



wwPDB X-ray Structure Validation Summary Report

Sep 17, 2014 – 03:11 PM EDT

PDB ID : 4L47
Title : Crystal Structure of Frameshift Suppressor tRNA SufA6 Bound to Codon CCC-U on the Ribosome
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-06-07
Resolution : 3.22 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>

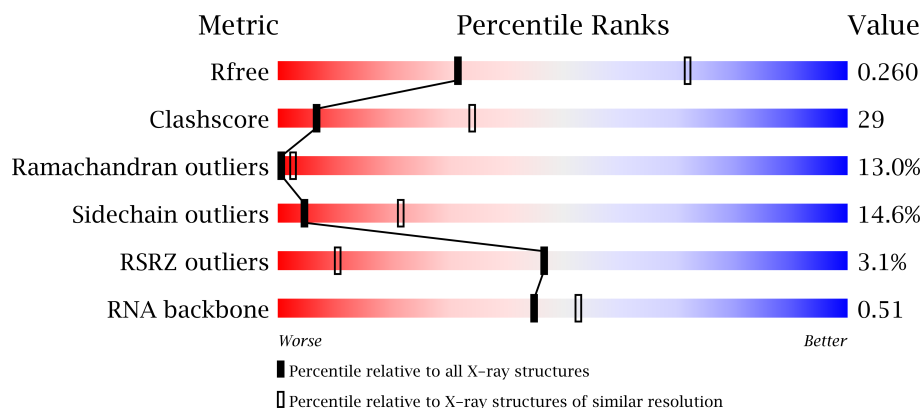
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.22 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	1205 (3.30-3.14)
Clashscore	79885	1072 (3.28-3.16)
Ramachandran outliers	78287	1052 (3.28-3.16)
Sidechain outliers	78261	1051 (3.28-3.16)
RSRZ outliers	66119	1206 (3.30-3.14)
RNA backbone	1838	1004 (3.74-2.70)

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

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

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Mol	Chain	Length	Quality of chain
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	25	
23	XX	25	
24	QY	18	
24	XY	18	
25	RA	2916	
25	YA	2916	
26	RB	122	
26	YB	122	
27	RD	276	

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

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

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291957 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	8	Total	C	N	O	P	0	0	0
			167	75	28	56	8			
23	XX	8	Total	C	N	O	P	0	0	0
			167	75	28	56	8			

- Molecule 24 is a RNA chain called messenger RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	66	Total	Mg	0	0
			66	66		
57	RP	2	Total	Mg	0	0
			2	2		
57	YA	269	Total	Mg	0	0
			269	269		
57	QM	1	Total	Mg	0	0
			1	1		
57	YD	1	Total	Mg	0	0
			1	1		

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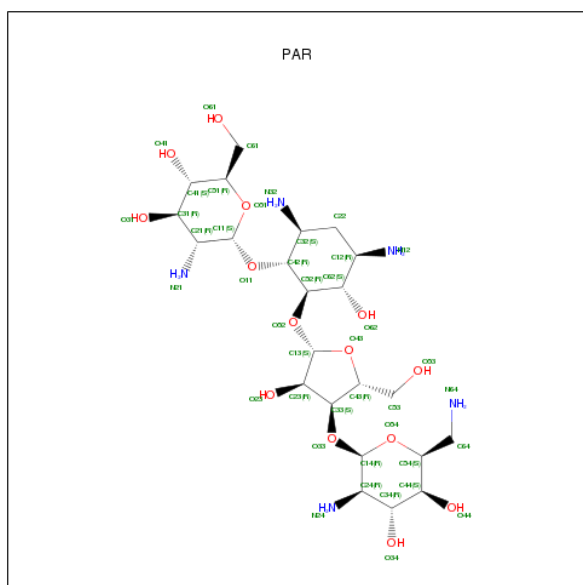
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	XX	1	Total 1	Mg 1	0	0
57	QV	2	Total 2	Mg 2	0	0
57	XA	72	Total 72	Mg 72	0	0
57	R0	1	Total 1	Mg 1	0	0
57	XT	1	Total 1	Mg 1	0	0
57	RU	1	Total 1	Mg 1	0	0
57	QH	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	YX	1	Total 1	Mg 1	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RD	1	Total 1	Mg 1	0	0
57	Y7	1	Total 1	Mg 1	0	0
57	QF	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	RA	241	Total 241	Mg 241	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	1	Total 1	Mg 1	0	0
57	RB	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	XM	1	Total	Mg	0	0
			1	1		
57	YE	2	Total	Mg	0	0
			2	2		

- 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		

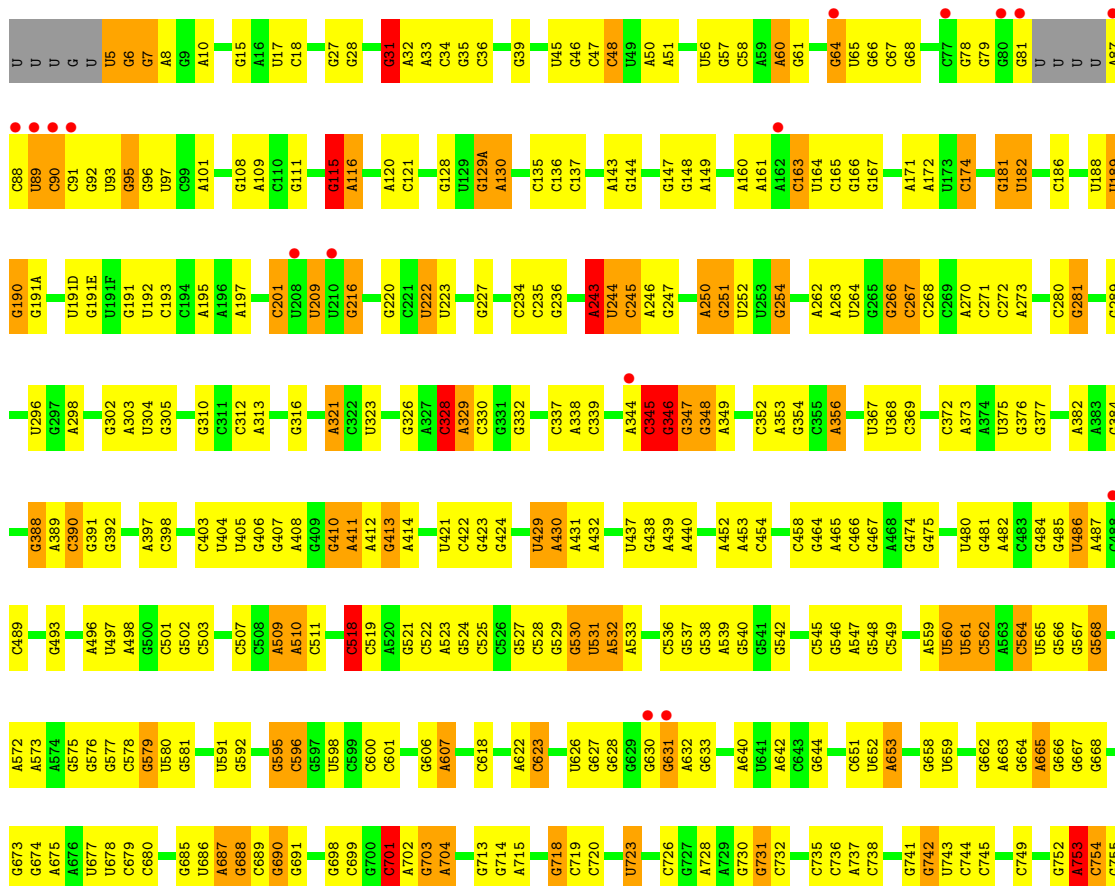
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

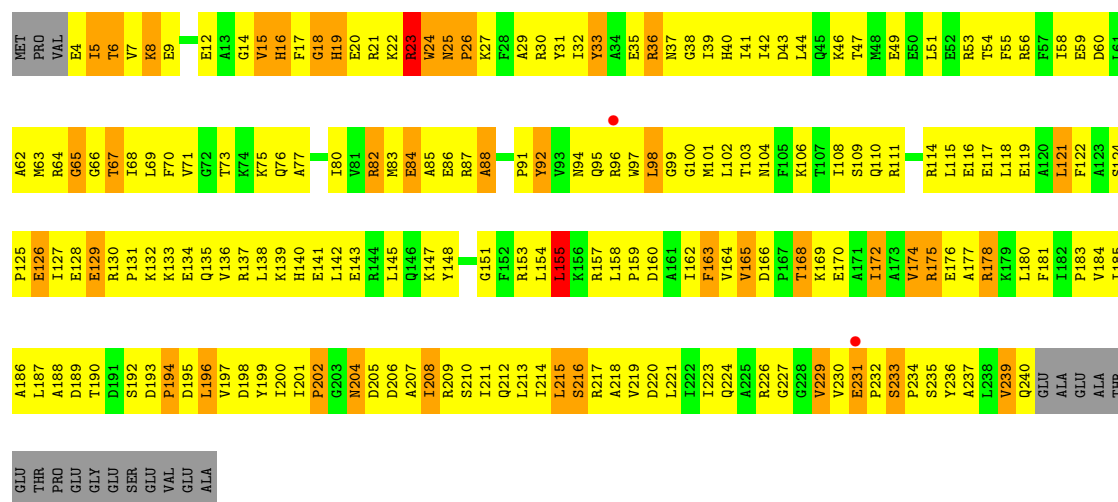
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	R9	1	Total	Zn	0	0
			1	1		

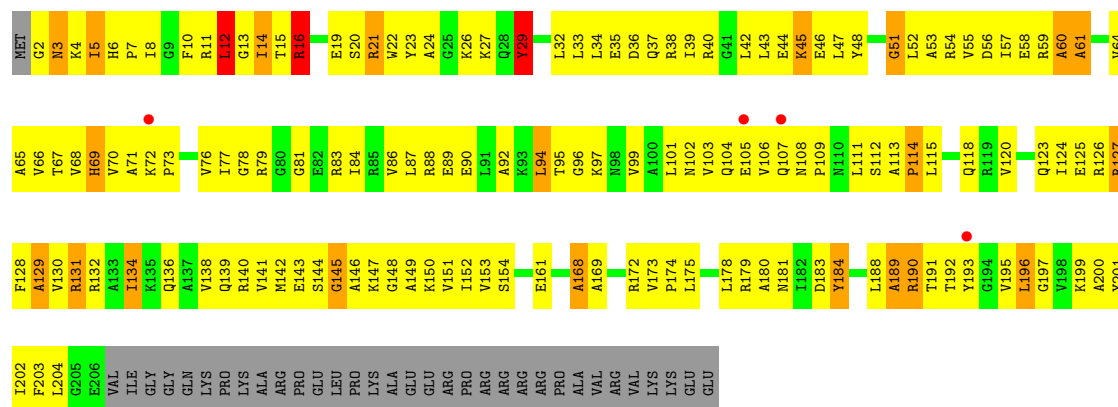






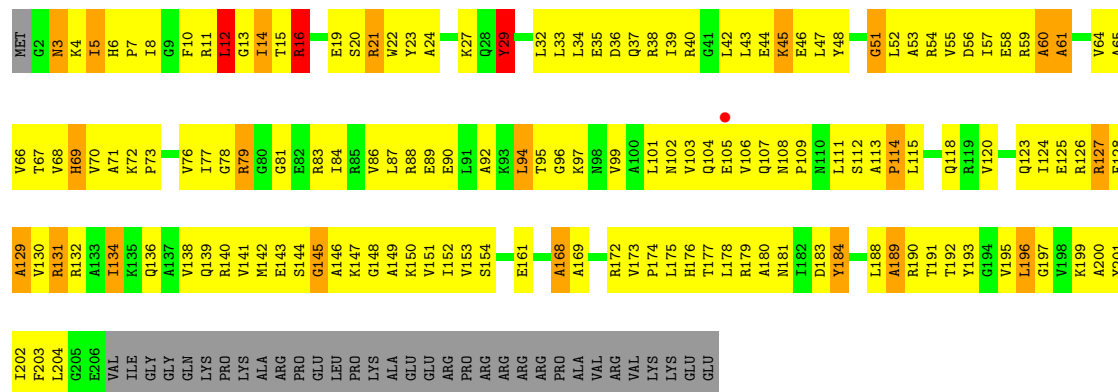
• Molecule 3: 30S ribosomal protein S3

Chain QC:



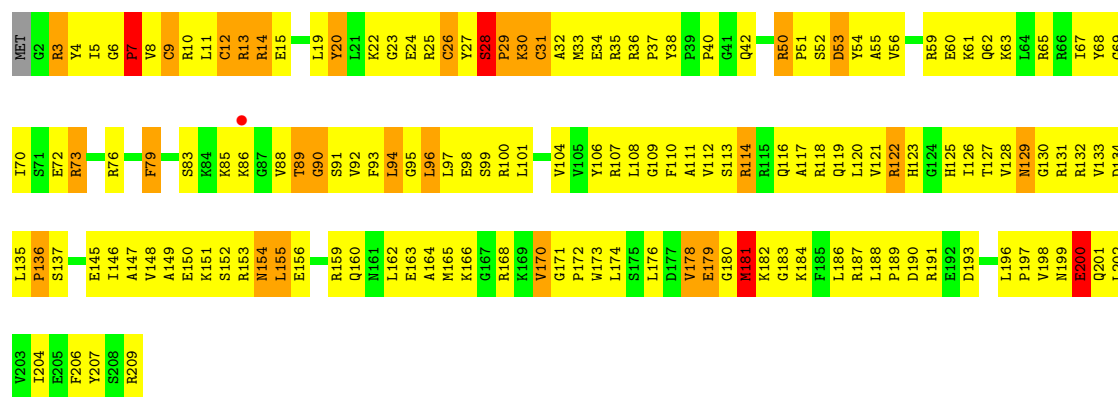
• Molecule 3: 30S ribosomal protein S3

Chain XC:



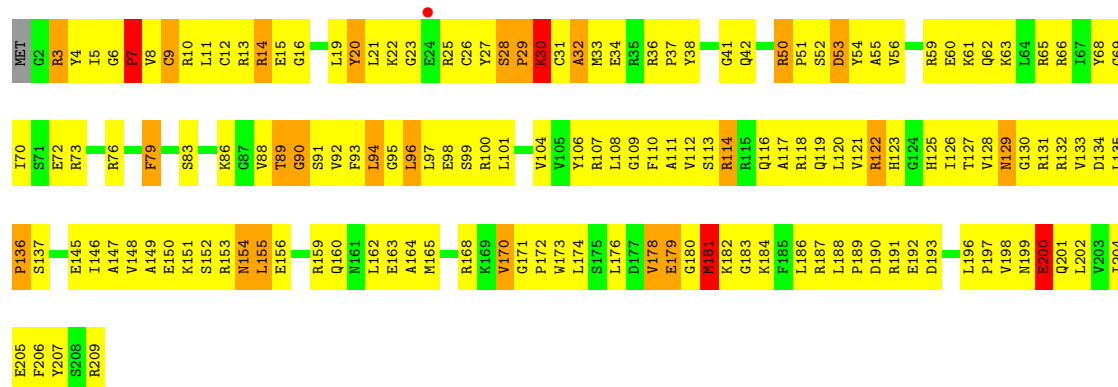
• Molecule 4: 30S ribosomal protein S4

Chain QD:



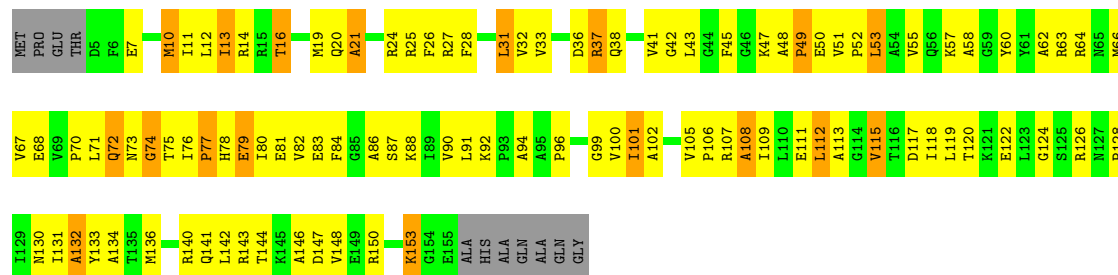
• Molecule 4: 30S ribosomal protein S4

Chain XD:



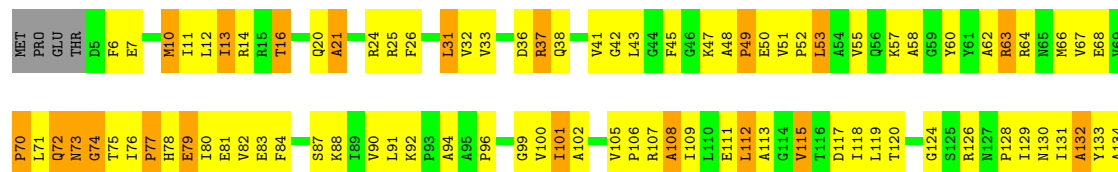
• Molecule 5: 30S ribosomal protein S5

Chain QE:



• Molecule 5: 30S ribosomal protein S5

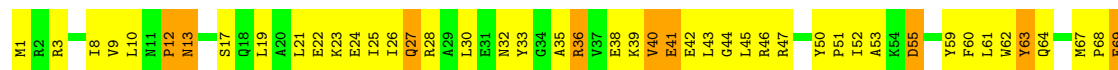
Chain XE:





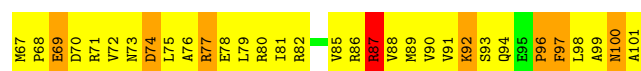
• Molecule 6: 30S ribosomal protein S6

Chain QF:



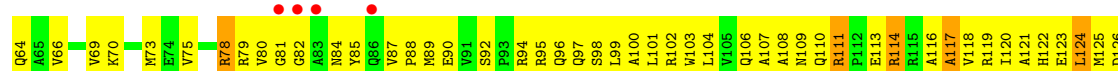
• Molecule 6: 30S ribosomal protein S6

Chain XF:



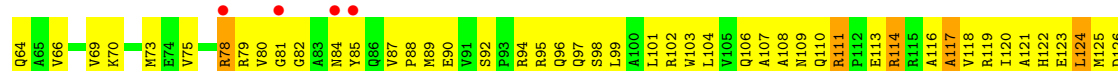
• Molecule 7: 30S ribosomal protein S7

Chain QG:



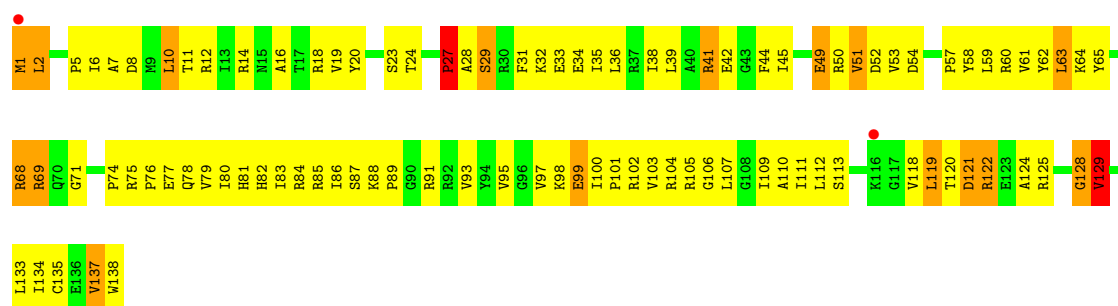
• Molecule 7: 30S ribosomal protein S7

Chain XG:



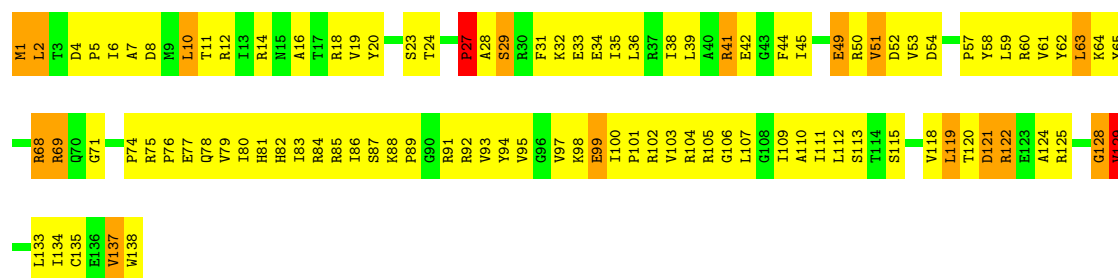
• Molecule 8: 30S ribosomal protein S8

Chain QH:



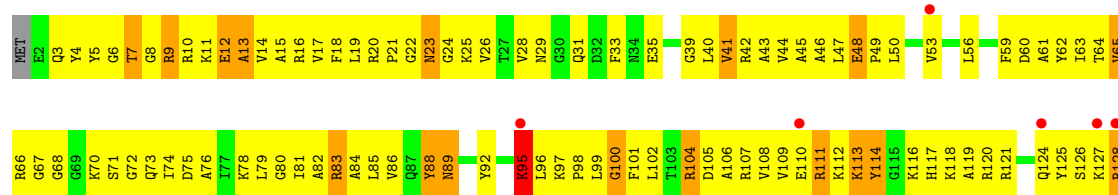
- Molecule 8: 30S ribosomal protein S8

Chain XH:



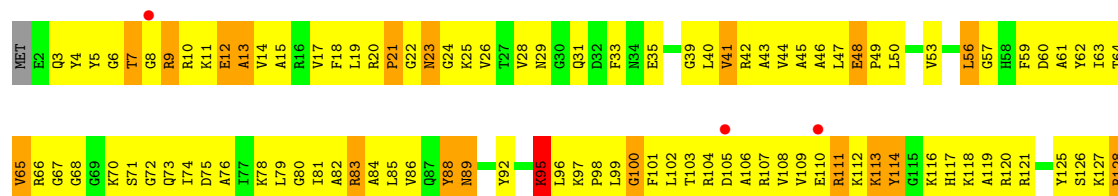
- Molecule 9: 30S ribosomal protein S9

Chain QI:



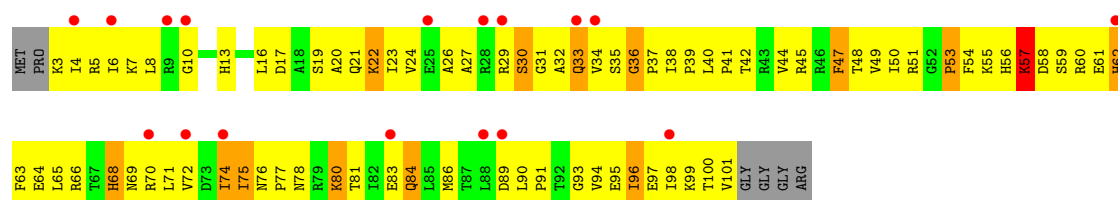
- Molecule 9: 30S ribosomal protein S9

Chain XI:



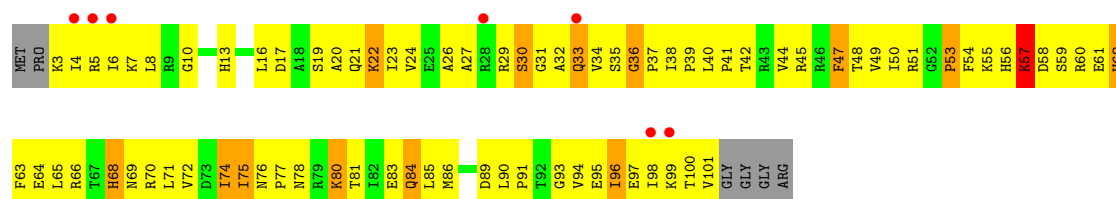
- Molecule 10: 30S ribosomal protein S10

Chain QJ:



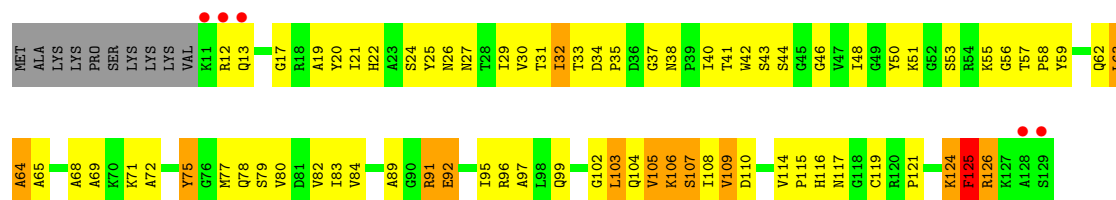
- Molecule 10: 30S ribosomal protein S10

Chain XJ:



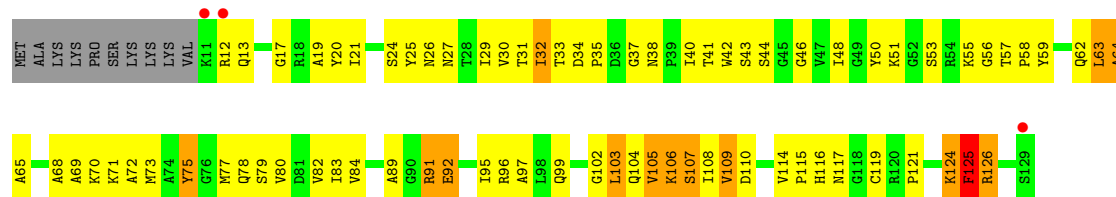
- Molecule 11: 30S ribosomal protein S11

Chain QK:



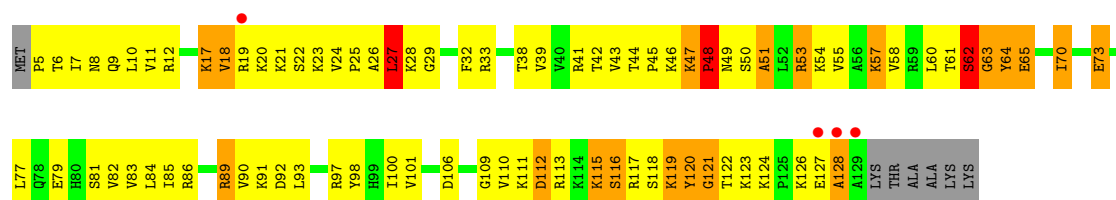
- Molecule 11: 30S ribosomal protein S11

Chain XK:



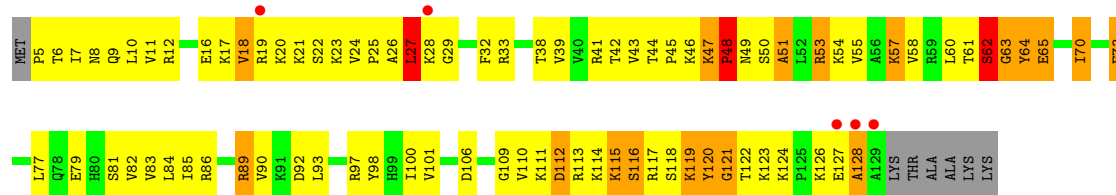
- Molecule 12: 30S ribosomal protein S12

Chain QL:



- Molecule 12: 30S ribosomal protein S12

Chain XL:



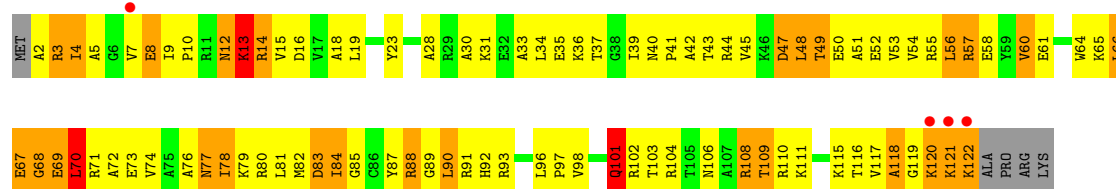
- Molecule 13: 30S ribosomal protein S13

Chain QM:



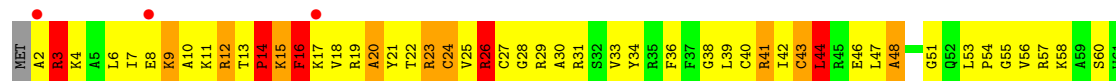
- Molecule 13: 30S ribosomal protein S13

Chain XM:



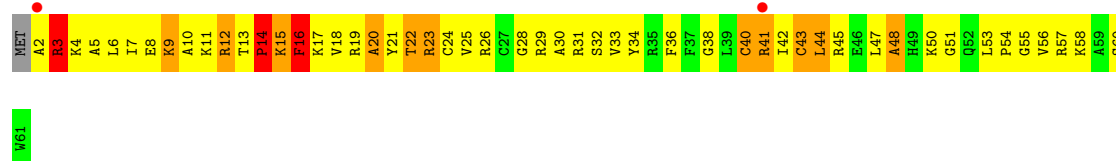
- Molecule 14: 30S ribosomal protein S14

Chain QN:



- Molecule 14: 30S ribosomal protein S14

Chain XN:



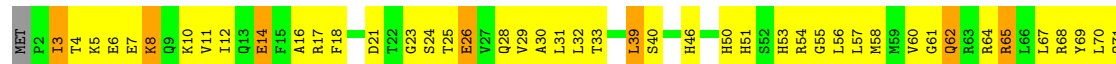
- Molecule 15: 30S ribosomal protein S15

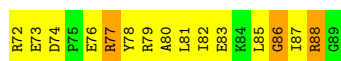
Chain QO:



- Molecule 15: 30S ribosomal protein S15

Chain XO:





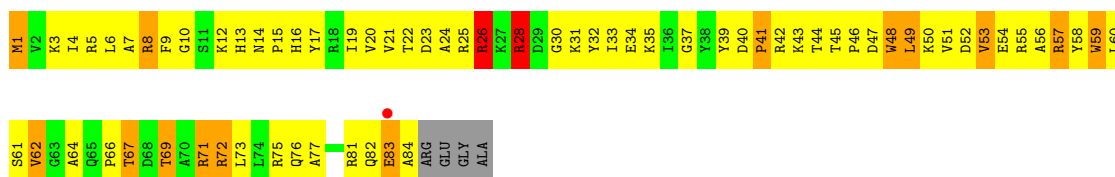
- Molecule 16: 30S ribosomal protein S16

Chain QP:



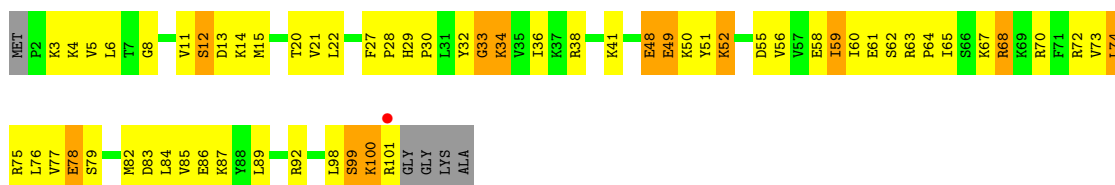
- Molecule 16: 30S ribosomal protein S16

Chain XP:



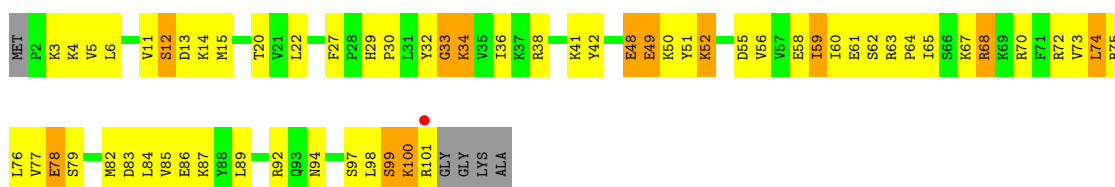
- Molecule 17: 30S ribosomal protein S17

Chain QQ:



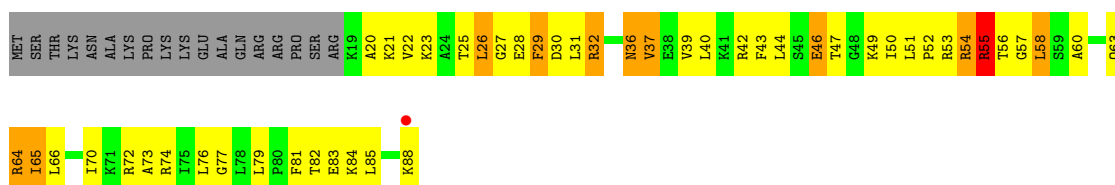
- Molecule 17: 30S ribosomal protein S17

Chain XQ:



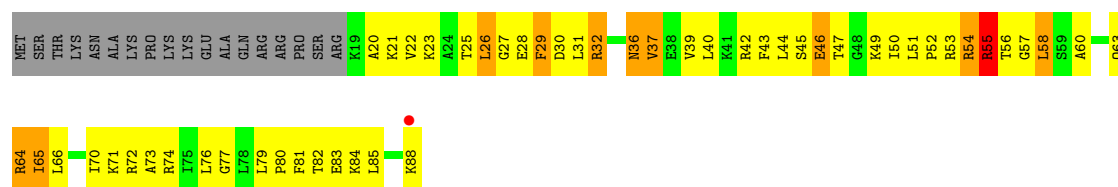
- Molecule 18: 30S ribosomal protein S18

Chain QR:



- Molecule 18: 30S ribosomal protein S18

Chain XR:



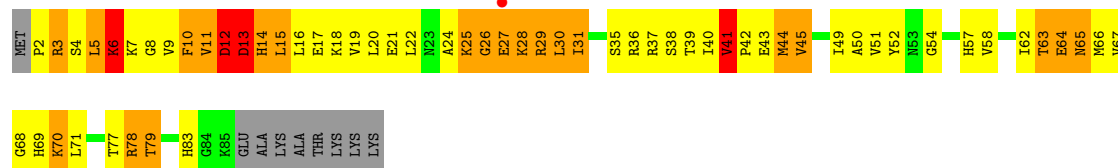
- Molecule 19: 30S ribosomal protein S19

Chain QS:



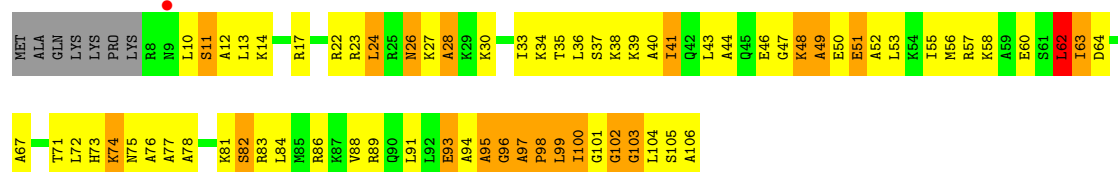
- Molecule 19: 30S ribosomal protein S19

Chain XS:



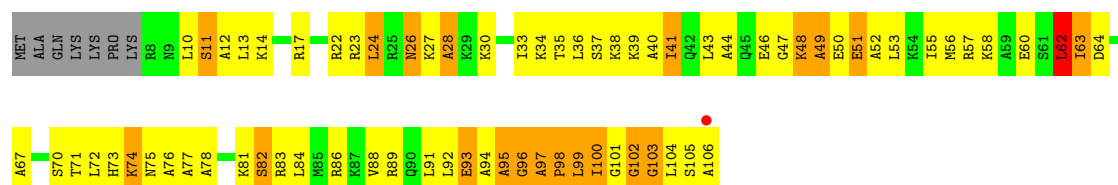
- Molecule 20: 30S ribosomal protein S20

Chain QT:



- Molecule 20: 30S ribosomal protein S20

Chain XT:



- Molecule 21: 30S ribosomal protein S21

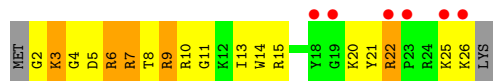
Chain QU:





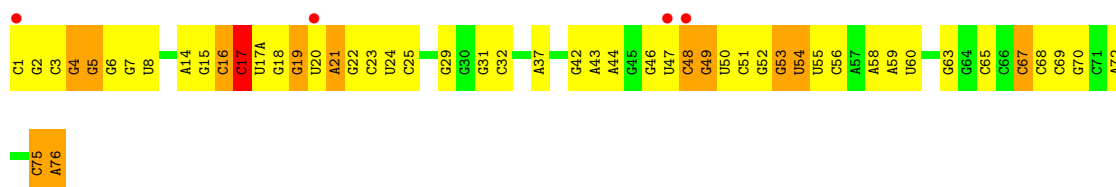
- Molecule 21: 30S ribosomal protein S21

Chain XU:



- Molecule 22: P-site tRNA fMet

Chain QV:



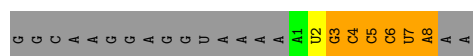
- Molecule 22: P-site tRNA fMet

Chain XV:



- Molecule 23: A-site ASL SufA6

Chain QX:



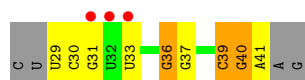
- Molecule 23: A-site ASL SufA6

Chain XX:



- Molecule 24: messenger RNA

Chain QY:



- Molecule 24: messenger RNA

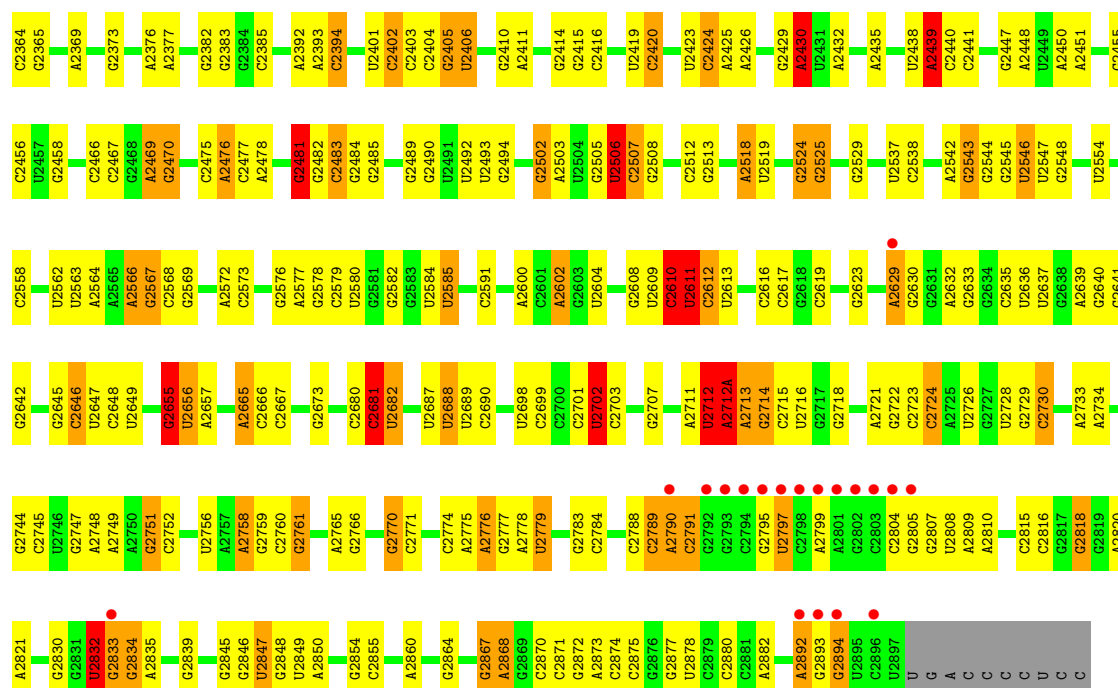
Chain XY:



C2507	C2508	U2423	A2346	U2244	G2152	A2062	U2244	G2152	A1847	C1754	A1637	G1521	G1422	G1328	G1239	U1141
U2528	G2506	C2424	C2347	U2245	G2153	C2063	U2246	G2154	A1848	A1755	C1640	G1522	A1427	U1329	U1240	U1142
A2426	C2517	A2426	U2348	G2246	G2155	C2065	G2247	G2156	G1849	U1756	G1641	G1523	A1428	C1330	A1241	A1142A
G2429	A2518	C2350	G2349	G2250	G2157	C2066	G2251	G2158	U1853	G1758	G1642	A1528	C1429	G1332	G1250	G1149
A2430	U2519	A2352	G2351	C2264	G2159	U2068	C2265	A2158	A1854	G1763	G1643	G1534	C1430	U1335	C1251	C1150
U2431	C2527	C2355	A2352	C2266	G2160	G2069	C2267	A2159	A1858	G1764	G1644	U1535	U1431	A1283	G1252	G1151
A2432	U2528	C2356	C2347	A2269	G2161	U2074	U2075	G2162	G1862	C1771	C1645	U1536	G1436	U1340	G1256	C1153
A2433	A2530	U2357	U2358	C2276	C2163	U2075	U2076	C2164	G1863	G1772	G1646	A1536	A1444A	U1342	C1257	G1154
A2434	G2537	G2358	G2359	G2277	G2165	U2086	U2087	G2166	U1864	A1773	C1647	C1537	C1445	G1348	C1258	A1155
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A2450	C2558	C2374	C2375	C2376	A2180	G2010	U2114	A2181	A1889	U1796	G1674	G1560	G1463	G1370	G1278	U1177
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U2464	A2565	G2380	C2381	C2382	G2185	A2015	U2119	A2186	A1901	G1802	U1688	A1580	A1477	A1384	C1291	G1184
A2465	A2566	C2381	C2382	C2383	G2186	A2016	U2120	A2187	A1902	A1803	A1689	A1581	U1482	A1395	G1297	G1187
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U2467	C2568	C2383	C2384	C2385	G2188	U2022	U2122	A2189	G1904	A1812	C1694	A1586	G1484	U1397	G1299	A1189
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G2470	C2573	C2385	C2386	C2387	A2191	G2024	U2124	A2191	G1906	G1814	A1698	C1588	G1486	C1398	U1301	C1201
C2471	A2577	C2386	C2387	C2388	G2192	U2025	U2125	A2192	G1907	G1815	G1699	U1590	G1487	C1399	A1302	C1202
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C2473	C2579	C2388	C2389	C2390	G2194	C2027	U2127	A2194	G1909	U1701	A1701	G1592	C1493	C1402	G1304	A1204
U2474	U2580	C2389	C2390	C2391	U2195	G2028	U2128	A2195	G1910	U1702	A1702	G1593	C1494	C1403	C1305	U1205
G2481	G2582	C2390	C2391	C2392	G2196	U2029	U2129	A2196	G1911	U1703	U1703	G1594	A1496	C1404	G1306	G1206
U2482	A2583	C2391	C2392	C2393	G2197	U2030	U2130	A2197	G1912	U1704	U1704	G1595	A1497	U1405	G1309	A1210
C2483	C2584	C2392	C2393	C2394	G2198	U2031	U2131	A2198	G1913	G1824	G1725	C1607	C1498	U1406	G1310	U1211
U2484	G2585	C2393	C2394	C2395	G2199	U2032	U2132	A2199	G1914	G1825	G1726	A1608	C1505	U1407	U1312	G1212
G2485	C2586	C2394	C2395	C2396	G2200	U2033	U2133	A2200	G1915	G1826	G1727	A1609	C1506	C1408	U1313	G1216
U2486	C2587	C2395	C2396	C2397	G2201	U2034	U2134	A2201	G1916	G1827	G1728	A1610	C1507	C1409	C1314	G1217
C2487	G2588	C2396	C2397	C2398	G2202	U2035	U2135	A2202	G1917	G1828	G1729	A1611	C1508	C1410	C1315	A1220
U2488	U2589	C2397	C2398	C2399	G2203	U2036	U2136	A2203	G1918	G1829	U1730	A1612	C1509	C1411	C1316	C1221
G2490	C2591	C2398	C2399	C2400	G2204	U2037	U2137	A2204	G1919	G1830	G1731	A1613	C1510	C1412	G1317	G1224
U2491	G2592	C2399	C2401	C2402	G2205	U2038	U2138	A2205	G1920	G1831	G1732	A1614	C1511	C1413	G1318	U1225
C2492	A2593	C2403	C2404	C2405	G2206	U2039	U2139	A2206	G1921	G1832	G1733	A1615	C1512	C1414	C1319	G1226
U2493	C2594	C2404	C2405	C2406	G2207	U2040	U2140	A2207	G1922	G1833	G1734	A1616	C1513	C1415	G1320	U1227
G2494	U2595	C2405	C2406	C2407	G2208	U2041	U2141	A2208	G1923	G1834	G1735	A1617	C1514	C1416	G1321	G1228
C2495	A2596	C2406	C2407	C2408	G2209	U2042	U2142	A2209	G1924	G1835	G1736	A1618	C1515	C1417	C1322	G1229
U2496	G2597	C2407	C2408	C2409	G2210	U2043	U2143	A2210	G1925	G1836	G1737	A1619	C1516	C1418	G1323	U1230
G2497	C2598	C2408	C2409	C2410	G2211	U2044	U2144	A2211	G1926	G1837	G1738	A1620	C1517	C1419	C1324	G1231
C2498	U2599	C2409	C2410	C2411	G2212	U2045	U2145	A2212	G1927	G1838	G1739	A1621	C1518	C1420	G1325	G1232
U2499	A2600	C2410	C2411	C2412	G2213	U2046	U2146	A2213	G1928	G1839	G1740	A1622	C1519	C1421	C1326	U1233
G2500	C2601	C2411	C2412	C2413	G2214	U2047	U2147	A2214	G1929	G1840	G1741	A1623	C1520	C1422	G1327	G1234
A2501	U2602	C2412	C2413	C2414	G2215	U2048	U2148	A2215	G1930	G1841	G1742	A1624	C1521	C1423	C1328	G1235
C2502	C2603	C2413	C2414	C2415	G2216	U2049	U2149	A2216	G1931	G1842	G1743	A1625	C1522	C1424	G1329	U1234
U2503	G2604	C2414	C2415	C2416	G2217	U2050	U2150	A2217	G1932	G1843	G1744	A1626	C1523	C1425	C1330	G1236
A2504	U2605	C2415	C2416	C2417	G2218	U2051	U2151	A2218	G1933	G1844	G1745	A1627	C1524	C1426	G1331	G1237
C2505	G2606	C2416	C2417	C2418	G2219	U2052	U2152	A2219	G1934	G1845	G1746	A1628	C1525	C1427	C1332	U1235
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		C2418	C2419	C2420	G2221	U2054	U2154	A2221	G1936	G1847	G1748	A1630	C1527	C1429	C1334	G1239
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		C2422	C2423	C2424	G2225	U2058	U2158	A2225	G1940	G1851	G1752	A1634	C1531	C1433	C1338	G1243
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		C2428	C2429	C2430	G2231	U2064	U2164	A2231	G1946	G1857	G1758	A1640	C1537	C1439	C1344	G1249
		C2429	C2430	C2431	G2232	U2065	U2165	A2232	G1947	G1858	G1759	A1641	C1538	C1440	C1345	G1250
		C2430	C2431	C2432	G2233	U2066	U2166	A2233	G1948	G1859	G1760	A1642	C1539	C1441	C1346	G1251
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		C2432	C2433	C2434	G2235	U2068	U2168	A2235	G1950	G1861	G1762	A1644	C1541	C1443	C1348	G1253
		C2433	C2434	C2435	G2236	U2069	U2169	A2236	G1951	G1862	G1763	A1645	C1542	C1444	C1349	G1254
		C2434	C2435	C2436	G2237	U2070	U2170	A2237	G1952	G1863	G1764	A1646	C1543	C1445	C1350	G1255
		C2435	C2436	C2437	G2238	U2071	U2171	A2238	G1953	G1864	G1765	A1647	C1544	C1446	C1351	G1256
		C2436	C2437	C2438	G2239	U2072	U2172	A2239	G1954	G1865	G1766	A1648	C1545	C1447	C1352	G1257
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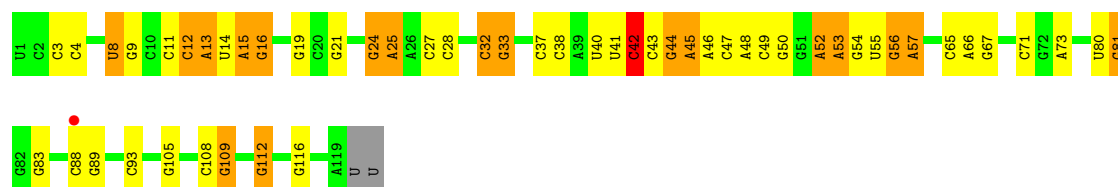






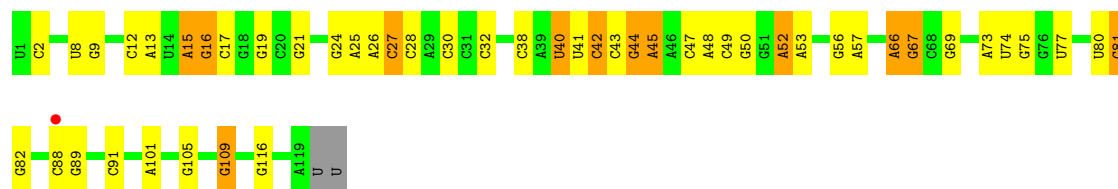
• Molecule 26: 5S rRNA

Chain RB:



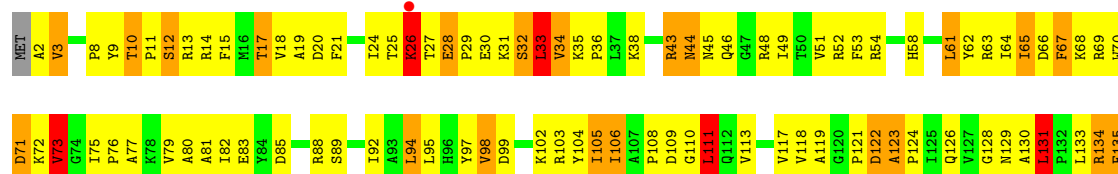
• Molecule 26: 5S rRNA

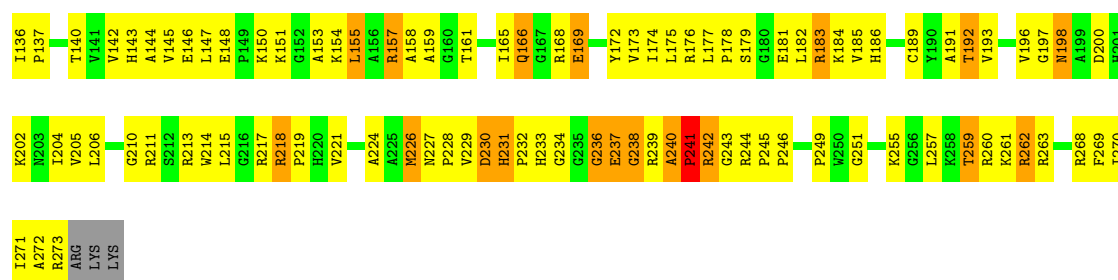
Chain YB:



• Molecule 27: 50S ribosomal protein L2

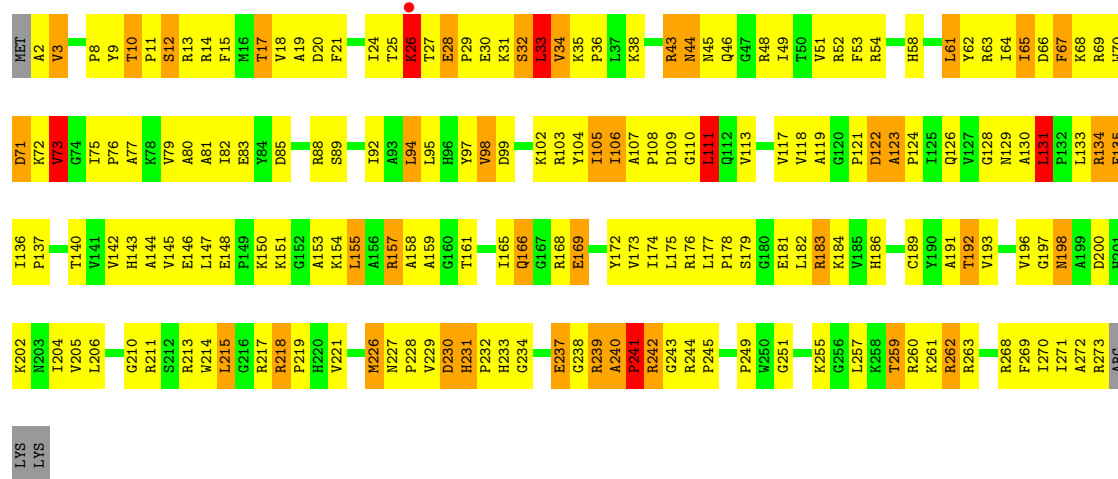
Chain RD:





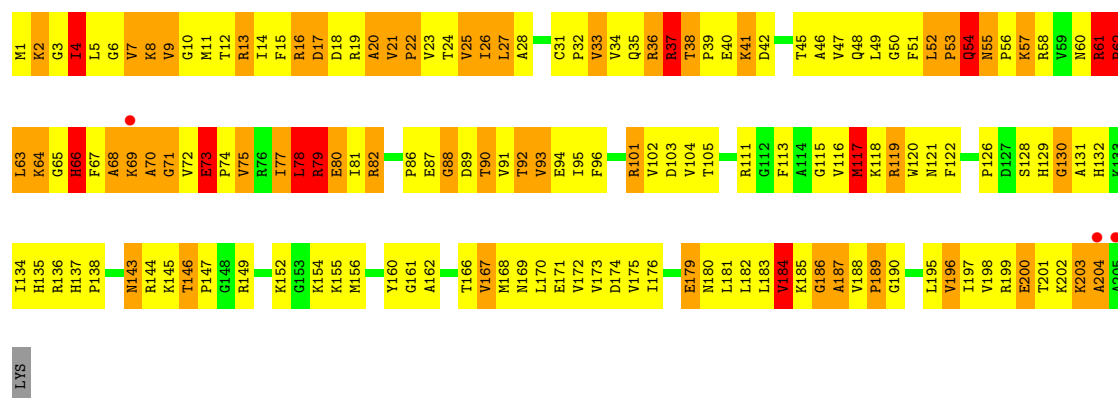
• Molecule 27: 50S ribosomal protein L2

Chain YD:



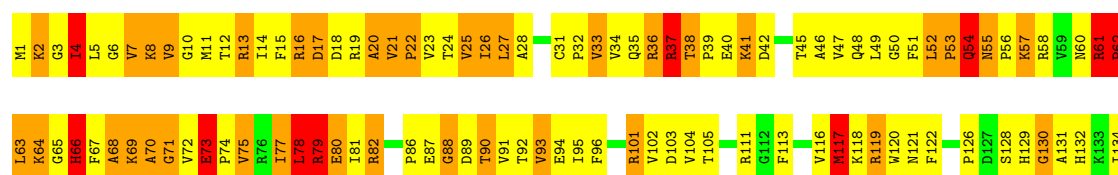
• Molecule 28: 50S ribosomal protein L3

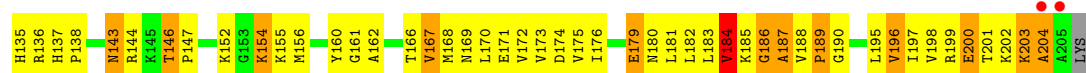
Chain RE:



• Molecule 28: 50S ribosomal protein L3

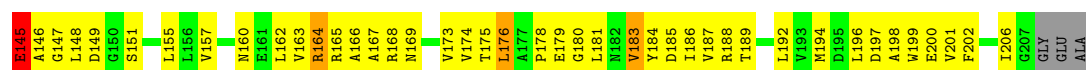
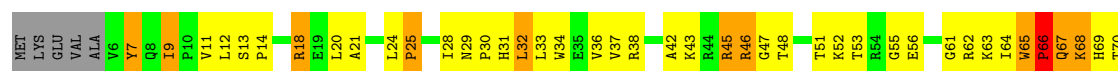
Chain YE:





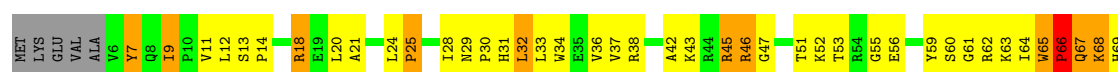
• Molecule 29: 50S ribosomal protein L4

Chain RF:



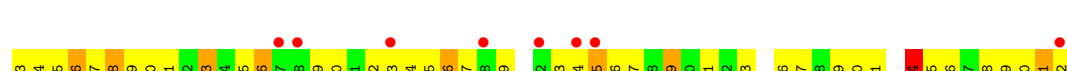
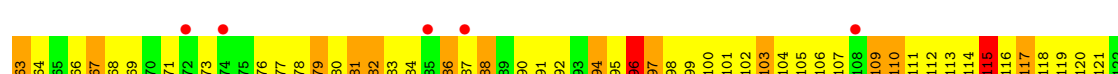
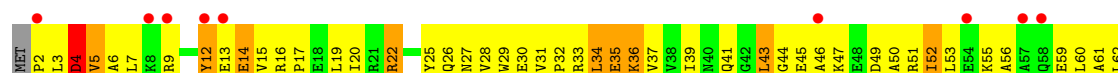
• Molecule 29: 50S ribosomal protein L4

Chain YF:



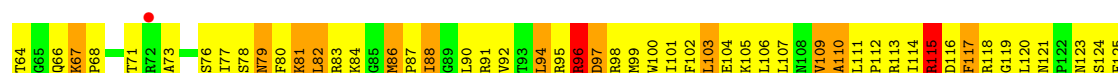
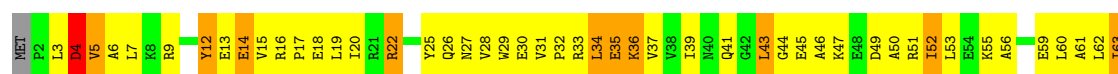
• Molecule 30: 50S ribosomal protein L5

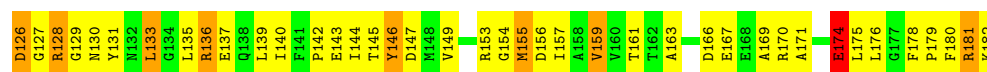
Chain RG:



• Molecule 30: 50S ribosomal protein L5

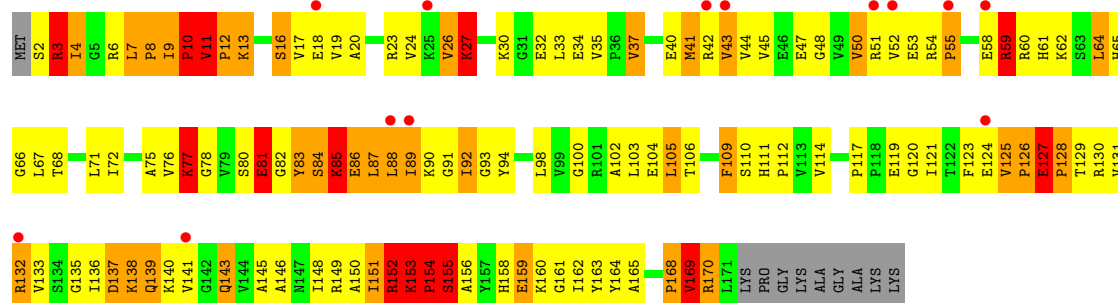
Chain YG:





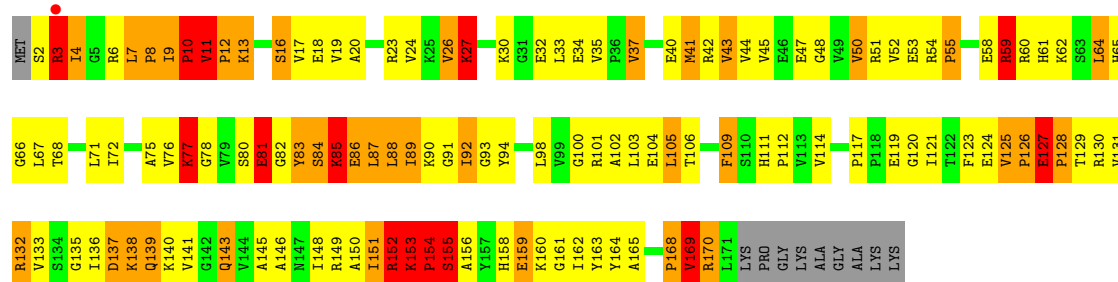
• Molecule 31: 50S ribosomal protein L6

Chain RH:



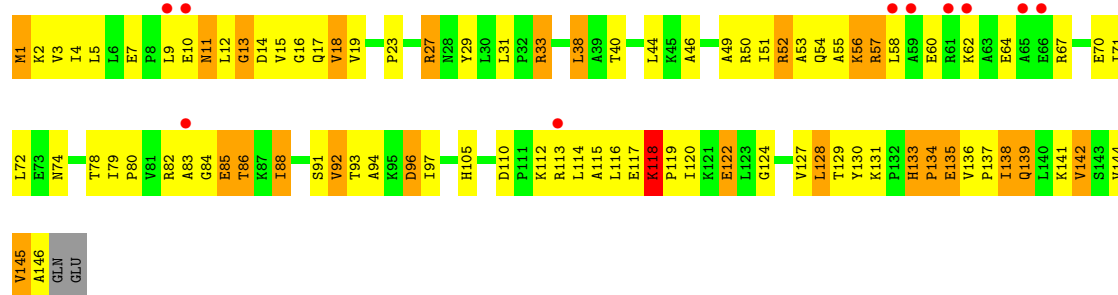
• Molecule 31: 50S ribosomal protein L6

Chain YH:



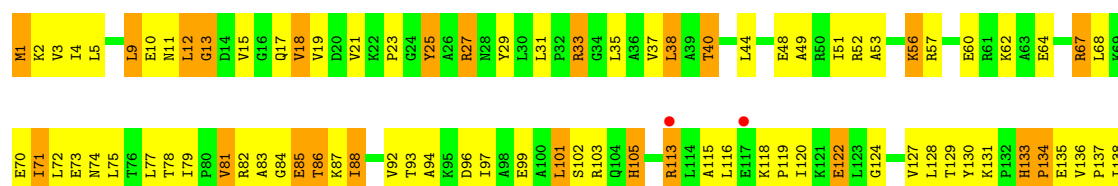
• Molecule 32: 50S ribosomal protein L9

Chain RI:



• Molecule 32: 50S ribosomal protein L9

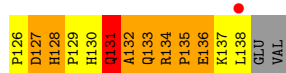
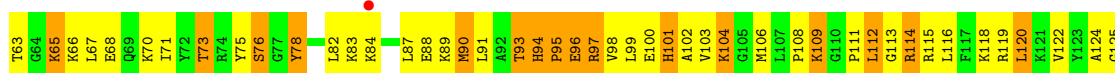
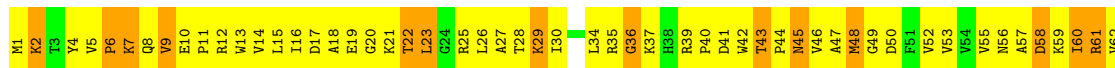
Chain YI:





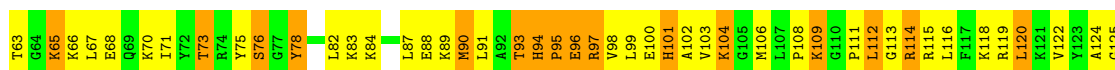
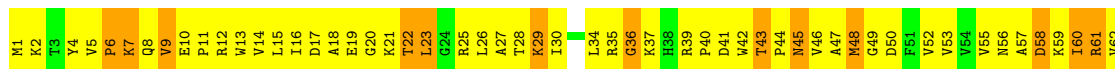
- Molecule 33: 50S ribosomal protein L13

Chain RN:



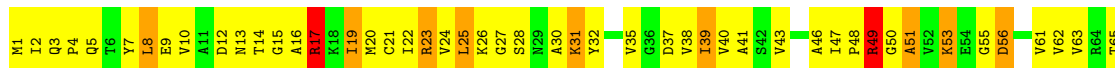
- Molecule 33: 50S ribosomal protein L13

Chain YN:



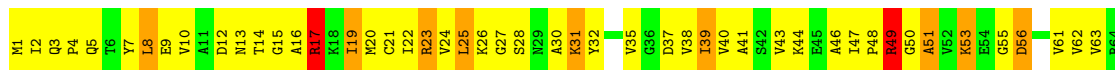
- Molecule 34: 50S ribosomal protein L14

Chain RO:



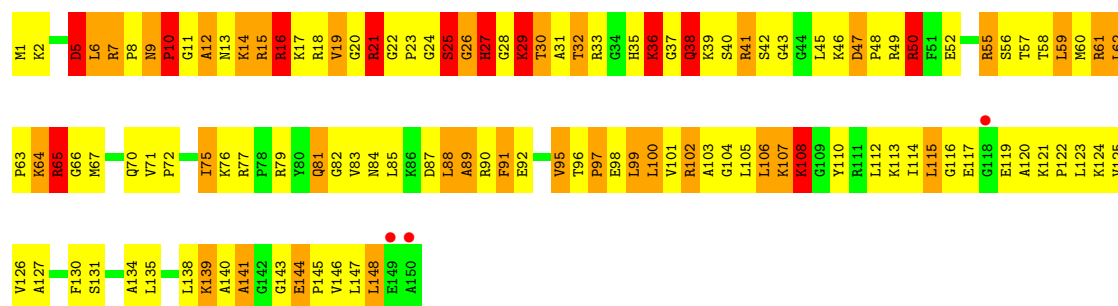
- Molecule 34: 50S ribosomal protein L14

Chain YO:



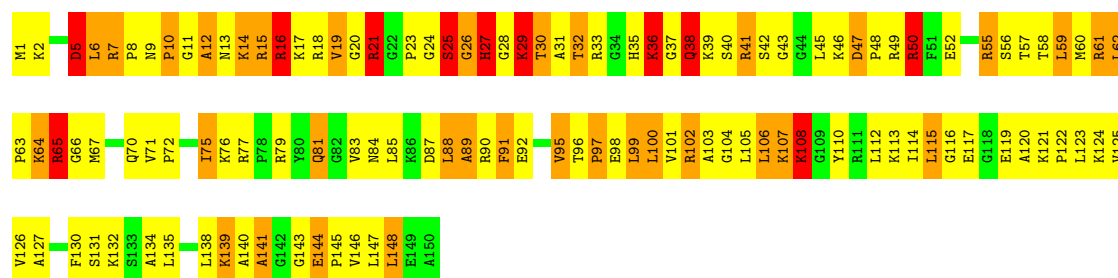
- Molecule 35: 50S ribosomal protein L15

Chain RP:



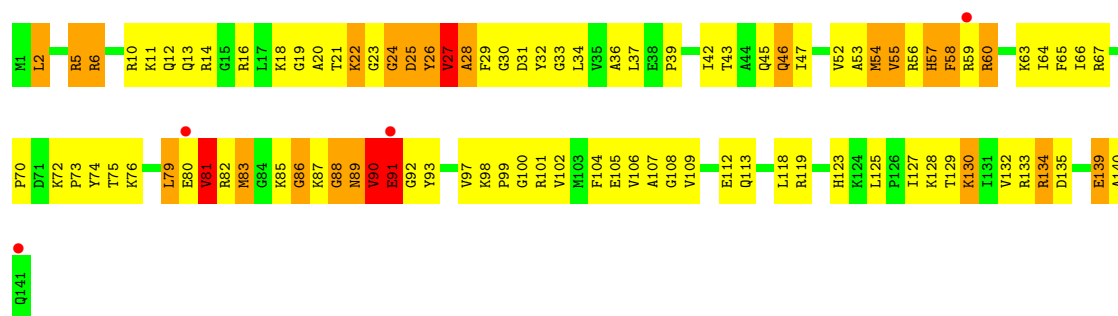
- Molecule 35: 50S ribosomal protein L15

Chain YP:



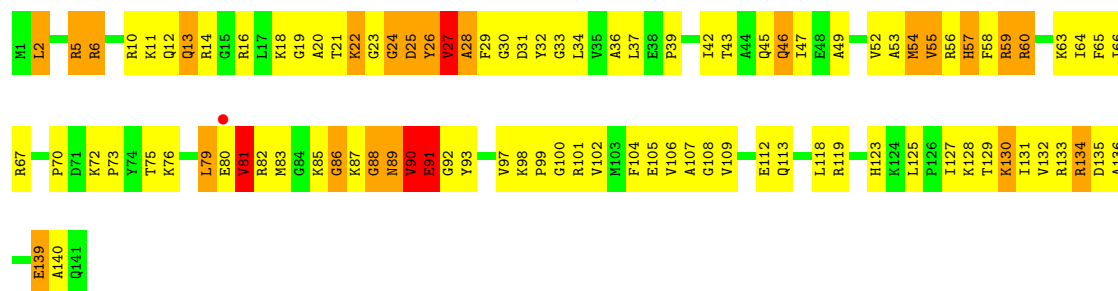
- Molecule 36: 50S ribosomal protein L16

Chain RQ:



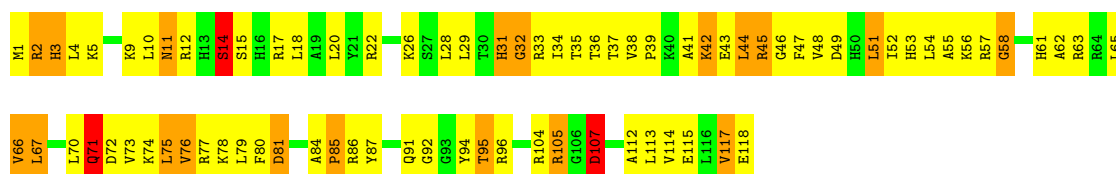
- Molecule 36: 50S ribosomal protein L16

Chain YQ:



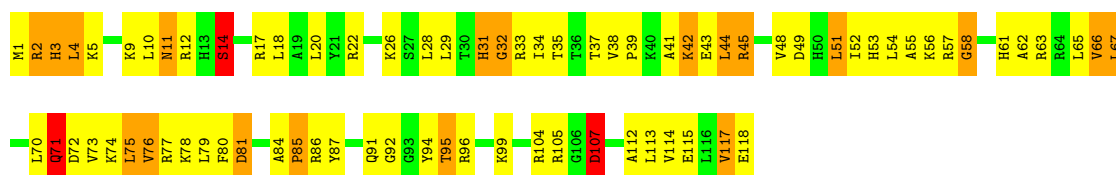
- Molecule 37: 50S ribosomal protein L17

Chain RR:



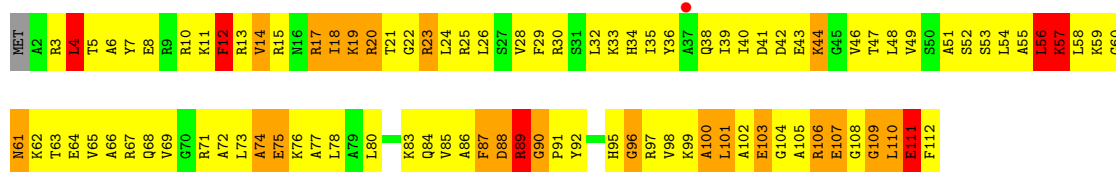
- Molecule 37: 50S ribosomal protein L17

Chain YR:



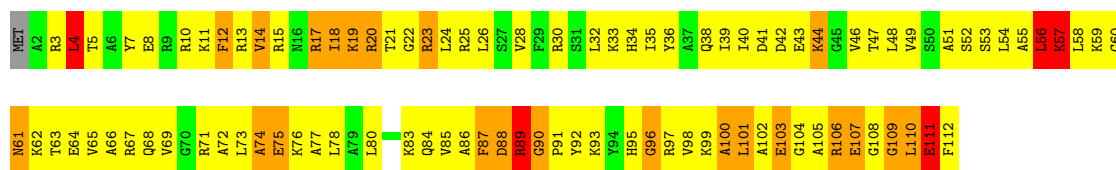
- Molecule 38: 50S ribosomal protein L18

Chain RS:



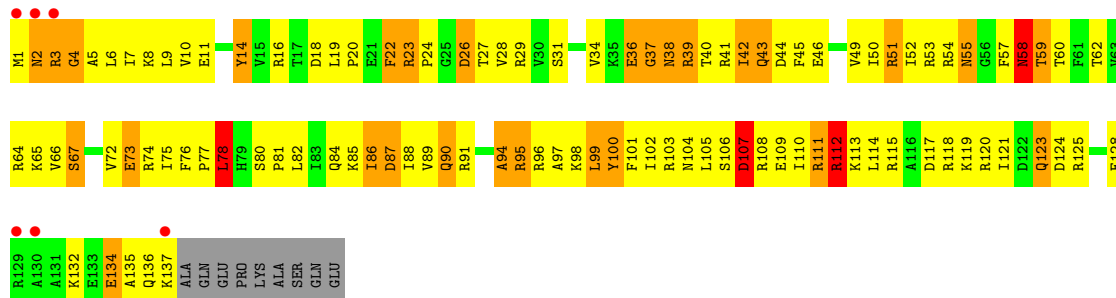
- Molecule 38: 50S ribosomal protein L18

Chain YS:



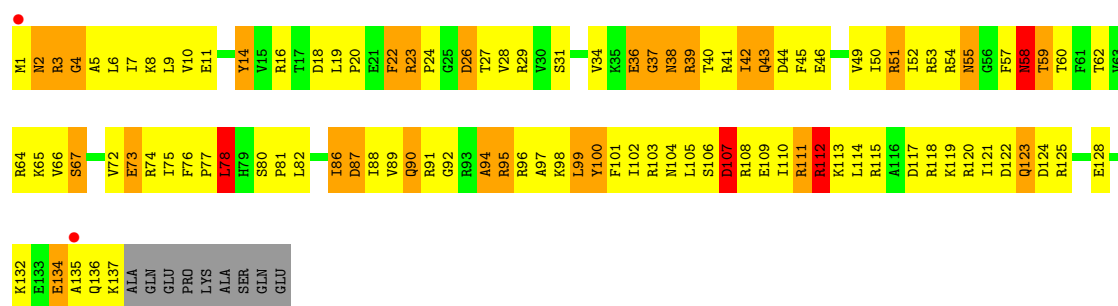
- Molecule 39: 50S ribosomal protein L19

Chain RT:



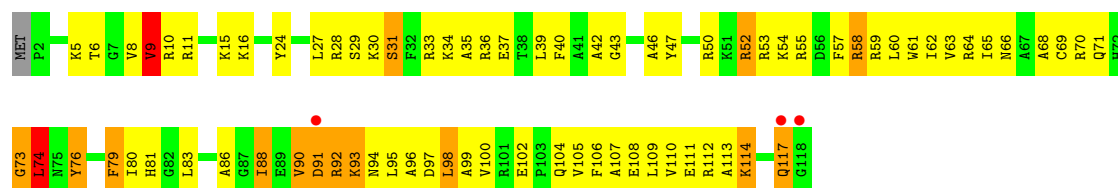
- Molecule 39: 50S ribosomal protein L19

Chain YT:



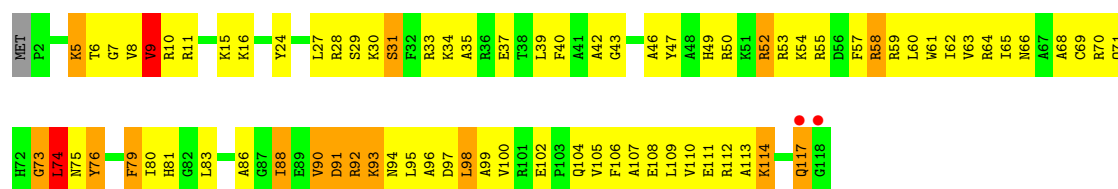
- Molecule 40: 50S ribosomal protein L20

Chain RU:



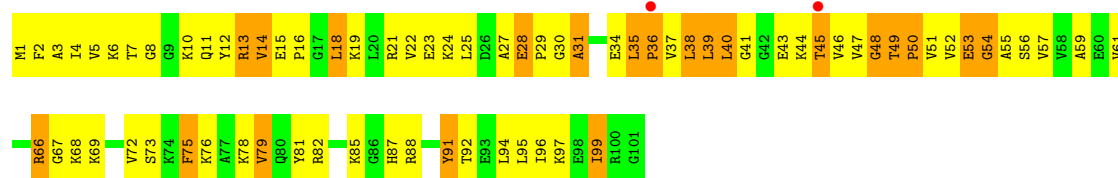
- Molecule 40: 50S ribosomal protein L20

Chain YU:



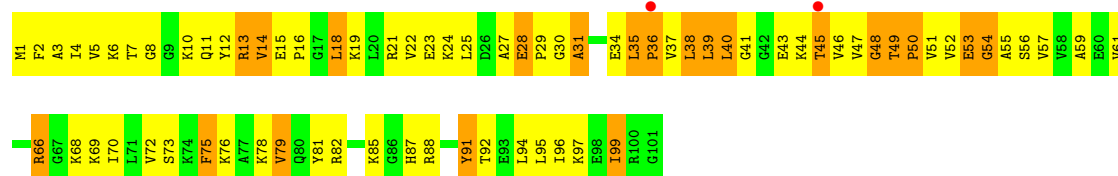
- Molecule 41: 50S ribosomal protein L21

Chain RV:



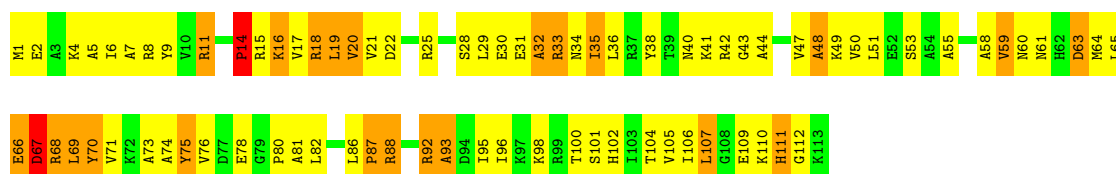
- Molecule 41: 50S ribosomal protein L21

Chain YV:



- Molecule 42: 50S ribosomal protein L22

Chain RW:



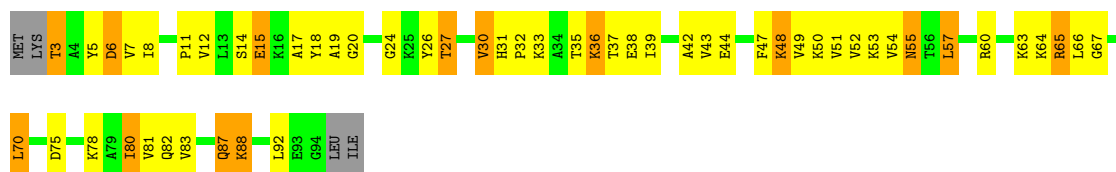
- Molecule 42: 50S ribosomal protein L22

Chain YW:



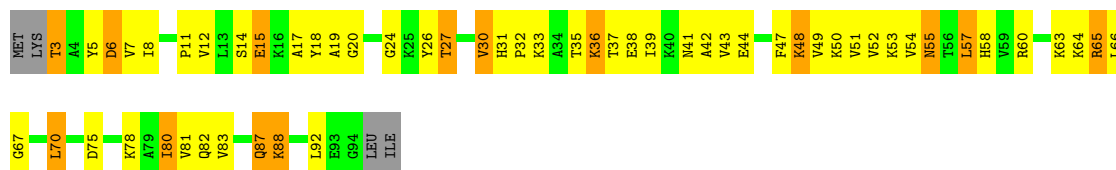
- Molecule 43: 50S ribosomal protein L23

Chain RX:



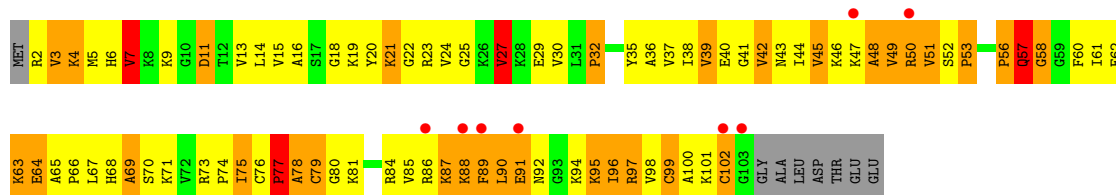
- Molecule 43: 50S ribosomal protein L23

Chain YX:



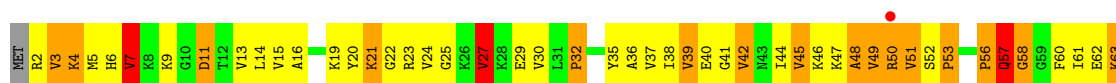
- Molecule 44: 50S ribosomal protein L24

Chain RY:



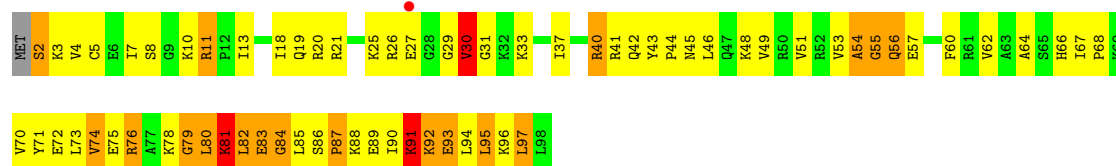
- Molecule 44: 50S ribosomal protein L24

Chain YY:



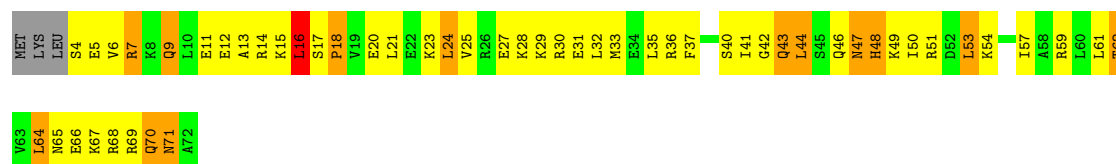
- Molecule 47: 50S ribosomal protein L28

Chain Y1:



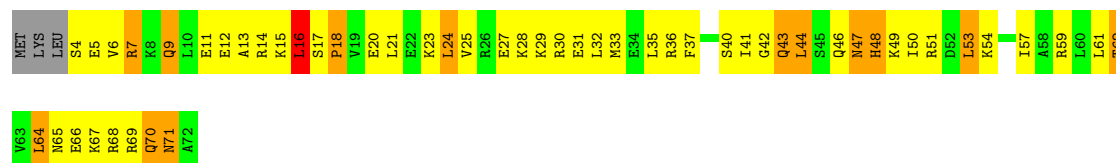
- Molecule 48: 50S ribosomal protein L29

Chain R2:



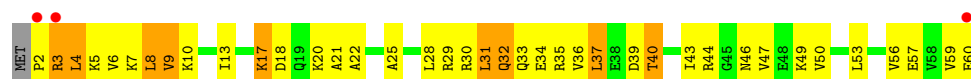
- Molecule 48: 50S ribosomal protein L29

Chain Y2:



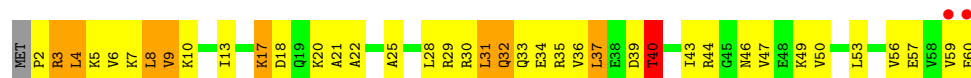
- Molecule 49: 50S ribosomal protein L30

Chain R3:



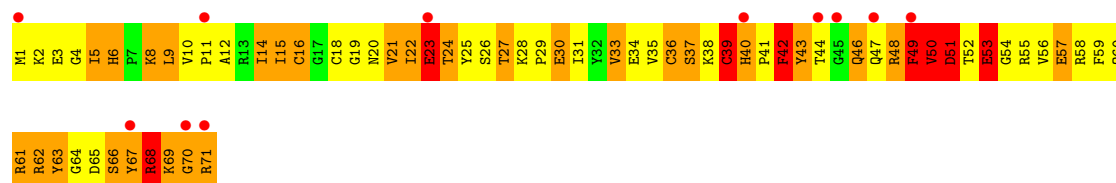
- Molecule 49: 50S ribosomal protein L30

Chain Y3:



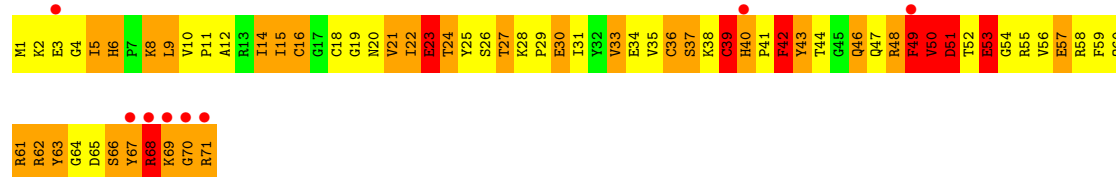
- Molecule 50: 50S ribosomal protein L31

Chain R4:



- Molecule 50: 50S ribosomal protein L31

Chain Y4: 



- Molecule 51: 50S ribosomal protein L32

Chain R5: 



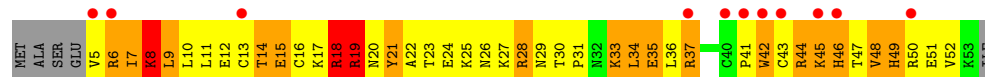
- Molecule 51: 50S ribosomal protein L32

Chain Y5: 



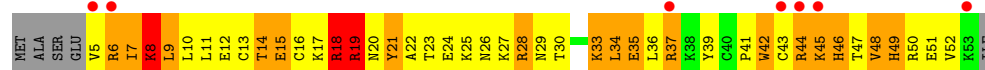
- Molecule 52: 50S ribosomal protein L33

Chain R6: 



- Molecule 52: 50S ribosomal protein L33

Chain Y6: 



- Molecule 53: 50S ribosomal protein L34

Chain R7: 



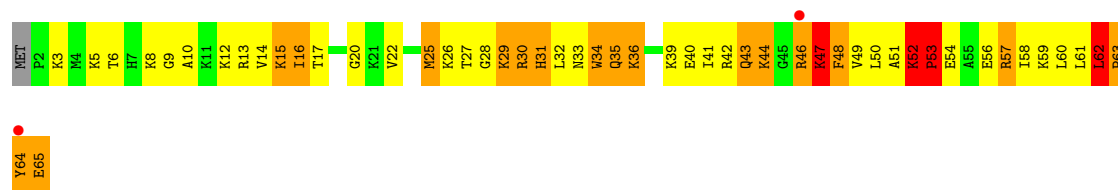
- Molecule 53: 50S ribosomal protein L34

Chain Y7: 



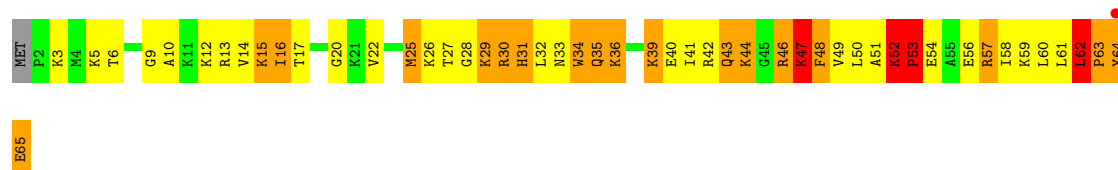
- Molecule 54: 50S ribosomal protein L35

Chain R8: 



- Molecule 54: 50S ribosomal protein L35

Chain Y8:



- Molecule 55: 50S ribosomal protein L36

Chain R9:



- Molecule 55: 50S ribosomal protein L36

Chain Y9:



- Molecule 56: tRNA acceptor end mimic

Chain Z6:



- Molecule 56: tRNA acceptor end mimic

Chain Z8:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.20Å 450.23Å 621.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.97 – 3.22 34.97 – 3.18	Depositor EDS
% Data completeness (in resolution range)	98.5 (34.97-3.22) 98.6 (34.97-3.18)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.18Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.229 , 0.260 0.229 , 0.260	Depositor DCC
R_{free} test set	43396 reflections (4.68%)	DCC
Wilson B-factor (Å ²)	67.8	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 42.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 962803 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	291957	wwPDB-VP
Average B, all atoms (Å ²)	91.0	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	0.31	0/36098	0.86	46/56341 (0.1%)
1	XA	0.34	1/36101 (0.0%)	0.89	66/56346 (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	0.42	0/856	0.68	0/1154
7	QG	0.37	0/1276	0.60	0/1709
7	XG	0.36	0/1276	0.60	0/1709
8	QH	0.40	0/1136	0.69	0/1527
8	XH	0.40	0/1136	0.69	0/1527
9	QI	0.36	0/1029	0.67	0/1379
9	XI	0.36	0/1029	0.67	0/1379
10	QJ	0.35	0/814	0.61	0/1095
10	XJ	0.36	0/814	0.61	0/1095
11	QK	0.40	0/900	0.67	0/1213
11	XK	0.40	0/900	0.67	0/1213
12	QL	0.45	0/991	1.00	4/1327 (0.3%)
12	XL	0.46	0/991	1.00	4/1327 (0.3%)
13	QM	0.34	0/974	0.66	0/1303
13	XM	0.34	0/974	0.66	0/1303
14	QN	0.42	0/501	0.68	0/664
14	XN	0.52	0/501	0.67	0/664
15	QO	0.39	0/745	0.67	0/992
15	XO	0.39	0/745	0.67	0/992
16	QP	0.36	0/721	0.67	0/970
16	XP	0.36	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	0.69	0/1007
20	XT	0.34	0/765	0.69	0/1007
21	QU	0.37	0/221	0.63	0/288
21	XU	0.37	0/221	0.63	0/288
22	QV	0.52	0/1836	0.99	5/2859 (0.2%)
22	XV	0.52	0/1836	0.99	6/2859 (0.2%)
23	QX	0.39	0/185	0.72	0/285
23	XX	0.86	1/185 (0.5%)	1.12	1/285 (0.4%)
24	QY	0.52	0/311	0.88	0/483
24	XY	0.53	0/311	0.89	0/483
25	RA	0.39	1/69521 (0.0%)	0.91	95/108529 (0.1%)
25	YA	0.44	3/69543 (0.0%)	0.94	121/108563 (0.1%)
26	RB	0.34	0/2878	0.89	3/4490 (0.1%)
26	YB	0.35	0/2878	0.89	0/4490
27	RD	0.59	2/2165 (0.1%)	0.90	4/2919 (0.1%)
27	YD	0.56	1/2165 (0.0%)	0.90	4/2919 (0.1%)
28	RE	0.52	0/1601	0.91	2/2160 (0.1%)
28	YE	0.52	0/1601	0.91	2/2160 (0.1%)
29	RF	0.50	0/1620	0.76	0/2194
29	YF	0.50	0/1620	0.76	0/2194
30	RG	0.40	0/1499	0.66	0/2016
30	YG	0.40	0/1499	0.66	0/2016
31	RH	0.45	0/1332	0.85	3/1802 (0.2%)
31	YH	0.45	0/1332	0.85	4/1802 (0.2%)
32	RI	0.29	0/1151	0.63	0/1558
32	YI	0.30	0/1151	0.63	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	0.53	0/943	0.71	0/1269
34	YO	0.53	0/943	0.71	0/1269
35	RP	0.50	0/1162	0.94	3/1544 (0.2%)
35	YP	0.49	0/1162	0.95	3/1544 (0.2%)
36	RQ	0.54	0/1143	0.90	3/1527 (0.2%)
36	YQ	0.54	0/1143	0.89	3/1527 (0.2%)
37	RR	0.45	0/982	0.80	1/1312 (0.1%)
37	YR	0.45	0/982	0.80	1/1312 (0.1%)
38	RS	0.46	0/892	0.82	1/1187 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YS	0.45	0/892	0.82	1/1187 (0.1%)
39	RT	0.47	0/1155	0.73	2/1542 (0.1%)
39	YT	0.46	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	0.32	0/1493	0.60	0/2026
45	YZ	0.33	0/1493	0.63	0/2026
46	R0	0.30	0/657	0.56	0/874
46	Y0	0.31	0/657	0.53	0/874
47	R1	0.49	0/770	0.85	1/1022 (0.1%)
47	Y1	0.49	0/770	0.85	1/1022 (0.1%)
48	R2	0.51	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	1.79	1/60 (1.7%)
56	Z8	0.78	0/40	1.81	1/60 (1.7%)
All	All	0.41	9/316323 (0.0%)	0.87	408/472911 (0.1%)

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	RD	236	GLY	C-N	8.55	1.53	1.34
25	YA	1762	A	N9-C4	6.24	1.41	1.37
23	XX	8	A	C6-N6	6.10	1.38	1.33
25	RA	654(T)	C	C1'-N1	5.71	1.57	1.48
1	XA	518	C	N3-C4	-5.32	1.30	1.33

The worst 5 of 408 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	QL	47	LYS	C-N-CD	-20.48	75.56	120.60
12	XL	47	LYS	C-N-CD	-20.46	75.59	120.60
1	XA	518	C	C5-C4-N4	15.43	131.00	120.20
1	XA	518	C	C6-N1-C1'	12.95	136.34	120.80
1	XA	518	C	C2-N1-C1'	-11.78	105.84	118.80

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	492	0
1	XA	32249	0	16279	531	1
2	QB	1924	0	1975	287	0
2	XB	1924	0	1975	289	0
3	QC	1605	0	1668	207	0
3	XC	1605	0	1668	207	1
4	QD	1703	0	1764	253	0
4	XD	1703	0	1765	215	0
5	QE	1155	0	1213	136	0
5	XE	1155	0	1213	131	0
6	QF	843	0	857	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	XF	843	0	857	100	0
7	QG	1257	0	1296	145	0
7	XG	1257	0	1296	141	0
8	QH	1116	0	1175	140	0
8	XH	1116	0	1177	144	0
9	QI	1010	0	1037	141	0
9	XI	1010	0	1037	153	0
10	QJ	801	0	849	149	0
10	XJ	801	0	849	135	0
11	QK	885	0	904	100	1
11	XK	885	0	904	103	0
12	QL	975	0	1062	104	0
12	XL	975	0	1062	108	0
13	QM	964	0	1034	161	0
13	XM	964	0	1034	161	0
14	QN	492	0	530	98	0
14	XN	492	0	529	100	0
15	QO	734	0	771	75	0
15	XO	734	0	771	72	0
16	QP	705	0	725	112	0
16	XP	705	0	725	110	0
17	QQ	834	0	904	83	0
17	XQ	834	0	904	75	0
18	QR	574	0	644	66	0
18	XR	574	0	644	69	0
19	QS	674	0	699	113	0
19	XS	674	0	699	152	0
20	QT	763	0	860	105	0
20	XT	763	0	861	101	0
21	QU	217	0	234	26	0
21	XU	217	0	234	26	0
22	QV	1644	0	836	25	0
22	XV	1644	0	836	28	0
23	QX	167	0	87	12	0
23	XX	167	0	87	13	0
24	QY	303	0	154	11	0
24	XY	303	0	154	11	0
25	RA	62071	0	31285	855	0
25	YA	62091	0	31296	839	0
26	RB	2573	0	1306	58	0
26	YB	2573	0	1306	35	0
27	RD	2115	0	2195	317	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	YD	2115	0	2195	320	0
28	RE	1568	0	1634	271	0
28	YE	1568	0	1634	264	0
29	RF	1585	0	1632	177	0
29	YF	1585	0	1632	174	0
30	RG	1474	0	1535	205	0
30	YG	1474	0	1535	183	0
31	RH	1307	0	1382	226	0
31	YH	1307	0	1382	226	0
32	RI	1136	0	1223	69	1
32	YI	1136	0	1223	50	0
33	RN	1104	0	1180	194	0
33	YN	1104	0	1180	189	0
34	RO	933	0	996	122	0
34	YO	933	0	996	123	0
35	RP	1145	0	1227	245	0
35	YP	1145	0	1228	242	0
36	RQ	1122	0	1179	158	0
36	YQ	1122	0	1179	154	0
37	RR	968	0	1033	112	0
37	YR	968	0	1033	111	0
38	RS	882	0	943	160	0
38	YS	882	0	943	154	0
39	RT	1141	0	1202	150	0
39	YT	1141	0	1202	157	0
40	RU	964	0	1022	129	0
40	YU	964	0	1022	135	0
41	RV	779	0	852	129	0
41	YV	779	0	852	135	1
42	RW	900	0	964	98	0
42	YW	900	0	964	98	0
43	RX	725	0	778	67	0
43	YX	725	0	778	68	0
44	RY	785	0	878	168	0
44	YY	785	0	878	152	0
45	RZ	1461	0	1493	77	0
45	YZ	1461	0	1493	59	0
46	R0	648	0	672	27	0
46	Y0	648	0	672	20	0
47	R1	763	0	848	138	0
47	Y1	763	0	848	140	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	76	0
49	R3	469	0	518	39	0
49	Y3	469	0	518	42	0
50	R4	581	0	574	155	0
50	Y4	581	0	574	188	0
51	R5	459	0	480	74	0
51	Y5	459	0	480	75	1
52	R6	424	0	450	92	0
52	Y6	424	0	450	88	0
53	R7	430	0	480	43	0
53	Y7	430	0	480	41	0
54	R8	517	0	582	103	0
54	Y8	517	0	582	103	0
55	R9	307	0	335	18	0
55	Y9	307	0	336	16	0
56	Z6	74	0	51	4	0
56	Z8	74	0	51	6	0
57	QA	66	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	2	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	241	0	0	0	0
57	RB	2	0	0	0	0
57	RD	1	0	0	0	0
57	RE	2	0	0	0	0
57	RF	1	0	0	0	0
57	RP	2	0	0	0	0
57	RR	1	0	0	0	0
57	RU	1	0	0	0	0
57	XA	72	0	0	0	0
57	XM	1	0	0	0	0
57	XT	1	0	0	0	0
57	XV	1	0	0	0	0
57	XX	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y7	1	0	0	0	0
57	YA	269	0	0	0	0
57	YB	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	YD	1	0	0	0	0
57	YE	2	0	0	0	0
57	YX	1	0	0	0	0
58	QA	42	0	45	1	0
58	XA	42	0	45	1	0
59	QD	1	0	0	0	0
59	QN	1	0	0	0	0
59	R9	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y9	1	0	0	0	0
All	All	291957	0	198335	14232	3

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 29.

The worst 5 of 14232 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:YN:32:SER:CB	14:YN:41:ARG:HB3	1.23	1.55
14:YN:32:SER:HB3	14:YN:41:ARG:CB	1.28	1.54
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.36	1.53
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.36	1.52
4:XD:22:LYS:CG	4:XD:26:CYS:SG	2.01	1.49

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
41:YV:51:VAL:N	51:Y5:60:VAL:O[4_445]	2.16	0.04
32:RI:91:SER:OG	1:XA:368:U:OP1[4_555]	2.17	0.03
11:QK:99:GLN:NE2	3:XC:79:ARG:NH2[4_555]	2.19	0.01

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%)	128 (63%)	56 (28%)	19 (9%)	1	8
3	XC	203/239 (85%)	129 (64%)	55 (27%)	19 (9%)	1	8
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	7
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	11
11	XK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	11
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%)	28 (24%)	20 (17%)	0	1
13	XM	119/126 (94%)	71 (60%)	26 (22%)	22 (18%)	0	1
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%)	60 (70%)	20 (23%)	6 (7%)	2	14
16	QP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	2
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%)	46 (68%)	14 (21%)	8 (12%)	1	4
18	XR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	1	4
19	QS	82/93 (88%)	47 (57%)	17 (21%)	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	1
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	1
21	XU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	1
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	7
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	7
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%)	101 (70%)	26 (18%)	17 (12%)	1	4
32	YI	144/148 (97%)	103 (72%)	24 (17%)	17 (12%)	1	4
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	7
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	1	7
37	RR	116/118 (98%)	82 (71%)	20 (17%)	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	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	YS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	1
39	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	1
39	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	1
40	RU	115/118 (98%)	86 (75%)	20 (17%)	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	7
41	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	7
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	23
43	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	3	23
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%)	118 (65%)	39 (22%)	24 (13%)	0	2
45	YZ	181/206 (88%)	130 (72%)	34 (19%)	17 (9%)	1	8
46	R0	80/85 (94%)	69 (86%)	8 (10%)	3 (4%)	5	34
46	Y0	80/85 (94%)	70 (88%)	9 (11%)	1 (1%)	18	68
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%)	47 (70%)	11 (16%)	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	1
54	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	1
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%)	7647 (67%)	2334 (20%)	1489 (13%)	0	3

5 of 1489 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	34
2	XB	205/220 (93%)	181 (88%)	24 (12%)	8	34
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	58
6	QF	90/90 (100%)	76 (84%)	14 (16%)	4	17
6	XF	90/90 (100%)	76 (84%)	14 (16%)	4	17
7	QG	126/127 (99%)	114 (90%)	12 (10%)	12	44
7	XG	126/127 (99%)	115 (91%)	11 (9%)	15	51
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	48
10	XJ	89/92 (97%)	81 (91%)	8 (9%)	14	48
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	26
12	XL	104/109 (95%)	90 (86%)	14 (14%)	6	26
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	30
16	XP	72/74 (97%)	63 (88%)	9 (12%)	7	30
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	35
18	XR	61/77 (79%)	54 (88%)	7 (12%)	8	35
19	QS	73/80 (91%)	62 (85%)	11 (15%)	4	19
19	XS	73/80 (91%)	62 (85%)	11 (15%)	4	19
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%)	127 (77%)	38 (23%)	1	5
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	28
29	YF	161/166 (97%)	140 (87%)	21 (13%)	6	28
30	RG	155/156 (99%)	130 (84%)	25 (16%)	3	16
30	YG	155/156 (99%)	130 (84%)	25 (16%)	3	16
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%)	94 (77%)	28 (23%)	1	5
32	YI	122/124 (98%)	93 (76%)	29 (24%)	1	4
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	14
37	YR	101/101 (100%)	84 (83%)	17 (17%)	3	14
38	RS	87/88 (99%)	74 (85%)	13 (15%)	4	20
38	YS	87/88 (99%)	74 (85%)	13 (15%)	4	20
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	24
40	YU	93/94 (99%)	80 (86%)	13 (14%)	5	24
41	RV	82/82 (100%)	71 (87%)	11 (13%)	6	26
41	YV	82/82 (100%)	71 (87%)	11 (13%)	6	26
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	20
43	YX	74/78 (95%)	63 (85%)	11 (15%)	4	20
44	RY	85/91 (93%)	70 (82%)	15 (18%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	YY	85/91 (93%)	70 (82%)	15 (18%)	3	13
45	RZ	162/179 (90%)	140 (86%)	22 (14%)	5	26
45	YZ	162/179 (90%)	140 (86%)	22 (14%)	5	26
46	R0	65/67 (97%)	60 (92%)	5 (8%)	18	59
46	Y0	65/67 (97%)	61 (94%)	4 (6%)	26	70
47	R1	82/83 (99%)	67 (82%)	15 (18%)	2	12
47	Y1	82/83 (99%)	67 (82%)	15 (18%)	2	12
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	4
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	4
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	63
53	Y7	42/42 (100%)	39 (93%)	3 (7%)	21	63
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	2
54	Y8	54/55 (98%)	39 (72%)	15 (28%)	0	2
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%)	8287 (85%)	1415 (15%)	5	21

5 of 1415 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	R3	4	LEU
7	XG	78	ARG
45	YZ	112	ARG
50	R4	48	ARG
2	XB	36	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
46	R0	29	GLN
5	XE	72	GLN
43	YX	87	GLN
47	R1	56	GLN
49	R3	32	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	296 (19%)	46 (3%)
1	XA	1499/1522 (98%)	294 (19%)	52 (3%)
22	QV	76/77 (98%)	30 (39%)	1 (1%)
22	XV	76/77 (98%)	30 (39%)	1 (1%)
23	QX	7/25 (28%)	5 (71%)	1 (14%)
23	XX	7/25 (28%)	5 (71%)	0
24	QY	13/18 (72%)	5 (38%)	1 (7%)
24	XY	13/18 (72%)	5 (38%)	1 (7%)
25	RA	2879/2916 (98%)	623 (21%)	73 (2%)
25	YA	2880/2916 (98%)	626 (21%)	70 (2%)
26	RB	119/122 (97%)	25 (21%)	2 (1%)
26	YB	119/122 (97%)	30 (25%)	1 (0%)
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9189/9366 (98%)	1974 (21%)	249 (2%)

5 of 1974 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	7	G
1	QA	8	A
1	QA	9	G
1	QA	32	A

5 of 249 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2518	A
1	XA	412	A
25	YA	1992	G

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Mol	Chain	Res	Type
25	RA	2689	U
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	$\# Z > 2$
24	1MG	QY	37	24	24,26,27	3.02	6 (25%)	34,39,42	3.99	12 (35%)
24	1MG	XY	37	24	24,26,27	3.03	6 (25%)	34,39,42	3.75	12 (35%)
56	PPU	Z6	76	25,56	38,40,41	2.43	9 (23%)	54,57,60	2.61	14 (25%)
56	PPU	Z8	76	25,56	38,40,41	2.42	9 (23%)	54,57,60	2.61	14 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	1MG	QY	37	24	-	0/8/25/26	0/3/3/3
24	1MG	XY	37	24	-	0/8/25/26	0/3/3/3
56	PPU	Z6	76	25,56	-	0/26/43/44	0/4/4/4
56	PPU	Z8	76	25,56	-	0/26/43/44	0/4/4/4

The worst 5 of 30 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	9.19	1.41	1.23
24	XY	37	1MG	C4-N3	8.25	1.49	1.35
24	QY	37	1MG	C4-N3	8.23	1.49	1.35
24	QY	37	1MG	C2-N1	7.46	1.47	1.37

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	QY	37	1MG	C6-C5-N7	-17.40	133.31	134.24
24	XY	37	1MG	C6-C5-N7	-15.50	133.41	134.24
24	QY	37	1MG	C6-N1-C2	11.86	123.96	120.71
24	XY	37	1MG	C6-N1-C2	11.68	123.91	120.71
56	Z8	76	PPU	N3-C2-N1	-8.55	121.37	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 687 ligands modelled in this entry, 685 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
58	PAR	QA	1667	-	45,45,45	1.31	7 (15%)	67,67,67	1.40	8 (11%)
58	PAR	XA	1673	-	45,45,45	1.36	6 (13%)	67,67,67	1.33	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	QA	1667	-	-	0/18/94/94	0/4/4/4
58	PAR	XA	1673	-	-	0/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	QA	1667	PAR	C52-C42	3.21	1.58	1.52
58	XA	1673	PAR	C52-C42	3.09	1.58	1.52
58	XA	1673	PAR	O54-C14	2.90	1.49	1.41
58	QA	1667	PAR	C64-C54	2.90	1.59	1.51
58	QA	1667	PAR	O54-C14	2.87	1.49	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	QA	1667	PAR	O52-C13-C23	4.73	115.94	107.50
58	XA	1673	PAR	C14-O54-C54	4.34	122.14	113.73
58	XA	1673	PAR	O52-C13-C23	4.26	115.10	107.50
58	XA	1673	PAR	O33-C14-C24	4.16	116.30	108.08
58	QA	1667	PAR	C14-O54-C54	3.86	121.19	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%)	-0.02	34 (2%) 57 15	49, 89, 176, 309	0
1	XA	1500/1522 (98%)	-0.05	31 (2%) 60 17	41, 81, 178, 324	0
2	QB	237/256 (92%)	0.30	8 (3%) 43 9	88, 147, 217, 264	0
2	XB	237/256 (92%)	0.18	2 (0%) 83 37	70, 122, 194, 242	0
3	QC	205/239 (85%)	0.26	4 (1%) 62 18	81, 126, 182, 248	0
3	XC	205/239 (85%)	0.03	1 (0%) 88 48	56, 100, 159, 208	0
4	QD	208/209 (99%)	0.12	1 (0%) 88 48	53, 96, 150, 208	0
4	XD	208/209 (99%)	0.17	1 (0%) 88 48	45, 95, 147, 226	0
5	QE	151/162 (93%)	0.23	0 100 100	54, 107, 156, 244	0
5	XE	151/162 (93%)	-0.01	2 (1%) 74 26	47, 84, 135, 167	0
6	QF	101/101 (100%)	0.06	1 (0%) 79 31	45, 90, 129, 174	0
6	XF	101/101 (100%)	0.03	0 100 100	48, 87, 125, 178	0
7	QG	155/156 (99%)	0.20	5 (3%) 45 10	66, 115, 166, 229	0
7	XG	155/156 (99%)	0.08	4 (2%) 53 12	68, 107, 155, 214	0
8	QH	138/138 (100%)	0.12	2 (1%) 72 24	55, 103, 153, 176	0
8	XH	138/138 (100%)	-0.06	0 100 100	53, 90, 130, 158	0
9	QI	127/128 (99%)	0.49	6 (4%) 30 6	71, 131, 193, 226	0
9	XI	127/128 (99%)	0.40	3 (2%) 56 14	58, 121, 176, 214	0
10	QJ	99/105 (94%)	0.98	17 (17%) 2 1	81, 161, 235, 275	0
10	XJ	99/105 (94%)	0.54	7 (7%) 16 4	59, 128, 180, 212	0
11	QK	119/129 (92%)	0.33	5 (4%) 35 7	56, 95, 161, 209	0
11	XK	119/129 (92%)	0.12	3 (2%) 54 13	47, 86, 151, 204	0
12	QL	125/132 (94%)	0.23	4 (3%) 45 10	56, 93, 157, 241	0
12	XL	125/132 (94%)	0.10	5 (4%) 36 7	33, 70, 130, 235	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	0.34	5 (4%) 35 7	59, 130, 190, 293	0
13	XM	121/126 (96%)	0.20	4 (3%) 44 10	63, 114, 165, 262	0
14	QN	60/61 (98%)	0.66	3 (5%) 28 6	72, 123, 164, 178	0
14	XN	60/61 (98%)	0.25	2 (3%) 44 10	59, 92, 132, 161	0
15	QO	88/89 (98%)	0.12	0 100 100	56, 98, 153, 188	0
15	XO	88/89 (98%)	0.19	0 100 100	46, 84, 134, 150	0
16	QP	84/88 (95%)	0.12	0 100 100	48, 87, 135, 191	0
16	XP	84/88 (95%)	0.10	1 (1%) 75 27	59, 97, 142, 225	0
17	QQ	100/105 (95%)	0.27	1 (1%) 79 31	60, 100, 144, 205	0
17	XQ	100/105 (95%)	0.16	1 (1%) 79 31	60, 100, 147, 175	0
18	QR	70/88 (79%)	0.16	1 (1%) 72 24	44, 94, 144, 177	0
18	XR	70/88 (79%)	0.06	1 (1%) 72 24	50, 88, 136, 179	0
19	QS	84/93 (90%)	0.47	2 (2%) 56 14	94, 142, 188, 229	0
19	XS	84/93 (90%)	0.29	1 (1%) 75 27	74, 117, 173, 225	0
20	QT	99/106 (93%)	0.22	1 (1%) 79 31	66, 105, 159, 206	0
20	XT	99/106 (93%)	0.14	1 (1%) 79 31	60, 108, 168, 201	0
21	QU	25/27 (92%)	1.80	8 (32%) 1 1	76, 114, 154, 186	0
21	XU	25/27 (92%)	1.22	6 (24%) 1 1	59, 101, 140, 155	0
22	QV	77/77 (100%)	0.33	4 (5%) 26 5	49, 107, 178, 226	0
22	XV	77/77 (100%)	0.14	2 (2%) 53 12	43, 92, 154, 198	0
23	QX	8/25 (32%)	0.75	0 100 100	66, 95, 136, 155	0
23	XX	8/25 (32%)	0.52	1 (12%) 5 1	56, 74, 96, 136	0
24	QY	14/18 (77%)	1.65	3 (21%) 1 1	98, 170, 239, 259	0
24	XY	14/18 (77%)	1.67	6 (42%) 1 0	71, 145, 218, 228	0
25	RA	2882/2916 (98%)	0.01	141 (4%) 28 6	37, 67, 225, 362	0
25	YA	2883/2916 (98%)	-0.12	105 (3%) 41 8	28, 58, 202, 336	0
26	RB	120/122 (98%)	-0.01	1 (0%) 83 37	70, 97, 127, 172	0
26	YB	120/122 (98%)	-0.13	1 (0%) 83 37	57, 84, 112, 160	0
27	RD	272/276 (98%)	-0.06	1 (0%) 90 54	30, 64, 103, 185	0
27	YD	272/276 (98%)	-0.16	1 (0%) 90 54	21, 55, 91, 213	0
28	RE	205/206 (99%)	0.01	3 (1%) 70 23	37, 75, 150, 272	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YE	205/206 (99%)	-0.01	2 (0%) 79 31	33, 73, 141, 240	0
29	RF	202/210 (96%)	-0.05	0 100 100	35, 81, 142, 186	0
29	YF	202/210 (96%)	-0.15	0 100 100	19, 62, 127, 157	0
30	RG	181/182 (99%)	1.06	22 (12%) 5 2	79, 152, 236, 277	0
30	YG	181/182 (99%)	0.27	1 (0%) 86 43	59, 103, 159, 224	0
31	RH	170/180 (94%)	0.77	13 (7%) 14 4	89, 159, 219, 257	0
31	YH	170/180 (94%)	0.15	1 (0%) 86 43	50, 97, 137, 194	0
32	RI	146/148 (98%)	0.37	10 (6%) 17 4	53, 122, 189, 282	0
32	YI	146/148 (98%)	0.04	2 (1%) 72 24	48, 107, 166, 198	0
33	RN	138/140 (98%)	0.15	2 (1%) 72 24	52, 90, 138, 201	0
33	YN	138/140 (98%)	-0.09	0 100 100	45, 73, 129, 177	0
34	RO	122/122 (100%)	-0.04	0 100 100	39, 77, 111, 136	0
34	YO	122/122 (100%)	-0.16	0 100 100	36, 67, 96, 125	0
35	RP	150/150 (100%)	0.22	3 (2%) 62 18	34, 88, 161, 221	0
35	YP	150/150 (100%)	0.07	0 100 100	24, 73, 137, 220	0
36	RQ	141/141 (100%)	0.13	4 (2%) 50 11	45, 87, 138, 207	0
36	YQ	141/141 (100%)	-0.01	1 (0%) 84 40	35, 69, 135, 176	0
37	RR	118/118 (100%)	-0.11	0 100 100	40, 70, 105, 146	0
37	YR	118/118 (100%)	-0.12	0 100 100	39, 69, 108, 143	0
38	RS	111/112 (99%)	0.11	1 (0%) 81 35	61, 98, 149, 192	0
38	YS	111/112 (99%)	-0.04	0 100 100	51, 87, 133, 188	0
39	RT	137/146 (93%)	0.20	6 (4%) 33 7	46, 85, 188, 243	0
39	YT	137/146 (93%)	0.05	2 (1%) 70 23	47, 77, 174, 265	0
40	RU	117/118 (99%)	0.09	3 (2%) 53 12	36, 76, 134, 205	0
40	YU	117/118 (99%)	-0.10	2 (1%) 67 20	26, 59, 118, 220	0
41	RV	101/101 (100%)	0.06	2 (1%) 62 18	42, 96, 169, 265	0
41	YV	101/101 (100%)	-0.12	2 (1%) 62 18	38, 85, 145, 208	0
42	RW	113/113 (100%)	-0.00	0 100 100	39, 63, 114, 239	0
42	YW	113/113 (100%)	-0.03	1 (0%) 81 35	35, 60, 116, 221	0
43	RX	92/96 (95%)	0.10	0 100 100	49, 75, 117, 147	0
43	YX	92/96 (95%)	-0.06	0 100 100	38, 61, 99, 127	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RY	102/110 (92%)	0.58	8 (7%) 13 3	63, 121, 197, 242	0
44	YY	102/110 (92%)	0.14	2 (1%) 62 18	46, 89, 170, 226	0
45	RZ	183/206 (88%)	0.35	7 (3%) 38 8	66, 122, 199, 239	0
45	YZ	183/206 (88%)	0.28	2 (1%) 77 29	54, 112, 199, 258	0
46	R0	82/85 (96%)	0.04	1 (1%) 75 27	52, 75, 101, 157	0
46	Y0	82/85 (96%)	-0.12	0 100 100	43, 71, 90, 104	0
47	R1	97/98 (98%)	0.39	5 (5%) 26 5	44, 76, 158, 289	0
47	Y1	97/98 (98%)	0.22	1 (1%) 79 31	36, 65, 174, 221	0
48	R2	69/72 (95%)	0.05	0 100 100	53, 99, 158, 195	0
48	Y2	69/72 (95%)	0.05	0 100 100	32, 74, 159, 183	0
49	R3	59/60 (98%)	0.32	3 (5%) 27 5	51, 87, 139, 197	0
49	Y3	59/60 (98%)	0.03	2 (3%) 43 9	49, 74, 125, 182	0
50	R4	71/71 (100%)	1.05	11 (15%) 3 1	126, 200, 274, 317	0
50	Y4	71/71 (100%)	0.58	8 (11%) 6 2	88, 160, 235, 285	0
51	R5	59/60 (98%)	0.58	6 (10%) 7 2	39, 79, 219, 237	0
51	Y5	59/60 (98%)	0.23	4 (6%) 17 4	32, 77, 222, 240	0
52	R6	49/54 (90%)	1.25	11 (22%) 1 1	93, 153, 224, 237	0
52	Y6	49/54 (90%)	1.10	7 (14%) 3 1	83, 146, 203, 230	0
53	R7	49/49 (100%)	0.10	1 (2%) 62 18	36, 52, 107, 191	0
53	Y7	49/49 (100%)	0.03	2 (4%) 35 7	29, 41, 104, 206	0
54	R8	64/65 (98%)	0.31	2 (3%) 47 10	48, 73, 141, 217	0
54	Y8	64/65 (98%)	0.18	1 (1%) 68 22	36, 66, 121, 208	0
55	R9	37/37 (100%)	2.40	20 (54%) 0 0	86, 127, 179, 254	0
55	Y9	37/37 (100%)	1.43	8 (21%) 1 1	72, 109, 161, 206	0
56	Z6	3/3 (100%)	2.10	1 (33%) 1 0	57, 57, 57, 66	0
56	Z8	3/3 (100%)	1.70	1 (33%) 1 0	46, 46, 47, 55	0
All	All	20875/21494 (97%)	0.09	647 (3%) 47 10	19, 84, 183, 362	0

The worst 5 of 647 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	RA	1096	A	16.8
25	RA	2116	G	11.8

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Mol	Chain	Res	Type	RSRZ
25	RA	1097	U	11.6
25	RA	1058	G	11.5
25	RA	1065	U	11.2

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

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	PPU	Z6	76	37/38	0.24	-	57,57,57,57	0
56	PPU	Z8	76	37/38	0.24	-	45,45,45,45	0
24	1MG	XY	37	24/25	0.15	-	79,79,79,79	0
24	1MG	QY	37	24/25	0.15	-	98,98,98,98	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	3198	1/1	0.17	-	56,56,56,56	0
57	MG	YA	3131	1/1	0.21	-	25,25,25,25	0
57	MG	YA	3079	1/1	0.38	-	25,25,25,25	0
57	MG	QA	1648	1/1	0.11	-	60,60,60,60	0
57	MG	RA	3059	1/1	0.33	-	19,19,19,19	0
57	MG	XA	1666	1/1	0.16	-	54,54,54,54	0
57	MG	YA	3171	1/1	0.19	-	49,49,49,49	0
57	MG	XA	1632	1/1	0.38	-	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	RA	3026	1/1	0.34	-	18,18,18,18	0
57	MG	RA	3074	1/1	0.10	-	51,51,51,51	0
57	MG	YA	3083	1/1	0.23	-	24,24,24,24	0
57	MG	RA	3209	1/1	0.18	-	67,67,67,67	0
57	MG	RA	3106	1/1	0.23	-	47,47,47,47	0
57	MG	QA	1656	1/1	0.28	-	65,65,65,65	0
57	MG	YA	3084	1/1	0.38	-	25,25,25,25	0
57	MG	YA	3269	1/1	0.58	-	52,52,52,52	0
57	MG	YA	3130	1/1	0.19	-	40,40,40,40	0
57	MG	YA	3032	1/1	0.36	-	22,22,22,22	0
57	MG	QA	1630	1/1	0.15	-	52,52,52,52	0
57	MG	XA	1618	1/1	0.43	-	41,41,41,41	0
57	MG	XA	1612	1/1	0.17	-	31,31,31,31	0
57	MG	YA	3145	1/1	0.34	-	40,40,40,40	0
57	MG	YA	3170	1/1	0.07	-	39,39,39,39	0
57	MG	RA	3015	1/1	0.36	-	22,22,22,22	0
57	MG	QA	1636	1/1	0.23	-	46,46,46,46	0
59	ZN	QN	100	1/1	0.13	-	100,100,100,100	0
57	MG	YA	3134	1/1	0.46	-	28,28,28,28	0
57	MG	RA	3150	1/1	0.22	-	47,47,47,47	0
57	MG	RA	3086	1/1	0.31	-	45,45,45,45	0
57	MG	YA	3163	1/1	0.12	-	47,47,47,47	0
57	MG	YA	3241	1/1	0.35	-	56,56,56,56	0
57	MG	YA	3224	1/1	0.17	-	51,51,51,51	0
57	MG	RA	3081	1/1	0.55	-	46,46,46,46	0
57	MG	YA	3166	1/1	0.23	-	44,44,44,44	0
57	MG	YA	3175	1/1	0.12	-	49,49,49,49	0
57	MG	YA	3202	1/1	0.13	-	55,55,55,55	0
57	MG	QA	1612	1/1	0.32	-	32,32,32,32	0
57	MG	QA	1609	1/1	0.16	-	62,62,62,62	0
57	MG	XA	1664	1/1	0.35	-	61,61,61,61	0
57	MG	RA	3063	1/1	0.49	-	31,31,31,31	0
57	MG	YA	3057	1/1	0.21	-	10,10,10,10	0
57	MG	QA	1643	1/1	0.27	-	46,46,46,46	0
57	MG	YA	3137	1/1	0.19	-	30,30,30,30	0
57	MG	XA	1607	1/1	0.23	-	49,49,49,49	0
57	MG	YA	3151	1/1	0.06	-	60,60,60,60	0
57	MG	RA	3098	1/1	0.40	-	25,25,25,25	0
57	MG	YA	3236	1/1	0.11	-	43,43,43,43	0
57	MG	QA	1644	1/1	0.38	-	54,54,54,54	0
57	MG	RE	301	1/1	0.17	-	31,31,31,31	0
57	MG	YA	3247	1/1	0.71	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3099	1/1	0.12	-	37,37,37,37	0
57	MG	RA	3223	1/1	0.28	-	98,98,98,98	0
57	MG	RA	3004	1/1	0.42	-	34,34,34,34	0
57	MG	XA	1663	1/1	0.31	-	55,55,55,55	0
57	MG	YA	3237	1/1	0.36	-	59,59,59,59	0
57	MG	XA	1646	1/1	0.17	-	55,55,55,55	0
57	MG	YA	3127	1/1	0.32	-	45,45,45,45	0
57	MG	RA	3082	1/1	0.52	-	39,39,39,39	0
57	MG	RA	3180	1/1	0.14	-	34,34,34,34	0
57	MG	YA	3055	1/1	0.12	-	52,52,52,52	0
57	MG	YA	3063	1/1	0.27	-	23,23,23,23	0
57	MG	QA	1662	1/1	0.27	-	119,119,119,119	0
57	MG	YA	3040	1/1	0.25	-	19,19,19,19	0
57	MG	XA	1652	1/1	0.13	-	105,105,105,105	0
57	MG	RA	3208	1/1	0.13	-	31,31,31,31	0
57	MG	YA	3221	1/1	0.52	-	65,65,65,65	0
57	MG	RA	3210	1/1	0.38	-	76,76,76,76	0
57	MG	RA	3077	1/1	0.40	-	42,42,42,42	0
57	MG	RA	3233	1/1	0.23	-	57,57,57,57	0
57	MG	RA	3216	1/1	0.23	-	47,47,47,47	0
57	MG	RA	3144	1/1	0.33	-	45,45,45,45	0
57	MG	YA	3121	1/1	0.36	-	76,76,76,76	0
57	MG	RA	3090	1/1	0.54	-	71,71,71,71	0
57	MG	RA	3047	1/1	0.36	-	19,19,19,19	0
57	MG	YA	3258	1/1	0.24	-	28,28,28,28	0
57	MG	RA	3183	1/1	0.17	-	49,49,49,49	0
57	MG	YA	3251	1/1	0.34	-	60,60,60,60	0
57	MG	YA	3015	1/1	0.54	-	18,18,18,18	0
57	MG	RA	3201	1/1	0.24	-	49,49,49,49	0
57	MG	YA	3220	1/1	0.12	-	38,38,38,38	0
57	MG	QA	1627	1/1	0.12	-	38,38,38,38	0
57	MG	YA	3261	1/1	0.30	-	29,29,29,29	0
57	MG	RA	3049	1/1	0.45	-	38,38,38,38	0
57	MG	YA	3216	1/1	0.20	-	57,57,57,57	0
57	MG	XA	1649	1/1	0.16	-	61,61,61,61	0
57	MG	RA	3065	1/1	0.33	-	36,36,36,36	0
57	MG	RA	3078	1/1	0.34	-	46,46,46,46	0
57	MG	RA	3239	1/1	0.49	-	37,37,37,37	0
57	MG	RA	3186	1/1	0.09	-	27,27,27,27	0
57	MG	YA	3187	1/1	0.21	-	36,36,36,36	0
57	MG	YA	3072	1/1	0.39	-	52,52,52,52	0
57	MG	XA	1662	1/1	0.61	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	QA	1602	1/1	0.37	-	37,37,37,37	0
57	MG	RB	202	1/1	0.08	-	63,63,63,63	0
57	MG	RA	3131	1/1	0.53	-	46,46,46,46	0
57	MG	RA	3062	1/1	0.45	-	18,18,18,18	0
57	MG	YA	3014	1/1	0.36	-	22,22,22,22	0
57	MG	YA	3154	1/1	0.24	-	36,36,36,36	0
57	MG	RA	3050	1/1	0.32	-	25,25,25,25	0
57	MG	YE	301	1/1	0.19	-	21,21,21,21	0
57	MG	YA	3027	1/1	0.20	-	21,21,21,21	0
57	MG	YA	3035	1/1	0.28	-	18,18,18,18	0
57	MG	XA	1620	1/1	0.26	-	33,33,33,33	0
57	MG	YA	3098	1/1	0.23	-	34,34,34,34	0
57	MG	YA	3096	1/1	0.38	-	33,33,33,33	0
57	MG	YA	3066	1/1	0.12	-	23,23,23,23	0
57	MG	QA	1637	1/1	0.29	-	72,72,72,72	0
57	MG	YA	3234	1/1	0.18	-	52,52,52,52	0
57	MG	YA	3006	1/1	0.38	-	11,11,11,11	0
57	MG	YA	3174	1/1	0.11	-	64,64,64,64	0
57	MG	RA	3222	1/1	0.27	-	67,67,67,67	0
57	MG	RA	3084	1/1	0.21	-	45,45,45,45	0
57	MG	RA	3236	1/1	0.36	-	44,44,44,44	0
57	MG	XA	1628	1/1	0.24	-	29,29,29,29	0
57	MG	XA	1610	1/1	0.30	-	32,32,32,32	0
57	MG	QA	1631	1/1	0.17	-	53,53,53,53	0
57	MG	YA	3146	1/1	0.42	-	48,48,48,48	0
57	MG	XA	1611	1/1	0.33	-	28,28,28,28	0
57	MG	XA	1665	1/1	0.22	-	53,53,53,53	0
57	MG	RB	201	1/1	0.09	-	76,76,76,76	0
57	MG	YA	3197	1/1	0.46	-	47,47,47,47	0
57	MG	YA	3092	1/1	0.30	-	44,44,44,44	0
57	MG	RA	3174	1/1	0.25	-	39,39,39,39	0
57	MG	XA	1631	1/1	0.17	-	50,50,50,50	0
57	MG	QA	1617	1/1	0.26	-	40,40,40,40	0
57	MG	QA	1659	1/1	0.23	-	84,84,84,84	0
57	MG	RA	3214	1/1	0.25	-	47,47,47,47	0
57	MG	RA	3069	1/1	0.38	-	40,40,40,40	0
57	MG	YB	203	1/1	0.07	-	47,47,47,47	0
57	MG	YA	3103	1/1	0.27	-	32,32,32,32	0
57	MG	QA	1645	1/1	0.14	-	43,43,43,43	0
57	MG	YA	3112	1/1	0.14	-	36,36,36,36	0
57	MG	QA	1611	1/1	0.25	-	27,27,27,27	0
57	MG	YA	3177	1/1	0.19	-	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	RA	3020	1/1	0.44	-	20,20,20,20	0
57	MG	RA	3199	1/1	0.17	-	58,58,58,58	0
57	MG	QA	1650	1/1	0.30	-	72,72,72,72	0
57	MG	RA	3060	1/1	0.20	-	31,31,31,31	0
57	MG	RA	3192	1/1	0.24	-	81,81,81,81	0
57	MG	YA	3033	1/1	0.41	-	30,30,30,30	0
57	MG	YA	3263	1/1	0.32	-	31,31,31,31	0
57	MG	YA	3111	1/1	0.17	-	28,28,28,28	0
57	MG	YA	3249	1/1	0.37	-	74,74,74,74	0
57	MG	RA	3095	1/1	0.42	-	37,37,37,37	0
57	MG	QA	1646	1/1	0.11	-	52,52,52,52	0
57	MG	RA	3179	1/1	0.15	-	32,32,32,32	0
57	MG	YA	3060	1/1	0.25	-	25,25,25,25	0
57	MG	YA	3053	1/1	0.28	-	27,27,27,27	0
57	MG	YA	3003	1/1	0.26	-	18,18,18,18	0
57	MG	RA	3017	1/1	0.21	-	29,29,29,29	0
57	MG	QA	1658	1/1	0.25	-	58,58,58,58	0
57	MG	YA	3152	1/1	0.45	-	41,41,41,41	0
57	MG	YA	3238	1/1	0.46	-	62,62,62,62	0
57	MG	R5	101	1/1	0.21	-	38,38,38,38	0
57	MG	YA	3192	1/1	0.07	-	38,38,38,38	0
57	MG	YA	3148	1/1	0.12	-	33,33,33,33	0
57	MG	YA	3181	1/1	0.20	-	60,60,60,60	0
57	MG	RA	3240	1/1	0.48	-	34,34,34,34	0
57	MG	RA	3043	1/1	0.24	-	43,43,43,43	0
57	MG	YA	3031	1/1	0.39	-	24,24,24,24	0
57	MG	XA	1645	1/1	0.36	-	49,49,49,49	0
57	MG	RA	3005	1/1	0.44	-	38,38,38,38	0
57	MG	RA	3200	1/1	0.42	-	43,43,43,43	0
57	MG	RA	3146	1/1	0.09	-	31,31,31,31	0
57	MG	RA	3229	1/1	0.30	-	80,80,80,80	0
57	MG	YA	3086	1/1	0.20	-	45,45,45,45	0
57	MG	YA	3082	1/1	0.34	-	23,23,23,23	0
57	MG	YA	3210	1/1	0.26	-	60,60,60,60	0
57	MG	YA	3117	1/1	0.43	-	73,73,73,73	0
57	MG	YD	301	1/1	0.12	-	32,32,32,32	0
57	MG	RA	3054	1/1	0.16	-	30,30,30,30	0
57	MG	YA	3250	1/1	0.49	-	45,45,45,45	0
57	MG	YA	3223	1/1	0.37	-	67,67,67,67	0
57	MG	YA	3005	1/1	0.19	-	20,20,20,20	0
57	MG	RA	3093	1/1	0.33	-	32,32,32,32	0
57	MG	RA	3076	1/1	0.36	-	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	3166	1/1	0.14	-	44,44,44,44	0
57	MG	YA	3262	1/1	0.38	-	35,35,35,35	0
57	MG	RA	3083	1/1	0.38	-	40,40,40,40	0
57	MG	YA	3186	1/1	0.24	-	43,43,43,43	0
57	MG	RA	3215	1/1	0.21	-	50,50,50,50	0
57	MG	XA	1621	1/1	0.53	-	48,48,48,48	0
57	MG	RA	3035	1/1	0.27	-	24,24,24,24	0
57	MG	YA	3071	1/1	0.12	-	17,17,17,17	0
57	MG	RA	3124	1/1	0.47	-	59,59,59,59	0
57	MG	RA	3241	1/1	0.17	-	34,34,34,34	0
57	MG	YA	3001	1/1	0.42	-	21,21,21,21	0
57	MG	RA	3138	1/1	0.28	-	59,59,59,59	0
57	MG	YA	3189	1/1	0.14	-	57,57,57,57	0
57	MG	YA	3081	1/1	0.38	-	28,28,28,28	0
57	MG	RA	3011	1/1	0.21	-	31,31,31,31	0
57	MG	YA	3232	1/1	0.16	-	50,50,50,50	0
57	MG	RA	3016	1/1	0.31	-	16,16,16,16	0
57	MG	YA	3231	1/1	0.16	-	45,45,45,45	0
57	MG	YA	3087	1/1	0.27	-	27,27,27,27	0
57	MG	XA	1605	1/1	0.34	-	37,37,37,37	0
57	MG	QA	1641	1/1	0.36	-	45,45,45,45	0
57	MG	RA	3193	1/1	0.41	-	73,73,73,73	0
57	MG	RA	3165	1/1	0.18	-	61,61,61,61	0
57	MG	YA	3156	1/1	0.31	-	50,50,50,50	0
59	ZN	R9	101	1/1	0.23	-	179,179,179,179	0
57	MG	RA	3189	1/1	0.11	-	45,45,45,45	0
57	MG	RA	3038	1/1	0.25	-	26,26,26,26	0
57	MG	QA	1601	1/1	0.20	-	44,44,44,44	0
57	MG	RA	3143	1/1	0.34	-	37,37,37,37	0
57	MG	YA	3034	1/1	0.39	-	19,19,19,19	0
57	MG	YA	3069	1/1	0.46	-	42,42,42,42	0
57	MG	XA	1650	1/1	0.23	-	39,39,39,39	0
57	MG	YB	201	1/1	0.36	-	71,71,71,71	0
57	MG	XA	1660	1/1	0.11	-	26,26,26,26	0
57	MG	YA	3078	1/1	0.19	-	27,27,27,27	0
57	MG	QA	1632	1/1	0.10	-	58,58,58,58	0
57	MG	RR	201	1/1	0.26	-	34,34,34,34	0
57	MG	YA	3042	1/1	0.28	-	19,19,19,19	0
57	MG	RA	3109	1/1	0.31	-	43,43,43,43	0
57	MG	RA	3190	1/1	0.25	-	48,48,48,48	0
57	MG	YA	3161	1/1	0.26	-	36,36,36,36	0
57	MG	YA	3012	1/1	0.40	-	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3023	1/1	0.16	-	26,26,26,26	0
57	MG	RA	3158	1/1	0.13	-	41,41,41,41	0
57	MG	RA	3156	1/1	0.14	-	47,47,47,47	0
57	MG	YA	3018	1/1	0.40	-	30,30,30,30	0
57	MG	YA	3212	1/1	0.23	-	62,62,62,62	0
57	MG	QA	1616	1/1	0.18	-	66,66,66,66	0
57	MG	YA	3198	1/1	0.20	-	57,57,57,57	0
57	MG	RA	3073	1/1	0.26	-	35,35,35,35	0
57	MG	RA	3220	1/1	0.24	-	72,72,72,72	0
57	MG	XA	1636	1/1	0.35	-	46,46,46,46	0
57	MG	RA	3013	1/1	0.25	-	14,14,14,14	0
57	MG	QA	1653	1/1	0.15	-	53,53,53,53	0
57	MG	RA	3021	1/1	0.34	-	27,27,27,27	0
57	MG	RA	3181	1/1	0.19	-	54,54,54,54	0
57	MG	YA	3147	1/1	0.29	-	54,54,54,54	0
57	MG	YA	3124	1/1	0.27	-	35,35,35,35	0
57	MG	RA	3164	1/1	0.11	-	32,32,32,32	0
57	MG	YA	3139	1/1	0.15	-	35,35,35,35	0
57	MG	YA	3191	1/1	0.18	-	34,34,34,34	0
57	MG	XA	1633	1/1	0.22	-	50,50,50,50	0
57	MG	YA	3157	1/1	0.38	-	48,48,48,48	0
57	MG	RA	3066	1/1	0.34	-	28,28,28,28	0
57	MG	YA	3150	1/1	0.22	-	52,52,52,52	0
57	MG	RA	3125	1/1	0.28	-	41,41,41,41	0
57	MG	QV	101	1/1	0.23	-	36,36,36,36	0
57	MG	QA	1622	1/1	0.19	-	46,46,46,46	0
57	MG	YA	3235	1/1	0.38	-	69,69,69,69	0
57	MG	QA	1666	1/1	0.20	-	52,52,52,52	0
57	MG	RA	3032	1/1	0.33	-	21,21,21,21	0
57	MG	YA	3110	1/1	0.34	-	29,29,29,29	0
57	MG	YA	3135	1/1	0.13	-	45,45,45,45	0
57	MG	XA	1604	1/1	0.60	-	40,40,40,40	0
57	MG	YA	3168	1/1	0.55	-	57,57,57,57	0
57	MG	RA	3079	1/1	0.47	-	39,39,39,39	0
57	MG	YA	3133	1/1	0.08	-	37,37,37,37	0
57	MG	YA	3207	1/1	0.44	-	61,61,61,61	0
57	MG	RA	3207	1/1	0.07	-	93,93,93,93	0
57	MG	YA	3104	1/1	0.15	-	31,31,31,31	0
57	MG	RA	3212	1/1	0.22	-	64,64,64,64	0
57	MG	YA	3209	1/1	0.31	-	71,71,71,71	0
57	MG	RA	3225	1/1	0.11	-	59,59,59,59	0
57	MG	QA	1606	1/1	0.20	-	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	QA	1634	1/1	0.45	-	39,39,39,39	0
57	MG	YA	3047	1/1	0.31	-	23,23,23,23	0
57	MG	Y7	101	1/1	0.32	-	48,48,48,48	0
57	MG	RA	3075	1/1	0.17	-	21,21,21,21	0
57	MG	RA	3153	1/1	0.28	-	50,50,50,50	0
57	MG	YA	3205	1/1	0.07	-	48,48,48,48	0
57	MG	RA	3196	1/1	0.09	-	62,62,62,62	0
57	MG	YA	3149	1/1	0.19	-	40,40,40,40	0
57	MG	XT	201	1/1	0.34	-	77,77,77,77	0
57	MG	RA	3133	1/1	0.28	-	73,73,73,73	0
57	MG	RA	3168	1/1	0.37	-	45,45,45,45	0
57	MG	YA	3142	1/1	0.31	-	54,54,54,54	0
57	MG	RA	3046	1/1	0.39	-	26,26,26,26	0
57	MG	YA	3254	1/1	0.47	-	32,32,32,32	0
57	MG	YA	3240	1/1	0.16	-	60,60,60,60	0
57	MG	YA	3125	1/1	0.29	-	33,33,33,33	0
57	MG	QM	201	1/1	0.09	-	81,81,81,81	0
57	MG	YA	3002	1/1	0.30	-	16,16,16,16	0
57	MG	RA	3226	1/1	0.20	-	44,44,44,44	0
57	MG	RA	3113	1/1	0.21	-	27,27,27,27	0
57	MG	RA	3119	1/1	0.41	-	66,66,66,66	0
57	MG	YA	3022	1/1	0.29	-	34,34,34,34	0
57	MG	R0	101	1/1	0.25	-	37,37,37,37	0
57	MG	QA	1633	1/1	0.35	-	73,73,73,73	0
57	MG	YA	3119	1/1	0.41	-	36,36,36,36	0
57	MG	RF	301	1/1	0.20	-	50,50,50,50	0
57	MG	RA	3203	1/1	0.20	-	73,73,73,73	0
57	MG	XA	1615	1/1	0.36	-	33,33,33,33	0
57	MG	QA	1608	1/1	0.09	-	41,41,41,41	0
57	MG	YA	3155	1/1	0.17	-	33,33,33,33	0
57	MG	RA	3051	1/1	0.30	-	26,26,26,26	0
57	MG	RA	3205	1/1	0.26	-	38,38,38,38	0
57	MG	RA	3123	1/1	0.35	-	53,53,53,53	0
57	MG	YA	3062	1/1	0.15	-	30,30,30,30	0
57	MG	RA	3014	1/1	0.20	-	25,25,25,25	0
57	MG	XA	1617	1/1	0.20	-	36,36,36,36	0
57	MG	RA	3048	1/1	0.23	-	30,30,30,30	0
57	MG	RA	3163	1/1	0.57	-	45,45,45,45	0
57	MG	XA	1622	1/1	0.13	-	37,37,37,37	0
59	ZN	XD	301	1/1	0.30	-	52,52,52,52	0
57	MG	YA	3046	1/1	0.29	-	27,27,27,27	0
57	MG	YA	3019	1/1	0.33	-	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3219	1/1	0.10	-	37,37,37,37	0
57	MG	YA	3020	1/1	0.51	-	18,18,18,18	0
57	MG	XA	1651	1/1	0.21	-	55,55,55,55	0
57	MG	XA	1672	1/1	0.29	-	44,44,44,44	0
57	MG	QA	1619	1/1	0.38	-	45,45,45,45	0
57	MG	YA	3089	1/1	0.43	-	30,30,30,30	0
57	MG	YA	3167	1/1	0.35	-	61,61,61,61	0
57	MG	RA	3204	1/1	0.31	-	68,68,68,68	0
57	MG	RA	3155	1/1	0.35	-	45,45,45,45	0
57	MG	RD	301	1/1	0.24	-	64,64,64,64	0
57	MG	XA	1602	1/1	0.24	-	26,26,26,26	0
57	MG	YA	3183	1/1	0.14	-	45,45,45,45	0
57	MG	YA	3007	1/1	0.15	-	21,21,21,21	0
57	MG	YA	3229	1/1	0.36	-	33,33,33,33	0
57	MG	XA	1647	1/1	0.23	-	58,58,58,58	0
57	MG	RA	3136	1/1	0.26	-	33,33,33,33	0
57	MG	RA	3116	1/1	0.17	-	77,77,77,77	0
57	MG	YA	3128	1/1	0.53	-	62,62,62,62	0
57	MG	YA	3024	1/1	0.29	-	21,21,21,21	0
57	MG	QA	1614	1/1	0.38	-	38,38,38,38	0
57	MG	RA	3227	1/1	0.30	-	55,55,55,55	0
57	MG	YA	3144	1/1	0.12	-	54,54,54,54	0
57	MG	RA	3053	1/1	0.10	-	19,19,19,19	0
57	MG	YA	3080	1/1	0.25	-	33,33,33,33	0
57	MG	QA	1647	1/1	0.65	-	50,50,50,50	0
57	MG	YA	3064	1/1	0.25	-	25,25,25,25	0
57	MG	RA	3039	1/1	0.28	-	30,30,30,30	0
57	MG	RA	3232	1/1	0.46	-	33,33,33,33	0
57	MG	RA	3030	1/1	0.29	-	31,31,31,31	0
57	MG	RA	3187	1/1	0.23	-	63,63,63,63	0
57	MG	YA	3217	1/1	0.22	-	70,70,70,70	0
57	MG	YA	3050	1/1	0.37	-	27,27,27,27	0
57	MG	RA	3145	1/1	0.19	-	53,53,53,53	0
57	MG	XA	1661	1/1	0.11	-	67,67,67,67	0
57	MG	RA	3045	1/1	0.10	-	28,28,28,28	0
57	MG	QA	1651	1/1	0.33	-	57,57,57,57	0
57	MG	RA	3080	1/1	0.20	-	36,36,36,36	0
57	MG	YA	3008	1/1	0.30	-	20,20,20,20	0
57	MG	YA	3036	1/1	0.19	-	19,19,19,19	0
57	MG	YA	3190	1/1	0.48	-	53,53,53,53	0
57	MG	XA	1635	1/1	0.42	-	40,40,40,40	0
57	MG	XA	1653	1/1	0.21	-	66,66,66,66	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	0.17	-	39,39,39,39	0
57	MG	YA	3028	1/1	0.17	-	17,17,17,17	0
57	MG	YA	3113	1/1	0.08	-	35,35,35,35	0
57	MG	YA	3048	1/1	0.24	-	26,26,26,26	0
57	MG	YA	3253	1/1	0.78	-	57,57,57,57	0
57	MG	RA	3238	1/1	0.16	-	34,34,34,34	0
57	MG	YA	3132	1/1	0.15	-	41,41,41,41	0
57	MG	RA	3094	1/1	0.44	-	34,34,34,34	0
57	MG	RA	3085	1/1	0.37	-	32,32,32,32	0
57	MG	XA	1608	1/1	0.14	-	57,57,57,57	0
57	MG	RA	3142	1/1	0.17	-	60,60,60,60	0
57	MG	YA	3245	1/1	0.26	-	60,60,60,60	0
57	MG	YA	3068	1/1	0.14	-	35,35,35,35	0
57	MG	RA	3211	1/1	0.18	-	50,50,50,50	0
57	MG	QA	1649	1/1	0.23	-	49,49,49,49	0
57	MG	RA	3126	1/1	0.23	-	53,53,53,53	0
57	MG	XA	1624	1/1	0.42	-	47,47,47,47	0
57	MG	RA	3089	1/1	0.49	-	35,35,35,35	0
57	MG	QA	1620	1/1	0.59	-	52,52,52,52	0
57	MG	RA	3130	1/1	0.31	-	43,43,43,43	0
57	MG	XA	1654	1/1	0.34	-	60,60,60,60	0
57	MG	RA	3213	1/1	0.20	-	40,40,40,40	0
57	MG	XA	1669	1/1	0.10	-	75,75,75,75	0
57	MG	YA	3129	1/1	0.38	-	35,35,35,35	0
59	ZN	QD	301	1/1	0.28	-	54,54,54,54	0
57	MG	QA	1638	1/1	0.27	-	47,47,47,47	0
57	MG	QA	1604	1/1	0.36	-	36,36,36,36	0
57	MG	YA	3061	1/1	0.36	-	19,19,19,19	0
57	MG	YA	3122	1/1	0.31	-	41,41,41,41	0
57	MG	RA	3161	1/1	0.25	-	34,34,34,34	0
57	MG	YA	3118	1/1	0.28	-	27,27,27,27	0
57	MG	RA	3088	1/1	0.30	-	30,30,30,30	0
57	MG	RA	3134	1/1	0.32	-	36,36,36,36	0
57	MG	YA	3182	1/1	0.39	-	64,64,64,64	0
57	MG	QA	1621	1/1	0.08	-	36,36,36,36	0
57	MG	RA	3072	1/1	0.23	-	34,34,34,34	0
57	MG	RA	3040	1/1	0.40	-	22,22,22,22	0
57	MG	YA	3158	1/1	0.24	-	40,40,40,40	0
57	MG	YA	3051	1/1	0.29	-	20,20,20,20	0
57	MG	XM	201	1/1	0.14	-	79,79,79,79	0
57	MG	RA	3178	1/1	0.38	-	48,48,48,48	0
57	MG	XA	1623	1/1	0.12	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3118	1/1	0.28	-	40,40,40,40	0
57	MG	YA	3193	1/1	0.41	-	39,39,39,39	0
57	MG	RA	3231	1/1	0.50	-	27,27,27,27	0
57	MG	RA	3003	1/1	0.43	-	28,28,28,28	0
57	MG	YA	3227	1/1	0.34	-	27,27,27,27	0
57	MG	YA	3226	1/1	0.16	-	41,41,41,41	0
57	MG	YA	3091	1/1	0.40	-	27,27,27,27	0
57	MG	RA	3169	1/1	0.21	-	51,51,51,51	0
57	MG	YA	3093	1/1	0.19	-	37,37,37,37	0
57	MG	YA	3108	1/1	0.39	-	34,34,34,34	0
57	MG	QA	1654	1/1	0.08	-	77,77,77,77	0
57	MG	YA	3030	1/1	0.46	-	30,30,30,30	0
57	MG	RA	3111	1/1	0.27	-	45,45,45,45	0
57	MG	RA	3097	1/1	0.26	-	26,26,26,26	0
57	MG	RA	3120	1/1	0.54	-	39,39,39,39	0
57	MG	YA	3169	1/1	0.23	-	43,43,43,43	0
57	MG	YA	3054	1/1	0.29	-	26,26,26,26	0
57	MG	YA	3109	1/1	0.33	-	27,27,27,27	0
57	MG	YA	3225	1/1	0.16	-	36,36,36,36	0
57	MG	QH	201	1/1	0.17	-	81,81,81,81	0
57	MG	RA	3091	1/1	0.33	-	28,28,28,28	0
57	MG	YA	3021	1/1	0.33	-	22,22,22,22	0
57	MG	YA	3255	1/1	0.48	-	33,33,33,33	0
57	MG	RA	3175	1/1	0.31	-	58,58,58,58	0
57	MG	YA	3143	1/1	0.22	-	35,35,35,35	0
57	MG	YA	3085	1/1	0.28	-	35,35,35,35	0
57	MG	YA	3252	1/1	0.45	-	70,70,70,70	0
57	MG	QA	1618	1/1	0.45	-	45,45,45,45	0
57	MG	YA	3099	1/1	0.19	-	28,28,28,28	0
57	MG	XA	1671	1/1	0.15	-	52,52,52,52	0
57	MG	YB	202	1/1	0.37	-	50,50,50,50	0
57	MG	YA	3159	1/1	0.17	-	25,25,25,25	0
57	MG	YA	3120	1/1	0.30	-	52,52,52,52	0
57	MG	YA	3026	1/1	0.42	-	12,12,12,12	0
57	MG	YA	3067	1/1	0.45	-	33,33,33,33	0
57	MG	RA	3188	1/1	0.29	-	41,41,41,41	0
57	MG	RA	3149	1/1	0.21	-	53,53,53,53	0
57	MG	QA	1639	1/1	0.32	-	35,35,35,35	0
57	MG	YA	3172	1/1	0.15	-	65,65,65,65	0
57	MG	RA	3202	1/1	0.43	-	52,52,52,52	0
57	MG	YA	3123	1/1	0.16	-	22,22,22,22	0
57	MG	XA	1640	1/1	0.54	-	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	RA	3122	1/1	0.20	-	61,61,61,61	0
57	MG	RA	3068	1/1	0.25	-	30,30,30,30	0
57	MG	YA	3153	1/1	0.66	-	67,67,67,67	0
57	MG	YA	3075	1/1	0.11	-	23,23,23,23	0
57	MG	Y5	101	1/1	0.18	-	35,35,35,35	0
57	MG	RA	3162	1/1	0.26	-	61,61,61,61	0
57	MG	RA	3129	1/1	0.15	-	71,71,71,71	0
57	MG	XA	1648	1/1	0.34	-	40,40,40,40	0
57	MG	YA	3044	1/1	0.21	-	15,15,15,15	0
57	MG	YA	3178	1/1	0.29	-	44,44,44,44	0
57	MG	YA	3233	1/1	0.34	-	55,55,55,55	0
57	MG	RA	3176	1/1	0.22	-	57,57,57,57	0
57	MG	RA	3105	1/1	0.26	-	30,30,30,30	0
57	MG	YA	3088	1/1	0.39	-	35,35,35,35	0
57	MG	YA	3059	1/1	0.29	-	13,13,13,13	0
57	MG	RA	3191	1/1	0.35	-	51,51,51,51	0
57	MG	YA	3056	1/1	0.22	-	20,20,20,20	0
57	MG	YE	302	1/1	0.29	-	35,35,35,35	0
57	MG	YA	3266	1/1	0.20	-	37,37,37,37	0
57	MG	YA	3162	1/1	0.28	-	71,71,71,71	0
57	MG	XA	1614	1/1	0.22	-	38,38,38,38	0
57	MG	RA	3218	1/1	0.38	-	66,66,66,66	0
57	MG	XA	1630	1/1	0.33	-	38,38,38,38	0
57	MG	RA	3052	1/1	0.30	-	18,18,18,18	0
57	MG	RA	3019	1/1	0.30	-	26,26,26,26	0
57	MG	QA	1664	1/1	0.07	-	118,118,118,118	0
57	MG	RA	3041	1/1	0.24	-	23,23,23,23	0
57	MG	RA	3110	1/1	0.29	-	32,32,32,32	0
57	MG	RA	3108	1/1	0.12	-	29,29,29,29	0
57	MG	XA	1626	1/1	0.30	-	40,40,40,40	0
57	MG	RU	201	1/1	0.24	-	90,90,90,90	0
57	MG	YA	3203	1/1	0.19	-	28,28,28,28	0
57	MG	XA	1657	1/1	0.54	-	56,56,56,56	0
57	MG	QA	1615	1/1	0.25	-	47,47,47,47	0
57	MG	QA	1640	1/1	0.13	-	44,44,44,44	0
57	MG	RA	3230	1/1	0.29	-	22,22,22,22	0
57	MG	RE	302	1/1	0.28	-	43,43,43,43	0
57	MG	YA	3041	1/1	0.28	-	17,17,17,17	0
57	MG	RA	3137	1/1	0.27	-	31,31,31,31	0
57	MG	RA	3167	1/1	0.18	-	51,51,51,51	0
57	MG	YA	3100	1/1	0.43	-	20,20,20,20	0
57	MG	YA	3039	1/1	0.34	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	XA	1606	1/1	0.31	-	35,35,35,35	0
57	MG	RA	3027	1/1	0.24	-	27,27,27,27	0
57	MG	YA	3101	1/1	0.39	-	32,32,32,32	0
57	MG	RA	3096	1/1	0.29	-	25,25,25,25	0
57	MG	RA	3042	1/1	0.25	-	26,26,26,26	0
57	MG	YA	3070	1/1	0.27	-	33,33,33,33	0
57	MG	RA	3140	1/1	0.69	-	45,45,45,45	0
57	MG	RA	3185	1/1	0.13	-	44,44,44,44	0
57	MG	XA	1613	1/1	0.09	-	36,36,36,36	0
57	MG	YA	3115	1/1	0.32	-	31,31,31,31	0
57	MG	RA	3127	1/1	0.16	-	34,34,34,34	0
57	MG	YA	3222	1/1	0.27	-	56,56,56,56	0
57	MG	RA	3157	1/1	0.39	-	69,69,69,69	0
58	PAR	QA	1667	42/42	0.25	-	75,75,75,75	0
57	MG	RA	3092	1/1	0.39	-	27,27,27,27	0
57	MG	YA	3244	1/1	0.21	-	71,71,71,71	0
57	MG	YA	3077	1/1	0.43	-	26,26,26,26	0
57	MG	RA	3057	1/1	0.40	-	44,44,44,44	0
57	MG	RA	3024	1/1	0.16	-	25,25,25,25	0
57	MG	YA	3165	1/1	0.25	-	46,46,46,46	0
57	MG	RA	3194	1/1	0.45	-	40,40,40,40	0
57	MG	YA	3180	1/1	0.14	-	44,44,44,44	0
57	MG	RA	3055	1/1	0.51	-	27,27,27,27	0
57	MG	YA	3106	1/1	0.27	-	28,28,28,28	0
57	MG	RA	3028	1/1	0.33	-	28,28,28,28	0
57	MG	RA	3139	1/1	0.28	-	54,54,54,54	0
59	ZN	Y9	101	1/1	0.27	-	166,166,166,166	0
57	MG	YA	3090	1/1	0.27	-	11,11,11,11	0
57	MG	RA	3132	1/1	0.10	-	40,40,40,40	0
57	MG	QA	1661	1/1	0.30	-	56,56,56,56	0
57	MG	QA	1626	1/1	0.15	-	64,64,64,64	0
57	MG	YA	3260	1/1	0.25	-	26,26,26,26	0
57	MG	YA	3107	1/1	0.13	-	30,30,30,30	0
57	MG	XA	1659	1/1	0.41	-	71,71,71,71	0
57	MG	RA	3151	1/1	0.23	-	54,54,54,54	0
57	MG	XA	1629	1/1	0.17	-	62,62,62,62	0
57	MG	RA	3037	1/1	0.23	-	16,16,16,16	0
57	MG	RA	3160	1/1	0.21	-	53,53,53,53	0
57	MG	YA	3176	1/1	0.16	-	47,47,47,47	0
57	MG	QA	1623	1/1	0.28	-	54,54,54,54	0
57	MG	YA	3246	1/1	0.29	-	44,44,44,44	0
57	MG	XA	1637	1/1	0.47	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	QA	1652	1/1	0.34	-	38,38,38,38	0
57	MG	QA	1624	1/1	0.28	-	41,41,41,41	0
57	MG	RA	3217	1/1	0.08	-	74,74,74,74	0
57	MG	RA	3002	1/1	0.64	-	37,37,37,37	0
57	MG	QV	102	1/1	0.25	-	30,30,30,30	0
57	MG	RA	3008	1/1	0.39	-	46,46,46,46	0
57	MG	YA	3076	1/1	0.19	-	29,29,29,29	0
57	MG	XA	1616	1/1	0.24	-	25,25,25,25	0
57	MG	RA	3022	1/1	0.48	-	25,25,25,25	0
57	MG	QA	1635	1/1	0.20	-	47,47,47,47	0
57	MG	YX	101	1/1	0.17	-	109,109,109,109	0
57	MG	QA	1629	1/1	0.57	-	49,49,49,49	0
57	MG	RA	3141	1/1	0.33	-	61,61,61,61	0
57	MG	QA	1610	1/1	0.26	-	33,33,33,33	0
57	MG	QA	1655	1/1	0.24	-	62,62,62,62	0
57	MG	YA	3009	1/1	0.52	-	28,28,28,28	0
57	MG	YA	3211	1/1	0.24	-	32,32,32,32	0
57	MG	YA	3204	1/1	0.24	-	60,60,60,60	0
57	MG	RA	3012	1/1	0.32	-	28,28,28,28	0
57	MG	YA	3179	1/1	0.14	-	44,44,44,44	0
57	MG	YA	3160	1/1	0.19	-	47,47,47,47	0
57	MG	YA	3073	1/1	0.19	-	28,28,28,28	0
57	MG	RA	3009	1/1	0.23	-	77,77,77,77	0
57	MG	XA	1627	1/1	0.25	-	48,48,48,48	0
57	MG	YA	3029	1/1	0.32	-	20,20,20,20	0
57	MG	YA	3201	1/1	0.85	-	49,49,49,49	0
57	MG	RA	3154	1/1	0.20	-	31,31,31,31	0
57	MG	YA	3038	1/1	0.14	-	17,17,17,17	0
57	MG	YA	3065	1/1	0.40	-	52,52,52,52	0
57	MG	XA	1601	1/1	0.46	-	32,32,32,32	0
57	MG	RA	3171	1/1	0.24	-	56,56,56,56	0
57	MG	YA	3218	1/1	0.35	-	63,63,63,63	0
57	MG	YA	3013	1/1	0.42	-	20,20,20,20	0
57	MG	RA	3036	1/1	0.27	-	23,23,23,23	0
57	MG	QA	1663	1/1	0.15	-	95,95,95,95	0
57	MG	YA	3095	1/1	0.36	-	24,24,24,24	0
57	MG	YA	3194	1/1	0.20	-	40,40,40,40	0
57	MG	XA	1670	1/1	0.12	-	52,52,52,52	0
57	MG	XA	1603	1/1	0.22	-	32,32,32,32	0
57	MG	RA	3104	1/1	0.34	-	29,29,29,29	0
57	MG	YA	3264	1/1	0.46	-	52,52,52,52	0
57	MG	XA	1667	1/1	0.30	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3103	1/1	0.23	-	28,28,28,28	0
57	MG	XX	101	1/1	0.20	-	79,79,79,79	0
57	MG	RA	3064	1/1	0.27	-	34,34,34,34	0
57	MG	QA	1628	1/1	0.12	-	44,44,44,44	0
57	MG	RA	3219	1/1	0.16	-	49,49,49,49	0
57	MG	XA	1643	1/1	0.28	-	45,45,45,45	0
57	MG	YA	3213	1/1	0.13	-	35,35,35,35	0
57	MG	YA	3141	1/1	0.42	-	41,41,41,41	0
57	MG	RA	3197	1/1	0.36	-	37,37,37,37	0
57	MG	QA	1603	1/1	0.60	-	36,36,36,36	0
57	MG	YA	3097	1/1	0.31	-	36,36,36,36	0
57	MG	RA	3044	1/1	0.46	-	43,43,43,43	0
57	MG	RA	3007	1/1	0.21	-	34,34,34,34	0
57	MG	RA	3107	1/1	0.34	-	45,45,45,45	0
57	MG	RA	3177	1/1	0.23	-	45,45,45,45	0
57	MG	RA	3237	1/1	0.35	-	51,51,51,51	0
57	MG	YA	3116	1/1	0.24	-	42,42,42,42	0
57	MG	XA	1641	1/1	0.28	-	39,39,39,39	0
57	MG	RA	3029	1/1	0.27	-	32,32,32,32	0
57	MG	YA	3102	1/1	0.32	-	26,26,26,26	0
58	PAR	XA	1673	42/42	0.22	-	64,64,64,64	0
57	MG	RA	3070	1/1	0.41	-	32,32,32,32	0
57	MG	YA	3043	1/1	0.37	-	17,17,17,17	0
57	MG	RA	3135	1/1	0.18	-	38,38,38,38	0
57	MG	RA	3235	1/1	0.52	-	57,57,57,57	0
57	MG	RA	3058	1/1	0.28	-	19,19,19,19	0
57	MG	QF	201	1/1	0.40	-	68,68,68,68	0
57	MG	YA	3016	1/1	0.24	-	29,29,29,29	0
57	MG	RA	3112	1/1	0.23	-	44,44,44,44	0
57	MG	YA	3199	1/1	0.15	-	45,45,45,45	0
57	MG	YA	3114	1/1	0.17	-	39,39,39,39	0
57	MG	RA	3184	1/1	0.20	-	41,41,41,41	0
57	MG	YA	3105	1/1	0.28	-	24,24,24,24	0
57	MG	RA	3010	1/1	0.56	-	56,56,56,56	0
57	MG	RA	3152	1/1	0.15	-	56,56,56,56	0
57	MG	XA	1656	1/1	0.41	-	48,48,48,48	0
57	MG	YA	3052	1/1	0.55	-	68,68,68,68	0
57	MG	YA	3256	1/1	0.31	-	32,32,32,32	0
57	MG	YA	3228	1/1	0.27	-	36,36,36,36	0
57	MG	YA	3206	1/1	0.28	-	56,56,56,56	0
57	MG	YA	3017	1/1	0.21	-	25,25,25,25	0
57	MG	XA	1609	1/1	0.36	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	XA	1634	1/1	0.22	-	33,33,33,33	0
57	MG	YA	3185	1/1	0.23	-	40,40,40,40	0
57	MG	YA	3058	1/1	0.49	-	24,24,24,24	0
57	MG	XA	1619	1/1	0.30	-	33,33,33,33	0
57	MG	QA	1625	1/1	0.26	-	53,53,53,53	0
57	MG	R8	101	1/1	0.23	-	33,33,33,33	0
57	MG	RA	3206	1/1	0.22	-	76,76,76,76	0
57	MG	RA	3006	1/1	0.52	-	30,30,30,30	0
57	MG	RA	3101	1/1	0.30	-	38,38,38,38	0
57	MG	XA	1625	1/1	0.12	-	32,32,32,32	0
57	MG	RA	3018	1/1	0.26	-	23,23,23,23	0
57	MG	YA	3004	1/1	0.28	-	11,11,11,11	0
57	MG	XA	1639	1/1	0.14	-	49,49,49,49	0
57	MG	RA	3025	1/1	0.20	-	18,18,18,18	0
57	MG	YA	3265	1/1	0.50	-	39,39,39,39	0
57	MG	XA	1644	1/1	0.20	-	54,54,54,54	0
57	MG	RA	3061	1/1	0.17	-	68,68,68,68	0
57	MG	YA	3045	1/1	0.29	-	20,20,20,20	0
57	MG	RA	3121	1/1	0.38	-	50,50,50,50	0
57	MG	RA	3159	1/1	0.10	-	38,38,38,38	0
57	MG	QA	1605	1/1	0.54	-	32,32,32,32	0
57	MG	RA	3117	1/1	0.16	-	35,35,35,35	0
57	MG	RA	3172	1/1	0.20	-	51,51,51,51	0
57	MG	YA	3049	1/1	0.41	-	30,30,30,30	0
57	MG	YA	3248	1/1	0.48	-	38,38,38,38	0
57	MG	XA	1658	1/1	0.36	-	51,51,51,51	0
57	MG	YA	3200	1/1	0.39	-	76,76,76,76	0
57	MG	YA	3023	1/1	0.27	-	21,21,21,21	0
57	MG	YA	3136	1/1	0.07	-	30,30,30,30	0
57	MG	RA	3170	1/1	0.34	-	46,46,46,46	0
57	MG	RA	3087	1/1	0.39	-	35,35,35,35	0
57	MG	RA	3031	1/1	0.31	-	35,35,35,35	0
57	MG	YA	3173	1/1	0.75	-	52,52,52,52	0
57	MG	YA	3126	1/1	0.32	-	38,38,38,38	0
57	MG	RA	3001	1/1	0.42	-	42,42,42,42	0
57	MG	YA	3011	1/1	0.42	-	27,27,27,27	0
57	MG	YA	3037	1/1	0.33	-	26,26,26,26	0
57	MG	YA	3010	1/1	0.23	-	17,17,17,17	0
57	MG	YA	3242	1/1	0.11	-	55,55,55,55	0
57	MG	YA	3257	1/1	0.22	-	12,12,12,12	0
57	MG	RA	3071	1/1	0.34	-	51,51,51,51	0
57	MG	RA	3182	1/1	0.19	-	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	QA	1660	1/1	0.35	-	59,59,59,59	0
57	MG	XA	1668	1/1	0.59	-	68,68,68,68	0
57	MG	RA	3114	1/1	0.24	-	31,31,31,31	0
57	MG	RA	3228	1/1	0.23	-	52,52,52,52	0
57	MG	YA	3215	1/1	0.47	-	66,66,66,66	0
57	MG	RA	3221	1/1	0.39	-	65,65,65,65	0
57	MG	XV	101	1/1	0.19	-	31,31,31,31	0
57	MG	QA	1657	1/1	0.33	-	55,55,55,55	0
57	MG	YA	3230	1/1	0.29	-	47,47,47,47	0
57	MG	QA	1642	1/1	0.19	-	55,55,55,55	0
57	MG	YA	3268	1/1	0.56	-	72,72,72,72	0
57	MG	RA	3056	1/1	0.36	-	28,28,28,28	0
57	MG	YA	3188	1/1	0.12	-	47,47,47,47	0
57	MG	YA	3259	1/1	0.46	-	28,28,28,28	0
57	MG	YA	3208	1/1	0.16	-	39,39,39,39	0
57	MG	QA	1613	1/1	0.42	-	39,39,39,39	0
57	MG	RA	3147	1/1	0.26	-	45,45,45,45	0
57	MG	YA	3267	1/1	0.34	-	40,40,40,40	0
57	MG	XA	1638	1/1	0.19	-	50,50,50,50	0
57	MG	YA	3239	1/1	0.51	-	74,74,74,74	0
57	MG	YA	3074	1/1	0.34	-	35,35,35,35	0
57	MG	RA	3173	1/1	0.08	-	47,47,47,47	0
57	MG	YA	3243	1/1	0.22	-	46,46,46,46	0
57	MG	RA	3100	1/1	0.21	-	26,26,26,26	0
57	MG	RA	3234	1/1	0.48	-	44,44,44,44	0
57	MG	RA	3034	1/1	0.50	-	29,29,29,29	0
57	MG	XA	1642	1/1	0.32	-	41,41,41,41	0
57	MG	YA	3196	1/1	0.26	-	45,45,45,45	0
57	MG	YA	3140	1/1	0.30	-	81,81,81,81	0
57	MG	YA	3184	1/1	0.29	-	67,67,67,67	0
59	ZN	XN	101	1/1	0.22	-	97,97,97,97	0
57	MG	RA	3148	1/1	0.24	-	52,52,52,52	0
57	MG	RA	3033	1/1	0.39	-	34,34,34,34	0
57	MG	RA	3195	1/1	0.19	-	48,48,48,48	0
57	MG	RP	201	1/1	0.41	-	41,41,41,41	0
57	MG	QA	1665	1/1	0.18	-	50,50,50,50	0
57	MG	RP	202	1/1	0.20	-	157,157,157,157	0
57	MG	RA	3128	1/1	0.11	-	39,39,39,39	0
57	MG	RA	3224	1/1	0.22	-	59,59,59,59	0
57	MG	RA	3067	1/1	0.27	-	44,44,44,44	0
57	MG	RA	3102	1/1	0.14	-	34,34,34,34	0
57	MG	YA	3025	1/1	0.20	-	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	3115	1/1	0.16	-	25,25,25,25	0
57	MG	XA	1655	1/1	0.23	-	44,44,44,44	0
57	MG	QA	1607	1/1	0.09	-	61,61,61,61	0
57	MG	YA	3138	1/1	0.25	-	33,33,33,33	0
57	MG	YA	3094	1/1	0.28	-	27,27,27,27	0
57	MG	YA	3214	1/1	0.18	-	49,49,49,49	0
57	MG	YA	3195	1/1	0.21	-	32,32,32,32	0

6.5 Other polymers ⓘ

There are no such residues in this entry.