



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2026 – 08:20 PM UTC

PDB ID : 6OXI / pdb_00006oxi
Title : Dimeric E.coli YoeB bound to Thermus thermophilus 70S post-cleavage (UAA)
Authors : Pavelich, I.J.; Hoffer, E.D.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2019-05-13
Resolution : 3.50 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

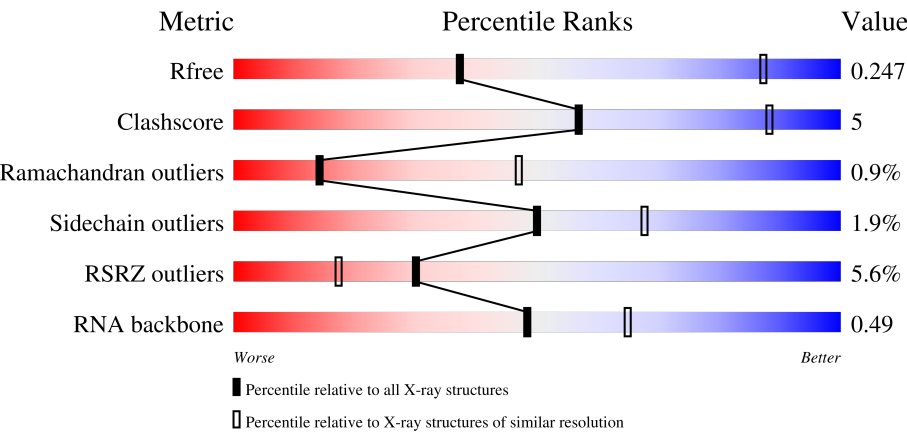
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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	2% 62%32%5%
1	XA	1521	2% 64%30%5%
2	QB	256	2% 67%18%5%8%
2	XB	256	5% 72%16%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	20	
23	XX	20	
24	QY	84	
24	QZ	84	
24	XY	84	
24	XZ	84	
25	R0	85	
25	Y0	85	
26	R1	98	
26	Y1	98	

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Mol	Chain	Length	Quality of chain
27	R2	72	
27	Y2	72	
28	R3	60	
28	Y3	60	
29	R4	71	
29	Y4	71	
30	R5	60	
30	Y5	60	
31	R6	54	
31	Y6	54	
32	R7	49	
32	Y7	49	
33	R8	65	
33	Y8	65	
34	R9	37	
34	Y9	37	
35	RA	2915	
35	YA	2915	
36	RB	124	
36	YB	124	
37	RD	276	
37	YD	276	
38	RE	206	
38	YE	206	
39	RF	210	

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Mol	Chain	Length	Quality of chain
39	YF	210	4% 75% 20% • •
40	RG	182	5% 75% 21% • • •
40	YG	182	8% 75% 23% • • •
41	RH	180	17% 73% 18% • • •
41	YH	180	12% 81% 15% • •
42	RI	148	15% 68% 22% 5% • •
42	YI	148	6% 81% 14% • •
43	RN	140	16% 76% 19% • •
43	YN	140	8% 79% 17% • •
44	RO	122	• 74% 26%
44	YO	122	3% 79% 21%
45	RP	150	11% 69% 27% • •
45	YP	150	7% 77% 22% • •
46	RQ	141	9% 70% 26% • •
46	YQ	141	4% 79% 21%
47	RR	118	3% 79% 19% • •
47	YR	118	9% 77% 20% • • •
48	RS	112	14% 74% 24% • •
48	YS	112	12% 76% 21% • •
49	RT	146	8% 66% 25% • 6%
49	YT	146	8% 71% 19% • 6%
50	RU	118	5% 77% 19% • • •
50	YU	118	11% 81% 15% • • •
51	RV	101	3% 69% 25% • •
51	YV	101	16% 70% 25% 5%

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Mol	Chain	Length	Quality of chain
52	RW	113	
52	YW	113	
53	RX	96	
53	YX	96	
54	RY	110	
54	YY	110	
55	RZ	206	
55	YZ	206	
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	QY	101	-	-	-	X
57	MG	RA	3302	-	-	-	X
57	MG	XA	1651	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 295153 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	1510	Total	C	N	O	P	0	0	0
			32452	14444	6009	10489	1510			
1	XA	1507	Total	C	N	O	P	0	0	0
			32389	14416	5999	10467	1507			

- 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	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	XE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	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	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	XK	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	QL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	XL	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	120	Total	C	N	O	S	0	0	0
			955	591	197	165	2			
13	XM	119	Total	C	N	O	S	0	0	0
			946	585	195	164	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	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	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
			656	418	123	113	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	XV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	18	Total	C	N	O	P	0	0	0
			394	176	79	121	18			
23	XX	18	Total	C	N	O	P	0	0	0
			394	176	79	121	18			

- Molecule 24 is a protein called Addiction module toxin, Txe/YoeB family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
24	QZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
24	XY	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
24	XZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			
25	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R1	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			
26	Y1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 27 is a protein called 50S ribosomal protein L29.

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

- Molecule 28 is a protein called 50S ribosomal protein L30.

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

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	R4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			
29	Y4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			

- Molecule 30 is a protein called 50S ribosomal protein L32.

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

- Molecule 31 is a protein called 50S ribosomal protein L33.

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

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

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	R7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
32	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 33 is a protein called 50S ribosomal protein L35.

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

- Molecule 34 is a protein called 50S ribosomal protein L36.

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

- Molecule 35 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RA	2891	Total	C	N	O	P	0	0	0
			62266	27713	11649	20014	2890			
35	YA	2878	Total	C	N	O	P	0	0	0
			61981	27587	11589	19928	2877			

- Molecule 36 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			
36	YB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			

- Molecule 37 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
37	YD	274	Total	C	N	O	S	0	0	0
			2135	1347	426	359	3			

- Molecule 38 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
38	YE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 39 is a protein called 50S ribosomal protein L4.

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

- Molecule 40 is a protein called 50S ribosomal protein L5.

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

- Molecule 41 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
41	YH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 42 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RI	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
42	YI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 43 is a protein called 50S ribosomal protein L13.

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

- Molecule 44 is a protein called 50S ribosomal protein L14.

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

- Molecule 45 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
45	YP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 46 is a protein called 50S ribosomal protein L16.

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

- Molecule 47 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	RR	117	Total	C	N	O	0	0	0
			960	599	202	159			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	YR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 48 is a protein called 50S ribosomal protein L18.

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

- Molecule 49 is a protein called 50S ribosomal protein L19.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L21.

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

- Molecule 52 is a protein called 50S ribosomal protein L22.

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

- Molecule 53 is a protein called 50S ribosomal protein L23.

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

- Molecule 54 is a protein called 50S ribosomal protein L24.

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

- Molecule 55 is a protein called 50S ribosomal protein L25.

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

- Molecule 56 is a RNA chain called CCPuro.

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	93	Total	Mg	0	0
			93	93		
57	QD	1	Total	Mg	0	0
			1	1		
57	QE	1	Total	Mg	0	0
			1	1		
57	QV	3	Total	Mg	0	0
			3	3		

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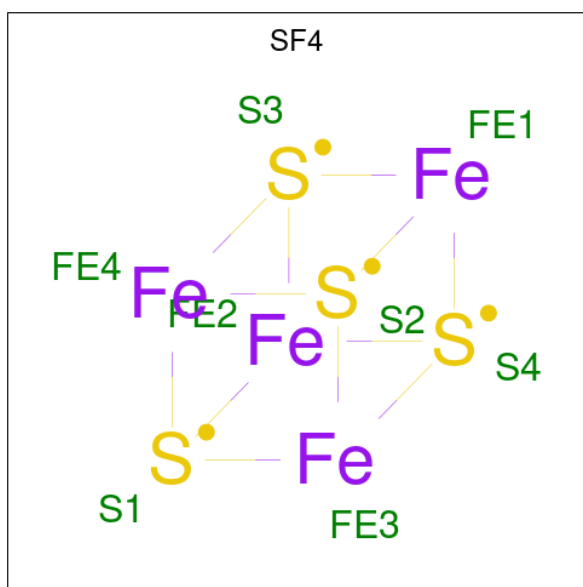
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QY	1	Total 1	Mg 1	0	0
57	R0	2	Total 2	Mg 2	0	0
57	R3	1	Total 1	Mg 1	0	0
57	RA	302	Total 302	Mg 302	0	0
57	RB	3	Total 3	Mg 3	0	0
57	RD	2	Total 2	Mg 2	0	0
57	RE	1	Total 1	Mg 1	0	0
57	RN	1	Total 1	Mg 1	0	0
57	RO	1	Total 1	Mg 1	0	0
57	RP	1	Total 1	Mg 1	0	0
57	RQ	4	Total 4	Mg 4	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RY	1	Total 1	Mg 1	0	0
57	XA	99	Total 99	Mg 99	0	0
57	XE	1	Total 1	Mg 1	0	0
57	XF	1	Total 1	Mg 1	0	0
57	XL	1	Total 1	Mg 1	0	0
57	XM	1	Total 1	Mg 1	0	0
57	XV	4	Total 4	Mg 4	0	0
57	Y0	2	Total 2	Mg 2	0	0
57	Y1	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y3	1	Total 1	Mg 1	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	Y9	1	Total 1	Mg 1	0	0
57	YA	335	Total 335	Mg 335	0	0
57	YB	3	Total 3	Mg 3	0	0
57	YD	4	Total 4	Mg 4	0	0
57	YE	5	Total 5	Mg 5	0	0
57	YF	1	Total 1	Mg 1	0	0
57	YG	1	Total 1	Mg 1	0	0
57	YO	1	Total 1	Mg 1	0	0
57	YP	1	Total 1	Mg 1	0	0
57	YQ	5	Total 5	Mg 5	0	0
57	YR	1	Total 1	Mg 1	0	0
57	YV	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		

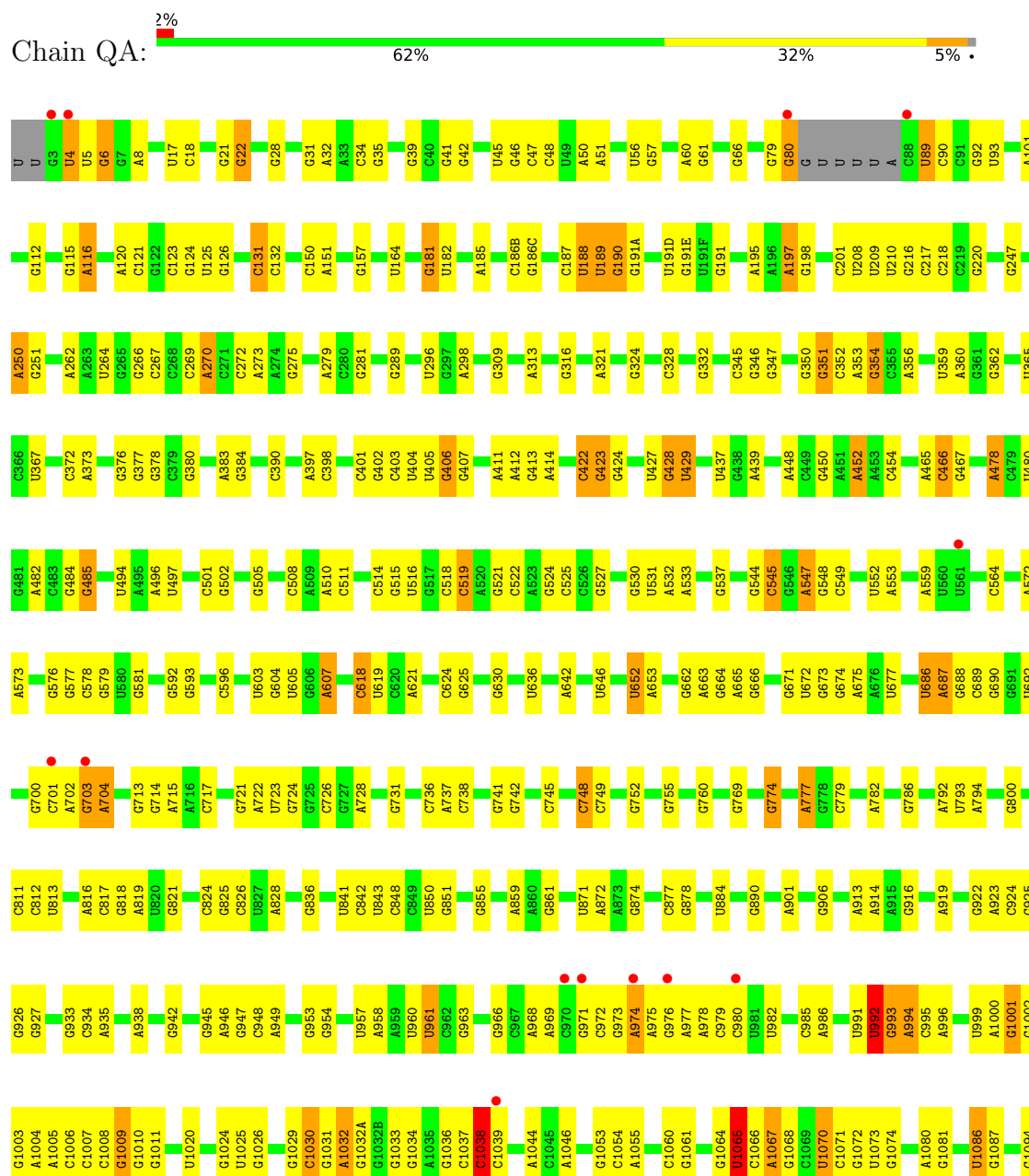
- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

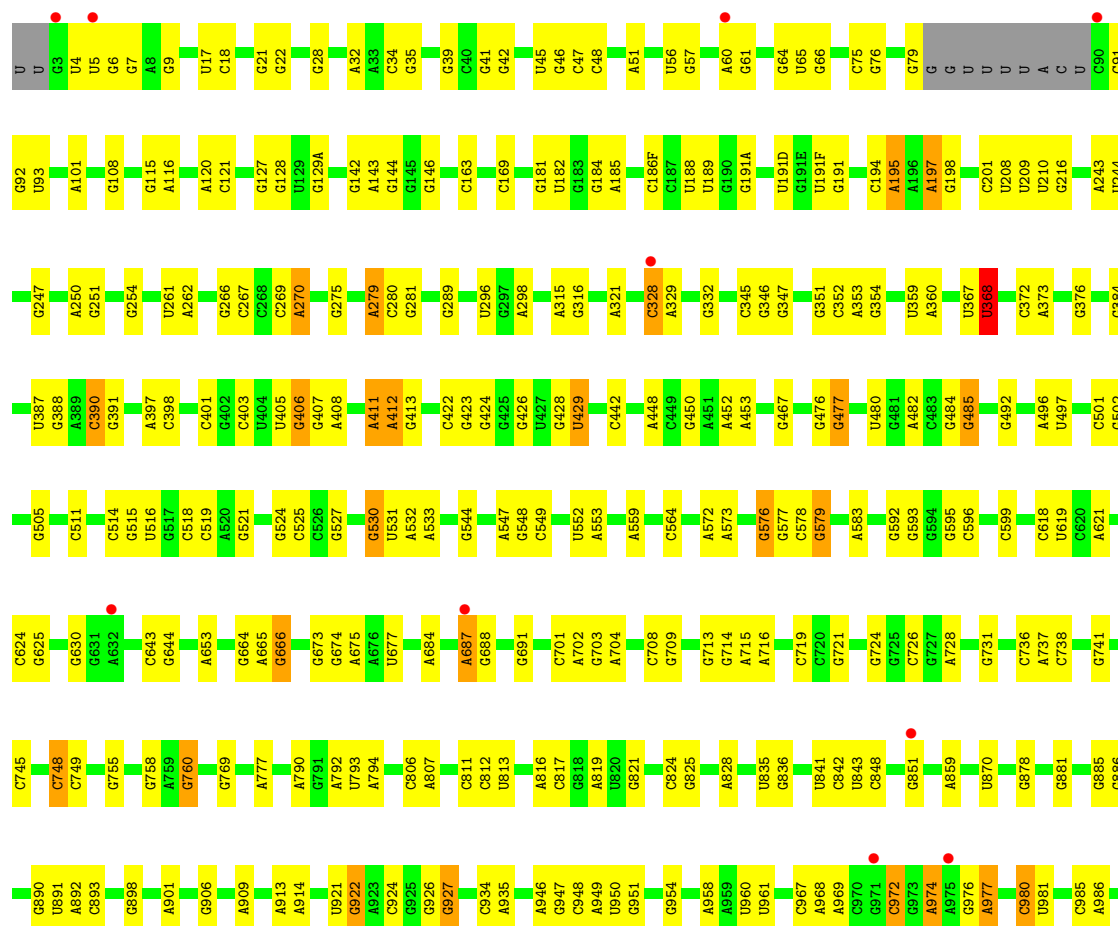
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	QN	1	Total	Zn	0	0
			1	1		
59	R4	1	Total	Zn	0	0
			1	1		
59	R5	1	Total	Zn	0	0
			1	1		
59	R6	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		
59	Y4	1	Total	Zn	0	0
			1	1		
59	Y6	1	Total	Zn	0	0
			1	1		

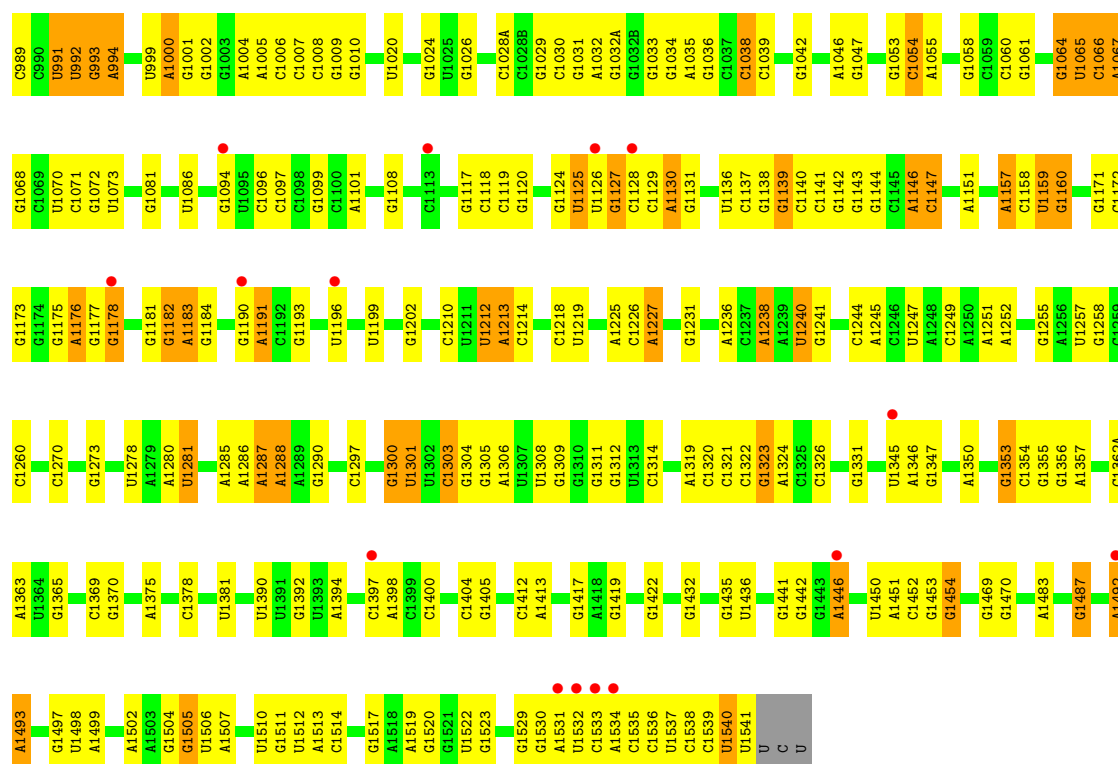
3 Residue-property plots

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.

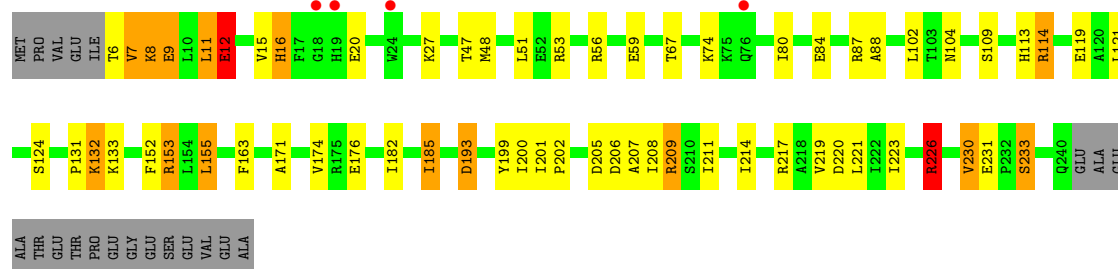
• Molecule 1: 16S rRNA



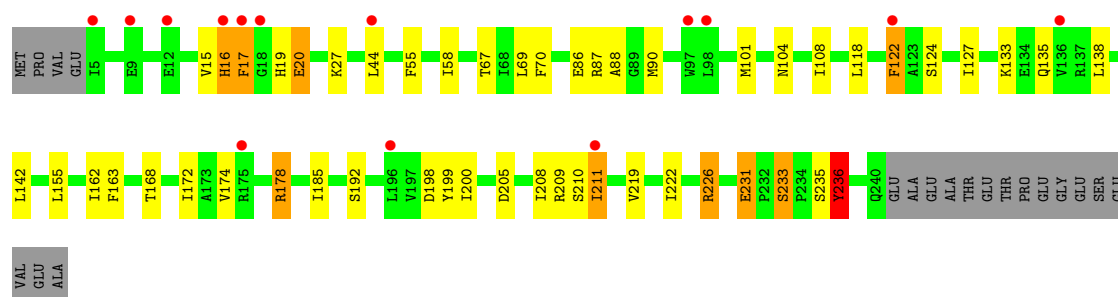
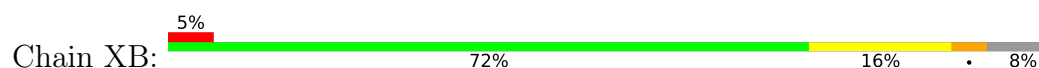




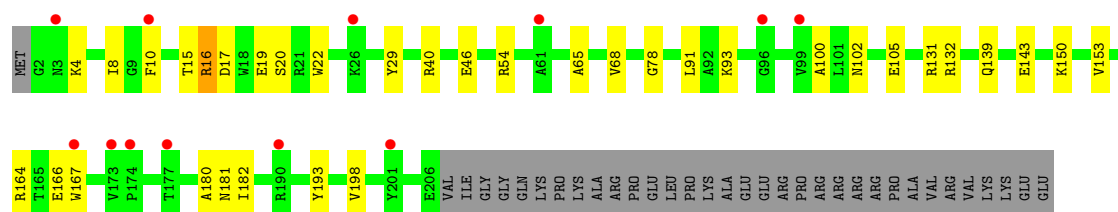
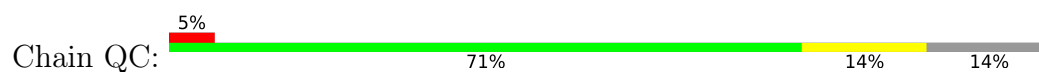
• Molecule 2: 30S ribosomal protein S2



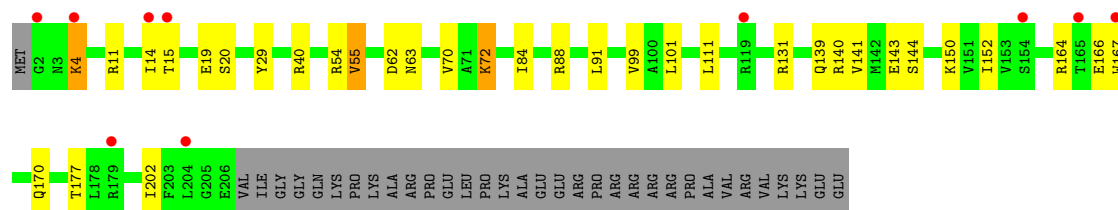
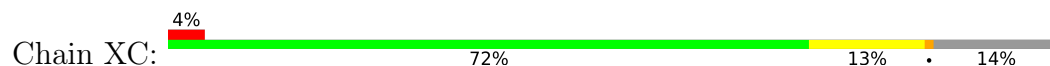
• Molecule 2: 30S ribosomal protein S2



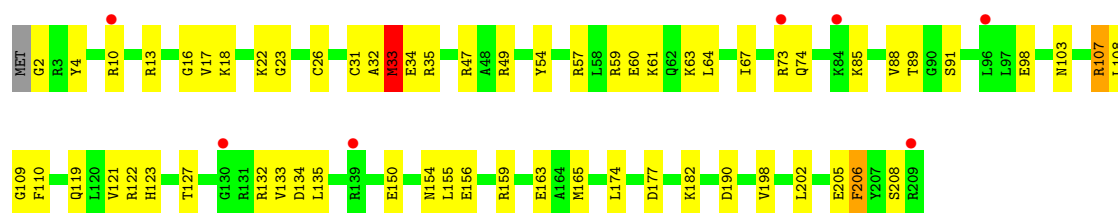
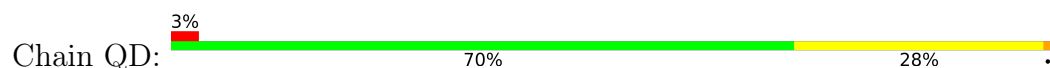
• Molecule 3: 30S ribosomal protein S3



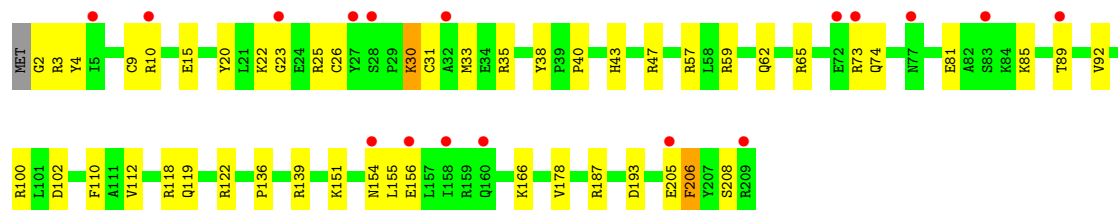
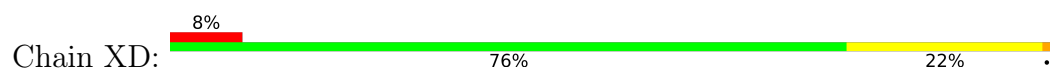
• Molecule 3: 30S ribosomal protein S3



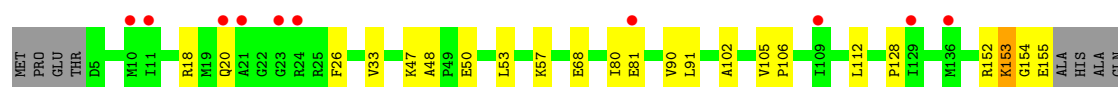
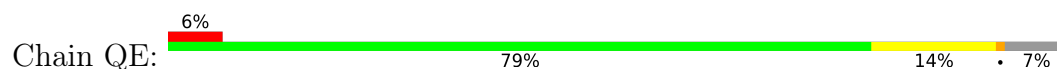
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5



ALA
GLN
GLY

- Molecule 5: 30S ribosomal protein S5

Chain XE:  5% 77% 15% 7%

MET PRO GLU THR D5 M10 I11 M19 Q20 A21 G22 G23 R24 R25 F26 V51 P52 L53 Q56 R63 M66 V69 I80 E81 G85 V90 L91 A102 V105 P106 R107 E111 T120 G124 P128 T135 G154 E155 ALA HIS ALA GLN

ALA
GLN
GLY

- Molecule 6: 30S ribosomal protein S6

Chain QF:  3% 79% 21%

M1 R2 R3 V6 V9 L10 N13 L14 D15 Q16 S17 R46 K54 Y59 F60 L61 W62 Y63 Q64 Y65 E66 E69 A76 L79 R80 R87 V88 M89 V90 S93 A101

- Molecule 6: 30S ribosomal protein S6

Chain XF:  83% 16%

M1 R2 V9 L10 E22 L30 V37 L45 R46 Y59 F60 L61 V65 V72 L75 R82 R87 E95 N100 A101

- Molecule 7: 30S ribosomal protein S7

Chain QG:  5% 81% 17%

MET A2 R3 R4 E8 V9 R10 D15 L16 V17 Y18 G19 D20 V23 N28 F29 I30 M31 D45 L59 F60 V61 F62 V75 R78 R79 V80 Y85 Q86 V87 P88 R94 R119 L124 A150 Y151 A152 H153 Y154 W156

- Molecule 7: 30S ribosomal protein S7

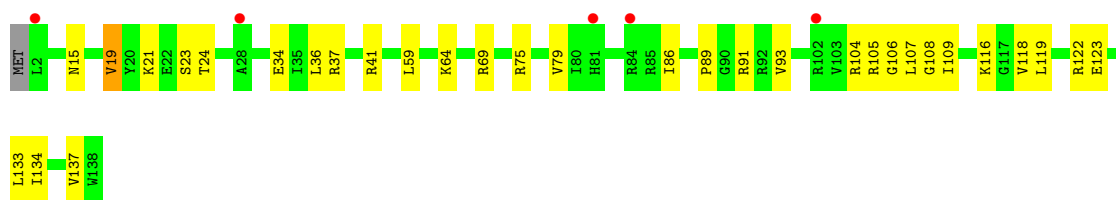
Chain XG:  10% 81% 16%

MET A2 R3 R4 Q13 P14 D15 L16 G19 D20 V23 F26 K29 R32 D33 N37 T42 F43 Y44 E57 R76 S77 R78 R79 V80 G81 G82 A83 N84 V87 R94 S98 L101 R113 R114 R119 M125 D126 A150 Y151 A152

H153 Y154 R155 W156

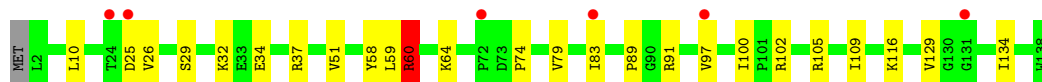
- Molecule 8: 30S ribosomal protein S8

Chain QH:  4% 76% 22%



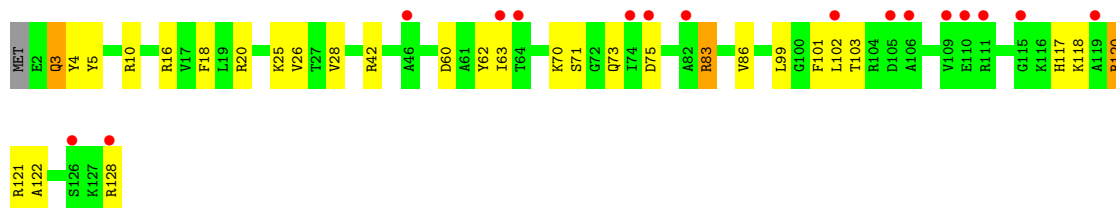
- Molecule 8: 30S ribosomal protein S8

Chain XH: 4% 81% 17% ..



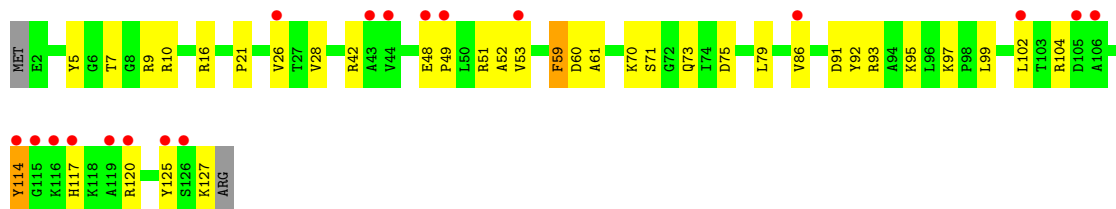
- Molecule 9: 30S ribosomal protein S9

Chain QI: 12% 76% 21% ..



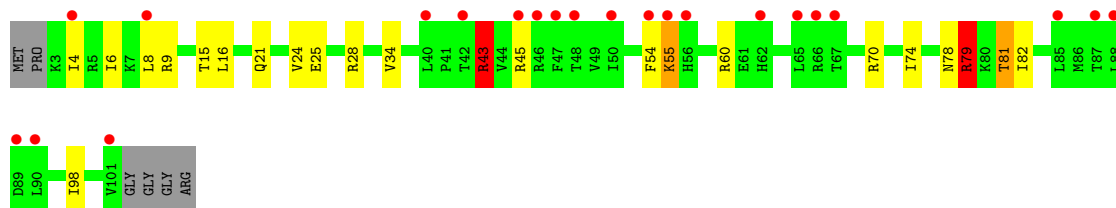
- Molecule 9: 30S ribosomal protein S9

Chain XI: 14% 70% 27% ..



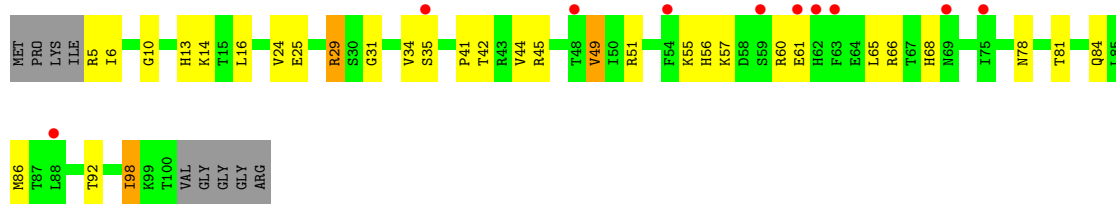
- Molecule 10: 30S ribosomal protein S10

Chain QJ: 21% 72% 18% 6%

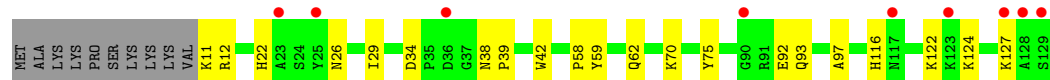
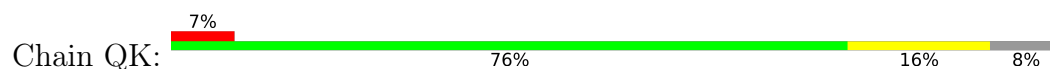


- Molecule 10: 30S ribosomal protein S10

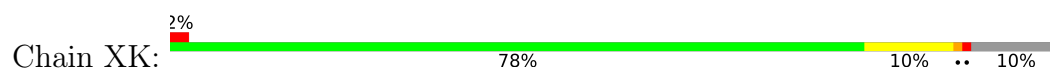
Chain XJ: 10% 61% 28% 9%



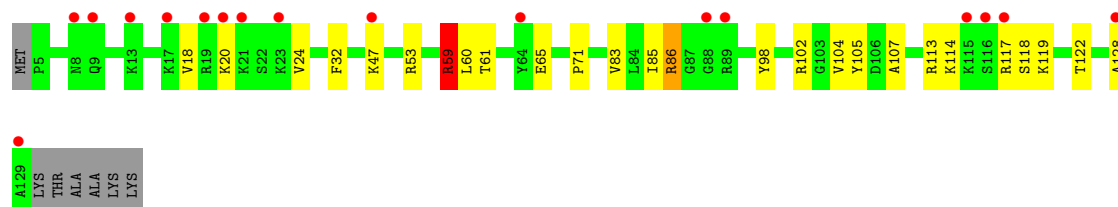
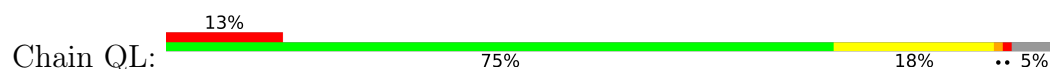
- Molecule 11: 30S ribosomal protein S11



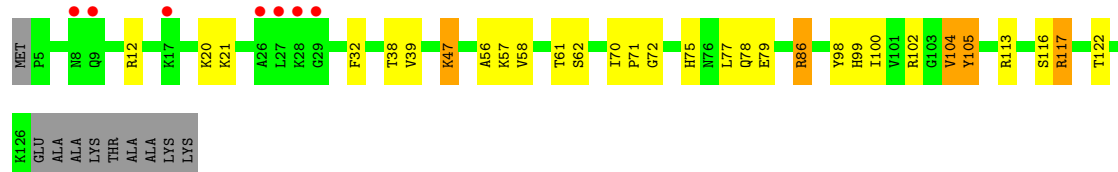
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12

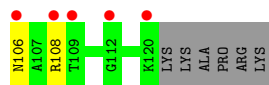
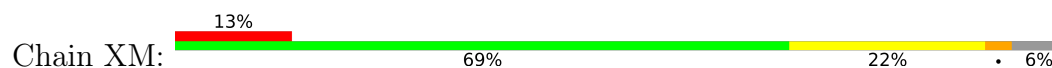


- Molecule 13: 30S ribosomal protein S13

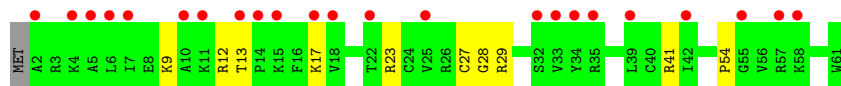
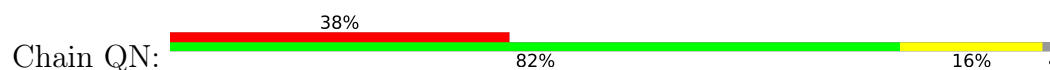




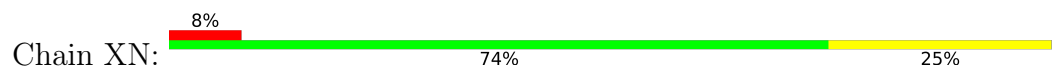
- Molecule 13: 30S ribosomal protein S13



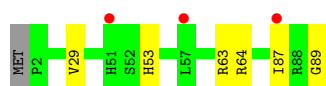
- Molecule 14: 30S ribosomal protein S14 type Z



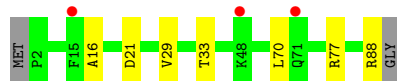
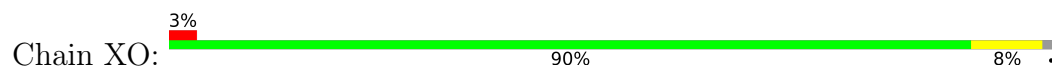
- Molecule 14: 30S ribosomal protein S14 type Z



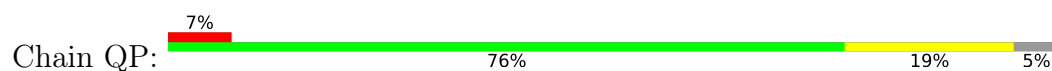
- Molecule 15: 30S ribosomal protein S15

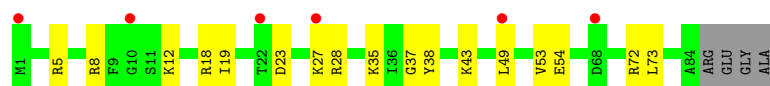


- Molecule 15: 30S ribosomal protein S15

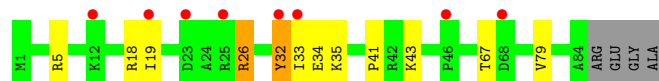
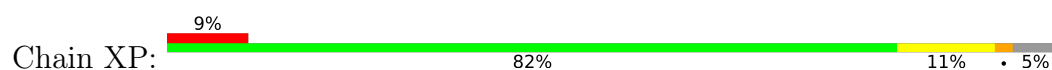


- Molecule 16: 30S ribosomal protein S16

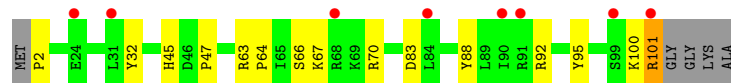
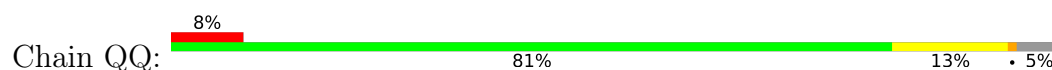




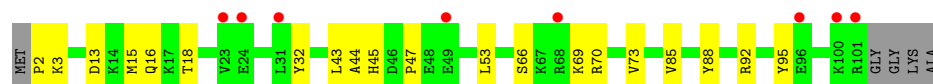
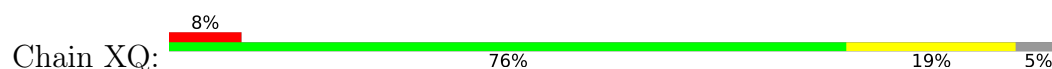
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



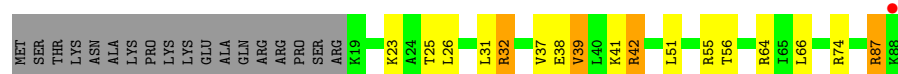
- Molecule 17: 30S ribosomal protein S17



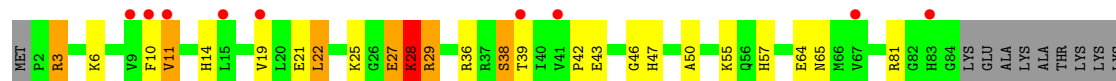
- Molecule 18: 30S ribosomal protein S18



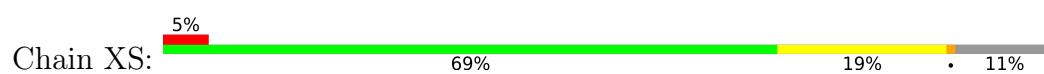
- Molecule 18: 30S ribosomal protein S18



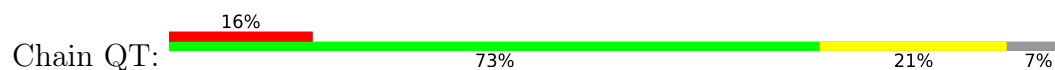
- Molecule 19: 30S ribosomal protein S19



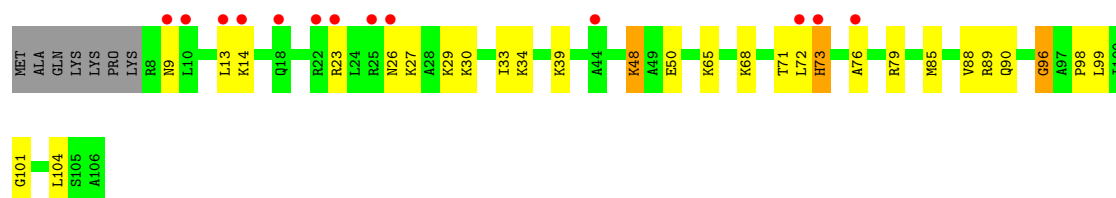
- Molecule 19: 30S ribosomal protein S19



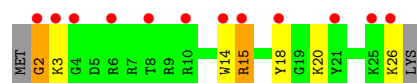
- Molecule 20: 30S ribosomal protein S20



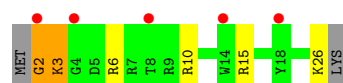
- Molecule 20: 30S ribosomal protein S20



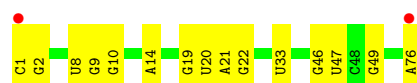
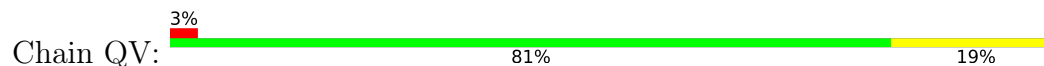
- Molecule 21: 30S ribosomal protein Thx



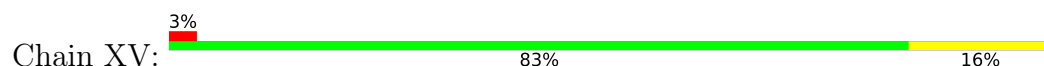
- Molecule 21: 30S ribosomal protein Thx

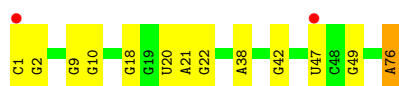


- Molecule 22: P-site tRNA-fMet

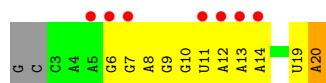


- Molecule 22: P-site tRNA-fMet

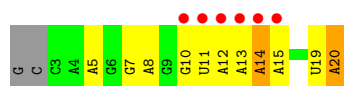




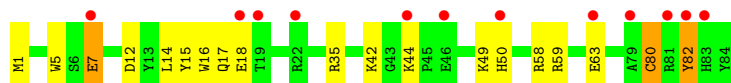
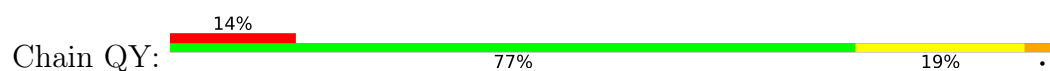
- Molecule 23: mRNA



- Molecule 23: mRNA



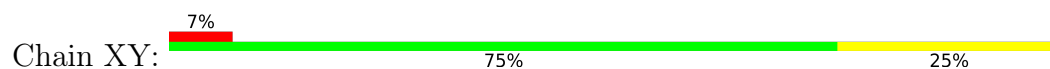
- Molecule 24: Addiction module toxin, Txe/YoeB family



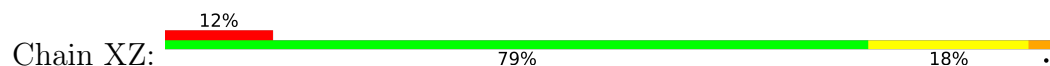
- Molecule 24: Addiction module toxin, Txe/YoeB family



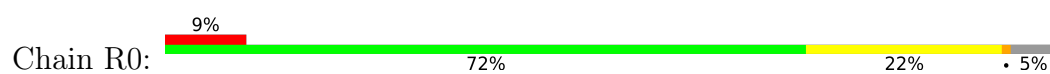
- Molecule 24: Addiction module toxin, Txe/YoeB family



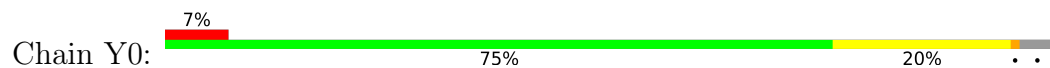
- Molecule 24: Addiction module toxin, Txe/YoeB family



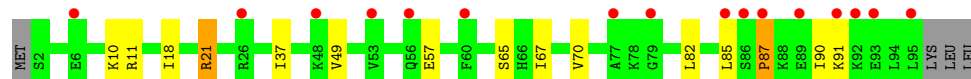
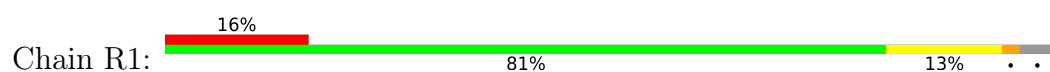
- Molecule 25: 50S ribosomal protein L27



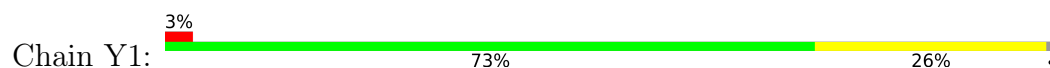
- Molecule 25: 50S ribosomal protein L27



- Molecule 26: 50S ribosomal protein L28



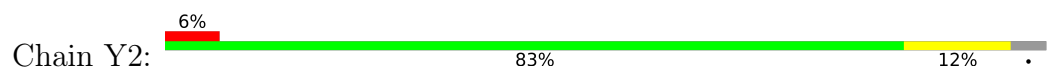
- Molecule 26: 50S ribosomal protein L28



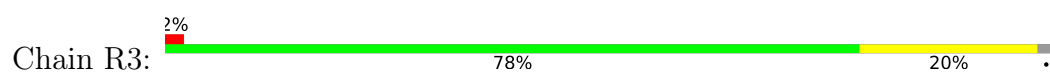
- Molecule 27: 50S ribosomal protein L29



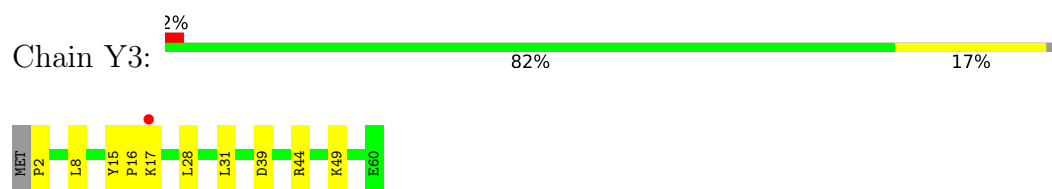
- Molecule 27: 50S ribosomal protein L29



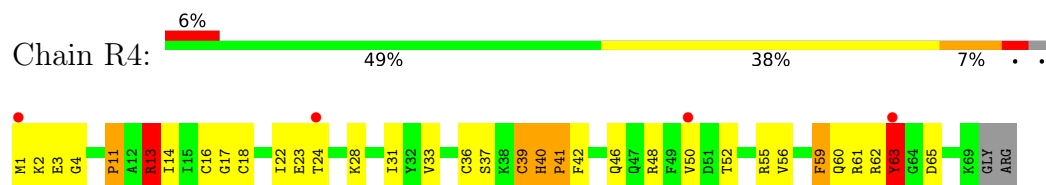
- Molecule 28: 50S ribosomal protein L30



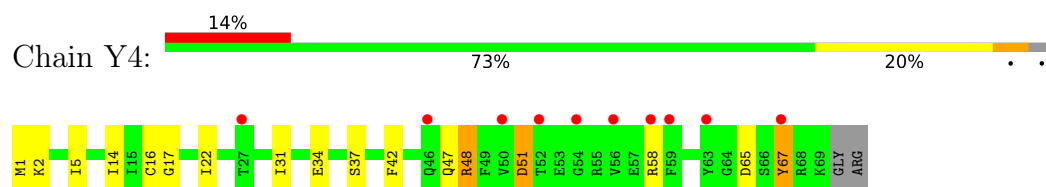
- Molecule 28: 50S ribosomal protein L30



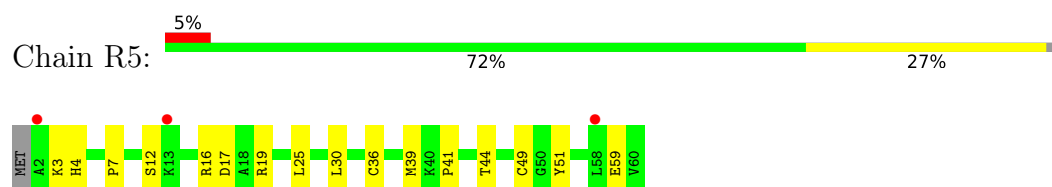
- Molecule 29: 50S ribosomal protein L31



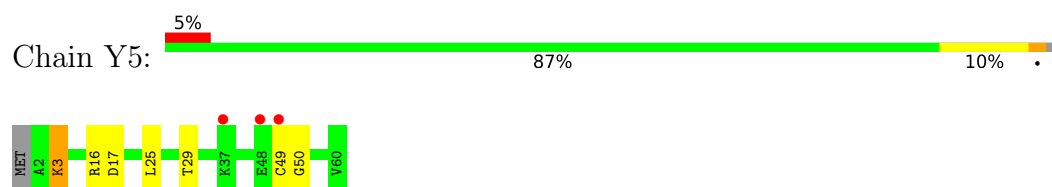
- Molecule 29: 50S ribosomal protein L31



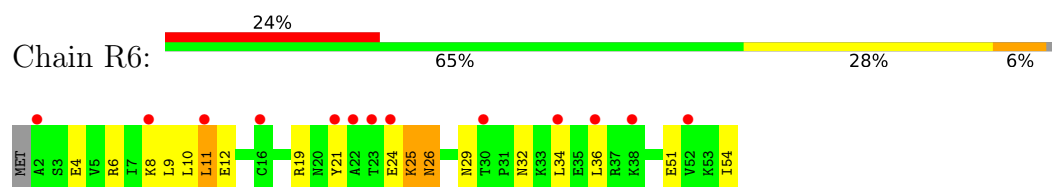
- Molecule 30: 50S ribosomal protein L32



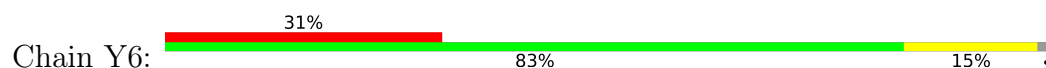
- Molecule 30: 50S ribosomal protein L32

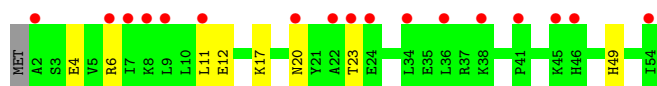


- Molecule 31: 50S ribosomal protein L33

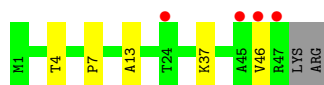
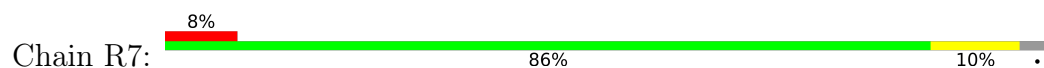


- Molecule 31: 50S ribosomal protein L33

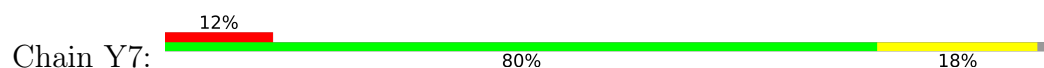




- Molecule 32: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L34



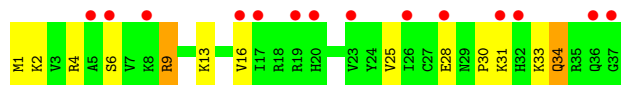
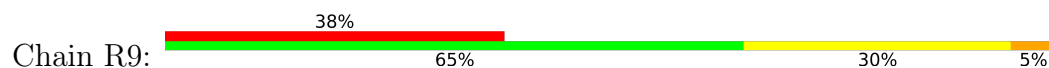
- Molecule 33: 50S ribosomal protein L35



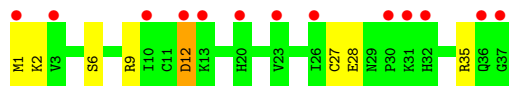
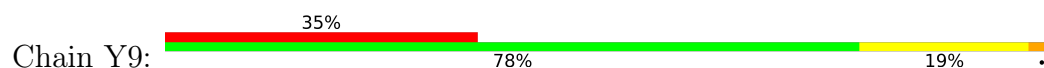
- Molecule 33: 50S ribosomal protein L35



- Molecule 34: 50S ribosomal protein L36



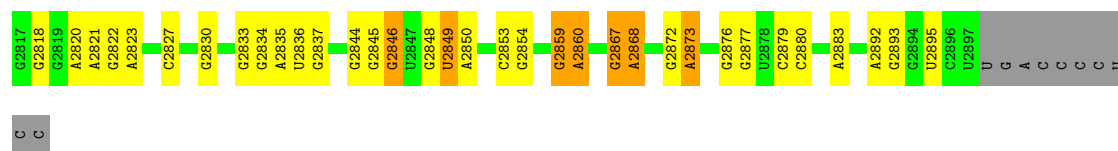
- Molecule 34: 50S ribosomal protein L36



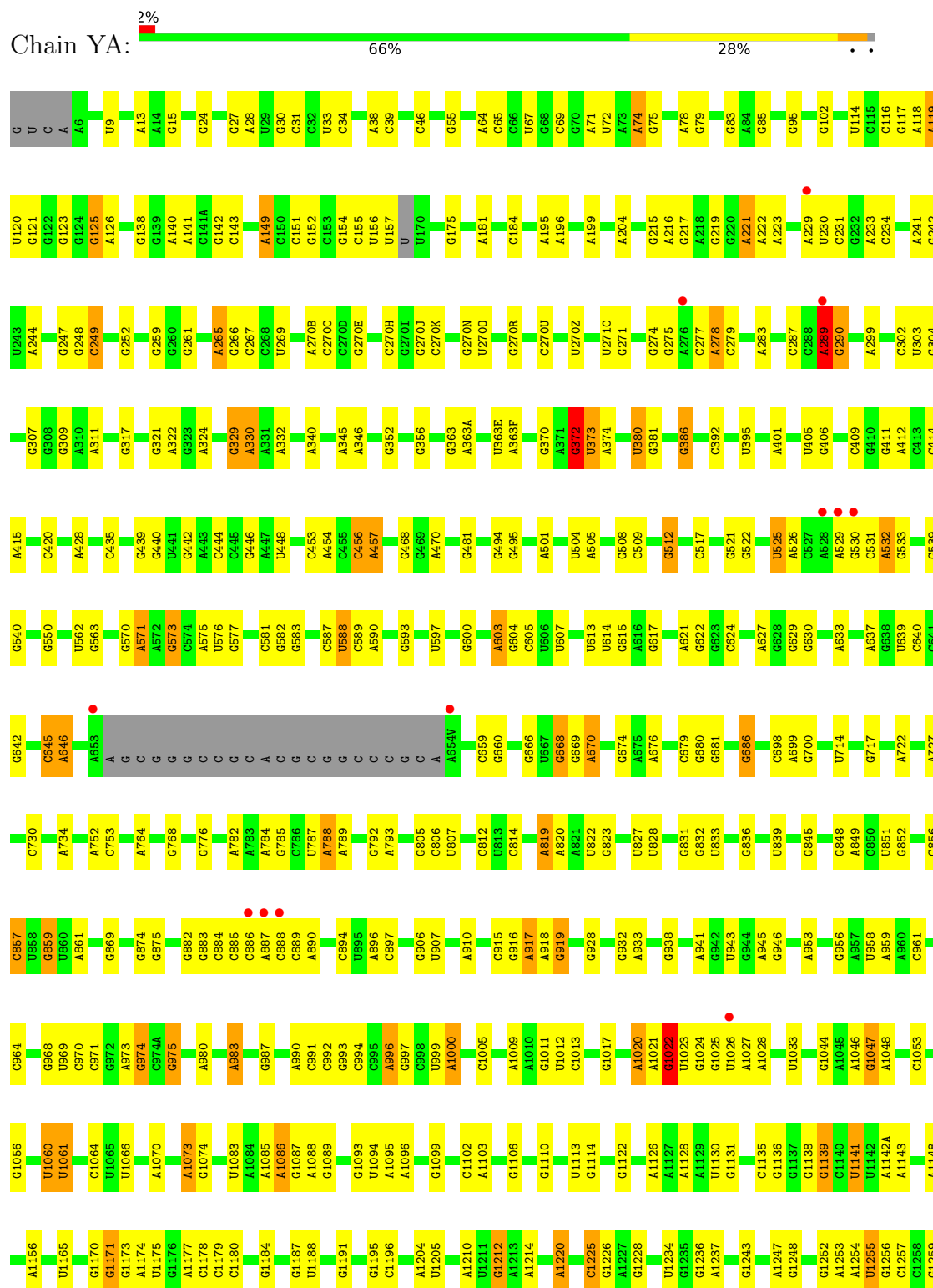
- Molecule 35: 23S rRNA



G2724	G2588	G2470	G2358	G2147	G2056	A1819	G1687	A1554	G1368
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G2726	C2592	U2472	G2473	G2149	A2060	G1824	A1689	A1558	A1379
U2728	G2597	C2474	G2373	U2150	G2061	C1827	C1694	G1560	G1380
G2729	A2598	A2475	G2374	G2153	C2063	G1828	G1696	C1565	A1384
G2732	A2602	C2477	G2374	C2161	G2069	A1829	G1697	A1566	G1385
A2733	G2481	G2482	G2382	G2165	U2074	G1830	A1698	A1567	A1471
C2743	U2609	G2482	G2383	U2167	U2074	G1831	G1699	A1568	G1388
G2744	C2610	G2482	G2384	G2168	U2075	G1842	A1701	A1571	U1391
U2747	U2491	U2491	G2385	A2169	U2079	A1847	G1725	A1572	A1392
G2748	G2502	G2502	A2392	A2170	G2080	A1853	G1728	U1578	A1393
A2749	A2503	A2503	A2393	A2171	A2082	C2081	A1729	A1579	U1396
G2750	G2504	G2504	C2394	U2172	U2086	G1857	U1730	A1580	C1399
G2751	U2505	U2505	C2402	U2173	U2089	G1858	G1731	C1585	G1400
C2752	C2403	C2403	C2403	C2174	U2092	G1863	A1732	A1586	A1401
A2629	G2404	G2404	U2291	C2177	G2093	U1864	G1733	A1587	C1402
G2630	G2405	G2405	C2292	C2178	U2092	G1869	G1733	C1592	C1403
G2638	U2406	U2406	A2298	C2179	G2093	G1872	G1733	C1598	G1407
C2646	G2410	G2410	G2302	C2180	U2102	G1878	A1762	C1599	C1408
A2654	A2411	A2411	G2303	G2181	G2104	C1881	G1764	C1600	C1409
G2655	A2412	A2412	C2304	G2182	C2104	G1888	G1769	A1603	G1410
A2665	C2416	C2416	C2305	C2183	C2111	C1889	G1770	C1518	G1416
G2673	G2422	G2422	G2307	C2184	C2112	A1890	G1771	G1520	C1417
C2680	U2423	U2423	C2308	G2185	C2113	G1895	G1772	G1521	G1418
U2778	C2424	C2424	C2310	C2186	U2113	G1898	G1773	G1522	A1419
G2779	A2425	A2425	U2311	G2189	G2116	A1899	G1776	G1523	U1420
U2682	A2426	A2426	U2312	G2190	A2117	A1890	G1779	G1524	G1421
G2780	C2427	C2427	C2313	G2191	C2118	G1906	A1780	G1536	G1422
A2781	G2428	G2428	C2314	G2192	A2119	A1900	G1781	G1537	U1431
U2689	G2429	G2429	G2315	C2193	G2120	A1913	C1782	G1538	A1434
C2690	A2430	A2430	G2318	U2198	G2124	C1914	A1783	G1539	A1444
C2691	G2435	G2435	G2319	G2199	G2124	A1927	A1784	U1535	U1449
A2693	U2438	U2438	A2320	G2210	C2127	G1935	G1801	U1541	G1449A
U2696	A2439	A2439	G2321	G2211	C2128	A1937	A1802	A1543	C1450
G2697	C2440	C2440	G2325	G2212	U2130	G1936	G1811	C1544	C1451
C2701	G2441	G2441	A2328	G2213	C2136	A1937	A1812	A1545	U1454
U2702	G2445	G2445	G2329	G2215	C2139	A1937	G1811	G1674	G1455
C2703	G2446	G2446	G2334	G2226	G2141	A1937	A1812	C1547	A1456
U2712	G2447	G2447	A2335	G2230	G2142	A1938	G1816	C1550	U1457
A2712A	A2448	A2448	C2343	U2233	C2143	C1941	G1817	G1681	C1458
G2802	C2573	C2573	C2347	G2238	U2144	G1948	A1817		
C2803	G2574	G2574	C2347	G2239	C2145				
G2804	U2457	U2457	C2350	U2243	C2146				
U2805	G2578	G2578	G2350	U2244	C2146				
G2807	U2584	U2584	G2353	U2245	C2146				
U2808	U2585	U2585	G2354	G2246	C2146				
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C2816	C2587	C2587							



• Molecule 35: 23S rRNA







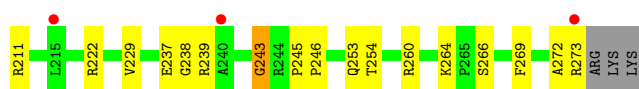
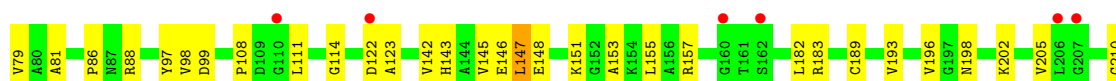
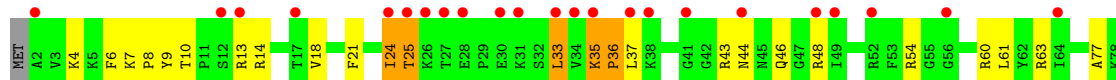
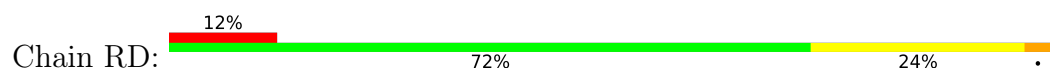
• Molecule 36: 5S rRNA



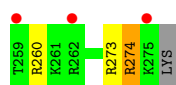
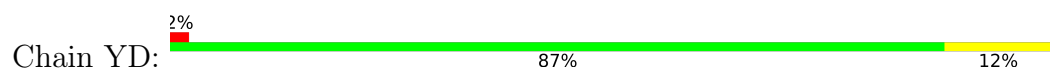
• Molecule 36: 5S rRNA



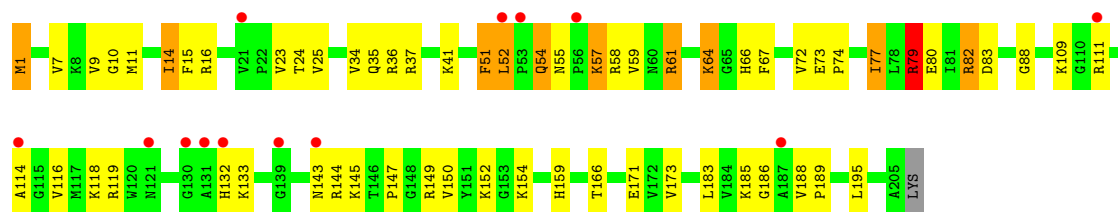
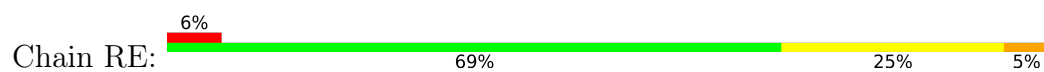
• Molecule 37: 50S ribosomal protein L2



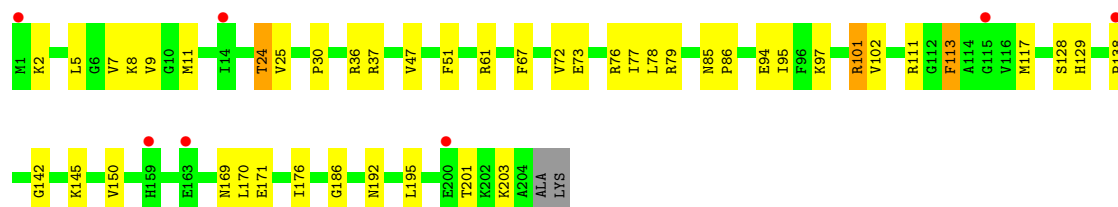
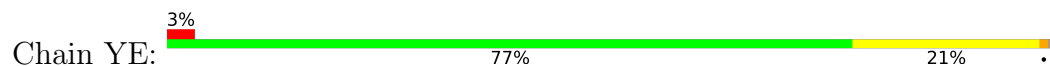
• Molecule 37: 50S ribosomal protein L2



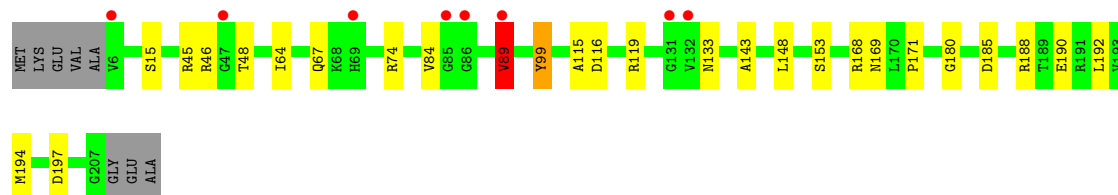
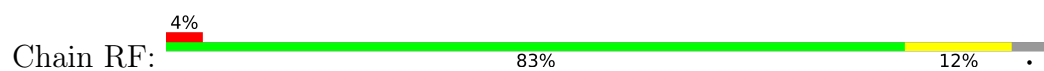
• Molecule 38: 50S ribosomal protein L3



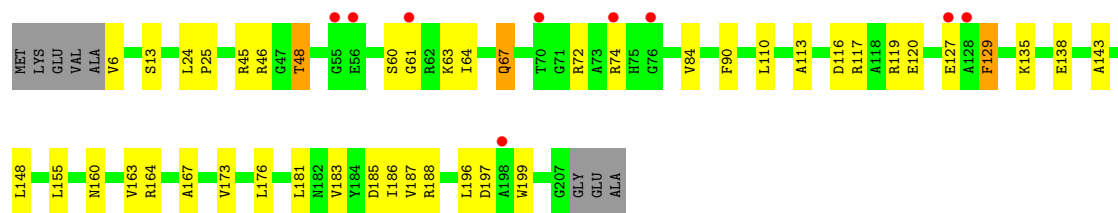
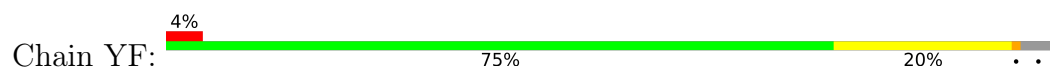
• Molecule 38: 50S ribosomal protein L3



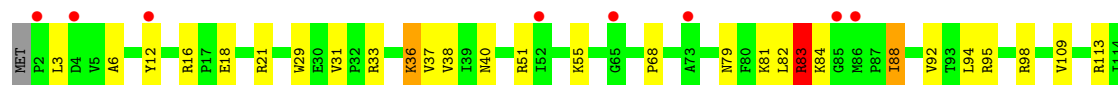
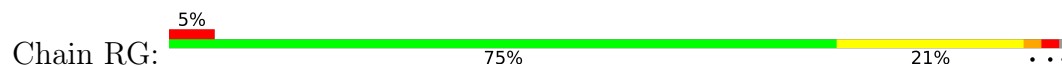
• Molecule 39: 50S ribosomal protein L4

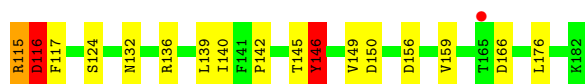


• Molecule 39: 50S ribosomal protein L4

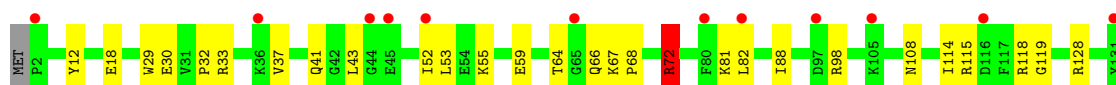
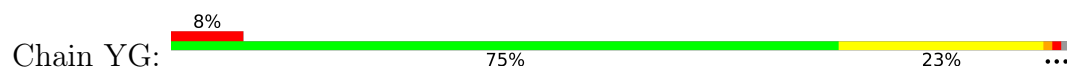


• Molecule 40: 50S ribosomal protein L5

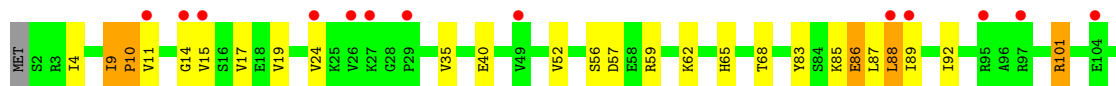
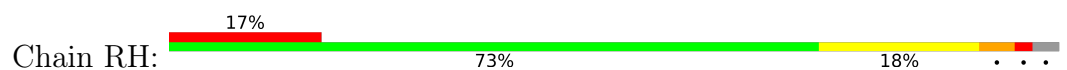




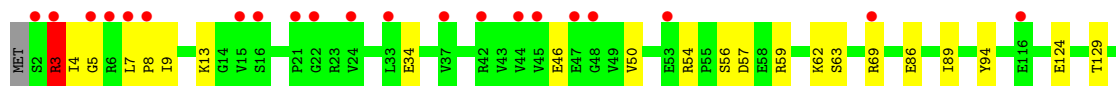
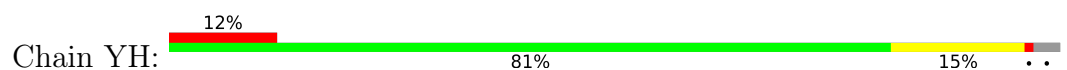
- Molecule 40: 50S ribosomal protein L5



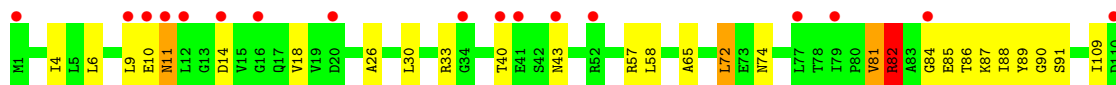
- Molecule 41: 50S ribosomal protein L6



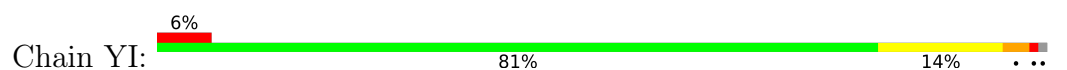
- Molecule 41: 50S ribosomal protein L6

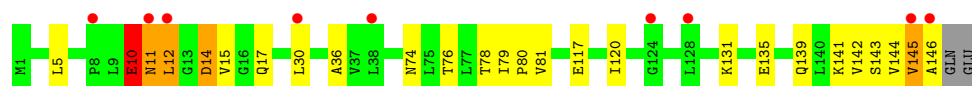


- Molecule 42: 50S ribosomal protein L9

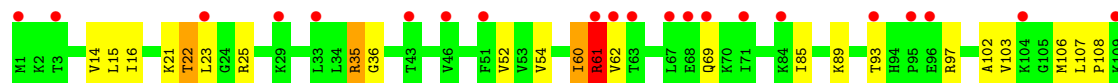
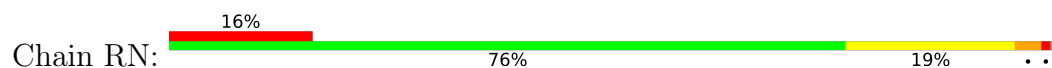


- Molecule 42: 50S ribosomal protein L9

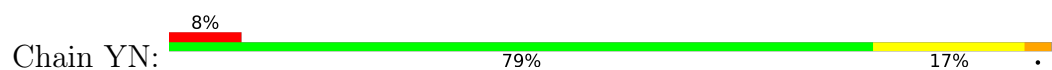




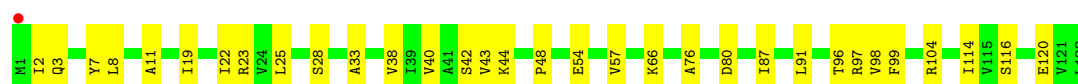
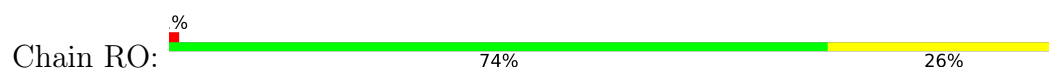
- Molecule 43: 50S ribosomal protein L13



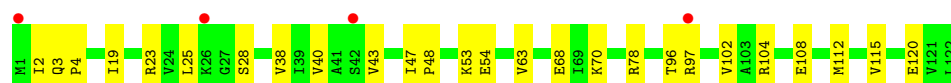
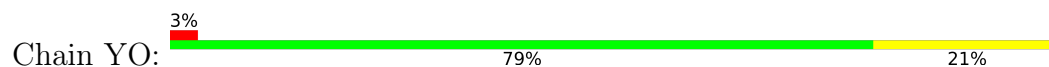
- Molecule 43: 50S ribosomal protein L13



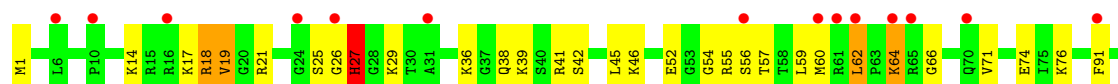
- Molecule 44: 50S ribosomal protein L14



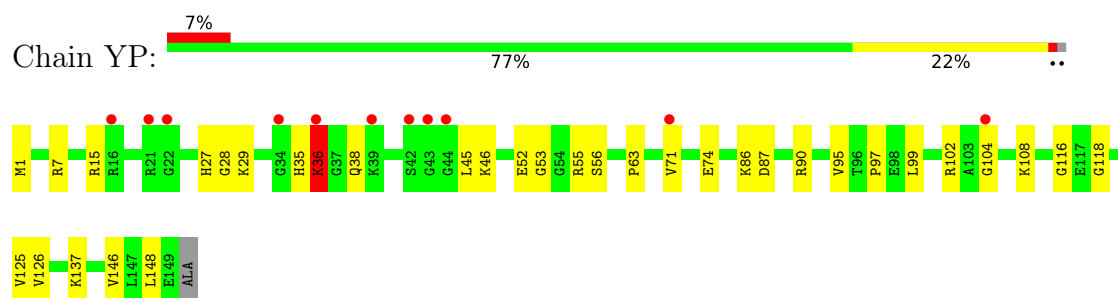
- Molecule 44: 50S ribosomal protein L14



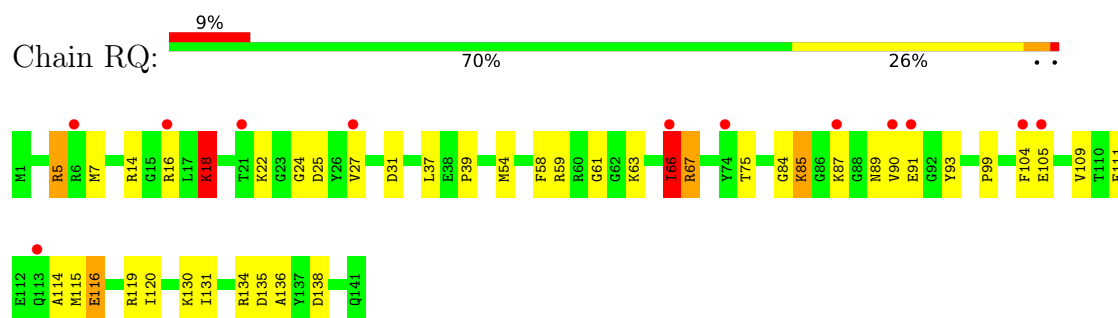
- Molecule 45: 50S ribosomal protein L15



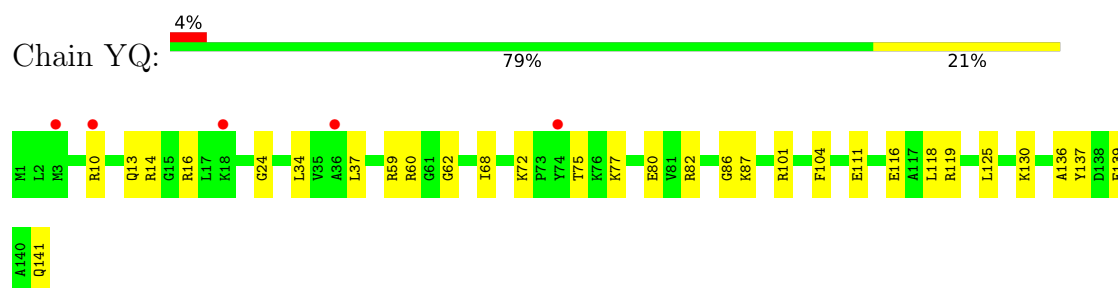
- Molecule 45: 50S ribosomal protein L15



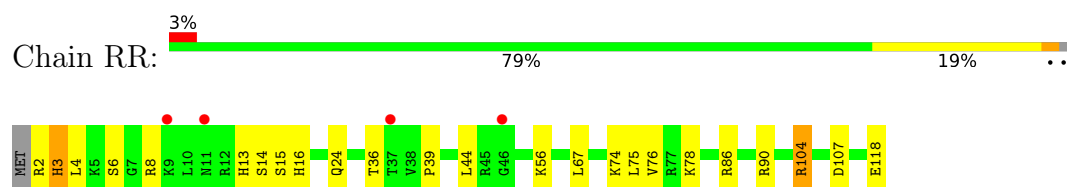
- Molecule 46: 50S ribosomal protein L16



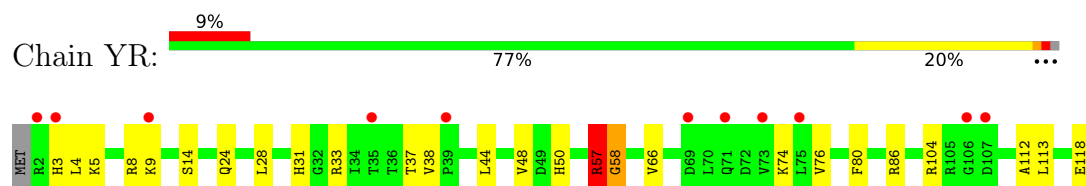
- Molecule 46: 50S ribosomal protein L16



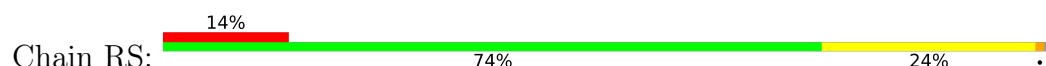
- Molecule 47: 50S ribosomal protein L17

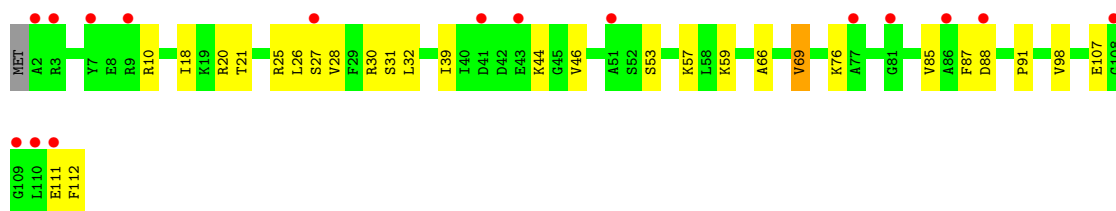


- Molecule 47: 50S ribosomal protein L17

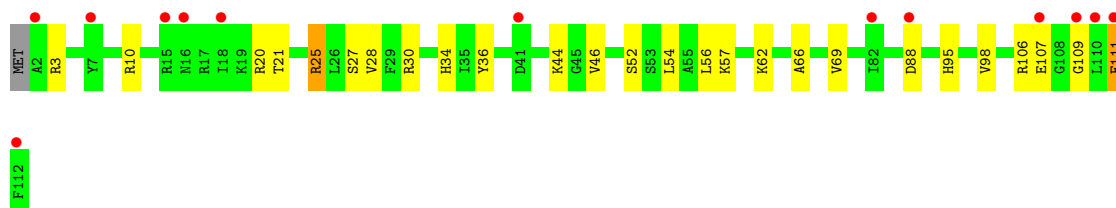
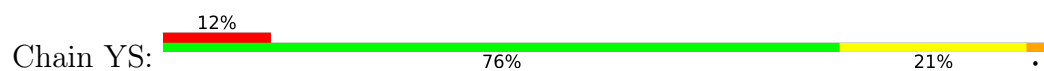


- Molecule 48: 50S ribosomal protein L18

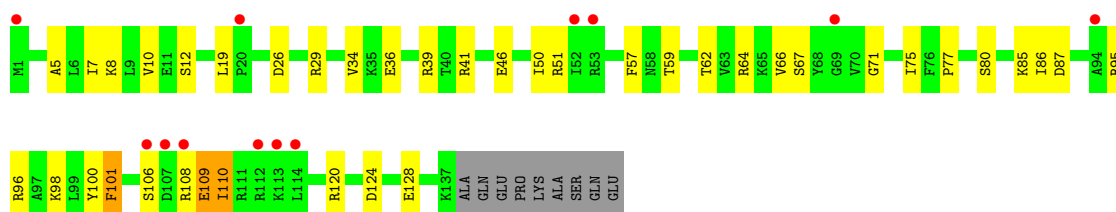




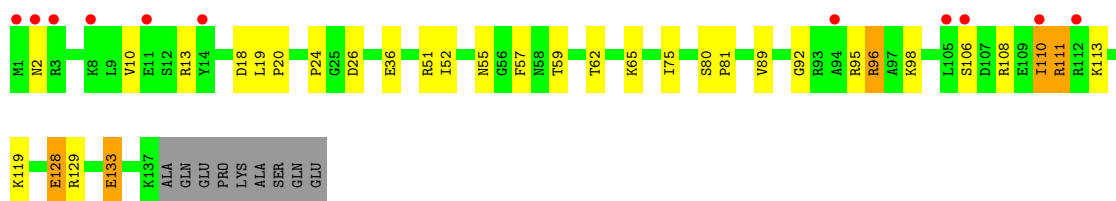
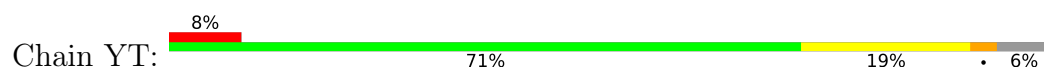
- Molecule 48: 50S ribosomal protein L18



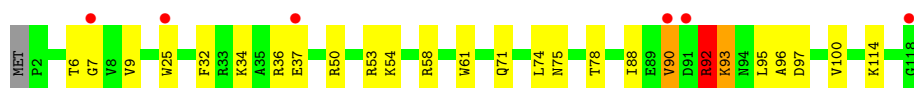
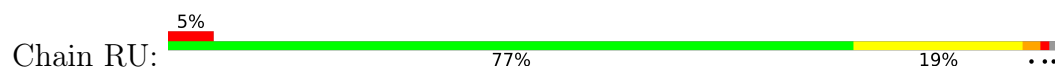
- Molecule 49: 50S ribosomal protein L19



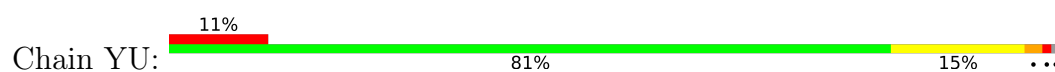
- Molecule 49: 50S ribosomal protein L19

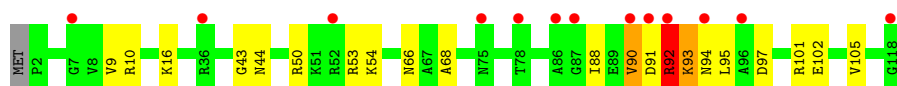


- Molecule 50: 50S ribosomal protein L20

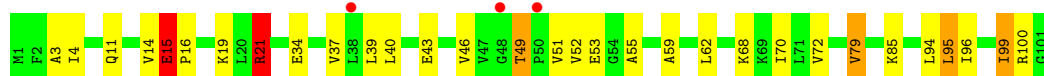


- Molecule 50: 50S ribosomal protein L20

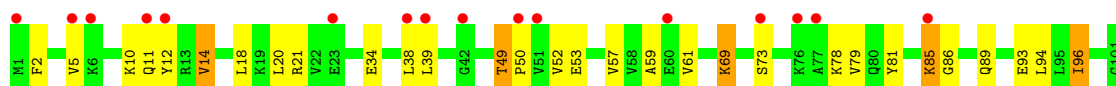
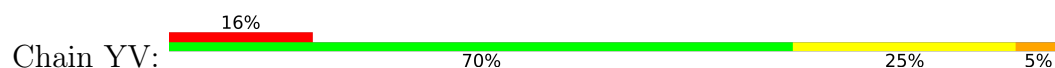




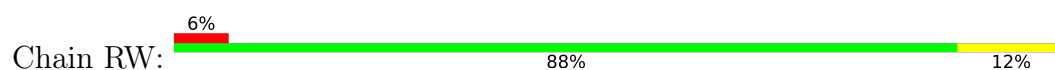
- Molecule 51: 50S ribosomal protein L21



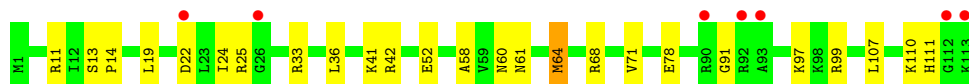
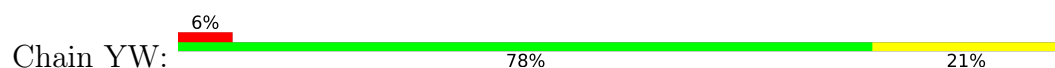
- Molecule 51: 50S ribosomal protein L21



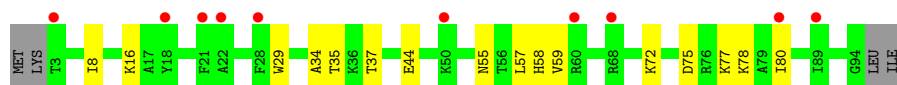
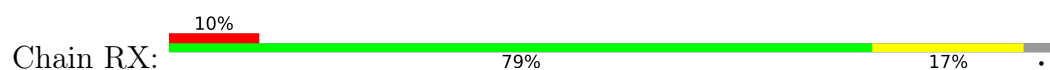
- Molecule 52: 50S ribosomal protein L22



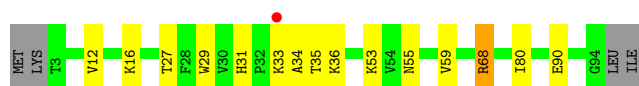
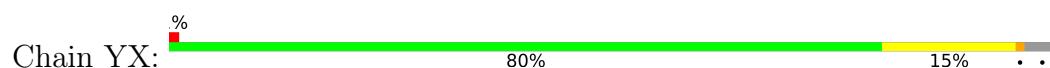
- Molecule 52: 50S ribosomal protein L22



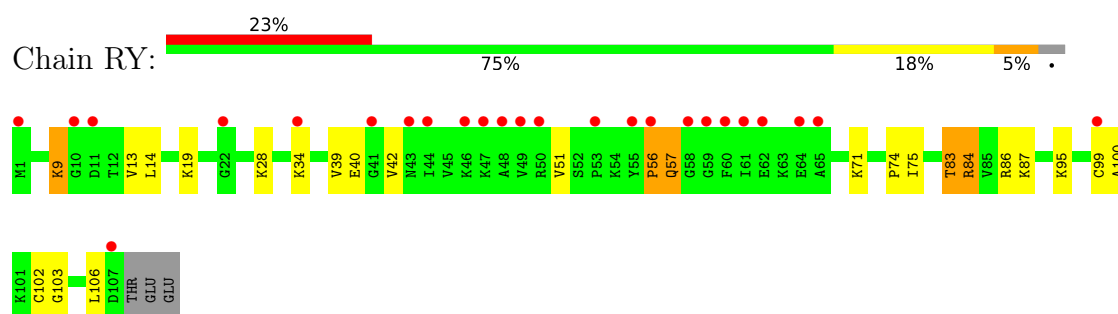
- Molecule 53: 50S ribosomal protein L23



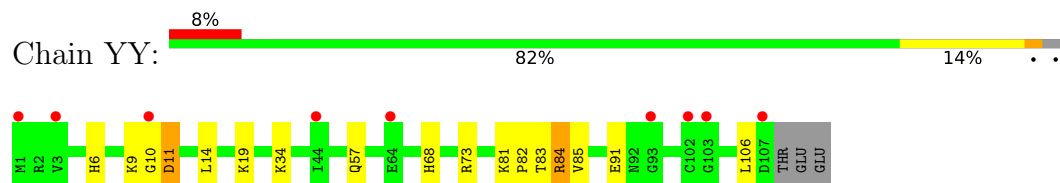
- Molecule 53: 50S ribosomal protein L23



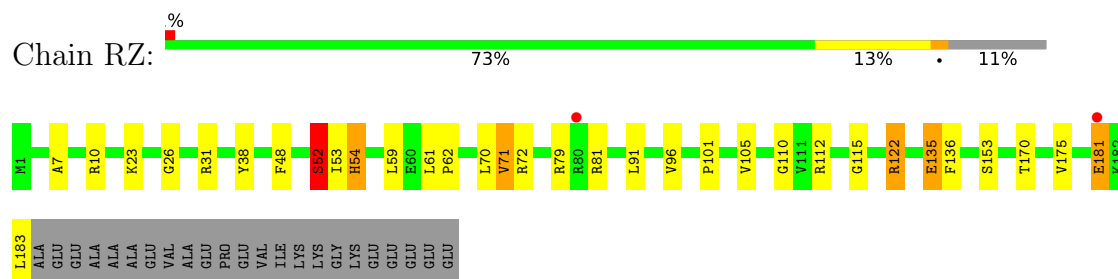
- Molecule 54: 50S ribosomal protein L24



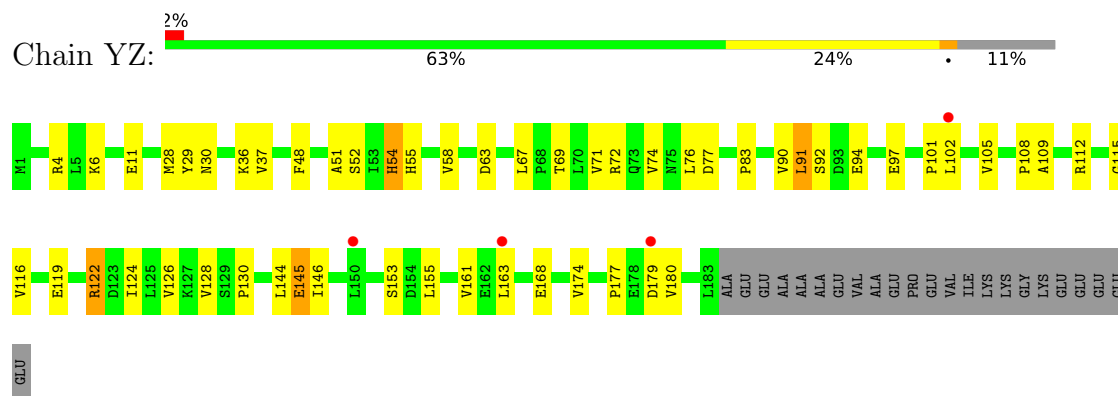
- Molecule 54: 50S ribosomal protein L24



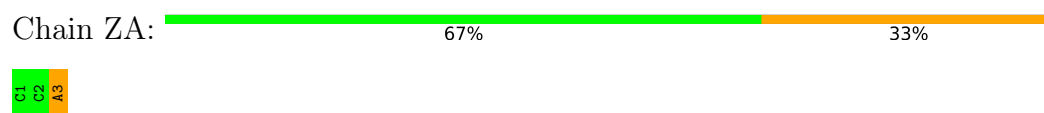
- Molecule 55: 50S ribosomal protein L25



- Molecule 55: 50S ribosomal protein L25



- Molecule 56: CCPuro



- Molecule 56: CCPuro





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	214.68Å 453.51Å 609.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.72 – 3.50 146.72 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (146.72-3.50) 98.0 (146.72-3.50)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.216 , 0.246 0.218 , 0.247	Depositor DCC
R_{free} test set	33274 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	89.9	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 86.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	295153	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% 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: MG, ZN, A3P, PPU, SF4

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	0.20	0/36324	0.43	11/56690 (0.0%)
1	XA	0.57	6/36254 (0.0%)	0.44	11/56581 (0.0%)
2	QB	0.63	6/1942 (0.3%)	1.15	21/2619 (0.8%)
2	XB	0.34	0/1950	1.07	18/2630 (0.7%)
3	QC	0.33	0/1629	1.05	12/2195 (0.5%)
3	XC	0.33	0/1629	0.97	5/2195 (0.2%)
4	QD	0.32	0/1733	1.03	13/2318 (0.6%)
4	XD	0.33	0/1733	1.12	19/2318 (0.8%)
5	QE	0.33	0/1171	0.94	3/1576 (0.2%)
5	XE	0.27	0/1171	0.88	3/1576 (0.2%)
6	QF	0.25	0/856	0.83	1/1154 (0.1%)
6	XF	0.27	0/856	0.87	2/1154 (0.2%)
7	QG	0.36	0/1276	1.10	12/1709 (0.7%)
7	XG	0.33	0/1276	0.93	5/1709 (0.3%)
8	QH	0.27	0/1128	0.99	4/1517 (0.3%)
8	XH	0.25	0/1128	0.92	6/1517 (0.4%)
9	QI	0.45	0/1029	1.20	9/1379 (0.7%)
9	XI	0.32	0/1017	1.11	12/1365 (0.9%)
10	QJ	0.42	0/814	1.12	8/1095 (0.7%)
10	XJ	0.35	0/790	1.13	9/1063 (0.8%)
11	QK	0.32	0/900	0.97	4/1213 (0.3%)
11	XK	0.32	0/879	0.98	4/1187 (0.3%)
12	QL	0.30	0/991	1.15	11/1327 (0.8%)
12	XL	0.37	0/972	1.18	15/1301 (1.2%)
13	QM	0.41	0/965	1.29	10/1292 (0.8%)
13	XM	0.35	0/956	1.17	11/1281 (0.9%)
14	QN	0.35	0/501	1.19	3/664 (0.5%)
14	XN	0.26	0/501	0.91	1/664 (0.2%)
15	QO	0.28	0/745	0.85	1/992 (0.1%)
15	XO	0.25	0/740	0.72	0/987
16	QP	0.31	0/721	1.09	6/970 (0.6%)
16	XP	0.28	0/721	1.00	4/970 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.30	0/847	1.04	5/1131 (0.4%)
17	XQ	0.28	0/847	0.84	1/1131 (0.1%)
18	QR	0.34	0/579	1.16	4/768 (0.5%)
18	XR	0.34	0/579	1.08	6/768 (0.8%)
19	QS	0.42	0/680	1.27	15/915 (1.6%)
19	XS	0.30	0/671	1.19	7/904 (0.8%)
20	QT	0.36	0/765	1.27	9/1007 (0.9%)
20	XT	0.35	0/765	1.16	8/1007 (0.8%)
21	QU	0.39	0/221	1.11	3/288 (1.0%)
21	XU	0.26	0/221	1.04	2/288 (0.7%)
22	QV	0.19	0/1832	0.40	0/2855
22	XV	0.19	0/1832	0.39	0/2855
23	QX	0.22	0/414	0.58	0/645
23	XX	0.19	0/414	0.48	0/645
24	QY	0.41	0/743	1.09	7/1002 (0.7%)
24	QZ	0.60	2/743 (0.3%)	1.39	11/1002 (1.1%)
24	XY	0.31	0/743	1.07	5/1002 (0.5%)
24	XZ	0.38	0/743	1.25	11/1002 (1.1%)
25	R0	0.37	0/652	1.17	5/867 (0.6%)
25	Y0	0.28	0/657	0.99	1/874 (0.1%)
26	R1	0.40	0/744	1.07	8/989 (0.8%)
26	Y1	0.36	0/770	1.01	2/1022 (0.2%)
27	R2	0.41	0/583	1.33	11/771 (1.4%)
27	Y2	0.30	0/583	0.93	0/771
28	R3	0.28	0/474	0.96	2/635 (0.3%)
28	Y3	0.31	0/474	1.02	3/635 (0.5%)
29	R4	0.59	0/578	1.59	15/776 (1.9%)
29	Y4	0.37	0/578	1.29	6/776 (0.8%)
30	R5	0.32	0/473	0.92	2/639 (0.3%)
30	Y5	0.39	0/473	1.02	1/639 (0.2%)
31	R6	0.32	0/460	1.18	5/613 (0.8%)
31	Y6	0.33	0/460	0.99	1/613 (0.2%)
32	R7	0.27	0/417	0.84	1/550 (0.2%)
32	Y7	0.29	0/426	0.88	2/561 (0.4%)
33	R8	0.48	0/525	1.28	8/691 (1.2%)
33	Y8	0.50	0/525	1.11	6/691 (0.9%)
34	R9	0.41	0/310	1.10	3/407 (0.7%)
34	Y9	0.32	0/310	1.15	2/407 (0.5%)
35	RA	0.21	0/69739	0.44	8/108870 (0.0%)
35	YA	0.21	0/69419	0.44	9/108369 (0.0%)
36	RB	0.23	0/2881	0.45	1/4494 (0.0%)
36	YB	0.28	0/2881	0.47	1/4494 (0.0%)
37	RD	0.35	0/2165	1.27	25/2919 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	YD	0.29	0/2185	1.01	11/2944 (0.4%)
38	RE	0.45	0/1601	1.24	20/2160 (0.9%)
38	YE	0.35	0/1592	1.16	14/2149 (0.7%)
39	RF	0.27	0/1620	0.94	9/2194 (0.4%)
39	YF	0.31	0/1620	1.06	9/2194 (0.4%)
40	RG	0.35	0/1499	1.21	21/2016 (1.0%)
40	YG	0.48	3/1499 (0.2%)	1.13	13/2016 (0.6%)
41	RH	0.44	0/1362	1.48	40/1841 (2.2%)
41	YH	0.35	0/1356	0.96	5/1834 (0.3%)
42	RI	2.65	3/1146 (0.3%)	1.65	31/1551 (2.0%)
42	YI	0.44	0/1151	1.26	20/1558 (1.3%)
43	RN	0.41	0/1131	1.17	10/1525 (0.7%)
43	YN	0.28	0/1131	1.05	10/1525 (0.7%)
44	RO	0.26	0/943	0.96	6/1269 (0.5%)
44	YO	0.29	0/943	0.96	3/1269 (0.2%)
45	RP	0.43	0/1162	1.34	20/1544 (1.3%)
45	YP	0.31	0/1152	1.13	12/1533 (0.8%)
46	RQ	0.46	0/1143	1.19	11/1527 (0.7%)
46	YQ	0.27	0/1143	1.04	6/1527 (0.4%)
47	RR	0.30	0/974	1.20	6/1302 (0.5%)
47	YR	0.35	0/974	1.09	13/1302 (1.0%)
48	RS	0.36	0/892	1.21	7/1187 (0.6%)
48	YS	0.40	0/892	1.21	9/1187 (0.8%)
49	RT	0.41	0/1155	1.16	6/1542 (0.4%)
49	YT	0.41	0/1155	1.16	14/1542 (0.9%)
50	RU	0.34	0/982	1.08	9/1306 (0.7%)
50	YU	0.33	0/982	0.96	5/1306 (0.4%)
51	RV	0.59	1/790 (0.1%)	1.24	6/1057 (0.6%)
51	YV	1.29	6/790 (0.8%)	1.34	10/1057 (0.9%)
52	RW	0.28	0/911	0.96	2/1220 (0.2%)
52	YW	0.28	0/911	0.91	2/1220 (0.2%)
53	RX	0.27	0/739	0.94	2/993 (0.2%)
53	YX	0.31	0/739	0.92	2/993 (0.2%)
54	RY	0.33	0/831	1.10	11/1108 (1.0%)
54	YY	0.29	0/831	1.11	12/1108 (1.1%)
55	RZ	0.37	0/1493	1.15	17/2026 (0.8%)
55	YZ	0.30	0/1493	1.08	13/2026 (0.6%)
56	ZA	0.28	0/40	0.52	0/60
56	ZB	0.27	0/40	0.47	0/60
All	All	0.36	27/319487 (0.0%)	0.69	893/477274 (0.2%)

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
2	QB	0	1
7	XG	0	1
8	XH	0	1
10	QJ	0	1
11	XK	0	1
24	QZ	0	1
37	RD	0	2
37	YD	0	1
38	RE	0	1
40	RG	0	2
40	YG	0	1
41	RH	0	2
41	YH	0	1
42	RI	0	4
47	RR	0	1
47	YR	0	1
51	RV	0	1
All	All	0	23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	RI	82	ARG	CZ-NH1	87.21	2.54	1.32
1	XA	368	U	N3-C4	47.56	2.33	1.38
1	XA	368	U	C2-N3	46.00	2.29	1.37
1	XA	368	U	N1-C2	41.62	2.21	1.38
1	XA	368	U	N1-C6	40.83	2.19	1.38

The worst 5 of 893 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	RR	76	VAL	N-CA-C	-19.67	93.29	112.96
37	RD	35	LYS	N-CA-C	-17.68	92.31	108.22
42	RI	11	ASN	CA-C-N	15.29	149.12	122.67
42	RI	11	ASN	C-N-CA	15.29	149.12	122.67
48	RS	107	GLU	N-CA-C	-15.26	92.38	112.68

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	12	GLU	Sidechain
10	QJ	79	ARG	Sidechain
24	QZ	50	HIS	Peptide
37	RD	33	LEU	Peptide
37	RD	35	LYS	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	32452	0	16383	245	0
1	XA	32389	0	16350	221	0
2	QB	1907	0	1958	31	0
2	XB	1915	0	1969	27	0
3	QC	1605	0	1668	13	0
3	XC	1605	0	1668	17	0
4	QD	1703	0	1767	32	0
4	XD	1703	0	1767	24	0
5	QE	1155	0	1213	12	0
5	XE	1155	0	1213	15	0
6	QF	843	0	857	13	0
6	XF	843	0	857	10	0
7	QG	1257	0	1296	10	0
7	XG	1257	0	1296	17	0
8	QH	1108	0	1165	21	0
8	XH	1108	0	1165	13	0
9	QI	1010	0	1037	17	0
9	XI	998	0	1024	20	0
10	QJ	801	0	849	11	0
10	XJ	777	0	816	18	0
11	QK	885	0	904	12	0
11	XK	864	0	881	9	0
12	QL	975	0	1062	11	0
12	XL	956	0	1046	13	0
13	QM	955	0	1021	27	0
13	XM	946	0	1008	16	0
14	QN	492	0	529	5	0
14	XN	492	0	529	12	0
15	QO	734	0	771	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	XO	729	0	768	4	0
16	QP	705	0	725	12	0
16	XP	705	0	725	6	0
17	QQ	834	0	904	9	0
17	XQ	834	0	904	12	0
18	QR	574	0	644	9	0
18	XR	574	0	644	12	0
19	QS	665	0	686	15	0
19	XS	656	0	666	9	0
20	QT	763	0	861	9	0
20	XT	763	0	861	15	0
21	QU	217	0	234	5	0
21	XU	217	0	234	7	0
22	QV	1640	0	837	4	0
22	XV	1640	0	837	3	0
23	QX	394	0	196	2	0
23	XX	394	0	196	4	0
24	QY	723	0	713	11	0
24	QZ	723	0	713	11	0
24	XY	723	0	713	9	0
24	XZ	723	0	713	7	0
25	R0	643	0	667	13	0
25	Y0	648	0	672	15	0
26	R1	737	0	813	6	0
26	Y1	763	0	848	18	0
27	R2	581	0	629	8	0
27	Y2	581	0	629	4	0
28	R3	469	0	518	5	0
28	Y3	469	0	518	5	0
29	R4	565	0	561	26	0
29	Y4	565	0	559	10	0
30	R5	459	0	476	11	0
30	Y5	459	0	480	6	0
31	R6	453	0	474	10	0
31	Y6	453	0	474	4	0
32	R7	409	0	454	3	0
32	Y7	418	0	467	6	0
33	R8	517	0	582	11	0
33	Y8	517	0	582	12	0
34	R9	307	0	337	10	0
34	Y9	307	0	336	5	0
35	RA	62266	0	31392	354	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	YA	61981	0	31243	341	0
36	RB	2576	0	1303	28	0
36	YB	2576	0	1305	19	0
37	RD	2115	0	2195	39	0
37	YD	2135	0	2221	19	0
38	RE	1568	0	1634	38	0
38	YE	1559	0	1617	25	0
39	RF	1585	0	1632	15	0
39	YF	1585	0	1632	25	0
40	RG	1474	0	1535	23	0
40	YG	1474	0	1535	20	0
41	RH	1336	0	1418	12	0
41	YH	1330	0	1407	18	0
42	RI	1131	0	1218	16	0
42	YI	1136	0	1223	9	0
43	RN	1104	0	1180	17	0
43	YN	1104	0	1180	15	0
44	RO	933	0	996	17	0
44	YO	933	0	996	16	0
45	RP	1145	0	1228	29	0
45	YP	1135	0	1212	17	0
46	RQ	1122	0	1179	27	0
46	YQ	1122	0	1179	20	0
47	RR	960	0	1021	12	0
47	YR	960	0	1021	11	0
48	RS	882	0	943	14	0
48	YS	882	0	943	15	0
49	RT	1141	0	1202	21	0
49	YT	1141	0	1202	14	0
50	RU	964	0	1022	19	0
50	YU	964	0	1022	22	0
51	RV	779	0	852	16	0
51	YV	779	0	852	26	0
52	RW	900	0	964	8	0
52	YW	900	0	964	16	0
53	RX	725	0	778	11	0
53	YX	725	0	778	8	0
54	RY	818	0	913	12	0
54	YY	818	0	913	5	0
55	RZ	1461	0	1493	17	0
55	YZ	1461	0	1493	27	0
56	ZA	74	0	51	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	ZB	74	0	51	7	0
57	QA	93	0	0	0	0
57	QD	1	0	0	0	0
57	QE	1	0	0	0	0
57	QV	3	0	0	0	0
57	QY	1	0	0	0	0
57	R0	2	0	0	0	0
57	R3	1	0	0	0	0
57	RA	302	0	0	0	0
57	RB	3	0	0	0	0
57	RD	2	0	0	0	0
57	RE	1	0	0	0	0
57	RN	1	0	0	0	0
57	RO	1	0	0	0	0
57	RP	1	0	0	0	0
57	RQ	4	0	0	0	0
57	RR	1	0	0	0	0
57	RY	1	0	0	0	0
57	XA	99	0	0	0	0
57	XE	1	0	0	0	0
57	XF	1	0	0	0	0
57	XL	1	0	0	0	0
57	XM	1	0	0	0	0
57	XV	4	0	0	0	0
57	Y0	2	0	0	0	0
57	Y1	1	0	0	0	0
57	Y3	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YA	335	0	0	0	0
57	YB	3	0	0	0	0
57	YD	4	0	0	0	0
57	YE	5	0	0	0	0
57	YF	1	0	0	0	0
57	YG	1	0	0	0	0
57	YO	1	0	0	0	0
57	YP	1	0	0	0	0
57	YQ	5	0	0	0	0
57	YR	1	0	0	0	0
57	YV	1	0	0	0	0
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	QN	1	0	0	0	0
59	R4	1	0	0	0	0
59	R5	1	0	0	0	0
59	R6	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
59	Y6	1	0	0	0	0
All	All	295153	0	201057	2224	0

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 5.

The worst 5 of 2224 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)
51:YV:85:LYS:CG	51:YV:85:LYS:CD	1.86	1.53
51:YV:85:LYS:CG	51:YV:85:LYS:CB	1.82	1.50
1:XA:368:U:C5	1:XA:368:U:C6	2.05	1.45
51:YV:85:LYS:NZ	51:YV:85:LYS:CE	1.87	1.36
51:YV:85:LYS:CD	51:YV:85:LYS:CE	2.10	1.30

There are no symmetry-related clashes.

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%)	202 (87%)	27 (12%)	4 (2%)	7	35
2	XB	234/256 (91%)	211 (90%)	21 (9%)	2 (1%)	14	47
3	QC	203/239 (85%)	186 (92%)	17 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	XC	203/239 (85%)	188 (93%)	14 (7%)	1 (0%)	24	57
4	QD	206/209 (99%)	193 (94%)	11 (5%)	2 (1%)	12	44
4	XD	206/209 (99%)	187 (91%)	17 (8%)	2 (1%)	12	44
5	QE	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
5	XE	149/162 (92%)	142 (95%)	7 (5%)	0	100	100
6	QF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
6	XF	99/101 (98%)	99 (100%)	0	0	100	100
7	QG	153/156 (98%)	144 (94%)	8 (5%)	1 (1%)	18	51
7	XG	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
8	QH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
8	XH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
9	QI	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
9	XI	124/128 (97%)	113 (91%)	11 (9%)	0	100	100
10	QJ	97/105 (92%)	85 (88%)	12 (12%)	0	100	100
10	XJ	94/105 (90%)	80 (85%)	13 (14%)	1 (1%)	11	43
11	QK	117/129 (91%)	107 (92%)	10 (8%)	0	100	100
11	XK	114/129 (88%)	105 (92%)	9 (8%)	0	100	100
12	QL	123/132 (93%)	110 (89%)	11 (9%)	2 (2%)	7	36
12	XL	120/132 (91%)	103 (86%)	16 (13%)	1 (1%)	16	49
13	QM	118/126 (94%)	102 (86%)	13 (11%)	3 (2%)	4	28
13	XM	117/126 (93%)	96 (82%)	21 (18%)	0	100	100
14	QN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	35
14	XN	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7	35
15	QO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
15	XO	85/89 (96%)	84 (99%)	1 (1%)	0	100	100
16	QP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
17	XQ	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	QR	68/88 (77%)	64 (94%)	4 (6%)	0	100	100
18	XR	68/88 (77%)	64 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	QS	81/93 (87%)	69 (85%)	11 (14%)	1 (1%)	10	41
19	XS	81/93 (87%)	75 (93%)	6 (7%)	0	100	100
20	QT	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
20	XT	97/106 (92%)	88 (91%)	6 (6%)	3 (3%)	3	25
21	QU	23/27 (85%)	20 (87%)	2 (9%)	1 (4%)	2	18
21	XU	23/27 (85%)	22 (96%)	0	1 (4%)	2	18
24	QY	82/84 (98%)	70 (85%)	10 (12%)	2 (2%)	4	29
24	QZ	82/84 (98%)	72 (88%)	10 (12%)	0	100	100
24	XY	82/84 (98%)	71 (87%)	8 (10%)	3 (4%)	2	21
24	XZ	82/84 (98%)	70 (85%)	11 (13%)	1 (1%)	10	41
25	R0	79/85 (93%)	72 (91%)	6 (8%)	1 (1%)	9	39
25	Y0	80/85 (94%)	72 (90%)	8 (10%)	0	100	100
26	R1	92/98 (94%)	82 (89%)	10 (11%)	0	100	100
26	Y1	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11	43
27	R2	67/72 (93%)	61 (91%)	5 (8%)	1 (2%)	8	37
27	Y2	67/72 (93%)	63 (94%)	2 (3%)	2 (3%)	3	25
28	R3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
28	Y3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
29	R4	67/71 (94%)	46 (69%)	17 (25%)	4 (6%)	1	12
29	Y4	67/71 (94%)	54 (81%)	12 (18%)	1 (2%)	8	37
30	R5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
30	Y5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
31	R6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
31	Y6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
32	R7	45/49 (92%)	45 (100%)	0	0	100	100
32	Y7	46/49 (94%)	46 (100%)	0	0	100	100
33	R8	62/65 (95%)	54 (87%)	6 (10%)	2 (3%)	3	24
33	Y8	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	3	24
34	R9	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
34	Y9	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
37	RD	270/276 (98%)	244 (90%)	22 (8%)	4 (2%)	8	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	YD	272/276 (99%)	263 (97%)	9 (3%)	0	100	100
38	RE	203/206 (98%)	179 (88%)	20 (10%)	4 (2%)	6	32
38	YE	202/206 (98%)	191 (95%)	9 (4%)	2 (1%)	12	44
39	RF	200/210 (95%)	195 (98%)	5 (2%)	0	100	100
39	YF	200/210 (95%)	184 (92%)	14 (7%)	2 (1%)	12	44
40	RG	179/182 (98%)	152 (85%)	24 (13%)	3 (2%)	7	35
40	YG	179/182 (98%)	151 (84%)	26 (14%)	2 (1%)	11	43
41	RH	172/180 (96%)	137 (80%)	29 (17%)	6 (4%)	3	23
41	YH	172/180 (96%)	164 (95%)	8 (5%)	0	100	100
42	RI	143/148 (97%)	117 (82%)	20 (14%)	6 (4%)	2	19
42	YI	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	9	38
43	RN	136/140 (97%)	117 (86%)	17 (12%)	2 (2%)	8	37
43	YN	136/140 (97%)	118 (87%)	16 (12%)	2 (2%)	8	37
44	RO	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
44	YO	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	16	49
45	RP	148/150 (99%)	125 (84%)	19 (13%)	4 (3%)	4	27
45	YP	147/150 (98%)	138 (94%)	7 (5%)	2 (1%)	9	38
46	RQ	139/141 (99%)	121 (87%)	13 (9%)	5 (4%)	2	22
46	YQ	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
47	RR	115/118 (98%)	108 (94%)	6 (5%)	1 (1%)	14	47
47	YR	115/118 (98%)	103 (90%)	11 (10%)	1 (1%)	14	47
48	RS	109/112 (97%)	93 (85%)	15 (14%)	1 (1%)	14	47
48	YS	109/112 (97%)	93 (85%)	16 (15%)	0	100	100
49	RT	135/146 (92%)	119 (88%)	15 (11%)	1 (1%)	18	51
49	YT	135/146 (92%)	119 (88%)	16 (12%)	0	100	100
50	RU	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	14	47
50	YU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	47
51	RV	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
51	YV	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	12	44
52	RW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
52	YW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	RX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
53	YX	90/96 (94%)	86 (96%)	3 (3%)	1 (1%)	11	43
54	RY	105/110 (96%)	94 (90%)	11 (10%)	0	100	100
54	YY	105/110 (96%)	101 (96%)	3 (3%)	1 (1%)	12	44
55	RZ	181/206 (88%)	166 (92%)	13 (7%)	2 (1%)	11	43
55	YZ	181/206 (88%)	168 (93%)	13 (7%)	0	100	100
All	All	11789/12464 (95%)	10734 (91%)	950 (8%)	105 (1%)	14	47

5 of 105 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	208	ILE
14	QN	17	LYS
21	QU	3	LYS
24	QY	82	TYR
27	R2	47	ASN

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%)	196 (97%)	7 (3%)	32	57
2	XB	204/220 (93%)	201 (98%)	3 (2%)	57	71
3	QC	159/188 (85%)	155 (98%)	4 (2%)	42	63
3	XC	159/188 (85%)	156 (98%)	3 (2%)	50	68
4	QD	180/181 (99%)	175 (97%)	5 (3%)	38	61
4	XD	180/181 (99%)	180 (100%)	0	100	100
5	QE	116/123 (94%)	115 (99%)	1 (1%)	70	76
5	XE	116/123 (94%)	115 (99%)	1 (1%)	70	76
6	QF	90/90 (100%)	89 (99%)	1 (1%)	65	74
6	XF	90/90 (100%)	89 (99%)	1 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	QG	126/127 (99%)	123 (98%)	3 (2%)	43	64
7	XG	126/127 (99%)	124 (98%)	2 (2%)	55	70
8	QH	118/119 (99%)	118 (100%)	0	100	100
8	XH	118/119 (99%)	117 (99%)	1 (1%)	73	77
9	QI	98/99 (99%)	93 (95%)	5 (5%)	21	48
9	XI	97/99 (98%)	95 (98%)	2 (2%)	47	66
10	QJ	89/92 (97%)	84 (94%)	5 (6%)	19	46
10	XJ	86/92 (94%)	85 (99%)	1 (1%)	63	73
11	QK	90/99 (91%)	88 (98%)	2 (2%)	45	65
11	XK	88/99 (89%)	87 (99%)	1 (1%)	65	74
12	QL	104/109 (95%)	103 (99%)	1 (1%)	68	75
12	XL	103/109 (94%)	102 (99%)	1 (1%)	68	75
13	QM	96/101 (95%)	95 (99%)	1 (1%)	68	75
13	XM	95/101 (94%)	93 (98%)	2 (2%)	47	66
14	QN	49/50 (98%)	48 (98%)	1 (2%)	48	67
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	70 (97%)	2 (3%)	38	61
17	QQ	95/97 (98%)	94 (99%)	1 (1%)	65	74
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	58 (95%)	3 (5%)	22	48
18	XR	61/77 (79%)	60 (98%)	1 (2%)	55	70
19	QS	72/80 (90%)	70 (97%)	2 (3%)	38	61
19	XS	69/80 (86%)	69 (100%)	0	100	100
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	74 (97%)	2 (3%)	40	62
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
24	QY	78/78 (100%)	76 (97%)	2 (3%)	40	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	QZ	78/78 (100%)	74 (95%)	4 (5%)	21	48
24	XY	78/78 (100%)	78 (100%)	0	100	100
24	XZ	78/78 (100%)	76 (97%)	2 (3%)	40	62
25	R0	65/67 (97%)	65 (100%)	0	100	100
25	Y0	65/67 (97%)	63 (97%)	2 (3%)	35	59
26	R1	79/83 (95%)	77 (98%)	2 (2%)	42	63
26	Y1	82/83 (99%)	81 (99%)	1 (1%)	63	73
27	R2	64/67 (96%)	62 (97%)	2 (3%)	35	59
27	Y2	64/67 (96%)	63 (98%)	1 (2%)	55	70
28	R3	51/52 (98%)	50 (98%)	1 (2%)	48	67
28	Y3	51/52 (98%)	51 (100%)	0	100	100
29	R4	62/63 (98%)	54 (87%)	8 (13%)	4	21
29	Y4	62/63 (98%)	60 (97%)	2 (3%)	34	59
30	R5	51/52 (98%)	51 (100%)	0	100	100
30	Y5	51/52 (98%)	51 (100%)	0	100	100
31	R6	51/52 (98%)	48 (94%)	3 (6%)	18	44
31	Y6	51/52 (98%)	49 (96%)	2 (4%)	28	54
32	R7	40/42 (95%)	40 (100%)	0	100	100
32	Y7	41/42 (98%)	41 (100%)	0	100	100
33	R8	54/55 (98%)	50 (93%)	4 (7%)	13	37
33	Y8	54/55 (98%)	52 (96%)	2 (4%)	30	56
34	R9	34/34 (100%)	33 (97%)	1 (3%)	37	60
34	Y9	34/34 (100%)	34 (100%)	0	100	100
37	RD	214/218 (98%)	210 (98%)	4 (2%)	50	68
37	YD	216/218 (99%)	215 (100%)	1 (0%)	81	80
38	RE	165/166 (99%)	157 (95%)	8 (5%)	23	49
38	YE	164/166 (99%)	163 (99%)	1 (1%)	78	79
39	RF	161/166 (97%)	159 (99%)	2 (1%)	63	73
39	YF	161/166 (97%)	160 (99%)	1 (1%)	78	79
40	RG	155/156 (99%)	151 (97%)	4 (3%)	40	62
40	YG	155/156 (99%)	153 (99%)	2 (1%)	61	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	RH	145/148 (98%)	142 (98%)	3 (2%)	47	66
41	YH	144/148 (97%)	141 (98%)	3 (2%)	47	66
42	RI	122/124 (98%)	116 (95%)	6 (5%)	22	48
42	YI	122/124 (98%)	119 (98%)	3 (2%)	42	63
43	RN	117/119 (98%)	116 (99%)	1 (1%)	70	76
43	YN	117/119 (98%)	116 (99%)	1 (1%)	70	76
44	RO	100/100 (100%)	100 (100%)	0	100	100
44	YO	100/100 (100%)	99 (99%)	1 (1%)	68	75
45	RP	116/116 (100%)	114 (98%)	2 (2%)	53	70
45	YP	115/116 (99%)	113 (98%)	2 (2%)	53	70
46	RQ	111/111 (100%)	106 (96%)	5 (4%)	24	50
46	YQ	111/111 (100%)	111 (100%)	0	100	100
47	RR	100/101 (99%)	99 (99%)	1 (1%)	68	75
47	YR	100/101 (99%)	99 (99%)	1 (1%)	68	75
48	RS	87/88 (99%)	84 (97%)	3 (3%)	32	57
48	YS	87/88 (99%)	86 (99%)	1 (1%)	65	74
49	RT	120/127 (94%)	115 (96%)	5 (4%)	26	52
49	YT	120/127 (94%)	117 (98%)	3 (2%)	42	63
50	RU	93/94 (99%)	92 (99%)	1 (1%)	65	74
50	YU	93/94 (99%)	91 (98%)	2 (2%)	45	65
51	RV	82/82 (100%)	73 (89%)	9 (11%)	6	26
51	YV	82/82 (100%)	80 (98%)	2 (2%)	43	64
52	RW	92/92 (100%)	92 (100%)	0	100	100
52	YW	92/92 (100%)	90 (98%)	2 (2%)	45	65
53	RX	74/78 (95%)	74 (100%)	0	100	100
53	YX	74/78 (95%)	73 (99%)	1 (1%)	59	71
54	RY	88/91 (97%)	88 (100%)	0	100	100
54	YY	88/91 (97%)	88 (100%)	0	100	100
55	RZ	162/179 (90%)	161 (99%)	1 (1%)	78	79
55	YZ	162/179 (90%)	159 (98%)	3 (2%)	50	68
All	All	10001/10378 (96%)	9812 (98%)	189 (2%)	50	68

5 of 189 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
51	RV	21	ARG
16	XP	32	TYR
51	RV	72	VAL
5	XE	155	GLU
25	Y0	82	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
48	RS	61	ASN
7	XG	109	ASN
46	YQ	57	HIS
49	RT	90	GLN
53	RX	55	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1508/1521 (99%)	293 (19%)	33 (2%)
1	XA	1505/1521 (98%)	302 (20%)	40 (2%)
22	QV	77/77 (100%)	8 (10%)	1 (1%)
22	XV	77/77 (100%)	9 (11%)	1 (1%)
23	QX	16/20 (80%)	7 (43%)	2 (12%)
23	XX	16/20 (80%)	8 (50%)	0
35	RA	2888/2915 (99%)	623 (21%)	37 (1%)
35	YA	2875/2915 (98%)	579 (20%)	28 (0%)
36	RB	119/124 (95%)	24 (20%)	1 (0%)
36	YB	119/124 (95%)	17 (14%)	1 (0%)
56	ZA	1/3 (33%)	0	0
56	ZB	1/3 (33%)	0	0
All	All	9202/9320 (98%)	1870 (20%)	144 (1%)

5 of 1870 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	4	U
1	QA	5	U
1	QA	6	G
1	QA	22	G
1	QA	32	A

5 of 144 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	YA	119	A
36	YB	66	A
35	YA	752	A
35	YA	2144	U
35	RA	1022	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	A3P	QX	20	23	25,28,29	3.31	9 (36%)	37,42,45	2.18	11 (29%)
56	PPU	ZB	3	35,56	37,40,41	1.24	5 (13%)	47,57,60	2.40	19 (40%)
56	PPU	ZA	3	35,56	37,40,41	1.25	6 (16%)	47,57,60	2.29	14 (29%)
23	A3P	XX	20	23	25,28,29	3.32	8 (32%)	37,42,45	2.12	9 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	A3P	QX	20	23	-	3/12/30/31	0/3/3/3
56	PPU	ZB	3	35,56	-	13/25/43/44	0/4/4/4
56	PPU	ZA	3	35,56	-	6/25/43/44	0/4/4/4
23	A3P	XX	20	23	-	1/12/30/31	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	QX	20	A3P	O4'-C1'	11.03	1.67	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	XX	20	A3P	O4'-C1'	10.74	1.66	1.42
23	XX	20	A3P	C2'-C1'	-6.54	1.32	1.53
23	QX	20	A3P	C2'-C1'	-6.40	1.33	1.53
23	XX	20	A3P	O4'-C4'	-5.95	1.31	1.45

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	QX	20	A3P	C5-C4-N3	-6.47	117.81	126.72
56	ZB	3	PPU	C5-C4-N3	-6.28	118.07	126.72
23	XX	20	A3P	C5-C4-N3	-6.07	118.35	126.72
56	ZA	3	PPU	C5-C4-N3	-6.05	118.39	126.72
23	XX	20	A3P	N3-C2-N1	-5.02	120.98	128.58

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	ZA	3	PPU	N-CA-CB-CG
56	ZA	3	PPU	C-CA-CB-CG
56	ZB	3	PPU	N3'-C-CA-N
56	ZB	3	PPU	O-C-CA-CB
56	ZB	3	PPU	N3'-C-CA-CB

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	QX	20	A3P	1	0
56	ZB	3	PPU	7	0
56	ZA	3	PPU	2	0
23	XX	20	A3P	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 900 ligands modelled in this entry, 898 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	302	4	0,12,12	-	-	-		
58	SF4	XD	301	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	302	4	-	-	0/6/5/5
58	SF4	XD	301	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.

No monomer is involved in short contacts.

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	1510/1521 (99%)	0.21	28 (1%) 66 41	49, 98, 212, 355	0
1	XA	1507/1521 (99%)	0.08	25 (1%) 69 43	45, 94, 192, 357	0
2	QB	235/256 (91%)	0.30	4 (1%) 69 43	74, 129, 195, 233	0
2	XB	236/256 (92%)	0.65	14 (5%) 28 16	70, 117, 191, 215	0
3	QC	205/239 (85%)	0.58	12 (5%) 28 16	78, 124, 163, 185	0
3	XC	205/239 (85%)	0.51	10 (4%) 35 19	66, 105, 158, 211	0
4	QD	208/209 (99%)	0.56	7 (3%) 48 27	56, 89, 122, 140	0
4	XD	208/209 (99%)	0.70	17 (8%) 17 11	54, 94, 137, 176	0
5	QE	151/162 (93%)	0.66	10 (6%) 24 15	51, 89, 126, 167	0
5	XE	151/162 (93%)	0.55	8 (5%) 32 18	59, 85, 129, 186	0
6	QF	101/101 (100%)	0.38	3 (2%) 52 30	75, 108, 147, 204	0
6	XF	101/101 (100%)	0.20	0 100 100	52, 85, 118, 164	0
7	QG	155/156 (99%)	0.49	8 (5%) 33 19	88, 127, 172, 241	0
7	XG	155/156 (99%)	0.67	15 (9%) 13 9	75, 113, 160, 233	0
8	QH	137/138 (99%)	0.45	5 (3%) 46 25	58, 91, 125, 158	0
8	XH	137/138 (99%)	0.61	6 (4%) 39 21	60, 90, 128, 156	0
9	QI	127/128 (99%)	1.04	16 (12%) 8 6	86, 142, 179, 263	0
9	XI	126/128 (98%)	0.98	18 (14%) 6 5	66, 121, 162, 174	0
10	QJ	99/105 (94%)	1.21	22 (22%) 2 2	95, 143, 201, 251	0
10	XJ	96/105 (91%)	0.87	10 (10%) 11 8	87, 133, 196, 223	0
11	QK	119/129 (92%)	0.84	9 (7%) 20 13	61, 109, 164, 270	0
11	XK	116/129 (89%)	0.44	2 (1%) 69 43	48, 93, 136, 182	0
12	QL	125/132 (94%)	0.73	17 (13%) 7 5	49, 80, 121, 230	0
12	XL	122/132 (92%)	0.62	7 (5%) 29 17	46, 78, 112, 193	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	120/126 (95%)	0.91	18 (15%) 5 5	74, 129, 179, 206	0
13	XM	119/126 (94%)	0.92	17 (14%) 6 5	75, 113, 158, 172	0
14	QN	60/61 (98%)	1.72	23 (38%) 1 1	81, 121, 159, 212	0
14	XN	60/61 (98%)	0.83	5 (8%) 17 11	75, 102, 144, 214	0
15	QO	88/89 (98%)	0.74	3 (3%) 48 27	59, 96, 131, 139	0
15	XO	87/89 (97%)	0.70	3 (3%) 48 27	52, 88, 118, 147	0
16	QP	84/88 (95%)	0.78	6 (7%) 22 14	58, 87, 127, 181	0
16	XP	84/88 (95%)	0.87	8 (9%) 14 9	64, 100, 143, 184	0
17	QQ	100/105 (95%)	0.70	8 (8%) 18 12	60, 92, 126, 153	0
17	XQ	100/105 (95%)	0.72	8 (8%) 18 12	62, 93, 118, 175	0
18	QR	70/88 (79%)	0.45	0 100 100	70, 110, 153, 155	0
18	XR	70/88 (79%)	0.09	1 (1%) 73 48	48, 85, 130, 156	0
19	QS	83/93 (89%)	0.80	9 (10%) 11 8	91, 135, 185, 224	0
19	XS	83/93 (89%)	0.63	5 (6%) 27 16	84, 116, 169, 214	0
20	QT	99/106 (93%)	0.97	17 (17%) 4 4	68, 104, 173, 248	0
20	XT	99/106 (93%)	0.95	13 (13%) 7 6	72, 115, 173, 205	0
21	QU	25/27 (92%)	1.64	12 (48%) 0 1	97, 124, 152, 161	0
21	XU	25/27 (92%)	1.27	5 (20%) 3 3	92, 120, 141, 153	0
22	QV	77/77 (100%)	-0.05	2 (2%) 57 33	51, 103, 134, 192	0
22	XV	77/77 (100%)	-0.13	2 (2%) 57 33	56, 88, 122, 191	0
23	QX	17/20 (85%)	1.83	7 (41%) 0 1	76, 258, 314, 321	0
23	XX	17/20 (85%)	1.68	6 (35%) 1 1	57, 237, 321, 369	0
24	QY	84/84 (100%)	0.85	12 (14%) 6 5	65, 97, 131, 170	0
24	QZ	84/84 (100%)	0.31	1 (1%) 76 52	94, 149, 209, 227	0
24	XY	84/84 (100%)	0.65	6 (7%) 22 14	58, 91, 129, 154	0
24	XZ	84/84 (100%)	0.97	10 (11%) 9 6	88, 145, 204, 270	0
25	R0	81/85 (95%)	0.81	8 (9%) 13 8	52, 80, 104, 153	0
25	Y0	82/85 (96%)	0.93	6 (7%) 21 13	48, 83, 110, 131	0
26	R1	94/98 (95%)	1.21	16 (17%) 4 4	39, 83, 137, 200	0
26	Y1	97/98 (98%)	0.60	3 (3%) 51 29	34, 72, 113, 185	0
27	R2	69/72 (95%)	0.82	5 (7%) 21 14	54, 95, 135, 193	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
27	Y2	69/72 (95%)	0.57	4 (5%)	29	17	49, 83, 118, 238	0
28	R3	59/60 (98%)	0.45	1 (1%)	69	43	50, 82, 140, 155	0
28	Y3	59/60 (98%)	0.44	1 (1%)	69	43	52, 83, 125, 170	0
29	R4	69/71 (97%)	0.71	4 (5%)	29	17	105, 164, 223, 306	0
29	Y4	69/71 (97%)	0.97	10 (14%)	6	5	95, 131, 211, 285	0
30	R5	59/60 (98%)	0.74	3 (5%)	33	19	46, 81, 150, 183	0
30	Y5	59/60 (98%)	0.76	3 (5%)	33	19	42, 87, 154, 179	0
31	R6	53/54 (98%)	1.44	13 (24%)	2	2	147, 191, 254, 315	0
31	Y6	53/54 (98%)	1.53	17 (32%)	1	1	153, 180, 229, 243	0
32	R7	47/49 (95%)	0.60	4 (8%)	16	11	37, 57, 98, 138	0
32	Y7	48/49 (97%)	0.93	6 (12%)	8	6	38, 57, 88, 136	0
33	R8	64/65 (98%)	1.10	10 (15%)	5	5	42, 75, 121, 168	0
33	Y8	64/65 (98%)	1.02	11 (17%)	4	4	48, 75, 112, 154	0
34	R9	37/37 (100%)	1.61	14 (37%)	1	1	122, 162, 209, 225	0
34	Y9	37/37 (100%)	1.64	13 (35%)	1	1	135, 156, 195, 222	0
35	RA	2891/2915 (99%)	0.02	54 (1%)	66	41	39, 76, 264, 453	0
35	YA	2878/2915 (98%)	-0.06	66 (2%)	61	37	34, 73, 271, 478	0
36	RB	120/124 (96%)	0.18	5 (4%)	40	22	74, 122, 167, 189	0
36	YB	120/124 (96%)	0.11	2 (1%)	69	43	74, 109, 162, 192	0
37	RD	272/276 (98%)	0.91	32 (11%)	9	6	33, 74, 112, 258	0
37	YD	274/276 (99%)	0.32	5 (1%)	67	42	31, 57, 86, 130	0
38	RE	205/206 (99%)	0.74	13 (6%)	26	15	48, 88, 136, 200	0
38	YE	204/206 (99%)	0.60	7 (3%)	48	27	44, 83, 122, 169	0
39	RF	202/210 (96%)	0.42	8 (3%)	42	23	29, 67, 117, 227	0
39	YF	202/210 (96%)	0.56	9 (4%)	38	20	38, 76, 135, 191	0
40	RG	181/182 (99%)	0.61	9 (4%)	34	19	80, 123, 166, 244	0
40	YG	181/182 (99%)	0.86	15 (8%)	17	11	64, 111, 158, 189	0
41	RH	174/180 (96%)	1.15	30 (17%)	4	4	91, 141, 215, 280	0
41	YH	174/180 (96%)	0.69	21 (12%)	8	6	77, 128, 184, 219	0
42	RI	145/148 (97%)	1.03	22 (15%)	5	5	72, 115, 152, 209	0
42	YI	146/148 (98%)	0.58	9 (6%)	26	16	61, 103, 147, 217	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	RN	138/140 (98%)	1.07	23 (16%) 4 4	58, 96, 143, 175	0
43	YN	138/140 (98%)	0.90	11 (7%) 18 12	50, 88, 135, 171	0
44	RO	122/122 (100%)	0.48	1 (0%) 82 60	37, 73, 103, 126	0
44	YO	122/122 (100%)	0.64	4 (3%) 49 28	36, 68, 97, 137	0
45	RP	150/150 (100%)	0.91	16 (10%) 11 8	44, 85, 129, 206	0
45	YP	149/150 (99%)	0.60	11 (7%) 20 13	40, 78, 107, 144	0
46	RQ	141/141 (100%)	0.94	12 (8%) 16 11	45, 87, 131, 190	0
46	YQ	141/141 (100%)	0.43	5 (3%) 47 26	53, 82, 113, 137	0
47	RR	117/118 (99%)	0.57	4 (3%) 48 27	50, 79, 110, 218	0
47	YR	117/118 (99%)	0.68	11 (9%) 14 9	47, 77, 114, 162	0
48	RS	111/112 (99%)	1.04	16 (14%) 6 5	79, 116, 157, 259	0
48	YS	111/112 (99%)	0.87	13 (11%) 9 6	72, 100, 145, 293	0
49	RT	137/146 (93%)	0.71	12 (8%) 15 10	57, 89, 152, 199	0
49	YT	137/146 (93%)	0.66	11 (8%) 18 12	52, 86, 169, 273	0
50	RU	117/118 (99%)	0.72	6 (5%) 33 19	41, 74, 125, 172	0
50	YU	117/118 (99%)	0.93	13 (11%) 10 7	51, 82, 124, 170	0
51	RV	101/101 (100%)	0.44	3 (2%) 52 30	46, 87, 139, 175	0
51	YV	101/101 (100%)	1.05	16 (15%) 5 4	53, 96, 137, 220	0
52	RW	113/113 (100%)	0.71	7 (6%) 26 16	47, 71, 121, 195	0
52	YW	113/113 (100%)	0.57	7 (6%) 26 16	44, 73, 126, 229	0
53	RX	92/96 (95%)	0.70	10 (10%) 10 7	54, 84, 118, 167	0
53	YX	92/96 (95%)	0.37	1 (1%) 78 54	39, 72, 106, 140	0
54	RY	107/110 (97%)	1.21	25 (23%) 2 2	54, 93, 163, 279	0
54	YY	107/110 (97%)	0.80	9 (8%) 17 11	57, 98, 152, 179	0
55	RZ	183/206 (88%)	0.49	2 (1%) 78 54	79, 118, 157, 207	0
55	YZ	183/206 (88%)	0.47	4 (2%) 62 37	70, 113, 152, 166	0
56	ZA	2/3 (66%)	-0.43	0 100 100	49, 49, 49, 58	0
56	ZB	2/3 (66%)	-0.30	0 100 100	53, 53, 53, 62	0
All	All	21211/21784 (97%)	0.43	1192 (5%) 30 17	29, 91, 181, 478	0

The worst 5 of 1192 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	QK	129	SER	9.6
12	XL	28	LYS	9.4
14	QN	13	THR	8.2
14	QN	2	ALA	7.6
49	RT	106	SER	7.4

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
23	A3P	QX	20	26/27	0.91	0.13	82,85,97,100	0
23	A3P	XX	20	26/27	0.91	0.11	71,76,82,84	0
56	PPU	ZA	3	37/38	0.91	0.15	41,59,68,71	0
56	PPU	ZB	3	37/38	0.94	0.13	38,56,67,69	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(Å ²)	Q<0.9
57	MG	Y9	101	1/1	0.33	0.27	122,122,122,122	0
59	ZN	Y6	101	1/1	0.36	0.25	229,229,229,229	0
57	MG	RA	3174	1/1	0.49	0.21	51,51,51,51	0
57	MG	QA	1673	1/1	0.51	0.26	69,69,69,69	0
57	MG	YA	3081	1/1	0.54	0.29	38,38,38,38	0
57	MG	QA	1645	1/1	0.57	0.17	81,81,81,81	0
57	MG	RA	3155	1/1	0.57	0.21	89,89,89,89	0
57	MG	XA	1651	1/1	0.58	0.69	81,81,81,81	0
57	MG	RA	3295	1/1	0.63	0.20	51,51,51,51	0
57	MG	XA	1636	1/1	0.63	0.22	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3235	1/1	0.65	0.19	208,208,208,208	0
59	ZN	R5	101	1/1	0.66	0.20	244,244,244,244	0
57	MG	XA	1676	1/1	0.67	0.32	53,53,53,53	0
57	MG	XA	1699	1/1	0.67	0.19	49,49,49,49	0
57	MG	RA	3164	1/1	0.67	0.24	57,57,57,57	0
57	MG	YA	3060	1/1	0.67	0.34	40,40,40,40	0
57	MG	RA	3012	1/1	0.67	0.17	48,48,48,48	0
57	MG	RA	3081	1/1	0.67	0.34	55,55,55,55	0
57	MG	RA	3112	1/1	0.67	0.23	41,41,41,41	0
57	MG	QA	1646	1/1	0.67	0.13	67,67,67,67	0
57	MG	XA	1644	1/1	0.68	0.11	76,76,76,76	0
57	MG	RQ	202	1/1	0.68	0.18	58,58,58,58	0
57	MG	RA	3058	1/1	0.69	0.35	46,46,46,46	0
57	MG	YA	3103	1/1	0.69	0.31	81,81,81,81	0
57	MG	RA	3190	1/1	0.69	0.11	55,55,55,55	0
57	MG	YA	3321	1/1	0.69	0.12	69,69,69,69	0
57	MG	RA	3242	1/1	0.69	0.26	47,47,47,47	0
57	MG	RA	3134	1/1	0.69	0.16	52,52,52,52	0
57	MG	XA	1674	1/1	0.70	0.12	28,28,28,28	0
57	MG	RA	3086	1/1	0.70	0.21	26,26,26,26	0
57	MG	XA	1685	1/1	0.70	0.20	62,62,62,62	0
57	MG	QA	1657	1/1	0.71	0.32	74,74,74,74	0
57	MG	QY	101	1/1	0.71	0.41	77,77,77,77	0
57	MG	YA	3175	1/1	0.72	0.19	57,57,57,57	0
57	MG	RA	3167	1/1	0.72	0.14	59,59,59,59	0
57	MG	XA	1603	1/1	0.72	0.20	48,48,48,48	0
57	MG	YA	3057	1/1	0.72	0.17	38,38,38,38	0
57	MG	YA	3149	1/1	0.72	0.19	76,76,76,76	0
57	MG	RA	3177	1/1	0.73	0.17	46,46,46,46	0
57	MG	RA	3296	1/1	0.73	0.22	40,40,40,40	0
57	MG	XA	1693	1/1	0.73	0.23	48,48,48,48	0
57	MG	YA	3194	1/1	0.74	0.13	61,61,61,61	0
57	MG	RA	3271	1/1	0.74	0.11	53,53,53,53	0
57	MG	YA	3305	1/1	0.74	0.20	50,50,50,50	0
57	MG	XA	1687	1/1	0.75	0.17	50,50,50,50	0
57	MG	RA	3189	1/1	0.75	0.21	58,58,58,58	0
57	MG	RA	3294	1/1	0.75	0.28	54,54,54,54	0
57	MG	RA	3248	1/1	0.75	0.18	28,28,28,28	0
57	MG	YA	3287	1/1	0.76	0.13	44,44,44,44	0
57	MG	YA	3168	1/1	0.76	0.15	62,62,62,62	0
57	MG	YA	3222	1/1	0.76	0.18	29,29,29,29	0
57	MG	RA	3301	1/1	0.76	0.24	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3246	1/1	0.76	0.14	61,61,61,61	0
57	MG	RA	3302	1/1	0.77	0.49	80,80,80,80	0
57	MG	RA	3143	1/1	0.77	0.22	59,59,59,59	0
57	MG	YA	3265	1/1	0.77	0.11	44,44,44,44	0
57	MG	RA	3133	1/1	0.77	0.20	51,51,51,51	0
57	MG	YA	3011	1/1	0.77	0.33	43,43,43,43	0
57	MG	YA	3019	1/1	0.77	0.29	32,32,32,32	0
57	MG	RA	3061	1/1	0.77	0.22	67,67,67,67	0
57	MG	RA	3165	1/1	0.77	0.12	47,47,47,47	0
57	MG	YA	3257	1/1	0.78	0.18	50,50,50,50	0
57	MG	QA	1628	1/1	0.78	0.08	74,74,74,74	0
57	MG	YA	3279	1/1	0.78	0.17	50,50,50,50	0
57	MG	RA	3283	1/1	0.78	0.32	61,61,61,61	0
57	MG	RA	3147	1/1	0.79	0.14	56,56,56,56	0
57	MG	YA	3066	1/1	0.79	0.12	38,38,38,38	0
57	MG	RA	3014	1/1	0.79	0.23	58,58,58,58	0
57	MG	YA	3091	1/1	0.79	0.17	36,36,36,36	0
57	MG	YA	3055	1/1	0.79	0.14	7,7,7,7	0
59	ZN	R4	101	1/1	0.79	0.20	176,176,176,176	0
57	MG	RA	3107	1/1	0.79	0.20	41,41,41,41	0
59	ZN	R6	101	1/1	0.79	0.28	227,227,227,227	0
57	MG	YA	3161	1/1	0.79	0.10	44,44,44,44	0
57	MG	YA	3273	1/1	0.80	0.12	58,58,58,58	0
57	MG	YA	3277	1/1	0.80	0.10	52,52,52,52	0
57	MG	RA	3182	1/1	0.80	0.15	44,44,44,44	0
57	MG	YA	3107	1/1	0.80	0.24	71,71,71,71	0
57	MG	YA	3288	1/1	0.80	0.10	28,28,28,28	0
57	MG	YA	3110	1/1	0.80	0.20	41,41,41,41	0
57	MG	YA	3117	1/1	0.80	0.11	55,55,55,55	0
57	MG	YE	303	1/1	0.80	0.18	69,69,69,69	0
57	MG	YA	3236	1/1	0.80	0.17	38,38,38,38	0
57	MG	YA	3034	1/1	0.80	0.18	75,75,75,75	0
57	MG	XA	1641	1/1	0.80	0.20	51,51,51,51	0
57	MG	RA	3072	1/1	0.80	0.24	14,14,14,14	0
57	MG	YA	3184	1/1	0.81	0.19	37,37,37,37	0
57	MG	YA	3143	1/1	0.81	0.09	60,60,60,60	0
57	MG	YA	3219	1/1	0.81	0.25	37,37,37,37	0
57	MG	YG	201	1/1	0.81	0.14	59,59,59,59	0
57	MG	YA	3084	1/1	0.81	0.24	24,24,24,24	0
57	MG	YA	3049	1/1	0.81	0.19	42,42,42,42	0
57	MG	YA	3002	1/1	0.81	0.21	32,32,32,32	0
57	MG	YA	3138	1/1	0.81	0.16	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	RA	3056	1/1	0.82	0.11	54,54,54,54	0
57	MG	RA	3237	1/1	0.82	0.20	40,40,40,40	0
57	MG	RA	3276	1/1	0.82	0.18	48,48,48,48	0
57	MG	YA	3311	1/1	0.82	0.17	45,45,45,45	0
57	MG	RA	3277	1/1	0.82	0.14	45,45,45,45	0
57	MG	RB	202	1/1	0.82	0.19	27,27,27,27	0
57	MG	YE	305	1/1	0.82	0.11	66,66,66,66	0
57	MG	YA	3261	1/1	0.82	0.15	35,35,35,35	0
57	MG	RA	3241	1/1	0.82	0.12	36,36,36,36	0
57	MG	QA	1617	1/1	0.82	0.13	57,57,57,57	0
57	MG	YA	3141	1/1	0.82	0.16	41,41,41,41	0
57	MG	YA	3220	1/1	0.82	0.14	22,22,22,22	0
57	MG	XA	1677	1/1	0.83	0.18	46,46,46,46	0
57	MG	YA	3281	1/1	0.83	0.18	37,37,37,37	0
57	MG	YA	3183	1/1	0.83	0.14	44,44,44,44	0
57	MG	YB	202	1/1	0.83	0.32	47,47,47,47	0
57	MG	YD	301	1/1	0.83	0.20	24,24,24,24	0
57	MG	RA	3020	1/1	0.83	0.23	39,39,39,39	0
57	MG	YA	3223	1/1	0.84	0.15	31,31,31,31	0
57	MG	RA	3035	1/1	0.84	0.12	34,34,34,34	0
57	MG	RA	3268	1/1	0.84	0.23	56,56,56,56	0
57	MG	QA	1693	1/1	0.84	0.12	50,50,50,50	0
57	MG	YA	3251	1/1	0.84	0.19	68,68,68,68	0
57	MG	RA	3108	1/1	0.84	0.12	43,43,43,43	0
57	MG	XA	1667	1/1	0.84	0.20	26,26,26,26	0
57	MG	XA	1670	1/1	0.84	0.13	46,46,46,46	0
57	MG	YA	3270	1/1	0.84	0.17	44,44,44,44	0
57	MG	XA	1672	1/1	0.84	0.14	30,30,30,30	0
57	MG	QA	1618	1/1	0.84	0.15	55,55,55,55	0
57	MG	XA	1675	1/1	0.84	0.20	35,35,35,35	0
57	MG	YA	3280	1/1	0.84	0.24	42,42,42,42	0
57	MG	RA	3126	1/1	0.84	0.15	60,60,60,60	0
57	MG	YA	3133	1/1	0.84	0.14	32,32,32,32	0
57	MG	RA	3059	1/1	0.84	0.19	27,27,27,27	0
57	MG	RA	3183	1/1	0.84	0.19	56,56,56,56	0
57	MG	QA	1642	1/1	0.84	0.10	64,64,64,64	0
57	MG	YA	3314	1/1	0.84	0.14	50,50,50,50	0
57	MG	YA	3319	1/1	0.84	0.18	57,57,57,57	0
57	MG	QA	1620	1/1	0.84	0.15	75,75,75,75	0
57	MG	RA	3236	1/1	0.84	0.25	47,47,47,47	0
57	MG	RA	3074	1/1	0.84	0.26	23,23,23,23	0
57	MG	RD	301	1/1	0.84	0.13	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YE	304	1/1	0.84	0.25	60,60,60,60	0
57	MG	YA	3010	1/1	0.84	0.11	35,35,35,35	0
57	MG	RN	201	1/1	0.84	0.31	72,72,72,72	0
57	MG	YQ	202	1/1	0.84	0.34	70,70,70,70	0
57	MG	RO	201	1/1	0.84	0.24	60,60,60,60	0
57	MG	QA	1682	1/1	0.84	0.08	33,33,33,33	0
57	MG	RQ	204	1/1	0.84	0.14	53,53,53,53	0
57	MG	RA	3160	1/1	0.84	0.26	33,33,33,33	0
57	MG	YA	3097	1/1	0.85	0.10	52,52,52,52	0
57	MG	QA	1649	1/1	0.85	0.11	53,53,53,53	0
57	MG	RA	3258	1/1	0.85	0.27	44,44,44,44	0
57	MG	QA	1664	1/1	0.85	0.24	46,46,46,46	0
57	MG	RA	3270	1/1	0.85	0.14	41,41,41,41	0
57	MG	YA	3127	1/1	0.85	0.26	66,66,66,66	0
57	MG	RA	3090	1/1	0.85	0.13	34,34,34,34	0
57	MG	YA	3135	1/1	0.85	0.12	34,34,34,34	0
57	MG	RA	3106	1/1	0.85	0.18	18,18,18,18	0
57	MG	XA	1613	1/1	0.85	0.33	52,52,52,52	0
57	MG	YA	3283	1/1	0.85	0.20	32,32,32,32	0
57	MG	XA	1617	1/1	0.85	0.10	30,30,30,30	0
57	MG	XA	1619	1/1	0.85	0.14	48,48,48,48	0
57	MG	YA	3290	1/1	0.85	0.19	57,57,57,57	0
57	MG	XA	1635	1/1	0.85	0.15	36,36,36,36	0
57	MG	YA	3309	1/1	0.85	0.16	52,52,52,52	0
57	MG	YA	3012	1/1	0.85	0.14	68,68,68,68	0
57	MG	YA	3312	1/1	0.85	0.09	43,43,43,43	0
57	MG	YA	3171	1/1	0.85	0.13	45,45,45,45	0
57	MG	RA	3188	1/1	0.85	0.15	57,57,57,57	0
57	MG	R0	102	1/1	0.85	0.14	31,31,31,31	0
57	MG	YA	3328	1/1	0.85	0.44	77,77,77,77	0
57	MG	YA	3046	1/1	0.85	0.24	31,31,31,31	0
57	MG	RA	3158	1/1	0.85	0.08	40,40,40,40	0
57	MG	YA	3210	1/1	0.85	0.18	34,34,34,34	0
57	MG	YA	3215	1/1	0.85	0.24	35,35,35,35	0
57	MG	RA	3191	1/1	0.85	0.18	118,118,118,118	0
57	MG	RA	3024	1/1	0.85	0.25	13,13,13,13	0
57	MG	RA	3298	1/1	0.85	0.12	57,57,57,57	0
57	MG	XA	1671	1/1	0.85	0.18	39,39,39,39	0
57	MG	RA	3009	1/1	0.85	0.19	41,41,41,41	0
57	MG	RA	3120	1/1	0.85	0.12	45,45,45,45	0
57	MG	RA	3047	1/1	0.85	0.20	19,19,19,19	0
57	MG	RA	3032	1/1	0.86	0.23	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3109	1/1	0.86	0.24	35,35,35,35	0
57	MG	QA	1679	1/1	0.86	0.14	35,35,35,35	0
57	MG	YA	3297	1/1	0.86	0.13	31,31,31,31	0
57	MG	YA	3115	1/1	0.86	0.17	18,18,18,18	0
57	MG	RA	3013	1/1	0.86	0.22	43,43,43,43	0
57	MG	XA	1618	1/1	0.86	0.11	42,42,42,42	0
57	MG	YA	3231	1/1	0.86	0.16	26,26,26,26	0
57	MG	YA	3042	1/1	0.86	0.21	9,9,9,9	0
57	MG	RA	3076	1/1	0.86	0.24	31,31,31,31	0
57	MG	XA	1630	1/1	0.86	0.09	66,66,66,66	0
57	MG	YA	3325	1/1	0.86	0.08	61,61,61,61	0
57	MG	XA	1632	1/1	0.86	0.12	47,47,47,47	0
57	MG	XA	1634	1/1	0.86	0.07	77,77,77,77	0
57	MG	R0	101	1/1	0.86	0.07	9,9,9,9	0
57	MG	QD	301	1/1	0.86	0.09	81,81,81,81	0
57	MG	QV	102	1/1	0.86	0.15	55,55,55,55	0
57	MG	XE	201	1/1	0.86	0.11	32,32,32,32	0
57	MG	RA	3170	1/1	0.86	0.17	74,74,74,74	0
57	MG	RA	3092	1/1	0.86	0.11	38,38,38,38	0
57	MG	YQ	203	1/1	0.86	0.20	64,64,64,64	0
57	MG	YA	3102	1/1	0.86	0.09	52,52,52,52	0
57	MG	RA	3100	1/1	0.86	0.14	39,39,39,39	0
57	MG	YA	3195	1/1	0.86	0.10	38,38,38,38	0
57	MG	YA	3284	1/1	0.86	0.15	36,36,36,36	0
57	MG	YA	3276	1/1	0.87	0.21	49,49,49,49	0
57	MG	QA	1612	1/1	0.87	0.26	33,33,33,33	0
57	MG	XA	1656	1/1	0.87	0.18	34,34,34,34	0
57	MG	YA	3152	1/1	0.87	0.10	44,44,44,44	0
57	MG	QA	1639	1/1	0.87	0.09	59,59,59,59	0
57	MG	RA	3178	1/1	0.87	0.25	63,63,63,63	0
57	MG	RA	3007	1/1	0.87	0.12	25,25,25,25	0
57	MG	RA	3097	1/1	0.87	0.09	36,36,36,36	0
57	MG	YA	3177	1/1	0.87	0.27	68,68,68,68	0
57	MG	RA	3261	1/1	0.87	0.18	44,44,44,44	0
57	MG	YA	3291	1/1	0.87	0.10	39,39,39,39	0
57	MG	RA	3186	1/1	0.87	0.13	36,36,36,36	0
57	MG	YA	3190	1/1	0.87	0.09	44,44,44,44	0
57	MG	QA	1665	1/1	0.87	0.19	31,31,31,31	0
57	MG	QA	1692	1/1	0.87	0.20	42,42,42,42	0
57	MG	YA	3087	1/1	0.87	0.28	22,22,22,22	0
57	MG	YA	3211	1/1	0.87	0.13	26,26,26,26	0
57	MG	RA	3274	1/1	0.87	0.22	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	3142	1/1	0.87	0.25	28,28,28,28	0
57	MG	RA	3169	1/1	0.87	0.09	63,63,63,63	0
57	MG	RA	3193	1/1	0.87	0.15	57,57,57,57	0
57	MG	RA	3286	1/1	0.87	0.16	51,51,51,51	0
57	MG	XL	201	1/1	0.87	0.08	66,66,66,66	0
57	MG	RA	3207	1/1	0.87	0.17	17,17,17,17	0
57	MG	YA	3112	1/1	0.87	0.17	65,65,65,65	0
57	MG	YA	3239	1/1	0.87	0.09	39,39,39,39	0
57	MG	RA	3210	1/1	0.87	0.14	19,19,19,19	0
57	MG	YA	3006	1/1	0.87	0.12	33,33,33,33	0
57	MG	YA	3009	1/1	0.87	0.15	41,41,41,41	0
57	MG	RA	3211	1/1	0.87	0.22	27,27,27,27	0
57	MG	XA	1638	1/1	0.87	0.12	41,41,41,41	0
57	MG	RA	3232	1/1	0.87	0.31	57,57,57,57	0
59	ZN	R9	101	1/1	0.87	0.34	127,127,127,127	0
57	MG	RA	3082	1/1	0.87	0.17	33,33,33,33	0
57	MG	RA	3041	1/1	0.88	0.19	18,18,18,18	0
57	MG	RA	3029	1/1	0.88	0.10	35,35,35,35	0
57	MG	XA	1673	1/1	0.88	0.17	45,45,45,45	0
57	MG	RA	3166	1/1	0.88	0.24	54,54,54,54	0
57	MG	XA	1606	1/1	0.88	0.21	29,29,29,29	0
57	MG	YA	3286	1/1	0.88	0.10	33,33,33,33	0
57	MG	XA	1609	1/1	0.88	0.22	19,19,19,19	0
57	MG	YA	3185	1/1	0.88	0.17	68,68,68,68	0
57	MG	RA	3131	1/1	0.88	0.14	61,61,61,61	0
57	MG	YA	3191	1/1	0.88	0.10	56,56,56,56	0
57	MG	YA	3294	1/1	0.88	0.16	57,57,57,57	0
57	MG	YA	3085	1/1	0.88	0.15	14,14,14,14	0
57	MG	YA	3301	1/1	0.88	0.14	33,33,33,33	0
57	MG	XA	1679	1/1	0.88	0.14	36,36,36,36	0
57	MG	RA	3208	1/1	0.88	0.11	37,37,37,37	0
57	MG	RA	3066	1/1	0.88	0.15	36,36,36,36	0
57	MG	RA	3103	1/1	0.88	0.12	24,24,24,24	0
57	MG	XA	1620	1/1	0.88	0.12	42,42,42,42	0
57	MG	YA	3316	1/1	0.88	0.16	66,66,66,66	0
57	MG	RA	3136	1/1	0.88	0.18	52,52,52,52	0
57	MG	RA	3289	1/1	0.88	0.27	56,56,56,56	0
57	MG	RA	3141	1/1	0.88	0.15	32,32,32,32	0
57	MG	RA	3085	1/1	0.88	0.14	15,15,15,15	0
57	MG	YA	3003	1/1	0.88	0.15	36,36,36,36	0
57	MG	YA	3005	1/1	0.88	0.17	34,34,34,34	0
57	MG	R3	101	1/1	0.88	0.22	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3088	1/1	0.88	0.14	33,33,33,33	0
57	MG	RA	3245	1/1	0.88	0.23	48,48,48,48	0
57	MG	RA	3111	1/1	0.88	0.17	41,41,41,41	0
57	MG	XA	1648	1/1	0.88	0.07	34,34,34,34	0
57	MG	QA	1689	1/1	0.88	0.16	70,70,70,70	0
57	MG	YV	301	1/1	0.88	0.08	68,68,68,68	0
57	MG	YA	3266	1/1	0.88	0.23	47,47,47,47	0
57	MG	RA	3115	1/1	0.88	0.23	25,25,25,25	0
57	MG	RA	3263	1/1	0.88	0.16	51,51,51,51	0
57	MG	RA	3264	1/1	0.88	0.16	41,41,41,41	0
57	MG	YA	3164	1/1	0.88	0.16	39,39,39,39	0
57	MG	YA	3165	1/1	0.89	0.07	49,49,49,49	0
57	MG	RA	3139	1/1	0.89	0.12	32,32,32,32	0
57	MG	YA	3169	1/1	0.89	0.17	44,44,44,44	0
57	MG	YA	3063	1/1	0.89	0.23	31,31,31,31	0
57	MG	RA	3096	1/1	0.89	0.12	38,38,38,38	0
57	MG	QA	1605	1/1	0.89	0.22	30,30,30,30	0
57	MG	RA	3045	1/1	0.89	0.18	40,40,40,40	0
57	MG	RA	3195	1/1	0.89	0.18	44,44,44,44	0
57	MG	RA	3205	1/1	0.89	0.26	16,16,16,16	0
57	MG	XA	1642	1/1	0.89	0.13	55,55,55,55	0
57	MG	XV	102	1/1	0.89	0.15	32,32,32,32	0
57	MG	YA	3193	1/1	0.89	0.17	38,38,38,38	0
57	MG	XV	103	1/1	0.89	0.18	57,57,57,57	0
57	MG	Y5	101	1/1	0.89	0.14	71,71,71,71	0
57	MG	YA	3302	1/1	0.89	0.22	50,50,50,50	0
57	MG	YA	3205	1/1	0.89	0.15	17,17,17,17	0
57	MG	RA	3173	1/1	0.89	0.13	29,29,29,29	0
57	MG	XA	1645	1/1	0.89	0.09	60,60,60,60	0
57	MG	RA	3025	1/1	0.89	0.18	15,15,15,15	0
57	MG	YA	3313	1/1	0.89	0.14	51,51,51,51	0
57	MG	RA	3209	1/1	0.89	0.20	26,26,26,26	0
57	MG	RA	3154	1/1	0.89	0.13	53,53,53,53	0
57	MG	YA	3221	1/1	0.89	0.20	27,27,27,27	0
57	MG	XA	1666	1/1	0.89	0.18	40,40,40,40	0
57	MG	YA	3322	1/1	0.89	0.12	71,71,71,71	0
57	MG	YA	3121	1/1	0.89	0.13	34,34,34,34	0
57	MG	YA	3228	1/1	0.89	0.14	34,34,34,34	0
57	MG	YA	3329	1/1	0.89	0.19	36,36,36,36	0
57	MG	XA	1604	1/1	0.89	0.18	21,21,21,21	0
57	MG	RA	3130	1/1	0.89	0.20	38,38,38,38	0
57	MG	RA	3223	1/1	0.89	0.16	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	QA	1671	1/1	0.89	0.21	34,34,34,34	0
57	MG	YA	3240	1/1	0.89	0.18	36,36,36,36	0
57	MG	YA	3140	1/1	0.89	0.14	27,27,27,27	0
57	MG	RA	3089	1/1	0.89	0.21	25,25,25,25	0
57	MG	RA	3185	1/1	0.89	0.14	33,33,33,33	0
57	MG	RA	3239	1/1	0.89	0.24	57,57,57,57	0
57	MG	YA	3150	1/1	0.89	0.15	58,58,58,58	0
57	MG	QA	1662	1/1	0.89	0.18	63,63,63,63	0
57	MG	YA	3154	1/1	0.89	0.09	56,56,56,56	0
57	MG	QA	1641	1/1	0.89	0.23	55,55,55,55	0
57	MG	XA	1678	1/1	0.89	0.19	35,35,35,35	0
57	MG	RY	201	1/1	0.90	0.13	51,51,51,51	0
57	MG	YA	3014	1/1	0.90	0.17	38,38,38,38	0
57	MG	QA	1651	1/1	0.90	0.09	81,81,81,81	0
57	MG	YA	3030	1/1	0.90	0.10	27,27,27,27	0
57	MG	YA	3275	1/1	0.90	0.19	53,53,53,53	0
57	MG	RA	3280	1/1	0.90	0.11	37,37,37,37	0
57	MG	RA	3282	1/1	0.90	0.29	28,28,28,28	0
57	MG	YA	3163	1/1	0.90	0.14	41,41,41,41	0
57	MG	RA	3161	1/1	0.90	0.10	34,34,34,34	0
57	MG	XA	1612	1/1	0.90	0.15	27,27,27,27	0
57	MG	YA	3052	1/1	0.90	0.09	40,40,40,40	0
57	MG	RA	3033	1/1	0.90	0.19	55,55,55,55	0
57	MG	QA	1684	1/1	0.90	0.26	51,51,51,51	0
57	MG	YA	3059	1/1	0.90	0.22	8,8,8,8	0
57	MG	RA	3293	1/1	0.90	0.21	26,26,26,26	0
57	MG	RA	3037	1/1	0.90	0.14	18,18,18,18	0
57	MG	XA	1680	1/1	0.90	0.10	45,45,45,45	0
57	MG	YA	3071	1/1	0.90	0.18	16,16,16,16	0
57	MG	YA	3187	1/1	0.90	0.11	33,33,33,33	0
57	MG	RA	3039	1/1	0.90	0.13	31,31,31,31	0
57	MG	XA	1686	1/1	0.90	0.13	47,47,47,47	0
57	MG	RA	3110	1/1	0.90	0.15	54,54,54,54	0
57	MG	XA	1689	1/1	0.90	0.06	27,27,27,27	0
57	MG	QA	1602	1/1	0.90	0.18	33,33,33,33	0
57	MG	YA	3203	1/1	0.90	0.18	15,15,15,15	0
57	MG	RA	3299	1/1	0.90	0.21	47,47,47,47	0
57	MG	YA	3207	1/1	0.90	0.20	36,36,36,36	0
57	MG	YA	3100	1/1	0.90	0.39	67,67,67,67	0
57	MG	QA	1630	1/1	0.90	0.24	36,36,36,36	0
57	MG	YA	3320	1/1	0.90	0.14	57,57,57,57	0
57	MG	XF	301	1/1	0.90	0.05	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3104	1/1	0.90	0.18	22,22,22,22	0
57	MG	YA	3324	1/1	0.90	0.19	47,47,47,47	0
57	MG	QA	1635	1/1	0.90	0.17	57,57,57,57	0
57	MG	YA	3327	1/1	0.90	0.36	71,71,71,71	0
57	MG	RB	201	1/1	0.90	0.08	41,41,41,41	0
57	MG	RA	3116	1/1	0.90	0.15	40,40,40,40	0
57	MG	YA	3331	1/1	0.90	0.11	30,30,30,30	0
57	MG	YA	3334	1/1	0.90	0.10	42,42,42,42	0
57	MG	YA	3335	1/1	0.90	0.28	44,44,44,44	0
57	MG	RB	203	1/1	0.90	0.13	21,21,21,21	0
57	MG	RA	3148	1/1	0.90	0.14	25,25,25,25	0
57	MG	YE	301	1/1	0.90	0.16	25,25,25,25	0
57	MG	YA	3230	1/1	0.90	0.15	34,34,34,34	0
57	MG	RA	3055	1/1	0.90	0.12	24,24,24,24	0
57	MG	RA	3099	1/1	0.90	0.15	37,37,37,37	0
57	MG	YA	3004	1/1	0.90	0.13	52,52,52,52	0
57	MG	XA	1649	1/1	0.90	0.24	55,55,55,55	0
57	MG	RQ	201	1/1	0.90	0.15	42,42,42,42	0
57	MG	YQ	204	1/1	0.90	0.18	86,86,86,86	0
57	MG	YA	3136	1/1	0.90	0.10	41,41,41,41	0
57	MG	RA	3227	1/1	0.90	0.12	31,31,31,31	0
57	MG	YA	3256	1/1	0.90	0.17	34,34,34,34	0
57	MG	RQ	203	1/1	0.90	0.14	32,32,32,32	0
57	MG	RA	3127	1/1	0.90	0.10	35,35,35,35	0
57	MG	YA	3262	1/1	0.90	0.11	55,55,55,55	0
57	MG	YA	3036	1/1	0.91	0.17	19,19,19,19	0
57	MG	XA	1607	1/1	0.91	0.10	51,51,51,51	0
57	MG	RA	3231	1/1	0.91	0.12	26,26,26,26	0
57	MG	YA	3048	1/1	0.91	0.19	9,9,9,9	0
57	MG	QA	1637	1/1	0.91	0.17	43,43,43,43	0
57	MG	YA	3162	1/1	0.91	0.18	42,42,42,42	0
57	MG	RA	3285	1/1	0.91	0.23	18,18,18,18	0
57	MG	RA	3031	1/1	0.91	0.16	29,29,29,29	0
57	MG	RA	3137	1/1	0.91	0.11	41,41,41,41	0
57	MG	YA	3282	1/1	0.91	0.10	24,24,24,24	0
57	MG	YA	3167	1/1	0.91	0.25	25,25,25,25	0
57	MG	RA	3138	1/1	0.91	0.15	46,46,46,46	0
57	MG	RA	3240	1/1	0.91	0.22	41,41,41,41	0
57	MG	YA	3061	1/1	0.91	0.16	23,23,23,23	0
57	MG	XA	1629	1/1	0.91	0.17	26,26,26,26	0
57	MG	QA	1619	1/1	0.91	0.14	55,55,55,55	0
57	MG	YA	3178	1/1	0.91	0.15	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1621	1/1	0.91	0.17	41,41,41,41	0
57	MG	XA	1696	1/1	0.91	0.08	55,55,55,55	0
57	MG	YA	3298	1/1	0.91	0.15	36,36,36,36	0
57	MG	YA	3082	1/1	0.91	0.21	21,21,21,21	0
57	MG	XA	1698	1/1	0.91	0.26	49,49,49,49	0
57	MG	RA	3297	1/1	0.91	0.16	45,45,45,45	0
57	MG	RA	3101	1/1	0.91	0.17	40,40,40,40	0
57	MG	YA	3310	1/1	0.91	0.14	27,27,27,27	0
57	MG	RA	3246	1/1	0.91	0.16	43,43,43,43	0
57	MG	YA	3095	1/1	0.91	0.14	22,22,22,22	0
57	MG	YA	3096	1/1	0.91	0.23	23,23,23,23	0
57	MG	RA	3247	1/1	0.91	0.15	31,31,31,31	0
57	MG	XA	1640	1/1	0.91	0.24	59,59,59,59	0
57	MG	RA	3069	1/1	0.91	0.22	20,20,20,20	0
57	MG	YA	3209	1/1	0.91	0.16	30,30,30,30	0
57	MG	RA	3201	1/1	0.91	0.18	14,14,14,14	0
57	MG	RA	3172	1/1	0.91	0.14	60,60,60,60	0
57	MG	QA	1623	1/1	0.91	0.09	41,41,41,41	0
57	MG	RA	3128	1/1	0.91	0.19	16,16,16,16	0
57	MG	RA	3266	1/1	0.91	0.16	37,37,37,37	0
57	MG	YA	3111	1/1	0.91	0.17	33,33,33,33	0
57	MG	RA	3176	1/1	0.91	0.12	26,26,26,26	0
57	MG	RA	3152	1/1	0.91	0.10	75,75,75,75	0
57	MG	YA	3224	1/1	0.91	0.14	24,24,24,24	0
57	MG	XA	1657	1/1	0.91	0.21	28,28,28,28	0
57	MG	YA	3119	1/1	0.91	0.17	50,50,50,50	0
57	MG	QA	1643	1/1	0.91	0.30	69,69,69,69	0
57	MG	YA	3124	1/1	0.91	0.18	40,40,40,40	0
57	MG	RA	3272	1/1	0.91	0.07	38,38,38,38	0
57	MG	RA	3057	1/1	0.91	0.20	15,15,15,15	0
57	MG	YA	3134	1/1	0.91	0.13	54,54,54,54	0
57	MG	RA	3226	1/1	0.91	0.12	32,32,32,32	0
57	MG	YA	3248	1/1	0.91	0.09	39,39,39,39	0
57	MG	RA	3094	1/1	0.91	0.15	24,24,24,24	0
57	MG	YA	3254	1/1	0.91	0.19	39,39,39,39	0
57	MG	YA	3024	1/1	0.91	0.21	23,23,23,23	0
57	MG	YA	3139	1/1	0.91	0.19	32,32,32,32	0
57	MG	YA	3260	1/1	0.91	0.13	28,28,28,28	0
57	MG	RA	3279	1/1	0.91	0.15	44,44,44,44	0
57	MG	YA	3033	1/1	0.91	0.22	25,25,25,25	0
59	ZN	Y4	101	1/1	0.91	0.09	230,230,230,230	0
57	MG	RA	3228	1/1	0.91	0.19	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3091	1/1	0.92	0.12	32,32,32,32	0
57	MG	YA	3269	1/1	0.92	0.11	24,24,24,24	0
57	MG	RA	3038	1/1	0.92	0.22	26,26,26,26	0
57	MG	YA	3054	1/1	0.92	0.16	14,14,14,14	0
57	MG	YA	3274	1/1	0.92	0.10	43,43,43,43	0
57	MG	RA	3149	1/1	0.92	0.07	69,69,69,69	0
57	MG	RA	3150	1/1	0.92	0.11	58,58,58,58	0
57	MG	RA	3288	1/1	0.92	0.19	38,38,38,38	0
57	MG	RA	3117	1/1	0.92	0.25	44,44,44,44	0
57	MG	XA	1624	1/1	0.92	0.14	30,30,30,30	0
57	MG	XA	1690	1/1	0.92	0.20	54,54,54,54	0
57	MG	RA	3093	1/1	0.92	0.16	30,30,30,30	0
57	MG	YA	3174	1/1	0.92	0.20	45,45,45,45	0
57	MG	XA	1695	1/1	0.92	0.18	61,61,61,61	0
57	MG	YA	3073	1/1	0.92	0.08	46,46,46,46	0
57	MG	QA	1650	1/1	0.92	0.27	53,53,53,53	0
57	MG	YA	3179	1/1	0.92	0.24	49,49,49,49	0
57	MG	YA	3289	1/1	0.92	0.19	42,42,42,42	0
57	MG	YA	3180	1/1	0.92	0.19	50,50,50,50	0
57	MG	XA	1631	1/1	0.92	0.22	45,45,45,45	0
57	MG	YA	3292	1/1	0.92	0.16	49,49,49,49	0
57	MG	QA	1675	1/1	0.92	0.08	33,33,33,33	0
57	MG	RA	3243	1/1	0.92	0.10	22,22,22,22	0
57	MG	RA	3244	1/1	0.92	0.19	34,34,34,34	0
57	MG	YA	3299	1/1	0.92	0.16	31,31,31,31	0
57	MG	YA	3089	1/1	0.92	0.09	45,45,45,45	0
57	MG	RA	3043	1/1	0.92	0.26	16,16,16,16	0
57	MG	YA	3303	1/1	0.92	0.08	38,38,38,38	0
57	MG	YA	3192	1/1	0.92	0.15	70,70,70,70	0
57	MG	XV	101	1/1	0.92	0.16	8,8,8,8	0
57	MG	QA	1677	1/1	0.92	0.07	22,22,22,22	0
57	MG	XA	1639	1/1	0.92	0.14	33,33,33,33	0
57	MG	XV	104	1/1	0.92	0.10	18,18,18,18	0
57	MG	YA	3101	1/1	0.92	0.12	28,28,28,28	0
57	MG	RA	3077	1/1	0.92	0.17	6,6,6,6	0
57	MG	RA	3197	1/1	0.92	0.23	13,13,13,13	0
57	MG	YA	3317	1/1	0.92	0.10	32,32,32,32	0
57	MG	RA	3250	1/1	0.92	0.11	36,36,36,36	0
57	MG	RA	3255	1/1	0.92	0.10	29,29,29,29	0
57	MG	RA	3198	1/1	0.92	0.21	22,22,22,22	0
57	MG	RA	3079	1/1	0.92	0.16	32,32,32,32	0
57	MG	QA	1626	1/1	0.92	0.23	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1650	1/1	0.92	0.07	76,76,76,76	0
57	MG	RA	3105	1/1	0.92	0.16	47,47,47,47	0
57	MG	QA	1613	1/1	0.92	0.18	44,44,44,44	0
57	MG	QA	1614	1/1	0.92	0.06	53,53,53,53	0
57	MG	QA	1686	1/1	0.92	0.21	55,55,55,55	0
57	MG	YA	3229	1/1	0.92	0.12	38,38,38,38	0
57	MG	YA	3015	1/1	0.92	0.24	13,13,13,13	0
57	MG	YA	3018	1/1	0.92	0.13	28,28,28,28	0
57	MG	YA	3232	1/1	0.92	0.10	34,34,34,34	0
57	MG	QA	1611	1/1	0.92	0.18	21,21,21,21	0
57	MG	YA	3020	1/1	0.92	0.09	29,29,29,29	0
57	MG	RA	3212	1/1	0.92	0.17	26,26,26,26	0
57	MG	RA	3219	1/1	0.92	0.13	35,35,35,35	0
57	MG	YA	3137	1/1	0.92	0.12	42,42,42,42	0
57	MG	QA	1610	1/1	0.92	0.13	23,23,23,23	0
57	MG	XA	1605	1/1	0.92	0.18	18,18,18,18	0
57	MG	RA	3175	1/1	0.92	0.14	47,47,47,47	0
57	MG	YA	3037	1/1	0.92	0.21	29,29,29,29	0
57	MG	YA	3142	1/1	0.92	0.28	41,41,41,41	0
57	MG	YA	3258	1/1	0.92	0.10	19,19,19,19	0
57	MG	QA	1625	1/1	0.92	0.12	40,40,40,40	0
57	MG	YA	3044	1/1	0.92	0.22	23,23,23,23	0
57	MG	RA	3146	1/1	0.92	0.15	17,17,17,17	0
57	MG	XA	1610	1/1	0.92	0.24	33,33,33,33	0
57	MG	YA	3072	1/1	0.93	0.09	47,47,47,47	0
57	MG	XA	1602	1/1	0.93	0.10	47,47,47,47	0
57	MG	YA	3272	1/1	0.93	0.23	35,35,35,35	0
57	MG	YA	3077	1/1	0.93	0.25	20,20,20,20	0
57	MG	XA	1652	1/1	0.93	0.18	24,24,24,24	0
57	MG	YA	3001	1/1	0.93	0.15	31,31,31,31	0
57	MG	RA	3050	1/1	0.93	0.16	22,22,22,22	0
57	MG	YA	3173	1/1	0.93	0.07	59,59,59,59	0
57	MG	RA	3053	1/1	0.93	0.14	19,19,19,19	0
57	MG	XA	1661	1/1	0.93	0.23	38,38,38,38	0
57	MG	YA	3088	1/1	0.93	0.12	20,20,20,20	0
57	MG	RA	3023	1/1	0.93	0.14	25,25,25,25	0
57	MG	QV	101	1/1	0.93	0.20	20,20,20,20	0
57	MG	YA	3092	1/1	0.93	0.14	26,26,26,26	0
57	MG	YA	3008	1/1	0.93	0.20	46,46,46,46	0
57	MG	QA	1634	1/1	0.93	0.16	42,42,42,42	0
57	MG	RA	3179	1/1	0.93	0.12	30,30,30,30	0
57	MG	RA	3234	1/1	0.93	0.19	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3189	1/1	0.93	0.16	34,34,34,34	0
57	MG	QA	1652	1/1	0.93	0.14	54,54,54,54	0
57	MG	QA	1656	1/1	0.93	0.17	37,37,37,37	0
57	MG	RA	3119	1/1	0.93	0.12	33,33,33,33	0
57	MG	YA	3295	1/1	0.93	0.13	41,41,41,41	0
57	MG	QA	1615	1/1	0.93	0.12	46,46,46,46	0
57	MG	YA	3105	1/1	0.93	0.20	90,90,90,90	0
57	MG	RA	3124	1/1	0.93	0.15	37,37,37,37	0
57	MG	YA	3196	1/1	0.93	0.21	48,48,48,48	0
57	MG	YA	3198	1/1	0.93	0.19	19,19,19,19	0
57	MG	YA	3108	1/1	0.93	0.15	10,10,10,10	0
57	MG	YA	3304	1/1	0.93	0.08	47,47,47,47	0
57	MG	QA	1624	1/1	0.93	0.08	40,40,40,40	0
57	MG	YA	3021	1/1	0.93	0.17	16,16,16,16	0
57	MG	YA	3023	1/1	0.93	0.16	10,10,10,10	0
57	MG	RA	3156	1/1	0.93	0.14	20,20,20,20	0
57	MG	YA	3113	1/1	0.93	0.15	75,75,75,75	0
57	MG	YA	3114	1/1	0.93	0.21	33,33,33,33	0
57	MG	YA	3029	1/1	0.93	0.18	10,10,10,10	0
57	MG	YA	3315	1/1	0.93	0.09	40,40,40,40	0
57	MG	QA	1607	1/1	0.93	0.05	44,44,44,44	0
57	MG	YA	3031	1/1	0.93	0.20	35,35,35,35	0
57	MG	XA	1683	1/1	0.93	0.07	63,63,63,63	0
57	MG	RA	3192	1/1	0.93	0.10	31,31,31,31	0
57	MG	RA	3071	1/1	0.93	0.11	30,30,30,30	0
57	MG	QA	1688	1/1	0.93	0.09	57,57,57,57	0
57	MG	YA	3323	1/1	0.93	0.18	39,39,39,39	0
57	MG	RA	3162	1/1	0.93	0.13	33,33,33,33	0
57	MG	QA	1648	1/1	0.93	0.10	73,73,73,73	0
57	MG	XA	1692	1/1	0.93	0.12	42,42,42,42	0
57	MG	RA	3254	1/1	0.93	0.15	39,39,39,39	0
57	MG	YA	3233	1/1	0.93	0.21	34,34,34,34	0
57	MG	RA	3132	1/1	0.93	0.17	34,34,34,34	0
57	MG	YA	3332	1/1	0.93	0.14	28,28,28,28	0
57	MG	YA	3051	1/1	0.93	0.11	11,11,11,11	0
57	MG	YA	3237	1/1	0.93	0.12	45,45,45,45	0
57	MG	RA	3203	1/1	0.93	0.16	11,11,11,11	0
57	MG	QA	1640	1/1	0.93	0.18	51,51,51,51	0
57	MG	YD	304	1/1	0.93	0.23	56,56,56,56	0
57	MG	YA	3241	1/1	0.93	0.05	6,6,6,6	0
57	MG	RA	3102	1/1	0.93	0.18	22,22,22,22	0
57	MG	RA	3168	1/1	0.93	0.11	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	QA	1672	1/1	0.93	0.12	52,52,52,52	0
57	MG	RA	3017	1/1	0.93	0.26	25,25,25,25	0
57	MG	YP	201	1/1	0.93	0.12	9,9,9,9	0
57	MG	YA	3151	1/1	0.93	0.20	25,25,25,25	0
57	MG	XA	1647	1/1	0.93	0.10	42,42,42,42	0
57	MG	RA	3171	1/1	0.93	0.11	45,45,45,45	0
57	MG	YQ	205	1/1	0.93	0.16	59,59,59,59	0
57	MG	YA	3156	1/1	0.93	0.13	36,36,36,36	0
57	MG	YA	3160	1/1	0.93	0.25	24,24,24,24	0
57	MG	QA	1633	1/1	0.93	0.15	49,49,49,49	0
57	MG	YA	3264	1/1	0.93	0.14	34,34,34,34	0
57	MG	YA	3068	1/1	0.93	0.19	16,16,16,16	0
57	MG	RA	3022	1/1	0.93	0.17	17,17,17,17	0
57	MG	YA	3267	1/1	0.93	0.13	51,51,51,51	0
57	MG	RR	201	1/1	0.94	0.20	33,33,33,33	0
57	MG	XA	1659	1/1	0.94	0.11	10,10,10,10	0
57	MG	RA	3224	1/1	0.94	0.16	26,26,26,26	0
57	MG	YA	3093	1/1	0.94	0.10	30,30,30,30	0
57	MG	RA	3028	1/1	0.94	0.13	20,20,20,20	0
57	MG	RA	3157	1/1	0.94	0.23	11,11,11,11	0
57	MG	XA	1668	1/1	0.94	0.18	24,24,24,24	0
57	MG	RA	3273	1/1	0.94	0.25	47,47,47,47	0
57	MG	RA	3129	1/1	0.94	0.17	37,37,37,37	0
57	MG	RA	3052	1/1	0.94	0.13	23,23,23,23	0
57	MG	QA	1608	1/1	0.94	0.12	45,45,45,45	0
57	MG	QA	1622	1/1	0.94	0.20	28,28,28,28	0
57	MG	RA	3235	1/1	0.94	0.05	22,22,22,22	0
57	MG	YA	3022	1/1	0.94	0.16	39,39,39,39	0
57	MG	QA	1616	1/1	0.94	0.12	43,43,43,43	0
57	MG	RA	3084	1/1	0.94	0.15	19,19,19,19	0
57	MG	YA	3025	1/1	0.94	0.09	2,2,2,2	0
57	MG	QA	1681	1/1	0.94	0.10	53,53,53,53	0
57	MG	RA	3194	1/1	0.94	0.23	46,46,46,46	0
57	MG	QA	1606	1/1	0.94	0.28	40,40,40,40	0
57	MG	YA	3032	1/1	0.94	0.15	21,21,21,21	0
57	MG	XA	1682	1/1	0.94	0.11	41,41,41,41	0
57	MG	YA	3116	1/1	0.94	0.31	28,28,28,28	0
57	MG	YA	3212	1/1	0.94	0.17	27,27,27,27	0
57	MG	RA	3015	1/1	0.94	0.24	29,29,29,29	0
57	MG	YA	3118	1/1	0.94	0.18	42,42,42,42	0
57	MG	XA	1622	1/1	0.94	0.17	15,15,15,15	0
57	MG	RA	3291	1/1	0.94	0.05	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3122	1/1	0.94	0.15	44,44,44,44	0
57	MG	YA	3039	1/1	0.94	0.19	13,13,13,13	0
57	MG	XA	1628	1/1	0.94	0.06	47,47,47,47	0
57	MG	YA	3130	1/1	0.94	0.11	31,31,31,31	0
57	MG	YA	3131	1/1	0.94	0.10	36,36,36,36	0
57	MG	RA	3060	1/1	0.94	0.16	10,10,10,10	0
57	MG	QA	1667	1/1	0.94	0.13	64,64,64,64	0
57	MG	YA	3047	1/1	0.94	0.15	33,33,33,33	0
57	MG	XA	1691	1/1	0.94	0.13	49,49,49,49	0
57	MG	RA	3202	1/1	0.94	0.24	20,20,20,20	0
57	MG	RA	3062	1/1	0.94	0.12	36,36,36,36	0
57	MG	XA	1694	1/1	0.94	0.13	20,20,20,20	0
57	MG	XA	1633	1/1	0.94	0.12	49,49,49,49	0
57	MG	RA	3204	1/1	0.94	0.14	26,26,26,26	0
57	MG	YA	3330	1/1	0.94	0.08	38,38,38,38	0
57	MG	QA	1638	1/1	0.94	0.11	32,32,32,32	0
57	MG	RA	3067	1/1	0.94	0.07	21,21,21,21	0
57	MG	RA	3300	1/1	0.94	0.12	38,38,38,38	0
57	MG	RA	3251	1/1	0.94	0.09	14,14,14,14	0
57	MG	RA	3118	1/1	0.94	0.16	33,33,33,33	0
57	MG	YA	3064	1/1	0.94	0.21	14,14,14,14	0
57	MG	YD	303	1/1	0.94	0.16	25,25,25,25	0
57	MG	QA	1653	1/1	0.94	0.14	38,38,38,38	0
57	MG	YA	3067	1/1	0.94	0.18	31,31,31,31	0
57	MG	YA	3157	1/1	0.94	0.23	4,4,4,4	0
57	MG	QA	1632	1/1	0.94	0.13	40,40,40,40	0
57	MG	RA	3260	1/1	0.94	0.27	46,46,46,46	0
57	MG	RA	3123	1/1	0.94	0.21	50,50,50,50	0
57	MG	Y1	101	1/1	0.94	0.12	44,44,44,44	0
57	MG	YA	3074	1/1	0.94	0.23	22,22,22,22	0
57	MG	RD	302	1/1	0.94	0.06	27,27,27,27	0
57	MG	YA	3166	1/1	0.94	0.13	42,42,42,42	0
57	MG	RA	3262	1/1	0.94	0.12	39,39,39,39	0
57	MG	YR	201	1/1	0.94	0.06	34,34,34,34	0
57	MG	RA	3003	1/1	0.94	0.13	30,30,30,30	0
57	MG	RA	3218	1/1	0.94	0.16	33,33,33,33	0
57	MG	RA	3265	1/1	0.94	0.12	41,41,41,41	0
57	MG	YA	3086	1/1	0.94	0.22	34,34,34,34	0
57	MG	RA	3098	1/1	0.94	0.20	49,49,49,49	0
57	MG	RA	3005	1/1	0.94	0.20	36,36,36,36	0
57	MG	YA	3278	1/1	0.94	0.10	37,37,37,37	0
57	MG	YA	3075	1/1	0.95	0.13	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1691	1/1	0.95	0.15	44,44,44,44	0
57	MG	YA	3079	1/1	0.95	0.11	12,12,12,12	0
57	MG	RA	3083	1/1	0.95	0.14	36,36,36,36	0
57	MG	YA	3271	1/1	0.95	0.11	26,26,26,26	0
57	MG	RA	3049	1/1	0.95	0.17	10,10,10,10	0
57	MG	RA	3200	1/1	0.95	0.18	10,10,10,10	0
57	MG	QA	1680	1/1	0.95	0.17	35,35,35,35	0
57	MG	RA	3006	1/1	0.95	0.11	35,35,35,35	0
57	MG	YA	3007	1/1	0.95	0.15	37,37,37,37	0
57	MG	XA	1655	1/1	0.95	0.16	24,24,24,24	0
57	MG	RA	3122	1/1	0.95	0.19	21,21,21,21	0
57	MG	YA	3090	1/1	0.95	0.14	21,21,21,21	0
57	MG	RA	3087	1/1	0.95	0.14	10,10,10,10	0
57	MG	YA	3176	1/1	0.95	0.16	30,30,30,30	0
57	MG	RA	3163	1/1	0.95	0.08	27,27,27,27	0
57	MG	RA	3026	1/1	0.95	0.27	12,12,12,12	0
57	MG	XA	1664	1/1	0.95	0.12	40,40,40,40	0
57	MG	XA	1601	1/1	0.95	0.09	17,17,17,17	0
57	MG	YA	3181	1/1	0.95	0.06	61,61,61,61	0
57	MG	YA	3016	1/1	0.95	0.20	4,4,4,4	0
57	MG	YA	3098	1/1	0.95	0.10	56,56,56,56	0
57	MG	YA	3017	1/1	0.95	0.11	1,1,1,1	0
57	MG	YA	3186	1/1	0.95	0.07	33,33,33,33	0
57	MG	QA	1654	1/1	0.95	0.16	22,22,22,22	0
57	MG	YA	3293	1/1	0.95	0.06	46,46,46,46	0
57	MG	RA	3008	1/1	0.95	0.11	31,31,31,31	0
57	MG	XA	1669	1/1	0.95	0.11	34,34,34,34	0
57	MG	YA	3296	1/1	0.95	0.15	40,40,40,40	0
57	MG	RA	3030	1/1	0.95	0.16	36,36,36,36	0
57	MG	QA	1636	1/1	0.95	0.11	33,33,33,33	0
57	MG	RA	3010	1/1	0.95	0.21	42,42,42,42	0
57	MG	RA	3213	1/1	0.95	0.10	25,25,25,25	0
57	MG	RA	3216	1/1	0.95	0.24	29,29,29,29	0
57	MG	QA	1683	1/1	0.95	0.25	51,51,51,51	0
57	MG	XA	1611	1/1	0.95	0.24	31,31,31,31	0
57	MG	YA	3199	1/1	0.95	0.18	10,10,10,10	0
57	MG	YA	3201	1/1	0.95	0.21	21,21,21,21	0
57	MG	YA	3202	1/1	0.95	0.24	22,22,22,22	0
57	MG	RA	3034	1/1	0.95	0.13	1,1,1,1	0
57	MG	QA	1603	1/1	0.95	0.05	33,33,33,33	0
57	MG	RA	3065	1/1	0.95	0.13	7,7,7,7	0
57	MG	RA	3225	1/1	0.95	0.13	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3135	1/1	0.95	0.08	34,34,34,34	0
57	MG	RA	3036	1/1	0.95	0.21	35,35,35,35	0
57	MG	XA	1621	1/1	0.95	0.12	10,10,10,10	0
57	MG	QA	1676	1/1	0.95	0.08	27,27,27,27	0
57	MG	YA	3120	1/1	0.95	0.11	24,24,24,24	0
57	MG	XA	1623	1/1	0.95	0.06	40,40,40,40	0
57	MG	YA	3045	1/1	0.95	0.09	11,11,11,11	0
57	MG	RA	3229	1/1	0.95	0.20	45,45,45,45	0
57	MG	XA	1626	1/1	0.95	0.07	38,38,38,38	0
57	MG	YA	3128	1/1	0.95	0.20	4,4,4,4	0
57	MG	YA	3326	1/1	0.95	0.15	22,22,22,22	0
57	MG	YA	3225	1/1	0.95	0.10	31,31,31,31	0
57	MG	QA	1687	1/1	0.95	0.06	46,46,46,46	0
57	MG	RA	3016	1/1	0.95	0.10	24,24,24,24	0
57	MG	RA	3140	1/1	0.95	0.10	23,23,23,23	0
57	MG	RA	3181	1/1	0.95	0.19	7,7,7,7	0
57	MG	QA	1660	1/1	0.95	0.10	25,25,25,25	0
57	MG	RA	3073	1/1	0.95	0.06	50,50,50,50	0
57	MG	RA	3184	1/1	0.95	0.16	45,45,45,45	0
57	MG	YA	3058	1/1	0.95	0.23	28,28,28,28	0
57	MG	RA	3042	1/1	0.95	0.12	24,24,24,24	0
57	MG	YD	302	1/1	0.95	0.18	1,1,1,1	0
57	MG	RA	3075	1/1	0.95	0.15	11,11,11,11	0
57	MG	XA	1637	1/1	0.95	0.14	43,43,43,43	0
57	MG	YA	3062	1/1	0.95	0.16	23,23,23,23	0
57	MG	QA	1661	1/1	0.95	0.14	26,26,26,26	0
57	MG	YA	3147	1/1	0.95	0.04	37,37,37,37	0
57	MG	RA	3044	1/1	0.95	0.12	5,5,5,5	0
57	MG	YA	3252	1/1	0.95	0.12	23,23,23,23	0
57	MG	YO	201	1/1	0.95	0.23	57,57,57,57	0
57	MG	YA	3253	1/1	0.95	0.10	23,23,23,23	0
57	MG	RA	3078	1/1	0.95	0.12	52,52,52,52	0
57	MG	YA	3255	1/1	0.95	0.05	35,35,35,35	0
57	MG	RA	3002	1/1	0.95	0.07	23,23,23,23	0
57	MG	RA	3151	1/1	0.95	0.20	36,36,36,36	0
57	MG	XA	1643	1/1	0.95	0.09	29,29,29,29	0
57	MG	YA	3259	1/1	0.95	0.06	19,19,19,19	0
57	MG	YA	3155	1/1	0.95	0.05	61,61,61,61	0
57	MG	Y3	101	1/1	0.95	0.15	11,11,11,11	0
57	MG	RA	3113	1/1	0.95	0.16	19,19,19,19	0
57	MG	YA	3263	1/1	0.95	0.13	28,28,28,28	0
57	MG	YA	3158	1/1	0.95	0.06	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3046	1/1	0.95	0.14	31,31,31,31	0
57	MG	RA	3217	1/1	0.96	0.11	21,21,21,21	0
57	MG	XA	1681	1/1	0.96	0.11	35,35,35,35	0
57	MG	YA	3053	1/1	0.96	0.16	25,25,25,25	0
57	MG	RA	3196	1/1	0.96	0.06	33,33,33,33	0
57	MG	RA	3104	1/1	0.96	0.18	12,12,12,12	0
57	MG	XA	1646	1/1	0.96	0.11	30,30,30,30	0
57	MG	YA	3300	1/1	0.96	0.19	56,56,56,56	0
57	MG	YA	3234	1/1	0.96	0.25	47,47,47,47	0
57	MG	XA	1614	1/1	0.96	0.06	66,66,66,66	0
57	MG	RA	3180	1/1	0.96	0.08	24,24,24,24	0
57	MG	XA	1688	1/1	0.96	0.14	49,49,49,49	0
57	MG	YA	3013	1/1	0.96	0.16	38,38,38,38	0
57	MG	QA	1669	1/1	0.96	0.09	38,38,38,38	0
57	MG	QA	1647	1/1	0.96	0.14	37,37,37,37	0
57	MG	YA	3243	1/1	0.96	0.18	33,33,33,33	0
57	MG	RA	3051	1/1	0.96	0.10	27,27,27,27	0
57	MG	YA	3247	1/1	0.96	0.08	29,29,29,29	0
57	MG	RA	3278	1/1	0.96	0.17	47,47,47,47	0
57	MG	RE	301	1/1	0.96	0.16	21,21,21,21	0
57	MG	QA	1631	1/1	0.96	0.11	64,64,64,64	0
57	MG	YA	3069	1/1	0.96	0.11	19,19,19,19	0
57	MG	RA	3109	1/1	0.96	0.12	35,35,35,35	0
57	MG	XA	1625	1/1	0.96	0.20	24,24,24,24	0
57	MG	YA	3182	1/1	0.96	0.23	19,19,19,19	0
57	MG	XA	1697	1/1	0.96	0.17	22,22,22,22	0
57	MG	QA	1685	1/1	0.96	0.06	34,34,34,34	0
57	MG	XA	1663	1/1	0.96	0.07	16,16,16,16	0
57	MG	YA	3076	1/1	0.96	0.09	21,21,21,21	0
57	MG	RA	3206	1/1	0.96	0.18	25,25,25,25	0
57	MG	YA	3078	1/1	0.96	0.13	31,31,31,31	0
57	MG	YA	3027	1/1	0.96	0.09	12,12,12,12	0
57	MG	RA	3257	1/1	0.96	0.07	36,36,36,36	0
57	MG	RA	3125	1/1	0.96	0.09	21,21,21,21	0
57	MG	YA	3083	1/1	0.96	0.07	17,17,17,17	0
57	MG	XM	201	1/1	0.96	0.04	52,52,52,52	0
57	MG	YA	3268	1/1	0.96	0.05	37,37,37,37	0
57	MG	RA	3233	1/1	0.96	0.24	28,28,28,28	0
57	MG	QA	1601	1/1	0.96	0.11	28,28,28,28	0
57	MG	YB	203	1/1	0.96	0.17	28,28,28,28	0
57	MG	QA	1627	1/1	0.96	0.07	34,34,34,34	0
57	MG	RA	3292	1/1	0.96	0.10	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	Y0	101	1/1	0.96	0.07	9,9,9,9	0
57	MG	YA	3145	1/1	0.96	0.12	14,14,14,14	0
57	MG	YA	3146	1/1	0.96	0.10	21,21,21,21	0
57	MG	YA	3204	1/1	0.96	0.12	18,18,18,18	0
57	MG	RA	3159	1/1	0.96	0.09	32,32,32,32	0
57	MG	YA	3148	1/1	0.96	0.14	23,23,23,23	0
57	MG	YA	3040	1/1	0.96	0.05	16,16,16,16	0
57	MG	YA	3041	1/1	0.96	0.13	20,20,20,20	0
57	MG	RA	3068	1/1	0.96	0.18	12,12,12,12	0
57	MG	RA	3114	1/1	0.96	0.10	29,29,29,29	0
57	MG	YA	3213	1/1	0.96	0.07	16,16,16,16	0
57	MG	YA	3153	1/1	0.96	0.05	30,30,30,30	0
57	MG	YA	3285	1/1	0.96	0.09	36,36,36,36	0
57	MG	RA	3018	1/1	0.96	0.15	10,10,10,10	0
57	MG	RA	3267	1/1	0.96	0.05	32,32,32,32	0
57	MG	XA	1608	1/1	0.96	0.11	28,28,28,28	0
57	MG	QE	201	1/1	0.96	0.21	42,42,42,42	0
57	MG	RA	3269	1/1	0.96	0.12	34,34,34,34	0
57	MG	YA	3159	1/1	0.96	0.10	23,23,23,23	0
57	MG	YA	3050	1/1	0.96	0.16	22,22,22,22	0
57	MG	YA	3226	1/1	0.96	0.16	27,27,27,27	0
57	MG	YA	3245	1/1	0.97	0.20	24,24,24,24	0
57	MG	RA	3249	1/1	0.97	0.11	28,28,28,28	0
57	MG	YA	3144	1/1	0.97	0.07	25,25,25,25	0
57	MG	XA	1658	1/1	0.97	0.18	34,34,34,34	0
57	MG	YA	3250	1/1	0.97	0.12	35,35,35,35	0
57	MG	YA	3306	1/1	0.97	0.14	48,48,48,48	0
57	MG	YA	3307	1/1	0.97	0.05	24,24,24,24	0
57	MG	YA	3308	1/1	0.97	0.11	30,30,30,30	0
57	MG	RA	3199	1/1	0.97	0.17	17,17,17,17	0
57	MG	XA	1660	1/1	0.97	0.06	23,23,23,23	0
57	MG	QA	1609	1/1	0.97	0.08	31,31,31,31	0
57	MG	XA	1662	1/1	0.97	0.06	22,22,22,22	0
57	MG	XA	1627	1/1	0.97	0.08	37,37,37,37	0
57	MG	YA	3197	1/1	0.97	0.04	42,42,42,42	0
57	MG	YA	3106	1/1	0.97	0.12	25,25,25,25	0
57	MG	RA	3252	1/1	0.97	0.06	29,29,29,29	0
57	MG	YA	3200	1/1	0.97	0.22	23,23,23,23	0
57	MG	YA	3318	1/1	0.97	0.13	41,41,41,41	0
57	MG	RA	3284	1/1	0.97	0.05	16,16,16,16	0
57	MG	RA	3144	1/1	0.97	0.04	27,27,27,27	0
57	MG	RA	3145	1/1	0.97	0.10	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	3070	1/1	0.97	0.09	25,25,25,25	0
57	MG	RA	3027	1/1	0.97	0.15	23,23,23,23	0
57	MG	QA	1629	1/1	0.97	0.05	33,33,33,33	0
57	MG	RA	3230	1/1	0.97	0.11	33,33,33,33	0
57	MG	RA	3040	1/1	0.97	0.12	10,10,10,10	0
57	MG	RA	3054	1/1	0.97	0.18	14,14,14,14	0
57	MG	RA	3187	1/1	0.97	0.14	5,5,5,5	0
57	MG	QA	1644	1/1	0.97	0.11	43,43,43,43	0
57	MG	RA	3001	1/1	0.97	0.13	8,8,8,8	0
57	MG	YA	3216	1/1	0.97	0.13	14,14,14,14	0
57	MG	YA	3217	1/1	0.97	0.05	37,37,37,37	0
57	MG	YA	3218	1/1	0.97	0.05	10,10,10,10	0
57	MG	RA	3019	1/1	0.97	0.11	13,13,13,13	0
57	MG	YA	3080	1/1	0.97	0.07	37,37,37,37	0
57	MG	QA	1663	1/1	0.97	0.16	36,36,36,36	0
57	MG	YA	3123	1/1	0.97	0.18	17,17,17,17	0
57	MG	RA	3011	1/1	0.97	0.05	30,30,30,30	0
57	MG	YA	3125	1/1	0.97	0.05	36,36,36,36	0
57	MG	YA	3126	1/1	0.97	0.11	15,15,15,15	0
57	MG	YA	3043	1/1	0.97	0.16	13,13,13,13	0
57	MG	YE	302	1/1	0.97	0.09	25,25,25,25	0
57	MG	YA	3227	1/1	0.97	0.20	36,36,36,36	0
57	MG	RA	3121	1/1	0.97	0.20	50,50,50,50	0
57	MG	RA	3214	1/1	0.97	0.17	35,35,35,35	0
57	MG	RA	3215	1/1	0.97	0.15	21,21,21,21	0
57	MG	XA	1615	1/1	0.97	0.11	28,28,28,28	0
57	MG	XA	1616	1/1	0.97	0.10	37,37,37,37	0
57	MG	YQ	201	1/1	0.97	0.12	58,58,58,58	0
57	MG	QA	1678	1/1	0.97	0.05	33,33,33,33	0
57	MG	RA	3004	1/1	0.97	0.10	26,26,26,26	0
57	MG	QA	1659	1/1	0.97	0.14	44,44,44,44	0
57	MG	RA	3275	1/1	0.97	0.23	40,40,40,40	0
57	MG	RA	3064	1/1	0.97	0.13	20,20,20,20	0
57	MG	YA	3238	1/1	0.97	0.16	27,27,27,27	0
57	MG	XA	1653	1/1	0.97	0.16	17,17,17,17	0
57	MG	RA	3220	1/1	0.97	0.13	34,34,34,34	0
57	MG	RA	3095	1/1	0.97	0.18	28,28,28,28	0
57	MG	YA	3242	1/1	0.97	0.14	10,10,10,10	0
59	ZN	XN	101	1/1	0.97	0.05	90,90,90,90	0
57	MG	YA	3188	1/1	0.97	0.17	8,8,8,8	0
57	MG	YA	3244	1/1	0.97	0.30	37,37,37,37	0
57	MG	RA	3070	1/1	0.98	0.12	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3035	1/1	0.98	0.17	2,2,2,2	0
57	MG	YA	3333	1/1	0.98	0.12	36,36,36,36	0
57	MG	RA	3259	1/1	0.98	0.15	26,26,26,26	0
57	MG	RA	3290	1/1	0.98	0.07	11,11,11,11	0
57	MG	YB	201	1/1	0.98	0.10	11,11,11,11	0
57	MG	YA	3206	1/1	0.98	0.12	14,14,14,14	0
57	MG	YA	3038	1/1	0.98	0.10	6,6,6,6	0
57	MG	YA	3208	1/1	0.98	0.18	17,17,17,17	0
57	MG	XA	1684	1/1	0.98	0.11	53,53,53,53	0
57	MG	YA	3065	1/1	0.98	0.07	38,38,38,38	0
57	MG	RA	3221	1/1	0.98	0.11	16,16,16,16	0
57	MG	XA	1665	1/1	0.98	0.05	34,34,34,34	0
57	MG	RA	3080	1/1	0.98	0.08	50,50,50,50	0
57	MG	YA	3214	1/1	0.98	0.15	22,22,22,22	0
57	MG	RA	3048	1/1	0.98	0.10	23,23,23,23	0
57	MG	RP	201	1/1	0.98	0.13	33,33,33,33	0
57	MG	YF	301	1/1	0.98	0.04	32,32,32,32	0
57	MG	RA	3063	1/1	0.98	0.22	12,12,12,12	0
57	MG	YA	3099	1/1	0.98	0.11	19,19,19,19	0
57	MG	QA	1674	1/1	0.98	0.15	36,36,36,36	0
57	MG	RA	3238	1/1	0.98	0.14	23,23,23,23	0
57	MG	YA	3129	1/1	0.98	0.09	25,25,25,25	0
57	MG	QA	1658	1/1	0.98	0.15	20,20,20,20	0
57	MG	RA	3281	1/1	0.98	0.18	44,44,44,44	0
57	MG	YA	3132	1/1	0.98	0.14	21,21,21,21	0
57	MG	XA	1654	1/1	0.98	0.15	28,28,28,28	0
57	MG	QA	1666	1/1	0.98	0.07	22,22,22,22	0
58	SF4	QD	302	8/8	0.98	0.07	59,76,106,109	0
58	SF4	XD	301	8/8	0.98	0.07	68,75,103,103	0
57	MG	YA	3028	1/1	0.98	0.05	14,14,14,14	0
57	MG	RA	3021	1/1	0.98	0.10	19,19,19,19	0
57	MG	QV	103	1/1	0.98	0.14	33,33,33,33	0
57	MG	RA	3256	1/1	0.98	0.19	37,37,37,37	0
57	MG	YA	3056	1/1	0.98	0.14	15,15,15,15	0
57	MG	QA	1670	1/1	0.98	0.12	37,37,37,37	0
57	MG	RA	3287	1/1	0.98	0.07	42,42,42,42	0
57	MG	RA	3253	1/1	0.99	0.06	10,10,10,10	0
57	MG	QA	1690	1/1	0.99	0.05	13,13,13,13	0
57	MG	RA	3153	1/1	0.99	0.04	23,23,23,23	0
57	MG	YA	3026	1/1	0.99	0.19	16,16,16,16	0
57	MG	YA	3170	1/1	0.99	0.03	56,56,56,56	0
57	MG	QA	1604	1/1	0.99	0.06	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	ZN	QN	101	1/1	0.99	0.05	112,112,112,112	0
57	MG	YA	3172	1/1	0.99	0.09	21,21,21,21	0
57	MG	QA	1655	1/1	0.99	0.11	33,33,33,33	0
57	MG	Y0	102	1/1	0.99	0.18	24,24,24,24	0
57	MG	QA	1668	1/1	0.99	0.06	44,44,44,44	0
57	MG	YA	3094	1/1	0.99	0.09	27,27,27,27	0
57	MG	YA	3249	1/1	0.99	0.05	18,18,18,18	0
57	MG	RA	3222	1/1	0.99	0.09	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.