	MG	RA	3072	1/1	0.22	-	13,13,13,13	0
57	MG	RA	3097	1/1	0.29	-	14,14,14,14	0
57	MG	QA	1612	1/1	0.18	-	13,13,13,13	0
57	MG	XA	1641	1/1	0.12	-	40,40,40,40	0
57	MG	RA	3138	1/1	0.29	-	12,12,12,12	0
57	MG	XA	1671	1/1	0.13	-	71,71,71,71	0
57	MG	RA	3184	1/1	0.34	-	13,13,13,13	0
57	MG	XA	1651	1/1	0.15	-	12,12,12,12	0
57	MG	QA	1669	1/1	0.09	-	45,45,45,45	0
57	MG	RA	3041	1/1	0.18	-	2,2,2,2	0
57	MG	YA	3262	1/1	0.19	-	38,38,38,38	0
57	MG	YA	3054	1/1	0.26	-	49,49,49,49	0
57	MG	XA	1618	1/1	0.14	-	7,7,7,7	0
57	MG	QA	1665	1/1	0.13	-	18,18,18,18	0
57	MG	RA	3201	1/1	0.17	-	24,24,24,24	0
57	MG	YA	3152	1/1	0.29	-	51,51,51,51	0
57	MG	RA	3084	1/1	0.13	-	9,9,9,9	0
57	MG	XA	1656	1/1	0.13	-	31,31,31,31	0
57	MG	YA	3120	1/1	0.64	-	63,63,63,63	0
57	MG	QA	1613	1/1	0.20	-	21,21,21,21	0
57	MG	RA	3039	1/1	0.19	-	2,2,2,2	0
57	MG	YA	3001	1/1	0.20	-	9,9,9,9	0
57	MG	RA	3121	1/1	0.19	-	29,29,29,29	0
57	MG	RA	3082	1/1	0.12	-	42,42,42,42	0
57	MG	RA	3126	1/1	0.27	-	33,33,33,33	0
57	MG	RA	3141	1/1	0.17	-	33,33,33,33	0
57	MG	YA	3056	1/1	0.13	-	8,8,8,8	0
57	MG	XA	1667	1/1	0.14	-	32,32,32,32	0
57	MG	XA	1662	1/1	0.07	-	11,11,11,11	0
57	MG	RA	3089	1/1	0.16	-	8,8,8,8	0
57	MG	QA	1634	1/1	0.23	-	20,20,20,20	0
57	MG	YA	3239	1/1	0.44	-	46,46,46,46	0
57	MG	YA	3222	1/1	0.29	-	34,34,34,34	0
57	MG	YA	3005	1/1	0.06	-	1,1,1,1	0
57	MG	RA	3155	1/1	0.24	-	24,24,24,24	0
57	MG	YA	3058	1/1	0.17	-	12,12,12,12	0
57	MG	QA	1666	1/1	0.15	-	36,36,36,36	0
57	MG	RA	3186	1/1	0.06	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3043	1/1	0.34	-	15,15,15,15	0
57	MG	RA	3068	1/1	0.17	-	21,21,21,21	0
57	MG	XA	1614	1/1	0.20	-	7,7,7,7	0
57	MG	YA	3036	1/1	0.18	-	5,5,5,5	0
57	MG	RA	3063	1/1	0.42	-	6,6,6,6	0
57	MG	YA	3124	1/1	0.22	-	9,9,9,9	0
57	MG	QA	1608	1/1	0.06	-	13,13,13,13	0
57	MG	RA	3077	1/1	0.30	-	6,6,6,6	0
57	MG	RA	3191	1/1	0.09	-	21,21,21,21	0
57	MG	RA	3236	1/1	0.25	-	33,33,33,33	0
57	MG	RA	3047	1/1	0.31	-	9,9,9,9	0
57	MG	YA	3123	1/1	0.20	-	9,9,9,9	0
57	MG	YA	3067	1/1	0.17	-	22,22,22,22	0
59	ZN	XN	101	1/1	0.20	-	65,65,65,65	0
57	MG	QA	1651	1/1	0.27	-	35,35,35,35	0
57	MG	RD	301	1/1	0.21	-	41,41,41,41	0
57	MG	YA	3052	1/1	0.19	-	21,21,21,21	0
57	MG	YA	3174	1/1	0.16	-	19,19,19,19	0
57	MG	YA	3027	1/1	0.29	-	0,0,0,0	0
57	MG	YA	3048	1/1	0.19	-	10,10,10,10	0
57	MG	XA	1644	1/1	0.15	-	27,27,27,27	0
57	MG	YA	3135	1/1	0.14	-	21,21,21,21	0
57	MG	RA	3017	1/1	0.25	-	8,8,8,8	0
57	MG	RA	3204	1/1	0.34	-	82,82,82,82	0
57	MG	YA	3071	1/1	0.16	-	10,10,10,10	0
57	MG	R5	101	1/1	0.17	-	19,19,19,19	0
57	MG	YA	3157	1/1	0.17	-	30,30,30,30	0
57	MG	RA	3228	1/1	0.69	-	58,58,58,58	0
57	MG	RA	3107	1/1	0.13	-	25,25,25,25	0
57	MG	YA	3046	1/1	0.21	-	8,8,8,8	0
57	MG	YA	3182	1/1	0.22	-	24,24,24,24	0
58	PAR	XA	1675	42/42	0.33	-	49,49,49,49	0
57	MG	XA	1605	1/1	0.19	-	16,16,16,16	0
57	MG	YA	3165	1/1	0.31	-	54,54,54,54	0
57	MG	RA	3028	1/1	0.21	-	4,4,4,4	0
57	MG	QA	1645	1/1	0.30	-	53,53,53,53	0
57	MG	RA	3018	1/1	0.12	-	9,9,9,9	0
57	MG	YA	3253	1/1	0.29	-	18,18,18,18	0
57	MG	YA	3210	1/1	0.19	-	37,37,37,37	0
57	MG	YA	3033	1/1	0.24	-	4,4,4,4	0
57	MG	YA	3143	1/1	0.16	-	17,17,17,17	0
57	MG	RA	3143	1/1	0.23	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3099	1/1	0.28	-	7,7,7,7	0
57	MG	YA	3140	1/1	0.30	-	20,20,20,20	0
57	MG	XA	1626	1/1	0.15	-	19,19,19,19	0
57	MG	YA	3047	1/1	0.24	-	6,6,6,6	0
57	MG	YA	3096	1/1	0.21	-	10,10,10,10	0
57	MG	RA	3104	1/1	0.13	-	16,16,16,16	0
57	MG	RA	3234	1/1	0.18	-	48,48,48,48	0
57	MG	YA	3119	1/1	0.25	-	31,31,31,31	0
57	MG	YA	3010	1/1	0.18	-	4,4,4,4	0
57	MG	YA	3207	1/1	0.37	-	80,80,80,80	0
57	MG	RA	3240	1/1	0.27	-	25,25,25,25	0
57	MG	XA	1621	1/1	0.14	-	29,29,29,29	0
57	MG	YA	3198	1/1	0.33	-	59,59,59,59	0
57	MG	RA	3210	1/1	0.16	-	30,30,30,30	0
57	MG	RA	3014	1/1	0.21	-	9,9,9,9	0
57	MG	RA	3030	1/1	0.26	-	12,12,12,12	0
57	MG	YA	3087	1/1	0.23	-	15,15,15,15	0
57	MG	XA	1642	1/1	0.16	-	23,23,23,23	0
57	MG	RA	3021	1/1	0.30	-	2,2,2,2	0
57	MG	RA	3233	1/1	0.20	-	24,24,24,24	0
57	MG	XA	1625	1/1	0.10	-	16,16,16,16	0
57	MG	RA	3112	1/1	0.11	-	25,25,25,25	0
57	MG	RA	3003	1/1	0.30	-	14,14,14,14	0
57	MG	RA	3136	1/1	0.09	-	9,9,9,9	0
57	MG	RA	3013	1/1	0.26	-	20,20,20,20	0
57	MG	YA	3153	1/1	0.16	-	21,21,21,21	0
57	MG	RA	3001	1/1	0.26	-	11,11,11,11	0
57	MG	XA	1673	1/1	0.18	-	26,26,26,26	0
57	MG	QA	1603	1/1	0.15	-	7,7,7,7	0
57	MG	RA	3085	1/1	0.22	-	16,16,16,16	0
57	MG	YA	3003	1/1	0.21	-	10,10,10,10	0
57	MG	XA	1668	1/1	0.36	-	19,19,19,19	0
57	MG	RA	3177	1/1	0.44	-	38,38,38,38	0
57	MG	QA	1605	1/1	0.28	-	30,30,30,30	0
57	MG	YA	3156	1/1	0.25	-	33,33,33,33	0
57	MG	YA	3028	1/1	0.26	-	9,9,9,9	0
57	MG	YA	3236	1/1	0.20	-	40,40,40,40	0
57	MG	RA	3056	1/1	0.30	-	17,17,17,17	0
57	MG	YA	3243	1/1	0.17	-	42,42,42,42	0
57	MG	QA	1615	1/1	0.16	-	23,23,23,23	0
57	MG	YA	3155	1/1	0.15	-	53,53,53,53	0
57	MG	RA	3105	1/1	0.33	-	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3164	1/1	0.29	-	36,36,36,36	0
57	MG	XA	1661	1/1	0.17	-	48,48,48,48	0
57	MG	XA	1640	1/1	0.21	-	31,31,31,31	0
59	ZN	XD	301	1/1	0.35	-	45,45,45,45	0
57	MG	YA	3220	1/1	0.20	-	52,52,52,52	0
57	MG	RA	3157	1/1	0.28	-	49,49,49,49	0
57	MG	QA	1644	1/1	0.24	-	40,40,40,40	0
57	MG	RA	3187	1/1	0.27	-	63,63,63,63	0
57	MG	RA	3198	1/1	0.13	-	20,20,20,20	0
57	MG	RA	3232	1/1	0.15	-	30,30,30,30	0
57	MG	XA	1623	1/1	0.26	-	40,40,40,40	0
57	MG	YA	3144	1/1	0.26	-	35,35,35,35	0
57	MG	QA	1624	1/1	0.21	-	27,27,27,27	0
57	MG	XA	1657	1/1	0.18	-	31,31,31,31	0
57	MG	RA	3040	1/1	0.32	-	21,21,21,21	0
57	MG	YA	3118	1/1	0.32	-	25,25,25,25	0
57	MG	YA	3097	1/1	0.21	-	19,19,19,19	0
57	MG	RA	3215	1/1	0.13	-	48,48,48,48	0
57	MG	RA	3227	1/1	0.29	-	73,73,73,73	0
57	MG	YA	3138	1/1	0.13	-	10,10,10,10	0
57	MG	YA	3104	1/1	0.27	-	24,24,24,24	0
57	MG	XA	1613	1/1	0.26	-	13,13,13,13	0
57	MG	YA	3023	1/1	0.26	-	16,16,16,16	0
57	MG	YA	3173	1/1	0.27	-	43,43,43,43	0
57	MG	XA	1602	1/1	0.12	-	30,30,30,30	0
57	MG	RA	3172	1/1	0.10	-	23,23,23,23	0
57	MG	RA	3117	1/1	0.20	-	3,3,3,3	0
57	MG	YA	3136	1/1	0.17	-	18,18,18,18	0
57	MG	YA	3238	1/1	0.12	-	24,24,24,24	0
57	MG	RA	3135	1/1	0.17	-	16,16,16,16	0
57	MG	YA	3258	1/1	0.40	-	11,11,11,11	0
57	MG	YA	3032	1/1	0.23	-	4,4,4,4	0
57	MG	QA	1629	1/1	0.26	-	43,43,43,43	0
57	MG	YA	3233	1/1	0.12	-	34,34,34,34	0
57	MG	XA	1649	1/1	0.18	-	30,30,30,30	0
57	MG	RA	3207	1/1	0.35	-	47,47,47,47	0
57	MG	RA	3088	1/1	0.28	-	19,19,19,19	0
57	MG	RA	3235	1/1	0.26	-	22,22,22,22	0
57	MG	YA	3057	1/1	0.23	-	6,6,6,6	0
57	MG	RA	3057	1/1	0.26	-	11,11,11,11	0
57	MG	YA	3208	1/1	0.20	-	55,55,55,55	0
57	MG	RA	3171	1/1	0.16	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3012	1/1	0.39	-	9,9,9,9	0
57	MG	YA	3196	1/1	0.27	-	28,28,28,28	0
57	MG	QA	1607	1/1	0.11	-	40,40,40,40	0
57	MG	YA	3113	1/1	0.15	-	19,19,19,19	0
57	MG	XA	1635	1/1	0.16	-	41,41,41,41	0
57	MG	YA	3031	1/1	0.17	-	2,2,2,2	0
57	MG	YA	3248	1/1	0.26	-	26,26,26,26	0
57	MG	YA	3115	1/1	0.15	-	17,17,17,17	0
57	MG	RA	3049	1/1	0.10	-	8,8,8,8	0
57	MG	XA	1617	1/1	0.15	-	14,14,14,14	0
57	MG	YA	3093	1/1	0.15	-	13,13,13,13	0
57	MG	XA	1645	1/1	0.09	-	29,29,29,29	0
57	MG	XA	1611	1/1	0.15	-	23,23,23,23	0
57	MG	QA	1642	1/1	0.07	-	21,21,21,21	0
57	MG	YA	3175	1/1	0.17	-	37,37,37,37	0
57	MG	RF	301	1/1	0.12	-	40,40,40,40	0
57	MG	RA	3102	1/1	0.20	-	14,14,14,14	0
57	MG	RA	3190	1/1	0.16	-	38,38,38,38	0
57	MG	YA	3122	1/1	0.11	-	9,9,9,9	0
57	MG	YA	3065	1/1	0.12	-	8,8,8,8	0
57	MG	RA	3116	1/1	0.15	-	1,1,1,1	0
57	MG	XA	1622	1/1	0.16	-	26,26,26,26	0
57	MG	RR	201	1/1	0.21	-	7,7,7,7	0
57	MG	RA	3015	1/1	0.16	-	2,2,2,2	0
57	MG	XA	1610	1/1	0.18	-	42,42,42,42	0
57	MG	YA	3014	1/1	0.13	-	3,3,3,3	0
57	MG	YA	3091	1/1	0.17	-	21,21,21,21	0
57	MG	YA	3013	1/1	0.20	-	1,1,1,1	0
57	MG	YA	3131	1/1	0.18	-	35,35,35,35	0
57	MG	RA	3213	1/1	0.26	-	29,29,29,29	0
57	MG	XA	1633	1/1	0.20	-	37,37,37,37	0
57	MG	XA	1620	1/1	0.21	-	17,17,17,17	0
57	MG	QA	1664	1/1	0.15	-	40,40,40,40	0
57	MG	QA	1661	1/1	0.06	-	38,38,38,38	0
57	MG	RA	3079	1/1	0.14	-	17,17,17,17	0
57	MG	YA	3235	1/1	0.15	-	29,29,29,29	0
57	MG	RA	3209	1/1	0.38	-	50,50,50,50	0
57	MG	XV	101	1/1	0.16	-	9,9,9,9	0
57	MG	YA	3044	1/1	0.28	-	7,7,7,7	0
57	MG	YA	3247	1/1	0.13	-	30,30,30,30	0
57	MG	YA	3086	1/1	0.26	-	6,6,6,6	0
57	MG	YA	3177	1/1	0.10	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3122	1/1	0.17	-	29,29,29,29	0
57	MG	YA	3075	1/1	0.24	-	28,28,28,28	0
57	MG	RA	3011	1/1	0.49	-	32,32,32,32	0
57	MG	XA	1660	1/1	0.15	-	30,30,30,30	0
57	MG	YA	3206	1/1	0.14	-	15,15,15,15	0
57	MG	RA	3151	1/1	0.09	-	18,18,18,18	0
57	MG	RA	3016	1/1	0.22	-	1,1,1,1	0
57	MG	RA	3071	1/1	0.16	-	19,19,19,19	0
57	MG	RA	3043	1/1	0.15	-	4,4,4,4	0
57	MG	RA	3118	1/1	0.09	-	33,33,33,33	0
57	MG	RB	202	1/1	0.14	-	54,54,54,54	0
57	MG	XA	1652	1/1	0.18	-	32,32,32,32	0
57	MG	XA	1624	1/1	0.11	-	55,55,55,55	0
57	MG	QA	1658	1/1	0.19	-	63,63,63,63	0
57	MG	YA	3192	1/1	0.22	-	30,30,30,30	0
57	MG	YA	3114	1/1	0.20	-	8,8,8,8	0
57	MG	YA	3125	1/1	0.17	-	11,11,11,11	0
57	MG	YA	3197	1/1	0.10	-	44,44,44,44	0
57	MG	RA	3031	1/1	0.17	-	16,16,16,16	0
57	MG	XA	1601	1/1	0.18	-	4,4,4,4	0
57	MG	YA	3100	1/1	0.33	-	13,13,13,13	0
57	MG	QA	1647	1/1	0.10	-	23,23,23,23	0
57	MG	YQ	201	1/1	0.15	-	25,25,25,25	0
57	MG	YA	3127	1/1	0.29	-	26,26,26,26	0
57	MG	YA	3085	1/1	0.12	-	71,71,71,71	0
57	MG	XA	1603	1/1	0.17	-	38,38,38,38	0
57	MG	RA	3033	1/1	0.25	-	3,3,3,3	0
57	MG	YA	3066	1/1	0.20	-	16,16,16,16	0
57	MG	YA	3149	1/1	0.11	-	16,16,16,16	0
57	MG	QA	1656	1/1	0.22	-	52,52,52,52	0
57	MG	YA	3263	1/1	0.14	-	33,33,33,33	0
57	MG	RA	3038	1/1	0.29	-	9,9,9,9	0
57	MG	QA	1606	1/1	0.13	-	22,22,22,22	0
57	MG	RA	3050	1/1	0.27	-	31,31,31,31	0
57	MG	RA	3100	1/1	0.26	-	9,9,9,9	0
57	MG	RA	3048	1/1	0.10	-	1,1,1,1	0
57	MG	YA	3170	1/1	0.13	-	38,38,38,38	0
57	MG	YA	3045	1/1	0.18	-	2,2,2,2	0
57	MG	YA	3084	1/1	0.20	-	10,10,10,10	0
57	MG	YA	3117	1/1	0.11	-	18,18,18,18	0
57	MG	RA	3133	1/1	0.21	-	28,28,28,28	0
57	MG	YA	3133	1/1	0.11	-	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	XA	1639	1/1	0.07	-	35,35,35,35	0
57	MG	RA	3123	1/1	0.16	-	28,28,28,28	0
57	MG	XA	1619	1/1	0.08	-	18,18,18,18	0
57	MG	RA	3130	1/1	0.24	-	46,46,46,46	0
57	MG	QA	1625	1/1	0.09	-	36,36,36,36	0
57	MG	YA	3204	1/1	0.14	-	19,19,19,19	0
57	MG	RA	3217	1/1	0.13	-	28,28,28,28	0
57	MG	YA	3188	1/1	0.12	-	32,32,32,32	0
57	MG	XA	1663	1/1	0.10	-	44,44,44,44	0
57	MG	YA	3089	1/1	0.22	-	8,8,8,8	0
57	MG	RA	3109	1/1	0.08	-	8,8,8,8	0
57	MG	YA	3088	1/1	0.18	-	1,1,1,1	0
57	MG	YA	3021	1/1	0.27	-	9,9,9,9	0
57	MG	QA	1622	1/1	0.07	-	32,32,32,32	0
57	MG	YA	3172	1/1	0.18	-	43,43,43,43	0
57	MG	RA	3086	1/1	0.21	-	14,14,14,14	0
57	MG	RA	3069	1/1	0.11	-	21,21,21,21	0
57	MG	YA	3185	1/1	0.12	-	10,10,10,10	0
57	MG	QA	1641	1/1	0.18	-	24,24,24,24	0
57	MG	RA	3230	1/1	0.34	-	18,18,18,18	0
57	MG	YA	3068	1/1	0.26	-	17,17,17,17	0
57	MG	YA	3037	1/1	0.22	-	1,1,1,1	0
57	MG	YA	3203	1/1	0.18	-	27,27,27,27	0
57	MG	QA	1626	1/1	0.18	-	59,59,59,59	0
57	MG	YA	3254	1/1	0.22	-	7,7,7,7	0
57	MG	RA	3195	1/1	0.34	-	31,31,31,31	0
57	MG	RA	3078	1/1	0.21	-	22,22,22,22	0
57	MG	RA	3019	1/1	0.27	-	19,19,19,19	0
57	MG	XA	1638	1/1	0.09	-	16,16,16,16	0
57	MG	RA	3222	1/1	0.45	-	93,93,93,93	0
57	MG	RA	3153	1/1	0.20	-	51,51,51,51	0
57	MG	YA	3232	1/1	0.09	-	23,23,23,23	0
57	MG	YA	3223	1/1	0.19	-	25,25,25,25	0
57	MG	QA	1668	1/1	0.10	-	42,42,42,42	0
57	MG	RA	3064	1/1	0.23	-	5,5,5,5	0
57	MG	Y0	101	1/1	0.20	-	7,7,7,7	0
57	MG	RA	3007	1/1	0.23	-	6,6,6,6	0
59	ZN	QD	301	1/1	0.26	-	47,47,47,47	0
57	MG	RA	3181	1/1	0.30	-	48,48,48,48	0
57	MG	RA	3099	1/1	0.31	-	24,24,24,24	0
57	MG	YA	3116	1/1	0.18	-	36,36,36,36	0
57	MG	RA	3062	1/1	0.15	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3018	1/1	0.29	-	13,13,13,13	0
57	MG	XA	1631	1/1	0.15	-	35,35,35,35	0
57	MG	YA	3024	1/1	0.18	-	16,16,16,16	0
57	MG	RA	3206	1/1	0.31	-	15,15,15,15	0
57	MG	RA	3022	1/1	0.20	-	16,16,16,16	0
57	MG	RA	3058	1/1	0.30	-	37,37,37,37	0
57	MG	RA	3051	1/1	0.15	-	3,3,3,3	0
57	MG	QA	1662	1/1	0.10	-	53,53,53,53	0
57	MG	QA	1643	1/1	0.13	-	22,22,22,22	0
57	MG	RA	3185	1/1	0.17	-	25,25,25,25	0
57	MG	QA	1650	1/1	0.21	-	49,49,49,49	0
57	MG	RA	3103	1/1	0.11	-	8,8,8,8	0
57	MG	QA	1648	1/1	0.16	-	12,12,12,12	0
57	MG	RA	3211	1/1	0.38	-	43,43,43,43	0
57	MG	RA	3114	1/1	0.24	-	20,20,20,20	0
57	MG	YA	3142	1/1	0.23	-	28,28,28,28	0
57	MG	RA	3094	1/1	0.07	-	9,9,9,9	0
57	MG	QA	1611	1/1	0.22	-	14,14,14,14	0
57	MG	YA	3202	1/1	0.21	-	59,59,59,59	0
57	MG	QA	1620	1/1	0.16	-	28,28,28,28	0
57	MG	RA	3221	1/1	0.33	-	62,62,62,62	0
57	MG	RA	3134	1/1	0.33	-	44,44,44,44	0
57	MG	RA	3164	1/1	0.23	-	36,36,36,36	0
57	MG	YA	3128	1/1	0.30	-	26,26,26,26	0
57	MG	RA	3216	1/1	0.30	-	43,43,43,43	0
57	MG	RA	3124	1/1	0.17	-	23,23,23,23	0
57	MG	RA	3081	1/1	0.07	-	30,30,30,30	0
57	MG	YA	3229	1/1	0.14	-	24,24,24,24	0
57	MG	XA	1643	1/1	0.13	-	29,29,29,29	0
57	MG	RA	3146	1/1	0.11	-	33,33,33,33	0
57	MG	RA	3035	1/1	0.24	-	11,11,11,11	0
57	MG	R0	101	1/1	0.19	-	11,11,11,11	0
57	MG	XA	1608	1/1	0.32	-	23,23,23,23	0
57	MG	QA	1601	1/1	0.18	-	33,33,33,33	0
57	MG	YA	3260	1/1	0.16	-	14,14,14,14	0
57	MG	YA	3219	1/1	0.96	-	52,52,52,52	0
57	MG	RA	3144	1/1	0.23	-	17,17,17,17	0
57	MG	YA	3073	1/1	0.18	-	7,7,7,7	0
57	MG	RA	3208	1/1	0.14	-	19,19,19,19	0
57	MG	YA	3006	1/1	0.23	-	9,9,9,9	0
57	MG	RA	3002	1/1	0.51	-	36,36,36,36	0
57	MG	RA	3203	1/1	0.18	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3109	1/1	0.24	-	10,10,10,10	0
57	MG	YA	3042	1/1	0.17	-	19,19,19,19	0
57	MG	YA	3242	1/1	0.15	-	72,72,72,72	0
57	MG	QA	1619	1/1	0.07	-	33,33,33,33	0
57	MG	YA	3205	1/1	0.18	-	38,38,38,38	0
57	MG	QA	1609	1/1	0.15	-	34,34,34,34	0
57	MG	YA	3213	1/1	0.19	-	29,29,29,29	0
57	MG	RA	3111	1/1	0.40	-	22,22,22,22	0
57	MG	YB	203	1/1	0.17	-	37,37,37,37	0
57	MG	RA	3106	1/1	0.18	-	11,11,11,11	0
57	MG	YA	3060	1/1	0.13	-	4,4,4,4	0
57	MG	RA	3060	1/1	0.26	-	8,8,8,8	0
57	MG	RA	3059	1/1	0.16	-	2,2,2,2	0
57	MG	YA	3095	1/1	0.24	-	7,7,7,7	0
57	MG	QA	1632	1/1	0.16	-	35,35,35,35	0
57	MG	QA	1638	1/1	0.23	-	27,27,27,27	0
57	MG	RA	3029	1/1	0.23	-	2,2,2,2	0
57	MG	RA	3045	1/1	0.19	-	16,16,16,16	0
57	MG	YA	3191	1/1	0.29	-	24,24,24,24	0
57	MG	RP	201	1/1	0.20	-	30,30,30,30	0
57	MG	RA	3214	1/1	0.19	-	18,18,18,18	0
57	MG	QA	1646	1/1	0.07	-	39,39,39,39	0
57	MG	YA	3105	1/1	0.24	-	21,21,21,21	0
57	MG	QM	201	1/1	0.04	-	55,55,55,55	0
57	MG	RE	301	1/1	0.06	-	1,1,1,1	0
57	MG	YA	3150	1/1	0.35	-	61,61,61,61	0
57	MG	RA	3073	1/1	0.21	-	24,24,24,24	0
57	MG	YA	3218	1/1	0.09	-	10,10,10,10	0
57	MG	QA	1621	1/1	0.08	-	14,14,14,14	0
57	MG	YA	3163	1/1	0.17	-	28,28,28,28	0
57	MG	RA	3158	1/1	0.25	-	51,51,51,51	0
57	MG	RA	3087	1/1	0.19	-	34,34,34,34	0
57	MG	YA	3025	1/1	0.20	-	8,8,8,8	0
57	MG	XA	1616	1/1	0.11	-	17,17,17,17	0
57	MG	YA	3252	1/1	0.41	-	25,25,25,25	0
57	MG	RA	3179	1/1	0.21	-	15,15,15,15	0
57	MG	YA	3040	1/1	0.24	-	8,8,8,8	0
57	MG	RA	3147	1/1	0.20	-	21,21,21,21	0
57	MG	YA	3259	1/1	0.45	-	43,43,43,43	0
57	MG	YA	3083	1/1	0.18	-	7,7,7,7	0
57	MG	QA	1637	1/1	0.24	-	57,57,57,57	0
57	MG	QA	1623	1/1	0.18	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3205	1/1	0.17	-	46,46,46,46	0
57	MG	YA	3181	1/1	0.25	-	34,34,34,34	0
57	MG	YA	3107	1/1	0.30	-	11,11,11,11	0
57	MG	YA	3110	1/1	0.08	-	15,15,15,15	0
57	MG	RA	3101	1/1	0.20	-	7,7,7,7	0
57	MG	YA	3049	1/1	0.31	-	14,14,14,14	0
57	MG	RA	3026	1/1	0.18	-	8,8,8,8	0
57	MG	RA	3156	1/1	0.29	-	44,44,44,44	0
57	MG	RA	3199	1/1	0.13	-	29,29,29,29	0
57	MG	YA	3017	1/1	0.14	-	2,2,2,2	0
57	MG	RA	3231	1/1	0.35	-	9,9,9,9	0
57	MG	YA	3081	1/1	0.15	-	5,5,5,5	0
57	MG	YA	3241	1/1	0.23	-	46,46,46,46	0
57	MG	XA	1607	1/1	0.34	-	31,31,31,31	0
57	MG	YA	3256	1/1	0.23	-	7,7,7,7	0
57	MG	YA	3079	1/1	0.09	-	12,12,12,12	0
57	MG	QA	1663	1/1	0.09	-	82,82,82,82	0
57	MG	RA	3108	1/1	0.19	-	24,24,24,24	0
57	MG	YA	3251	1/1	0.28	-	20,20,20,20	0
57	MG	YA	3216	1/1	0.20	-	59,59,59,59	0
57	MG	YA	3166	1/1	0.20	-	58,58,58,58	0
57	MG	RA	3193	1/1	0.40	-	51,51,51,51	0
57	MG	QA	1627	1/1	0.14	-	26,26,26,26	0
57	MG	RA	3010	1/1	0.26	-	78,78,78,78	0
57	MG	YA	3186	1/1	0.15	-	39,39,39,39	0
57	MG	QA	1602	1/1	0.20	-	18,18,18,18	0
57	MG	QA	1657	1/1	0.28	-	58,58,58,58	0
57	MG	RA	3012	1/1	0.25	-	8,8,8,8	0
57	MG	XA	1670	1/1	0.11	-	29,29,29,29	0
57	MG	RA	3070	1/1	0.23	-	26,26,26,26	0
57	MG	RA	3239	1/1	0.18	-	19,19,19,19	0
57	MG	RA	3139	1/1	0.22	-	49,49,49,49	0
57	MG	XA	1655	1/1	0.25	-	81,81,81,81	0
57	MG	RA	3061	1/1	0.25	-	9,9,9,9	0
57	MG	YA	3092	1/1	0.19	-	30,30,30,30	0
57	MG	RA	3092	1/1	0.11	-	9,9,9,9	0
57	MG	XA	1664	1/1	0.26	-	51,51,51,51	0
57	MG	YA	3121	1/1	0.09	-	18,18,18,18	0
57	MG	YA	3244	1/1	0.17	-	25,25,25,25	0
57	MG	YA	3090	1/1	0.23	-	5,5,5,5	0
57	MG	RA	3219	1/1	0.51	-	63,63,63,63	0
57	MG	XA	1648	1/1	0.12	-	39,39,39,39	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	0.13	-	8,8,8,8	0
57	MG	YA	3190	1/1	0.07	-	2,2,2,2	0
57	MG	RA	3165	1/1	0.09	-	19,19,19,19	0
57	MG	QA	1639	1/1	0.18	-	36,36,36,36	0
57	MG	QA	1660	1/1	0.17	-	35,35,35,35	0
57	MG	RA	3037	1/1	0.16	-	11,11,11,11	0
57	MG	RA	3162	1/1	0.14	-	18,18,18,18	0
57	MG	RA	3192	1/1	0.32	-	79,79,79,79	0
57	MG	XA	1609	1/1	0.23	-	22,22,22,22	0
57	MG	YA	3002	1/1	0.27	-	9,9,9,9	0
57	MG	YA	3230	1/1	0.13	-	32,32,32,32	0
57	MG	QA	1630	1/1	0.17	-	48,48,48,48	0
57	MG	RA	3149	1/1	0.11	-	32,32,32,32	0
57	MG	YA	3200	1/1	0.23	-	26,26,26,26	0
57	MG	RA	3188	1/1	0.19	-	39,39,39,39	0
57	MG	YA	3020	1/1	0.38	-	7,7,7,7	0
57	MG	RA	3095	1/1	0.26	-	14,14,14,14	0
57	MG	RA	3166	1/1	0.17	-	43,43,43,43	0
57	MG	RA	3220	1/1	0.22	-	56,56,56,56	0
57	MG	RA	3046	1/1	0.15	-	12,12,12,12	0
57	MG	YA	3261	1/1	0.26	-	8,8,8,8	0
57	MG	RA	3083	1/1	0.16	-	11,11,11,11	0
57	MG	QA	1618	1/1	0.20	-	42,42,42,42	0
57	MG	YA	3022	1/1	0.26	-	7,7,7,7	0
57	MG	XA	1629	1/1	0.19	-	29,29,29,29	0
57	MG	RA	3202	1/1	0.15	-	21,21,21,21	0
57	MG	YA	3167	1/1	0.10	-	21,21,21,21	0
57	MG	YA	3072	1/1	0.21	-	17,17,17,17	0
57	MG	XA	1636	1/1	0.15	-	5,5,5,5	0
57	MG	RA	3091	1/1	0.39	-	73,73,73,73	0
57	MG	YA	3183	1/1	0.19	-	30,30,30,30	0
57	MG	YA	3059	1/1	0.13	-	6,6,6,6	0
57	MG	RA	3218	1/1	0.17	-	29,29,29,29	0
57	MG	YA	3074	1/1	0.09	-	6,6,6,6	0
57	MG	XA	1669	1/1	0.15	-	41,41,41,41	0
57	MG	RA	3044	1/1	0.21	-	24,24,24,24	0
57	MG	RA	3032	1/1	0.24	-	15,15,15,15	0
57	MG	YA	3108	1/1	0.13	-	3,3,3,3	0
57	MG	RA	3120	1/1	0.33	-	60,60,60,60	0
57	MG	YA	3034	1/1	0.26	-	9,9,9,9	0
57	MG	YA	3160	1/1	0.17	-	12,12,12,12	0
57	MG	QA	1616	1/1	0.07	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YB	201	1/1	0.35	-	35,35,35,35	0
57	MG	XA	1653	1/1	0.14	-	60,60,60,60	0
57	MG	YA	3112	1/1	0.07	-	15,15,15,15	0
57	MG	RA	3212	1/1	0.15	-	42,42,42,42	0
57	MG	RA	3140	1/1	0.35	-	26,26,26,26	0
57	MG	Y5	101	1/1	0.12	-	26,26,26,26	0
57	MG	RA	3132	1/1	0.29	-	22,22,22,22	0
57	MG	YA	3080	1/1	0.20	-	10,10,10,10	0
57	MG	YA	3168	1/1	0.09	-	13,13,13,13	0
57	MG	XA	1612	1/1	0.11	-	13,13,13,13	0
57	MG	YA	3184	1/1	0.21	-	20,20,20,20	0
57	MG	RA	3160	1/1	0.22	-	51,51,51,51	0
57	MG	YA	3051	1/1	0.19	-	2,2,2,2	0
57	MG	YA	3199	1/1	0.33	-	18,18,18,18	0
57	MG	YE	301	1/1	0.17	-	7,7,7,7	0
57	MG	YA	3011	1/1	0.22	-	20,20,20,20	0
58	PAR	QA	1670	42/42	0.41	-	56,56,56,56	0
57	MG	RA	3115	1/1	0.18	-	7,7,7,7	0
57	MG	QA	1640	1/1	0.17	-	51,51,51,51	0
57	MG	YA	3062	1/1	0.11	-	9,9,9,9	0
57	MG	QA	1653	1/1	0.12	-	36,36,36,36	0
57	MG	QF	201	1/1	0.12	-	39,39,39,39	0
57	MG	RA	3066	1/1	0.13	-	24,24,24,24	0
57	MG	RA	3225	1/1	0.10	-	27,27,27,27	0
57	MG	RA	3119	1/1	0.16	-	56,56,56,56	0
57	MG	YA	3029	1/1	0.22	-	12,12,12,12	0
57	MG	YA	3134	1/1	0.17	-	21,21,21,21	0
57	MG	YA	3106	1/1	0.13	-	9,9,9,9	0
57	MG	YA	3245	1/1	0.12	-	38,38,38,38	0
57	MG	QA	1631	1/1	0.31	-	46,46,46,46	0
57	MG	XA	1634	1/1	0.14	-	15,15,15,15	0
57	MG	YA	3169	1/1	0.14	-	20,20,20,20	0
57	MG	RA	3142	1/1	0.22	-	39,39,39,39	0
57	MG	RA	3023	1/1	0.17	-	14,14,14,14	0
57	MG	RA	3054	1/1	0.08	-	0,0,0,0	0
57	MG	RA	3008	1/1	0.18	-	27,27,27,27	0
57	MG	RA	3009	1/1	0.07	-	9,9,9,9	0
57	MG	RA	3197	1/1	0.23	-	55,55,55,55	0
57	MG	YA	3195	1/1	0.20	-	35,35,35,35	0
57	MG	YA	3179	1/1	0.23	-	35,35,35,35	0
57	MG	RA	3076	1/1	0.30	-	15,15,15,15	0
57	MG	YA	3076	1/1	0.27	-	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3221	1/1	0.21	-	19,19,19,19	0
57	MG	RA	3176	1/1	0.17	-	24,24,24,24	0
57	MG	RA	3170	1/1	0.11	-	25,25,25,25	0
57	MG	RA	3075	1/1	0.08	-	15,15,15,15	0
57	MG	YA	3193	1/1	0.18	-	27,27,27,27	0
57	MG	YA	3246	1/1	0.18	-	21,21,21,21	0
57	MG	RA	3189	1/1	0.12	-	34,34,34,34	0
57	MG	RA	3129	1/1	0.12	-	21,21,21,21	0
57	MG	YA	3141	1/1	0.10	-	16,16,16,16	0
57	MG	YA	3227	1/1	0.25	-	13,13,13,13	0
57	MG	YA	3264	1/1	0.12	-	24,24,24,24	0
57	MG	YA	3064	1/1	0.20	-	39,39,39,39	0
57	MG	YA	3228	1/1	0.17	-	22,22,22,22	0
57	MG	RA	3137	1/1	0.17	-	10,10,10,10	0
57	MG	YA	3148	1/1	0.14	-	14,14,14,14	0
57	MG	QA	1652	1/1	0.16	-	37,37,37,37	0
57	MG	YA	3038	1/1	0.12	-	6,6,6,6	0
57	MG	YA	3103	1/1	0.24	-	31,31,31,31	0
57	MG	YA	3250	1/1	0.12	-	40,40,40,40	0
57	MG	RA	3224	1/1	0.11	-	52,52,52,52	0
57	MG	RA	3090	1/1	0.18	-	23,23,23,23	0
57	MG	RA	3161	1/1	0.13	-	27,27,27,27	0
57	MG	XA	1628	1/1	0.14	-	27,27,27,27	0
57	MG	RA	3093	1/1	0.22	-	9,9,9,9	0
57	MG	XA	1666	1/1	0.32	-	43,43,43,43	0
57	MG	YA	3101	1/1	0.28	-	8,8,8,8	0
57	MG	YA	3231	1/1	0.09	-	19,19,19,19	0
57	MG	YA	3212	1/1	0.07	-	9,9,9,9	0
57	MG	XX	101	1/1	0.14	-	22,22,22,22	0
57	MG	QA	1655	1/1	0.13	-	51,51,51,51	0
57	MG	YA	3176	1/1	0.17	-	6,6,6,6	0
57	MG	YA	3137	1/1	0.15	-	6,6,6,6	0
57	MG	XA	1665	1/1	0.24	-	44,44,44,44	0
57	MG	RA	3194	1/1	0.21	-	44,44,44,44	0
57	MG	YA	3154	1/1	0.23	-	9,9,9,9	0
57	MG	QA	1649	1/1	0.20	-	39,39,39,39	0
57	MG	RA	3173	1/1	0.15	-	15,15,15,15	0
57	MG	RA	3163	1/1	0.17	-	38,38,38,38	0
57	MG	XA	1632	1/1	0.17	-	17,17,17,17	0
57	MG	RB	201	1/1	0.10	-	59,59,59,59	0
57	MG	Y7	101	1/1	0.36	-	38,38,38,38	0
57	MG	RA	3006	1/1	0.36	-	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3169	1/1	0.35	-	35,35,35,35	0
57	MG	YA	3030	1/1	0.41	-	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.