



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 03:45 AM EDT

PDB ID : 6NDK / pdb_00006ndk
Title : Structure of ASLSufA6 A37.5 bound to the 70S A site
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Deposited on : 2018-12-13
Resolution : 3.64 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

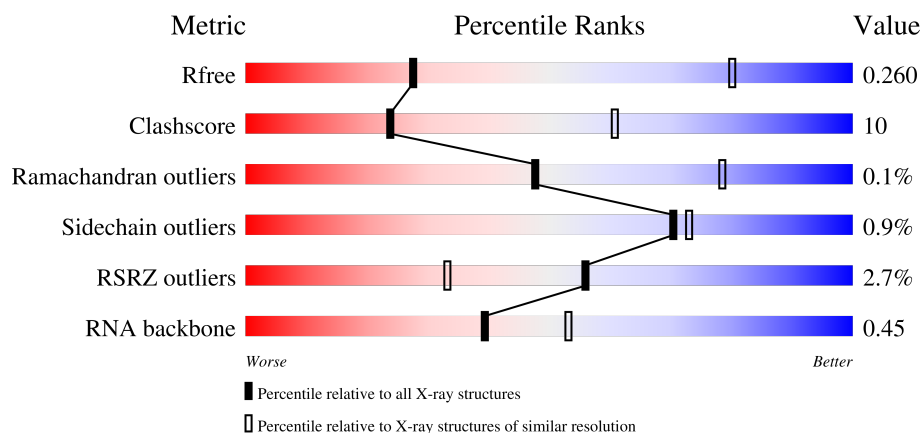
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.64 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}	180053	1132 (3.76-3.52)
Clashscore	190562	1014 (3.74-3.54)
Ramachandran outliers	187476	1123 (3.76-3.52)
Sidechain outliers	187428	1121 (3.76-3.52)
RSRZ outliers	180081	1130 (3.76-3.52)
RNA backbone	3983	1026 (4.22-3.06)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	QA	1521	42% 47% 10%
1	XA	1521	46% 44% 9%
2	QB	256	4% 57% 32% 8%
2	XB	256	4% 61% 29% 8%

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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
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	

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Mol	Chain	Length	Quality of chain
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	26	
23	XX	26	
24	QY	18	
24	XY	18	
25	RA	2915	
25	YA	2915	
26	RB	122	
26	YB	122	
27	RD	276	
27	YD	276	

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Mol	Chain	Length	Quality of chain
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	

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Mol	Chain	Length	Quality of chain
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	
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	

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Mol	Chain	Length	Quality of chain
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	
56	ZA	3	
56	ZB	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	QN	101	-	-	X	-
57	MG	RA	3098	-	-	-	X
57	MG	RA	3234	-	-	-	X
57	MG	RB	203	-	-	X	-
57	MG	RD	303	-	-	X	-
57	MG	RN	202	-	-	-	X
57	MG	RP	202	-	-	-	X
57	MG	YA	3516	-	-	-	X
57	MG	YA	3536	-	-	-	X
58	SF4	QD	303	-	-	X	-
58	SF4	XD	302	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291822 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			32246	14358	5975	10413	1500			
1	XA	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	235	Total	C	N	O	S	0	0	0
			1907	1217	342	343	5			
2	XB	236	Total	C	N	O	S	0	0	0
			1915	1223	343	344	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	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			
5	XE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	QF	100	Total	C	N	O	S	0	0	0
			837	528	154	152	3			
6	XF	100	Total	C	N	O	S	0	0	0
			837	528	154	152	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	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			
8	XH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			

- 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	126	Total	C	N	O		0	0	0
			998	633	193	172				

- 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	96	Total	C	N	O	S	0	0	0
			777	487	153	136	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	114	Total	C	N	O	S	0	0	0
			844	525	158	158	3			
11	XK	114	Total	C	N	O	S	0	0	0
			844	525	158	158	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	QL	122	Total	C	N	O	S	0	0	0
			958	604	193	159	2			
12	XL	122	Total	C	N	O	S	0	0	0
			958	604	193	159	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
13	XM	114	Total	C	N	O	S	0	0	0
			916	566	189	159	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	QP	82	Total	C	N	O	S	0	0	0
			691	438	138	114	1			
16	XP	82	Total	C	N	O	S	0	0	0
			691	438	138	114	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	QQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	XQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	68	Total	C	N	O	0	0	0
			555	355	108	92			
18	XR	68	Total	C	N	O	0	0	0
			555	355	108	92			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	XS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	96	Total	C	N	O	S	0	0	0
			743	458	159	124	2			
20	XT	98	Total	C	N	O	S	0	0	0
			759	469	162	126	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	QU	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	XU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- 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 mRNA.

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	11	Total	C	N	O	P	0	0	0
			233	105	43	74	11			

- Molecule 24 is a RNA chain called A-site ASLSufA6 A37.5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	14	Total	C	N	O	P	0	0	0
			301	134	55	98	14			
24	XY	16	Total	C	N	O	P	0	0	0
			341	153	63	110	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	RA	2870	Total	C	N	O	P	0	0	0
			61819	27519	11565	19867	2868			
25	YA	2870	Total	C	N	O	P	0	0	0
			61822	27520	11565	19869	2868			

- 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
			2572	1145	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	275	Total	C	N	O	S	0	0	0
			2144	1353	428	360	3			
27	YD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	RE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
28	YE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	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	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
31	YH	173	Total	C	N	O	S	0	0	0
			1330	845	250	234	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	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
33	YN	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	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	149	Total	C	N	O	S	0	0	0
			1139	709	231	196	3			
35	YP	149	Total	C	N	O	S	0	0	0
			1139	709	231	196	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	110	Total	C	N	O	S	0	0	0
			877	553	175	149				
38	YS	110	Total	C	N	O	S	0	0	0
			877	553	175	149				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
39	YT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
40	YU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	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	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	YW	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	RX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
43	YX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	RY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			
44	YY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RZ	196	Total	C	N	O	S	0	0	0
			1552	988	273	288	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	77	Total	C	N	O	S	0	0	0
			611	378	129	103	1			
46	Y0	77	Total	C	N	O	S	0	0	0
			611	378	129	103	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	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			
48	Y2	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

- 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
			468	298	90	80			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	R4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			
50	Y4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	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	58	Total	C	N	O	S	0	0	0
			451	283	89	74	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
52	Y6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	R7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
53	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	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	ZA	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
56	ZB	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	124	Total	Mg	0	0
			124	124		
57	QC	1	Total	Mg	0	0
			1	1		
57	QD	2	Total	Mg	0	0
			2	2		
57	QE	2	Total	Mg	0	0
			2	2		
57	QL	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QM	2	Total 2	Mg 2	0	0
57	QN	2	Total 2	Mg 2	0	0
57	QO	1	Total 1	Mg 1	0	0
57	QV	3	Total 3	Mg 3	0	0
57	RA	414	Total 414	Mg 414	0	0
57	RB	8	Total 8	Mg 8	0	0
57	RD	5	Total 5	Mg 5	0	0
57	RE	5	Total 5	Mg 5	0	0
57	RF	5	Total 5	Mg 5	0	0
57	RN	2	Total 2	Mg 2	0	0
57	RO	1	Total 1	Mg 1	0	0
57	RP	2	Total 2	Mg 2	0	0
57	RQ	1	Total 1	Mg 1	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RV	1	Total 1	Mg 1	0	0
57	RW	1	Total 1	Mg 1	0	0
57	RX	1	Total 1	Mg 1	0	0
57	RZ	1	Total 1	Mg 1	0	0
57	R0	2	Total 2	Mg 2	0	0
57	R1	1	Total 1	Mg 1	0	0
57	R3	1	Total 1	Mg 1	0	0

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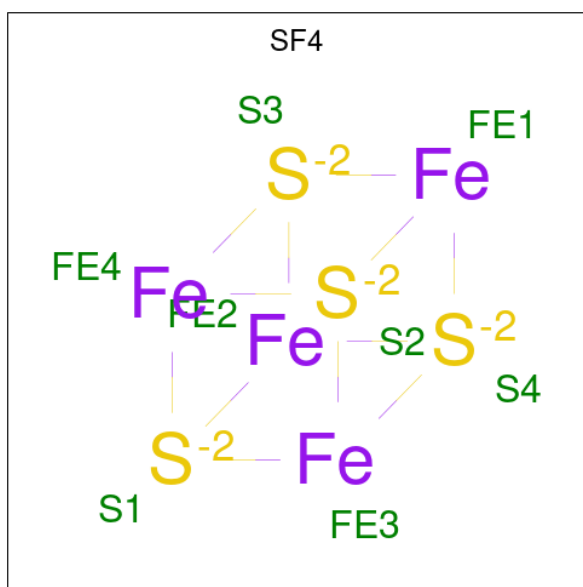
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	R5	1	Total 1	Mg 1	0	0
57	R6	1	Total 1	Mg 1	0	0
57	R7	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	R9	1	Total 1	Mg 1	0	0
57	XA	128	Total 128	Mg 128	0	0
57	XD	1	Total 1	Mg 1	0	0
57	XJ	1	Total 1	Mg 1	0	0
57	XK	2	Total 2	Mg 2	0	0
57	XN	1	Total 1	Mg 1	0	0
57	XV	1	Total 1	Mg 1	0	0
57	XX	1	Total 1	Mg 1	0	0
57	YA	544	Total 544	Mg 544	0	0
57	YB	8	Total 8	Mg 8	0	0
57	YD	8	Total 8	Mg 8	0	0
57	YE	7	Total 7	Mg 7	0	0
57	YF	1	Total 1	Mg 1	0	0
57	YG	1	Total 1	Mg 1	0	0
57	YP	3	Total 3	Mg 3	0	0
57	YQ	2	Total 2	Mg 2	0	0
57	YR	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YT	1	Total 1	Mg 1	0	0
57	YU	1	Total 1	Mg 1	0	0
57	YV	1	Total 1	Mg 1	0	0
57	YW	1	Total 1	Mg 1	0	0
57	YX	1	Total 1	Mg 1	0	0
57	Y0	1	Total 1	Mg 1	0	0
57	Y1	3	Total 3	Mg 3	0	0
57	Y3	1	Total 1	Mg 1	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	Y6	1	Total 1	Mg 1	0	0
57	Y7	1	Total 1	Mg 1	0	0
57	Y8	1	Total 1	Mg 1	0	0
57	Y9	1	Total 1	Mg 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	QD	1	Total	Fe	S	0	0
			8	4	4		
58	XD	1	Total	Fe	S	0	0
			8	4	4		

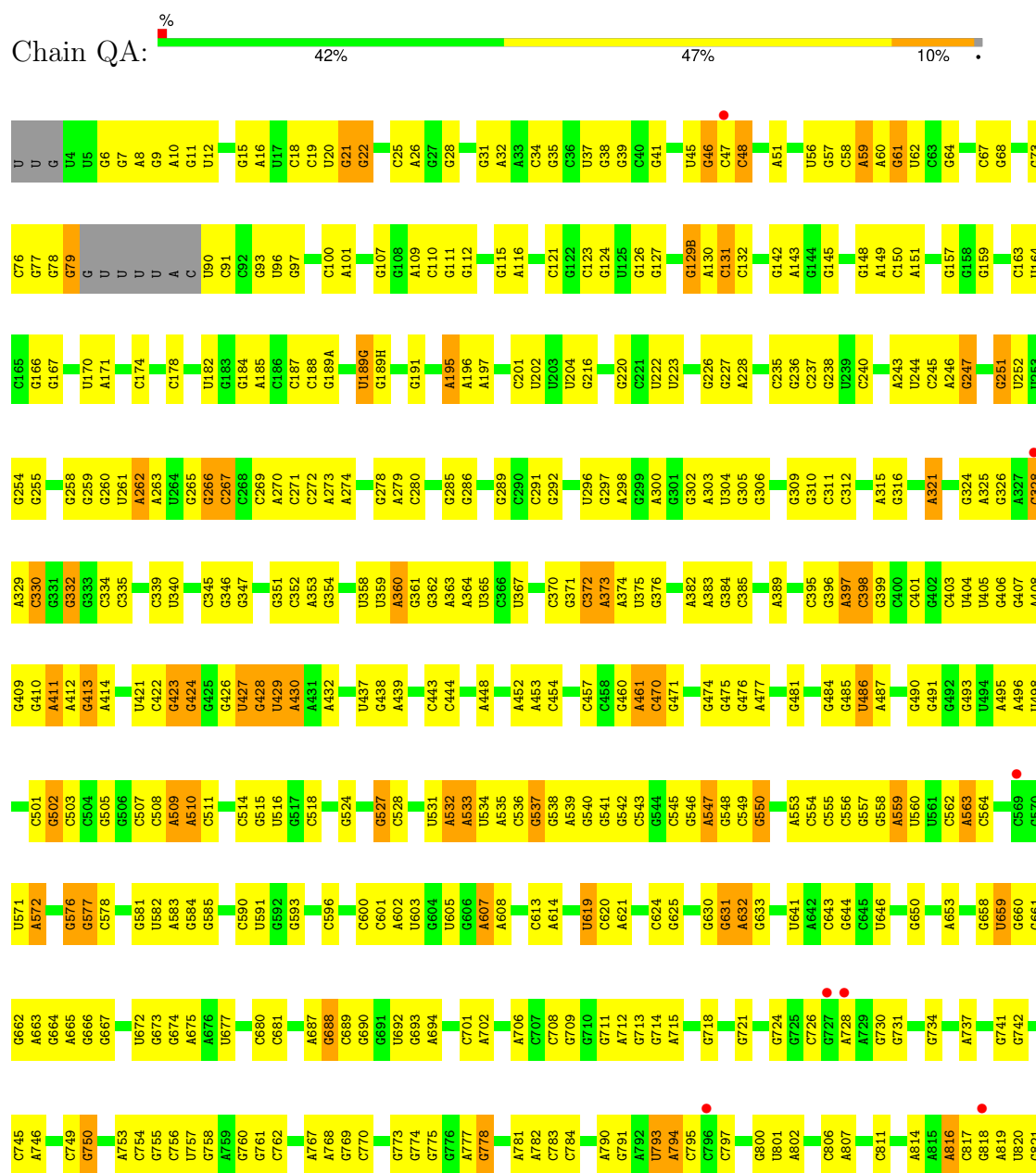
- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	QN	1	Total	Zn	0	0
			1	1		
59	R4	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		
59	Y4	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

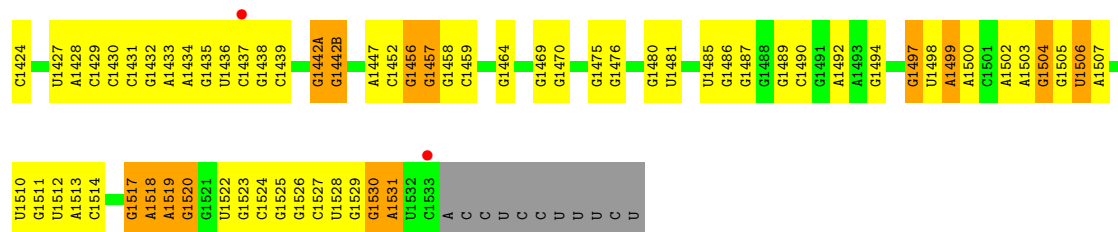
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S rRNA

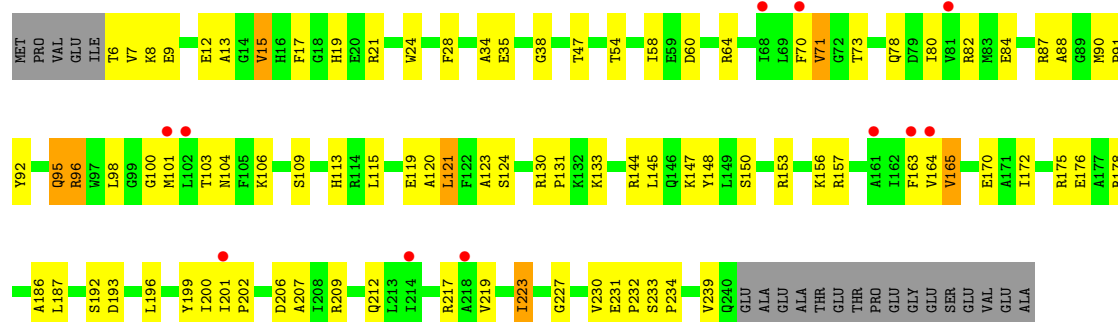




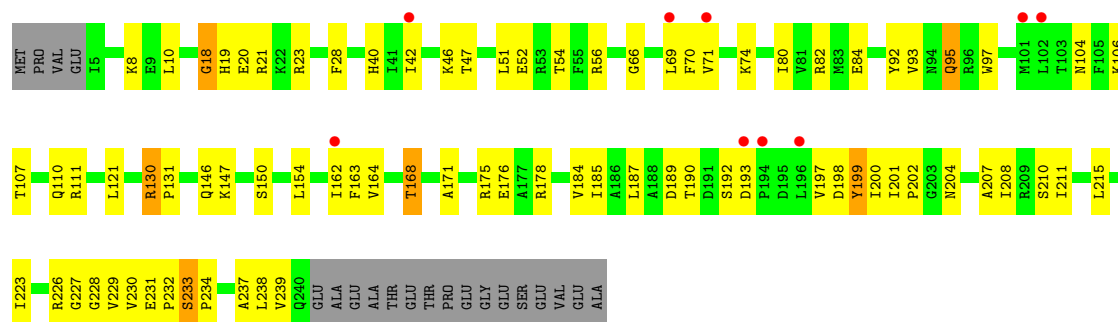
U1348	U1275	C1203	C1114	G1036	U955	G961	C770	G683	U582	C506	A412	C345	G266
C1352	U1278	A1204	C1115	G1039	U960	A864	G773	A684	A583	A509	G412	G346	C267
G1353	A1279	G1207	C1117	C1039	U961	A865	G774	A687	G584	A510	G416	G347	C268
G1356	U1281	C1208	C1118	U1040	G966	C966	G775	G688	G585	C511	C417	A349	C269
A1357	C1282	G1209	C1119	C1043	G967	C968	G776	C689	C586	U512	U421	G350	C271
A1360	A1285	U1211	G1120	A1044	A968	G969	A777	A695	C601	C513	C422	G351	C272
C1363A	A1286	U1212	U1121	C1045	A969	U970	G778	A696	G593	C514	C423	C352	A273
A1363B	A1287	C1213	A1123	A1046	G971	U971	A781	A702	C602	U516	G424	G353	C276
U1364	A1288	G1215	G1124	G1047	C972	A872	G785	C707	A603	C517	G425	C355	A279
G1365	U1126	C1218	U1125	G1053	G973	A873	G786	G711	U608	C518	G426	A356	C280
G1366	G1290	U1219	G1127	C1054	A974	G874	G787	G712	A609	A520	U427	G357	G281
C1367	G1291	G1220	C1128	A1055	A975	G877	A790	A713	A610	G521	U429	U358	
G1368	U1292	G1221	C1129	G1058	A977	G878	G791	G714	G610	G524	A430	U359	G285
C1369	G1293	G1222	A1130	C1059	C980	C883	A792	G715	A611	C525	A431	G361	G286
G1370	G1294	C1223	U1136	C1060	U981	U884	U793	A716	C618	C526	C432	U367	A288
G1371	C1295	G1224	C1137	G1061	U982	U891	A794	G717	U619	G527	C433	U368	G289
U1372	C1297	A1227	G1138	U1062	C985	A892	G797	G718	A620	A532	U434	G371	C290
G1373	C1298	C1228	C1139	C1063	A986	A893	G798	G719	A621	A533	C435	C372	C291
A1374	A1299	G1229	C1140	C1064	C988	C993	C799	G720	G630	A534	C436	A373	G292
A1375	G1300	C1230	G1141	C1067	U991	U894	C799	A721	G631	U535	U437	A374	G293
U1380	U1301	G1231	G1142	G1068	G902	G903	A802	G722	G624	A536	A438	A375	G297
C1384	C1303	A1236	C1147	C1069	U992	A908	G803	G723	G625	A539	A448	G376	G301
G1385	G1304	C1237	U1148	C1070	A994	C909	U804	G725	G630	G540	G377	G377	G302
G1386	A1306	A1238	C1149	C1071	G1001B	A910	C805	A631	G631	C543	A452	G378	G303
G1387	U1307	G1239	U1150	C1072	G1002	C910	C806	A728	A632	C544	A453	G379	G304
U1390	U1308	U1240	A1151	C1073	G1003	U911	U813	A729	G635	G546	A461	G380	G310
U1391	G1309	G1241	C1152	C1075	U1004	C912	A814	G730	U636	C547	C470	A381	C311
G1392	G1312	C1244	U1159	U1078	A1005	A913	C817	G731	G637	A547	G471	A382	C312
A1396	C1314	A1245	G1160	G1079	C1006	U914	U819	G734	G639	U552	A472	A383	C313
C1397	U1315	G1246	C1161	A1080	G1010	U920	A819	G735	A640	C554	G473	A315	G316
A1398	G1316	U1247	G1164	G1081	G1011	U921	U820	C736	U641	C555	G474	C385	A321
C1399	C1317	A1248	U1165	U1085	A1014	A923	G821	A737	A642	C556	G475	U387	C322
C1400	A1318	C1249	A1170	U1086	A1015	C924	G822	C738	U646	C557	G476	G388	U323
C1401	A1319	A1251	G1178	U1092	A1016	G925	G823	C739	U646	G558	C477	A389	G324
C1402	C1320	G1255	A1179	A1093	U1017	G926	A828	U740	A653	A559	U480	C391	A325
C1403	G1323	A1256	C1183	G1094	U1020	G927	G829	G741	G661	U560	A481	G392	G326
C1404	A1324	U1257	G1184	U1095	G1021	A946	U835	C745	G662	U561	G482	A327	A327
U1405	C1325	G1258	G1185	C1096	G1022	G947	G836	A746	A663	C564	G485	C328	C328
C1407	C1326	C1259	G1186	C1097	G1023	C948	U837	C747	A664	U565	U486	A329	C329
A1408	C1260	A1261	G1187	C1098	G1024	C949	C840	C748	G665	U566	A487	G330	C330
C1409	U1261	C1262	G1190	C1100	U1025	A935	U841	G750	A666	C566	C488	G331	G331
G1410	C1263	U1263	A1191	A1101	G1026	A946	C848	G755	G673	A572	C489	C401	G332
C1412	C1264	C1192	C1192	A1102	C1028	G947	G851	C756	G674	A573	G490	G402	C334
A1413	G1265	U1196	G1197	G1103	C1029	C948	U854	U757	A675	U576	A495	C403	C335
U1414	A1269	G1197	G1197	G1104	C1030A	A949	G854	G761	A676	C577	A496	U405	C336
G1419	C1270	G1197	G1197	G1108	C1030C	U950	G855	C762	U677	C578	U498	A338	C337
C1422	G1271	C1200	A1201	C1112	G1031	U952	A859	G763	C680	U579	C501	G407	A339
G1423	G1347	G1202	G1202	C1113	G1032	U954	A860	A766		G581	G502	A408	C342
											G505	G410	A344



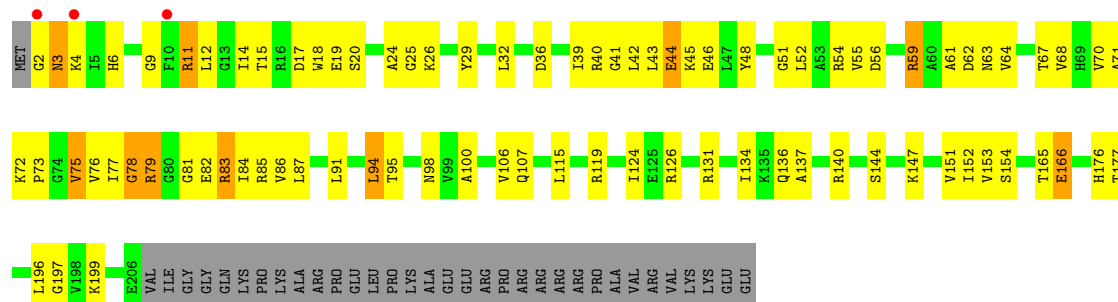
• Molecule 2: 30S ribosomal protein S2



• Molecule 2: 30S ribosomal protein S2

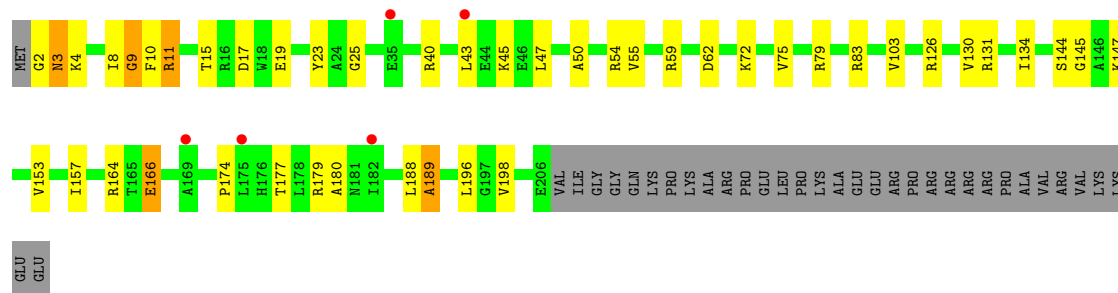


• Molecule 3: 30S ribosomal protein S3



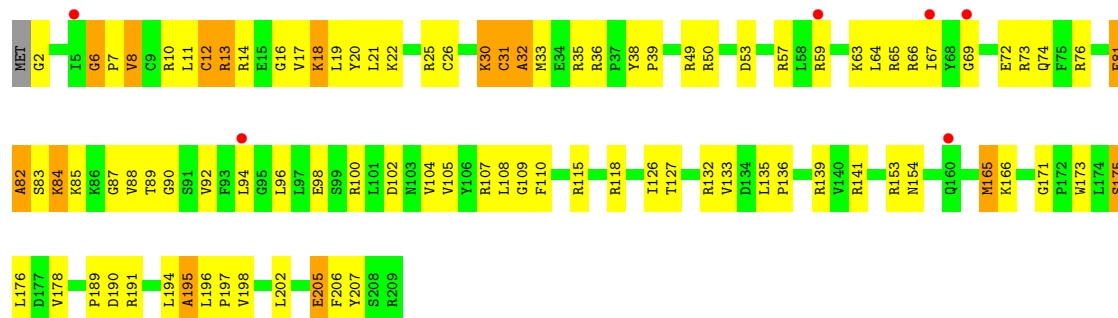
- Molecule 3: 30S ribosomal protein S3

Chain XC: 



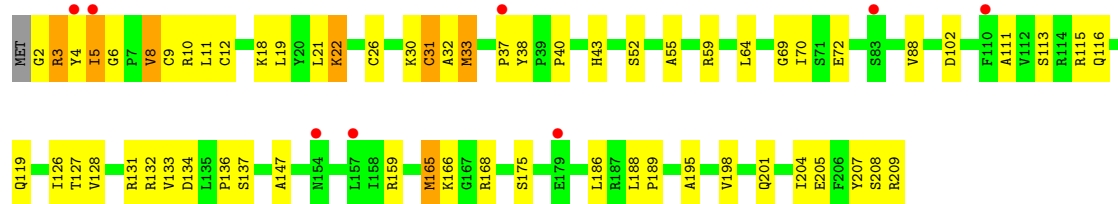
- Molecule 4: 30S ribosomal protein S4

Chain QD: 



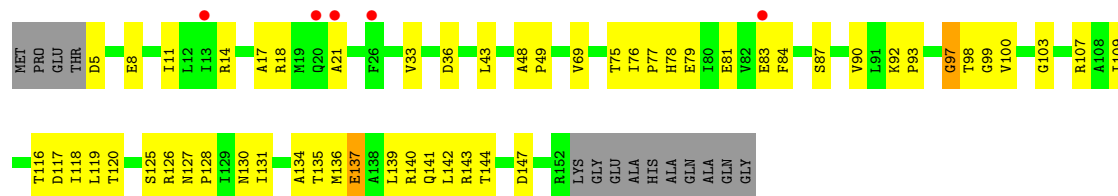
- Molecule 4: 30S ribosomal protein S4

Chain XD: 

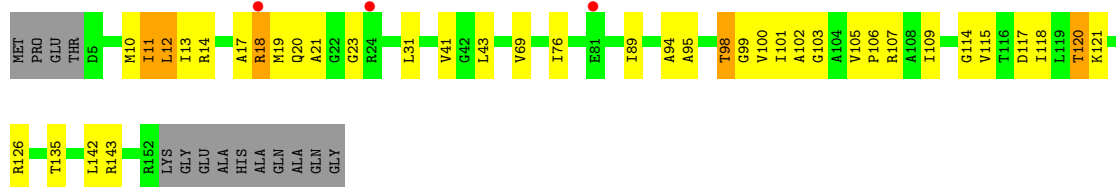


- Molecule 5: 30S ribosomal protein S5

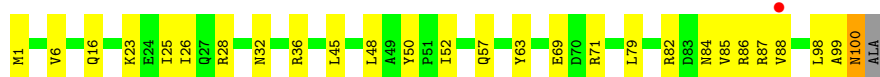
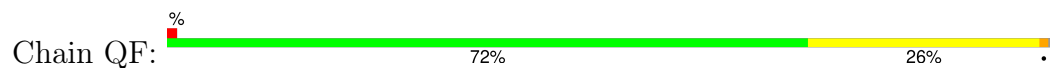
Chain QE: 



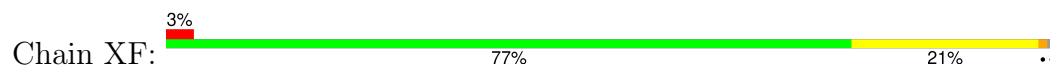
- Molecule 5: 30S ribosomal protein S5



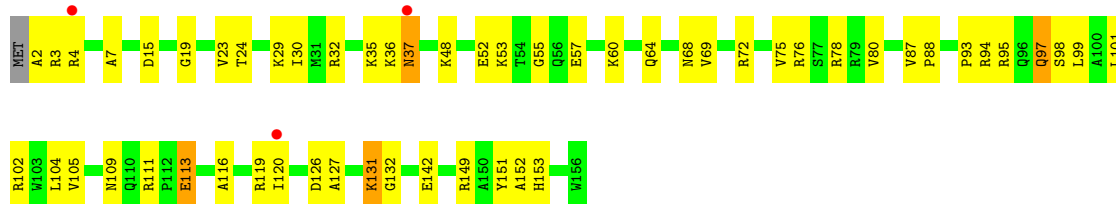
- Molecule 6: 30S ribosomal protein S6



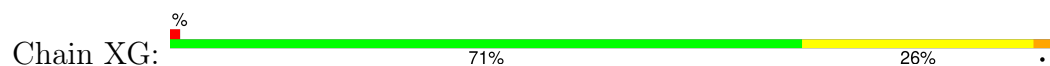
- Molecule 6: 30S ribosomal protein S6



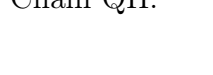
- Molecule 7: 30S ribosomal protein S7

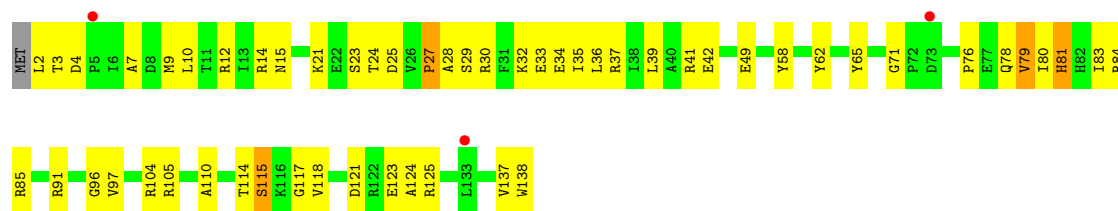


- Molecule 7: 30S ribosomal protein S7

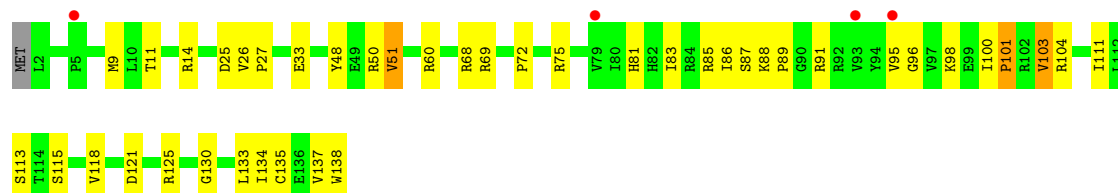


- Molecule 8: 30S ribosomal protein S8

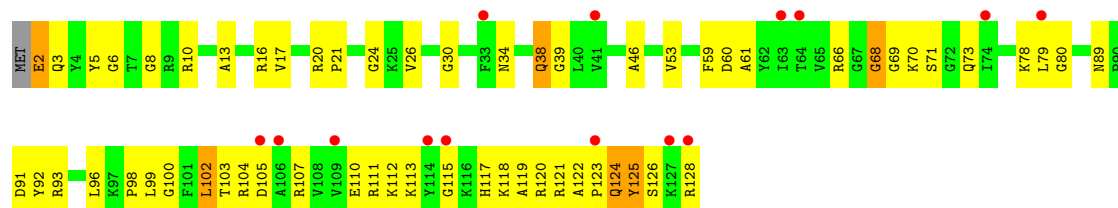




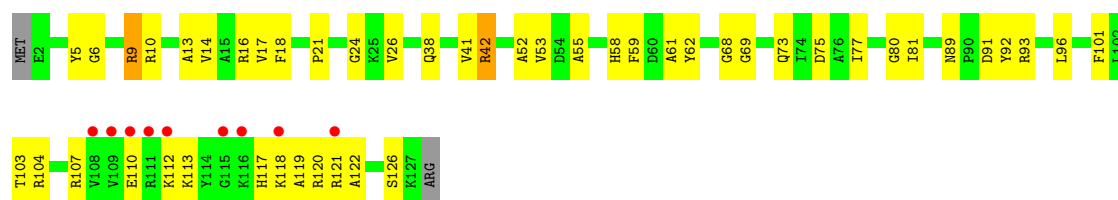
• Molecule 8: 30S ribosomal protein S8



• Molecule 9: 30S ribosomal protein S9



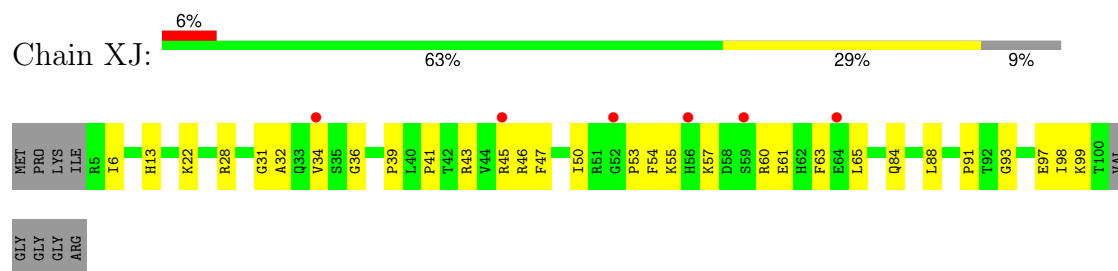
• Molecule 9: 30S ribosomal protein S9



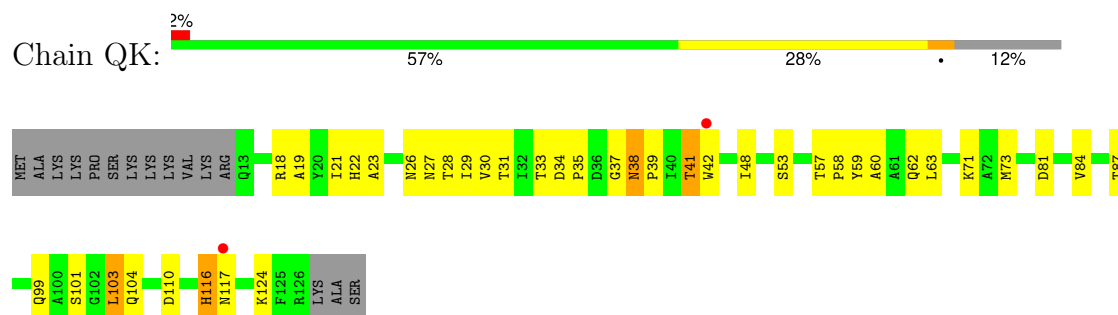
• Molecule 10: 30S ribosomal protein S10



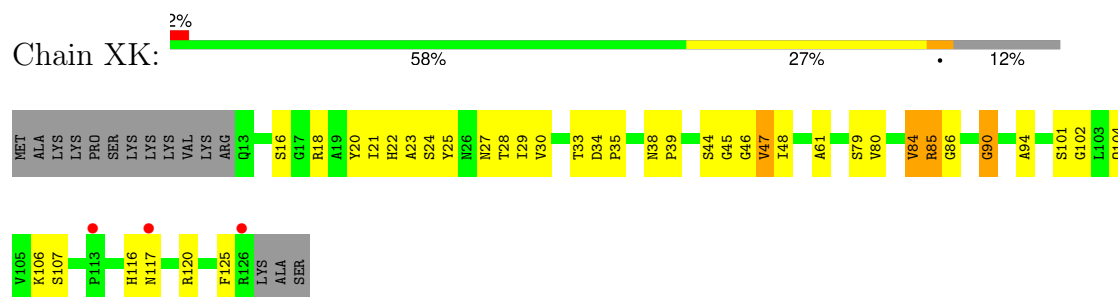
- Molecule 10: 30S ribosomal protein S10



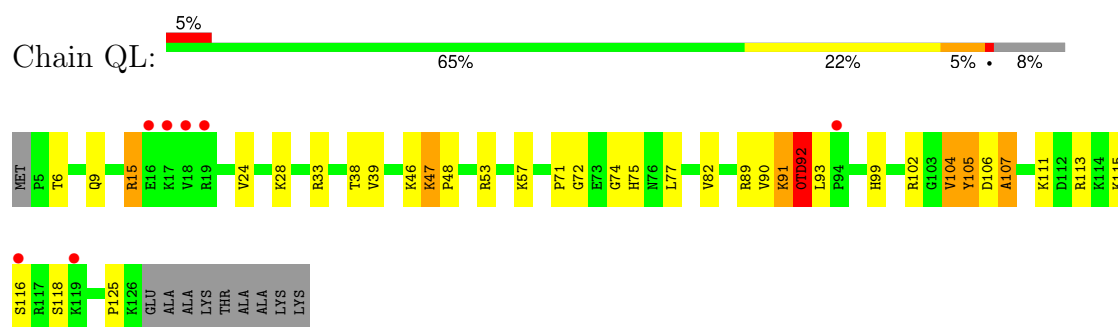
- Molecule 11: 30S ribosomal protein S11



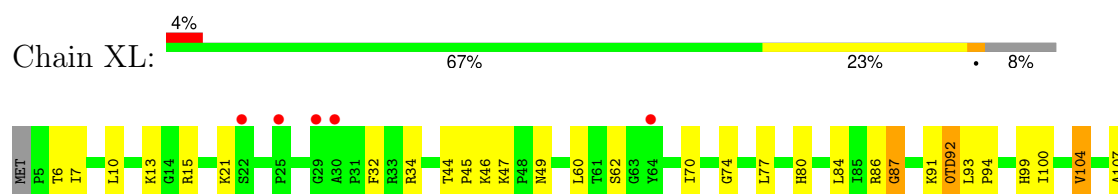
- Molecule 11: 30S ribosomal protein S11

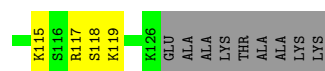


- Molecule 12: 30S ribosomal protein S12

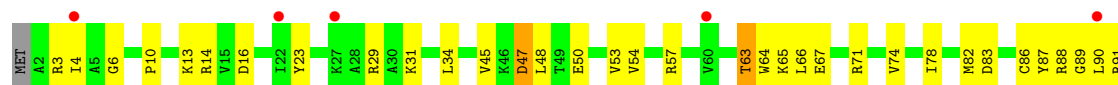


- Molecule 12: 30S ribosomal protein S12

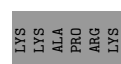




- Molecule 13: 30S ribosomal protein S13



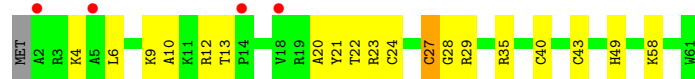
- Molecule 13: 30S ribosomal protein S13



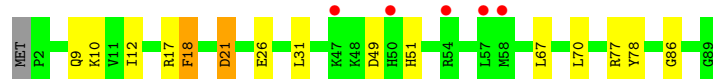
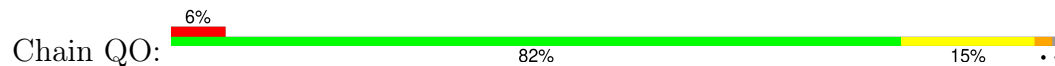
- Molecule 14: 30S ribosomal protein S14 type Z



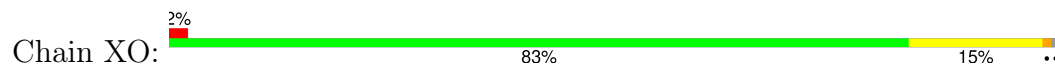
- Molecule 14: 30S ribosomal protein S14 type Z

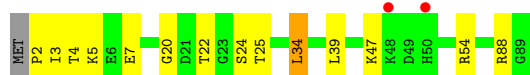


- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15

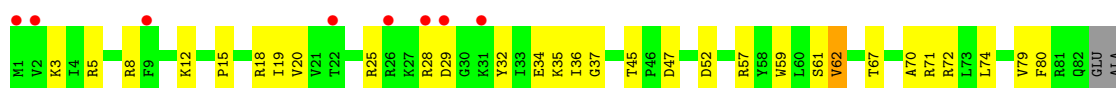




- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



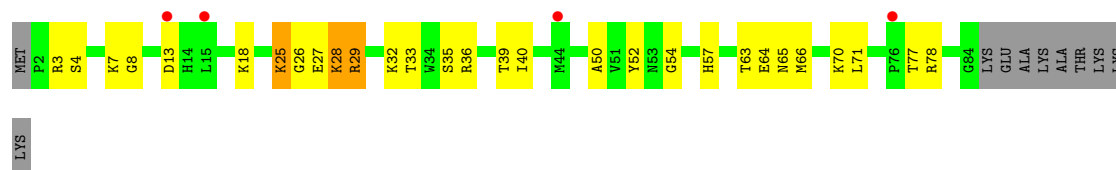
- Molecule 18: 30S ribosomal protein S18



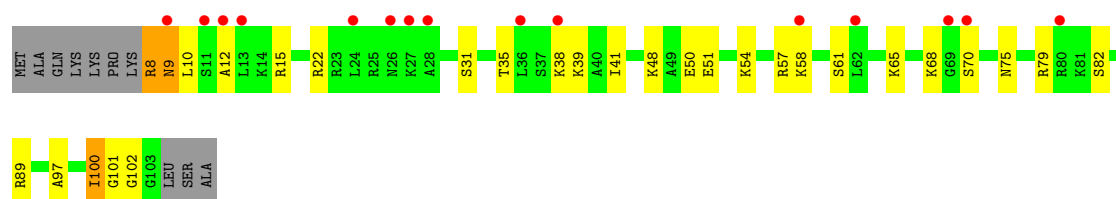
- Molecule 19: 30S ribosomal protein S19



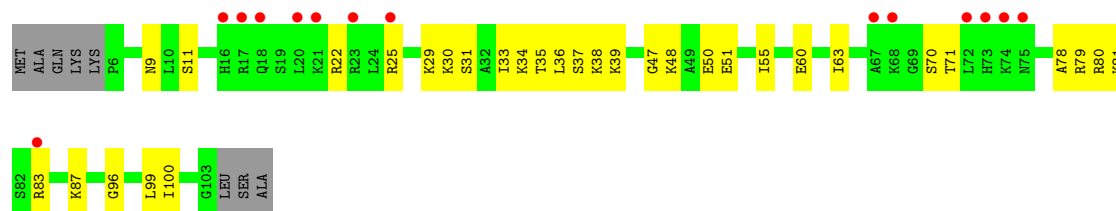
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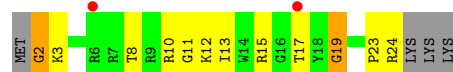
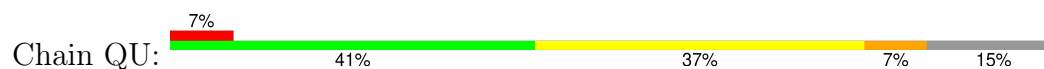
- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20



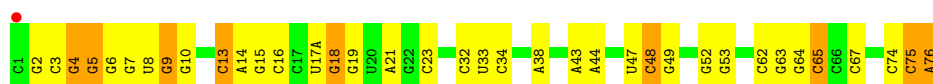
- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: P-site tRNAfMet



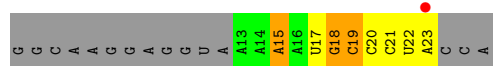
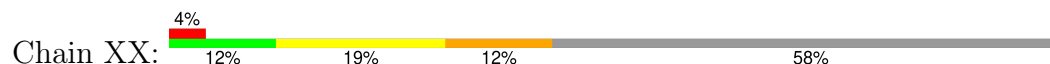
- Molecule 22: P-site tRNAfMet



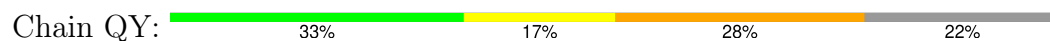
- Molecule 23: mRNA



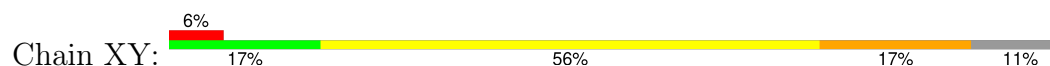
- Molecule 23: mRNA



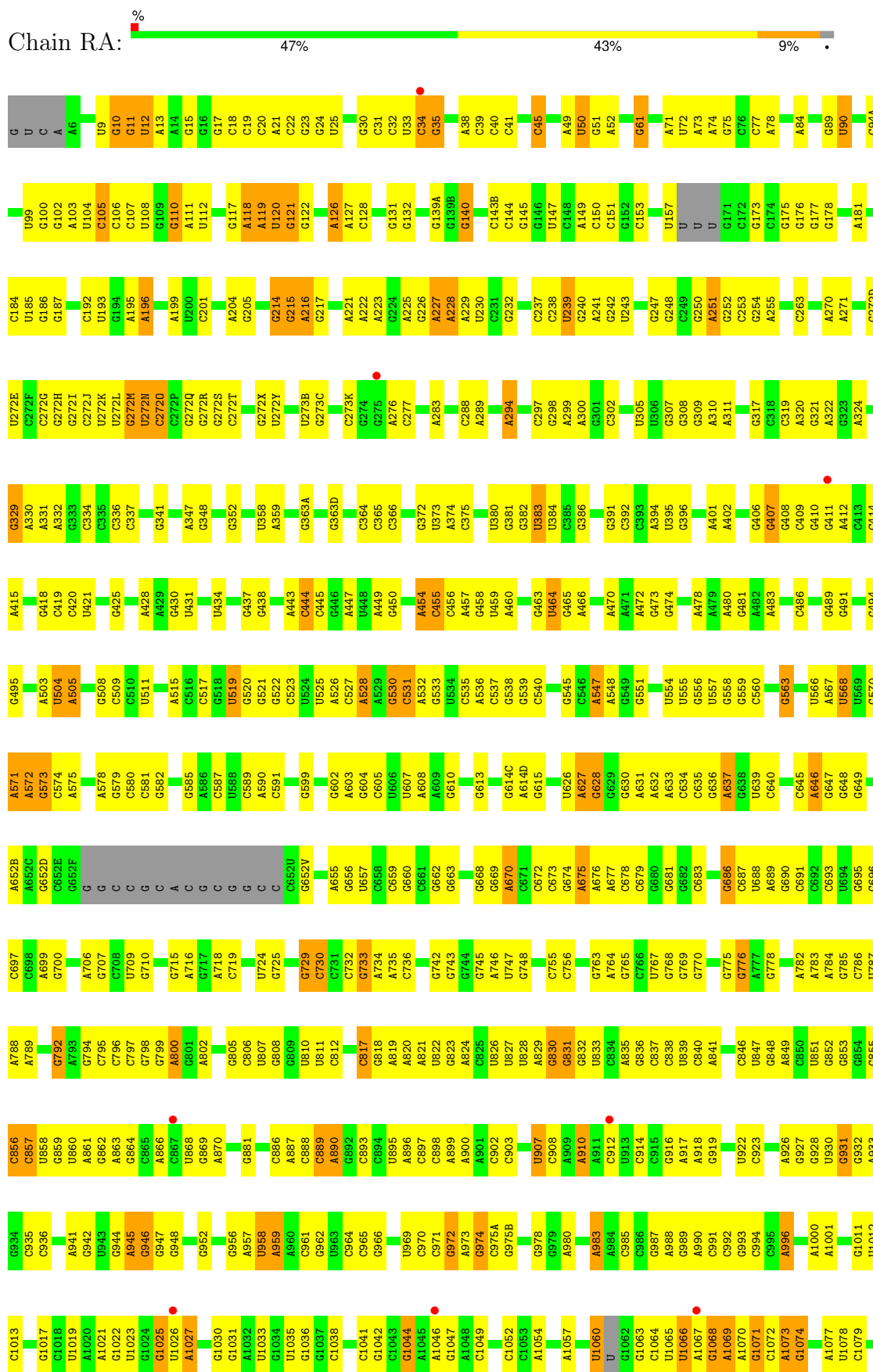
- Molecule 24: A-site ASLSufA6 A37.5



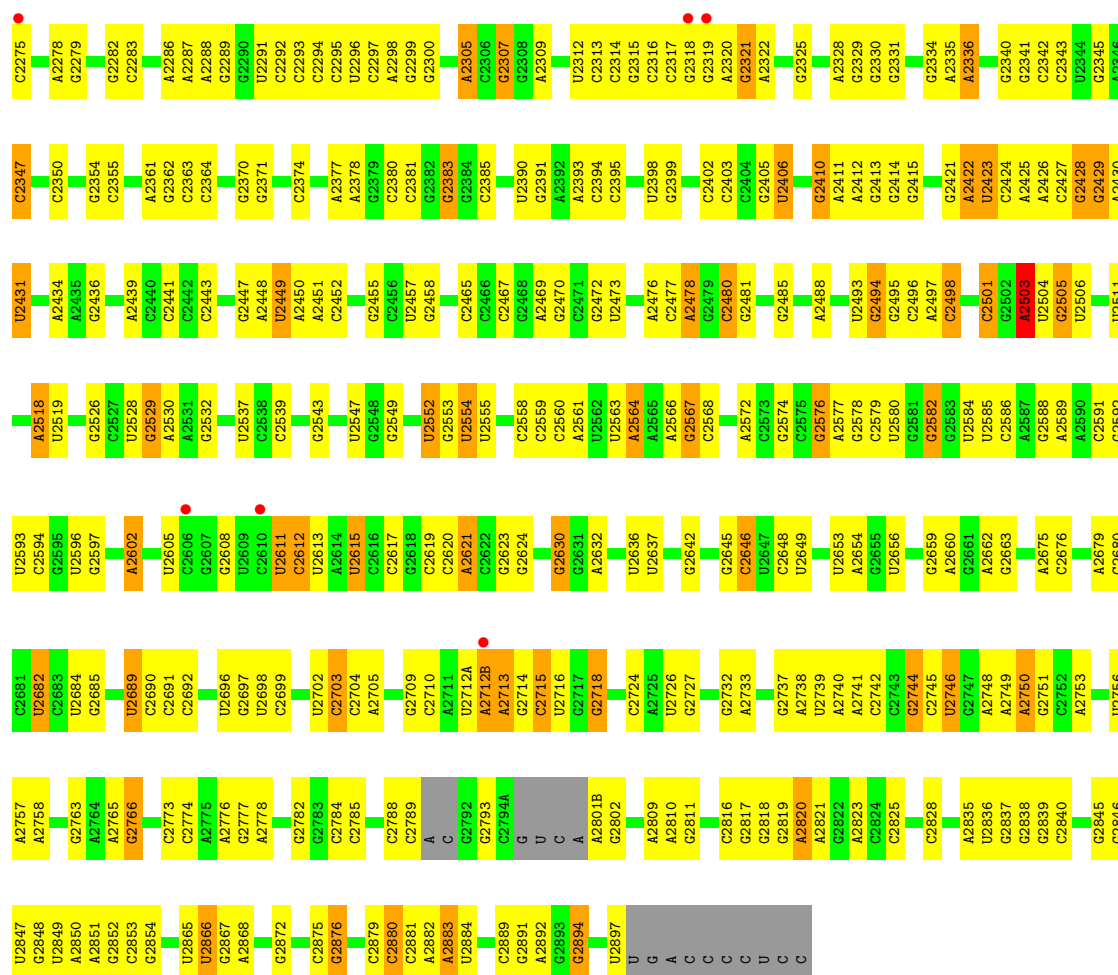
- Molecule 24: A-site ASLSufA6 A37.5



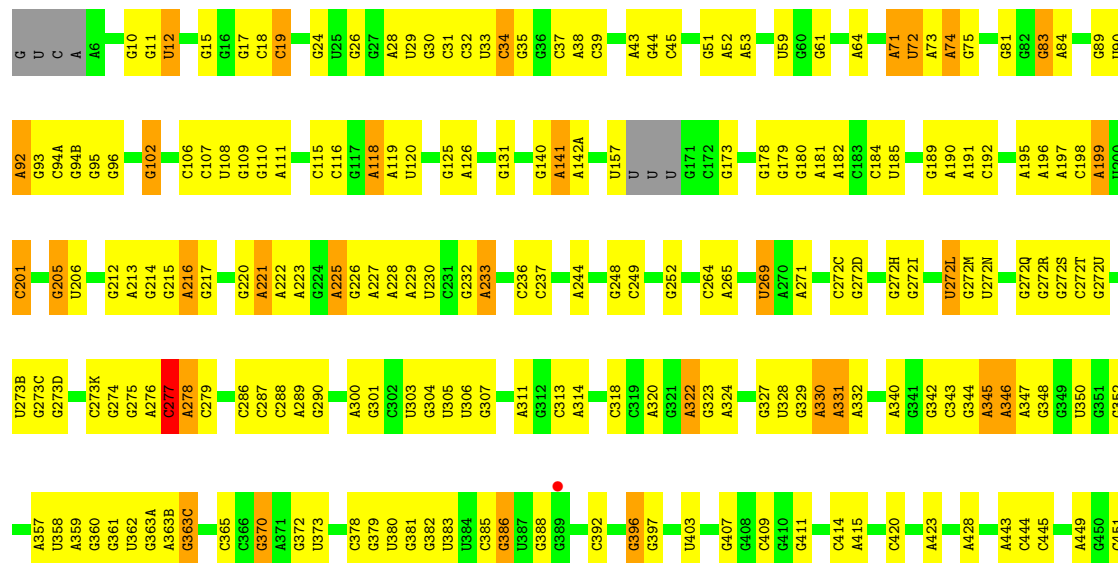
- Molecule 25: 23S rRNA



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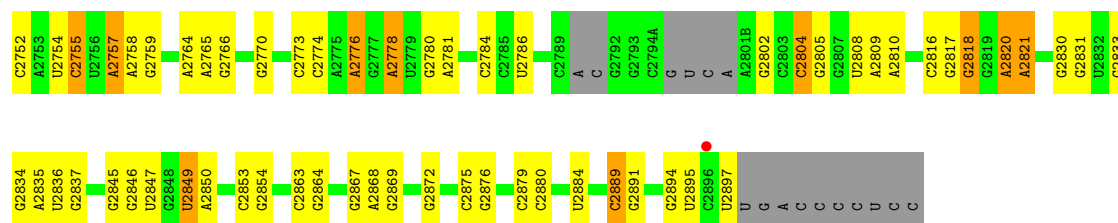


- Molecule 25: 23S rRNA



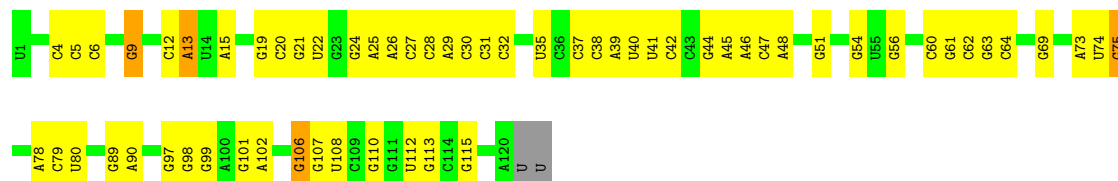
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C1546	G1443	C1354	G1271	C1195	C1117</																				

U2682	C2683	U2684	G2685	U2686	G2687	U2688	G2689	C2690	C2691	C2692	C2693	C2694	C2695	U2696	C2697	U2698	C2699	U2702	C2703	C2704	A2705	G2706	A2711	U2712A	A2712B	A2713	G2714	A2715	G2716	G2717	G2718	G2719	C2723	U2726	G2727	C2730	G2731	G2732	A2733	G2737	A2738	U2739	A2740	A2741	G2742	G2743	G2744	G2747	A2748	A2749	A2750	G2751																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
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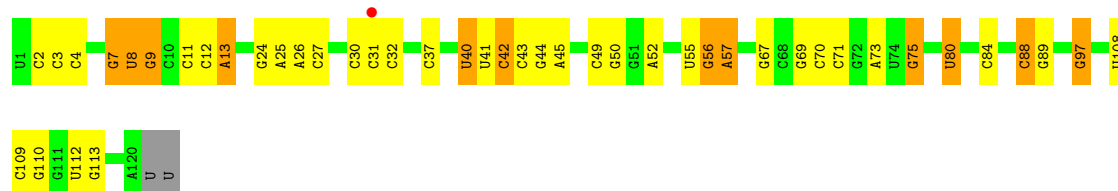
• Molecule 26: 5S rRNA

Chain RB: 48% 47%



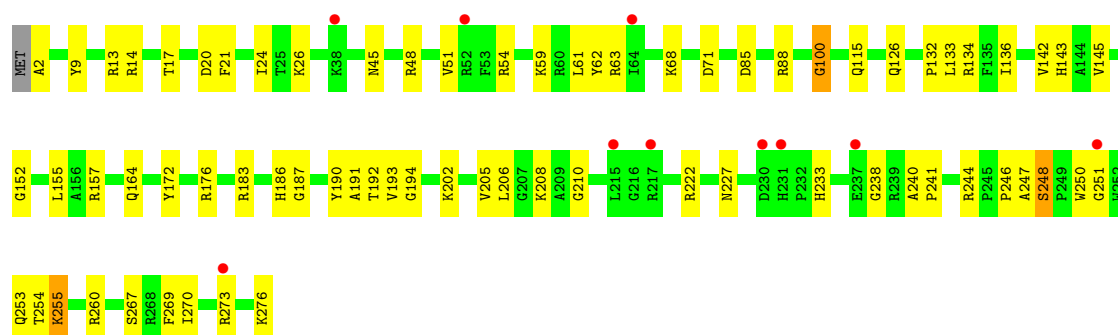
• Molecule 26: 5S rRNA

Chain YB: 61% 27% 10%



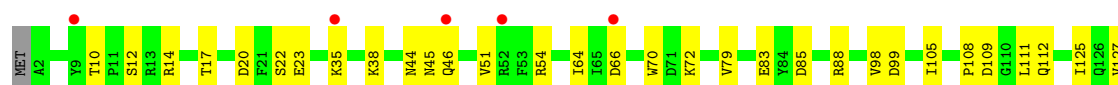
• Molecule 27: 50S ribosomal protein L2

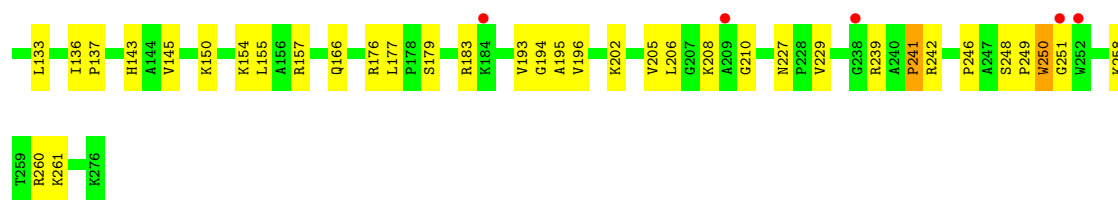
Chain RD: 4% 74% 25%



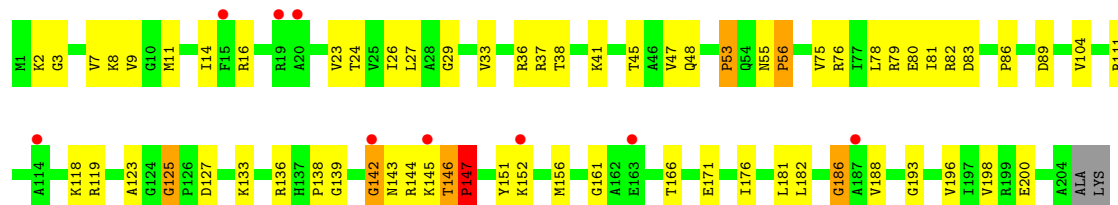
• Molecule 27: 50S ribosomal protein L2

Chain YD: 4% 75% 24%

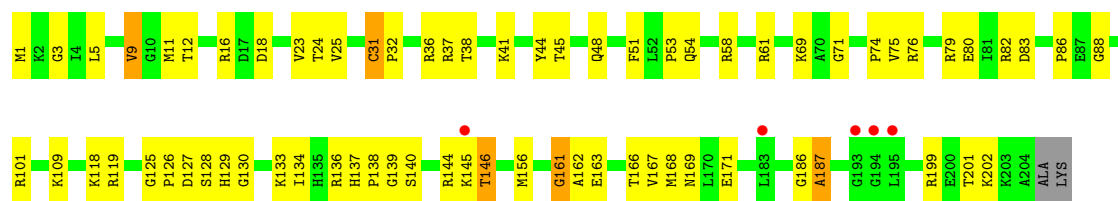




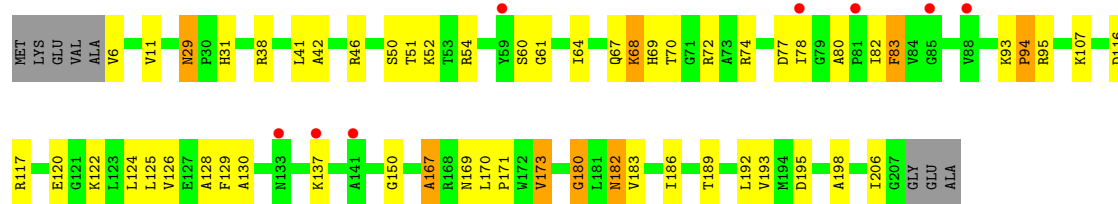
• Molecule 28: 50S ribosomal protein L3



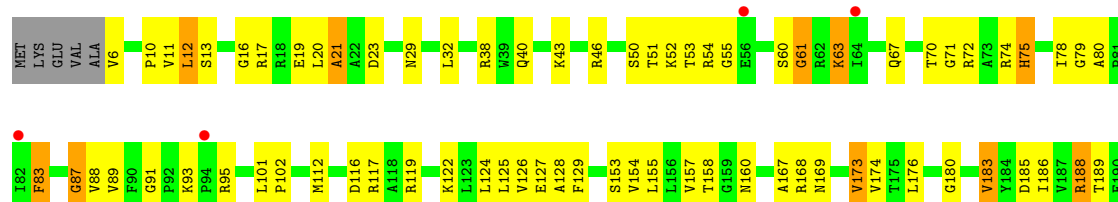
• Molecule 28: 50S ribosomal protein L3

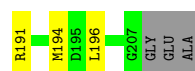


• Molecule 29: 50S ribosomal protein L4

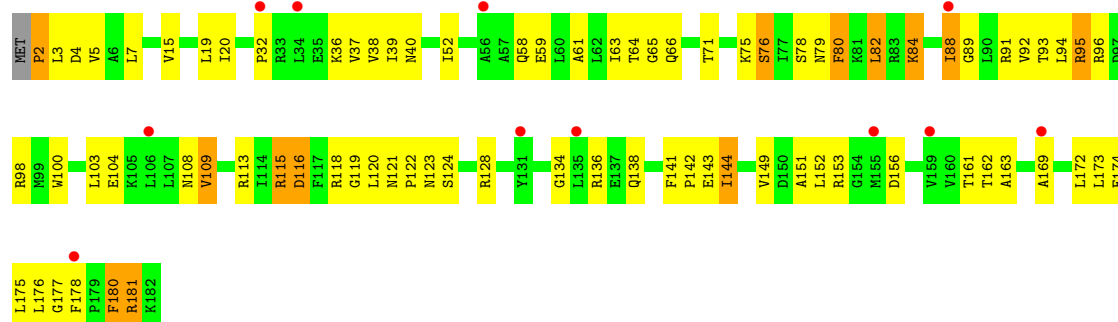


• Molecule 29: 50S ribosomal protein L4

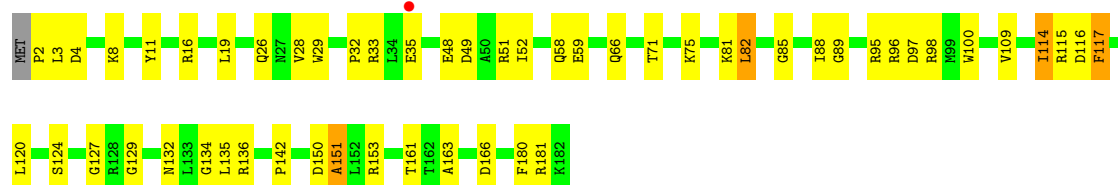
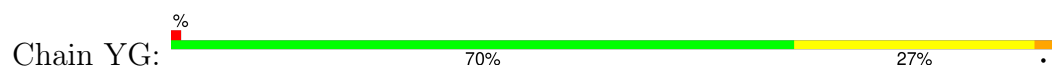




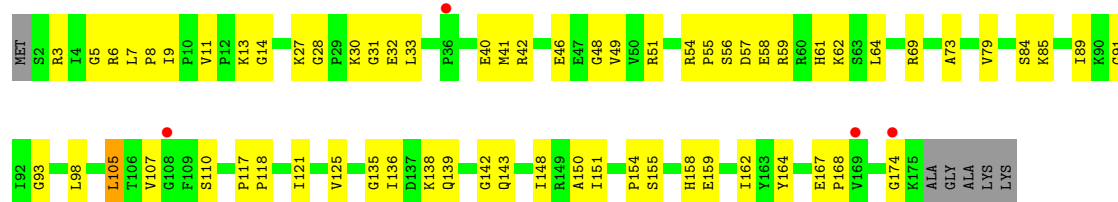
- Molecule 30: 50S ribosomal protein L5



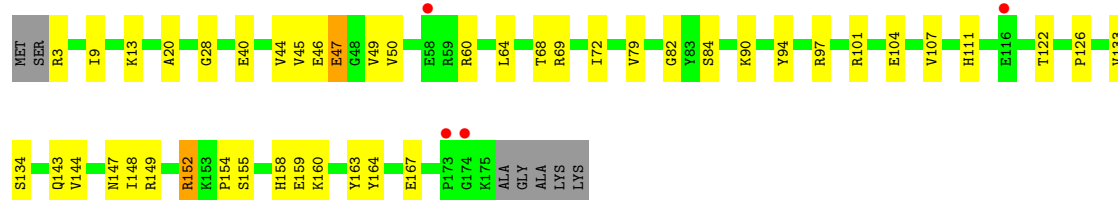
- Molecule 30: 50S ribosomal protein L5



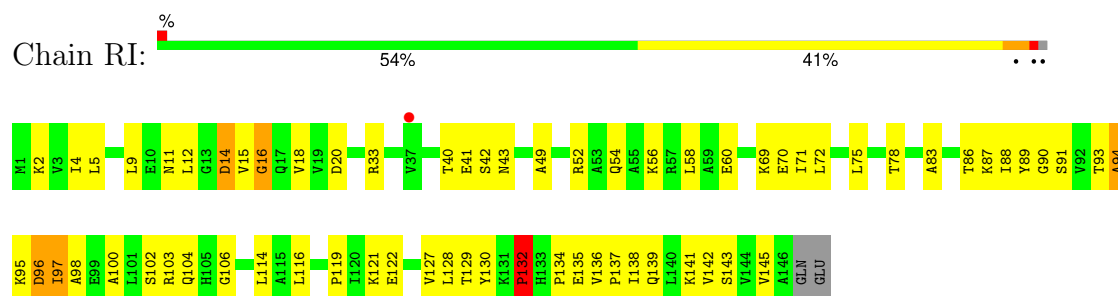
- Molecule 31: 50S ribosomal protein L6



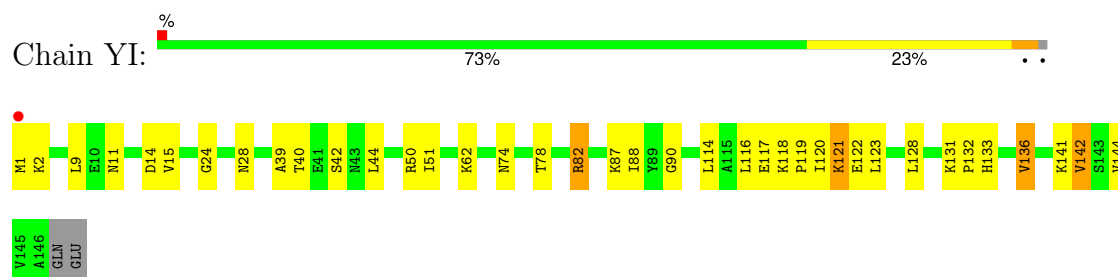
- Molecule 31: 50S ribosomal protein L6



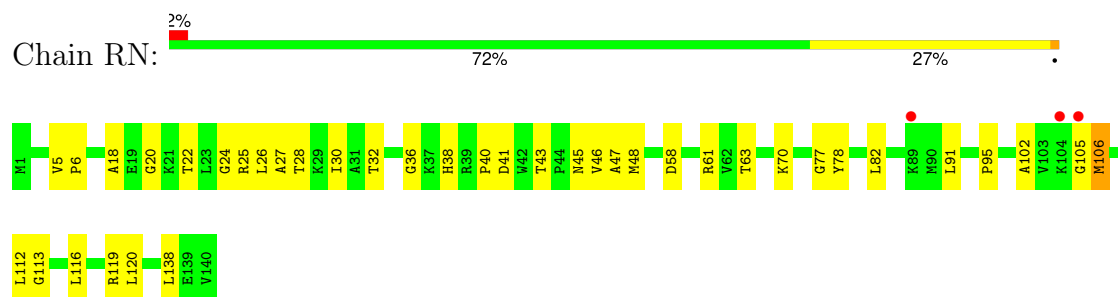
- Molecule 32: 50S ribosomal protein L9



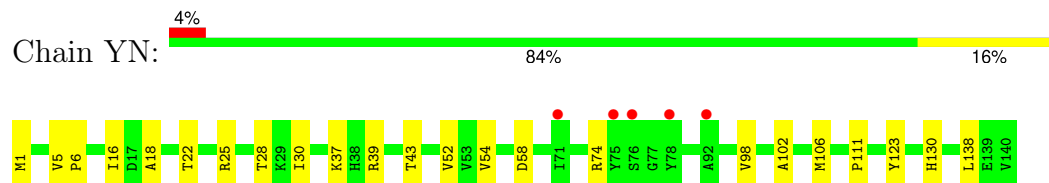
- Molecule 32: 50S ribosomal protein L9



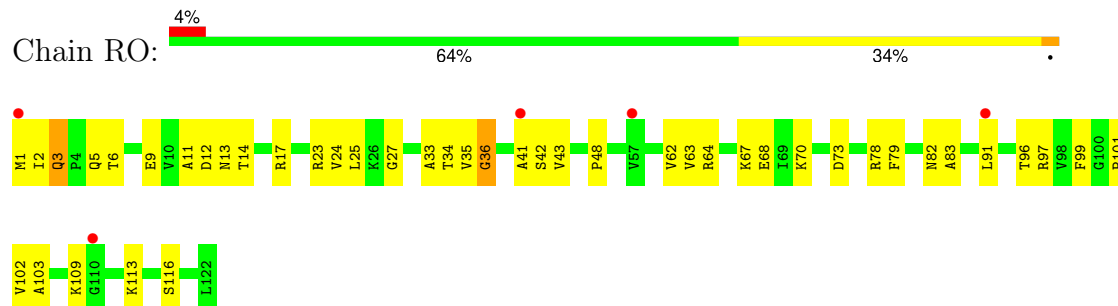
- Molecule 33: 50S ribosomal protein L13



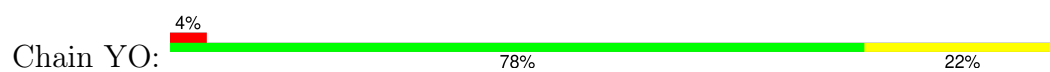
- Molecule 33: 50S ribosomal protein L13



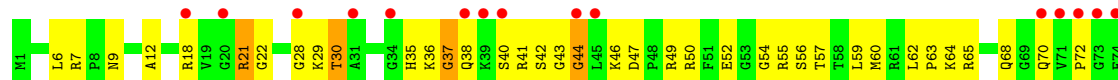
- Molecule 34: 50S ribosomal protein L14



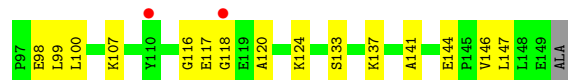
- Molecule 34: 50S ribosomal protein L14



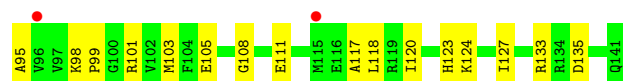
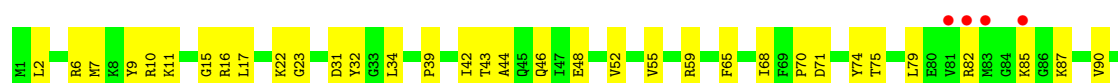
• Molecule 35: 50S ribosomal protein L15



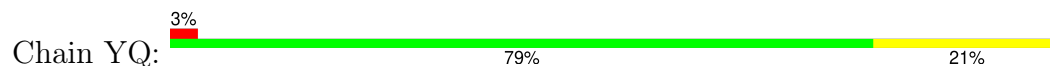
• Molecule 35: 50S ribosomal protein L15



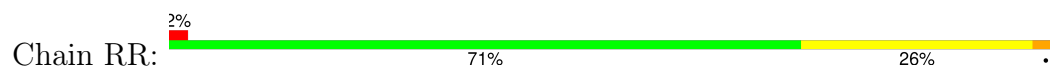
• Molecule 36: 50S ribosomal protein L16



• Molecule 36: 50S ribosomal protein L16

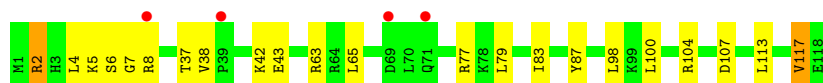
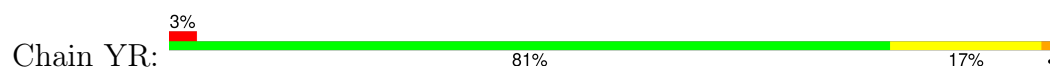


• Molecule 37: 50S ribosomal protein L17

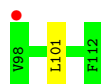




- Molecule 37: 50S ribosomal protein L17



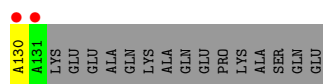
- Molecule 38: 50S ribosomal protein L18



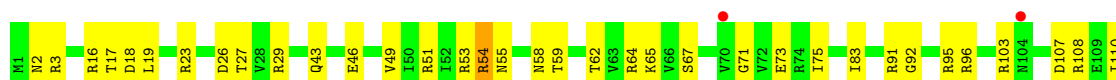
- Molecule 38: 50S ribosomal protein L18

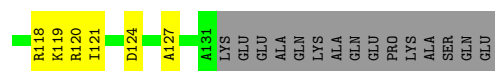


- Molecule 39: 50S ribosomal protein L19

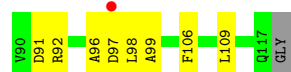
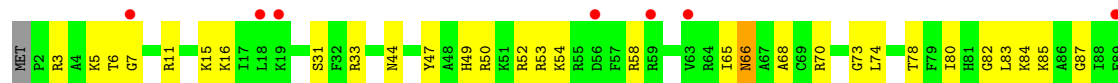


- Molecule 39: 50S ribosomal protein L19

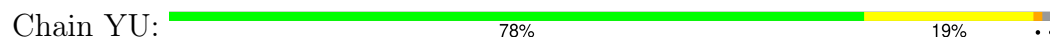




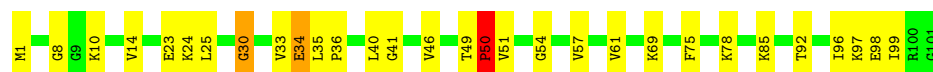
- Molecule 40: 50S ribosomal protein L20



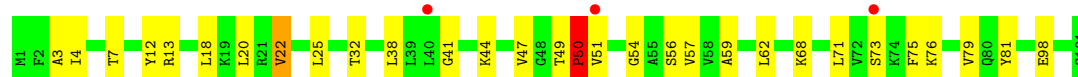
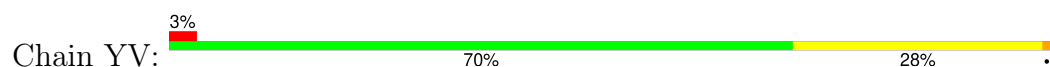
- Molecule 40: 50S ribosomal protein L20



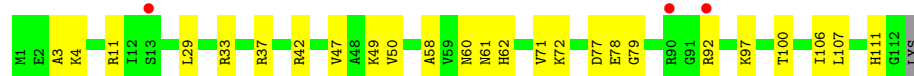
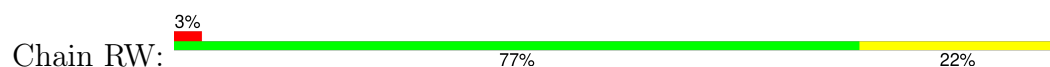
- Molecule 41: 50S ribosomal protein L21



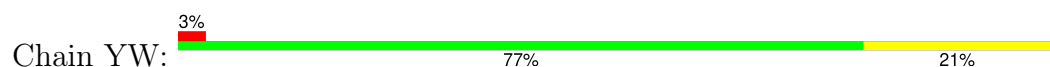
- Molecule 41: 50S ribosomal protein L21



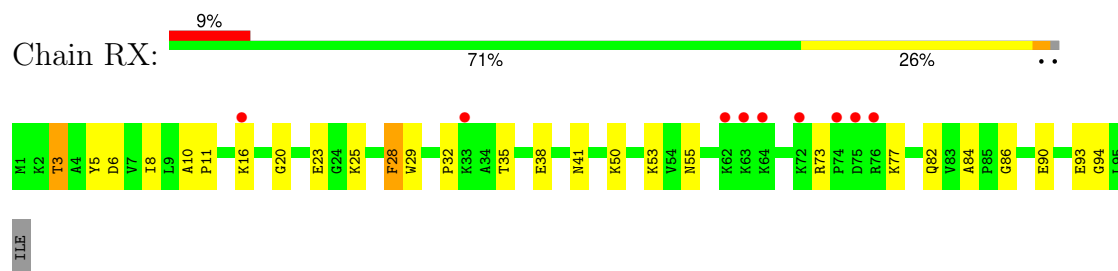
- Molecule 42: 50S ribosomal protein L22



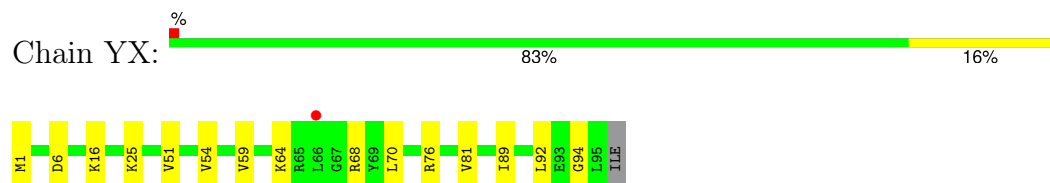
- Molecule 42: 50S ribosomal protein L22



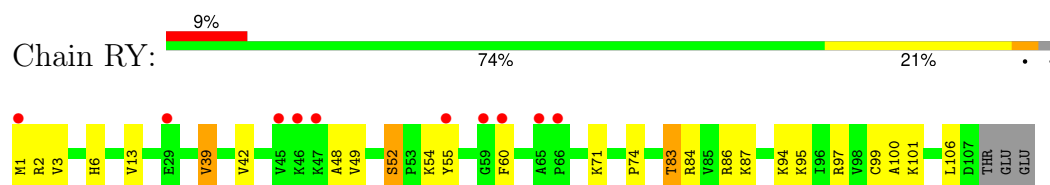
• Molecule 43: 50S ribosomal protein L23



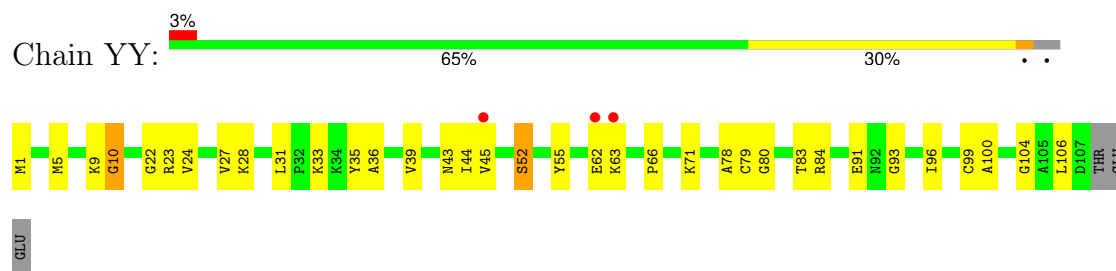
• Molecule 43: 50S ribosomal protein L23



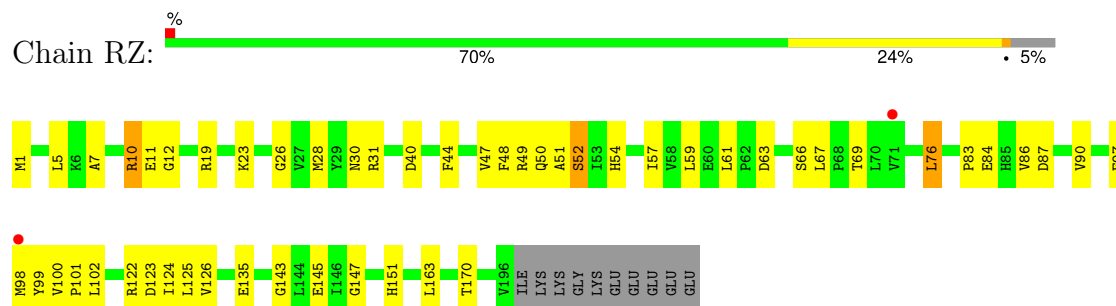
• Molecule 44: 50S ribosomal protein L24



• Molecule 44: 50S ribosomal protein L24

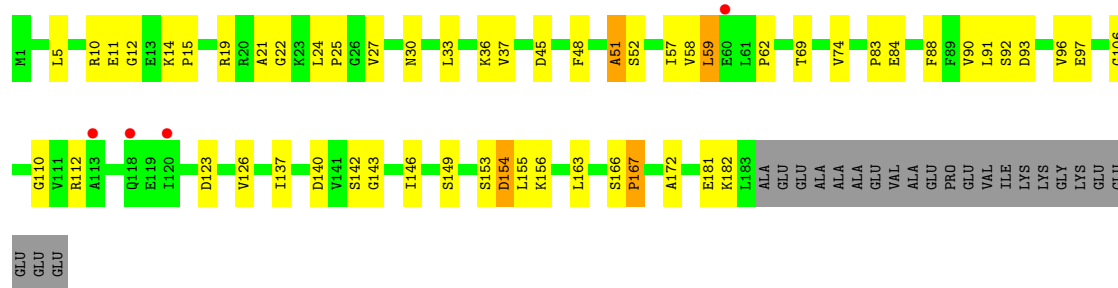


• Molecule 45: 50S ribosomal protein L25

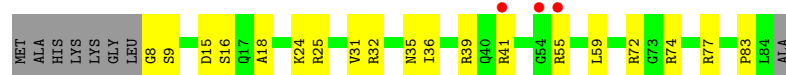


• Molecule 45: 50S ribosomal protein L25

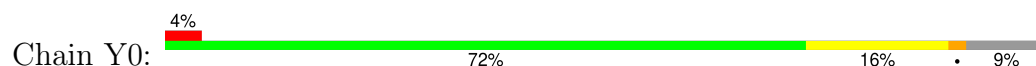




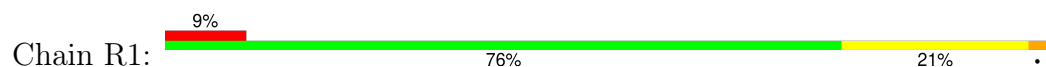
- Molecule 46: 50S ribosomal protein L27



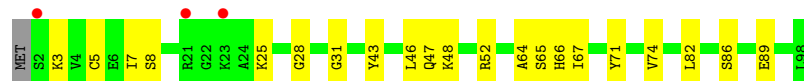
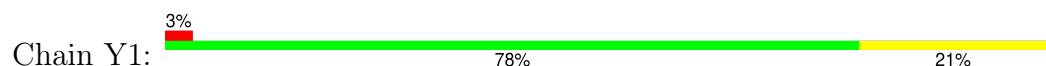
- Molecule 46: 50S ribosomal protein L27



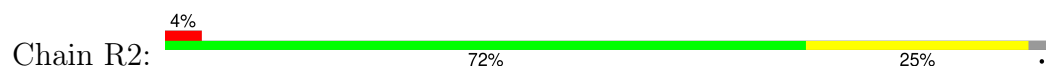
- Molecule 47: 50S ribosomal protein L28



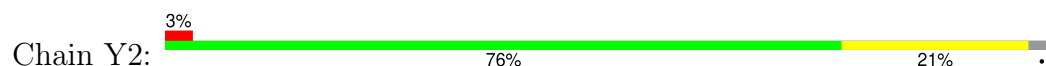
- Molecule 47: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L29

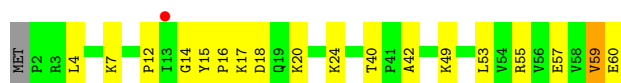


- Molecule 48: 50S ribosomal protein L29





- Molecule 49: 50S ribosomal protein L30



- Molecule 49: 50S ribosomal protein L30



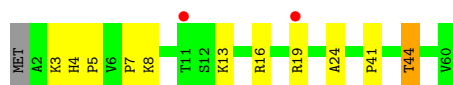
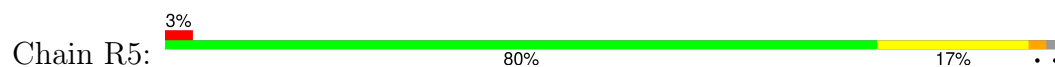
- Molecule 50: 50S ribosomal protein L31



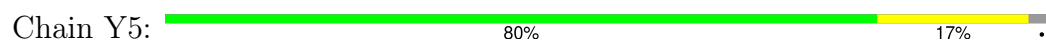
- Molecule 50: 50S ribosomal protein L31



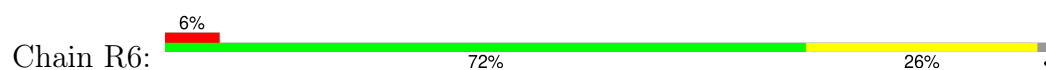
- Molecule 51: 50S ribosomal protein L32



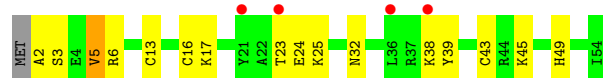
- Molecule 51: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L33



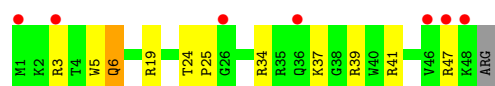
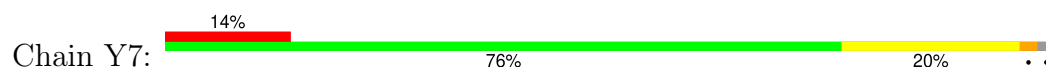
- Molecule 52: 50S ribosomal protein L33



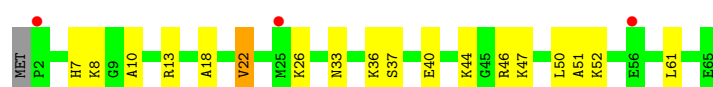
- Molecule 53: 50S ribosomal protein L34



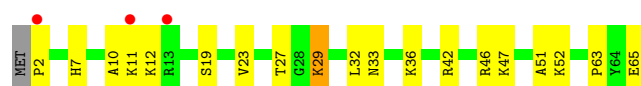
- Molecule 53: 50S ribosomal protein L34



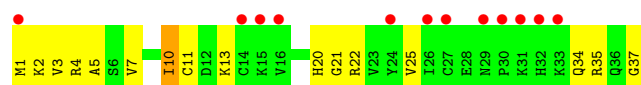
- Molecule 54: 50S ribosomal protein L35



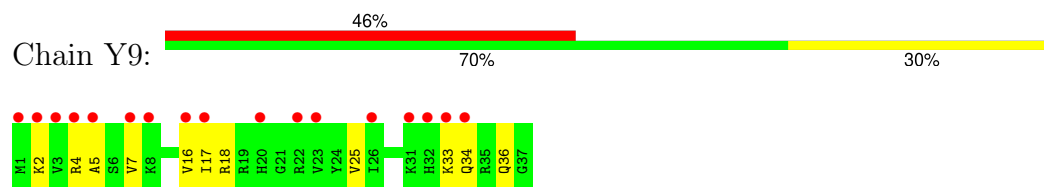
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: tRNA acceptor end mimic



- Molecule 56: tRNA acceptor end mimic



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.91Å 445.91Å 617.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.17 – 3.64 49.17 – 3.64	Depositor EDS
% Data completeness (in resolution range)	93.4 (49.17-3.64) 93.3 (49.17-3.64)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.208 , 0.250 0.228 , 0.260	Depositor DCC
R_{free} test set	27131 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	123.8	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 124.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	291822	wwPDB-VP
Average B, all atoms (Å ²)	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 0TD, 2MG, OMU, PSU, MG, 5MC, G7M, OMC, 4OC, OMG, 2MA, PPU, UR3, 5MU, MA6, ZN, M2G

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	0.44	0/35795	0.54	0/55864
1	XA	0.49	4/35890 (0.0%)	0.58	9/56012 (0.0%)
2	QB	0.33	0/1942	0.71	0/2619
2	XB	0.36	0/1950	0.64	0/2630
3	QC	0.31	0/1629	0.63	0/2195
3	XC	0.39	0/1629	0.62	0/2195
4	QD	0.48	0/1733	0.80	5/2318 (0.2%)
4	XD	0.47	0/1733	0.72	0/2318
5	QE	0.40	0/1149	0.66	0/1548
5	XE	0.48	0/1149	0.66	0/1548
6	QF	0.38	0/850	0.59	0/1147
6	XF	0.45	0/850	0.63	0/1147
7	QG	0.32	0/1276	0.62	0/1709
7	XG	0.39	0/1276	0.65	0/1709
8	QH	0.39	0/1128	0.61	0/1517
8	XH	0.43	0/1128	0.61	0/1517
9	QI	0.33	0/1029	0.66	0/1379
9	XI	0.39	0/1017	0.71	1/1365 (0.1%)
10	QJ	0.32	0/814	0.67	0/1095
10	XJ	0.37	0/790	0.53	0/1063
11	QK	0.39	0/859	0.58	0/1162
11	XK	0.40	0/859	0.62	0/1162
12	QL	0.48	1/963 (0.1%)	0.71	0/1287
12	XL	0.50	0/963	0.67	0/1287
13	QM	0.38	0/938	0.74	0/1258
13	XM	0.43	0/926	0.68	0/1241
14	QN	0.37	0/501	0.65	0/664
14	XN	0.43	0/501	0.66	0/664
15	QO	0.39	0/745	0.59	0/992
15	XO	0.43	0/745	0.65	0/992
16	QP	0.49	0/707	0.66	1/951 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	XP	0.43	0/707	0.63	0/951
17	QQ	0.42	0/836	0.59	0/1117
17	XQ	0.41	0/836	0.57	0/1117
18	QR	0.37	0/560	0.66	0/746
18	XR	0.47	0/560	0.61	0/746
19	QS	0.29	0/680	0.60	0/915
19	XS	0.41	0/680	0.62	0/915
20	QT	0.47	0/745	0.62	0/981
20	XT	0.35	0/762	0.73	0/1003
21	QU	0.34	0/203	0.56	0/266
21	XU	0.39	0/203	0.58	0/266
22	QV	0.42	0/1836	0.55	0/2859
22	XV	0.55	0/1836	0.67	0/2859
23	QX	0.37	0/185	0.66	0/285
23	XX	0.45	0/260	0.70	0/402
24	QY	0.36	0/336	0.55	0/522
24	XY	0.38	0/381	0.58	0/593
25	RA	0.57	0/68971	0.64	3/107656 (0.0%)
25	YA	0.66	0/68976	0.72	5/107668 (0.0%)
26	RB	0.38	0/2876	0.52	0/4486
26	YB	0.52	0/2878	0.61	0/4490
27	RD	0.62	0/2194	0.63	0/2955
27	YD	0.68	0/2195	0.68	0/2955
28	RE	0.57	0/1596	0.66	0/2153
28	YE	0.58	0/1596	0.73	0/2153
29	RF	0.58	0/1620	0.62	0/2194
29	YF	0.61	0/1620	0.66	0/2194
30	RG	0.38	0/1499	0.77	4/2016 (0.2%)
30	YG	0.55	0/1499	0.72	0/2016
31	RH	0.31	0/1362	0.59	0/1841
31	YH	0.53	0/1356	0.61	0/1833
32	RI	0.40	0/1151	0.73	2/1558 (0.1%)
32	YI	0.44	0/1151	0.75	0/1558
33	RN	0.54	0/1148	0.62	0/1547
33	YN	0.59	0/1148	0.57	0/1547
34	RO	0.56	0/943	0.69	1/1269 (0.1%)
34	YO	0.64	0/943	0.68	1/1269 (0.1%)
35	RP	0.51	0/1156	0.66	0/1537
35	YP	0.59	0/1156	0.69	0/1537
36	RQ	0.50	1/1143 (0.1%)	0.62	0/1527
36	YQ	0.56	0/1143	0.65	0/1527
37	RR	0.59	0/982	0.72	0/1312
37	YR	0.58	0/982	0.68	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	RS	0.35	0/887	0.62	0/1180
38	YS	0.46	0/887	0.65	0/1180
39	RT	0.50	0/1105	0.59	0/1477
39	YT	0.57	0/1105	0.61	0/1477
40	RU	0.51	0/977	0.62	0/1301
40	YU	0.58	0/977	0.59	0/1301
41	RV	0.46	0/790	0.65	2/1057 (0.2%)
41	YV	0.55	0/790	0.71	1/1057 (0.1%)
42	RW	0.58	0/901	0.61	0/1209
42	YW	0.61	0/901	0.59	0/1209
43	RX	0.51	0/764	0.58	0/1025
43	YX	0.60	0/764	0.59	0/1025
44	RY	0.45	0/831	0.64	0/1108
44	YY	0.53	0/831	0.67	0/1108
45	RZ	0.38	0/1585	0.62	0/2153
45	YZ	0.47	0/1493	0.71	0/2026
46	R0	0.47	0/619	0.59	0/825
46	Y0	0.60	0/619	0.59	0/825
47	R1	0.53	0/770	0.62	0/1022
47	Y1	0.60	0/770	0.65	0/1022
48	R2	0.44	0/594	0.59	0/785
48	Y2	0.49	0/594	0.54	0/785
49	R3	0.51	1/474 (0.2%)	0.67	0/635
49	Y3	0.55	0/473	0.70	1/635 (0.2%)
50	R4	0.31	0/578	0.70	0/776
50	Y4	0.39	0/578	0.76	2/776 (0.3%)
51	R5	0.57	0/473	0.67	0/639
51	Y5	0.57	0/465	0.63	0/629
52	R6	0.26	0/460	0.57	0/613
52	Y6	0.28	0/460	0.68	0/613
53	R7	0.65	0/426	0.71	0/561
53	Y7	0.65	0/426	0.73	0/561
54	R8	0.54	0/525	0.65	0/691
54	Y8	0.64	0/525	0.74	0/691
55	R9	0.27	0/310	0.59	0/407
55	Y9	0.33	0/310	0.64	0/407
56	ZA	0.50	0/40	0.82	0/60
56	ZB	0.70	0/40	1.09	0/60
All	All	0.54	7/314471 (0.0%)	0.65	38/470119 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	XA	0	1
2	QB	0	30
2	XB	0	23
3	QC	0	24
3	XC	0	16
4	QD	0	18
4	XD	0	8
5	QE	0	13
5	XE	0	15
6	QF	0	6
6	XF	0	5
7	QG	0	10
7	XG	0	10
8	QH	0	14
8	XH	0	6
9	QI	0	22
9	XI	0	9
10	QJ	0	10
10	XJ	0	8
11	QK	0	6
11	XK	0	11
12	QL	0	13
12	XL	0	10
13	QM	0	12
13	XM	0	7
14	QN	0	5
14	XN	0	6
15	QO	0	4
15	XO	0	3
16	QP	0	10
16	XP	0	4
17	QQ	0	7
17	XQ	0	5
18	QR	0	3
18	XR	0	1
19	QS	0	10
19	XS	0	8
20	QT	0	6
20	XT	0	4
21	QU	0	3
21	XU	0	2
25	YA	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
27	RD	0	17
27	YD	0	9
28	RE	0	14
28	YE	0	16
29	RF	0	15
29	YF	0	19
30	RG	0	29
30	YG	0	19
31	RH	0	20
31	YH	0	5
32	RI	0	26
32	YI	0	19
33	RN	0	7
33	YN	0	5
34	RO	0	5
34	YO	0	1
35	RP	0	23
35	YP	0	18
36	RQ	0	4
36	YQ	0	4
37	RR	0	5
37	YR	0	5
38	RS	0	5
38	YS	0	5
39	RT	0	5
39	YT	0	5
40	RU	0	6
40	YU	0	1
41	RV	0	8
41	YV	0	9
42	RW	0	2
42	YW	0	5
43	RX	0	4
43	YX	0	3
44	RY	0	6
44	YY	0	6
45	RZ	0	13
45	YZ	0	22
46	R0	0	5
46	Y0	0	3
47	R1	0	5
47	Y1	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
48	R2	0	3
48	Y2	0	1
49	R3	0	2
49	Y3	0	4
50	R4	0	10
50	Y4	0	11
51	R5	0	2
51	Y5	0	3
52	R6	0	5
52	Y6	0	5
53	R7	0	4
53	Y7	0	2
54	R8	0	1
54	Y8	0	4
55	R9	0	4
55	Y9	0	1
All	All	0	858

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	XA	88	A	C3'-C2'	8.79	1.66	1.52
1	XA	88	A	C1'-N9	8.49	1.59	1.47
36	RQ	124	LYS	C-N	-5.90	1.24	1.33
1	XA	88	A	C4'-O4'	5.87	1.54	1.45
1	XA	358	U	C3'-O3'	5.85	1.50	1.42

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	88	A	O4'-C1'-C2'	16.62	122.42	105.80
1	XA	358	U	N1-C1'-C2'	-9.77	97.35	112.00
25	YA	1281	G	N9-C1'-C2'	-8.44	99.35	112.00
1	XA	359	U	P-O5'-C5'	7.90	132.75	120.90
1	XA	367	U	N1-C1'-C2'	-7.43	102.85	114.00

There are no chirality outliers.

5 of 858 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	13	ALA	Peptide

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Mol	Chain	Res	Type	Group
2	QB	15	VAL	Peptide
2	QB	17	PHE	Peptide
2	QB	19	HIS	Peptide
2	QB	21	ARG	Peptide

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32246	0	16294	686	0
1	XA	32331	0	16338	599	12
2	QB	1907	0	1958	42	0
2	XB	1915	0	1969	45	0
3	QC	1605	0	1668	48	0
3	XC	1605	0	1668	20	1
4	QD	1703	0	1762	85	0
4	XD	1703	0	1763	54	6
5	QE	1133	0	1190	33	0
5	XE	1133	0	1191	23	0
6	QF	837	0	852	12	1
6	XF	837	0	852	15	0
7	QG	1257	0	1296	34	0
7	XG	1257	0	1296	27	0
8	QH	1108	0	1165	31	0
8	XH	1108	0	1165	27	0
9	QI	1010	0	1037	35	0
9	XI	998	0	1024	29	0
10	QJ	801	0	849	32	0
10	XJ	777	0	815	17	0
11	QK	844	0	855	28	1
11	XK	844	0	855	24	0
12	QL	958	0	1047	24	0
12	XL	958	0	1047	18	0
13	QM	928	0	987	38	0
13	XM	916	0	973	21	0
14	QN	492	0	530	30	0
14	XN	492	0	528	11	0
15	QO	734	0	771	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	XO	734	0	771	10	0
16	QP	691	0	714	17	0
16	XP	691	0	714	19	0
17	QQ	823	0	891	25	0
17	XQ	823	0	891	20	0
18	QR	555	0	618	13	0
18	XR	555	0	618	8	0
19	QS	665	0	686	14	0
19	XS	665	0	686	20	0
20	QT	743	0	840	23	0
20	XT	759	0	861	25	0
21	QU	199	0	208	10	0
21	XU	199	0	208	8	0
22	QV	1644	0	835	29	0
22	XV	1644	0	836	26	0
23	QX	167	0	86	2	0
23	XX	233	0	120	4	0
24	QY	301	0	152	5	0
24	XY	341	0	175	8	0
25	RA	61819	0	31179	962	3
25	YA	61822	0	31176	968	3
26	RB	2572	0	1305	44	0
26	YB	2573	0	1306	28	0
27	RD	2144	0	2233	55	3
27	YD	2145	0	2234	54	0
28	RE	1563	0	1629	45	0
28	YE	1563	0	1628	45	0
29	RF	1585	0	1632	35	0
29	YF	1585	0	1632	44	0
30	RG	1474	0	1535	43	0
30	YG	1474	0	1535	31	0
31	RH	1336	0	1418	30	0
31	YH	1330	0	1413	28	13
32	RI	1136	0	1223	26	12
32	YI	1136	0	1223	15	0
33	RN	1121	0	1195	26	0
33	YN	1121	0	1195	15	0
34	RO	933	0	996	33	0
34	YO	933	0	996	22	0
35	RP	1139	0	1222	36	0
35	YP	1139	0	1222	37	0
36	RQ	1122	0	1179	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	YQ	1122	0	1179	20	0
37	RR	968	0	1033	23	0
37	YR	968	0	1033	18	0
38	RS	877	0	938	26	0
38	YS	877	0	938	28	0
39	RT	1091	0	1151	26	0
39	YT	1091	0	1151	32	0
40	RU	959	0	1019	29	0
40	YU	959	0	1019	25	0
41	RV	779	0	852	16	0
41	YV	779	0	852	13	6
42	RW	890	0	951	17	1
42	YW	890	0	951	18	0
43	RX	750	0	814	17	0
43	YX	750	0	814	9	0
44	RY	818	0	913	15	0
44	YY	818	0	911	18	14
45	RZ	1552	0	1573	32	0
45	YZ	1461	0	1493	23	0
46	R0	611	0	631	12	0
46	Y0	611	0	631	13	0
47	R1	763	0	848	15	0
47	Y1	763	0	848	11	0
48	R2	592	0	654	10	0
48	Y2	592	0	654	8	1
49	R3	469	0	518	12	0
49	Y3	468	0	518	16	0
50	R4	565	0	556	14	0
50	Y4	565	0	557	13	0
51	R5	459	0	480	9	0
51	Y5	451	0	471	5	3
52	R6	453	0	477	6	0
52	Y6	453	0	477	8	0
53	R7	418	0	467	13	0
53	Y7	418	0	467	8	0
54	R8	517	0	582	15	0
54	Y8	517	0	582	12	0
55	R9	307	0	335	11	0
55	Y9	307	0	338	8	0
56	ZA	74	0	51	13	0
56	ZB	74	0	51	5	0
57	QA	124	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	QC	1	0	0	0	0
57	QD	2	0	0	0	0
57	QE	2	0	0	0	0
57	QL	2	0	0	0	0
57	QM	2	0	0	0	0
57	QN	2	0	0	2	0
57	QO	1	0	0	0	0
57	QV	3	0	0	0	0
57	R0	2	0	0	0	0
57	R1	1	0	0	0	0
57	R3	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R7	1	0	0	0	0
57	R8	1	0	0	0	0
57	R9	1	0	0	0	0
57	RA	414	0	0	2	0
57	RB	8	0	0	2	0
57	RD	5	0	0	2	0
57	RE	5	0	0	2	0
57	RF	5	0	0	0	0
57	RN	2	0	0	0	0
57	RO	1	0	0	0	0
57	RP	2	0	0	0	0
57	RQ	1	0	0	0	0
57	RR	1	0	0	0	0
57	RV	1	0	0	0	0
57	RW	1	0	0	0	0
57	RX	1	0	0	0	0
57	RZ	1	0	0	0	0
57	XA	128	0	0	0	0
57	XD	1	0	0	0	0
57	XJ	1	0	0	0	0
57	XK	2	0	0	0	0
57	XN	1	0	0	0	0
57	XV	1	0	0	0	0
57	XX	1	0	0	0	0
57	Y0	1	0	0	0	0
57	Y1	3	0	0	0	0
57	Y3	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	Y7	1	0	0	0	0
57	Y8	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YA	544	0	0	1	0
57	YB	8	0	0	0	0
57	YD	8	0	0	0	0
57	YE	7	0	0	1	0
57	YF	1	0	0	0	0
57	YG	1	0	0	0	0
57	YP	3	0	0	0	0
57	YQ	2	0	0	0	0
57	YR	1	0	0	0	0
57	YT	1	0	0	0	0
57	YU	1	0	0	0	0
57	YV	1	0	0	0	0
57	YW	1	0	0	0	0
57	YX	1	0	0	0	0
58	QD	8	0	0	6	0
58	XD	8	0	0	4	0
59	QN	1	0	0	1	0
59	R4	1	0	0	0	0
59	R9	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y4	1	0	0	0	0
All	All	291822	0	197739	4783	40

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 4783 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:RE:152:LYS:HG3	33:RN:77:GLY:O	1.40	1.18
49:Y3:10:LYS:NZ	49:Y3:15:TYR:OH	1.81	1.13
25:YA:2228:G:OP1	27:YD:261:LYS:NZ	1.83	1.12
1:QA:982:U:H3	1:QA:1223:C:N4	1.52	1.08
1:QA:1055:A:H62	1:QA:1200:C:N4	1.56	1.04

The worst 5 of 40 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	Interatomic distance (Å)	Clash overlap (Å)
31:YH:46:GLU:CG	44:YY:22:GLY:O[4_445]	1.23	0.97
31:YH:46:GLU:CB	44:YY:22:GLY:O[4_445]	1.41	0.79
27:RD:134:ARG:NE	4:XD:166:LYS:NZ[4_555]	1.53	0.67
6:QF:16:GLN:O	4:XD:195:ALA:CB[4_555]	1.62	0.58
31:YH:13:LYS:NZ	44:YY:78:ALA:O[4_445]	1.64	0.56

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	233/256 (91%)	204 (88%)	29 (12%)	0	100	100
2	XB	234/256 (91%)	204 (87%)	30 (13%)	0	100	100
3	QC	203/239 (85%)	184 (91%)	19 (9%)	0	100	100
3	XC	203/239 (85%)	183 (90%)	20 (10%)	0	100	100
4	QD	206/209 (99%)	183 (89%)	21 (10%)	2 (1%)	12	41
4	XD	206/209 (99%)	196 (95%)	10 (5%)	0	100	100
5	QE	146/162 (90%)	134 (92%)	12 (8%)	0	100	100
5	XE	146/162 (90%)	134 (92%)	12 (8%)	0	100	100
6	QF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
6	XF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
7	QG	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	XG	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
8	QH	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
8	XH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
9	QI	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
9	XI	124/128 (97%)	110 (89%)	14 (11%)	0	100	100
10	QJ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
10	XJ	94/105 (90%)	83 (88%)	11 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	QK	112/129 (87%)	105 (94%)	7 (6%)	0	100	100
11	XK	112/129 (87%)	104 (93%)	8 (7%)	0	100	100
12	QL	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
12	XL	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
13	QM	114/126 (90%)	108 (95%)	6 (5%)	0	100	100
13	XM	112/126 (89%)	102 (91%)	10 (9%)	0	100	100
14	QN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
14	XN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
15	QO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
15	XO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
16	QP	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
16	XP	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
17	QQ	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
17	XQ	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
18	QR	66/88 (75%)	66 (100%)	0	0	100	100
18	XR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
19	QS	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
19	XS	81/93 (87%)	78 (96%)	3 (4%)	0	100	100
20	QT	94/106 (89%)	89 (95%)	5 (5%)	0	100	100
20	XT	96/106 (91%)	91 (95%)	5 (5%)	0	100	100
21	QU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
21	XU	21/27 (78%)	21 (100%)	0	0	100	100
27	RD	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
27	YD	273/276 (99%)	252 (92%)	21 (8%)	0	100	100
28	RE	202/206 (98%)	184 (91%)	17 (8%)	1 (0%)	24	55
28	YE	202/206 (98%)	181 (90%)	21 (10%)	0	100	100
29	RF	200/210 (95%)	192 (96%)	8 (4%)	0	100	100
29	YF	200/210 (95%)	188 (94%)	12 (6%)	0	100	100
30	RG	179/182 (98%)	156 (87%)	23 (13%)	0	100	100
30	YG	179/182 (98%)	151 (84%)	27 (15%)	1 (1%)	21	51
31	RH	172/180 (96%)	166 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	YH	171/180 (95%)	162 (95%)	8 (5%)	1 (1%)	21	51
32	RI	144/148 (97%)	115 (80%)	28 (19%)	1 (1%)	18	48
32	YI	144/148 (97%)	125 (87%)	19 (13%)	0	100	100
33	RN	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
33	YN	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
34	RO	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
34	YO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
35	RP	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	18	48
35	YP	147/150 (98%)	135 (92%)	12 (8%)	0	100	100
36	RQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
36	YQ	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
37	RR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
37	YR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
38	RS	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
38	YS	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
39	RT	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
39	YT	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
40	RU	114/118 (97%)	107 (94%)	7 (6%)	0	100	100
40	YU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
41	RV	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12	41
41	YV	99/101 (98%)	88 (89%)	10 (10%)	1 (1%)	12	41
42	RW	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
42	YW	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
43	RX	93/96 (97%)	84 (90%)	9 (10%)	0	100	100
43	YX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
44	RY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
44	YY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
45	RZ	194/206 (94%)	181 (93%)	13 (7%)	0	100	100
45	YZ	181/206 (88%)	154 (85%)	27 (15%)	0	100	100
46	R0	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
46	Y0	75/85 (88%)	72 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	R1	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
47	Y1	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
48	R2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
48	Y2	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
49	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
49	Y3	57/60 (95%)	57 (100%)	0	0	100	100
50	R4	67/71 (94%)	53 (79%)	14 (21%)	0	100	100
50	Y4	67/71 (94%)	53 (79%)	14 (21%)	0	100	100
51	R5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
51	Y5	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
52	R6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
52	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
53	R7	46/49 (94%)	42 (91%)	4 (9%)	0	100	100
53	Y7	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
54	R8	62/65 (95%)	55 (89%)	7 (11%)	0	100	100
54	Y8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
55	R9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
55	Y9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
All	All	11420/12128 (94%)	10610 (93%)	801 (7%)	9 (0%)	48	78

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	QD	32	ALA
4	QD	31	CYS
30	YG	81	LYS
32	RI	132	PRO
41	RV	50	PRO

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	203/220 (92%)	201 (99%)	2 (1%)	68	72
2	XB	204/220 (93%)	203 (100%)	1 (0%)	81	78
3	QC	159/188 (85%)	158 (99%)	1 (1%)	78	77
3	XC	159/188 (85%)	158 (99%)	1 (1%)	78	77
4	QD	180/181 (99%)	176 (98%)	4 (2%)	45	61
4	XD	180/181 (99%)	174 (97%)	6 (3%)	33	54
5	QE	114/123 (93%)	112 (98%)	2 (2%)	51	64
5	XE	114/123 (93%)	112 (98%)	2 (2%)	51	64
6	QF	90/90 (100%)	89 (99%)	1 (1%)	65	71
6	XF	90/90 (100%)	88 (98%)	2 (2%)	45	61
7	QG	126/127 (99%)	125 (99%)	1 (1%)	73	74
7	XG	126/127 (99%)	125 (99%)	1 (1%)	73	74
8	QH	118/119 (99%)	117 (99%)	1 (1%)	73	74
8	XH	118/119 (99%)	117 (99%)	1 (1%)	73	74
9	QI	98/99 (99%)	97 (99%)	1 (1%)	68	72
9	XI	97/99 (98%)	97 (100%)	0	100	100
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	86 (100%)	0	100	100
11	QK	86/99 (87%)	85 (99%)	1 (1%)	63	70
11	XK	86/99 (87%)	86 (100%)	0	100	100
12	QL	102/108 (94%)	102 (100%)	0	100	100
12	XL	102/108 (94%)	102 (100%)	0	100	100
13	QM	94/101 (93%)	93 (99%)	1 (1%)	65	71
13	XM	93/101 (92%)	93 (100%)	0	100	100
14	QN	49/50 (98%)	48 (98%)	1 (2%)	48	63
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	78 (99%)	1 (1%)	61	69
15	XO	79/80 (99%)	78 (99%)	1 (1%)	61	69
16	QP	71/74 (96%)	71 (100%)	0	100	100
16	XP	71/74 (96%)	71 (100%)	0	100	100
17	QQ	94/97 (97%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	XQ	94/97 (97%)	94 (100%)	0	100	100
18	QR	59/77 (77%)	58 (98%)	1 (2%)	53	65
18	XR	59/77 (77%)	58 (98%)	1 (2%)	53	65
19	QS	72/80 (90%)	72 (100%)	0	100	100
19	XS	72/80 (90%)	72 (100%)	0	100	100
20	QT	74/82 (90%)	74 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	18/22 (82%)	18 (100%)	0	100	100
21	XU	18/22 (82%)	18 (100%)	0	100	100
27	RD	217/218 (100%)	216 (100%)	1 (0%)	81	78
27	YD	217/218 (100%)	216 (100%)	1 (0%)	81	78
28	RE	165/166 (99%)	163 (99%)	2 (1%)	63	70
28	YE	165/166 (99%)	163 (99%)	2 (1%)	63	70
29	RF	161/166 (97%)	161 (100%)	0	100	100
29	YF	161/166 (97%)	158 (98%)	3 (2%)	50	64
30	RG	155/156 (99%)	154 (99%)	1 (1%)	78	77
30	YG	155/156 (99%)	153 (99%)	2 (1%)	61	69
31	RH	145/148 (98%)	145 (100%)	0	100	100
31	YH	144/148 (97%)	142 (99%)	2 (1%)	59	68
32	RI	122/124 (98%)	121 (99%)	1 (1%)	73	74
32	YI	122/124 (98%)	121 (99%)	1 (1%)	73	74
33	RN	119/119 (100%)	116 (98%)	3 (2%)	42	59
33	YN	119/119 (100%)	117 (98%)	2 (2%)	53	65
34	RO	100/100 (100%)	100 (100%)	0	100	100
34	YO	100/100 (100%)	99 (99%)	1 (1%)	68	72
35	RP	116/116 (100%)	113 (97%)	3 (3%)	40	58
35	YP	116/116 (100%)	115 (99%)	1 (1%)	70	73
36	RQ	111/111 (100%)	111 (100%)	0	100	100
36	YQ	111/111 (100%)	109 (98%)	2 (2%)	51	64
37	RR	101/101 (100%)	98 (97%)	3 (3%)	36	55
37	YR	101/101 (100%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	RS	87/88 (99%)	86 (99%)	1 (1%)	65	71
38	YS	87/88 (99%)	87 (100%)	0	100	100
39	RT	115/127 (91%)	115 (100%)	0	100	100
39	YT	115/127 (91%)	113 (98%)	2 (2%)	53	65
40	RU	93/94 (99%)	93 (100%)	0	100	100
40	YU	93/94 (99%)	91 (98%)	2 (2%)	45	61
41	RV	82/82 (100%)	82 (100%)	0	100	100
41	YV	82/82 (100%)	80 (98%)	2 (2%)	43	60
42	RW	91/92 (99%)	91 (100%)	0	100	100
42	YW	91/92 (99%)	91 (100%)	0	100	100
43	RX	77/78 (99%)	77 (100%)	0	100	100
43	YX	77/78 (99%)	76 (99%)	1 (1%)	61	69
44	RY	88/91 (97%)	88 (100%)	0	100	100
44	YY	88/91 (97%)	88 (100%)	0	100	100
45	RZ	170/179 (95%)	170 (100%)	0	100	100
45	YZ	162/179 (90%)	159 (98%)	3 (2%)	50	64
46	R0	62/67 (92%)	61 (98%)	1 (2%)	55	65
46	Y0	62/67 (92%)	61 (98%)	1 (2%)	55	65
47	R1	82/83 (99%)	82 (100%)	0	100	100
47	Y1	82/83 (99%)	82 (100%)	0	100	100
48	R2	66/67 (98%)	65 (98%)	1 (2%)	57	66
48	Y2	66/67 (98%)	65 (98%)	1 (2%)	57	66
49	R3	51/52 (98%)	50 (98%)	1 (2%)	48	63
49	Y3	51/52 (98%)	50 (98%)	1 (2%)	48	63
50	R4	62/63 (98%)	61 (98%)	1 (2%)	55	65
50	Y4	62/63 (98%)	62 (100%)	0	100	100
51	R5	51/52 (98%)	50 (98%)	1 (2%)	48	63
51	Y5	50/52 (96%)	49 (98%)	1 (2%)	48	63
52	R6	51/52 (98%)	51 (100%)	0	100	100
52	Y6	51/52 (98%)	50 (98%)	1 (2%)	48	63
53	R7	41/42 (98%)	41 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	Y7	41/42 (98%)	41 (100%)	0	100	100
54	R8	54/55 (98%)	53 (98%)	1 (2%)	50	64
54	Y8	54/55 (98%)	53 (98%)	1 (2%)	50	64
55	R9	34/34 (100%)	33 (97%)	1 (3%)	37	56
55	Y9	34/34 (100%)	33 (97%)	1 (3%)	37	56
All	All	9676/10064 (96%)	9586 (99%)	90 (1%)	70	73

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	YE	9	VAL
36	YQ	66	ILE
29	YF	78	ILE
31	YH	47	GLU
40	YU	8	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
37	YR	13	HIS
41	YV	80	GLN
55	Y9	34	GLN
50	R4	47	GLN
48	R2	38	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1497/1521 (98%)	295 (19%)	14 (0%)
1	XA	1501/1521 (98%)	289 (19%)	14 (0%)
22	QV	76/77 (98%)	18 (23%)	0
22	XV	76/77 (98%)	17 (22%)	1 (1%)
23	QX	7/26 (26%)	1 (14%)	1 (14%)
23	XX	10/26 (38%)	7 (70%)	1 (10%)
24	QY	13/18 (72%)	5 (38%)	2 (15%)
24	XY	15/18 (83%)	9 (60%)	1 (6%)
25	RA	2862/2915 (98%)	600 (20%)	21 (0%)
25	YA	2862/2915 (98%)	580 (20%)	19 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	RB	119/122 (97%)	17 (14%)	0
26	YB	119/122 (97%)	24 (20%)	0
56	ZA	1/3 (33%)	0	0
56	ZB	1/3 (33%)	1 (100%)	0
All	All	9159/9364 (97%)	1863 (20%)	74 (0%)

5 of 1863 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	11	G
1	QA	21	G
1	QA	22	G
1	QA	32	A
1	QA	39	G

5 of 74 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	YA	752	A
25	YA	2439	A
25	YA	856	C
25	YA	1900	A
25	RA	1073	A

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

50 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
25	PSU	RA	2605	25	18,21,22	1.70	4 (22%)	21,30,33	2.27	5 (23%)
1	4OC	XA	1402	1	20,23,24	0.86	1 (5%)	25,32,35	0.93	1 (4%)
12	0TD	QL	92	12	8,9,10	3.48	2 (25%)	6,11,13	2.20	3 (50%)
25	5MC	RA	1962	25,57	19,22,23	1.04	1 (5%)	26,32,35	1.62	7 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	XA	1400	1	19,22,23	1.30	3 (15%)	26,32,35	1.22	2 (7%)
25	PSU	YA	1911	25	18,21,22	1.58	6 (33%)	21,30,33	2.02	4 (19%)
12	0TD	XL	92	12	8,9,10	4.33	3 (37%)	6,11,13	1.43	1 (16%)
1	5MC	XA	1404	1	19,22,23	1.21	2 (10%)	26,32,35	1.35	3 (11%)
1	5MC	QA	1400	1	19,22,23	1.36	2 (10%)	26,32,35	1.20	1 (3%)
25	2MA	RA	2503	25,57	22,25,26	1.46	7 (31%)	32,37,40	2.42	7 (21%)
1	MA6	QA	1519	1	23,26,27	1.50	5 (21%)	33,38,41	2.37	11 (33%)
1	G7M	QA	527	1	23,26,27	2.38	5 (21%)	34,39,42	3.21	10 (29%)
25	OMU	RA	2552	25	19,22,23	1.40	3 (15%)	25,31,34	2.05	6 (24%)
25	5MU	RA	1939	25,57	19,22,23	1.45	4 (21%)	27,32,35	2.33	6 (22%)
25	5MC	YA	1962	25,57	19,22,23	1.10	2 (10%)	26,32,35	2.29	8 (30%)
25	PSU	RA	1911	25	18,21,22	1.57	5 (27%)	21,30,33	2.17	4 (19%)
25	OMU	YA	2552	25,57	19,22,23	1.46	3 (15%)	25,31,34	2.12	7 (28%)
1	MA6	QA	1518	1	23,26,27	1.49	5 (21%)	33,38,41	2.38	14 (42%)
1	PSU	XA	516	1,57	18,21,22	1.38	5 (27%)	21,30,33	1.95	5 (23%)
1	5MC	XA	1407	1	19,22,23	1.20	3 (15%)	26,32,35	1.41	5 (19%)
25	5MC	RA	1942	25	19,22,23	1.21	2 (10%)	26,32,35	1.40	2 (7%)
1	5MC	QA	1404	1	19,22,23	1.29	2 (10%)	26,32,35	1.42	4 (15%)
1	M2G	XA	966	1	24,27,28	1.31	4 (16%)	33,40,43	1.79	6 (18%)
1	5MC	XA	967	1	19,22,23	1.23	2 (10%)	26,32,35	1.33	3 (11%)
25	OMG	YA	2251	22,25,57	23,26,27	1.43	4 (17%)	32,38,41	2.22	8 (25%)
25	PSU	YA	2605	25	18,21,22	1.63	5 (27%)	21,30,33	2.36	5 (23%)
1	UR3	QA	1498	1	19,22,23	0.97	2 (10%)	26,32,35	1.63	3 (11%)
25	PSU	RA	1917	25	18,21,22	1.49	5 (27%)	21,30,33	2.24	4 (19%)
25	OMC	YA	1920	25	19,22,23	0.90	1 (5%)	25,31,34	1.87	5 (20%)
25	5MU	YA	1939	25,57	19,22,23	1.51	3 (15%)	27,32,35	2.24	6 (22%)
25	5MU	RA	1915	25	19,22,23	1.57	5 (26%)	27,32,35	2.48	8 (29%)
56	PPU	ZA	3	25,56,57	37,40,41	1.26	6 (16%)	47,57,60	2.32	14 (29%)
1	5MC	QA	1407	1	19,22,23	1.19	3 (15%)	26,32,35	1.10	3 (11%)
1	2MG	XA	1207	1	23,26,27	1.38	4 (17%)	33,38,41	2.28	7 (21%)
1	MA6	XA	1518	1	23,26,27	1.57	5 (21%)	33,38,41	2.34	12 (36%)
1	MA6	XA	1519	1	23,26,27	1.41	4 (17%)	33,38,41	2.52	11 (33%)
25	5MU	YA	1915	25	19,22,23	1.52	5 (26%)	27,32,35	2.55	9 (33%)
56	PPU	ZB	3	25,56	37,40,41	1.25	6 (16%)	47,57,60	2.21	13 (27%)
1	PSU	QA	516	1	18,21,22	1.38	4 (22%)	21,30,33	2.07	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	5MC	YA	1942	25	19,22,23	1.25	3 (15%)	26,32,35	1.54	2 (7%)
25	OMG	RA	2251	22,25,57	23,26,27	1.38	3 (13%)	32,38,41	2.14	6 (18%)
25	PSU	YA	1917	25	18,21,22	1.46	4 (22%)	21,30,33	2.17	5 (23%)
25	OMC	RA	1920	25	19,22,23	0.92	1 (5%)	25,31,34	1.93	7 (28%)
25	2MA	YA	2503	25,57	22,25,26	1.58	5 (22%)	32,37,40	2.65	9 (28%)
1	M2G	QA	966	1	24,27,28	1.33	5 (20%)	33,40,43	1.85	6 (18%)
1	5MC	QA	967	1	19,22,23	1.44	3 (15%)	26,32,35	1.28	2 (7%)
1	2MG	QA	1207	1	23,26,27	1.34	4 (17%)	33,38,41	2.27	9 (27%)
1	G7M	XA	527	1	23,26,27	2.34	5 (21%)	34,39,42	3.16	11 (32%)
1	UR3	XA	1498	1	19,22,23	1.02	2 (10%)	26,32,35	1.61	3 (11%)
1	4OC	QA	1402	1	20,23,24	0.78	0	25,32,35	0.94	0

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
25	PSU	RA	2605	25	-	0/7/25/26	0/2/2/2
1	4OC	XA	1402	1	-	2/9/29/30	0/2/2/2
12	0TD	QL	92	12	-	4/7/12/14	-
25	5MC	RA	1962	25,57	-	0/7/25/26	0/2/2/2
1	5MC	XA	1400	1	-	4/7/25/26	0/2/2/2
25	PSU	YA	1911	25	-	0/7/25/26	0/2/2/2
12	0TD	XL	92	12	-	4/7/12/14	-
1	5MC	XA	1404	1	-	0/7/25/26	0/2/2/2
1	5MC	QA	1400	1	-	5/7/25/26	0/2/2/2
25	2MA	RA	2503	25,57	-	3/7/25/26	0/3/3/3
1	MA6	QA	1519	1	-	5/11/29/30	0/3/3/3
1	G7M	QA	527	1	-	2/7/25/26	0/3/3/3
25	OMU	RA	2552	25	-	3/9/27/28	0/2/2/2
25	5MU	RA	1939	25,57	-	0/7/25/26	0/2/2/2
25	5MC	YA	1962	25,57	-	4/7/25/26	0/2/2/2
25	PSU	RA	1911	25	-	0/7/25/26	0/2/2/2
25	OMU	YA	2552	25,57	-	2/9/27/28	0/2/2/2
1	MA6	QA	1518	1	-	2/11/29/30	0/3/3/3
1	PSU	XA	516	1,57	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	XA	1407	1	-	0/7/25/26	0/2/2/2
25	5MC	RA	1942	25	-	0/7/25/26	0/2/2/2
1	5MC	QA	1404	1	-	0/7/25/26	0/2/2/2
1	M2G	XA	966	1	-	2/11/29/30	0/3/3/3
1	5MC	XA	967	1	-	0/7/25/26	0/2/2/2
25	OMG	YA	2251	22,25,57	-	0/9/27/28	0/3/3/3
25	PSU	YA	2605	25	-	0/7/25/26	0/2/2/2
1	UR3	QA	1498	1	-	2/7/25/26	0/2/2/2
25	PSU	RA	1917	25	-	0/7/25/26	0/2/2/2
25	OMC	YA	1920	25	-	4/9/27/28	0/2/2/2
25	5MU	YA	1939	25,57	-	0/7/25/26	0/2/2/2
25	5MU	RA	1915	25	-	3/7/25/26	0/2/2/2
56	PPU	ZA	3	25,56,57	-	5/25/43/44	0/4/4/4
1	5MC	QA	1407	1	-	0/7/25/26	0/2/2/2
1	2MG	XA	1207	1	-	0/9/27/28	0/3/3/3
1	MA6	XA	1518	1	-	1/11/29/30	0/3/3/3
1	MA6	XA	1519	1	-	6/11/29/30	0/3/3/3
25	5MU	YA	1915	25	-	4/7/25/26	0/2/2/2
56	PPU	ZB	3	25,56	-	5/25/43/44	0/4/4/4
1	PSU	QA	516	1	-	0/7/25/26	0/2/2/2
25	5MC	YA	1942	25	-	0/7/25/26	0/2/2/2
25	OMG	RA	2251	22,25,57	-	0/9/27/28	0/3/3/3
25	PSU	YA	1917	25	-	0/7/25/26	0/2/2/2
25	OMC	RA	1920	25	-	4/9/27/28	0/2/2/2
25	2MA	YA	2503	25,57	-	4/7/25/26	0/3/3/3
1	M2G	QA	966	1	-	0/11/29/30	0/3/3/3
1	5MC	QA	967	1	-	0/7/25/26	0/2/2/2
1	2MG	QA	1207	1	-	0/9/27/28	0/3/3/3
1	G7M	XA	527	1	-	2/7/25/26	0/3/3/3
1	UR3	XA	1498	1	-	0/7/25/26	0/2/2/2
1	4OC	QA	1402	1	-	2/9/29/30	0/2/2/2

The worst 5 of 178 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	XL	92	0TD	CB-CA	-11.66	1.51	1.54
12	QL	92	0TD	CB-CA	-9.10	1.51	1.54
1	QA	527	G7M	C8-N7	7.07	1.45	1.33
1	XA	527	G7M	C8-N7	6.65	1.44	1.33
1	QA	527	G7M	C5-N7	-5.68	1.32	1.39

The worst 5 of 298 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	2503	2MA	C5-C4-N3	-9.78	116.88	127.18
25	RA	2503	2MA	C5-C4-N3	-9.19	117.50	127.18
1	XA	527	G7M	CN7-N7-C8	-9.10	111.01	124.79
1	QA	527	G7M	CN7-N7-C8	-8.93	111.26	124.79
25	YA	2503	2MA	N3-C4-N9	8.10	137.26	126.99

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	QL	92	0TD	O-C-CA-CB
12	QL	92	0TD	CA-CB-SB-CSB
12	QL	92	0TD	CG-CB-SB-CSB
1	QA	527	G7M	O4'-C4'-C5'-O5'
1	QA	527	G7M	C3'-C4'-C5'-O5'

There are no ring outliers.

26 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	XA	1402	4OC	1	0
12	QL	92	0TD	2	0
12	XL	92	0TD	1	0
1	XA	1404	5MC	2	0
1	QA	1400	5MC	1	0
25	RA	2503	2MA	2	0
1	QA	1519	MA6	1	0
25	RA	2552	OMU	3	0
25	YA	1962	5MC	1	0
25	YA	2552	OMU	2	0
1	XA	1407	5MC	1	0
25	RA	1942	5MC	1	0
1	XA	967	5MC	1	0
25	YA	2251	OMG	1	0
25	YA	1920	OMC	2	0
25	YA	1939	5MU	1	0
56	ZA	3	PPU	10	0
1	XA	1207	2MG	2	0
1	XA	1518	MA6	1	0
56	ZB	3	PPU	4	0
25	RA	2251	OMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	YA	1917	PSU	1	0
25	RA	1920	OMC	1	0
25	YA	2503	2MA	1	0
1	QA	966	M2G	1	0
1	QA	1402	4OC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1328 ligands modelled in this entry, 1326 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	SF4	QD	303	4	0,12,12	-	-	-		
58	SF4	XD	302	4	0,12,12	-	-	-		

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	SF4	QD	303	4	-	-	0/6/5/5
58	SF4	XD	302	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	QD	303	SF4	6	0
58	XD	302	SF4	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	1488/1521 (97%)	-0.10	16 (1%) 78 53	109, 169, 287, 424	0
1	XA	1492/1521 (98%)	-0.20	9 (0%) 85 65	91, 149, 251, 393	0
2	QB	235/256 (91%)	0.07	11 (4%) 36 22	147, 231, 284, 346	0
2	XB	236/256 (92%)	-0.04	9 (3%) 44 26	124, 194, 257, 317	0
3	QC	205/239 (85%)	0.09	3 (1%) 72 45	147, 229, 305, 353	0
3	XC	205/239 (85%)	-0.09	5 (2%) 59 35	117, 172, 217, 259	0
4	QD	208/209 (99%)	0.18	6 (2%) 53 31	108, 165, 220, 245	0
4	XD	208/209 (99%)	0.12	8 (3%) 44 26	98, 159, 205, 232	0
5	QE	148/162 (91%)	0.15	5 (3%) 48 28	129, 179, 220, 236	0
5	XE	148/162 (91%)	-0.00	3 (2%) 65 39	97, 160, 207, 246	0
6	QF	100/101 (99%)	-0.21	1 (1%) 79 54	122, 174, 219, 246	0
6	XF	100/101 (99%)	-0.13	3 (3%) 52 31	104, 162, 210, 242	0
7	QG	155/156 (99%)	0.02	3 (1%) 66 40	151, 206, 296, 361	0
7	XG	155/156 (99%)	-0.18	1 (0%) 85 65	111, 172, 227, 280	0
8	QH	137/138 (99%)	0.08	3 (2%) 62 37	137, 182, 216, 269	0
8	XH	137/138 (99%)	0.09	4 (2%) 53 31	117, 169, 213, 272	0
9	QI	127/128 (99%)	0.56	14 (11%) 10 10	153, 234, 286, 339	0
9	XI	126/128 (98%)	0.35	9 (7%) 22 15	119, 179, 237, 329	0
10	QJ	99/105 (94%)	0.59	11 (11%) 10 9	189, 230, 306, 324	0
10	XJ	96/105 (91%)	0.20	6 (6%) 26 17	127, 180, 236, 270	0
11	QK	114/129 (88%)	-0.10	2 (1%) 67 41	128, 173, 243, 273	0
11	XK	114/129 (88%)	-0.01	3 (2%) 57 34	112, 163, 223, 296	0
12	QL	121/132 (91%)	0.43	7 (5%) 29 18	117, 159, 205, 221	0
12	XL	121/132 (91%)	0.29	5 (4%) 41 24	94, 135, 170, 204	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	QM	116/126 (92%)	0.34	8 (6%)	23 15	149, 203, 261, 333	0
13	XM	114/126 (90%)	0.11	3 (2%)	57 34	110, 157, 203, 235	0
14	QN	60/61 (98%)	0.93	9 (15%)	5 6	186, 216, 284, 315	0
14	XN	60/61 (98%)	0.46	4 (6%)	24 16	123, 166, 215, 238	0
15	QO	88/89 (98%)	0.17	5 (5%)	29 18	115, 161, 207, 215	0
15	XO	88/89 (98%)	-0.04	2 (2%)	61 37	111, 154, 200, 223	0
16	QP	82/88 (93%)	0.38	4 (4%)	35 21	102, 149, 180, 219	0
16	XP	82/88 (93%)	0.74	8 (9%)	13 11	132, 183, 216, 244	0
17	QQ	99/105 (94%)	-0.03	0	100 100	113, 163, 205, 215	0
17	XQ	99/105 (94%)	0.19	2 (2%)	65 39	105, 152, 201, 249	0
18	QR	68/88 (77%)	0.02	1 (1%)	72 45	152, 191, 237, 243	0
18	XR	68/88 (77%)	-0.24	0	100 100	114, 149, 197, 207	0
19	QS	83/93 (89%)	0.61	12 (14%)	6 6	180, 239, 284, 336	0
19	XS	83/93 (89%)	0.14	4 (4%)	35 22	120, 167, 228, 276	0
20	QT	96/106 (90%)	0.70	15 (15%)	5 5	95, 146, 191, 239	0
20	XT	98/106 (92%)	0.83	14 (14%)	6 6	150, 188, 236, 285	0
21	QU	23/27 (85%)	1.08	2 (8%)	16 12	184, 214, 262, 287	0
21	XU	23/27 (85%)	0.97	3 (13%)	7 7	133, 151, 184, 194	0
22	QV	77/77 (100%)	-0.15	1 (1%)	75 49	105, 176, 213, 291	0
22	XV	77/77 (100%)	-0.49	0	100 100	100, 136, 202, 247	0
23	QX	8/26 (30%)	0.45	0	100 100	159, 174, 192, 215	0
23	XX	11/26 (42%)	0.86	1 (9%)	15 11	127, 152, 261, 262	0
24	QY	14/18 (77%)	0.20	0	100 100	178, 226, 271, 289	0
24	XY	16/18 (88%)	-0.03	1 (6%)	26 17	196, 234, 278, 300	0
25	RA	2859/2915 (98%)	-0.24	25 (0%)	81 57	73, 124, 264, 398	0
25	YA	2859/2915 (98%)	-0.29	11 (0%)	88 71	64, 107, 253, 410	0
26	RB	120/122 (98%)	0.02	0	100 100	134, 206, 259, 316	0
26	YB	120/122 (98%)	-0.23	1 (0%)	82 60	109, 145, 180, 228	0
27	RD	275/276 (99%)	0.26	10 (3%)	46 27	78, 116, 157, 200	0
27	YD	275/276 (99%)	0.24	10 (3%)	46 27	69, 104, 150, 199	0
28	RE	204/206 (99%)	0.18	9 (4%)	39 23	83, 129, 169, 227	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YE	204/206 (99%)	0.04	5 (2%) 58 35	79, 116, 169, 224	0
29	RF	202/210 (96%)	0.18	8 (3%) 42 25	90, 131, 192, 214	0
29	YF	202/210 (96%)	0.24	4 (1%) 65 39	73, 122, 188, 231	0
30	RG	181/182 (99%)	0.32	11 (6%) 27 17	140, 209, 252, 313	0
30	YG	181/182 (99%)	-0.23	1 (0%) 85 65	82, 142, 202, 249	0
31	RH	174/180 (96%)	0.00	4 (2%) 61 37	141, 215, 271, 348	0
31	YH	173/180 (96%)	-0.01	4 (2%) 61 37	76, 124, 173, 210	0
32	RI	146/148 (98%)	-0.16	1 (0%) 84 62	102, 171, 219, 267	0
32	YI	146/148 (98%)	-0.15	1 (0%) 84 62	94, 159, 224, 262	0
33	RN	140/140 (100%)	0.06	3 (2%) 63 38	87, 141, 191, 225	0
33	YN	140/140 (100%)	0.10	5 (3%) 46 27	62, 117, 179, 216	0
34	RO	122/122 (100%)	0.27	5 (4%) 41 24	86, 125, 169, 203	0
34	YO	122/122 (100%)	0.08	5 (4%) 41 24	66, 115, 150, 243	0
35	RP	149/150 (99%)	0.42	18 (12%) 8 8	79, 145, 196, 235	0
35	YP	149/150 (99%)	0.53	14 (9%) 14 11	83, 121, 174, 229	0
36	RQ	141/141 (100%)	0.33	6 (4%) 40 23	114, 150, 194, 254	0
36	YQ	141/141 (100%)	0.31	4 (2%) 55 32	67, 116, 154, 174	0
37	RR	118/118 (100%)	0.28	2 (1%) 69 42	76, 116, 163, 219	0
37	YR	118/118 (100%)	0.31	4 (3%) 48 28	76, 113, 161, 193	0
38	RS	110/112 (98%)	0.67	8 (7%) 21 15	113, 182, 229, 253	0
38	YS	110/112 (98%)	0.16	1 (0%) 81 57	94, 139, 174, 199	0
39	RT	131/146 (89%)	-0.02	2 (1%) 72 45	78, 131, 202, 244	0
39	YT	131/146 (89%)	-0.03	2 (1%) 72 45	79, 121, 167, 194	0
40	RU	116/118 (98%)	0.46	8 (6%) 23 15	87, 149, 210, 239	0
40	YU	116/118 (98%)	0.26	0 100 100	74, 114, 176, 210	0
41	RV	101/101 (100%)	-0.22	0 100 100	99, 157, 199, 234	0
41	YV	101/101 (100%)	0.08	3 (2%) 52 31	71, 139, 190, 232	0
42	RW	112/113 (99%)	0.20	3 (2%) 56 33	72, 116, 163, 245	0
42	YW	112/113 (99%)	0.07	3 (2%) 56 33	69, 101, 164, 229	0
43	RX	95/96 (98%)	0.35	9 (9%) 14 11	78, 128, 173, 227	0
43	YX	95/96 (98%)	0.21	1 (1%) 78 53	75, 109, 163, 224	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RY	107/110 (97%)	0.45	10 (9%) 14 11	93, 159, 200, 236	0
44	YY	107/110 (97%)	0.22	3 (2%) 55 32	92, 136, 194, 270	0
45	RZ	196/206 (95%)	-0.09	2 (1%) 79 54	136, 190, 246, 271	0
45	YZ	183/206 (88%)	0.01	4 (2%) 62 37	94, 144, 211, 256	0
46	R0	77/85 (90%)	0.27	3 (3%) 43 26	102, 151, 176, 187	0
46	Y0	77/85 (90%)	0.23	3 (3%) 43 26	89, 122, 146, 180	0
47	R1	97/98 (98%)	0.59	9 (9%) 14 11	83, 134, 192, 221	0
47	Y1	97/98 (98%)	0.30	3 (3%) 51 30	74, 124, 179, 211	0
48	R2	70/72 (97%)	0.22	3 (4%) 40 23	68, 152, 193, 217	0
48	Y2	70/72 (97%)	0.17	2 (2%) 53 31	77, 121, 166, 206	0
49	R3	59/60 (98%)	-0.07	1 (1%) 69 42	102, 154, 208, 222	0
49	Y3	59/60 (98%)	0.17	1 (1%) 69 42	92, 119, 178, 208	0
50	R4	69/71 (97%)	-0.02	2 (2%) 53 31	170, 232, 315, 373	0
50	Y4	69/71 (97%)	-0.30	0 100 100	139, 188, 262, 312	0
51	R5	59/60 (98%)	0.09	2 (3%) 48 28	81, 129, 205, 229	0
51	Y5	58/60 (96%)	0.08	0 100 100	66, 120, 223, 251	0
52	R6	53/54 (98%)	0.40	3 (5%) 29 18	207, 303, 328, 345	0
52	Y6	53/54 (98%)	0.70	4 (7%) 20 14	218, 320, 351, 372	0
53	R7	48/49 (97%)	0.73	3 (6%) 26 17	75, 115, 148, 200	0
53	Y7	48/49 (97%)	0.74	7 (14%) 6 6	73, 103, 170, 201	0
54	R8	64/65 (98%)	0.32	3 (4%) 36 22	92, 122, 179, 215	0
54	Y8	64/65 (98%)	0.73	3 (4%) 36 22	82, 114, 154, 221	0
55	R9	37/37 (100%)	1.54	12 (32%) 1 1	186, 253, 325, 353	0
55	Y9	37/37 (100%)	1.90	17 (45%) 0 1	204, 229, 284, 316	0
56	ZA	2/3 (66%)	0.78	0 100 100	116, 116, 116, 152	0
56	ZB	2/3 (66%)	0.51	0 100 100	86, 86, 86, 97	0
All	All	20761/21492 (96%)	0.01	557 (2%) 56 33	62, 144, 253, 424	0

The worst 5 of 557 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	RY	29	GLU	9.4
20	QT	9	ASN	7.3

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Mol	Chain	Res	Type	RSRZ
47	R1	2	SER	7.0
2	QB	163	PHE	6.8
35	RP	74	GLU	6.8

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	M2G	QA	966	25/26	0.84	0.16	174,183,189,190	0
1	PSU	QA	516	20/21	0.85	0.07	180,194,201,203	0
1	2MG	QA	1207	24/25	0.86	0.11	205,208,210,211	0
1	PSU	XA	516	20/21	0.87	0.07	127,131,141,143	0
25	5MU	RA	1915	21/22	0.87	0.07	143,150,164,165	0
1	5MC	QA	1407	21/22	0.89	0.11	155,163,168,170	0
1	4OC	QA	1402	22/23	0.90	0.11	176,191,194,194	0
1	5MC	QA	967	21/22	0.90	0.11	148,156,167,184	0
1	2MG	XA	1207	24/25	0.90	0.08	111,119,125,126	0
25	5MU	YA	1915	21/22	0.90	0.06	128,133,136,138	0
25	OMC	RA	1920	21/22	0.90	0.10	135,144,149,152	0
25	OMU	RA	2552	21/22	0.90	0.12	88,98,119,122	0
25	PSU	YA	1911	20/21	0.91	0.09	103,114,117,119	0
1	5MC	QA	1404	21/22	0.92	0.08	128,135,138,139	0
1	G7M	XA	527	24/25	0.92	0.13	115,119,125,128	0
1	UR3	QA	1498	21/22	0.92	0.11	119,128,137,144	0
25	PSU	RA	1917	20/21	0.92	0.06	116,122,126,129	0
1	UR3	XA	1498	21/22	0.92	0.10	105,112,124,129	0
25	PSU	RA	1911	20/21	0.92	0.07	101,115,132,143	0
25	OMC	YA	1920	21/22	0.93	0.07	87,99,104,105	0
25	2MA	RA	2503	23/24	0.93	0.13	104,116,121,123	0
1	MA6	QA	1518	24/25	0.93	0.16	145,152,155,162	0
1	4OC	XA	1402	22/23	0.94	0.10	105,111,116,118	0
25	5MC	RA	1942	21/22	0.94	0.07	95,102,111,116	0
25	5MC	YA	1942	21/22	0.94	0.07	81,90,107,118	0
25	OMG	RA	2251	24/25	0.94	0.12	79,94,101,115	0
1	5MC	XA	967	21/22	0.94	0.09	124,129,137,147	0
1	G7M	QA	527	24/25	0.94	0.10	154,155,159,160	0
25	OMU	YA	2552	21/22	0.94	0.09	68,80,91,105	0
25	PSU	RA	2605	20/21	0.94	0.13	91,99,103,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	PPU	ZB	3	37/38	0.94	0.16	69,89,143,149	0
1	5MC	XA	1400	21/22	0.95	0.07	116,122,130,134	0
1	5MC	XA	1407	21/22	0.95	0.07	94,99,108,113	0
25	5MC	RA	1962	21/22	0.95	0.07	117,122,129,136	0
12	0TD	QL	92	10/11	0.95	0.16	168,188,192,195	0
25	OMG	YA	2251	24/25	0.95	0.15	68,77,89,100	0
1	M2G	XA	966	25/26	0.95	0.09	120,129,137,138	0
25	2MA	YA	2503	23/24	0.95	0.09	66,80,90,97	0
1	5MC	QA	1400	21/22	0.95	0.08	160,166,172,174	0
1	MA6	XA	1518	24/25	0.95	0.10	97,106,122,125	0
1	MA6	QA	1519	24/25	0.95	0.14	144,152,161,162	0
25	PSU	YA	2605	20/21	0.95	0.09	71,80,89,89	0
25	5MU	YA	1939	21/22	0.95	0.09	78,85,94,95	0
1	MA6	XA	1519	24/25	0.96	0.11	81,94,109,113	0
1	5MC	XA	1404	21/22	0.96	0.07	92,106,113,114	0
25	5MC	YA	1962	21/22	0.96	0.08	86,98,104,109	0
25	5MU	RA	1939	21/22	0.96	0.11	89,108,119,121	0
12	0TD	XL	92	10/11	0.96	0.14	143,157,176,178	0
56	PPU	ZA	3	37/38	0.96	0.13	65,80,98,115	0
25	PSU	YA	1917	20/21	0.96	0.06	105,118,129,129	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3333	1/1	0.06	0.23	94,94,94,94	0
57	MG	RA	3341	1/1	0.22	0.16	86,86,86,86	0
57	MG	XA	1648	1/1	0.39	0.24	118,118,118,118	0
57	MG	RA	3356	1/1	0.40	0.12	180,180,180,180	0
59	ZN	R9	102	1/1	0.44	0.37	209,209,209,209	0
57	MG	XA	1665	1/1	0.47	0.14	98,98,98,98	0
57	MG	RA	3390	1/1	0.47	0.12	129,129,129,129	0
57	MG	RA	3342	1/1	0.49	0.16	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QD	301	1/1	0.51	0.13	117,117,117,117	0
57	MG	YD	301	1/1	0.53	0.26	65,65,65,65	0
57	MG	QA	1650	1/1	0.53	0.17	107,107,107,107	0
57	MG	YA	3388	1/1	0.54	0.18	78,78,78,78	0
57	MG	RA	3365	1/1	0.54	0.14	96,96,96,96	0
57	MG	RA	3361	1/1	0.54	0.10	92,92,92,92	0
57	MG	YA	3109	1/1	0.56	0.17	199,199,199,199	0
57	MG	YA	3147	1/1	0.57	0.14	82,82,82,82	0
57	MG	QA	1681	1/1	0.57	0.14	97,97,97,97	0
57	MG	QA	1688	1/1	0.57	0.11	100,100,100,100	0
57	MG	XA	1615	1/1	0.57	0.31	78,78,78,78	0
57	MG	YA	3011	1/1	0.58	0.19	110,110,110,110	0
57	MG	YA	3026	1/1	0.58	0.32	83,83,83,83	0
57	MG	YA	3305	1/1	0.58	0.12	74,74,74,74	0
57	MG	RA	3196	1/1	0.59	0.22	96,96,96,96	0
57	MG	RA	3199	1/1	0.60	0.20	78,78,78,78	0
57	MG	RA	3369	1/1	0.60	0.11	51,51,51,51	0
57	MG	YA	3080	1/1	0.60	0.10	82,82,82,82	0
57	MG	RA	3252	1/1	0.61	0.26	76,76,76,76	0
57	MG	RA	3394	1/1	0.61	0.14	70,70,70,70	0
57	MG	RA	3258	1/1	0.62	0.21	93,93,93,93	0
57	MG	XA	1690	1/1	0.62	0.16	82,82,82,82	0
57	MG	XX	101	1/1	0.62	0.16	105,105,105,105	0
57	MG	RB	201	1/1	0.62	0.20	90,90,90,90	0
57	MG	QA	1637	1/1	0.62	0.09	83,83,83,83	0
57	MG	QA	1666	1/1	0.62	0.21	87,87,87,87	0
57	MG	YA	3363	1/1	0.63	0.11	94,94,94,94	0
57	MG	YA	3492	1/1	0.63	0.13	72,72,72,72	0
57	MG	YA	3453	1/1	0.64	0.21	72,72,72,72	0
57	MG	R0	101	1/1	0.64	0.11	58,58,58,58	0
57	MG	RA	3098	1/1	0.64	0.56	86,86,86,86	0
57	MG	YA	3060	1/1	0.64	0.12	88,88,88,88	0
57	MG	XA	1660	1/1	0.65	0.17	96,96,96,96	0
57	MG	YA	3475	1/1	0.65	0.18	95,95,95,95	0
57	MG	YA	3073	1/1	0.65	0.22	71,71,71,71	0
57	MG	RZ	301	1/1	0.65	0.07	101,101,101,101	0
57	MG	QA	1620	1/1	0.65	0.08	74,74,74,74	0
57	MG	QA	1715	1/1	0.66	0.08	96,96,96,96	0
57	MG	XA	1671	1/1	0.66	0.10	110,110,110,110	0
57	MG	YA	3356	1/1	0.66	0.13	59,59,59,59	0
57	MG	YA	3039	1/1	0.66	0.17	76,76,76,76	0
57	MG	YA	3058	1/1	0.66	0.21	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3092	1/1	0.67	0.08	93,93,93,93	0
57	MG	YA	3458	1/1	0.67	0.14	111,111,111,111	0
57	MG	RB	208	1/1	0.67	0.13	97,97,97,97	0
57	MG	YA	3128	1/1	0.67	0.20	87,87,87,87	0
57	MG	RF	302	1/1	0.67	0.15	74,74,74,74	0
57	MG	YA	3428	1/1	0.67	0.37	78,78,78,78	0
57	MG	YA	3341	1/1	0.68	0.07	83,83,83,83	0
57	MG	RA	3331	1/1	0.68	0.28	119,119,119,119	0
57	MG	XA	1712	1/1	0.68	0.21	101,101,101,101	0
57	MG	QA	1711	1/1	0.68	0.19	100,100,100,100	0
57	MG	YA	3001	1/1	0.68	0.13	191,191,191,191	0
57	MG	RA	3216	1/1	0.68	0.16	96,96,96,96	0
57	MG	YA	3013	1/1	0.68	0.32	90,90,90,90	0
57	MG	RA	3261	1/1	0.68	0.16	96,96,96,96	0
57	MG	YA	3181	1/1	0.68	0.38	87,87,87,87	0
57	MG	YA	3190	1/1	0.68	0.09	67,67,67,67	0
57	MG	XA	1689	1/1	0.68	0.24	79,79,79,79	0
57	MG	YA	3327	1/1	0.69	0.19	106,106,106,106	0
57	MG	QA	1669	1/1	0.69	0.12	79,79,79,79	0
57	MG	XK	201	1/1	0.69	0.12	116,116,116,116	0
57	MG	RA	3317	1/1	0.69	0.28	89,89,89,89	0
59	ZN	Y4	101	1/1	0.69	0.15	305,305,305,305	0
57	MG	QA	1706	1/1	0.70	0.13	84,84,84,84	0
57	MG	RA	3151	1/1	0.70	0.15	80,80,80,80	0
57	MG	YA	3087	1/1	0.70	0.06	93,93,93,93	0
57	MG	RP	202	1/1	0.70	0.61	52,52,52,52	0
57	MG	RA	3266	1/1	0.70	0.13	97,97,97,97	0
57	MG	YA	3137	1/1	0.70	0.32	96,96,96,96	0
57	MG	RA	3409	1/1	0.70	0.17	80,80,80,80	0
57	MG	RA	3277	1/1	0.70	0.12	96,96,96,96	0
57	MG	YA	3049	1/1	0.70	0.18	99,99,99,99	0
57	MG	XA	1635	1/1	0.70	0.10	82,82,82,82	0
57	MG	YA	3323	1/1	0.70	0.24	51,51,51,51	0
57	MG	XA	1646	1/1	0.70	0.18	90,90,90,90	0
57	MG	YA	3431	1/1	0.71	0.17	74,74,74,74	0
57	MG	YA	3447	1/1	0.71	0.11	62,62,62,62	0
57	MG	RA	3206	1/1	0.71	0.27	118,118,118,118	0
57	MG	RR	201	1/1	0.71	0.16	85,85,85,85	0
57	MG	RW	201	1/1	0.71	0.10	82,82,82,82	0
57	MG	RA	3110	1/1	0.71	0.16	73,73,73,73	0
57	MG	QA	1654	1/1	0.71	0.19	89,89,89,89	0
57	MG	RD	304	1/1	0.71	0.25	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3398	1/1	0.71	0.20	67,67,67,67	0
57	MG	YA	3008	1/1	0.72	0.24	92,92,92,92	0
57	MG	YA	3194	1/1	0.72	0.12	36,36,36,36	0
57	MG	RA	3267	1/1	0.72	0.15	101,101,101,101	0
57	MG	YA	3312	1/1	0.72	0.07	56,56,56,56	0
57	MG	RA	3207	1/1	0.72	0.22	134,134,134,134	0
57	MG	QA	1662	1/1	0.72	0.20	98,98,98,98	0
57	MG	RA	3329	1/1	0.72	0.21	84,84,84,84	0
57	MG	YA	3516	1/1	0.72	0.49	54,54,54,54	0
57	MG	YA	3519	1/1	0.72	0.20	66,66,66,66	0
57	MG	XA	1659	1/1	0.72	0.16	77,77,77,77	0
57	MG	QA	1682	1/1	0.72	0.11	119,119,119,119	0
57	MG	XA	1608	1/1	0.72	0.17	68,68,68,68	0
57	MG	RA	3230	1/1	0.73	0.14	64,64,64,64	0
57	MG	QA	1636	1/1	0.73	0.14	111,111,111,111	0
57	MG	XA	1708	1/1	0.73	0.24	98,98,98,98	0
57	MG	RA	3254	1/1	0.73	0.16	98,98,98,98	0
57	MG	YA	3340	1/1	0.73	0.09	42,42,42,42	0
57	MG	QA	1724	1/1	0.73	0.18	70,70,70,70	0
57	MG	YA	3304	1/1	0.73	0.22	79,79,79,79	0
57	MG	RA	3239	1/1	0.74	0.23	62,62,62,62	0
57	MG	QM	202	1/1	0.74	0.15	72,72,72,72	0
57	MG	RA	3343	1/1	0.74	0.15	91,91,91,91	0
57	MG	RA	3393	1/1	0.74	0.24	112,112,112,112	0
57	MG	YA	3065	1/1	0.74	0.09	102,102,102,102	0
57	MG	RA	3221	1/1	0.74	0.14	80,80,80,80	0
57	MG	RN	201	1/1	0.74	0.12	83,83,83,83	0
57	MG	YA	3538	1/1	0.74	0.17	72,72,72,72	0
57	MG	YA	3398	1/1	0.74	0.12	81,81,81,81	0
57	MG	RN	202	1/1	0.74	0.46	101,101,101,101	0
57	MG	RA	3086	1/1	0.74	0.23	56,56,56,56	0
57	MG	YA	3314	1/1	0.75	0.16	91,91,91,91	0
57	MG	RA	3101	1/1	0.75	0.11	84,84,84,84	0
57	MG	QA	1667	1/1	0.75	0.10	62,62,62,62	0
57	MG	YA	3002	1/1	0.75	0.26	54,54,54,54	0
57	MG	RA	3120	1/1	0.75	0.15	90,90,90,90	0
57	MG	QA	1624	1/1	0.75	0.08	85,85,85,85	0
57	MG	YA	3502	1/1	0.75	0.11	112,112,112,112	0
57	MG	YA	3512	1/1	0.75	0.12	67,67,67,67	0
57	MG	QA	1691	1/1	0.75	0.23	82,82,82,82	0
57	MG	YA	3081	1/1	0.75	0.09	58,58,58,58	0
57	MG	YA	3394	1/1	0.75	0.35	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1630	1/1	0.75	0.16	111,111,111,111	0
57	MG	YA	3418	1/1	0.75	0.15	64,64,64,64	0
57	MG	RA	3270	1/1	0.75	0.15	82,82,82,82	0
57	MG	YA	3462	1/1	0.76	0.23	69,69,69,69	0
57	MG	YA	3247	1/1	0.76	0.24	69,69,69,69	0
57	MG	QA	1615	1/1	0.76	0.10	93,93,93,93	0
57	MG	RA	3351	1/1	0.76	0.09	87,87,87,87	0
57	MG	RA	3244	1/1	0.76	0.08	85,85,85,85	0
57	MG	RA	3227	1/1	0.76	0.08	74,74,74,74	0
57	MG	YA	3153	1/1	0.76	0.15	83,83,83,83	0
57	MG	QA	1694	1/1	0.76	0.09	67,67,67,67	0
57	MG	RA	3404	1/1	0.76	0.23	79,79,79,79	0
57	MG	YA	3191	1/1	0.76	0.23	82,82,82,82	0
57	MG	YA	3102	1/1	0.76	0.09	96,96,96,96	0
57	MG	RA	3211	1/1	0.77	0.12	58,58,58,58	0
57	MG	RA	3133	1/1	0.77	0.16	86,86,86,86	0
57	MG	YA	3066	1/1	0.77	0.15	70,70,70,70	0
57	MG	YA	3040	1/1	0.77	0.07	93,93,93,93	0
57	MG	Y8	101	1/1	0.77	0.19	74,74,74,74	0
57	MG	RA	3251	1/1	0.77	0.07	94,94,94,94	0
57	MG	RA	3219	1/1	0.77	0.15	64,64,64,64	0
57	MG	YA	3286	1/1	0.78	0.37	76,76,76,76	0
57	MG	RA	3379	1/1	0.78	0.28	115,115,115,115	0
57	MG	XA	1723	1/1	0.78	0.09	74,74,74,74	0
57	MG	RA	3289	1/1	0.78	0.15	99,99,99,99	0
57	MG	YA	3456	1/1	0.78	0.10	64,64,64,64	0
57	MG	RA	3339	1/1	0.78	0.07	88,88,88,88	0
57	MG	YA	3317	1/1	0.78	0.22	94,94,94,94	0
57	MG	YA	3041	1/1	0.78	0.10	50,50,50,50	0
57	MG	YA	3285	1/1	0.78	0.26	90,90,90,90	0
57	MG	YA	3068	1/1	0.79	0.12	49,49,49,49	0
57	MG	QN	103	1/1	0.79	0.20	88,88,88,88	0
57	MG	RA	3357	1/1	0.79	0.10	81,81,81,81	0
57	MG	XA	1716	1/1	0.79	0.15	74,74,74,74	0
57	MG	YA	3459	1/1	0.79	0.10	83,83,83,83	0
57	MG	YA	3239	1/1	0.79	0.07	83,83,83,83	0
57	MG	YA	3349	1/1	0.79	0.16	62,62,62,62	0
57	MG	RA	3168	1/1	0.79	0.14	119,119,119,119	0
57	MG	YA	3493	1/1	0.79	0.12	50,50,50,50	0
57	MG	RA	3249	1/1	0.79	0.11	106,106,106,106	0
57	MG	YA	3365	1/1	0.79	0.14	39,39,39,39	0
57	MG	RA	3274	1/1	0.79	0.21	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3290	1/1	0.79	0.23	79,79,79,79	0
57	MG	XA	1687	1/1	0.79	0.10	67,67,67,67	0
57	MG	YA	3543	1/1	0.79	0.19	78,78,78,78	0
57	MG	RA	3372	1/1	0.79	0.11	125,125,125,125	0
57	MG	RA	3149	1/1	0.79	0.05	82,82,82,82	0
57	MG	XA	1704	1/1	0.79	0.25	74,74,74,74	0
57	MG	YA	3437	1/1	0.79	0.25	96,96,96,96	0
57	MG	XA	1678	1/1	0.80	0.06	97,97,97,97	0
57	MG	RA	3301	1/1	0.80	0.08	58,58,58,58	0
57	MG	YA	3296	1/1	0.80	0.08	49,49,49,49	0
57	MG	XA	1606	1/1	0.80	0.07	71,71,71,71	0
57	MG	RA	3304	1/1	0.80	0.08	78,78,78,78	0
57	MG	RA	3376	1/1	0.80	0.10	68,68,68,68	0
57	MG	RA	3309	1/1	0.80	0.10	78,78,78,78	0
57	MG	YA	3133	1/1	0.80	0.11	99,99,99,99	0
57	MG	YA	3136	1/1	0.80	0.23	65,65,65,65	0
57	MG	YA	3472	1/1	0.80	0.13	78,78,78,78	0
57	MG	XA	1645	1/1	0.80	0.09	65,65,65,65	0
57	MG	YA	3487	1/1	0.80	0.12	41,41,41,41	0
57	MG	YA	3138	1/1	0.80	0.07	73,73,73,73	0
57	MG	RA	3348	1/1	0.80	0.09	71,71,71,71	0
57	MG	YA	3343	1/1	0.80	0.13	92,92,92,92	0
57	MG	YA	3055	1/1	0.80	0.11	67,67,67,67	0
57	MG	QA	1604	1/1	0.80	0.18	79,79,79,79	0
57	MG	XA	1726	1/1	0.80	0.27	83,83,83,83	0
57	MG	YA	3536	1/1	0.80	0.41	85,85,85,85	0
57	MG	YA	3061	1/1	0.80	0.11	74,74,74,74	0
57	MG	RA	3242	1/1	0.80	0.12	53,53,53,53	0
57	MG	QE	201	1/1	0.80	0.26	76,76,76,76	0
57	MG	QA	1603	1/1	0.80	0.10	110,110,110,110	0
57	MG	YA	3410	1/1	0.80	0.16	59,59,59,59	0
57	MG	RA	3234	1/1	0.80	0.51	94,94,94,94	0
57	MG	QA	1677	1/1	0.81	0.08	58,58,58,58	0
57	MG	YA	3230	1/1	0.81	0.15	106,106,106,106	0
57	MG	RA	3018	1/1	0.81	0.25	35,35,35,35	0
57	MG	YA	3071	1/1	0.81	0.18	67,67,67,67	0
57	MG	YA	3281	1/1	0.81	0.13	61,61,61,61	0
57	MG	RA	3330	1/1	0.81	0.26	84,84,84,84	0
57	MG	YA	3452	1/1	0.81	0.13	51,51,51,51	0
57	MG	RF	305	1/1	0.81	0.10	82,82,82,82	0
57	MG	RA	3056	1/1	0.81	0.36	69,69,69,69	0
57	MG	RA	3139	1/1	0.81	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3273	1/1	0.81	0.22	75,75,75,75	0
57	MG	YA	3108	1/1	0.81	0.17	74,74,74,74	0
57	MG	QA	1629	1/1	0.81	0.25	77,77,77,77	0
57	MG	YA	3110	1/1	0.81	0.09	55,55,55,55	0
57	MG	YA	3117	1/1	0.81	0.14	56,56,56,56	0
57	MG	YA	3031	1/1	0.81	0.07	60,60,60,60	0
57	MG	QA	1608	1/1	0.81	0.27	97,97,97,97	0
57	MG	QA	1683	1/1	0.81	0.12	91,91,91,91	0
57	MG	RA	3195	1/1	0.81	0.09	85,85,85,85	0
57	MG	RA	3256	1/1	0.81	0.23	88,88,88,88	0
57	MG	QA	1684	1/1	0.81	0.16	84,84,84,84	0
57	MG	XA	1611	1/1	0.81	0.07	82,82,82,82	0
57	MG	YA	3154	1/1	0.81	0.06	92,92,92,92	0
57	MG	RA	3311	1/1	0.81	0.11	100,100,100,100	0
57	MG	YA	3369	1/1	0.81	0.09	61,61,61,61	0
57	MG	Y1	103	1/1	0.81	0.07	92,92,92,92	0
57	MG	Y3	101	1/1	0.81	0.22	70,70,70,70	0
57	MG	YA	3189	1/1	0.81	0.28	94,94,94,94	0
57	MG	RB	205	1/1	0.81	0.08	151,151,151,151	0
57	MG	XA	1644	1/1	0.81	0.14	86,86,86,86	0
57	MG	YA	3228	1/1	0.82	0.08	33,33,33,33	0
57	MG	YA	3417	1/1	0.82	0.07	55,55,55,55	0
57	MG	QA	1644	1/1	0.82	0.18	71,71,71,71	0
57	MG	QA	1647	1/1	0.82	0.10	67,67,67,67	0
57	MG	RA	3161	1/1	0.82	0.17	107,107,107,107	0
57	MG	YA	3252	1/1	0.82	0.12	55,55,55,55	0
57	MG	YA	3082	1/1	0.82	0.25	48,48,48,48	0
57	MG	RD	301	1/1	0.82	0.26	101,101,101,101	0
57	MG	QA	1692	1/1	0.82	0.13	75,75,75,75	0
57	MG	RA	3192	1/1	0.82	0.12	66,66,66,66	0
57	MG	RA	3223	1/1	0.82	0.26	76,76,76,76	0
57	MG	YA	3018	1/1	0.82	0.17	61,61,61,61	0
57	MG	QA	1676	1/1	0.82	0.14	68,68,68,68	0
57	MG	YA	3126	1/1	0.82	0.09	94,94,94,94	0
57	MG	RA	3375	1/1	0.82	0.10	55,55,55,55	0
57	MG	RA	3127	1/1	0.82	0.09	27,27,27,27	0
57	MG	QD	302	1/1	0.82	0.14	104,104,104,104	0
57	MG	YA	3326	1/1	0.82	0.15	71,71,71,71	0
57	MG	RA	3269	1/1	0.82	0.11	64,64,64,64	0
57	MG	RA	3201	1/1	0.82	0.17	48,48,48,48	0
57	MG	XA	1702	1/1	0.82	0.14	89,89,89,89	0
57	MG	RA	3205	1/1	0.82	0.11	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1633	1/1	0.82	0.14	68,68,68,68	0
57	MG	YA	3158	1/1	0.82	0.11	68,68,68,68	0
57	MG	YA	3160	1/1	0.82	0.29	65,65,65,65	0
57	MG	RA	3401	1/1	0.82	0.09	66,66,66,66	0
57	MG	YT	201	1/1	0.82	0.11	93,93,93,93	0
57	MG	YA	3368	1/1	0.82	0.15	61,61,61,61	0
57	MG	RA	3246	1/1	0.82	0.14	64,64,64,64	0
57	MG	RA	3286	1/1	0.82	0.11	60,60,60,60	0
59	ZN	R4	101	1/1	0.82	0.25	199,199,199,199	0
57	MG	XA	1627	1/1	0.82	0.07	72,72,72,72	0
57	MG	XJ	401	1/1	0.82	0.08	111,111,111,111	0
57	MG	QA	1704	1/1	0.83	0.11	108,108,108,108	0
57	MG	RA	3340	1/1	0.83	0.11	100,100,100,100	0
57	MG	RA	3175	1/1	0.83	0.19	61,61,61,61	0
57	MG	YA	3449	1/1	0.83	0.16	46,46,46,46	0
57	MG	R5	3600	1/1	0.83	0.16	96,96,96,96	0
57	MG	RA	3288	1/1	0.83	0.20	127,127,127,127	0
57	MG	RA	3255	1/1	0.83	0.19	79,79,79,79	0
57	MG	YA	3146	1/1	0.83	0.06	76,76,76,76	0
57	MG	RA	3290	1/1	0.83	0.21	75,75,75,75	0
57	MG	RA	3300	1/1	0.83	0.11	68,68,68,68	0
57	MG	QA	1660	1/1	0.83	0.08	63,63,63,63	0
57	MG	QA	1634	1/1	0.83	0.16	99,99,99,99	0
57	MG	YA	3331	1/1	0.83	0.10	69,69,69,69	0
57	MG	XA	1728	1/1	0.83	0.19	83,83,83,83	0
57	MG	XA	1636	1/1	0.83	0.12	81,81,81,81	0
57	MG	RA	3215	1/1	0.83	0.12	78,78,78,78	0
57	MG	RD	302	1/1	0.83	0.12	82,82,82,82	0
57	MG	RA	3152	1/1	0.83	0.06	51,51,51,51	0
57	MG	YA	3361	1/1	0.83	0.30	69,69,69,69	0
57	MG	RA	3313	1/1	0.83	0.08	105,105,105,105	0
57	MG	RA	3243	1/1	0.83	0.06	74,74,74,74	0
57	MG	YA	3539	1/1	0.83	0.12	94,94,94,94	0
57	MG	RA	3218	1/1	0.83	0.07	52,52,52,52	0
57	MG	YA	3235	1/1	0.83	0.36	85,85,85,85	0
57	MG	YA	3107	1/1	0.83	0.19	89,89,89,89	0
57	MG	Y1	102	1/1	0.83	0.12	74,74,74,74	0
57	MG	YA	3240	1/1	0.83	0.05	49,49,49,49	0
57	MG	RA	3154	1/1	0.83	0.17	77,77,77,77	0
57	MG	YA	3248	1/1	0.83	0.14	72,72,72,72	0
57	MG	XA	1667	1/1	0.83	0.14	75,75,75,75	0
57	MG	QA	1648	1/1	0.83	0.09	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3222	1/1	0.83	0.12	102,102,102,102	0
57	MG	XA	1710	1/1	0.84	0.17	73,73,73,73	0
57	MG	QA	1651	1/1	0.84	0.22	60,60,60,60	0
57	MG	RA	3405	1/1	0.84	0.08	93,93,93,93	0
57	MG	XA	1720	1/1	0.84	0.09	67,67,67,67	0
57	MG	XA	1658	1/1	0.84	0.07	62,62,62,62	0
57	MG	YA	3241	1/1	0.84	0.23	30,30,30,30	0
57	MG	YA	3490	1/1	0.84	0.07	64,64,64,64	0
57	MG	RA	3126	1/1	0.84	0.07	73,73,73,73	0
57	MG	QA	1717	1/1	0.84	0.14	69,69,69,69	0
57	MG	RA	3235	1/1	0.84	0.21	46,46,46,46	0
57	MG	YA	3273	1/1	0.84	0.21	86,86,86,86	0
57	MG	YA	3387	1/1	0.84	0.10	59,59,59,59	0
57	MG	RA	3336	1/1	0.84	0.07	66,66,66,66	0
57	MG	RA	3253	1/1	0.84	0.13	73,73,73,73	0
57	MG	XA	1675	1/1	0.84	0.17	65,65,65,65	0
57	MG	QA	1618	1/1	0.84	0.19	71,71,71,71	0
57	MG	RA	3305	1/1	0.84	0.12	111,111,111,111	0
57	MG	QA	1649	1/1	0.84	0.24	68,68,68,68	0
57	MG	QA	1626	1/1	0.84	0.11	61,61,61,61	0
57	MG	YW	201	1/1	0.84	0.09	104,104,104,104	0
57	MG	RA	3284	1/1	0.84	0.12	86,86,86,86	0
57	MG	YA	3169	1/1	0.84	0.07	32,32,32,32	0
57	MG	RA	3117	1/1	0.84	0.16	56,56,56,56	0
57	MG	Y5	101	1/1	0.84	0.11	82,82,82,82	0
57	MG	Y6	101	1/1	0.84	0.13	68,68,68,68	0
57	MG	YA	3089	1/1	0.84	0.05	79,79,79,79	0
57	MG	YA	3093	1/1	0.84	0.17	74,74,74,74	0
57	MG	RA	3327	1/1	0.84	0.11	64,64,64,64	0
57	MG	YA	3035	1/1	0.84	0.12	68,68,68,68	0
57	MG	RA	3399	1/1	0.85	0.15	77,77,77,77	0
57	MG	YA	3322	1/1	0.85	0.16	35,35,35,35	0
57	MG	RA	3292	1/1	0.85	0.13	65,65,65,65	0
57	MG	YA	3513	1/1	0.85	0.24	73,73,73,73	0
57	MG	RA	3203	1/1	0.85	0.12	52,52,52,52	0
57	MG	RA	3143	1/1	0.85	0.07	93,93,93,93	0
57	MG	YA	3525	1/1	0.85	0.10	65,65,65,65	0
57	MG	YA	3532	1/1	0.85	0.09	64,64,64,64	0
57	MG	YA	3534	1/1	0.85	0.11	42,42,42,42	0
57	MG	XA	1679	1/1	0.85	0.17	104,104,104,104	0
57	MG	XD	301	1/1	0.85	0.21	77,77,77,77	0
57	MG	YA	3047	1/1	0.85	0.14	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3268	1/1	0.85	0.07	86,86,86,86	0
57	MG	RF	304	1/1	0.85	0.15	106,106,106,106	0
57	MG	YE	306	1/1	0.85	0.17	48,48,48,48	0
57	MG	YA	3353	1/1	0.85	0.14	40,40,40,40	0
57	MG	R6	101	1/1	0.85	0.07	93,93,93,93	0
57	MG	RA	3077	1/1	0.85	0.17	54,54,54,54	0
57	MG	XA	1700	1/1	0.85	0.20	70,70,70,70	0
57	MG	QA	1686	1/1	0.85	0.11	72,72,72,72	0
57	MG	YA	3466	1/1	0.85	0.13	82,82,82,82	0
57	MG	XA	1610	1/1	0.85	0.05	72,72,72,72	0
57	MG	QA	1625	1/1	0.85	0.08	77,77,77,77	0
57	MG	XA	1663	1/1	0.85	0.09	86,86,86,86	0
57	MG	YA	3131	1/1	0.85	0.17	69,69,69,69	0
57	MG	RA	3189	1/1	0.85	0.19	100,100,100,100	0
57	MG	YA	3265	1/1	0.86	0.10	52,52,52,52	0
57	MG	YA	3267	1/1	0.86	0.05	69,69,69,69	0
57	MG	RE	305	1/1	0.86	0.07	85,85,85,85	0
57	MG	YA	3440	1/1	0.86	0.14	37,37,37,37	0
57	MG	YA	3272	1/1	0.86	0.09	80,80,80,80	0
57	MG	RA	3006	1/1	0.86	0.06	68,68,68,68	0
57	MG	QA	1628	1/1	0.86	0.15	106,106,106,106	0
57	MG	RA	3214	1/1	0.86	0.24	68,68,68,68	0
57	MG	XA	1666	1/1	0.86	0.08	73,73,73,73	0
57	MG	RA	3040	1/1	0.86	0.18	46,46,46,46	0
57	MG	XA	1669	1/1	0.86	0.12	54,54,54,54	0
57	MG	RA	3177	1/1	0.86	0.24	39,39,39,39	0
57	MG	RA	3377	1/1	0.86	0.27	82,82,82,82	0
57	MG	YA	3038	1/1	0.86	0.27	71,71,71,71	0
57	MG	RA	3378	1/1	0.86	0.07	93,93,93,93	0
57	MG	YA	3315	1/1	0.86	0.08	89,89,89,89	0
57	MG	RA	3280	1/1	0.86	0.14	80,80,80,80	0
57	MG	YA	3318	1/1	0.86	0.22	68,68,68,68	0
57	MG	RA	3184	1/1	0.86	0.21	90,90,90,90	0
57	MG	QA	1721	1/1	0.86	0.06	91,91,91,91	0
57	MG	QA	1638	1/1	0.86	0.13	67,67,67,67	0
57	MG	YA	3053	1/1	0.86	0.07	64,64,64,64	0
57	MG	YA	3330	1/1	0.86	0.15	59,59,59,59	0
57	MG	RA	3135	1/1	0.86	0.06	62,62,62,62	0
57	MG	YA	3523	1/1	0.86	0.14	62,62,62,62	0
57	MG	QA	1655	1/1	0.86	0.08	61,61,61,61	0
57	MG	RA	3291	1/1	0.86	0.11	74,74,74,74	0
57	MG	QA	1670	1/1	0.86	0.05	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3187	1/1	0.86	0.06	82,82,82,82	0
57	MG	RA	3299	1/1	0.86	0.16	99,99,99,99	0
57	MG	QA	1685	1/1	0.86	0.22	100,100,100,100	0
57	MG	YA	3067	1/1	0.86	0.12	76,76,76,76	0
57	MG	YB	207	1/1	0.86	0.06	73,73,73,73	0
57	MG	RA	3410	1/1	0.86	0.20	100,100,100,100	0
57	MG	YD	303	1/1	0.86	0.12	87,87,87,87	0
57	MG	YE	303	1/1	0.86	0.10	41,41,41,41	0
57	MG	RA	3411	1/1	0.86	0.20	86,86,86,86	0
57	MG	YQ	202	1/1	0.86	0.07	57,57,57,57	0
57	MG	RA	3099	1/1	0.86	0.10	70,70,70,70	0
57	MG	RA	3303	1/1	0.86	0.15	81,81,81,81	0
57	MG	YA	3371	1/1	0.86	0.09	66,66,66,66	0
57	MG	RA	3355	1/1	0.86	0.07	45,45,45,45	0
57	MG	QA	1643	1/1	0.86	0.07	79,79,79,79	0
57	MG	YA	3392	1/1	0.86	0.12	74,74,74,74	0
57	MG	QA	1623	1/1	0.86	0.04	95,95,95,95	0
57	MG	XA	1651	1/1	0.86	0.19	69,69,69,69	0
57	MG	XN	101	1/1	0.86	0.27	72,72,72,72	0
57	MG	RA	3307	1/1	0.86	0.14	73,73,73,73	0
57	MG	YA	3262	1/1	0.86	0.08	61,61,61,61	0
57	MG	RA	3121	1/1	0.87	0.13	51,51,51,51	0
57	MG	QA	1722	1/1	0.87	0.10	84,84,84,84	0
57	MG	XA	1724	1/1	0.87	0.08	86,86,86,86	0
57	MG	YA	3379	1/1	0.87	0.16	73,73,73,73	0
57	MG	YA	3383	1/1	0.87	0.10	70,70,70,70	0
57	MG	YA	3386	1/1	0.87	0.25	76,76,76,76	0
57	MG	YA	3295	1/1	0.87	0.12	73,73,73,73	0
57	MG	RA	3210	1/1	0.87	0.10	92,92,92,92	0
57	MG	YA	3104	1/1	0.87	0.07	36,36,36,36	0
57	MG	RA	3028	1/1	0.87	0.23	33,33,33,33	0
57	MG	YA	3528	1/1	0.87	0.08	64,64,64,64	0
57	MG	XA	1631	1/1	0.87	0.04	78,78,78,78	0
57	MG	YA	3408	1/1	0.87	0.14	64,64,64,64	0
57	MG	YA	3052	1/1	0.87	0.09	57,57,57,57	0
57	MG	QA	1673	1/1	0.87	0.14	76,76,76,76	0
57	MG	RA	3197	1/1	0.87	0.20	72,72,72,72	0
57	MG	YA	3232	1/1	0.87	0.10	79,79,79,79	0
57	MG	XA	1684	1/1	0.87	0.17	51,51,51,51	0
57	MG	QA	1718	1/1	0.87	0.07	111,111,111,111	0
57	MG	RA	3217	1/1	0.87	0.05	74,74,74,74	0
57	MG	QV	101	1/1	0.87	0.09	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3265	1/1	0.87	0.07	66,66,66,66	0
57	MG	RA	3083	1/1	0.87	0.08	50,50,50,50	0
57	MG	YA	3012	1/1	0.87	0.05	60,60,60,60	0
57	MG	YV	201	1/1	0.87	0.08	106,106,106,106	0
57	MG	YA	3455	1/1	0.87	0.15	51,51,51,51	0
57	MG	RA	3344	1/1	0.87	0.12	61,61,61,61	0
57	MG	QA	1709	1/1	0.87	0.14	81,81,81,81	0
57	MG	YA	3149	1/1	0.87	0.13	63,63,63,63	0
57	MG	YA	3152	1/1	0.87	0.09	104,104,104,104	0
57	MG	YA	3464	1/1	0.87	0.13	73,73,73,73	0
57	MG	R7	101	1/1	0.87	0.10	86,86,86,86	0
57	MG	RA	3391	1/1	0.87	0.05	43,43,43,43	0
57	MG	YA	3278	1/1	0.87	0.17	96,96,96,96	0
57	MG	RA	3325	1/1	0.87	0.17	89,89,89,89	0
57	MG	RA	3193	1/1	0.88	0.12	37,37,37,37	0
57	MG	YA	3483	1/1	0.88	0.09	103,103,103,103	0
57	MG	R1	101	1/1	0.88	0.08	86,86,86,86	0
57	MG	XA	1664	1/1	0.88	0.11	79,79,79,79	0
57	MG	YA	3142	1/1	0.88	0.06	65,65,65,65	0
57	MG	RA	3366	1/1	0.88	0.09	48,48,48,48	0
57	MG	YA	3063	1/1	0.88	0.10	66,66,66,66	0
57	MG	YA	3509	1/1	0.88	0.05	77,77,77,77	0
57	MG	YA	3511	1/1	0.88	0.09	24,24,24,24	0
57	MG	QA	1656	1/1	0.88	0.06	74,74,74,74	0
57	MG	YA	3150	1/1	0.88	0.11	58,58,58,58	0
57	MG	RA	3371	1/1	0.88	0.12	52,52,52,52	0
57	MG	R9	101	1/1	0.88	0.12	81,81,81,81	0
57	MG	YA	3521	1/1	0.88	0.17	69,69,69,69	0
57	MG	RA	3334	1/1	0.88	0.10	121,121,121,121	0
57	MG	RA	3114	1/1	0.88	0.13	45,45,45,45	0
57	MG	YA	3393	1/1	0.88	0.08	48,48,48,48	0
57	MG	RA	3115	1/1	0.88	0.14	75,75,75,75	0
57	MG	YA	3004	1/1	0.88	0.06	67,67,67,67	0
57	MG	RA	3198	1/1	0.88	0.09	52,52,52,52	0
57	MG	RA	3162	1/1	0.88	0.12	66,66,66,66	0
57	MG	XA	1622	1/1	0.88	0.05	71,71,71,71	0
57	MG	RD	305	1/1	0.88	0.09	93,93,93,93	0
57	MG	YA	3422	1/1	0.88	0.07	56,56,56,56	0
57	MG	YA	3316	1/1	0.88	0.07	76,76,76,76	0
57	MG	QA	1710	1/1	0.88	0.10	70,70,70,70	0
57	MG	RA	3057	1/1	0.88	0.19	34,34,34,34	0
57	MG	YA	3223	1/1	0.88	0.08	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3446	1/1	0.88	0.19	59,59,59,59	0
57	MG	RA	3144	1/1	0.88	0.31	97,97,97,97	0
57	MG	RA	3179	1/1	0.88	0.13	95,95,95,95	0
57	MG	YA	3231	1/1	0.88	0.21	57,57,57,57	0
57	MG	RA	3183	1/1	0.88	0.15	36,36,36,36	0
57	MG	RA	3354	1/1	0.88	0.12	58,58,58,58	0
57	MG	XA	1711	1/1	0.88	0.05	59,59,59,59	0
57	MG	RA	3145	1/1	0.88	0.08	75,75,75,75	0
57	MG	YA	3342	1/1	0.88	0.34	60,60,60,60	0
57	MG	XA	1715	1/1	0.88	0.09	64,64,64,64	0
57	MG	QA	1680	1/1	0.88	0.11	82,82,82,82	0
57	MG	RA	3035	1/1	0.88	0.08	42,42,42,42	0
57	MG	RA	3295	1/1	0.88	0.05	115,115,115,115	0
57	MG	YA	3024	1/1	0.89	0.26	82,82,82,82	0
57	MG	YA	3025	1/1	0.89	0.21	67,67,67,67	0
57	MG	RA	3247	1/1	0.89	0.05	92,92,92,92	0
57	MG	QO	101	1/1	0.89	0.30	92,92,92,92	0
57	MG	RA	3185	1/1	0.89	0.20	83,83,83,83	0
57	MG	XA	1682	1/1	0.89	0.04	62,62,62,62	0
57	MG	YA	3143	1/1	0.89	0.30	75,75,75,75	0
57	MG	YA	3307	1/1	0.89	0.09	73,73,73,73	0
57	MG	RA	3045	1/1	0.89	0.10	70,70,70,70	0
57	MG	RA	3051	1/1	0.89	0.20	36,36,36,36	0
57	MG	QA	1616	1/1	0.89	0.05	64,64,64,64	0
57	MG	RA	3297	1/1	0.89	0.12	102,102,102,102	0
57	MG	RA	3003	1/1	0.89	0.15	47,47,47,47	0
57	MG	YA	3050	1/1	0.89	0.20	65,65,65,65	0
57	MG	YA	3320	1/1	0.89	0.20	54,54,54,54	0
57	MG	YA	3051	1/1	0.89	0.07	52,52,52,52	0
57	MG	RA	3119	1/1	0.89	0.09	92,92,92,92	0
57	MG	YA	3491	1/1	0.89	0.12	60,60,60,60	0
57	MG	RA	3061	1/1	0.89	0.09	55,55,55,55	0
57	MG	XA	1620	1/1	0.89	0.10	58,58,58,58	0
57	MG	YA	3176	1/1	0.89	0.26	59,59,59,59	0
57	MG	YA	3179	1/1	0.89	0.16	57,57,57,57	0
57	MG	QA	1663	1/1	0.89	0.12	86,86,86,86	0
57	MG	YA	3184	1/1	0.89	0.07	50,50,50,50	0
57	MG	RB	203	1/1	0.89	0.06	90,90,90,90	0
57	MG	RA	3263	1/1	0.89	0.10	62,62,62,62	0
57	MG	XA	1632	1/1	0.89	0.11	75,75,75,75	0
57	MG	YA	3520	1/1	0.89	0.11	77,77,77,77	0
57	MG	RA	3225	1/1	0.89	0.18	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3124	1/1	0.89	0.16	63,63,63,63	0
57	MG	YA	3206	1/1	0.89	0.14	77,77,77,77	0
57	MG	RA	3308	1/1	0.89	0.08	60,60,60,60	0
57	MG	RA	3363	1/1	0.89	0.06	72,72,72,72	0
57	MG	RA	3007	1/1	0.89	0.21	54,54,54,54	0
57	MG	XA	1727	1/1	0.89	0.07	52,52,52,52	0
57	MG	RE	304	1/1	0.89	0.19	91,91,91,91	0
57	MG	YA	3374	1/1	0.89	0.12	69,69,69,69	0
57	MG	RA	3172	1/1	0.89	0.17	60,60,60,60	0
57	MG	XA	1656	1/1	0.89	0.07	73,73,73,73	0
57	MG	RA	3173	1/1	0.89	0.16	59,59,59,59	0
57	MG	RA	3236	1/1	0.89	0.12	95,95,95,95	0
57	MG	YA	3245	1/1	0.89	0.15	82,82,82,82	0
57	MG	YA	3391	1/1	0.89	0.07	64,64,64,64	0
57	MG	RA	3323	1/1	0.89	0.14	64,64,64,64	0
57	MG	XA	1662	1/1	0.89	0.06	58,58,58,58	0
57	MG	QA	1696	1/1	0.89	0.12	84,84,84,84	0
57	MG	YA	3261	1/1	0.89	0.12	21,21,21,21	0
57	MG	RA	3275	1/1	0.89	0.10	76,76,76,76	0
57	MG	YA	3264	1/1	0.89	0.11	22,22,22,22	0
57	MG	RA	3328	1/1	0.89	0.08	95,95,95,95	0
57	MG	QA	1703	1/1	0.89	0.08	81,81,81,81	0
57	MG	RA	3031	1/1	0.89	0.09	48,48,48,48	0
57	MG	QA	1610	1/1	0.89	0.06	90,90,90,90	0
57	MG	YA	3118	1/1	0.89	0.17	72,72,72,72	0
57	MG	YA	3017	1/1	0.89	0.18	78,78,78,78	0
57	MG	RA	3212	1/1	0.89	0.06	50,50,50,50	0
57	MG	YA	3141	1/1	0.90	0.09	62,62,62,62	0
57	MG	YA	3282	1/1	0.90	0.16	62,62,62,62	0
57	MG	YA	3284	1/1	0.90	0.23	52,52,52,52	0
57	MG	YA	3432	1/1	0.90	0.08	57,57,57,57	0
57	MG	XA	1693	1/1	0.90	0.11	85,85,85,85	0
57	MG	RD	303	1/1	0.90	0.61	59,59,59,59	0
57	MG	XA	1623	1/1	0.90	0.05	87,87,87,87	0
57	MG	YA	3291	1/1	0.90	0.22	66,66,66,66	0
57	MG	RA	3373	1/1	0.90	0.07	86,86,86,86	0
57	MG	YA	3148	1/1	0.90	0.09	91,91,91,91	0
57	MG	YA	3302	1/1	0.90	0.15	55,55,55,55	0
57	MG	XA	1629	1/1	0.90	0.09	67,67,67,67	0
57	MG	QA	1627	1/1	0.90	0.11	82,82,82,82	0
57	MG	RE	303	1/1	0.90	0.12	52,52,52,52	0
57	MG	RA	3084	1/1	0.90	0.14	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1678	1/1	0.90	0.06	77,77,77,77	0
57	MG	XA	1639	1/1	0.90	0.09	55,55,55,55	0
57	MG	RA	3146	1/1	0.90	0.08	70,70,70,70	0
57	MG	RF	303	1/1	0.90	0.16	60,60,60,60	0
57	MG	YA	3064	1/1	0.90	0.14	91,91,91,91	0
57	MG	RA	3245	1/1	0.90	0.15	90,90,90,90	0
57	MG	YA	3321	1/1	0.90	0.13	42,42,42,42	0
57	MG	QA	1601	1/1	0.90	0.18	54,54,54,54	0
57	MG	QA	1645	1/1	0.90	0.23	80,80,80,80	0
57	MG	YA	3325	1/1	0.90	0.07	63,63,63,63	0
57	MG	QA	1612	1/1	0.90	0.07	101,101,101,101	0
57	MG	RA	3027	1/1	0.90	0.09	56,56,56,56	0
57	MG	YA	3506	1/1	0.90	0.08	58,58,58,58	0
57	MG	YA	3508	1/1	0.90	0.16	51,51,51,51	0
57	MG	RA	3276	1/1	0.90	0.20	71,71,71,71	0
57	MG	RA	3350	1/1	0.90	0.10	68,68,68,68	0
57	MG	RA	3187	1/1	0.90	0.12	89,89,89,89	0
57	MG	YA	3203	1/1	0.90	0.20	32,32,32,32	0
57	MG	RA	3157	1/1	0.90	0.07	50,50,50,50	0
57	MG	YA	3218	1/1	0.90	0.09	71,71,71,71	0
57	MG	RA	3314	1/1	0.90	0.06	119,119,119,119	0
57	MG	YA	3352	1/1	0.90	0.12	64,64,64,64	0
57	MG	R3	101	1/1	0.90	0.20	69,69,69,69	0
57	MG	QA	1708	1/1	0.90	0.04	60,60,60,60	0
57	MG	YA	3101	1/1	0.90	0.10	59,59,59,59	0
57	MG	YA	3006	1/1	0.90	0.12	38,38,38,38	0
57	MG	RA	3318	1/1	0.90	0.10	71,71,71,71	0
57	MG	YA	3535	1/1	0.90	0.25	83,83,83,83	0
57	MG	YA	3367	1/1	0.90	0.10	90,90,90,90	0
57	MG	YA	3537	1/1	0.90	0.24	54,54,54,54	0
57	MG	YA	3238	1/1	0.90	0.29	98,98,98,98	0
57	MG	RA	3071	1/1	0.90	0.24	45,45,45,45	0
57	MG	RA	3412	1/1	0.90	0.18	58,58,58,58	0
57	MG	YB	205	1/1	0.90	0.05	73,73,73,73	0
57	MG	XA	1674	1/1	0.90	0.07	65,65,65,65	0
57	MG	RA	3213	1/1	0.90	0.16	70,70,70,70	0
57	MG	RA	3257	1/1	0.90	0.34	96,96,96,96	0
57	MG	YE	301	1/1	0.90	0.12	24,24,24,24	0
57	MG	YA	3384	1/1	0.90	0.15	80,80,80,80	0
57	MG	YE	305	1/1	0.90	0.07	68,68,68,68	0
57	MG	QA	1639	1/1	0.90	0.08	60,60,60,60	0
57	MG	YA	3120	1/1	0.90	0.09	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3260	1/1	0.90	0.17	58,58,58,58	0
57	MG	YA	3390	1/1	0.90	0.09	71,71,71,71	0
57	MG	YA	3121	1/1	0.90	0.06	82,82,82,82	0
57	MG	YA	3125	1/1	0.90	0.10	76,76,76,76	0
57	MG	XA	1680	1/1	0.90	0.06	86,86,86,86	0
57	MG	RA	3260	1/1	0.90	0.10	45,45,45,45	0
57	MG	RA	3238	1/1	0.90	0.09	106,106,106,106	0
57	MG	YA	3404	1/1	0.90	0.22	38,38,38,38	0
57	MG	XA	1686	1/1	0.90	0.23	41,41,41,41	0
57	MG	XA	1616	1/1	0.90	0.08	68,68,68,68	0
57	MG	XA	1618	1/1	0.90	0.06	51,51,51,51	0
57	MG	RA	3262	1/1	0.90	0.13	67,67,67,67	0
57	MG	RA	3176	1/1	0.91	0.14	71,71,71,71	0
57	MG	YA	3471	1/1	0.91	0.12	32,32,32,32	0
57	MG	RA	3414	1/1	0.91	0.08	68,68,68,68	0
57	MG	XA	1681	1/1	0.91	0.07	77,77,77,77	0
57	MG	YA	3478	1/1	0.91	0.11	67,67,67,67	0
57	MG	YA	3479	1/1	0.91	0.11	58,58,58,58	0
57	MG	YA	3480	1/1	0.91	0.14	47,47,47,47	0
57	MG	YA	3249	1/1	0.91	0.22	42,42,42,42	0
57	MG	QA	1679	1/1	0.91	0.09	82,82,82,82	0
57	MG	QA	1661	1/1	0.91	0.14	82,82,82,82	0
57	MG	YA	3069	1/1	0.91	0.10	41,41,41,41	0
57	MG	RA	3226	1/1	0.91	0.11	64,64,64,64	0
57	MG	YA	3151	1/1	0.91	0.28	60,60,60,60	0
57	MG	YA	3494	1/1	0.91	0.15	75,75,75,75	0
57	MG	RB	206	1/1	0.91	0.12	69,69,69,69	0
57	MG	YA	3505	1/1	0.91	0.13	52,52,52,52	0
57	MG	YA	3075	1/1	0.91	0.17	43,43,43,43	0
57	MG	RA	3049	1/1	0.91	0.09	66,66,66,66	0
57	MG	RA	3022	1/1	0.91	0.22	31,31,31,31	0
57	MG	RA	3319	1/1	0.91	0.09	55,55,55,55	0
57	MG	YA	3162	1/1	0.91	0.19	89,89,89,89	0
57	MG	YA	3382	1/1	0.91	0.11	85,85,85,85	0
57	MG	XA	1652	1/1	0.91	0.13	54,54,54,54	0
57	MG	YA	3019	1/1	0.91	0.11	68,68,68,68	0
57	MG	YA	3283	1/1	0.91	0.23	57,57,57,57	0
57	MG	YA	3023	1/1	0.91	0.05	57,57,57,57	0
57	MG	XA	1653	1/1	0.91	0.07	48,48,48,48	0
57	MG	XA	1703	1/1	0.91	0.09	57,57,57,57	0
57	MG	YA	3289	1/1	0.91	0.14	72,72,72,72	0
57	MG	RA	3381	1/1	0.91	0.08	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3250	1/1	0.91	0.09	47,47,47,47	0
57	MG	XA	1607	1/1	0.91	0.05	71,71,71,71	0
57	MG	RA	3352	1/1	0.91	0.09	69,69,69,69	0
57	MG	RE	302	1/1	0.91	0.09	90,90,90,90	0
57	MG	YA	3198	1/1	0.91	0.07	42,42,42,42	0
57	MG	YA	3199	1/1	0.91	0.06	62,62,62,62	0
57	MG	YA	3541	1/1	0.91	0.15	72,72,72,72	0
57	MG	YA	3415	1/1	0.91	0.29	52,52,52,52	0
57	MG	YB	202	1/1	0.91	0.07	63,63,63,63	0
57	MG	RA	3233	1/1	0.91	0.10	60,60,60,60	0
57	MG	YB	206	1/1	0.91	0.07	69,69,69,69	0
57	MG	RA	3200	1/1	0.91	0.08	61,61,61,61	0
57	MG	YA	3421	1/1	0.91	0.15	53,53,53,53	0
57	MG	RA	3271	1/1	0.91	0.09	56,56,56,56	0
57	MG	YA	3423	1/1	0.91	0.21	17,17,17,17	0
57	MG	YA	3220	1/1	0.91	0.21	25,25,25,25	0
57	MG	XA	1721	1/1	0.91	0.07	71,71,71,71	0
57	MG	RA	3055	1/1	0.91	0.05	74,74,74,74	0
57	MG	QA	1672	1/1	0.91	0.06	69,69,69,69	0
57	MG	XA	1668	1/1	0.91	0.06	64,64,64,64	0
57	MG	YU	201	1/1	0.91	0.09	65,65,65,65	0
57	MG	RA	3237	1/1	0.91	0.17	72,72,72,72	0
57	MG	QA	1705	1/1	0.91	0.05	61,61,61,61	0
57	MG	YA	3236	1/1	0.91	0.11	71,71,71,71	0
57	MG	YA	3237	1/1	0.91	0.11	66,66,66,66	0
57	MG	QA	1693	1/1	0.91	0.07	69,69,69,69	0
57	MG	RA	3278	1/1	0.91	0.05	90,90,90,90	0
57	MG	XA	1677	1/1	0.91	0.08	78,78,78,78	0
57	MG	QA	1607	1/1	0.91	0.12	133,133,133,133	0
59	ZN	QN	102	1/1	0.91	0.09	145,145,145,145	0
57	MG	YA	3336	1/1	0.91	0.18	42,42,42,42	0
57	MG	YA	3243	1/1	0.91	0.15	63,63,63,63	0
57	MG	YA	3244	1/1	0.91	0.07	51,51,51,51	0
57	MG	RV	201	1/1	0.92	0.24	86,86,86,86	0
57	MG	YA	3186	1/1	0.92	0.04	42,42,42,42	0
57	MG	YA	3313	1/1	0.92	0.30	77,77,77,77	0
57	MG	RA	3171	1/1	0.92	0.06	43,43,43,43	0
57	MG	RA	3316	1/1	0.92	0.07	79,79,79,79	0
57	MG	QA	1701	1/1	0.92	0.12	83,83,83,83	0
57	MG	XA	1661	1/1	0.92	0.07	78,78,78,78	0
57	MG	YA	3460	1/1	0.92	0.17	48,48,48,48	0
57	MG	YA	3192	1/1	0.92	0.07	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3079	1/1	0.92	0.06	90,90,90,90	0
57	MG	RA	3402	1/1	0.92	0.10	55,55,55,55	0
57	MG	YA	3467	1/1	0.92	0.22	82,82,82,82	0
57	MG	RA	3009	1/1	0.92	0.19	29,29,29,29	0
57	MG	QA	1617	1/1	0.92	0.07	118,118,118,118	0
57	MG	YA	3084	1/1	0.92	0.14	58,58,58,58	0
57	MG	YA	3212	1/1	0.92	0.09	65,65,65,65	0
57	MG	RA	3232	1/1	0.92	0.18	81,81,81,81	0
57	MG	RA	3358	1/1	0.92	0.06	67,67,67,67	0
57	MG	RA	3141	1/1	0.92	0.19	78,78,78,78	0
57	MG	YA	3333	1/1	0.92	0.17	57,57,57,57	0
57	MG	XA	1601	1/1	0.92	0.15	67,67,67,67	0
57	MG	YA	3005	1/1	0.92	0.08	61,61,61,61	0
57	MG	RA	3142	1/1	0.92	0.15	67,67,67,67	0
57	MG	RA	3364	1/1	0.92	0.17	73,73,73,73	0
57	MG	RA	3209	1/1	0.92	0.12	45,45,45,45	0
57	MG	YA	3347	1/1	0.92	0.17	60,60,60,60	0
57	MG	RA	3104	1/1	0.92	0.12	48,48,48,48	0
57	MG	RA	3368	1/1	0.92	0.15	59,59,59,59	0
57	MG	YA	3116	1/1	0.92	0.06	87,87,87,87	0
57	MG	YA	3354	1/1	0.92	0.11	86,86,86,86	0
57	MG	YA	3016	1/1	0.92	0.13	62,62,62,62	0
57	MG	YA	3359	1/1	0.92	0.15	63,63,63,63	0
57	MG	XA	1612	1/1	0.92	0.06	92,92,92,92	0
57	MG	XA	1614	1/1	0.92	0.21	68,68,68,68	0
57	MG	YA	3517	1/1	0.92	0.08	59,59,59,59	0
57	MG	RA	3105	1/1	0.92	0.09	59,59,59,59	0
57	MG	RA	3370	1/1	0.92	0.18	52,52,52,52	0
57	MG	QA	1611	1/1	0.92	0.11	63,63,63,63	0
57	MG	RA	3026	1/1	0.92	0.10	38,38,38,38	0
57	MG	YA	3370	1/1	0.92	0.09	73,73,73,73	0
57	MG	YA	3526	1/1	0.92	0.05	53,53,53,53	0
57	MG	XA	1685	1/1	0.92	0.09	75,75,75,75	0
57	MG	YA	3531	1/1	0.92	0.07	63,63,63,63	0
57	MG	YA	3372	1/1	0.92	0.05	68,68,68,68	0
57	MG	YA	3132	1/1	0.92	0.17	127,127,127,127	0
57	MG	YA	3378	1/1	0.92	0.10	59,59,59,59	0
57	MG	RA	3241	1/1	0.92	0.06	26,26,26,26	0
57	MG	YA	3254	1/1	0.92	0.06	33,33,33,33	0
57	MG	QA	1652	1/1	0.92	0.08	62,62,62,62	0
57	MG	YA	3037	1/1	0.92	0.11	40,40,40,40	0
57	MG	YA	3385	1/1	0.92	0.11	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3542	1/1	0.92	0.15	64,64,64,64	0
57	MG	RA	3337	1/1	0.92	0.06	63,63,63,63	0
57	MG	QA	1640	1/1	0.92	0.08	45,45,45,45	0
57	MG	RA	3029	1/1	0.92	0.19	41,41,41,41	0
57	MG	XA	1698	1/1	0.92	0.07	67,67,67,67	0
57	MG	YA	3144	1/1	0.92	0.12	53,53,53,53	0
57	MG	RA	3082	1/1	0.92	0.07	33,33,33,33	0
57	MG	YD	302	1/1	0.92	0.11	91,91,91,91	0
57	MG	QA	1641	1/1	0.92	0.09	39,39,39,39	0
57	MG	YD	308	1/1	0.92	0.12	42,42,42,42	0
57	MG	RA	3383	1/1	0.92	0.16	68,68,68,68	0
57	MG	RA	3384	1/1	0.92	0.26	25,25,25,25	0
57	MG	XA	1707	1/1	0.92	0.12	56,56,56,56	0
57	MG	XA	1641	1/1	0.92	0.07	87,87,87,87	0
57	MG	YQ	201	1/1	0.92	0.08	57,57,57,57	0
57	MG	RA	3160	1/1	0.92	0.17	65,65,65,65	0
57	MG	RA	3002	1/1	0.92	0.15	48,48,48,48	0
57	MG	RA	3392	1/1	0.92	0.20	87,87,87,87	0
57	MG	XA	1713	1/1	0.92	0.18	84,84,84,84	0
57	MG	YA	3420	1/1	0.92	0.15	51,51,51,51	0
57	MG	YA	3062	1/1	0.92	0.09	96,96,96,96	0
57	MG	QA	1609	1/1	0.92	0.20	52,52,52,52	0
57	MG	XA	1649	1/1	0.92	0.09	59,59,59,59	0
57	MG	RO	201	1/1	0.92	0.09	88,88,88,88	0
57	MG	YA	3297	1/1	0.92	0.11	39,39,39,39	0
57	MG	YA	3299	1/1	0.92	0.09	55,55,55,55	0
57	MG	QA	1668	1/1	0.92	0.11	79,79,79,79	0
57	MG	YA	3180	1/1	0.92	0.13	50,50,50,50	0
57	MG	RA	3395	1/1	0.92	0.09	25,25,25,25	0
57	MG	YA	3306	1/1	0.92	0.05	58,58,58,58	0
57	MG	YA	3338	1/1	0.93	0.08	57,57,57,57	0
57	MG	YA	3043	1/1	0.93	0.08	67,67,67,67	0
57	MG	YA	3046	1/1	0.93	0.24	71,71,71,71	0
57	MG	RA	3208	1/1	0.93	0.08	77,77,77,77	0
57	MG	YA	3048	1/1	0.93	0.12	73,73,73,73	0
57	MG	QA	1646	1/1	0.93	0.08	67,67,67,67	0
57	MG	YA	3474	1/1	0.93	0.12	33,33,33,33	0
57	MG	YA	3246	1/1	0.93	0.08	67,67,67,67	0
57	MG	YA	3350	1/1	0.93	0.06	55,55,55,55	0
57	MG	QE	202	1/1	0.93	0.07	108,108,108,108	0
57	MG	RA	3310	1/1	0.93	0.09	107,107,107,107	0
57	MG	RA	3240	1/1	0.93	0.11	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3180	1/1	0.93	0.05	48,48,48,48	0
57	MG	YA	3358	1/1	0.93	0.06	45,45,45,45	0
57	MG	XA	1719	1/1	0.93	0.25	74,74,74,74	0
57	MG	YA	3255	1/1	0.93	0.11	24,24,24,24	0
57	MG	YA	3362	1/1	0.93	0.18	40,40,40,40	0
57	MG	RA	3272	1/1	0.93	0.12	68,68,68,68	0
57	MG	RA	3315	1/1	0.93	0.05	82,82,82,82	0
57	MG	YA	3366	1/1	0.93	0.15	43,43,43,43	0
57	MG	RA	3066	1/1	0.93	0.04	60,60,60,60	0
57	MG	YA	3507	1/1	0.93	0.07	45,45,45,45	0
57	MG	RA	3005	1/1	0.93	0.16	48,48,48,48	0
57	MG	QA	1674	1/1	0.93	0.07	68,68,68,68	0
57	MG	YA	3510	1/1	0.93	0.07	27,27,27,27	0
57	MG	XA	1609	1/1	0.93	0.05	79,79,79,79	0
57	MG	RA	3081	1/1	0.93	0.09	39,39,39,39	0
57	MG	QN	101	1/1	0.93	0.07	66,66,66,66	0
57	MG	YA	3514	1/1	0.93	0.05	57,57,57,57	0
57	MG	RA	3191	1/1	0.93	0.10	64,64,64,64	0
57	MG	YA	3375	1/1	0.93	0.09	27,27,27,27	0
57	MG	YA	3275	1/1	0.93	0.18	40,40,40,40	0
57	MG	YA	3159	1/1	0.93	0.06	80,80,80,80	0
57	MG	YA	3280	1/1	0.93	0.18	63,63,63,63	0
57	MG	XA	1670	1/1	0.93	0.19	91,91,91,91	0
57	MG	RA	3279	1/1	0.93	0.14	64,64,64,64	0
57	MG	YA	3165	1/1	0.93	0.24	54,54,54,54	0
57	MG	XA	1672	1/1	0.93	0.07	52,52,52,52	0
57	MG	YA	3529	1/1	0.93	0.10	40,40,40,40	0
57	MG	YA	3172	1/1	0.93	0.06	50,50,50,50	0
57	MG	YA	3072	1/1	0.93	0.14	65,65,65,65	0
57	MG	YA	3533	1/1	0.93	0.11	57,57,57,57	0
57	MG	YA	3288	1/1	0.93	0.08	34,34,34,34	0
57	MG	YA	3178	1/1	0.93	0.22	35,35,35,35	0
57	MG	RA	3156	1/1	0.93	0.08	88,88,88,88	0
57	MG	QA	1716	1/1	0.93	0.11	74,74,74,74	0
57	MG	RA	3220	1/1	0.93	0.16	33,33,33,33	0
57	MG	YA	3395	1/1	0.93	0.07	71,71,71,71	0
57	MG	YA	3396	1/1	0.93	0.13	53,53,53,53	0
57	MG	RA	3016	1/1	0.93	0.07	27,27,27,27	0
57	MG	RA	3047	1/1	0.93	0.15	35,35,35,35	0
57	MG	YB	201	1/1	0.93	0.04	67,67,67,67	0
57	MG	RA	3087	1/1	0.93	0.16	31,31,31,31	0
57	MG	YA	3409	1/1	0.93	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3164	1/1	0.93	0.06	56,56,56,56	0
57	MG	XA	1628	1/1	0.93	0.05	85,85,85,85	0
57	MG	RF	301	1/1	0.93	0.05	66,66,66,66	0
57	MG	RA	3165	1/1	0.93	0.10	79,79,79,79	0
57	MG	YA	3097	1/1	0.93	0.04	68,68,68,68	0
57	MG	RA	3294	1/1	0.93	0.06	55,55,55,55	0
57	MG	RA	3090	1/1	0.93	0.09	66,66,66,66	0
57	MG	RA	3296	1/1	0.93	0.07	42,42,42,42	0
57	MG	YA	3426	1/1	0.93	0.15	40,40,40,40	0
57	MG	YA	3021	1/1	0.93	0.10	31,31,31,31	0
57	MG	YE	307	1/1	0.93	0.28	95,95,95,95	0
57	MG	YP	203	1/1	0.93	0.07	34,34,34,34	0
57	MG	YA	3211	1/1	0.93	0.08	54,54,54,54	0
57	MG	YA	3022	1/1	0.93	0.05	46,46,46,46	0
57	MG	QA	1675	1/1	0.93	0.14	80,80,80,80	0
57	MG	RA	3259	1/1	0.93	0.12	50,50,50,50	0
57	MG	YA	3445	1/1	0.93	0.08	34,34,34,34	0
57	MG	XA	1642	1/1	0.93	0.09	82,82,82,82	0
57	MG	RA	3020	1/1	0.93	0.14	33,33,33,33	0
57	MG	XA	1701	1/1	0.93	0.05	79,79,79,79	0
57	MG	RA	3204	1/1	0.93	0.18	41,41,41,41	0
57	MG	RA	3053	1/1	0.93	0.07	51,51,51,51	0
57	MG	YA	3454	1/1	0.93	0.15	66,66,66,66	0
57	MG	Y7	101	1/1	0.93	0.14	64,64,64,64	0
57	MG	YA	3124	1/1	0.93	0.06	53,53,53,53	0
57	MG	Y9	101	1/1	0.93	0.07	133,133,133,133	0
57	MG	QA	1605	1/1	0.93	0.05	68,68,68,68	0
57	MG	XA	1705	1/1	0.93	0.12	36,36,36,36	0
57	MG	RA	3400	1/1	0.93	0.06	82,82,82,82	0
57	MG	QV	103	1/1	0.93	0.41	92,92,92,92	0
57	MG	YA	3461	1/1	0.94	0.07	60,60,60,60	0
57	MG	YA	3029	1/1	0.94	0.06	66,66,66,66	0
57	MG	YA	3463	1/1	0.94	0.21	51,51,51,51	0
57	MG	RA	3046	1/1	0.94	0.07	63,63,63,63	0
57	MG	YA	3465	1/1	0.94	0.09	59,59,59,59	0
57	MG	YA	3034	1/1	0.94	0.18	54,54,54,54	0
57	MG	XA	1643	1/1	0.94	0.27	60,60,60,60	0
57	MG	YA	3470	1/1	0.94	0.08	55,55,55,55	0
57	MG	RA	3166	1/1	0.94	0.09	80,80,80,80	0
57	MG	YA	3348	1/1	0.94	0.10	59,59,59,59	0
57	MG	QL	202	1/1	0.94	0.10	70,70,70,70	0
57	MG	RA	3353	1/1	0.94	0.13	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3476	1/1	0.94	0.10	61,61,61,61	0
57	MG	RA	3169	1/1	0.94	0.04	79,79,79,79	0
57	MG	RA	3023	1/1	0.94	0.06	35,35,35,35	0
57	MG	RA	3130	1/1	0.94	0.13	63,63,63,63	0
57	MG	YA	3482	1/1	0.94	0.07	39,39,39,39	0
57	MG	YA	3355	1/1	0.94	0.13	78,78,78,78	0
57	MG	YA	3044	1/1	0.94	0.06	67,67,67,67	0
57	MG	YA	3488	1/1	0.94	0.17	42,42,42,42	0
57	MG	RA	3025	1/1	0.94	0.14	28,28,28,28	0
57	MG	QA	1712	1/1	0.94	0.15	88,88,88,88	0
57	MG	YA	3253	1/1	0.94	0.06	35,35,35,35	0
57	MG	XA	1655	1/1	0.94	0.07	84,84,84,84	0
57	MG	XA	1714	1/1	0.94	0.05	77,77,77,77	0
57	MG	YA	3498	1/1	0.94	0.13	25,25,25,25	0
57	MG	YA	3364	1/1	0.94	0.14	78,78,78,78	0
57	MG	YA	3503	1/1	0.94	0.03	45,45,45,45	0
57	MG	RA	3407	1/1	0.94	0.06	48,48,48,48	0
57	MG	XA	1657	1/1	0.94	0.05	51,51,51,51	0
57	MG	XA	1718	1/1	0.94	0.06	66,66,66,66	0
57	MG	RA	3360	1/1	0.94	0.04	53,53,53,53	0
57	MG	QA	1714	1/1	0.94	0.05	52,52,52,52	0
57	MG	YA	3057	1/1	0.94	0.16	66,66,66,66	0
57	MG	QA	1631	1/1	0.94	0.09	113,113,113,113	0
57	MG	XA	1722	1/1	0.94	0.17	49,49,49,49	0
57	MG	QA	1659	1/1	0.94	0.11	65,65,65,65	0
57	MG	XA	1602	1/1	0.94	0.10	55,55,55,55	0
57	MG	YA	3376	1/1	0.94	0.12	38,38,38,38	0
57	MG	YA	3276	1/1	0.94	0.07	32,32,32,32	0
57	MG	YA	3155	1/1	0.94	0.11	61,61,61,61	0
57	MG	YA	3279	1/1	0.94	0.31	70,70,70,70	0
57	MG	XA	1605	1/1	0.94	0.05	80,80,80,80	0
57	MG	YA	3522	1/1	0.94	0.17	56,56,56,56	0
57	MG	QA	1700	1/1	0.94	0.07	59,59,59,59	0
57	MG	YA	3524	1/1	0.94	0.10	82,82,82,82	0
57	MG	RA	3182	1/1	0.94	0.05	57,57,57,57	0
57	MG	RA	3367	1/1	0.94	0.03	74,74,74,74	0
57	MG	YA	3527	1/1	0.94	0.08	85,85,85,85	0
57	MG	RB	204	1/1	0.94	0.04	63,63,63,63	0
57	MG	YA	3166	1/1	0.94	0.15	34,34,34,34	0
57	MG	RA	3281	1/1	0.94	0.07	70,70,70,70	0
57	MG	RA	3282	1/1	0.94	0.05	74,74,74,74	0
57	MG	XV	101	1/1	0.94	0.06	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3063	1/1	0.94	0.06	68,68,68,68	0
57	MG	RA	3103	1/1	0.94	0.06	58,58,58,58	0
57	MG	RA	3017	1/1	0.94	0.08	48,48,48,48	0
57	MG	YA	3076	1/1	0.94	0.18	64,64,64,64	0
57	MG	YA	3397	1/1	0.94	0.12	79,79,79,79	0
57	MG	RA	3186	1/1	0.94	0.08	56,56,56,56	0
57	MG	YA	3399	1/1	0.94	0.04	53,53,53,53	0
57	MG	RA	3068	1/1	0.94	0.14	27,27,27,27	0
57	MG	YA	3407	1/1	0.94	0.18	51,51,51,51	0
57	MG	YA	3301	1/1	0.94	0.05	54,54,54,54	0
57	MG	RA	3109	1/1	0.94	0.07	70,70,70,70	0
57	MG	YB	203	1/1	0.94	0.09	34,34,34,34	0
57	MG	YB	204	1/1	0.94	0.04	81,81,81,81	0
57	MG	RA	3069	1/1	0.94	0.07	44,44,44,44	0
57	MG	YA	3413	1/1	0.94	0.07	48,48,48,48	0
57	MG	YA	3414	1/1	0.94	0.16	37,37,37,37	0
57	MG	QA	1635	1/1	0.94	0.08	59,59,59,59	0
57	MG	YA	3086	1/1	0.94	0.08	42,42,42,42	0
57	MG	XA	1625	1/1	0.94	0.05	53,53,53,53	0
57	MG	RA	3155	1/1	0.94	0.10	46,46,46,46	0
57	MG	RA	3072	1/1	0.94	0.10	47,47,47,47	0
57	MG	YA	3095	1/1	0.94	0.08	93,93,93,93	0
57	MG	YE	304	1/1	0.94	0.19	43,43,43,43	0
57	MG	RA	3042	1/1	0.94	0.08	26,26,26,26	0
57	MG	YA	3204	1/1	0.94	0.11	32,32,32,32	0
57	MG	YA	3427	1/1	0.94	0.08	20,20,20,20	0
57	MG	YA	3100	1/1	0.94	0.18	69,69,69,69	0
57	MG	YA	3430	1/1	0.94	0.20	40,40,40,40	0
57	MG	XA	1630	1/1	0.94	0.08	77,77,77,77	0
57	MG	RA	3118	1/1	0.94	0.09	44,44,44,44	0
57	MG	YA	3215	1/1	0.94	0.05	82,82,82,82	0
57	MG	YA	3020	1/1	0.94	0.23	76,76,76,76	0
57	MG	YA	3441	1/1	0.94	0.04	31,31,31,31	0
57	MG	RA	3387	1/1	0.94	0.07	18,18,18,18	0
57	MG	YA	3324	1/1	0.94	0.07	39,39,39,39	0
57	MG	XA	1633	1/1	0.94	0.05	70,70,70,70	0
57	MG	YA	3225	1/1	0.94	0.13	25,25,25,25	0
57	MG	RA	3079	1/1	0.94	0.16	31,31,31,31	0
57	MG	YA	3328	1/1	0.94	0.25	81,81,81,81	0
57	MG	RA	3080	1/1	0.94	0.11	37,37,37,37	0
57	MG	YA	3113	1/1	0.94	0.21	66,66,66,66	0
57	MG	RA	3163	1/1	0.94	0.07	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1719	1/1	0.94	0.15	83,83,83,83	0
57	MG	YA	3027	1/1	0.94	0.05	68,68,68,68	0
57	MG	YA	3339	1/1	0.94	0.08	36,36,36,36	0
57	MG	YA	3373	1/1	0.95	0.20	82,82,82,82	0
57	MG	YA	3183	1/1	0.95	0.13	72,72,72,72	0
57	MG	RA	3075	1/1	0.95	0.12	72,72,72,72	0
57	MG	RA	3158	1/1	0.95	0.19	65,65,65,65	0
57	MG	YA	3106	1/1	0.95	0.05	60,60,60,60	0
57	MG	RA	3076	1/1	0.95	0.10	35,35,35,35	0
57	MG	YA	3495	1/1	0.95	0.04	33,33,33,33	0
57	MG	YA	3381	1/1	0.95	0.07	64,64,64,64	0
57	MG	YA	3500	1/1	0.95	0.07	23,23,23,23	0
57	MG	YA	3501	1/1	0.95	0.15	44,44,44,44	0
57	MG	RA	3396	1/1	0.95	0.18	54,54,54,54	0
57	MG	RA	3326	1/1	0.95	0.07	60,60,60,60	0
57	MG	XA	1725	1/1	0.95	0.10	71,71,71,71	0
57	MG	RA	3136	1/1	0.95	0.04	44,44,44,44	0
57	MG	YA	3195	1/1	0.95	0.09	40,40,40,40	0
57	MG	YA	3292	1/1	0.95	0.06	47,47,47,47	0
57	MG	YA	3293	1/1	0.95	0.08	59,59,59,59	0
57	MG	RA	3033	1/1	0.95	0.10	52,52,52,52	0
57	MG	RA	3140	1/1	0.95	0.15	53,53,53,53	0
57	MG	YA	3200	1/1	0.95	0.11	31,31,31,31	0
57	MG	YA	3202	1/1	0.95	0.22	33,33,33,33	0
57	MG	QA	1720	1/1	0.95	0.04	64,64,64,64	0
57	MG	RA	3403	1/1	0.95	0.07	51,51,51,51	0
57	MG	RA	3097	1/1	0.95	0.06	55,55,55,55	0
57	MG	YA	3518	1/1	0.95	0.07	72,72,72,72	0
57	MG	YA	3207	1/1	0.95	0.15	19,19,19,19	0
57	MG	YA	3209	1/1	0.95	0.10	27,27,27,27	0
57	MG	YA	3123	1/1	0.95	0.08	43,43,43,43	0
57	MG	YA	3309	1/1	0.95	0.16	59,59,59,59	0
57	MG	YA	3311	1/1	0.95	0.11	60,60,60,60	0
57	MG	RA	3302	1/1	0.95	0.06	74,74,74,74	0
57	MG	YA	3214	1/1	0.95	0.16	23,23,23,23	0
57	MG	RA	3037	1/1	0.95	0.11	36,36,36,36	0
57	MG	YA	3054	1/1	0.95	0.06	79,79,79,79	0
57	MG	RA	3335	1/1	0.95	0.03	49,49,49,49	0
57	MG	YA	3222	1/1	0.95	0.10	66,66,66,66	0
57	MG	R0	102	1/1	0.95	0.04	58,58,58,58	0
57	MG	YA	3224	1/1	0.95	0.10	44,44,44,44	0
57	MG	QM	201	1/1	0.95	0.08	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3226	1/1	0.95	0.10	75,75,75,75	0
57	MG	RA	3014	1/1	0.95	0.09	28,28,28,28	0
57	MG	YA	3135	1/1	0.95	0.09	51,51,51,51	0
57	MG	XA	1688	1/1	0.95	0.04	60,60,60,60	0
57	MG	RA	3306	1/1	0.95	0.05	54,54,54,54	0
57	MG	YA	3233	1/1	0.95	0.19	38,38,38,38	0
57	MG	QA	1613	1/1	0.95	0.04	73,73,73,73	0
57	MG	YA	3329	1/1	0.95	0.20	33,33,33,33	0
57	MG	RA	3374	1/1	0.95	0.07	83,83,83,83	0
57	MG	R8	101	1/1	0.95	0.20	65,65,65,65	0
57	MG	RB	202	1/1	0.95	0.06	87,87,87,87	0
57	MG	YA	3335	1/1	0.95	0.10	68,68,68,68	0
57	MG	YA	3443	1/1	0.95	0.07	70,70,70,70	0
57	MG	YA	3015	1/1	0.95	0.22	67,67,67,67	0
57	MG	YA	3145	1/1	0.95	0.08	69,69,69,69	0
57	MG	QL	201	1/1	0.95	0.13	65,65,65,65	0
57	MG	YB	208	1/1	0.95	0.04	56,56,56,56	0
57	MG	YA	3242	1/1	0.95	0.05	57,57,57,57	0
57	MG	RA	3085	1/1	0.95	0.12	40,40,40,40	0
57	MG	XA	1654	1/1	0.95	0.05	47,47,47,47	0
57	MG	RA	3283	1/1	0.95	0.06	83,83,83,83	0
57	MG	YA	3346	1/1	0.95	0.04	60,60,60,60	0
57	MG	RA	3106	1/1	0.95	0.06	65,65,65,65	0
57	MG	XA	1706	1/1	0.95	0.08	67,67,67,67	0
57	MG	RA	3347	1/1	0.95	0.07	64,64,64,64	0
57	MG	RA	3312	1/1	0.95	0.08	46,46,46,46	0
57	MG	RA	3153	1/1	0.95	0.06	58,58,58,58	0
57	MG	YF	301	1/1	0.95	0.14	61,61,61,61	0
57	MG	YP	201	1/1	0.95	0.05	46,46,46,46	0
57	MG	RA	3287	1/1	0.95	0.04	59,59,59,59	0
57	MG	RA	3386	1/1	0.95	0.07	24,24,24,24	0
57	MG	RA	3128	1/1	0.95	0.09	58,58,58,58	0
57	MG	YA	3028	1/1	0.95	0.08	57,57,57,57	0
57	MG	RE	301	1/1	0.95	0.05	55,55,55,55	0
57	MG	YA	3030	1/1	0.95	0.19	71,71,71,71	0
57	MG	YA	3469	1/1	0.95	0.06	17,17,17,17	0
57	MG	YX	101	1/1	0.95	0.06	63,63,63,63	0
57	MG	Y1	101	1/1	0.95	0.08	42,42,42,42	0
57	MG	YA	3090	1/1	0.95	0.06	58,58,58,58	0
57	MG	YA	3091	1/1	0.95	0.07	81,81,81,81	0
57	MG	YA	3171	1/1	0.95	0.05	46,46,46,46	0
57	MG	YA	3092	1/1	0.95	0.08	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3269	1/1	0.95	0.24	24,24,24,24	0
57	MG	YA	3175	1/1	0.95	0.04	39,39,39,39	0
57	MG	RA	3388	1/1	0.95	0.09	50,50,50,50	0
57	MG	RA	3108	1/1	0.95	0.08	82,82,82,82	0
57	MG	RA	3131	1/1	0.95	0.05	56,56,56,56	0
57	MG	YA	3036	1/1	0.95	0.12	67,67,67,67	0
57	MG	RA	3268	1/1	0.95	0.11	38,38,38,38	0
59	ZN	XN	102	1/1	0.95	0.11	119,119,119,119	0
57	MG	YA	3182	1/1	0.95	0.07	90,90,90,90	0
57	MG	YA	3481	1/1	0.96	0.04	33,33,33,33	0
57	MG	YA	3257	1/1	0.96	0.05	42,42,42,42	0
57	MG	QA	1698	1/1	0.96	0.10	85,85,85,85	0
57	MG	RA	3038	1/1	0.96	0.07	30,30,30,30	0
57	MG	RA	3159	1/1	0.96	0.09	71,71,71,71	0
57	MG	RA	3293	1/1	0.96	0.04	77,77,77,77	0
57	MG	RA	3011	1/1	0.96	0.07	20,20,20,20	0
57	MG	RA	3078	1/1	0.96	0.05	56,56,56,56	0
57	MG	YA	3167	1/1	0.96	0.06	46,46,46,46	0
57	MG	QA	1713	1/1	0.96	0.04	78,78,78,78	0
57	MG	YA	3170	1/1	0.96	0.28	37,37,37,37	0
57	MG	YA	3496	1/1	0.96	0.13	32,32,32,32	0
57	MG	XA	1603	1/1	0.96	0.21	63,63,63,63	0
57	MG	XA	1604	1/1	0.96	0.04	66,66,66,66	0
57	MG	YA	3173	1/1	0.96	0.17	31,31,31,31	0
57	MG	YA	3277	1/1	0.96	0.08	49,49,49,49	0
57	MG	RA	3122	1/1	0.96	0.12	30,30,30,30	0
57	MG	YA	3083	1/1	0.96	0.04	48,48,48,48	0
57	MG	RA	3298	1/1	0.96	0.04	58,58,58,58	0
57	MG	RA	3406	1/1	0.96	0.07	39,39,39,39	0
57	MG	RA	3043	1/1	0.96	0.05	35,35,35,35	0
57	MG	RA	3408	1/1	0.96	0.05	68,68,68,68	0
57	MG	RA	3044	1/1	0.96	0.05	35,35,35,35	0
57	MG	QA	1699	1/1	0.96	0.09	79,79,79,79	0
57	MG	RA	3167	1/1	0.96	0.07	64,64,64,64	0
57	MG	YA	3287	1/1	0.96	0.08	57,57,57,57	0
57	MG	YA	3185	1/1	0.96	0.06	49,49,49,49	0
57	MG	QA	1687	1/1	0.96	0.05	69,69,69,69	0
57	MG	RA	3129	1/1	0.96	0.07	76,76,76,76	0
57	MG	XA	1683	1/1	0.96	0.17	53,53,53,53	0
57	MG	RA	3359	1/1	0.96	0.06	67,67,67,67	0
57	MG	RA	3170	1/1	0.96	0.11	55,55,55,55	0
57	MG	YA	3294	1/1	0.96	0.07	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1664	1/1	0.96	0.04	62,62,62,62	0
57	MG	RA	3048	1/1	0.96	0.06	32,32,32,32	0
57	MG	YA	3105	1/1	0.96	0.07	53,53,53,53	0
57	MG	QA	1702	1/1	0.96	0.05	85,85,85,85	0
57	MG	YA	3403	1/1	0.96	0.15	32,32,32,32	0
57	MG	YA	3300	1/1	0.96	0.14	38,38,38,38	0
57	MG	YA	3405	1/1	0.96	0.05	36,36,36,36	0
57	MG	XA	1624	1/1	0.96	0.08	53,53,53,53	0
57	MG	RA	3134	1/1	0.96	0.09	44,44,44,44	0
57	MG	XA	1626	1/1	0.96	0.13	52,52,52,52	0
57	MG	XA	1697	1/1	0.96	0.13	76,76,76,76	0
57	MG	RB	207	1/1	0.96	0.06	68,68,68,68	0
57	MG	YA	3115	1/1	0.96	0.07	46,46,46,46	0
57	MG	YA	3308	1/1	0.96	0.13	43,43,43,43	0
57	MG	YA	3416	1/1	0.96	0.05	70,70,70,70	0
57	MG	QA	1689	1/1	0.96	0.13	63,63,63,63	0
57	MG	YA	3208	1/1	0.96	0.13	43,43,43,43	0
57	MG	RA	3088	1/1	0.96	0.15	41,41,41,41	0
57	MG	RA	3178	1/1	0.96	0.08	65,65,65,65	0
57	MG	RA	3138	1/1	0.96	0.07	72,72,72,72	0
57	MG	YA	3213	1/1	0.96	0.06	47,47,47,47	0
57	MG	YA	3425	1/1	0.96	0.08	51,51,51,51	0
57	MG	QA	1690	1/1	0.96	0.04	64,64,64,64	0
57	MG	YA	3122	1/1	0.96	0.03	82,82,82,82	0
57	MG	RA	3054	1/1	0.96	0.16	61,61,61,61	0
57	MG	YA	3219	1/1	0.96	0.07	37,37,37,37	0
57	MG	RA	3024	1/1	0.96	0.10	34,34,34,34	0
57	MG	QA	1665	1/1	0.96	0.13	51,51,51,51	0
57	MG	YA	3433	1/1	0.96	0.03	55,55,55,55	0
57	MG	XA	1638	1/1	0.96	0.07	56,56,56,56	0
57	MG	YA	3127	1/1	0.96	0.06	41,41,41,41	0
57	MG	YD	305	1/1	0.96	0.27	75,75,75,75	0
57	MG	XA	1709	1/1	0.96	0.04	61,61,61,61	0
57	MG	YA	3130	1/1	0.96	0.06	60,60,60,60	0
57	MG	YA	3227	1/1	0.96	0.12	25,25,25,25	0
57	MG	RA	3229	1/1	0.96	0.07	52,52,52,52	0
57	MG	QA	1671	1/1	0.96	0.05	60,60,60,60	0
57	MG	RA	3231	1/1	0.96	0.16	66,66,66,66	0
57	MG	YA	3134	1/1	0.96	0.12	32,32,32,32	0
57	MG	RA	3058	1/1	0.96	0.08	40,40,40,40	0
57	MG	YA	3334	1/1	0.96	0.15	30,30,30,30	0
57	MG	QA	1658	1/1	0.96	0.05	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3188	1/1	0.96	0.04	56,56,56,56	0
57	MG	QA	1723	1/1	0.96	0.04	104,104,104,104	0
57	MG	XA	1717	1/1	0.96	0.19	54,54,54,54	0
57	MG	RA	3190	1/1	0.96	0.04	47,47,47,47	0
57	MG	RA	3148	1/1	0.96	0.07	37,37,37,37	0
57	MG	YA	3056	1/1	0.96	0.12	77,77,77,77	0
57	MG	RA	3385	1/1	0.96	0.20	40,40,40,40	0
57	MG	RA	3065	1/1	0.96	0.11	49,49,49,49	0
57	MG	RA	3332	1/1	0.96	0.09	91,91,91,91	0
57	MG	QA	1622	1/1	0.96	0.03	79,79,79,79	0
57	MG	RA	3389	1/1	0.96	0.05	73,73,73,73	0
57	MG	RA	3067	1/1	0.96	0.13	41,41,41,41	0
57	MG	YA	3351	1/1	0.96	0.12	78,78,78,78	0
57	MG	RA	3285	1/1	0.96	0.24	64,64,64,64	0
57	MG	QC	301	1/1	0.96	0.14	133,133,133,133	0
57	MG	YA	3250	1/1	0.96	0.12	36,36,36,36	0
57	MG	YA	3251	1/1	0.96	0.12	49,49,49,49	0
57	MG	RA	3032	1/1	0.96	0.11	51,51,51,51	0
57	MG	QA	1695	1/1	0.96	0.03	96,96,96,96	0
57	MG	QA	1657	1/1	0.96	0.06	75,75,75,75	0
57	MG	YA	3156	1/1	0.96	0.07	87,87,87,87	0
57	MG	QA	1606	1/1	0.97	0.11	93,93,93,93	0
57	MG	YA	3497	1/1	0.97	0.06	55,55,55,55	0
57	MG	RA	3050	1/1	0.97	0.08	55,55,55,55	0
57	MG	YA	3499	1/1	0.97	0.03	38,38,38,38	0
57	MG	YA	3077	1/1	0.97	0.12	49,49,49,49	0
57	MG	YA	3229	1/1	0.97	0.06	32,32,32,32	0
57	MG	XA	1694	1/1	0.97	0.11	61,61,61,61	0
57	MG	RA	3100	1/1	0.97	0.17	51,51,51,51	0
57	MG	RA	3074	1/1	0.97	0.03	34,34,34,34	0
57	MG	RA	3228	1/1	0.97	0.13	67,67,67,67	0
57	MG	RA	3102	1/1	0.97	0.08	49,49,49,49	0
57	MG	XA	1647	1/1	0.97	0.14	44,44,44,44	0
57	MG	YA	3085	1/1	0.97	0.10	48,48,48,48	0
57	MG	YA	3319	1/1	0.97	0.11	51,51,51,51	0
57	MG	YA	3157	1/1	0.97	0.08	43,43,43,43	0
57	MG	RA	3132	1/1	0.97	0.05	106,106,106,106	0
57	MG	RA	3034	1/1	0.97	0.06	34,34,34,34	0
57	MG	YA	3412	1/1	0.97	0.04	60,60,60,60	0
57	MG	YA	3515	1/1	0.97	0.10	40,40,40,40	0
57	MG	YA	3088	1/1	0.97	0.17	30,30,30,30	0
57	MG	RA	3413	1/1	0.97	0.06	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3163	1/1	0.97	0.05	72,72,72,72	0
57	MG	YA	3164	1/1	0.97	0.08	30,30,30,30	0
57	MG	QA	1621	1/1	0.97	0.06	60,60,60,60	0
57	MG	RA	3036	1/1	0.97	0.07	36,36,36,36	0
57	MG	YA	3419	1/1	0.97	0.11	60,60,60,60	0
57	MG	QA	1614	1/1	0.97	0.04	81,81,81,81	0
57	MG	QA	1619	1/1	0.97	0.05	57,57,57,57	0
57	MG	RA	3338	1/1	0.97	0.04	59,59,59,59	0
57	MG	RA	3039	1/1	0.97	0.10	41,41,41,41	0
57	MG	YA	3424	1/1	0.97	0.05	38,38,38,38	0
57	MG	YA	3032	1/1	0.97	0.07	75,75,75,75	0
57	MG	RA	3010	1/1	0.97	0.17	46,46,46,46	0
57	MG	YA	3530	1/1	0.97	0.08	39,39,39,39	0
57	MG	RA	3111	1/1	0.97	0.07	47,47,47,47	0
57	MG	YA	3103	1/1	0.97	0.05	43,43,43,43	0
57	MG	YA	3177	1/1	0.97	0.07	32,32,32,32	0
57	MG	RA	3112	1/1	0.97	0.08	65,65,65,65	0
57	MG	YA	3259	1/1	0.97	0.05	41,41,41,41	0
57	MG	RA	3382	1/1	0.97	0.09	33,33,33,33	0
57	MG	YA	3434	1/1	0.97	0.07	36,36,36,36	0
57	MG	RA	3113	1/1	0.97	0.03	56,56,56,56	0
57	MG	YA	3439	1/1	0.97	0.17	39,39,39,39	0
57	MG	YA	3344	1/1	0.97	0.09	8,8,8,8	0
57	MG	RA	3174	1/1	0.97	0.04	49,49,49,49	0
57	MG	XA	1613	1/1	0.97	0.08	59,59,59,59	0
57	MG	YA	3544	1/1	0.97	0.13	45,45,45,45	0
57	MG	RA	3345	1/1	0.97	0.10	90,90,90,90	0
57	MG	YA	3042	1/1	0.97	0.05	52,52,52,52	0
57	MG	YA	3111	1/1	0.97	0.03	74,74,74,74	0
57	MG	RA	3346	1/1	0.97	0.05	58,58,58,58	0
57	MG	YA	3271	1/1	0.97	0.05	41,41,41,41	0
57	MG	RA	3060	1/1	0.97	0.10	43,43,43,43	0
57	MG	YA	3188	1/1	0.97	0.04	29,29,29,29	0
57	MG	YA	3274	1/1	0.97	0.14	25,25,25,25	0
57	MG	QV	102	1/1	0.97	0.05	38,38,38,38	0
57	MG	YA	3457	1/1	0.97	0.13	70,70,70,70	0
57	MG	RA	3349	1/1	0.97	0.11	57,57,57,57	0
57	MG	RA	3116	1/1	0.97	0.09	37,37,37,37	0
57	MG	YD	307	1/1	0.97	0.11	109,109,109,109	0
57	MG	RA	3147	1/1	0.97	0.03	69,69,69,69	0
57	MG	RA	3062	1/1	0.97	0.15	52,52,52,52	0
57	MG	XA	1673	1/1	0.97	0.04	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3197	1/1	0.97	0.17	33,33,33,33	0
57	MG	RA	3012	1/1	0.97	0.05	36,36,36,36	0
57	MG	RA	3150	1/1	0.97	0.07	67,67,67,67	0
57	MG	XA	1676	1/1	0.97	0.05	49,49,49,49	0
57	MG	RA	3064	1/1	0.97	0.05	46,46,46,46	0
57	MG	YA	3468	1/1	0.97	0.10	65,65,65,65	0
57	MG	XK	202	1/1	0.97	0.09	41,41,41,41	0
57	MG	QA	1653	1/1	0.97	0.04	70,70,70,70	0
57	MG	RA	3397	1/1	0.97	0.05	11,11,11,11	0
57	MG	QA	1632	1/1	0.97	0.05	63,63,63,63	0
57	MG	YA	3473	1/1	0.97	0.06	53,53,53,53	0
57	MG	RA	3030	1/1	0.97	0.14	49,49,49,49	0
57	MG	RA	3123	1/1	0.97	0.04	53,53,53,53	0
57	MG	YA	3210	1/1	0.97	0.09	28,28,28,28	0
57	MG	Y0	101	1/1	0.97	0.09	27,27,27,27	0
57	MG	RQ	201	1/1	0.97	0.07	84,84,84,84	0
57	MG	XA	1634	1/1	0.97	0.05	60,60,60,60	0
57	MG	RA	3321	1/1	0.97	0.09	50,50,50,50	0
57	MG	YA	3380	1/1	0.97	0.05	70,70,70,70	0
57	MG	QA	1697	1/1	0.97	0.06	72,72,72,72	0
57	MG	YA	3009	1/1	0.97	0.08	67,67,67,67	0
57	MG	YA	3298	1/1	0.97	0.04	43,43,43,43	0
57	MG	YA	3140	1/1	0.97	0.06	60,60,60,60	0
57	MG	YA	3010	1/1	0.97	0.09	61,61,61,61	0
57	MG	RA	3362	1/1	0.97	0.08	111,111,111,111	0
57	MG	RA	3004	1/1	0.97	0.04	49,49,49,49	0
57	MG	XA	1640	1/1	0.97	0.16	37,37,37,37	0
57	MG	YA	3014	1/1	0.97	0.10	51,51,51,51	0
57	MG	YA	3074	1/1	0.97	0.13	45,45,45,45	0
57	MG	QA	1642	1/1	0.98	0.04	70,70,70,70	0
57	MG	RA	3001	1/1	0.98	0.11	83,83,83,83	0
57	MG	YA	3234	1/1	0.98	0.24	34,34,34,34	0
57	MG	RA	3194	1/1	0.98	0.13	23,23,23,23	0
57	MG	QA	1707	1/1	0.98	0.03	54,54,54,54	0
57	MG	QA	1602	1/1	0.98	0.03	71,71,71,71	0
57	MG	RA	3041	1/1	0.98	0.11	44,44,44,44	0
57	MG	YA	3345	1/1	0.98	0.03	50,50,50,50	0
57	MG	YA	3406	1/1	0.98	0.10	30,30,30,30	0
57	MG	YA	3112	1/1	0.98	0.08	43,43,43,43	0
57	MG	RA	3089	1/1	0.98	0.07	55,55,55,55	0
57	MG	YA	3114	1/1	0.98	0.03	68,68,68,68	0
57	MG	RP	201	1/1	0.98	0.06	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3411	1/1	0.98	0.08	31,31,31,31	0
57	MG	YA	3477	1/1	0.98	0.04	37,37,37,37	0
57	MG	YA	3196	1/1	0.98	0.09	20,20,20,20	0
57	MG	YA	3078	1/1	0.98	0.11	40,40,40,40	0
57	MG	YA	3045	1/1	0.98	0.05	61,61,61,61	0
57	MG	RA	3181	1/1	0.98	0.03	50,50,50,50	0
57	MG	YA	3119	1/1	0.98	0.07	64,64,64,64	0
57	MG	YA	3201	1/1	0.98	0.08	27,27,27,27	0
57	MG	RA	3073	1/1	0.98	0.05	60,60,60,60	0
57	MG	RA	3091	1/1	0.98	0.04	34,34,34,34	0
57	MG	YA	3489	1/1	0.98	0.04	59,59,59,59	0
57	MG	YA	3303	1/1	0.98	0.06	43,43,43,43	0
57	MG	YA	3360	1/1	0.98	0.06	26,26,26,26	0
57	MG	YA	3161	1/1	0.98	0.07	26,26,26,26	0
57	MG	YD	304	1/1	0.98	0.09	85,85,85,85	0
57	MG	YA	3205	1/1	0.98	0.09	27,27,27,27	0
57	MG	YD	306	1/1	0.98	0.07	60,60,60,60	0
57	MG	XA	1637	1/1	0.98	0.09	108,108,108,108	0
57	MG	XA	1691	1/1	0.98	0.03	53,53,53,53	0
57	MG	RA	3052	1/1	0.98	0.03	60,60,60,60	0
57	MG	YE	302	1/1	0.98	0.04	42,42,42,42	0
57	MG	RA	3107	1/1	0.98	0.11	96,96,96,96	0
57	MG	YA	3310	1/1	0.98	0.10	49,49,49,49	0
57	MG	YA	3429	1/1	0.98	0.09	35,35,35,35	0
57	MG	YA	3258	1/1	0.98	0.05	37,37,37,37	0
57	MG	XA	1695	1/1	0.98	0.07	29,29,29,29	0
57	MG	RX	101	1/1	0.98	0.07	107,107,107,107	0
57	MG	YA	3168	1/1	0.98	0.04	41,41,41,41	0
57	MG	YP	202	1/1	0.98	0.06	36,36,36,36	0
57	MG	RA	3137	1/1	0.98	0.03	59,59,59,59	0
57	MG	YA	3435	1/1	0.98	0.06	34,34,34,34	0
57	MG	YA	3436	1/1	0.98	0.05	49,49,49,49	0
57	MG	YA	3263	1/1	0.98	0.06	5,5,5,5	0
57	MG	XA	1699	1/1	0.98	0.04	47,47,47,47	0
57	MG	RA	3093	1/1	0.98	0.03	35,35,35,35	0
57	MG	YA	3216	1/1	0.98	0.03	37,37,37,37	0
57	MG	YA	3217	1/1	0.98	0.07	31,31,31,31	0
57	MG	RA	3320	1/1	0.98	0.03	61,61,61,61	0
57	MG	YA	3270	1/1	0.98	0.10	44,44,44,44	0
57	MG	XA	1617	1/1	0.98	0.07	78,78,78,78	0
57	MG	YA	3174	1/1	0.98	0.07	50,50,50,50	0
57	MG	YA	3221	1/1	0.98	0.09	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3094	1/1	0.98	0.04	42,42,42,42	0
57	MG	XA	1619	1/1	0.98	0.03	37,37,37,37	0
57	MG	YA	3098	1/1	0.98	0.10	90,90,90,90	0
57	MG	YA	3099	1/1	0.98	0.05	57,57,57,57	0
57	MG	RA	3264	1/1	0.98	0.07	35,35,35,35	0
57	MG	RA	3324	1/1	0.98	0.04	39,39,39,39	0
57	MG	RA	3096	1/1	0.98	0.10	48,48,48,48	0
57	MG	RA	3125	1/1	0.98	0.06	40,40,40,40	0
57	MG	YA	3003	1/1	0.98	0.05	43,43,43,43	0
57	MG	RA	3059	1/1	0.98	0.08	50,50,50,50	0
57	MG	YA	3504	1/1	0.99	0.09	14,14,14,14	0
57	MG	YA	3357	1/1	0.99	0.02	24,24,24,24	0
57	MG	XA	1692	1/1	0.99	0.05	53,53,53,53	0
57	MG	YA	3389	1/1	0.99	0.02	32,32,32,32	0
57	MG	RA	3095	1/1	0.99	0.04	45,45,45,45	0
57	MG	RA	3070	1/1	0.99	0.03	51,51,51,51	0
57	MG	YA	3332	1/1	0.99	0.04	21,21,21,21	0
57	MG	RA	3008	1/1	0.99	0.04	46,46,46,46	0
57	MG	YA	3094	1/1	0.99	0.03	44,44,44,44	0
57	MG	YA	3256	1/1	0.99	0.04	55,55,55,55	0
57	MG	XA	1696	1/1	0.99	0.03	36,36,36,36	0
57	MG	YA	3337	1/1	0.99	0.09	27,27,27,27	0
57	MG	YA	3139	1/1	0.99	0.04	94,94,94,94	0
57	MG	YA	3096	1/1	0.99	0.03	55,55,55,55	0
57	MG	YA	3400	1/1	0.99	0.03	20,20,20,20	0
57	MG	YA	3401	1/1	0.99	0.02	39,39,39,39	0
57	MG	YA	3402	1/1	0.99	0.07	46,46,46,46	0
57	MG	YA	3007	1/1	0.99	0.04	56,56,56,56	0
57	MG	YA	3438	1/1	0.99	0.09	39,39,39,39	0
57	MG	RA	3019	1/1	0.99	0.04	39,39,39,39	0
57	MG	YG	201	1/1	0.99	0.04	58,58,58,58	0
57	MG	YA	3059	1/1	0.99	0.10	32,32,32,32	0
57	MG	RA	3015	1/1	0.99	0.03	29,29,29,29	0
57	MG	YA	3442	1/1	0.99	0.03	50,50,50,50	0
57	MG	XA	1621	1/1	0.99	0.05	70,70,70,70	0
57	MG	YA	3484	1/1	0.99	0.03	39,39,39,39	0
57	MG	YR	201	1/1	0.99	0.03	51,51,51,51	0
57	MG	YA	3485	1/1	0.99	0.06	31,31,31,31	0
57	MG	YA	3486	1/1	0.99	0.03	50,50,50,50	0
57	MG	YA	3444	1/1	0.99	0.04	58,58,58,58	0
57	MG	RA	3202	1/1	0.99	0.08	50,50,50,50	0
57	MG	YA	3266	1/1	0.99	0.04	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3193	1/1	0.99	0.04	53,53,53,53	0
57	MG	YA	3448	1/1	0.99	0.05	26,26,26,26	0
57	MG	YA	3377	1/1	0.99	0.03	32,32,32,32	0
57	MG	YA	3450	1/1	0.99	0.05	47,47,47,47	0
57	MG	YA	3451	1/1	0.99	0.07	32,32,32,32	0
57	MG	RA	3380	1/1	0.99	0.03	21,21,21,21	0
57	MG	YA	3540	1/1	0.99	0.07	51,51,51,51	0
57	MG	RA	3248	1/1	0.99	0.02	43,43,43,43	0
57	MG	RA	3224	1/1	0.99	0.05	41,41,41,41	0
57	MG	XA	1650	1/1	0.99	0.05	50,50,50,50	0
58	SF4	QD	303	8/8	0.99	0.04	98,145,211,224	0
58	SF4	XD	302	8/8	0.99	0.03	105,135,155,248	0
57	MG	RA	3322	1/1	0.99	0.04	46,46,46,46	0
57	MG	YA	3129	1/1	0.99	0.06	60,60,60,60	0
57	MG	YA	3033	1/1	0.99	0.02	50,50,50,50	0
57	MG	RA	3021	1/1	0.99	0.06	67,67,67,67	0
57	MG	YA	3070	1/1	0.99	0.03	40,40,40,40	0
57	MG	RA	3013	1/1	1.00	0.02	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.