



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 07:33 AM EDT

PDB ID : 6BZ7 / pdb_00006bz7
Title : Thermus thermophilus 70S containing 16S G299A point mutation and near-cognate ASL Leucine in A site.
Authors : Hoffer, E.D.; Maehigashi, T.; Fagan, C.E.; Dunham, C.M.
Deposited on : 2017-12-22
Resolution : 3.68 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

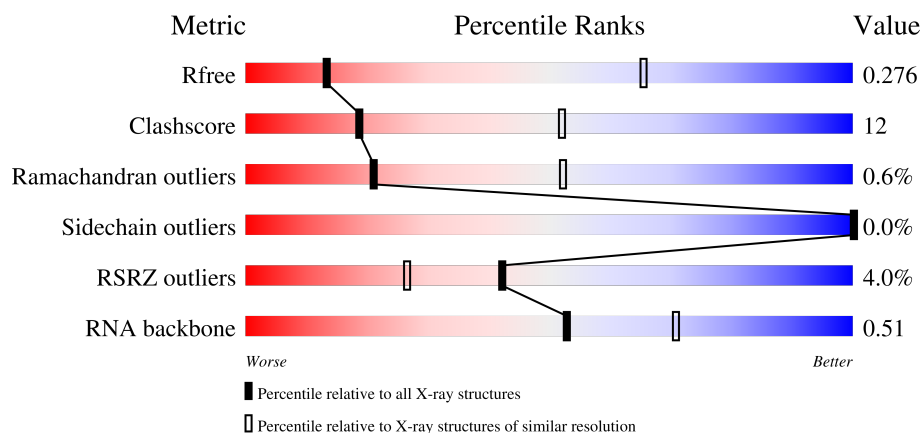
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.68 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	1263 (3.80-3.56)
Clashscore	190562	1305 (3.80-3.56)
Ramachandran outliers	187476	1259 (3.80-3.56)
Sidechain outliers	187428	1256 (3.80-3.56)
RSRZ outliers	180081	1262 (3.80-3.56)
RNA backbone	3983	1000 (4.26-3.08)

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	1508	45% 44% 10%
1	XA	1508	44% 46% 10%
2	QB	256	3% 61% 30% 8%
2	XB	256	4% 62% 29% 8%

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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	

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Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	QW	77	
22	XV	77	
22	XW	77	
23	QX	25	
23	XX	25	
24	QY	17	
24	XY	17	
25	RA	2915	
25	YA	2915	
26	RB	122	
26	YB	122	

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Mol	Chain	Length	Quality of chain
27	RD	276	
27	YD	276	
28	RE	206	
28	YE	206	
29	RF	210	
29	YF	210	
30	RG	182	
30	YG	182	
31	RH	180	
31	YH	180	
32	RI	148	
32	YI	148	
33	RN	140	
33	YN	140	
34	RO	122	
34	YO	122	
35	RP	150	
35	YP	150	
36	RQ	141	
36	YQ	141	
37	RR	118	
37	YR	118	
38	RS	112	
38	YS	112	
39	RT	146	

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Mol	Chain	Length	Quality of chain
39	YT	146	
40	RU	118	
40	YU	118	
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	71	
51	R5	60	
51	Y5	60	

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Mol	Chain	Length	Quality of chain
52	R6	54	
52	Y6	54	
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	

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
56	MG	QA	1610	-	-	-	X
56	MG	QA	1631	-	-	-	X
56	MG	QV	104	-	-	-	X
56	MG	R8	101	-	-	-	X
56	MG	RA	3012	-	-	-	X
56	MG	RA	3013	-	-	-	X
56	MG	RA	3016	-	-	-	X
56	MG	RA	3024	-	-	-	X
56	MG	RA	3037	-	-	-	X
56	MG	RA	3042	-	-	-	X
56	MG	RA	3044	-	-	-	X
56	MG	RA	3050	-	-	-	X
56	MG	RA	3056	-	-	-	X
56	MG	RA	3061	-	-	-	X
56	MG	RA	3071	-	-	-	X
56	MG	RA	3081	-	-	-	X
56	MG	RA	3096	-	-	-	X
56	MG	RA	3119	-	-	-	X
56	MG	RA	3148	-	-	-	X
56	MG	RA	3155	-	-	-	X
56	MG	RA	3243	-	-	-	X
56	MG	RA	3494	-	-	-	X
56	MG	XA	1603	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3017	-	-	-	X
56	MG	YA	3018	-	-	-	X
56	MG	YA	3020	-	-	-	X
56	MG	YA	3031	-	-	-	X
56	MG	YA	3035	-	-	-	X
56	MG	YA	3047	-	-	-	X
56	MG	YA	3078	-	-	-	X
56	MG	YA	3161	-	-	-	X
56	MG	YA	3260	-	-	-	X
56	MG	YA	3426	-	-	-	X
56	MG	YA	3528	-	-	-	X

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 295575 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1500	Total	C	N	O	P	0	0	0
			32246	14353	5981	10413	1499			
1	XA	1500	Total	C	N	O	P	0	0	0
			32248	14354	5984	10411	1499			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QA	299	A	G	engineered mutation	GB 55771382
XA	299	A	G	engineered mutation	GB 55771382

- 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			

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

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

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

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

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

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

- Molecule 22 is a RNA chain called tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	QW	76	Total	C	N	O	P	0	0	0
			1618	722	292	529	75			
22	XV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	XW	76	Total	C	N	O	P	0	0	0
			1618	722	292	529	75			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	8	Total	C	N	O	P	0	0	0
			169	76	29	56	8			
23	XX	10	Total	C	N	O	P	0	0	0
			210	96	39	66	9			

- Molecule 24 is a RNA chain called ASL Leu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	17	Total	C	N	O	P	0	0	0
			358	162	64	116	16			
24	XY	17	Total	C	N	O	P	0	0	0
			358	162	64	116	16			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
35	YP	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	Y0	75	Total	C	N	O	S	0	0	0
			599	370	127	101	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
47	Y1	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	68	Total	Mg	0	0
			68	68		
56	QC	1	Total	Mg	0	0
			1	1		
56	QE	1	Total	Mg	0	0
			1	1		
56	QF	1	Total	Mg	0	0
			1	1		

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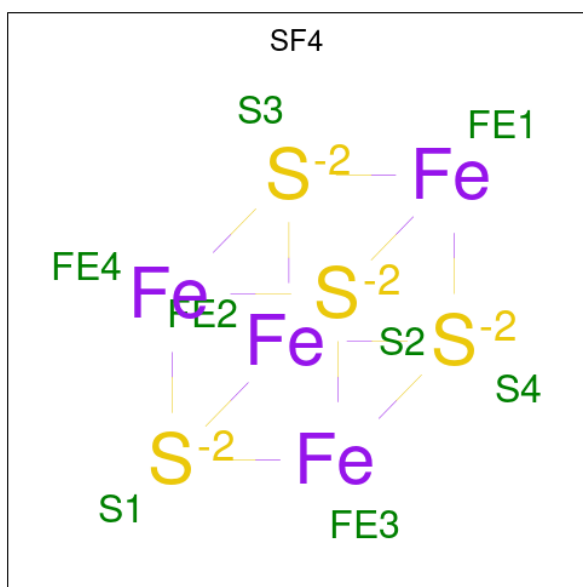
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QH	1	Total 1	Mg 1	0	0
56	QQ	1	Total 1	Mg 1	0	0
56	QV	6	Total 6	Mg 6	0	0
56	QY	1	Total 1	Mg 1	0	0
56	RA	508	Total 508	Mg 508	0	0
56	RB	7	Total 7	Mg 7	0	0
56	RE	2	Total 2	Mg 2	0	0
56	RF	1	Total 1	Mg 1	0	0
56	RN	1	Total 1	Mg 1	0	0
56	RO	2	Total 2	Mg 2	0	0
56	RP	2	Total 2	Mg 2	0	0
56	RQ	2	Total 2	Mg 2	0	0
56	RR	1	Total 1	Mg 1	0	0
56	RT	1	Total 1	Mg 1	0	0
56	RU	1	Total 1	Mg 1	0	0
56	RY	1	Total 1	Mg 1	0	0
56	R0	4	Total 4	Mg 4	0	0
56	R1	2	Total 2	Mg 2	0	0
56	R4	1	Total 1	Mg 1	0	0
56	R8	1	Total 1	Mg 1	0	0
56	R9	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	XA	82	Total 82	Mg 82	0	0
56	XE	1	Total 1	Mg 1	0	0
56	XL	1	Total 1	Mg 1	0	0
56	XM	1	Total 1	Mg 1	0	0
56	XQ	1	Total 1	Mg 1	0	0
56	XS	1	Total 1	Mg 1	0	0
56	XV	6	Total 6	Mg 6	0	0
56	YA	546	Total 546	Mg 546	0	0
56	YB	12	Total 12	Mg 12	0	0
56	YD	2	Total 2	Mg 2	0	0
56	YE	2	Total 2	Mg 2	0	0
56	YO	1	Total 1	Mg 1	0	0
56	YP	3	Total 3	Mg 3	0	0
56	YQ	3	Total 3	Mg 3	0	0
56	YX	2	Total 2	Mg 2	0	0
56	YY	1	Total 1	Mg 1	0	0
56	Y0	1	Total 1	Mg 1	0	0
56	Y7	1	Total 1	Mg 1	0	0
56	Y8	1	Total 1	Mg 1	0	0
56	Y9	1	Total 1	Mg 1	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	QN	1	Total	Zn	0	0
			1	1		
58	RY	1	Total	Zn	0	0
			1	1		
58	R4	1	Total	Zn	0	0
			1	1		
58	R5	1	Total	Zn	0	0
			1	1		
58	R6	1	Total	Zn	0	0
			1	1		
58	R9	1	Total	Zn	0	0
			1	1		
58	XN	1	Total	Zn	0	0
			1	1		
58	YY	1	Total	Zn	0	0
			1	1		
58	Y4	1	Total	Zn	0	0
			1	1		
58	Y5	1	Total	Zn	0	0
			1	1		

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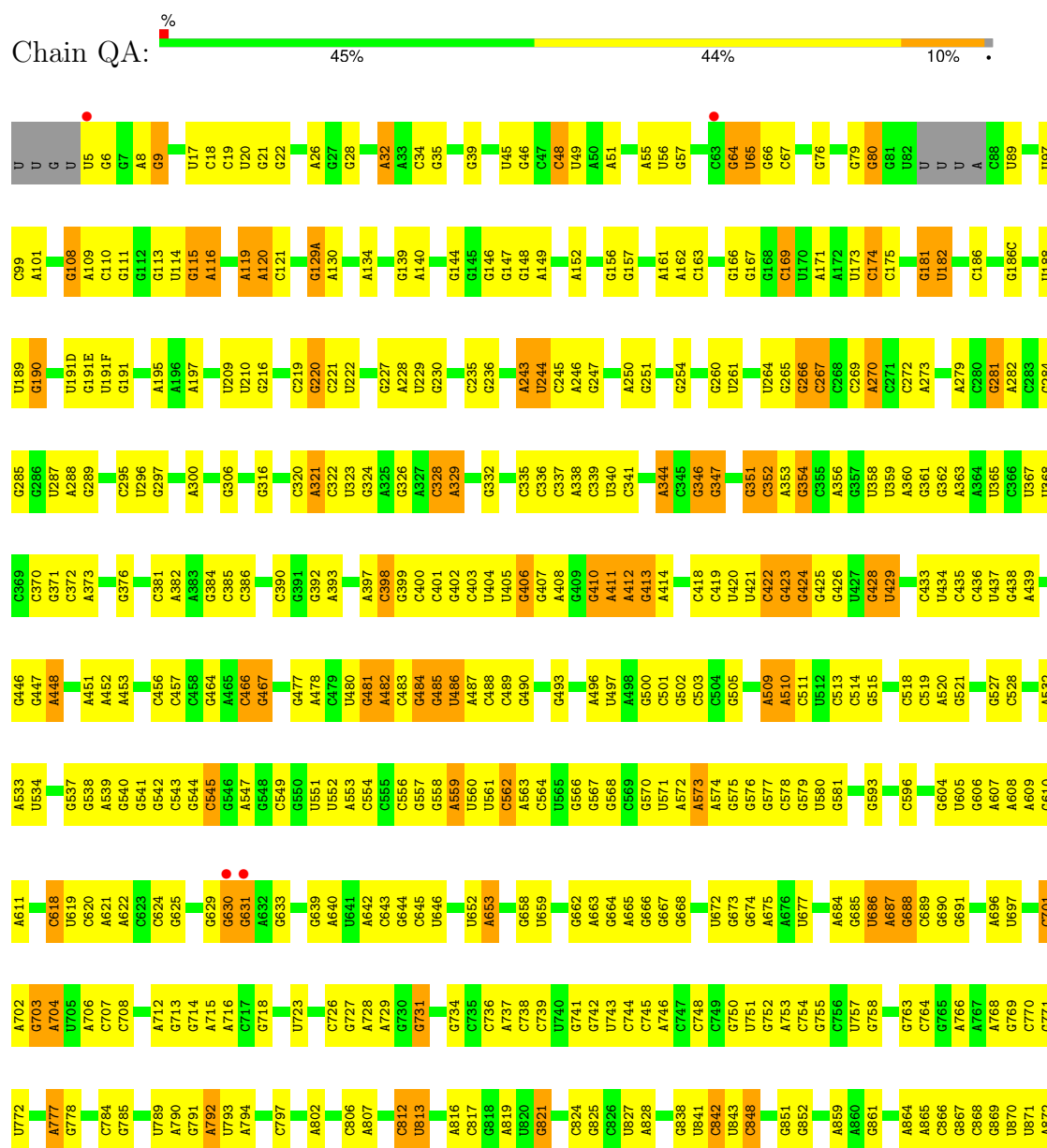
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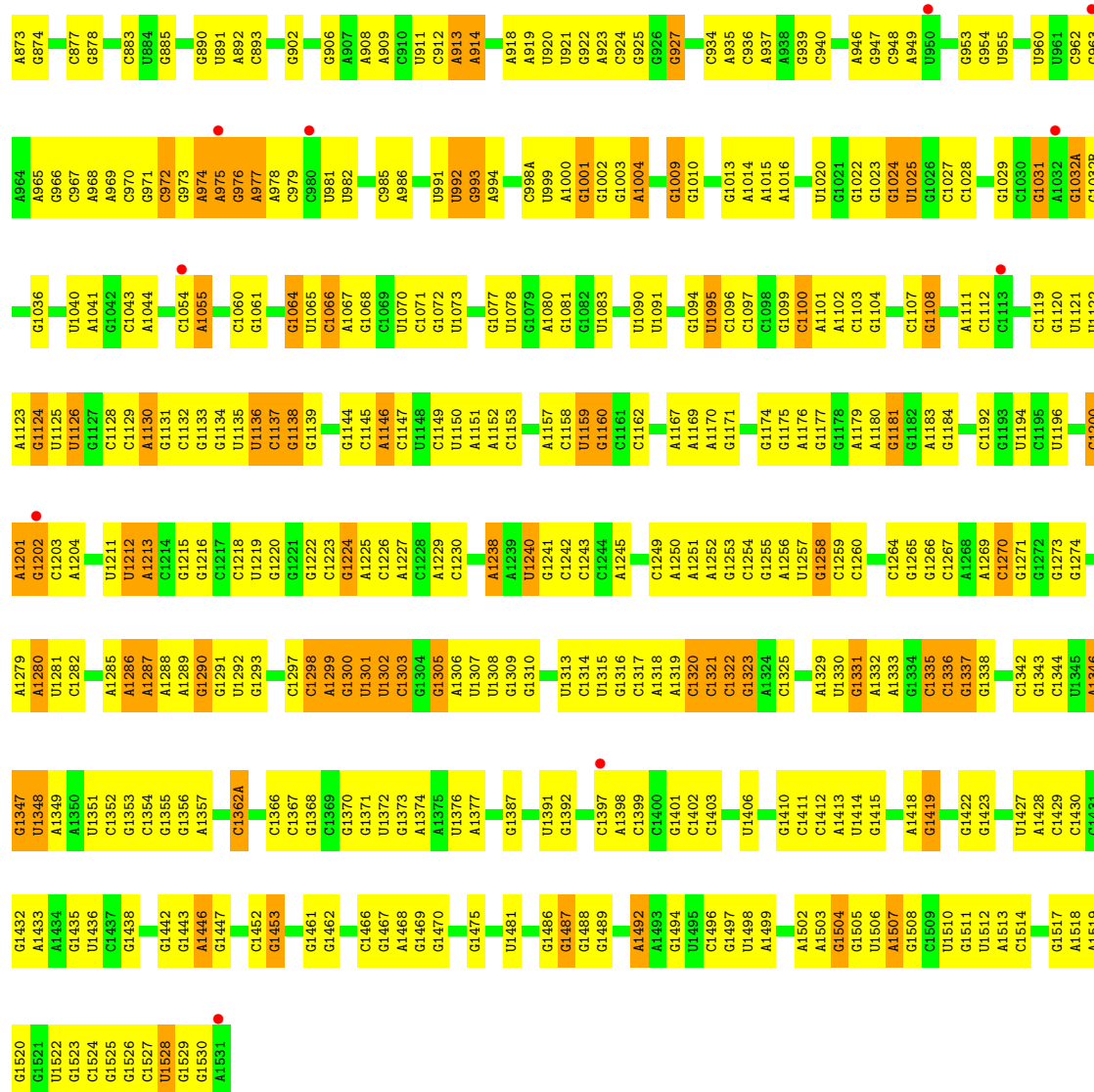
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	Y6	1	Total 1	Zn 1	0	0
58	Y9	1	Total 1	Zn 1	0	0

3 Residue-property plots

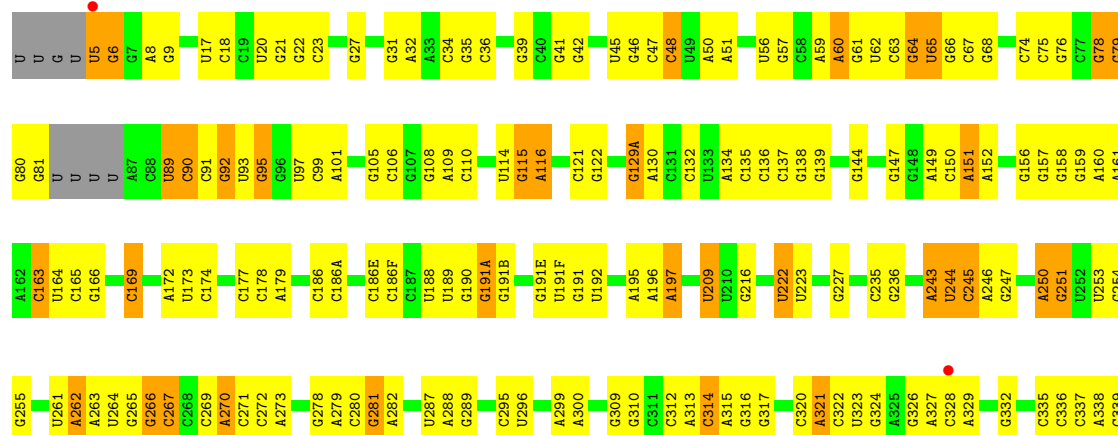
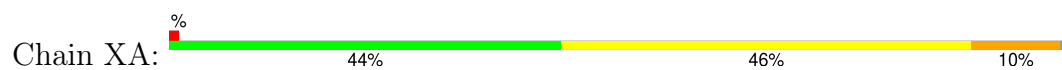
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



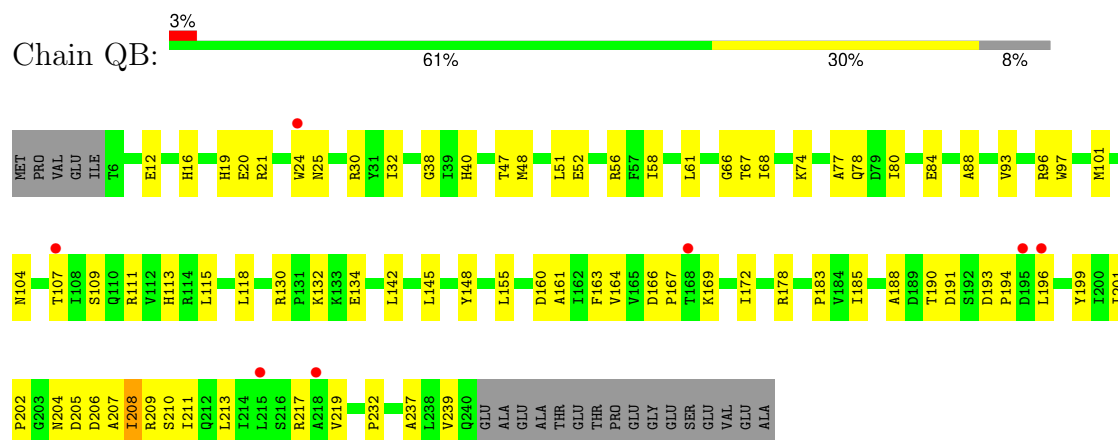


● Molecule 1: 16S rRNA

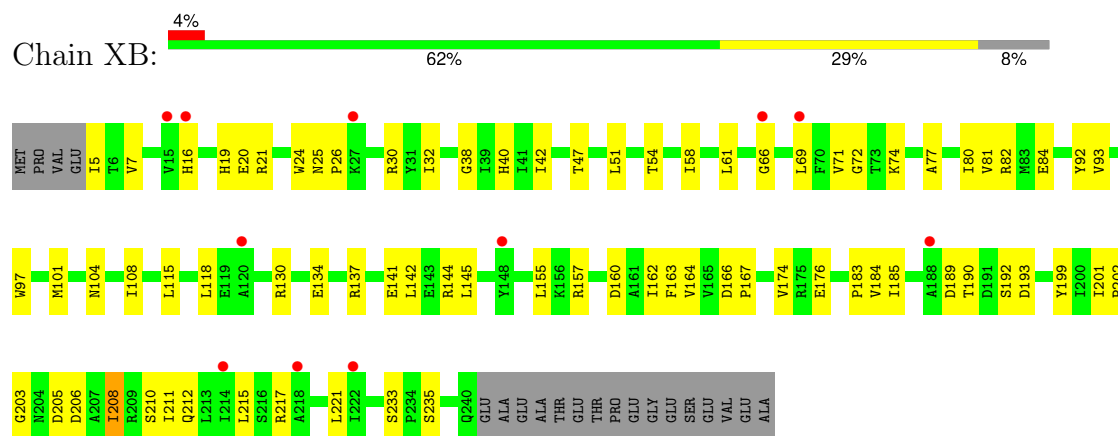


G1455	U1376	U1308	U1235	G1160	U1091	C1006	C932	A859	G755	A676	G584	A509	G409	U343
A1468	A1377	G1309	A1236	C1161	G1094	G1009	G953	A864	C756	U677	G585	A510	G410	A344
G1470	C1378	G1312	A1237	C1162	U1095	G1010	C934	A865	U757	U678	C596	A511	A411	C345
C1479	G1354	U1313	A1239	A1167	C1096	G1011	A935	C866	G758	C690	G587	C511	A412	G346
G1480	G1365	C1314	U1240	A1169	U1098	G1012	G939	C867	A768	C681	G592	C513	G413	G347
U1481	G1386	U1315	G1241	A1170	C1099	G1013	C940	C868	C769	C682	G595	C514	A414	
G1482	C1387	C1316	C1242	C1171	G1099	A1014	G941	C869	C770	G683	C596	C515		
	C1388	G1317	C1243	G1172	C1100	A1015	G942	U870	G771		C599	G518	U421	G351
	C1389	A1318	C1244	G1175	A1101	A1016	A946	A871	U772	U686	C600	C519	C422	C352
	U1390	A1319	A1245	G1176	G947	G1017	G947	A872	G773	C688	G600	G521	G423	A353
	U1391	C1320	A1250	G1177	A1105	G1023	U950	A873	G774	C689	U603	G524	G424	G354
	G1392	C1321	A1251	G1178	C1107	G1024	G951	C875	A777	C690	U604	G527	G425	C355
	U1393	C1322		A1179	G1108	U1025	U952	C876	G778	C691	G604	G528	U427	C357
		G1323	C1254	A1180	C1109	G1026	G953	C877	U779	U692	U605	G529	G428	U359
	C1397	C1324	G1255	G1181	G1112	C1027	A958	C878	A782	G700	G606	C530	A430	A360
	A1398	C1325	A1256	G1182	C1113	G1028	A959	A874	G783	C701	G610	U531	U437	G361
	C1399	C1326	U1257	A1183	G1117	G1028A	U960	A875	C784	A702	A611	A532	U438	C362
		C1327	G1258	G1184	G1117	G1029	G963	C882	G785	G703		A533	U439	A363
	G1404	C1328		G1185	G1120	A1032	G964	U884	U789	A704	C618	A539	A440	U367
	G1405	C1329	C1262	G1186	U1121	G1032A	A965	C885	A790	C708	U619	G540	C442	U368
	G1410	U1330	C1263	G1187	U1122		A966	C886	G791	G709	C624		A448	C369
	C1411	G1331	G1264	A1188	U1123	G1036	G967		A792	G710	G625	C543		C372
	C1412	A1332	C1265	C1189	U1124	C1037	A968	G890	A794	G711	G630	C544	A452	A373
	A1413	A1333	G1266	G1190	U1125	C1038	G969	C893	G800	G712	G631	C545	A453	A374
	U1414	C1335	C1267	C1191	U1126	C1039	C970	C894	G801	G713	A632	A547	G464	U375
	A1502	G1336	A1288	C1192	G1127	U1040	G971	C895	A807	G714	G633	G548	G465	G376
	G1504	C1337	U1196	U1199	U1129		C972	C896	C808	A715		C549	C466	G377
	G1505	G1417	C1270	C1200	A1130	A1044	G973	C897	C811	A716	U636	U552	G467	C378
	G1506	G1418		U1345	U1131		A974	G898	C812	C719	G637	A553	A468	G380
	A1507	G1419	G1273	C1201	C1132	U1049	A975	G900	U813	G720	G639	C554	G477	C381
	G1508	C1420	A1280	G1202	G1133	G1050	G976	A901	G817	G721	A640	C555	A478	A382
	A1509	G1421	U1281	C1203	G1136	G1053	A977	G902	C818	A722		C556	C479	A383
	U1510	C1422	C1282	G1206	U1137	C1054	C980	G903	G819	U723	C643		G481	A384
	G1511	G1423		G1207	G1138	A1055	U981	G906	G821	U728	G644	A559	U480	C385
	U1512		A1285	C1210	G1139		U982	A907	C824	A729	A648	U560	A482	C386
	A1513	U1425	A1286	C1211	C1140	C1060	A986	A908	C825	G730	G649	U561	C483	G388
	C1514	U1426	A1287	U1212	C1141	G1061	A987	A909	C826	G731	G650	C564	G484	A389
	G1516	A1428	A1288	U1213	G1142	U1062	G987	C910	C827		C651	U565	G485	C390
	G1517		A1289	C1214	G1143	C1063	U991	U911	U827	C736	G656	G566	G486	G391
	A1518	G1432	G1291	G1215	G1144	G1064	U992	C912	A828	A737	U652	G567	C489	C392
	G1520		G1292	C1218	C1145	U1065	U993	A913	C829	C738	A653	G568	G490	A393
	U1521	G1435	G1293	U1219	A1146	C1066	U994	A914	G836	U740	G662	A572	G493	A397
	U1522	C1437	C1294	U1220	C1147	U1067	A994	A918	U841	G741	A663	A573	G496	C398
	G1523	G1439	G1295	G1221	U1148	G1071		A919	U842		G664	A574	A496	G399
		C1440	C1296	G1222	C1149	G1072	U997	U920	C843	C745	A665	G575	U497	C400
	G1529	G1441	C1297	G1224	U1150	G1073	G998	U921	C844	G746	G666	G576	A498	G402
	A1530	G1442	A1298	C1225	A1151	G1077	G998A	U922	U845		G667	G577	G500	C403
		G1443	U1300	C1226	C1152	A1080	U999	A923	C848	C749	G671	G579	C501	U404
		A1446	U1302	G1154	G1153	G1081	A1000	C924			U672		G502	U405
	G1447	G1447	C1303	G1155	G1156	U1085	G1001	G925	G851	G752	G673	U582	G505	G406
			G1304	C1228	A1157	U1086	G1002	G926	C857	A753	G674	G588	G506	G407
		C1452	A1305	A1229	G1157		G1003	U927	G858	C754	A675			
	G1453	G1453	C1306	C1231	U1159		A1005							
	G1454	A1375	U1307											

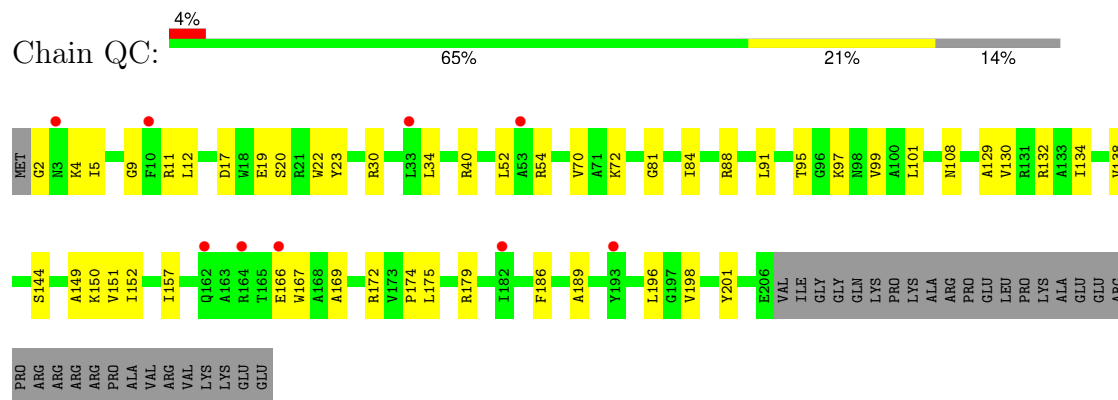
- Molecule 2: 30S ribosomal protein S2



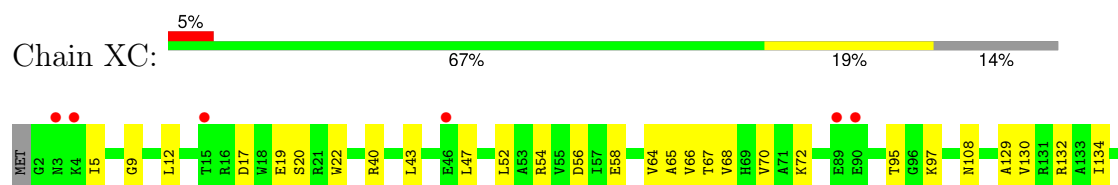
- Molecule 2: 30S ribosomal protein S2

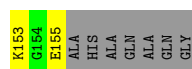


- Molecule 3: 30S ribosomal protein S3



- Molecule 3: 30S ribosomal protein S3

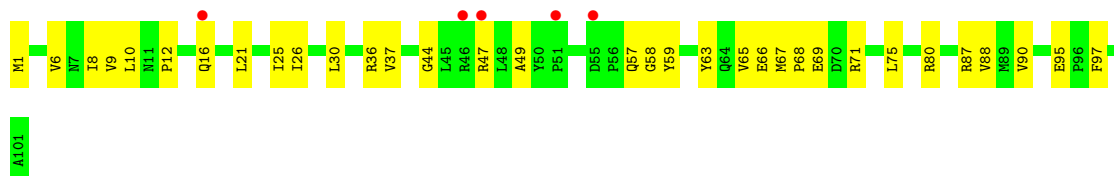




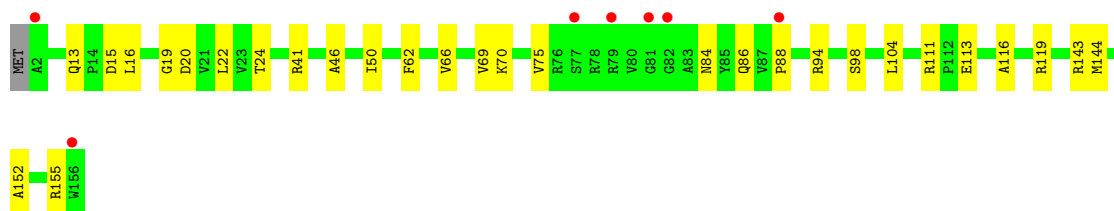
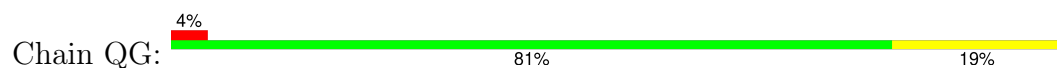
- Molecule 6: 30S ribosomal protein S6



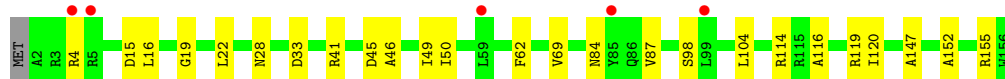
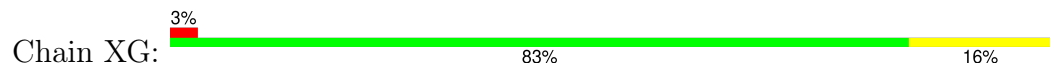
- Molecule 6: 30S ribosomal protein S6



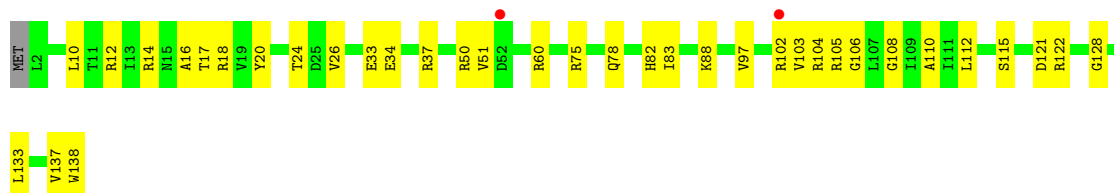
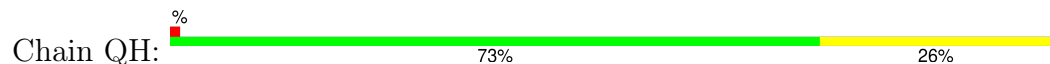
- Molecule 7: 30S ribosomal protein S7



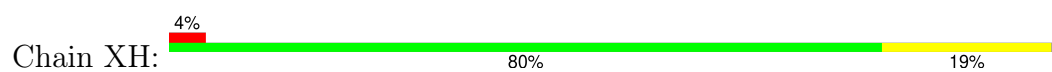
- Molecule 7: 30S ribosomal protein S7



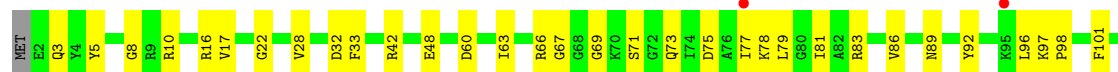
- Molecule 8: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S8



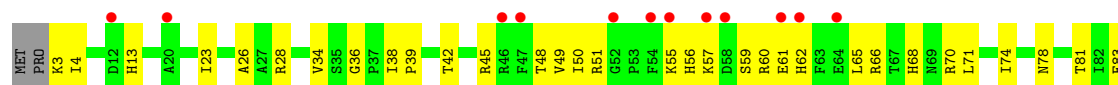
- Molecule 9: 30S ribosomal protein S9



- Molecule 9: 30S ribosomal protein S9



- Molecule 10: 30S ribosomal protein S10

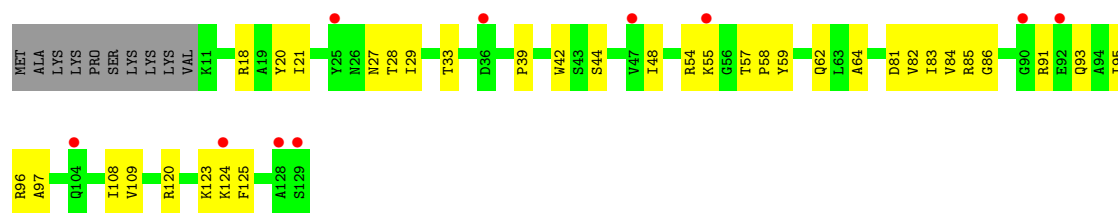


- Molecule 10: 30S ribosomal protein S10

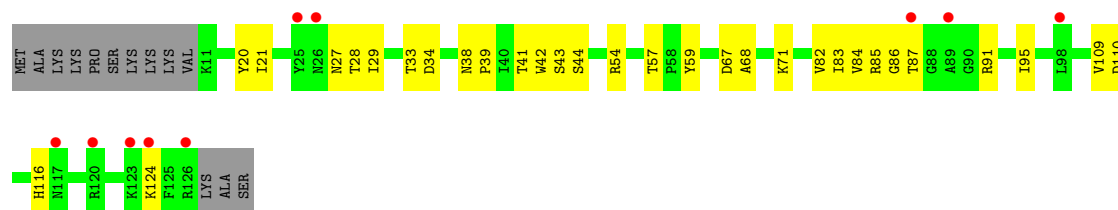


- Molecule 11: 30S ribosomal protein S11

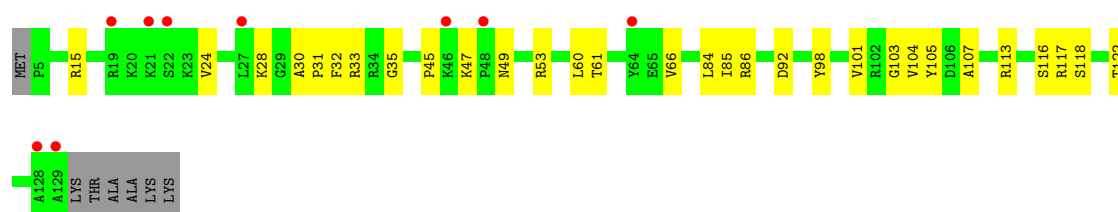
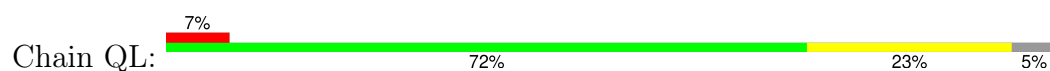




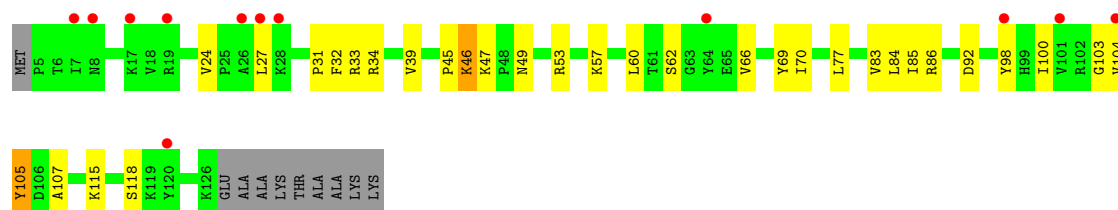
- Molecule 11: 30S ribosomal protein S11



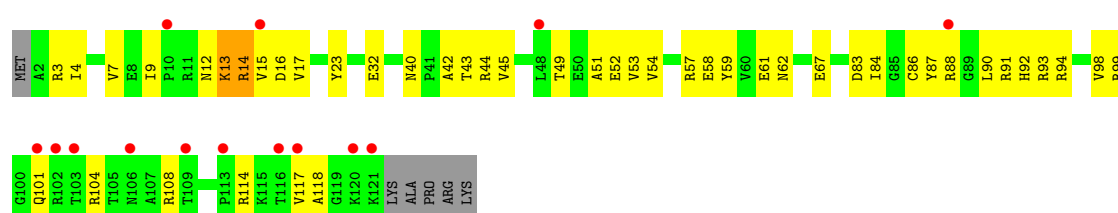
- Molecule 12: 30S ribosomal protein S12



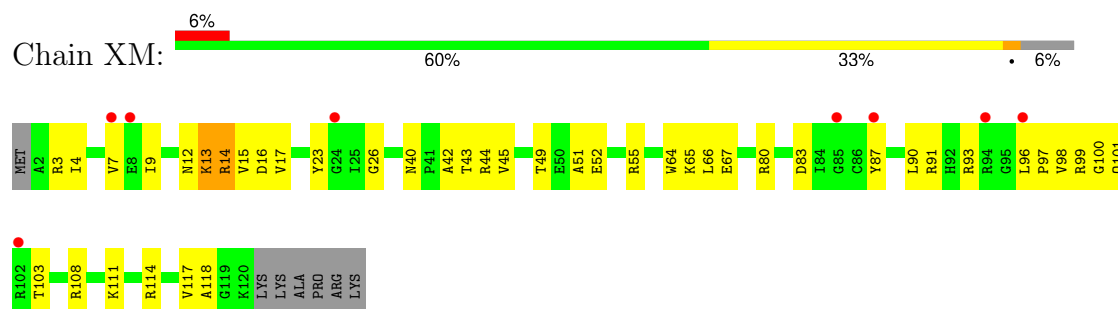
- Molecule 12: 30S ribosomal protein S12



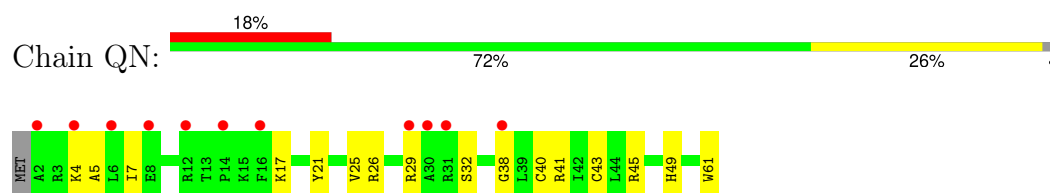
- Molecule 13: 30S ribosomal protein S13



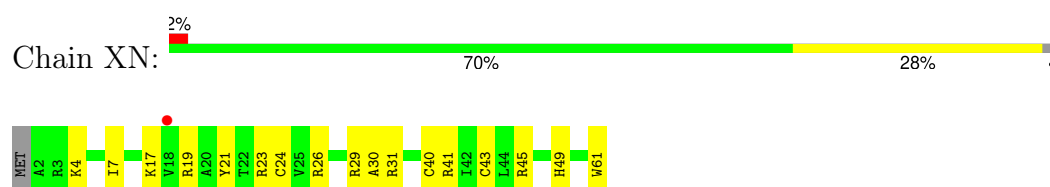
- Molecule 13: 30S ribosomal protein S13



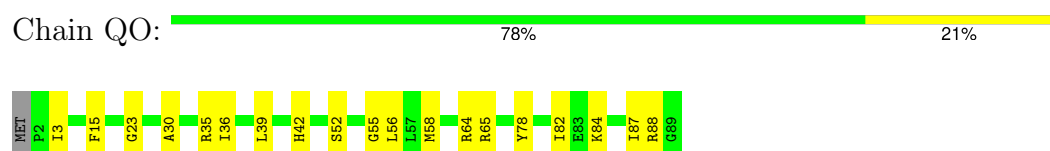
- Molecule 14: 30S ribosomal protein S14 type Z



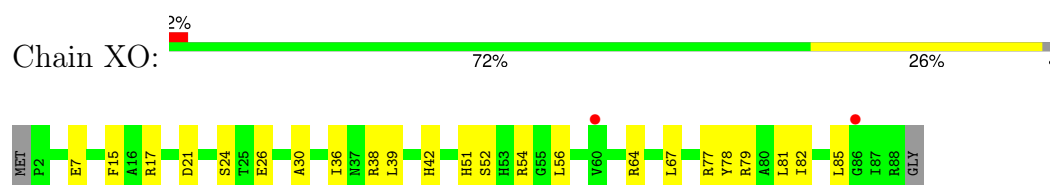
- Molecule 14: 30S ribosomal protein S14 type Z



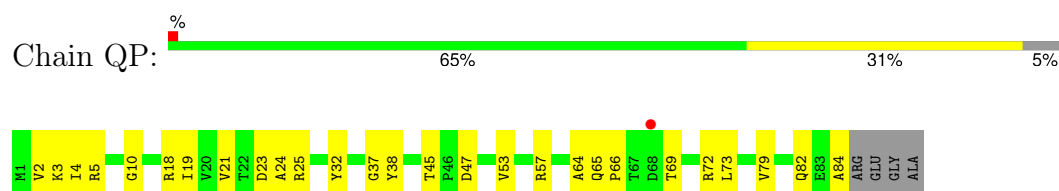
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16

Chain XP: 



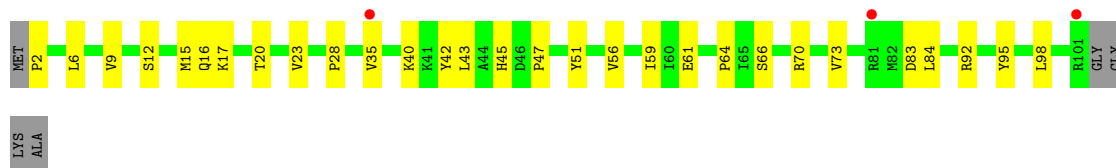
- Molecule 17: 30S ribosomal protein S17

Chain QQ: 



- Molecule 17: 30S ribosomal protein S17

Chain XQ: 



- Molecule 18: 30S ribosomal protein S18

Chain QR: 



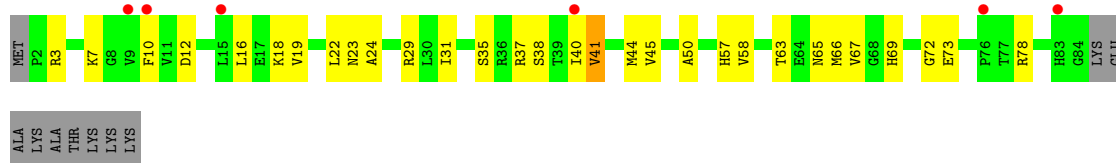
- Molecule 18: 30S ribosomal protein S18

Chain XR: 

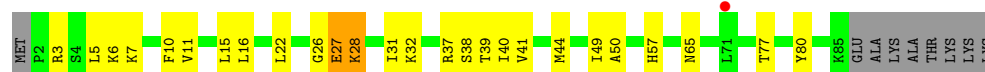


- Molecule 19: 30S ribosomal protein S19

Chain QS: 



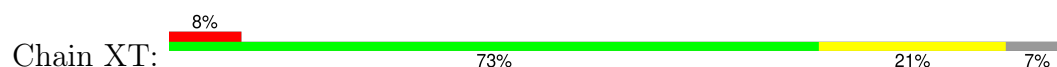
- Molecule 19: 30S ribosomal protein S19



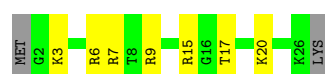
- Molecule 20: 30S ribosomal protein S20



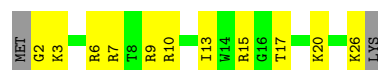
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx



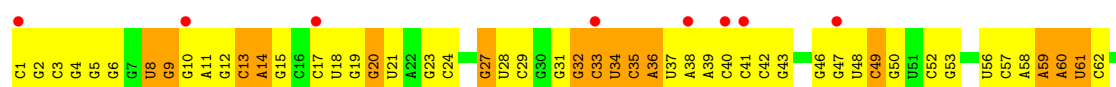
- Molecule 21: 30S ribosomal protein Thx

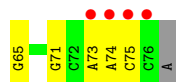


- Molecule 22: tRNA fMet

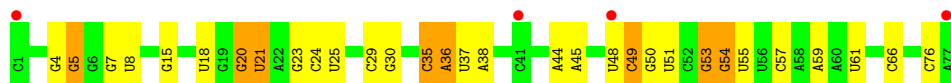


- Molecule 22: tRNA fMet

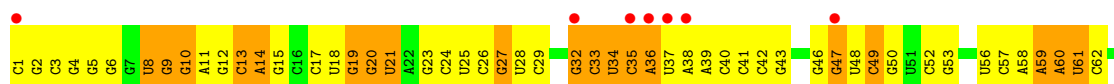




- Molecule 22: tRNA fMet



- Molecule 22: tRNA fMet



- Molecule 23: messenger RNA



- Molecule 23: messenger RNA



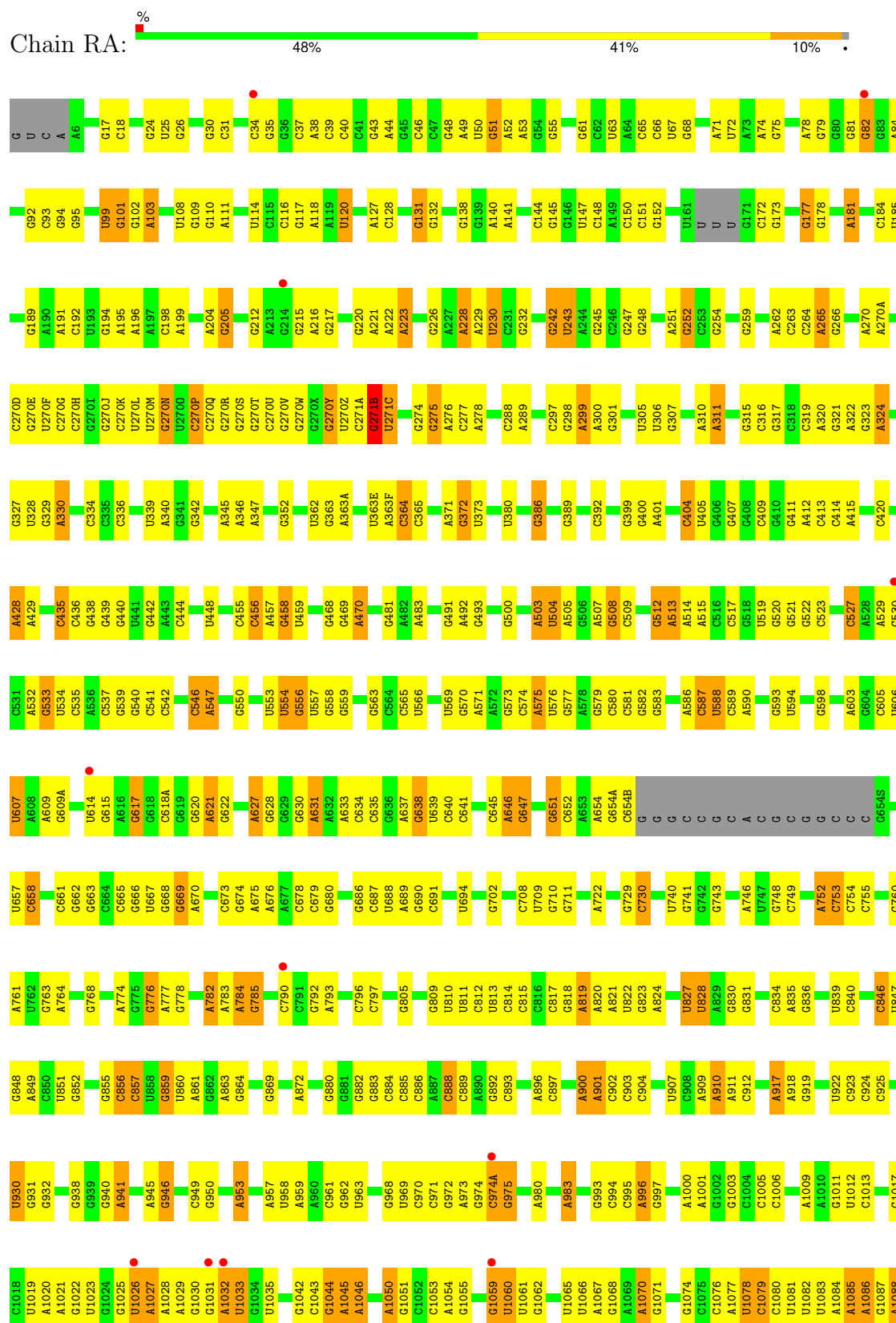
- Molecule 24: ASL Leu



- Molecule 24: ASL Leu



● Molecule 25: 23S rRNA

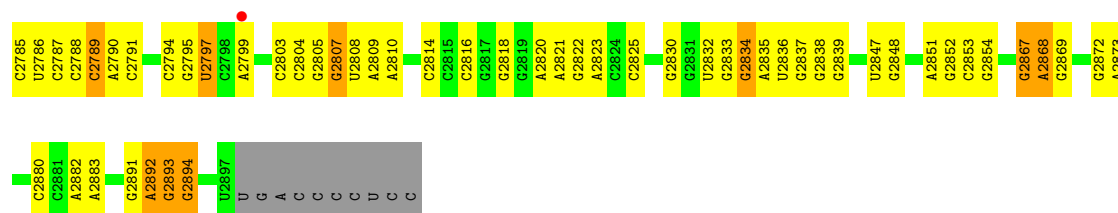


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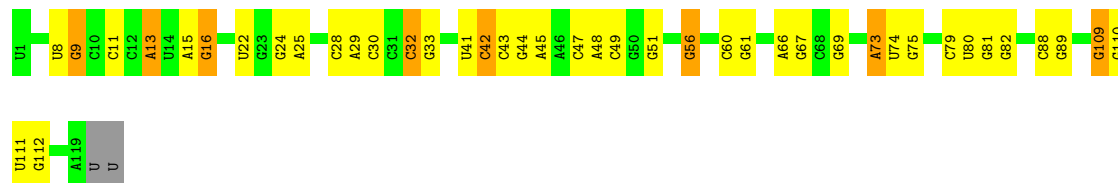
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• Molecule 26: 5S rRNA

Chain RB: 64% 28% 7% .



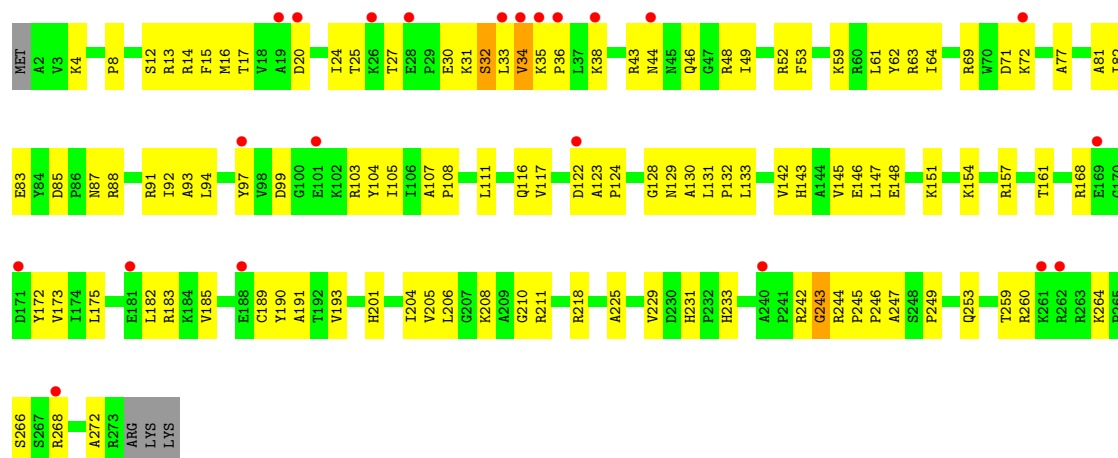
• Molecule 26: 5S rRNA

Chain YB: 52% 39% 7% .



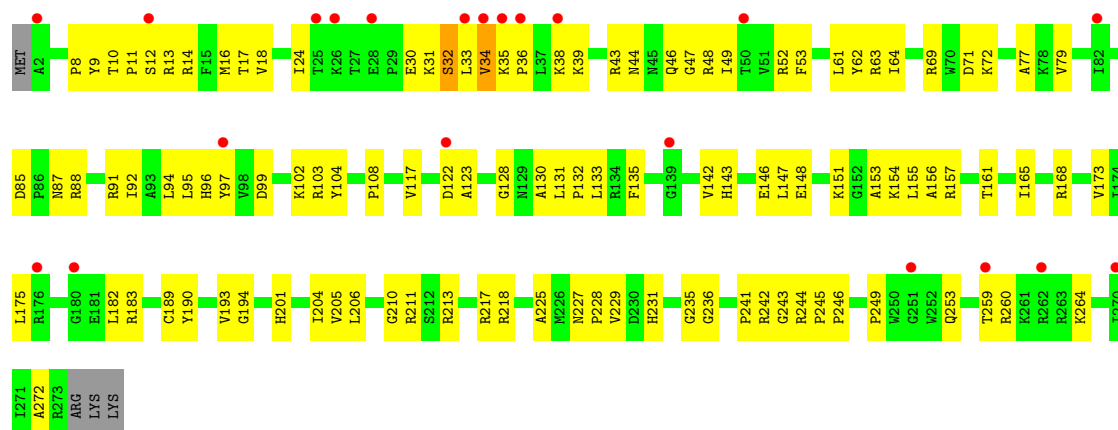
• Molecule 27: 50S ribosomal protein L2

Chain RD: 8% 58% 39% ..

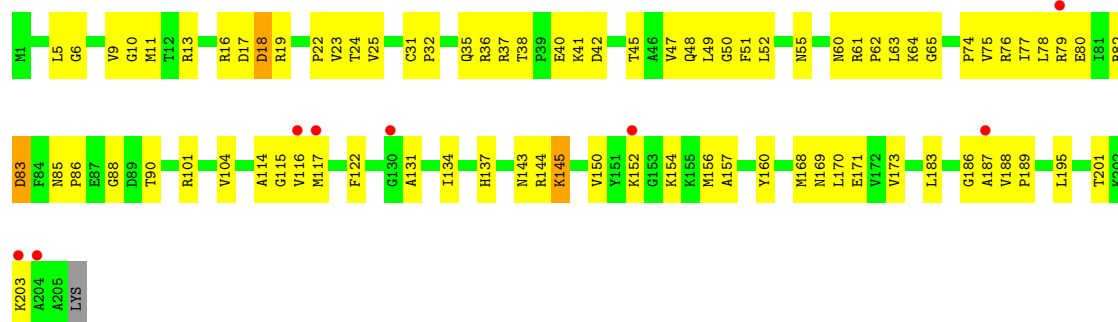


• Molecule 27: 50S ribosomal protein L2

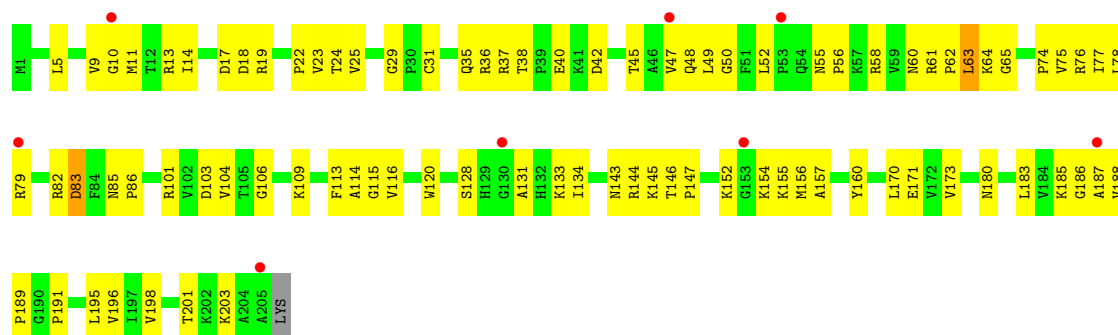
Chain YD: 8% 59% 39% ..



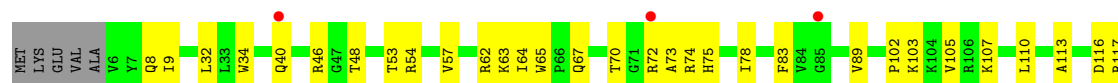
• Molecule 28: 50S ribosomal protein L3



• Molecule 28: 50S ribosomal protein L3

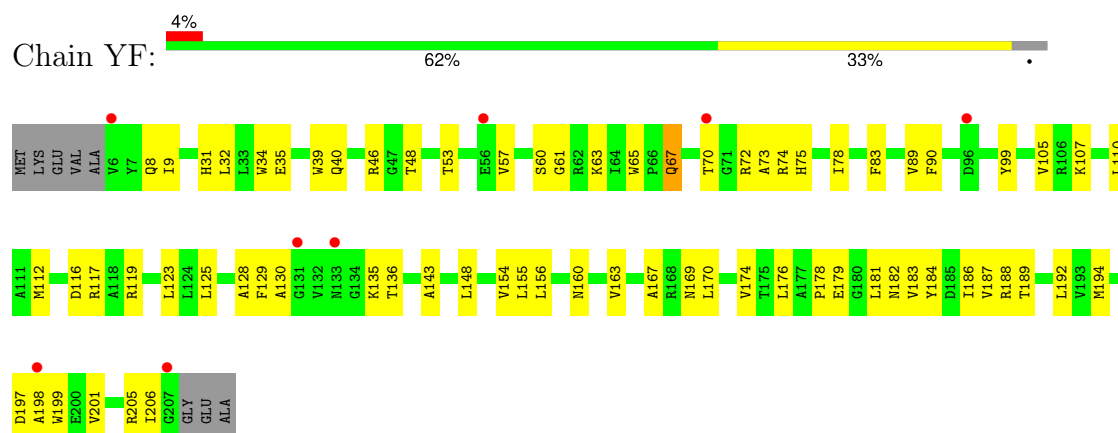


• Molecule 29: 50S ribosomal protein L4

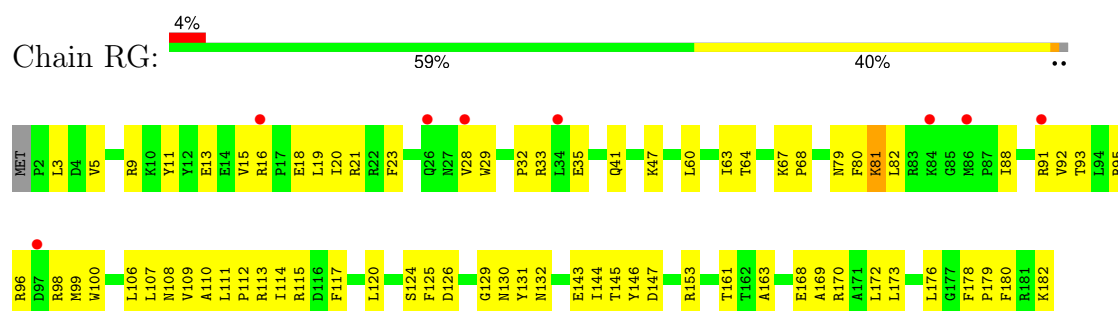




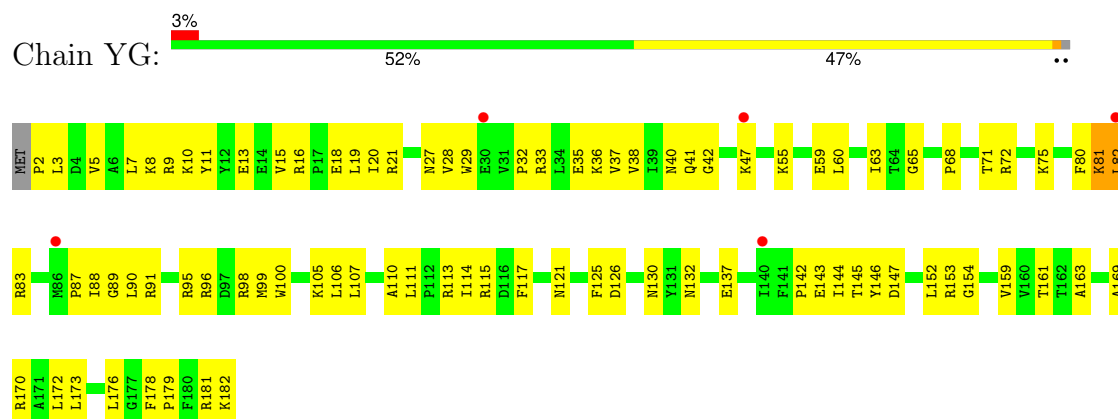
- Molecule 29: 50S ribosomal protein L4



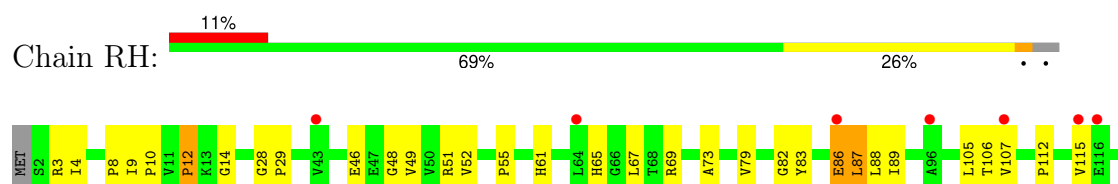
- Molecule 30: 50S ribosomal protein L5



- Molecule 30: 50S ribosomal protein L5

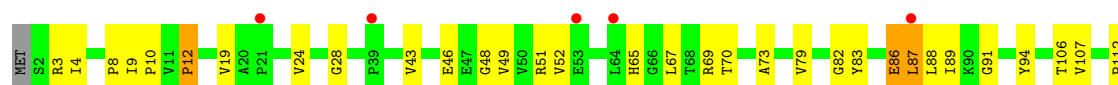


- Molecule 31: 50S ribosomal protein L6

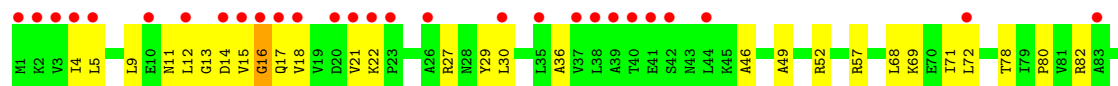




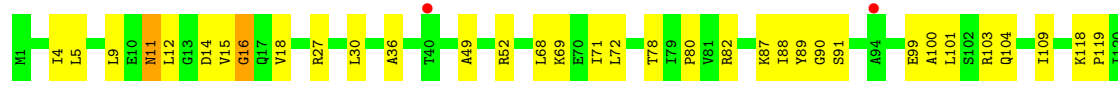
- Molecule 31: 50S ribosomal protein L6



- Molecule 32: 50S ribosomal protein L9



- Molecule 32: 50S ribosomal protein L9

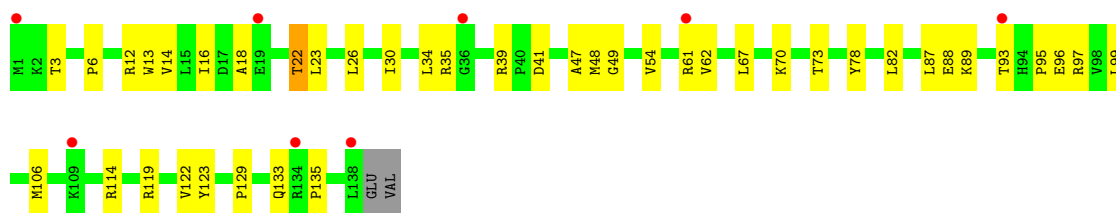


- Molecule 33: 50S ribosomal protein L13

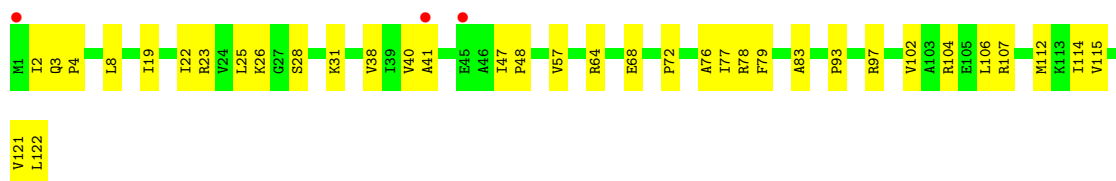
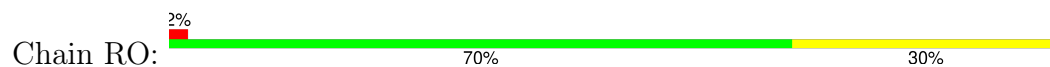


- Molecule 33: 50S ribosomal protein L13

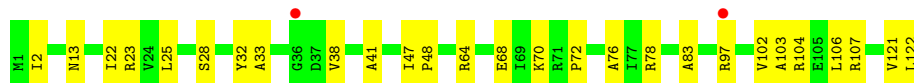
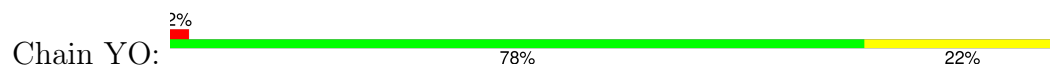




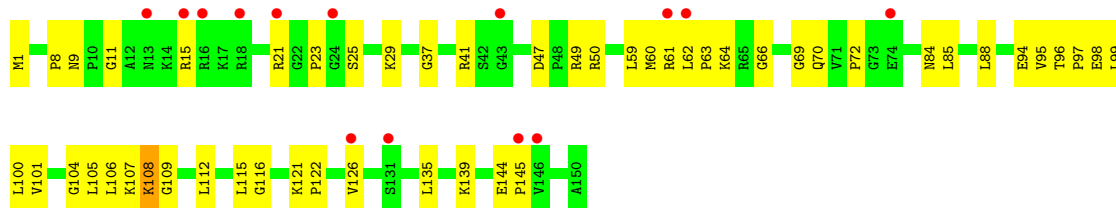
• Molecule 34: 50S ribosomal protein L14



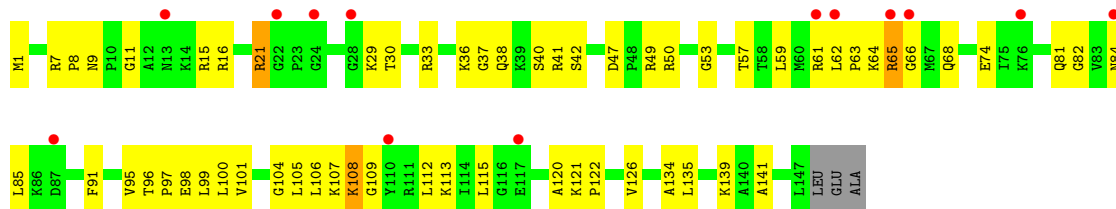
• Molecule 34: 50S ribosomal protein L14



• Molecule 35: 50S ribosomal protein L15

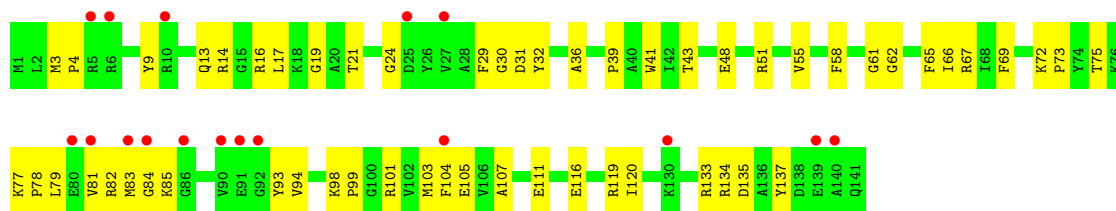


• Molecule 35: 50S ribosomal protein L15

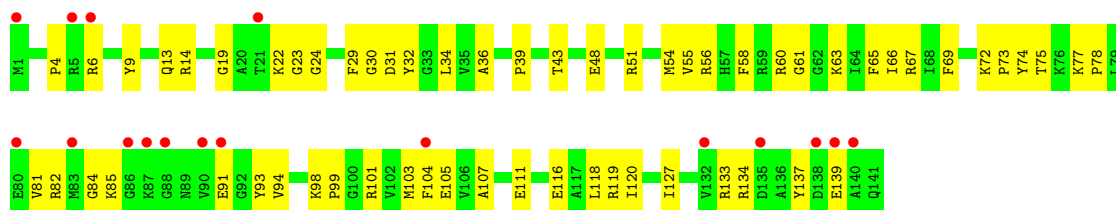


• Molecule 36: 50S ribosomal protein L16

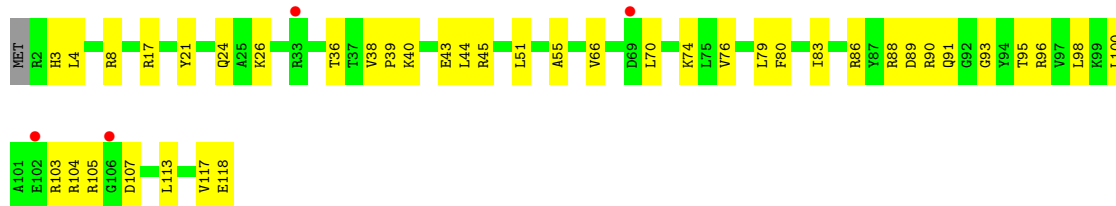




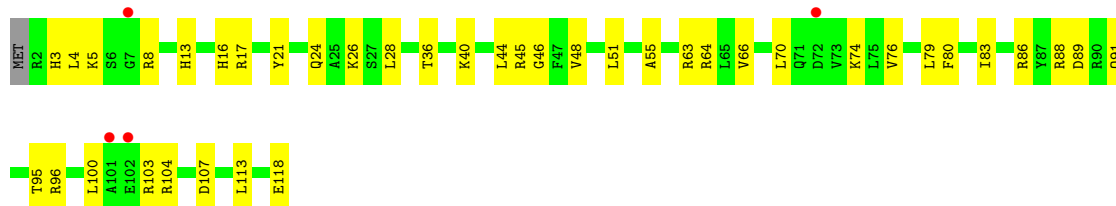
• Molecule 36: 50S ribosomal protein L16



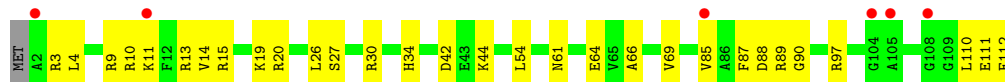
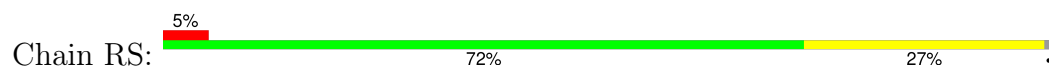
• Molecule 37: 50S ribosomal protein L17



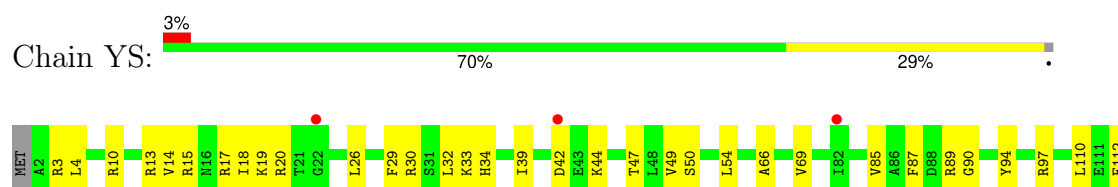
• Molecule 37: 50S ribosomal protein L17



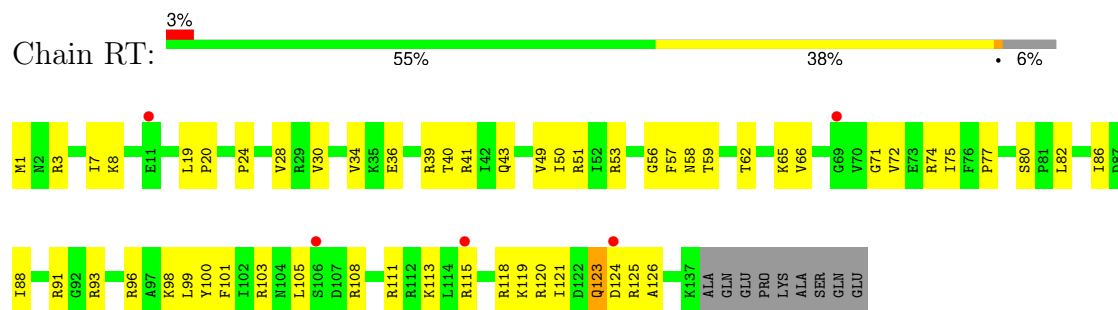
• Molecule 38: 50S ribosomal protein L18



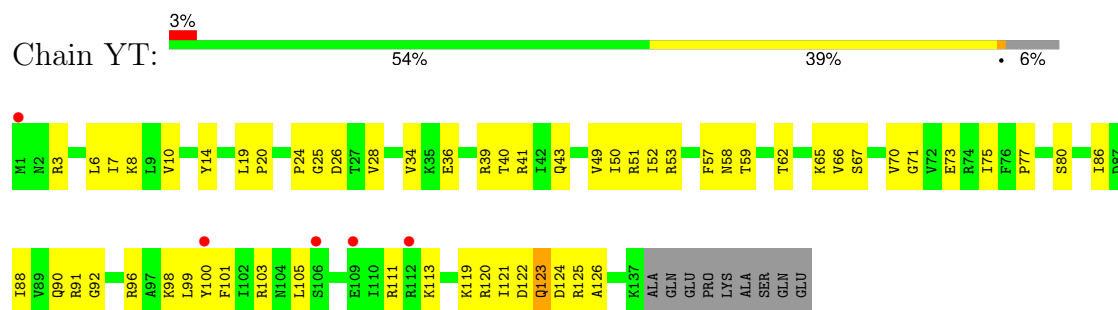
• Molecule 38: 50S ribosomal protein L18



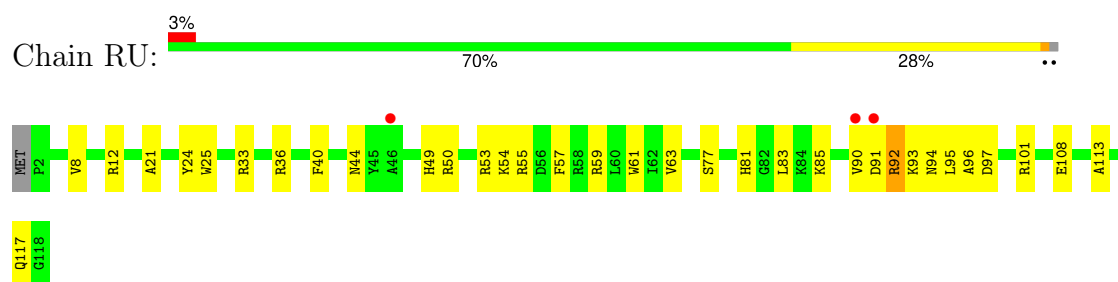
- Molecule 39: 50S ribosomal protein L19



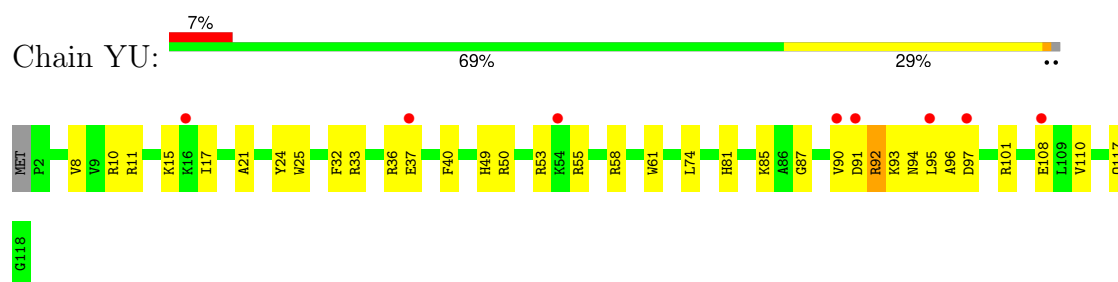
- Molecule 39: 50S ribosomal protein L19



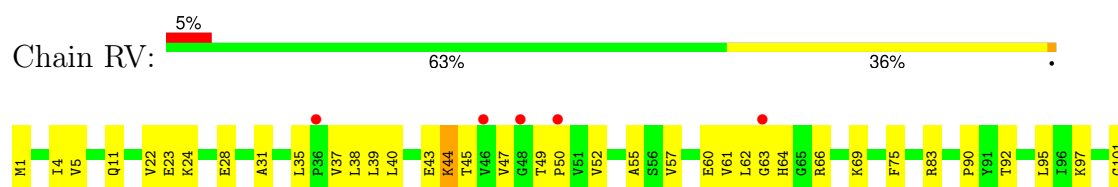
- Molecule 40: 50S ribosomal protein L20



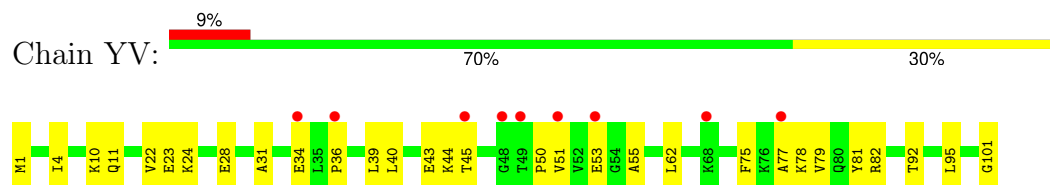
- Molecule 40: 50S ribosomal protein L20



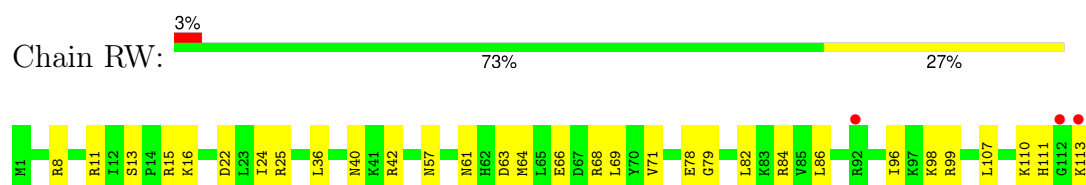
- Molecule 41: 50S ribosomal protein L21



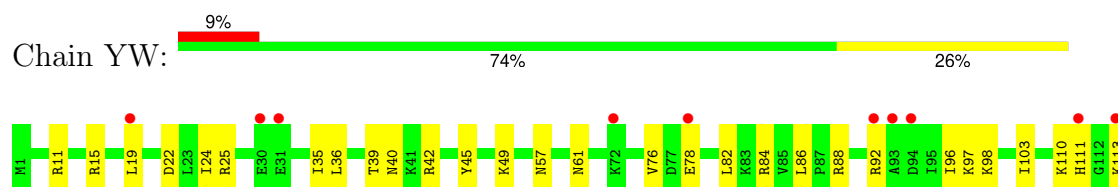
- Molecule 41: 50S ribosomal protein L21



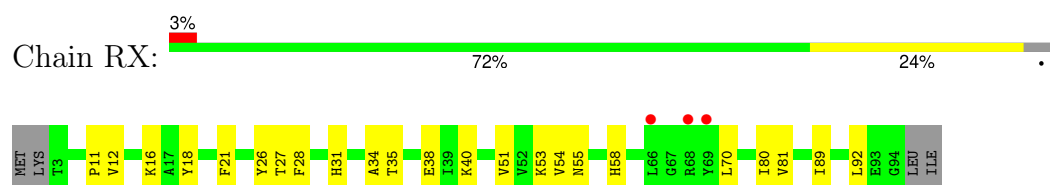
- Molecule 42: 50S ribosomal protein L22



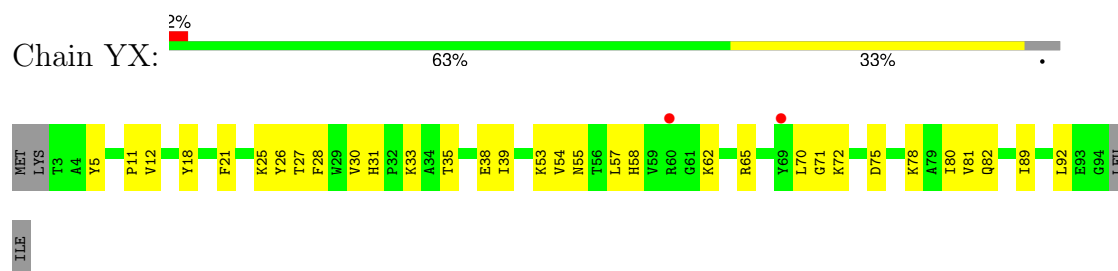
- Molecule 42: 50S ribosomal protein L22



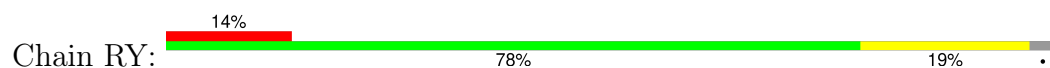
- Molecule 43: 50S ribosomal protein L23

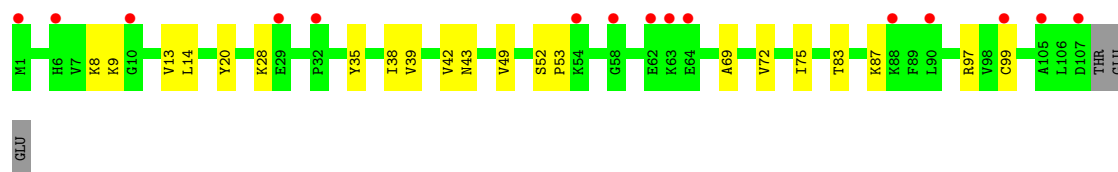


- Molecule 43: 50S ribosomal protein L23

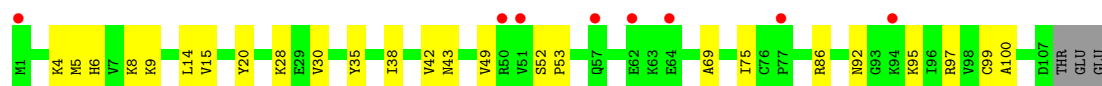
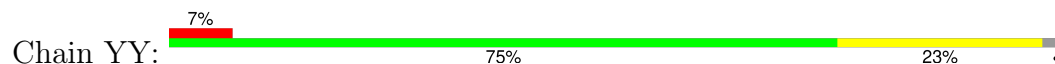


- Molecule 44: 50S ribosomal protein L24

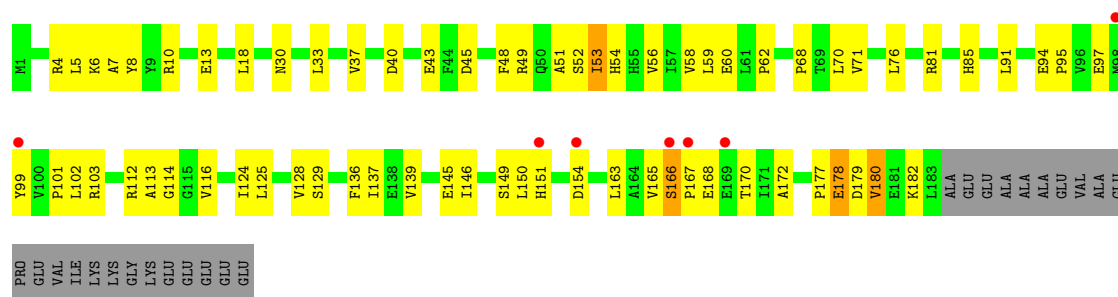




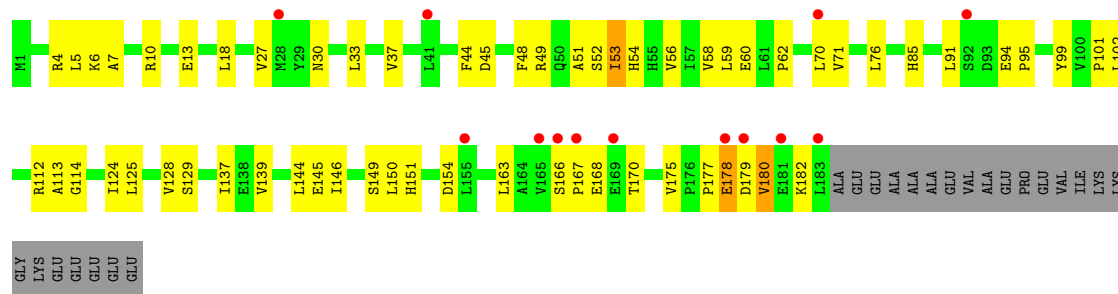
- Molecule 44: 50S ribosomal protein L24



- Molecule 45: 50S ribosomal protein L25



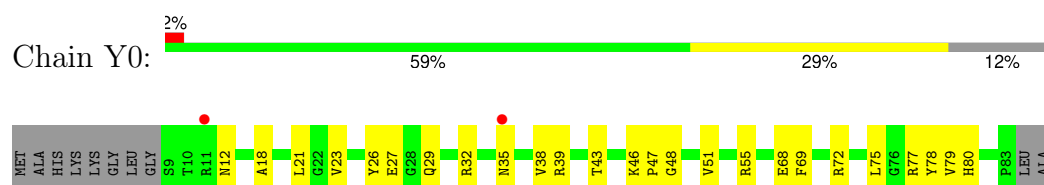
- Molecule 45: 50S ribosomal protein L25



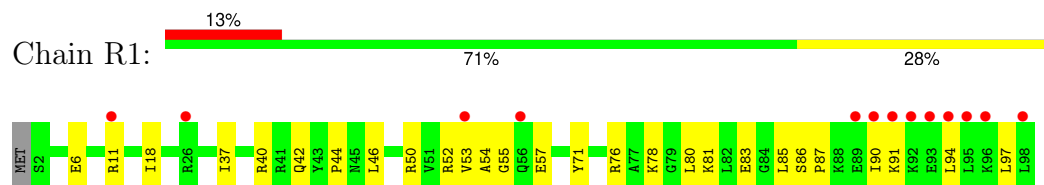
- Molecule 46: 50S ribosomal protein L27



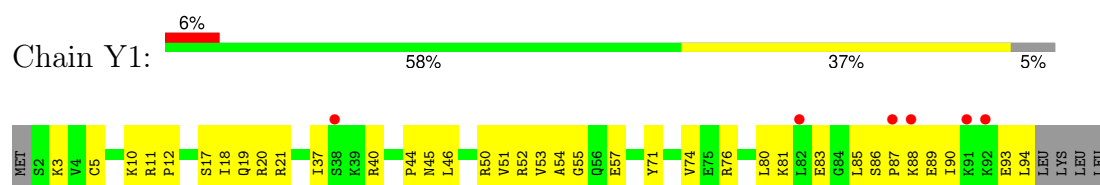
- Molecule 46: 50S ribosomal protein L27



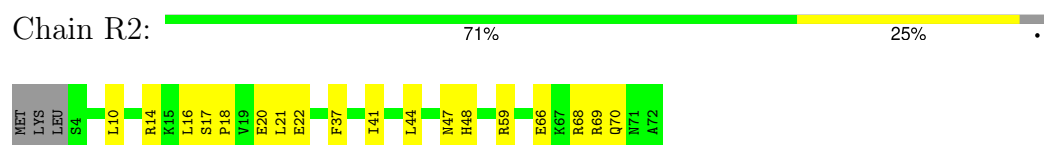
- Molecule 47: 50S ribosomal protein L28



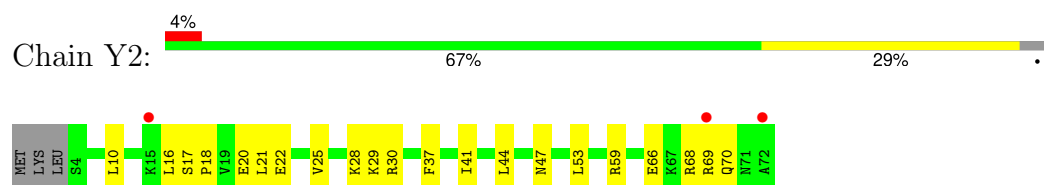
- Molecule 47: 50S ribosomal protein L28



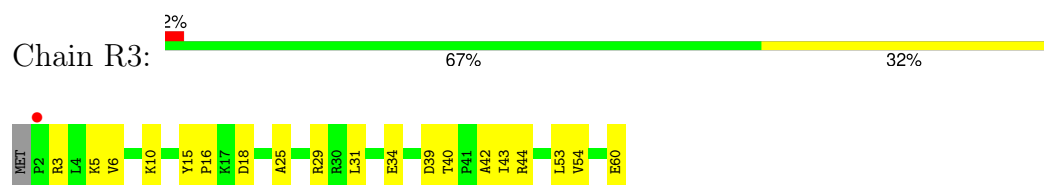
- Molecule 48: 50S ribosomal protein L29



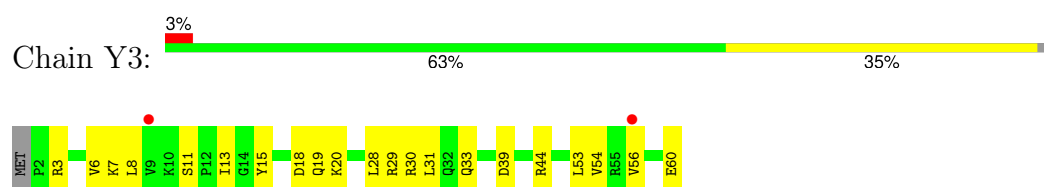
- Molecule 48: 50S ribosomal protein L29



- Molecule 49: 50S ribosomal protein L30



- Molecule 49: 50S ribosomal protein L30



- Molecule 50: 50S ribosomal protein L31

Chain R4:  68% 28% ..



- Molecule 50: 50S ribosomal protein L31

Chain Y4:  66% 28% . .



- Molecule 51: 50S ribosomal protein L32

Chain R5:  90% 8% .



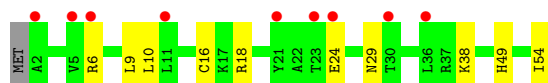
- Molecule 51: 50S ribosomal protein L32

Chain Y5:  85% 13% .



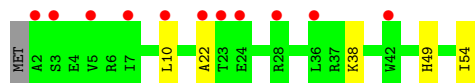
- Molecule 52: 50S ribosomal protein L33

Chain R6:  80% 19% .



- Molecule 52: 50S ribosomal protein L33

Chain Y6:  89% 9% .



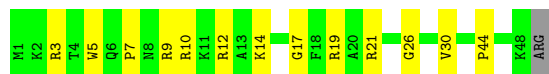
- Molecule 53: 50S ribosomal protein L34

Chain R7:  63% 33% .



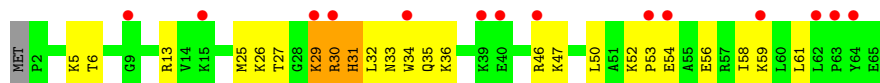
- Molecule 53: 50S ribosomal protein L34

Chain Y7:  71% 27% .



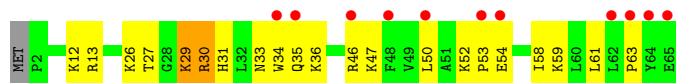
- Molecule 54: 50S ribosomal protein L35

Chain R8:  22% 62% 32% 5% .



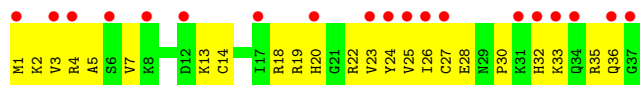
- Molecule 54: 50S ribosomal protein L35

Chain Y8:  17% 66% 29% . .

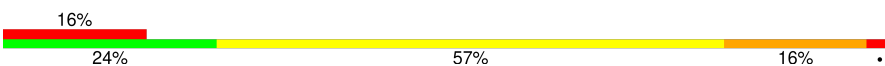


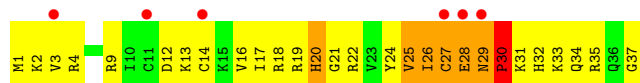
- Molecule 55: 50S ribosomal protein L36

Chain R9:  51% 38% 62%



- Molecule 55: 50S ribosomal protein L36

Chain Y9:  16% 24% 57% 16% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.70Å 446.14Å 616.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.57 – 3.68 145.57 – 3.68	Depositor EDS
% Data completeness (in resolution range)	99.3 (145.57-3.68) 99.3 (145.57-3.68)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.228 , 0.274 0.230 , 0.276	Depositor DCC
R_{free} test set	30649 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	89.7	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 103.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	295575	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% 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, SF4, ZN

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	0.12	0/36097	0.31	0/56339
1	XA	0.12	0/36100	0.31	0/56344
2	QB	0.15	0/1942	0.50	0/2619
2	XB	0.14	0/1950	0.48	0/2630
3	QC	0.14	0/1629	0.41	0/2195
3	XC	0.12	0/1629	0.39	0/2195
4	QD	0.27	1/1733 (0.1%)	0.55	2/2318 (0.1%)
4	XD	0.17	0/1733	0.49	0/2318
5	QE	0.13	0/1171	0.45	0/1576
5	XE	0.13	0/1171	0.45	0/1576
6	QF	0.15	0/856	0.44	0/1154
6	XF	0.13	0/856	0.42	0/1154
7	QG	0.13	0/1276	0.40	0/1709
7	XG	0.12	0/1276	0.40	0/1709
8	QH	0.12	0/1128	0.39	0/1517
8	XH	0.13	0/1128	0.41	0/1517
9	QI	0.14	0/1029	0.51	0/1379
9	XI	0.15	0/1017	0.49	0/1365
10	QJ	0.46	1/814 (0.1%)	0.66	5/1095 (0.5%)
10	XJ	0.14	0/790	0.47	0/1063
11	QK	0.12	0/900	0.35	0/1213
11	XK	0.12	0/879	0.37	0/1187
12	QL	0.16	0/991	0.61	0/1327
12	XL	0.17	0/972	0.69	5/1301 (0.4%)
13	QM	0.16	0/965	0.60	1/1292 (0.1%)
13	XM	0.16	0/956	0.60	1/1281 (0.1%)
14	QN	0.13	0/501	0.46	0/664
14	XN	0.14	0/501	0.48	0/664
15	QO	0.14	0/745	0.42	0/992
15	XO	0.12	0/740	0.39	0/987
16	QP	0.13	0/721	0.46	0/970
16	XP	0.13	0/721	0.45	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.11	0/847	0.39	0/1131
17	XQ	0.12	0/847	0.39	0/1131
18	QR	0.14	0/579	0.43	0/768
18	XR	0.14	0/579	0.44	0/768
19	QS	0.19	0/680	0.59	0/915
19	XS	0.17	0/689	0.57	1/926 (0.1%)
20	QT	0.18	0/765	0.56	0/1007
20	XT	0.18	0/765	0.53	0/1007
21	QU	0.11	0/221	0.43	0/288
21	XU	0.12	0/221	0.43	0/288
22	QV	0.12	0/1836	0.29	0/2859
22	QW	0.14	0/1807	0.37	0/2816
22	XV	0.12	0/1836	0.30	0/2859
22	XW	0.14	0/1807	0.35	0/2816
23	QX	0.09	0/188	0.20	0/290
23	XX	0.10	0/235	0.25	0/364
24	QY	0.09	0/400	0.26	0/621
24	XY	0.10	0/400	0.26	0/621
25	RA	0.13	0/69521	0.33	1/108529 (0.0%)
25	YA	0.15	1/69543 (0.0%)	0.34	11/108563 (0.0%)
26	RB	0.11	0/2878	0.27	0/4490
26	YB	0.12	0/2878	0.28	0/4490
27	RD	0.17	0/2165	0.56	2/2919 (0.1%)
27	YD	0.18	0/2165	0.56	2/2919 (0.1%)
28	RE	0.17	0/1601	0.64	0/2160
28	YE	0.18	0/1601	0.63	0/2160
29	RF	0.16	0/1620	0.49	0/2194
29	YF	0.17	0/1620	0.50	0/2194
30	RG	0.17	0/1499	0.57	0/2016
30	YG	0.17	0/1499	0.57	0/2016
31	RH	0.16	0/1362	0.59	1/1841 (0.1%)
31	YH	0.21	0/1362	0.71	2/1841 (0.1%)
32	RI	0.16	0/1151	0.58	0/1558
32	YI	0.17	0/1151	0.59	0/1558
33	RN	0.16	0/1131	0.61	1/1525 (0.1%)
33	YN	0.16	0/1131	0.59	1/1525 (0.1%)
34	RO	0.12	0/943	0.38	0/1269
34	YO	0.13	0/943	0.41	0/1269
35	RP	0.18	0/1162	0.66	0/1544
35	YP	0.20	0/1139	0.72	2/1514 (0.1%)
36	RQ	0.16	0/1143	0.60	0/1527
36	YQ	0.17	0/1143	0.62	0/1527
37	RR	0.18	0/974	0.55	0/1302

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	YR	0.15	0/974	0.52	0/1302
38	RS	0.15	0/892	0.51	0/1187
38	YS	0.16	0/892	0.51	0/1187
39	RT	0.16	0/1155	0.59	0/1542
39	YT	0.16	0/1155	0.59	0/1542
40	RU	0.17	0/982	0.59	0/1306
40	YU	0.17	0/982	0.59	0/1306
41	RV	0.14	0/790	0.51	0/1057
41	YV	0.13	0/790	0.52	0/1057
42	RW	0.15	0/911	0.48	0/1220
42	YW	0.14	0/911	0.48	0/1220
43	RX	0.14	0/739	0.43	0/993
43	YX	0.13	0/739	0.40	0/993
44	RY	0.12	0/831	0.41	0/1108
44	YY	0.12	0/831	0.44	0/1108
45	RZ	0.18	0/1493	0.69	4/2026 (0.2%)
45	YZ	0.19	0/1493	0.71	4/2026 (0.2%)
46	R0	0.13	0/652	0.41	0/867
46	Y0	0.14	0/607	0.43	0/809
47	R1	0.16	0/770	0.52	0/1022
47	Y1	0.23	0/736	0.47	0/978
48	R2	0.15	0/583	0.50	0/771
48	Y2	0.16	0/583	0.56	0/771
49	R3	0.14	0/474	0.44	0/635
49	Y3	0.14	0/474	0.44	0/635
50	R4	0.15	0/578	0.58	0/776
50	Y4	0.17	0/578	0.58	0/776
51	R5	0.18	0/473	0.46	0/639
51	Y5	0.13	0/473	0.42	0/639
52	R6	0.10	0/460	0.42	0/613
52	Y6	0.11	0/460	0.41	0/613
53	R7	0.15	0/417	0.51	0/550
53	Y7	0.16	0/426	0.54	0/561
54	R8	0.26	0/525	0.77	1/691 (0.1%)
54	Y8	0.26	0/525	0.80	0/691
55	R9	0.20	0/310	0.73	0/407
55	Y9	0.59	0/310	1.42	5/407 (1.2%)
All	All	0.14	3/319918 (0.0%)	0.39	52/478576 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
28	YE	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	QJ	84	GLN	CD-NE2	11.35	1.57	1.33
4	QD	119	GLN	CB-CG	8.74	1.78	1.52
25	YA	2743	C	C5'-C4'	5.85	1.60	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	QD	119	GLN	CB-CG-CD	-10.20	95.27	112.60
25	YA	2754	U	OP1-P-O3'	-9.57	79.29	108.00
25	YA	2743	C	O4'-C1'-N1	9.31	122.46	108.50
25	YA	2754	U	OP2-P-O3'	-9.17	80.50	108.00
25	YA	2741	A	P-O3'-C3'	7.75	131.83	120.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	YE	146	THR	Peptide,Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32246	0	16278	646	0
1	XA	32248	0	16279	621	0
2	QB	1907	0	1958	52	0
2	XB	1915	0	1969	48	0
3	QC	1605	0	1668	39	0
3	XC	1605	0	1668	32	0
4	QD	1703	0	1766	54	0
4	XD	1703	0	1767	47	0
5	QE	1155	0	1213	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	XE	1155	0	1213	19	0
6	QF	843	0	857	19	0
6	XF	843	0	857	23	0
7	QG	1257	0	1296	21	0
7	XG	1257	0	1296	18	0
8	QH	1108	0	1165	24	0
8	XH	1108	0	1165	20	0
9	QI	1010	0	1037	37	0
9	XI	998	0	1024	42	0
10	QJ	801	0	849	38	0
10	XJ	777	0	816	24	0
11	QK	885	0	904	35	0
11	XK	864	0	881	25	0
12	QL	975	0	1062	26	0
12	XL	956	0	1046	29	0
13	QM	955	0	1021	46	0
13	XM	946	0	1007	37	0
14	QN	492	0	529	15	0
14	XN	492	0	529	13	0
15	QO	734	0	771	14	0
15	XO	729	0	768	17	0
16	QP	705	0	725	20	0
16	XP	705	0	725	23	0
17	QQ	834	0	904	15	0
17	XQ	834	0	904	22	0
18	QR	574	0	644	20	0
18	XR	574	0	644	23	0
19	QS	665	0	686	27	0
19	XS	674	0	699	23	0
20	QT	763	0	861	18	0
20	XT	763	0	861	19	0
21	QU	217	0	234	6	0
21	XU	217	0	234	10	0
22	QV	1644	0	836	21	0
22	QW	1618	0	826	45	0
22	XV	1644	0	836	19	0
22	XW	1618	0	826	44	0
23	QX	169	0	86	0	0
23	XX	210	0	109	3	0
24	QY	358	0	183	3	0
24	XY	358	0	184	5	0
25	RA	62071	0	31291	1007	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	YA	62091	0	31297	1170	0
26	RB	2573	0	1306	30	0
26	YB	2573	0	1306	44	0
27	RD	2115	0	2195	103	0
27	YD	2115	0	2195	106	0
28	RE	1568	0	1634	70	0
28	YE	1568	0	1634	66	0
29	RF	1585	0	1632	55	0
29	YF	1585	0	1632	57	0
30	RG	1474	0	1535	60	0
30	YG	1474	0	1535	73	0
31	RH	1336	0	1418	38	0
31	YH	1336	0	1418	74	0
32	RI	1136	0	1223	29	0
32	YI	1136	0	1223	28	0
33	RN	1104	0	1180	31	0
33	YN	1104	0	1180	28	0
34	RO	933	0	996	33	0
34	YO	933	0	996	26	0
35	RP	1145	0	1228	52	0
35	YP	1122	0	1206	53	0
36	RQ	1122	0	1179	51	0
36	YQ	1122	0	1179	52	0
37	RR	960	0	1021	31	0
37	YR	960	0	1021	28	0
38	RS	882	0	943	23	0
38	YS	882	0	943	28	0
39	RT	1141	0	1202	48	0
39	YT	1141	0	1202	50	0
40	RU	964	0	1022	48	0
40	YU	964	0	1022	47	0
41	RV	779	0	852	32	0
41	YV	779	0	852	25	0
42	RW	900	0	964	22	1
42	YW	900	0	964	21	0
43	RX	725	0	778	16	0
43	YX	725	0	778	25	0
44	RY	818	0	910	13	0
44	YY	818	0	912	15	1
45	RZ	1461	0	1493	48	0
45	YZ	1461	0	1493	47	0
46	R0	643	0	667	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	Y0	599	0	617	23	0
47	R1	763	0	848	19	0
47	Y1	729	0	802	24	0
48	R2	581	0	629	12	0
48	Y2	581	0	629	14	0
49	R3	469	0	518	14	0
49	Y3	469	0	518	16	0
50	R4	565	0	557	20	0
50	Y4	565	0	558	25	0
51	R5	459	0	477	5	0
51	Y5	459	0	480	9	0
52	R6	453	0	474	8	0
52	Y6	453	0	473	3	0
53	R7	409	0	454	12	0
53	Y7	418	0	467	9	0
54	R8	517	0	582	25	0
54	Y8	517	0	582	24	0
55	R9	307	0	338	23	0
55	Y9	307	0	338	142	0
56	QA	68	0	0	0	0
56	QC	1	0	0	0	0
56	QE	1	0	0	0	0
56	QF	1	0	0	0	0
56	QH	1	0	0	0	0
56	QQ	1	0	0	0	0
56	QV	6	0	0	0	0
56	QY	1	0	0	0	0
56	R0	4	0	0	0	0
56	R1	2	0	0	0	0
56	R4	1	0	0	0	0
56	R8	1	0	0	0	0
56	R9	1	0	0	0	0
56	RA	508	0	0	0	0
56	RB	7	0	0	0	0
56	RE	2	0	0	0	0
56	RF	1	0	0	0	0
56	RN	1	0	0	0	0
56	RO	2	0	0	0	0
56	RP	2	0	0	0	0
56	RQ	2	0	0	0	0
56	RR	1	0	0	0	0
56	RT	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	RU	1	0	0	0	0
56	RY	1	0	0	0	0
56	XA	82	0	0	0	0
56	XE	1	0	0	0	0
56	XL	1	0	0	0	0
56	XM	1	0	0	0	0
56	XQ	1	0	0	0	0
56	XS	1	0	0	0	0
56	XV	6	0	0	0	0
56	Y0	1	0	0	0	0
56	Y7	1	0	0	0	0
56	Y8	1	0	0	0	0
56	Y9	1	0	0	0	0
56	YA	546	0	0	0	0
56	YB	12	0	0	0	0
56	YD	2	0	0	0	0
56	YE	2	0	0	0	0
56	YO	1	0	0	0	0
56	YP	3	0	0	0	0
56	YQ	3	0	0	0	0
56	YX	2	0	0	0	0
56	YY	1	0	0	0	0
57	QD	8	0	0	1	0
57	XD	8	0	0	0	0
58	QN	1	0	0	0	0
58	R4	1	0	0	0	0
58	R5	1	0	0	0	0
58	R6	1	0	0	0	0
58	R9	1	0	0	0	0
58	RY	1	0	0	0	0
58	XN	1	0	0	0	0
58	Y4	1	0	0	0	0
58	Y5	1	0	0	0	0
58	Y6	1	0	0	0	0
58	Y9	1	0	0	0	0
58	YY	1	0	0	0	0
All	All	295575	0	199664	5812	1

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 12.

The worst 5 of 5812 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)
4:QD:119:GLN:CG	4:QD:119:GLN:CB	1.78	1.55
25:YA:2755:C:H42	55:Y9:1:MET:HG2	1.08	1.16
25:RA:2747:G:N2	25:RA:2757:A:H62	1.43	1.15
25:YA:2742:C:H1'	55:Y9:26:ILE:HA	1.33	1.10
25:RA:2747:G:H21	25:RA:2757:A:N6	1.52	1.05

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:RW:63:ASP:OD1	44:YY:92:ASN:ND2[3_555]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	202 (87%)	29 (12%)	2 (1%)	14	45
2	XB	234/256 (91%)	202 (86%)	31 (13%)	1 (0%)	30	60
3	QC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
3	XC	203/239 (85%)	190 (94%)	13 (6%)	0	100	100
4	QD	206/209 (99%)	189 (92%)	17 (8%)	0	100	100
4	XD	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
5	QE	149/162 (92%)	141 (95%)	7 (5%)	1 (1%)	18	50
5	XE	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	18	50
6	QF	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
6	XF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
7	QG	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
7	XG	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
8	QH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	XH	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
9	QI	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
9	XI	124/128 (97%)	112 (90%)	12 (10%)	0	100	100
10	QJ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
10	XJ	94/105 (90%)	84 (89%)	10 (11%)	0	100	100
11	QK	117/129 (91%)	109 (93%)	8 (7%)	0	100	100
11	XK	114/129 (88%)	108 (95%)	6 (5%)	0	100	100
12	QL	123/132 (93%)	105 (85%)	18 (15%)	0	100	100
12	XL	120/132 (91%)	97 (81%)	22 (18%)	1 (1%)	16	47
13	QM	118/126 (94%)	96 (81%)	21 (18%)	1 (1%)	16	47
13	XM	117/126 (93%)	94 (80%)	22 (19%)	1 (1%)	14	45
14	QN	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7	33
14	XN	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7	33
15	QO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
15	XO	85/89 (96%)	84 (99%)	1 (1%)	0	100	100
16	QP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
17	XQ	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
18	QR	68/88 (77%)	64 (94%)	4 (6%)	0	100	100
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	81/93 (87%)	70 (86%)	11 (14%)	0	100	100
19	XS	82/93 (88%)	70 (85%)	11 (13%)	1 (1%)	10	39
20	QT	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
20	XT	97/106 (92%)	87 (90%)	10 (10%)	0	100	100
21	QU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
21	XU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
27	RD	270/276 (98%)	235 (87%)	33 (12%)	2 (1%)	18	50
27	YD	270/276 (98%)	239 (88%)	29 (11%)	2 (1%)	18	50
28	RE	203/206 (98%)	163 (80%)	37 (18%)	3 (2%)	8	35
28	YE	203/206 (98%)	158 (78%)	42 (21%)	3 (2%)	8	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	RF	200/210 (95%)	183 (92%)	17 (8%)	0	100	100
29	YF	200/210 (95%)	185 (92%)	13 (6%)	2 (1%)	12	43
30	RG	179/182 (98%)	149 (83%)	29 (16%)	1 (1%)	21	52
30	YG	179/182 (98%)	148 (83%)	29 (16%)	2 (1%)	11	41
31	RH	172/180 (96%)	141 (82%)	28 (16%)	3 (2%)	7	33
31	YH	172/180 (96%)	137 (80%)	32 (19%)	3 (2%)	7	33
32	RI	144/148 (97%)	119 (83%)	22 (15%)	3 (2%)	5	30
32	YI	144/148 (97%)	117 (81%)	24 (17%)	3 (2%)	5	30
33	RN	136/140 (97%)	117 (86%)	17 (12%)	2 (2%)	8	35
33	YN	136/140 (97%)	117 (86%)	18 (13%)	1 (1%)	18	50
34	RO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
34	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
35	RP	148/150 (99%)	114 (77%)	33 (22%)	1 (1%)	18	50
35	YP	145/150 (97%)	112 (77%)	32 (22%)	1 (1%)	18	50
36	RQ	139/141 (99%)	114 (82%)	24 (17%)	1 (1%)	18	50
36	YQ	139/141 (99%)	116 (84%)	21 (15%)	2 (1%)	9	36
37	RR	115/118 (98%)	102 (89%)	13 (11%)	0	100	100
37	YR	115/118 (98%)	103 (90%)	11 (10%)	1 (1%)	14	45
38	RS	109/112 (97%)	86 (79%)	23 (21%)	0	100	100
38	YS	109/112 (97%)	87 (80%)	22 (20%)	0	100	100
39	RT	135/146 (92%)	115 (85%)	18 (13%)	2 (2%)	8	35
39	YT	135/146 (92%)	115 (85%)	18 (13%)	2 (2%)	8	35
40	RU	115/118 (98%)	109 (95%)	5 (4%)	1 (1%)	14	45
40	YU	115/118 (98%)	109 (95%)	5 (4%)	1 (1%)	14	45
41	RV	99/101 (98%)	86 (87%)	12 (12%)	1 (1%)	12	43
41	YV	99/101 (98%)	86 (87%)	13 (13%)	0	100	100
42	RW	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
42	YW	111/113 (98%)	98 (88%)	13 (12%)	0	100	100
43	RX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
43	YX	90/96 (94%)	88 (98%)	2 (2%)	0	100	100
44	RY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	YY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
45	RZ	181/206 (88%)	144 (80%)	33 (18%)	4 (2%)	5	29
45	YZ	181/206 (88%)	142 (78%)	36 (20%)	3 (2%)	7	33
46	R0	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
46	Y0	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
47	R1	95/98 (97%)	85 (90%)	9 (10%)	1 (1%)	11	41
47	Y1	91/98 (93%)	77 (85%)	13 (14%)	1 (1%)	11	41
48	R2	67/72 (93%)	62 (92%)	4 (6%)	1 (2%)	8	35
48	Y2	67/72 (93%)	61 (91%)	5 (8%)	1 (2%)	8	35
49	R3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
49	Y3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
50	R4	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	8	35
50	Y4	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	8	35
51	R5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
51	Y5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
52	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
52	Y6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
53	R7	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
53	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
54	R8	62/65 (95%)	46 (74%)	14 (23%)	2 (3%)	3	24
54	Y8	62/65 (95%)	47 (76%)	13 (21%)	2 (3%)	3	24
55	R9	35/37 (95%)	25 (71%)	10 (29%)	0	100	100
55	Y9	35/37 (95%)	18 (51%)	15 (43%)	2 (6%)	1	15
All	All	11452/12128 (94%)	10130 (88%)	1249 (11%)	73 (1%)	21	52

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	RE	18	ASP
31	RH	87	LEU
32	RI	15	VAL
35	RP	108	LYS
39	RT	124	ASP

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%)	203 (100%)	0	100	100
2	XB	204/220 (93%)	204 (100%)	0	100	100
3	QC	159/188 (85%)	159 (100%)	0	100	100
3	XC	159/188 (85%)	159 (100%)	0	100	100
4	QD	180/181 (99%)	180 (100%)	0	100	100
4	XD	180/181 (99%)	180 (100%)	0	100	100
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	116 (100%)	0	100	100
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	118/119 (99%)	118 (100%)	0	100	100
8	XH	118/119 (99%)	118 (100%)	0	100	100
9	QI	98/99 (99%)	98 (100%)	0	100	100
9	XI	97/99 (98%)	97 (100%)	0	100	100
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	86 (100%)	0	100	100
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	104 (100%)	0	100	100
12	XL	103/109 (94%)	103 (100%)	0	100	100
13	QM	96/101 (95%)	96 (100%)	0	100	100
13	XM	95/101 (94%)	95 (100%)	0	100	100
14	QN	49/50 (98%)	49 (100%)	0	100	100
14	XN	49/50 (98%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	95 (100%)	0	100	100
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	72/80 (90%)	71 (99%)	1 (1%)	59	70
19	XS	73/80 (91%)	73 (100%)	0	100	100
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
27	RD	214/218 (98%)	214 (100%)	0	100	100
27	YD	214/218 (98%)	214 (100%)	0	100	100
28	RE	165/166 (99%)	165 (100%)	0	100	100
28	YE	165/166 (99%)	165 (100%)	0	100	100
29	RF	161/166 (97%)	161 (100%)	0	100	100
29	YF	161/166 (97%)	161 (100%)	0	100	100
30	RG	155/156 (99%)	155 (100%)	0	100	100
30	YG	155/156 (99%)	155 (100%)	0	100	100
31	RH	145/148 (98%)	145 (100%)	0	100	100
31	YH	145/148 (98%)	145 (100%)	0	100	100
32	RI	122/124 (98%)	122 (100%)	0	100	100
32	YI	122/124 (98%)	122 (100%)	0	100	100
33	RN	117/119 (98%)	117 (100%)	0	100	100
33	YN	117/119 (98%)	117 (100%)	0	100	100
34	RO	100/100 (100%)	100 (100%)	0	100	100
34	YO	100/100 (100%)	100 (100%)	0	100	100
35	RP	116/116 (100%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	YP	114/116 (98%)	114 (100%)	0	100	100
36	RQ	111/111 (100%)	111 (100%)	0	100	100
36	YQ	111/111 (100%)	111 (100%)	0	100	100
37	RR	100/101 (99%)	100 (100%)	0	100	100
37	YR	100/101 (99%)	100 (100%)	0	100	100
38	RS	87/88 (99%)	87 (100%)	0	100	100
38	YS	87/88 (99%)	87 (100%)	0	100	100
39	RT	120/127 (94%)	120 (100%)	0	100	100
39	YT	120/127 (94%)	120 (100%)	0	100	100
40	RU	93/94 (99%)	93 (100%)	0	100	100
40	YU	93/94 (99%)	93 (100%)	0	100	100
41	RV	82/82 (100%)	82 (100%)	0	100	100
41	YV	82/82 (100%)	82 (100%)	0	100	100
42	RW	92/92 (100%)	92 (100%)	0	100	100
42	YW	92/92 (100%)	92 (100%)	0	100	100
43	RX	74/78 (95%)	74 (100%)	0	100	100
43	YX	74/78 (95%)	74 (100%)	0	100	100
44	RY	88/91 (97%)	88 (100%)	0	100	100
44	YY	88/91 (97%)	88 (100%)	0	100	100
45	RZ	162/179 (90%)	162 (100%)	0	100	100
45	YZ	162/179 (90%)	162 (100%)	0	100	100
46	R0	65/67 (97%)	65 (100%)	0	100	100
46	Y0	61/67 (91%)	61 (100%)	0	100	100
47	R1	82/83 (99%)	82 (100%)	0	100	100
47	Y1	78/83 (94%)	78 (100%)	0	100	100
48	R2	64/67 (96%)	64 (100%)	0	100	100
48	Y2	64/67 (96%)	64 (100%)	0	100	100
49	R3	51/52 (98%)	51 (100%)	0	100	100
49	Y3	51/52 (98%)	51 (100%)	0	100	100
50	R4	62/63 (98%)	62 (100%)	0	100	100
50	Y4	62/63 (98%)	61 (98%)	1 (2%)	55	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	R5	51/52 (98%)	51 (100%)	0	100	100
51	Y5	51/52 (98%)	51 (100%)	0	100	100
52	R6	51/52 (98%)	51 (100%)	0	100	100
52	Y6	51/52 (98%)	51 (100%)	0	100	100
53	R7	40/42 (95%)	40 (100%)	0	100	100
53	Y7	41/42 (98%)	41 (100%)	0	100	100
54	R8	54/55 (98%)	54 (100%)	0	100	100
54	Y8	54/55 (98%)	54 (100%)	0	100	100
55	R9	34/34 (100%)	34 (100%)	0	100	100
55	Y9	34/34 (100%)	33 (97%)	1 (3%)	37	57
All	All	9687/10066 (96%)	9684 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	QS	41	VAL
50	Y4	56	VAL
55	Y9	27	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
31	YH	74	ASN
55	Y9	32	HIS
32	YI	105	HIS
37	YR	71	GLN
30	RG	40	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1508 (99%)	252 (16%)	34 (2%)
1	XA	1499/1508 (99%)	272 (18%)	37 (2%)
22	QV	76/77 (98%)	17 (22%)	3 (3%)
22	QW	75/77 (97%)	31 (41%)	2 (2%)
22	XV	76/77 (98%)	18 (23%)	3 (3%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	XW	75/77 (97%)	32 (42%)	2 (2%)
23	QX	7/25 (28%)	0	0
23	XX	9/25 (36%)	3 (33%)	0
24	QY	16/17 (94%)	2 (12%)	0
24	XY	16/17 (94%)	2 (12%)	0
25	RA	2879/2915 (98%)	599 (20%)	47 (1%)
25	YA	2880/2915 (98%)	570 (19%)	48 (1%)
26	RB	119/122 (97%)	17 (14%)	1 (0%)
26	YB	119/122 (97%)	19 (15%)	1 (0%)
All	All	9344/9482 (98%)	1834 (19%)	178 (1%)

5 of 1834 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	32	A
1	QA	39	G
1	QA	48	C

5 of 178 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	1027	C
25	YA	752	A
1	XA	1297	C
25	YA	195	A
25	YA	1026	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1301 ligands modelled in this entry, 1299 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	$\# Z > 2$
57	SF4	XD	301	4	0,12,12	-	-	-		
57	SF4	QD	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
57	SF4	XD	301	4	-	-	0/6/5/5
57	SF4	QD	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	QD	301	SF4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1500/1508 (99%)	-0.00	14 (0%) 81 57	53, 99, 184, 366	0
1	XA	1500/1508 (99%)	0.03	9 (0%) 85 65	51, 103, 201, 351	0
2	QB	235/256 (91%)	0.47	7 (2%) 52 32	89, 156, 228, 293	0
2	XB	236/256 (92%)	0.59	11 (4%) 36 23	66, 143, 208, 250	0
3	QC	205/239 (85%)	0.63	9 (4%) 39 24	76, 139, 197, 252	0
3	XC	205/239 (85%)	0.60	13 (6%) 26 18	72, 119, 188, 249	0
4	QD	208/209 (99%)	0.72	14 (6%) 24 17	67, 120, 188, 230	0
4	XD	208/209 (99%)	0.55	14 (6%) 24 17	56, 100, 153, 214	0
5	QE	151/162 (93%)	0.71	11 (7%) 21 16	70, 114, 162, 200	0
5	XE	151/162 (93%)	0.39	6 (3%) 42 26	48, 100, 152, 188	0
6	QF	101/101 (100%)	0.23	0 100 100	71, 106, 148, 187	0
6	XF	101/101 (100%)	0.49	5 (4%) 34 22	56, 108, 160, 225	0
7	QG	155/156 (99%)	0.43	7 (4%) 38 24	69, 122, 177, 218	0
7	XG	155/156 (99%)	0.55	5 (3%) 50 31	82, 137, 183, 233	0
8	QH	137/138 (99%)	0.28	2 (1%) 72 46	68, 112, 157, 196	0
8	XH	137/138 (99%)	0.44	5 (3%) 46 29	69, 112, 158, 198	0
9	QI	127/128 (99%)	0.52	10 (7%) 18 14	90, 149, 209, 294	0
9	XI	126/128 (98%)	0.77	14 (11%) 10 11	77, 141, 201, 223	0
10	QJ	99/105 (94%)	1.09	13 (13%) 7 8	126, 168, 245, 271	0
10	XJ	96/105 (91%)	0.92	12 (12%) 8 9	93, 143, 207, 249	0
11	QK	119/129 (92%)	0.63	10 (8%) 17 13	59, 110, 173, 201	0
11	XK	116/129 (89%)	0.72	10 (8%) 16 13	57, 112, 175, 202	0
12	QL	125/132 (94%)	0.59	9 (7%) 21 16	53, 92, 149, 227	0
12	XL	122/132 (92%)	0.69	12 (9%) 13 12	42, 87, 138, 224	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	120/126 (95%)	0.78	14 (11%) 9 10	105, 151, 207, 252	0
13	XM	119/126 (94%)	0.47	8 (6%) 24 17	78, 125, 180, 232	0
14	QN	60/61 (98%)	1.27	11 (18%) 3 4	115, 150, 215, 252	0
14	XN	60/61 (98%)	0.73	1 (1%) 69 43	66, 116, 175, 203	0
15	QO	88/89 (98%)	0.24	0 100 100	66, 106, 156, 181	0
15	XO	87/89 (97%)	0.33	2 (2%) 61 37	63, 97, 158, 203	0
16	QP	84/88 (95%)	0.41	1 (1%) 76 51	54, 97, 139, 208	0
16	XP	84/88 (95%)	0.62	2 (2%) 59 36	71, 113, 160, 187	0
17	QQ	100/105 (95%)	0.75	7 (7%) 22 16	61, 105, 145, 171	0
17	XQ	100/105 (95%)	0.64	3 (3%) 52 32	54, 110, 179, 207	0
18	QR	70/88 (79%)	0.11	0 100 100	59, 103, 140, 184	0
18	XR	70/88 (79%)	0.50	3 (4%) 40 25	67, 109, 173, 208	0
19	QS	83/93 (89%)	0.87	6 (7%) 21 16	103, 158, 216, 269	0
19	XS	84/93 (90%)	0.32	1 (1%) 76 51	77, 135, 192, 309	0
20	QT	99/106 (93%)	0.56	4 (4%) 42 26	62, 106, 167, 228	0
20	XT	99/106 (93%)	0.87	8 (8%) 18 14	68, 138, 223, 257	0
21	QU	25/27 (92%)	0.81	0 100 100	103, 152, 212, 213	0
21	XU	25/27 (92%)	0.40	0 100 100	97, 120, 167, 202	0
22	QV	77/77 (100%)	0.33	2 (2%) 57 35	64, 106, 171, 214	0
22	QW	76/77 (98%)	1.24	12 (15%) 5 6	158, 288, 392, 433	0
22	XV	77/77 (100%)	0.68	4 (5%) 33 21	63, 99, 150, 175	0
22	XW	76/77 (98%)	1.17	10 (13%) 7 8	167, 367, 436, 475	0
23	QX	8/25 (32%)	0.29	0 100 100	59, 74, 126, 131	0
23	XX	10/25 (40%)	0.83	3 (30%) 1 1	67, 82, 178, 179	0
24	QY	17/17 (100%)	0.05	0 100 100	84, 120, 193, 210	0
24	XY	17/17 (100%)	-0.02	0 100 100	79, 110, 181, 187	0
25	RA	2882/2915 (98%)	-0.00	25 (0%) 81 57	38, 73, 224, 388	0
25	YA	2883/2915 (98%)	0.02	28 (0%) 79 55	38, 73, 230, 444	0
26	RB	120/122 (98%)	-0.07	0 100 100	74, 114, 153, 206	0
26	YB	120/122 (98%)	0.01	1 (0%) 82 60	84, 128, 183, 206	0
27	RD	272/276 (98%)	0.66	22 (8%) 18 14	29, 64, 113, 186	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
27	YD	272/276 (98%)	0.59	21 (7%)	19 15	31, 66, 122, 251	0
28	RE	205/206 (99%)	0.50	8 (3%)	43 27	32, 81, 157, 251	0
28	YE	205/206 (99%)	0.56	8 (3%)	43 27	17, 96, 177, 238	0
29	RF	202/210 (96%)	0.52	7 (3%)	47 29	42, 86, 154, 228	0
29	YF	202/210 (96%)	0.38	8 (3%)	42 26	32, 75, 135, 196	0
30	RG	181/182 (99%)	0.41	8 (4%)	39 24	72, 123, 190, 214	0
30	YG	181/182 (99%)	0.54	5 (2%)	55 33	71, 128, 189, 250	0
31	RH	174/180 (96%)	0.98	20 (11%)	9 10	116, 185, 256, 288	0
31	YH	174/180 (96%)	0.69	17 (9%)	13 12	68, 122, 225, 348	0
32	RI	146/148 (98%)	1.36	38 (26%)	1 2	78, 147, 231, 273	0
32	YI	146/148 (98%)	0.62	4 (2%)	56 34	58, 131, 192, 250	0
33	RN	138/140 (98%)	0.47	2 (1%)	73 47	42, 88, 157, 212	0
33	YN	138/140 (98%)	0.71	8 (5%)	29 19	52, 93, 152, 215	0
34	RO	122/122 (100%)	0.30	3 (2%)	58 36	41, 78, 119, 154	0
34	YO	122/122 (100%)	0.39	2 (1%)	70 44	45, 73, 118, 145	0
35	RP	150/150 (100%)	0.92	14 (9%)	14 13	50, 99, 165, 218	0
35	YP	147/150 (98%)	0.88	13 (8%)	15 13	36, 85, 154, 201	0
36	RQ	141/141 (100%)	0.77	17 (12%)	8 9	53, 94, 174, 222	0
36	YQ	141/141 (100%)	0.73	17 (12%)	8 9	28, 83, 165, 218	0
37	RR	117/118 (99%)	0.19	4 (3%)	48 29	35, 68, 116, 179	0
37	YR	117/118 (99%)	0.57	4 (3%)	48 29	45, 87, 145, 196	0
38	RS	111/112 (99%)	0.51	6 (5%)	31 21	83, 120, 188, 214	0
38	YS	111/112 (99%)	0.39	3 (2%)	56 34	90, 129, 208, 296	0
39	RT	137/146 (93%)	0.49	5 (3%)	46 29	54, 92, 181, 245	0
39	YT	137/146 (93%)	0.37	5 (3%)	46 29	54, 100, 188, 219	0
40	RU	117/118 (99%)	0.37	3 (2%)	57 35	39, 84, 153, 216	0
40	YU	117/118 (99%)	0.70	8 (6%)	23 17	39, 81, 152, 278	0
41	RV	101/101 (100%)	0.59	5 (4%)	34 22	50, 107, 183, 274	0
41	YV	101/101 (100%)	0.75	9 (8%)	15 13	38, 97, 160, 282	0
42	RW	113/113 (100%)	0.28	3 (2%)	56 34	20, 62, 123, 201	0
42	YW	113/113 (100%)	0.52	10 (8%)	15 13	31, 67, 139, 226	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
43	RX	92/96 (95%)	0.22	3 (3%)	49	30	46, 76, 126, 170	0
43	YX	92/96 (95%)	0.17	2 (2%)	62	39	30, 67, 105, 153	0
44	RY	107/110 (97%)	0.98	15 (14%)	6	7	55, 98, 150, 219	0
44	YY	107/110 (97%)	0.58	8 (7%)	20	15	52, 88, 145, 185	0
45	RZ	183/206 (88%)	0.68	7 (3%)	44	28	82, 145, 213, 258	0
45	YZ	183/206 (88%)	0.62	13 (7%)	22	16	75, 130, 195, 234	0
46	R0	81/85 (95%)	0.86	7 (8%)	16	13	43, 93, 145, 197	0
46	Y0	75/85 (88%)	0.60	2 (2%)	56	34	54, 87, 146, 166	0
47	R1	97/98 (98%)	0.93	13 (13%)	7	8	33, 82, 168, 218	0
47	Y1	93/98 (94%)	0.53	6 (6%)	25	17	33, 77, 151, 185	0
48	R2	69/72 (95%)	0.33	0	100	100	51, 108, 175, 234	0
48	Y2	69/72 (95%)	0.57	3 (4%)	40	25	41, 77, 145, 212	0
49	R3	59/60 (98%)	0.53	1 (1%)	69	43	56, 89, 162, 202	0
49	Y3	59/60 (98%)	0.37	2 (3%)	48	29	48, 101, 157, 207	0
50	R4	69/71 (97%)	0.62	0	100	100	120, 178, 245, 302	0
50	Y4	69/71 (97%)	0.43	0	100	100	108, 152, 245, 300	0
51	R5	59/60 (98%)	0.18	0	100	100	33, 76, 168, 209	0
51	Y5	59/60 (98%)	0.71	5 (8%)	16	13	36, 91, 188, 216	0
52	R6	53/54 (98%)	1.38	9 (16%)	4	5	137, 226, 325, 346	0
52	Y6	53/54 (98%)	1.27	11 (20%)	2	3	140, 214, 285, 320	0
53	R7	47/49 (95%)	0.23	1 (2%)	63	40	26, 63, 90, 138	0
53	Y7	48/49 (97%)	0.10	0	100	100	20, 54, 97, 133	0
54	R8	64/65 (98%)	1.14	14 (21%)	2	3	45, 86, 143, 250	0
54	Y8	64/65 (98%)	0.90	11 (17%)	4	5	56, 83, 134, 258	0
55	R9	37/37 (100%)	2.04	19 (51%)	0	0	164, 238, 310, 331	0
55	Y9	37/37 (100%)	1.20	6 (16%)	4	6	146, 215, 372, 394	0
All	All	21011/21610 (97%)	0.35	843 (4%)	42	26	17, 98, 209, 475	0

The worst 5 of 843 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	RI	16	GLY	11.0
7	XG	5	ARG	10.1

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Mol	Chain	Res	Type	RSRZ
35	RP	13	ASN	8.1
46	R0	4	LYS	7.3
27	YD	2	ALA	7.2

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

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

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
56	MG	YA	3018	1/1	0.38	0.45	61,61,61,61	0
58	ZN	Y9	102	1/1	0.43	0.28	194,194,194,194	0
56	MG	RA	3438	1/1	0.46	0.14	58,58,58,58	0
56	MG	XM	201	1/1	0.47	0.12	87,87,87,87	0
56	MG	YA	3332	1/1	0.49	0.16	60,60,60,60	0
56	MG	YA	3220	1/1	0.53	0.12	59,59,59,59	0
56	MG	RA	3340	1/1	0.56	0.13	67,67,67,67	0
56	MG	YA	3268	1/1	0.56	0.36	56,56,56,56	0
56	MG	YA	3397	1/1	0.57	0.14	85,85,85,85	0
56	MG	RA	3257	1/1	0.58	0.24	51,51,51,51	0
56	MG	YA	3011	1/1	0.58	0.40	66,66,66,66	0
56	MG	YA	3017	1/1	0.58	0.49	63,63,63,63	0
56	MG	RA	3142	1/1	0.60	0.30	52,52,52,52	0
56	MG	YA	3260	1/1	0.60	0.42	56,56,56,56	0
56	MG	RA	3301	1/1	0.60	0.22	75,75,75,75	0
56	MG	YA	3402	1/1	0.61	0.12	53,53,53,53	0
56	MG	RA	3457	1/1	0.61	0.23	62,62,62,62	0
56	MG	RA	3482	1/1	0.62	0.23	94,94,94,94	0
56	MG	QQ	201	1/1	0.62	0.11	68,68,68,68	0
56	MG	RA	3350	1/1	0.62	0.12	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	ZN	R5	501	1/1	0.63	0.21	243,243,243,243	0
56	MG	RA	3318	1/1	0.64	0.17	62,62,62,62	0
56	MG	RA	3061	1/1	0.64	0.70	59,59,59,59	0
56	MG	RA	3484	1/1	0.64	0.19	70,70,70,70	0
56	MG	YA	3190	1/1	0.65	0.20	66,66,66,66	0
56	MG	YA	3405	1/1	0.65	0.12	65,65,65,65	0
56	MG	RA	3243	1/1	0.65	0.42	66,66,66,66	0
56	MG	YA	3086	1/1	0.65	0.40	63,63,63,63	0
56	MG	QV	104	1/1	0.66	0.45	58,58,58,58	0
56	MG	YA	3095	1/1	0.66	0.24	61,61,61,61	0
56	MG	RA	3016	1/1	0.67	0.41	54,54,54,54	0
56	MG	RA	3497	1/1	0.67	0.38	62,62,62,62	0
56	MG	YA	3161	1/1	0.67	0.47	64,64,64,64	0
56	MG	YA	3312	1/1	0.67	0.20	65,65,65,65	0
58	ZN	R9	102	1/1	0.67	0.31	211,211,211,211	0
56	MG	YA	3035	1/1	0.67	0.58	65,65,65,65	0
56	MG	RA	3494	1/1	0.68	0.58	61,61,61,61	0
56	MG	YA	3100	1/1	0.68	0.33	56,56,56,56	0
56	MG	YA	3455	1/1	0.68	0.12	63,63,63,63	0
56	MG	RA	3081	1/1	0.68	0.56	67,67,67,67	0
56	MG	RA	3024	1/1	0.68	0.53	49,49,49,49	0
56	MG	RA	3022	1/1	0.68	0.38	61,61,61,61	0
56	MG	YA	3048	1/1	0.69	0.37	54,54,54,54	0
56	MG	YA	3407	1/1	0.69	0.09	62,62,62,62	0
56	MG	YA	3180	1/1	0.69	0.27	55,55,55,55	0
56	MG	RA	3313	1/1	0.69	0.23	61,61,61,61	0
56	MG	QA	1660	1/1	0.69	0.27	69,69,69,69	0
56	MG	RA	3091	1/1	0.69	0.28	56,56,56,56	0
56	MG	RA	3468	1/1	0.70	0.11	57,57,57,57	0
56	MG	YA	3426	1/1	0.70	0.58	53,53,53,53	0
56	MG	YA	3394	1/1	0.70	0.15	67,67,67,67	0
56	MG	YA	3069	1/1	0.70	0.32	63,63,63,63	0
56	MG	YA	3031	1/1	0.70	0.42	63,63,63,63	0
56	MG	XS	101	1/1	0.70	0.09	66,66,66,66	0
56	MG	RA	3242	1/1	0.71	0.28	66,66,66,66	0
56	MG	RA	3206	1/1	0.71	0.21	63,63,63,63	0
56	MG	XA	1682	1/1	0.71	0.09	77,77,77,77	0
56	MG	YA	3535	1/1	0.71	0.18	66,66,66,66	0
56	MG	RA	3402	1/1	0.71	0.17	69,69,69,69	0
56	MG	RA	3212	1/1	0.71	0.23	56,56,56,56	0
56	MG	YA	3155	1/1	0.71	0.23	65,65,65,65	0
56	MG	YA	3231	1/1	0.72	0.17	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3246	1/1	0.72	0.21	66,66,66,66	0
56	MG	QA	1631	1/1	0.72	0.43	53,53,53,53	0
56	MG	XA	1611	1/1	0.72	0.23	63,63,63,63	0
56	MG	YA	3174	1/1	0.72	0.32	64,64,64,64	0
56	MG	YA	3020	1/1	0.72	0.54	51,51,51,51	0
56	MG	YA	3335	1/1	0.72	0.25	72,72,72,72	0
58	ZN	R6	101	1/1	0.72	0.21	211,211,211,211	0
56	MG	XV	101	1/1	0.72	0.27	50,50,50,50	0
56	MG	RA	3119	1/1	0.72	0.46	67,67,67,67	0
56	MG	RA	3014	1/1	0.73	0.30	61,61,61,61	0
56	MG	YA	3456	1/1	0.73	0.12	85,85,85,85	0
56	MG	YA	3502	1/1	0.73	0.10	59,59,59,59	0
56	MG	YA	3380	1/1	0.73	0.26	49,49,49,49	0
56	MG	RA	3466	1/1	0.74	0.18	54,54,54,54	0
56	MG	YA	3187	1/1	0.74	0.29	55,55,55,55	0
56	MG	YA	3047	1/1	0.74	0.60	48,48,48,48	0
56	MG	QA	1610	1/1	0.74	0.40	51,51,51,51	0
56	MG	YA	3222	1/1	0.74	0.23	47,47,47,47	0
56	MG	RA	3009	1/1	0.74	0.40	54,54,54,54	0
56	MG	YA	3005	1/1	0.74	0.27	56,56,56,56	0
56	MG	QA	1656	1/1	0.74	0.20	66,66,66,66	0
56	MG	RA	3035	1/1	0.74	0.22	60,60,60,60	0
56	MG	YA	3287	1/1	0.74	0.08	67,67,67,67	0
56	MG	YB	211	1/1	0.74	0.08	65,65,65,65	0
56	MG	RA	3039	1/1	0.74	0.31	65,65,65,65	0
56	MG	RA	3199	1/1	0.74	0.20	55,55,55,55	0
56	MG	YA	3168	1/1	0.74	0.10	66,66,66,66	0
56	MG	RA	3305	1/1	0.74	0.13	57,57,57,57	0
56	MG	YA	3453	1/1	0.75	0.16	67,67,67,67	0
56	MG	YA	3363	1/1	0.75	0.30	63,63,63,63	0
56	MG	YA	3118	1/1	0.75	0.34	67,67,67,67	0
56	MG	RA	3219	1/1	0.75	0.11	64,64,64,64	0
56	MG	YA	3022	1/1	0.75	0.28	64,64,64,64	0
56	MG	RA	3042	1/1	0.75	0.53	66,66,66,66	0
56	MG	RA	3122	1/1	0.75	0.40	52,52,52,52	0
56	MG	RA	3013	1/1	0.75	0.43	60,60,60,60	0
56	MG	YA	3361	1/1	0.75	0.08	59,59,59,59	0
56	MG	YA	3450	1/1	0.75	0.20	74,74,74,74	0
56	MG	QC	301	1/1	0.76	0.13	87,87,87,87	0
56	MG	YA	3024	1/1	0.76	0.35	55,55,55,55	0
56	MG	RA	3344	1/1	0.76	0.21	54,54,54,54	0
56	MG	YA	3399	1/1	0.76	0.14	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3056	1/1	0.76	0.54	57,57,57,57	0
56	MG	XA	1621	1/1	0.76	0.21	66,66,66,66	0
56	MG	RA	3207	1/1	0.76	0.16	60,60,60,60	0
56	MG	YA	3229	1/1	0.76	0.21	60,60,60,60	0
56	MG	YA	3054	1/1	0.76	0.22	57,57,57,57	0
56	MG	RA	3429	1/1	0.76	0.23	54,54,54,54	0
56	MG	RA	3208	1/1	0.76	0.25	58,58,58,58	0
56	MG	YA	3267	1/1	0.76	0.30	63,63,63,63	0
56	MG	RA	3453	1/1	0.76	0.12	54,54,54,54	0
56	MG	RA	3162	1/1	0.76	0.24	54,54,54,54	0
56	MG	RA	3178	1/1	0.76	0.15	58,58,58,58	0
56	MG	YA	3125	1/1	0.76	0.38	79,79,79,79	0
56	MG	RA	3317	1/1	0.76	0.16	62,62,62,62	0
56	MG	RA	3230	1/1	0.76	0.33	63,63,63,63	0
56	MG	RA	3322	1/1	0.76	0.19	62,62,62,62	0
56	MG	YA	3374	1/1	0.77	0.18	55,55,55,55	0
56	MG	RA	3351	1/1	0.77	0.29	57,57,57,57	0
56	MG	YA	3045	1/1	0.77	0.26	66,66,66,66	0
56	MG	RA	3001	1/1	0.77	0.32	84,84,84,84	0
56	MG	RA	3416	1/1	0.77	0.07	62,62,62,62	0
56	MG	RA	3008	1/1	0.77	0.26	68,68,68,68	0
56	MG	YA	3403	1/1	0.77	0.15	67,67,67,67	0
56	MG	YA	3226	1/1	0.77	0.11	70,70,70,70	0
56	MG	RA	3065	1/1	0.77	0.28	54,54,54,54	0
56	MG	RA	3441	1/1	0.77	0.12	53,53,53,53	0
56	MG	YA	3234	1/1	0.77	0.33	67,67,67,67	0
56	MG	YA	3093	1/1	0.77	0.27	60,60,60,60	0
56	MG	RA	3202	1/1	0.77	0.26	64,64,64,64	0
56	MG	RA	3072	1/1	0.77	0.37	55,55,55,55	0
56	MG	QA	1651	1/1	0.77	0.12	79,79,79,79	0
56	MG	YA	3526	1/1	0.77	0.39	61,61,61,61	0
56	MG	RA	3012	1/1	0.77	0.52	54,54,54,54	0
56	MG	RA	3037	1/1	0.77	0.48	63,63,63,63	0
56	MG	YA	3157	1/1	0.77	0.22	66,66,66,66	0
56	MG	QA	1603	1/1	0.77	0.25	67,67,67,67	0
56	MG	QA	1636	1/1	0.77	0.22	63,63,63,63	0
58	ZN	Y4	500	1/1	0.77	0.15	206,206,206,206	0
56	MG	RA	3148	1/1	0.77	0.41	65,65,65,65	0
56	MG	RA	3050	1/1	0.78	0.48	57,57,57,57	0
56	MG	RA	3096	1/1	0.78	0.46	63,63,63,63	0
56	MG	YA	3007	1/1	0.78	0.17	57,57,57,57	0
56	MG	RA	3238	1/1	0.78	0.33	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3104	1/1	0.78	0.24	60,60,60,60	0
56	MG	YA	3250	1/1	0.78	0.34	66,66,66,66	0
56	MG	RA	3196	1/1	0.78	0.32	64,64,64,64	0
56	MG	RA	3100	1/1	0.78	0.23	59,59,59,59	0
56	MG	YA	3129	1/1	0.78	0.34	63,63,63,63	0
56	MG	RA	3251	1/1	0.78	0.37	63,63,63,63	0
56	MG	RA	3397	1/1	0.78	0.22	49,49,49,49	0
56	MG	RA	3071	1/1	0.78	0.41	61,61,61,61	0
56	MG	RB	201	1/1	0.78	0.13	67,67,67,67	0
56	MG	R8	101	1/1	0.78	0.44	61,61,61,61	0
56	MG	QA	1663	1/1	0.78	0.12	61,61,61,61	0
56	MG	RA	3025	1/1	0.78	0.31	52,52,52,52	0
56	MG	RA	3086	1/1	0.78	0.39	51,51,51,51	0
56	MG	RA	3155	1/1	0.78	0.43	60,60,60,60	0
56	MG	RA	3446	1/1	0.78	0.16	60,60,60,60	0
56	MG	RA	3304	1/1	0.79	0.23	64,64,64,64	0
56	MG	RA	3448	1/1	0.79	0.09	65,65,65,65	0
56	MG	YA	3396	1/1	0.79	0.36	66,66,66,66	0
56	MG	YA	3478	1/1	0.79	0.15	53,53,53,53	0
56	MG	YA	3496	1/1	0.79	0.23	72,72,72,72	0
56	MG	RA	3274	1/1	0.79	0.33	58,58,58,58	0
56	MG	RA	3478	1/1	0.79	0.16	67,67,67,67	0
56	MG	YA	3528	1/1	0.79	0.48	65,65,65,65	0
56	MG	XA	1624	1/1	0.79	0.20	63,63,63,63	0
56	MG	XA	1635	1/1	0.79	0.21	50,50,50,50	0
58	ZN	R4	102	1/1	0.79	0.11	257,257,257,257	0
56	MG	YA	3027	1/1	0.79	0.28	53,53,53,53	0
56	MG	YA	3078	1/1	0.79	0.48	66,66,66,66	0
56	MG	YA	3422	1/1	0.79	0.06	63,63,63,63	0
56	MG	YA	3200	1/1	0.79	0.09	96,96,96,96	0
58	ZN	Y6	101	1/1	0.79	0.26	245,245,245,245	0
56	MG	YA	3375	1/1	0.79	0.32	62,62,62,62	0
56	MG	RA	3332	1/1	0.80	0.21	69,69,69,69	0
56	MG	RA	3087	1/1	0.80	0.36	62,62,62,62	0
56	MG	RA	3044	1/1	0.80	0.41	60,60,60,60	0
56	MG	RA	3067	1/1	0.80	0.28	50,50,50,50	0
56	MG	QA	1664	1/1	0.80	0.23	67,67,67,67	0
56	MG	RA	3106	1/1	0.80	0.26	63,63,63,63	0
56	MG	RE	302	1/1	0.80	0.10	107,107,107,107	0
56	MG	YA	3383	1/1	0.80	0.11	59,59,59,59	0
56	MG	YA	3150	1/1	0.80	0.38	59,59,59,59	0
56	MG	R0	103	1/1	0.80	0.11	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3050	1/1	0.80	0.44	63,63,63,63	0
56	MG	RA	3401	1/1	0.80	0.31	60,60,60,60	0
56	MG	XA	1603	1/1	0.80	0.40	65,65,65,65	0
56	MG	RA	3228	1/1	0.80	0.43	55,55,55,55	0
56	MG	YA	3176	1/1	0.80	0.20	64,64,64,64	0
56	MG	RA	3229	1/1	0.80	0.28	56,56,56,56	0
58	ZN	Y5	501	1/1	0.80	0.20	170,170,170,170	0
56	MG	YA	3183	1/1	0.80	0.19	58,58,58,58	0
56	MG	YA	3316	1/1	0.80	0.24	62,62,62,62	0
56	MG	YA	3249	1/1	0.81	0.25	56,56,56,56	0
56	MG	RA	3252	1/1	0.81	0.30	56,56,56,56	0
56	MG	RA	3256	1/1	0.81	0.18	66,66,66,66	0
56	MG	QA	1628	1/1	0.81	0.09	66,66,66,66	0
56	MG	YA	3432	1/1	0.81	0.38	56,56,56,56	0
56	MG	YA	3449	1/1	0.81	0.08	55,55,55,55	0
56	MG	YA	3040	1/1	0.81	0.32	49,49,49,49	0
56	MG	YA	3280	1/1	0.81	0.24	60,60,60,60	0
56	MG	RA	3220	1/1	0.81	0.16	67,67,67,67	0
56	MG	XA	1646	1/1	0.81	0.11	63,63,63,63	0
56	MG	RA	3286	1/1	0.81	0.14	66,66,66,66	0
56	MG	YA	3488	1/1	0.81	0.05	66,66,66,66	0
56	MG	RA	3377	1/1	0.81	0.31	59,59,59,59	0
56	MG	YA	3499	1/1	0.81	0.24	66,66,66,66	0
56	MG	YA	3501	1/1	0.81	0.16	59,59,59,59	0
56	MG	QH	201	1/1	0.81	0.07	71,71,71,71	0
56	MG	YA	3511	1/1	0.81	0.15	64,64,64,64	0
56	MG	YA	3519	1/1	0.81	0.31	67,67,67,67	0
56	MG	RA	3031	1/1	0.81	0.51	61,61,61,61	0
56	MG	YA	3076	1/1	0.81	0.20	59,59,59,59	0
56	MG	RA	3145	1/1	0.81	0.35	60,60,60,60	0
56	MG	RA	3098	1/1	0.81	0.14	62,62,62,62	0
56	MG	RA	3507	1/1	0.81	0.42	67,67,67,67	0
56	MG	RA	3417	1/1	0.81	0.07	54,54,54,54	0
56	MG	YA	3096	1/1	0.81	0.51	65,65,65,65	0
56	MG	RA	3316	1/1	0.81	0.16	68,68,68,68	0
56	MG	RA	3150	1/1	0.81	0.22	64,64,64,64	0
56	MG	RA	3062	1/1	0.81	0.31	66,66,66,66	0
56	MG	YA	3237	1/1	0.81	0.15	60,60,60,60	0
56	MG	QA	1616	1/1	0.81	0.10	51,51,51,51	0
56	MG	RA	3428	1/1	0.82	0.14	56,56,56,56	0
56	MG	RA	3033	1/1	0.82	0.44	65,65,65,65	0
56	MG	RA	3498	1/1	0.82	0.34	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3505	1/1	0.82	0.33	54,54,54,54	0
56	MG	YA	3002	1/1	0.82	0.32	63,63,63,63	0
56	MG	YA	3088	1/1	0.82	0.46	62,62,62,62	0
56	MG	YA	3423	1/1	0.82	0.15	68,68,68,68	0
56	MG	RA	3279	1/1	0.82	0.06	58,58,58,58	0
56	MG	RA	3354	1/1	0.82	0.30	52,52,52,52	0
56	MG	YA	3009	1/1	0.82	0.42	54,54,54,54	0
56	MG	RA	3372	1/1	0.82	0.14	54,54,54,54	0
56	MG	RR	201	1/1	0.82	0.12	58,58,58,58	0
56	MG	QA	1602	1/1	0.82	0.31	54,54,54,54	0
56	MG	RA	3090	1/1	0.82	0.52	59,59,59,59	0
56	MG	YA	3460	1/1	0.82	0.16	64,64,64,64	0
56	MG	YA	3476	1/1	0.82	0.19	61,61,61,61	0
56	MG	RA	3331	1/1	0.82	0.15	57,57,57,57	0
56	MG	YA	3486	1/1	0.82	0.21	64,64,64,64	0
56	MG	YA	3131	1/1	0.82	0.17	61,61,61,61	0
56	MG	YA	3283	1/1	0.82	0.29	64,64,64,64	0
56	MG	YA	3140	1/1	0.82	0.19	53,53,53,53	0
56	MG	YA	3145	1/1	0.82	0.34	50,50,50,50	0
56	MG	YA	3313	1/1	0.82	0.10	57,57,57,57	0
56	MG	YA	3315	1/1	0.82	0.10	49,49,49,49	0
56	MG	RA	3078	1/1	0.82	0.48	62,62,62,62	0
56	MG	RA	3403	1/1	0.82	0.23	60,60,60,60	0
56	MG	RA	3414	1/1	0.82	0.29	63,63,63,63	0
56	MG	YA	3033	1/1	0.82	0.31	66,66,66,66	0
56	MG	YA	3540	1/1	0.82	0.33	52,52,52,52	0
56	MG	XA	1628	1/1	0.82	0.21	56,56,56,56	0
56	MG	XA	1632	1/1	0.82	0.26	64,64,64,64	0
56	MG	QA	1612	1/1	0.82	0.25	57,57,57,57	0
56	MG	RA	3085	1/1	0.82	0.35	64,64,64,64	0
56	MG	YA	3381	1/1	0.82	0.08	73,73,73,73	0
56	MG	XA	1654	1/1	0.82	0.20	53,53,53,53	0
56	MG	YA	3049	1/1	0.82	0.32	54,54,54,54	0
56	MG	XA	1662	1/1	0.82	0.12	53,53,53,53	0
56	MG	YA	3198	1/1	0.82	0.37	57,57,57,57	0
56	MG	YA	3003	1/1	0.83	0.12	79,79,79,79	0
56	MG	QA	1604	1/1	0.83	0.24	54,54,54,54	0
56	MG	YA	3413	1/1	0.83	0.49	61,61,61,61	0
56	MG	RA	3028	1/1	0.83	0.21	58,58,58,58	0
56	MG	RA	3248	1/1	0.83	0.30	65,65,65,65	0
56	MG	YA	3425	1/1	0.83	0.09	48,48,48,48	0
56	MG	RB	204	1/1	0.83	0.23	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3030	1/1	0.83	0.55	62,62,62,62	0
56	MG	RA	3020	1/1	0.83	0.39	50,50,50,50	0
56	MG	YA	3126	1/1	0.83	0.41	65,65,65,65	0
56	MG	RA	3049	1/1	0.83	0.41	50,50,50,50	0
56	MG	RA	3160	1/1	0.83	0.36	62,62,62,62	0
56	MG	YA	3132	1/1	0.83	0.19	62,62,62,62	0
56	MG	YA	3136	1/1	0.83	0.19	62,62,62,62	0
56	MG	QA	1611	1/1	0.83	0.38	56,56,56,56	0
56	MG	RA	3227	1/1	0.83	0.13	58,58,58,58	0
56	MG	YA	3029	1/1	0.83	0.27	51,51,51,51	0
56	MG	RA	3282	1/1	0.83	0.24	66,66,66,66	0
56	MG	XA	1622	1/1	0.83	0.11	50,50,50,50	0
56	MG	YA	3325	1/1	0.83	0.33	58,58,58,58	0
56	MG	RA	3353	1/1	0.83	0.18	62,62,62,62	0
56	MG	QA	1622	1/1	0.83	0.12	56,56,56,56	0
56	MG	XA	1629	1/1	0.83	0.16	68,68,68,68	0
56	MG	YA	3515	1/1	0.83	0.15	62,62,62,62	0
56	MG	RA	3363	1/1	0.83	0.18	82,82,82,82	0
56	MG	YA	3364	1/1	0.83	0.20	70,70,70,70	0
56	MG	YA	3178	1/1	0.83	0.23	66,66,66,66	0
56	MG	RA	3371	1/1	0.83	0.38	61,61,61,61	0
56	MG	YA	3379	1/1	0.83	0.20	57,57,57,57	0
56	MG	YA	3544	1/1	0.83	0.12	62,62,62,62	0
56	MG	YB	207	1/1	0.83	0.06	58,58,58,58	0
56	MG	RA	3057	1/1	0.83	0.35	63,63,63,63	0
56	MG	YB	212	1/1	0.83	0.35	103,103,103,103	0
58	ZN	RY	202	1/1	0.83	0.17	258,258,258,258	0
56	MG	RA	3197	1/1	0.83	0.30	62,62,62,62	0
56	MG	RA	3380	1/1	0.83	0.15	50,50,50,50	0
56	MG	RA	3388	1/1	0.83	0.38	51,51,51,51	0
56	MG	RA	3492	1/1	0.83	0.46	55,55,55,55	0
56	MG	YA	3217	1/1	0.83	0.25	58,58,58,58	0
56	MG	RA	3395	1/1	0.83	0.15	56,56,56,56	0
56	MG	RA	3235	1/1	0.83	0.10	58,58,58,58	0
56	MG	RA	3036	1/1	0.83	0.25	49,49,49,49	0
56	MG	RA	3088	1/1	0.84	0.45	61,61,61,61	0
56	MG	YA	3401	1/1	0.84	0.13	56,56,56,56	0
56	MG	YA	3206	1/1	0.84	0.18	57,57,57,57	0
56	MG	YA	3080	1/1	0.84	0.23	47,47,47,47	0
56	MG	RA	3123	1/1	0.84	0.15	62,62,62,62	0
56	MG	XV	106	1/1	0.84	0.27	49,49,49,49	0
56	MG	RA	3339	1/1	0.84	0.18	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3136	1/1	0.84	0.23	56,56,56,56	0
56	MG	RB	205	1/1	0.84	0.17	58,58,58,58	0
56	MG	YA	3097	1/1	0.84	0.26	58,58,58,58	0
56	MG	RA	3427	1/1	0.84	0.32	48,48,48,48	0
56	MG	YA	3242	1/1	0.84	0.55	50,50,50,50	0
56	MG	YA	3243	1/1	0.84	0.18	64,64,64,64	0
56	MG	YA	3245	1/1	0.84	0.17	53,53,53,53	0
56	MG	RA	3018	1/1	0.84	0.47	54,54,54,54	0
56	MG	YA	3454	1/1	0.84	0.10	68,68,68,68	0
56	MG	RY	201	1/1	0.84	0.23	121,121,121,121	0
56	MG	RA	3349	1/1	0.84	0.21	67,67,67,67	0
56	MG	YA	3259	1/1	0.84	0.15	62,62,62,62	0
56	MG	YA	3465	1/1	0.84	0.10	62,62,62,62	0
56	MG	YA	3466	1/1	0.84	0.22	55,55,55,55	0
56	MG	R0	104	1/1	0.84	0.22	65,65,65,65	0
56	MG	YA	3128	1/1	0.84	0.33	54,54,54,54	0
56	MG	YA	3481	1/1	0.84	0.22	57,57,57,57	0
56	MG	RA	3079	1/1	0.84	0.33	60,60,60,60	0
56	MG	RA	3051	1/1	0.84	0.40	59,59,59,59	0
56	MG	RA	3084	1/1	0.84	0.34	57,57,57,57	0
56	MG	RA	3151	1/1	0.84	0.31	67,67,67,67	0
56	MG	RA	3224	1/1	0.84	0.24	59,59,59,59	0
56	MG	YA	3144	1/1	0.84	0.34	48,48,48,48	0
56	MG	QA	1626	1/1	0.84	0.16	60,60,60,60	0
56	MG	RA	3104	1/1	0.84	0.39	64,64,64,64	0
56	MG	RA	3105	1/1	0.84	0.18	50,50,50,50	0
56	MG	RA	3379	1/1	0.84	0.18	56,56,56,56	0
56	MG	YA	3158	1/1	0.84	0.27	59,59,59,59	0
56	MG	YA	3344	1/1	0.84	0.12	55,55,55,55	0
56	MG	YA	3349	1/1	0.84	0.07	57,57,57,57	0
56	MG	RA	3168	1/1	0.84	0.32	57,57,57,57	0
56	MG	RA	3234	1/1	0.84	0.26	56,56,56,56	0
56	MG	QE	201	1/1	0.84	0.20	59,59,59,59	0
56	MG	YA	3371	1/1	0.84	0.27	60,60,60,60	0
56	MG	YQ	203	1/1	0.84	0.31	58,58,58,58	0
56	MG	RA	3116	1/1	0.84	0.30	50,50,50,50	0
56	MG	YA	3177	1/1	0.84	0.14	63,63,63,63	0
56	MG	XA	1673	1/1	0.84	0.47	66,66,66,66	0
56	MG	YA	3179	1/1	0.84	0.26	57,57,57,57	0
56	MG	YA	3053	1/1	0.84	0.25	66,66,66,66	0
56	MG	RA	3239	1/1	0.84	0.21	54,54,54,54	0
56	MG	YA	3059	1/1	0.84	0.35	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XL	201	1/1	0.84	0.16	55,55,55,55	0
56	MG	QA	1661	1/1	0.84	0.37	61,61,61,61	0
56	MG	RA	3075	1/1	0.85	0.47	53,53,53,53	0
56	MG	RA	3063	1/1	0.85	0.23	53,53,53,53	0
56	MG	YA	3275	1/1	0.85	0.21	51,51,51,51	0
56	MG	YA	3444	1/1	0.85	0.15	50,50,50,50	0
56	MG	RA	3045	1/1	0.85	0.32	52,52,52,52	0
56	MG	RB	207	1/1	0.85	0.16	80,80,80,80	0
56	MG	YA	3160	1/1	0.85	0.32	47,47,47,47	0
56	MG	YA	3296	1/1	0.85	0.29	57,57,57,57	0
56	MG	YA	3300	1/1	0.85	0.25	60,60,60,60	0
56	MG	YA	3057	1/1	0.85	0.28	56,56,56,56	0
56	MG	YA	3163	1/1	0.85	0.26	55,55,55,55	0
56	MG	RA	3019	1/1	0.85	0.25	55,55,55,55	0
56	MG	YA	3061	1/1	0.85	0.36	52,52,52,52	0
56	MG	YA	3062	1/1	0.85	0.33	61,61,61,61	0
56	MG	YA	3326	1/1	0.85	0.24	65,65,65,65	0
56	MG	YA	3480	1/1	0.85	0.23	54,54,54,54	0
56	MG	RA	3137	1/1	0.85	0.25	52,52,52,52	0
56	MG	YA	3071	1/1	0.85	0.29	63,63,63,63	0
56	MG	YA	3337	1/1	0.85	0.31	50,50,50,50	0
56	MG	RA	3385	1/1	0.85	0.13	65,65,65,65	0
56	MG	RA	3269	1/1	0.85	0.24	49,49,49,49	0
56	MG	YA	3355	1/1	0.85	0.18	54,54,54,54	0
56	MG	RA	3461	1/1	0.85	0.16	57,57,57,57	0
56	MG	RA	3002	1/1	0.85	0.16	53,53,53,53	0
56	MG	RA	3167	1/1	0.85	0.22	52,52,52,52	0
56	MG	YA	3516	1/1	0.85	0.14	65,65,65,65	0
56	MG	XA	1605	1/1	0.85	0.23	59,59,59,59	0
56	MG	YA	3094	1/1	0.85	0.35	50,50,50,50	0
56	MG	RA	3472	1/1	0.85	0.17	50,50,50,50	0
56	MG	YA	3529	1/1	0.85	0.38	59,59,59,59	0
56	MG	XA	1619	1/1	0.85	0.18	64,64,64,64	0
56	MG	YA	3537	1/1	0.85	0.09	70,70,70,70	0
56	MG	RA	3236	1/1	0.85	0.39	63,63,63,63	0
56	MG	RA	3144	1/1	0.85	0.15	70,70,70,70	0
56	MG	YB	205	1/1	0.85	0.14	48,48,48,48	0
56	MG	RA	3215	1/1	0.85	0.32	55,55,55,55	0
56	MG	YA	3108	1/1	0.85	0.39	65,65,65,65	0
56	MG	YA	3025	1/1	0.85	0.36	54,54,54,54	0
56	MG	RA	3491	1/1	0.85	0.47	60,60,60,60	0
56	MG	RA	3407	1/1	0.85	0.14	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3029	1/1	0.85	0.30	61,61,61,61	0
56	MG	RA	3181	1/1	0.85	0.25	65,65,65,65	0
56	MG	RA	3312	1/1	0.85	0.29	54,54,54,54	0
56	MG	RA	3504	1/1	0.85	0.21	51,51,51,51	0
56	MG	XA	1656	1/1	0.85	0.13	51,51,51,51	0
56	MG	YA	3046	1/1	0.85	0.26	55,55,55,55	0
56	MG	RA	3247	1/1	0.85	0.17	52,52,52,52	0
56	MG	RA	3368	1/1	0.85	0.21	63,63,63,63	0
56	MG	YA	3323	1/1	0.86	0.22	54,54,54,54	0
56	MG	RB	203	1/1	0.86	0.18	49,49,49,49	0
56	MG	QA	1635	1/1	0.86	0.22	64,64,64,64	0
56	MG	YA	3099	1/1	0.86	0.45	66,66,66,66	0
56	MG	YA	3038	1/1	0.86	0.56	59,59,59,59	0
56	MG	YA	3102	1/1	0.86	0.30	61,61,61,61	0
56	MG	YA	3039	1/1	0.86	0.34	51,51,51,51	0
56	MG	YA	3348	1/1	0.86	0.12	63,63,63,63	0
56	MG	XA	1666	1/1	0.86	0.04	56,56,56,56	0
56	MG	RA	3156	1/1	0.86	0.22	59,59,59,59	0
56	MG	YA	3356	1/1	0.86	0.07	78,78,78,78	0
56	MG	YA	3484	1/1	0.86	0.18	60,60,60,60	0
56	MG	RA	3097	1/1	0.86	0.23	52,52,52,52	0
56	MG	YA	3487	1/1	0.86	0.20	54,54,54,54	0
56	MG	YA	3362	1/1	0.86	0.07	61,61,61,61	0
56	MG	RA	3463	1/1	0.86	0.07	68,68,68,68	0
56	MG	YA	3127	1/1	0.86	0.35	66,66,66,66	0
56	MG	RA	3298	1/1	0.86	0.38	60,60,60,60	0
56	MG	RA	3040	1/1	0.86	0.28	64,64,64,64	0
56	MG	YA	3507	1/1	0.86	0.18	60,60,60,60	0
56	MG	RA	3469	1/1	0.86	0.09	64,64,64,64	0
56	MG	YA	3051	1/1	0.86	0.40	48,48,48,48	0
56	MG	RA	3213	1/1	0.86	0.28	69,69,69,69	0
56	MG	RA	3352	1/1	0.86	0.25	68,68,68,68	0
56	MG	YA	3525	1/1	0.86	0.51	54,54,54,54	0
56	MG	RA	3041	1/1	0.86	0.29	67,67,67,67	0
56	MG	RA	3027	1/1	0.86	0.33	57,57,57,57	0
56	MG	RA	3176	1/1	0.86	0.11	66,66,66,66	0
56	MG	YA	3151	1/1	0.86	0.19	67,67,67,67	0
56	MG	RA	3424	1/1	0.86	0.28	55,55,55,55	0
56	MG	RA	3143	1/1	0.86	0.19	70,70,70,70	0
56	MG	RA	3073	1/1	0.86	0.28	52,52,52,52	0
56	MG	RA	3015	1/1	0.86	0.26	59,59,59,59	0
56	MG	RA	3499	1/1	0.86	0.16	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3501	1/1	0.86	0.07	78,78,78,78	0
56	MG	YA	3408	1/1	0.86	0.09	51,51,51,51	0
56	MG	YA	3411	1/1	0.86	0.38	55,55,55,55	0
56	MG	RA	3108	1/1	0.86	0.18	53,53,53,53	0
56	MG	YA	3087	1/1	0.86	0.30	54,54,54,54	0
56	MG	YA	3298	1/1	0.86	0.19	57,57,57,57	0
56	MG	RA	3007	1/1	0.86	0.23	66,66,66,66	0
56	MG	YA	3089	1/1	0.86	0.17	61,61,61,61	0
56	MG	QA	1657	1/1	0.86	0.07	61,61,61,61	0
56	MG	XA	1653	1/1	0.86	0.17	57,57,57,57	0
56	MG	RA	3338	1/1	0.86	0.21	65,65,65,65	0
56	MG	YA	3322	1/1	0.86	0.27	56,56,56,56	0
56	MG	RA	3034	1/1	0.87	0.29	51,51,51,51	0
56	MG	RA	3149	1/1	0.87	0.36	61,61,61,61	0
56	MG	YA	3240	1/1	0.87	0.34	56,56,56,56	0
56	MG	YA	3101	1/1	0.87	0.36	53,53,53,53	0
56	MG	RA	3237	1/1	0.87	0.31	67,67,67,67	0
56	MG	YA	3026	1/1	0.87	0.36	49,49,49,49	0
56	MG	YA	3106	1/1	0.87	0.22	60,60,60,60	0
56	MG	YA	3248	1/1	0.87	0.52	49,49,49,49	0
56	MG	RA	3311	1/1	0.87	0.30	61,61,61,61	0
56	MG	YA	3115	1/1	0.87	0.33	65,65,65,65	0
56	MG	YA	3255	1/1	0.87	0.45	63,63,63,63	0
56	MG	RA	3038	1/1	0.87	0.42	63,63,63,63	0
56	MG	YA	3439	1/1	0.87	0.21	49,49,49,49	0
56	MG	YA	3443	1/1	0.87	0.15	64,64,64,64	0
56	MG	RA	3475	1/1	0.87	0.21	63,63,63,63	0
56	MG	QA	1653	1/1	0.87	0.05	58,58,58,58	0
56	MG	RA	3315	1/1	0.87	0.12	47,47,47,47	0
56	MG	RA	3153	1/1	0.87	0.30	58,58,58,58	0
56	MG	RA	3489	1/1	0.87	0.16	57,57,57,57	0
56	MG	RA	3076	1/1	0.87	0.24	53,53,53,53	0
56	MG	YA	3042	1/1	0.87	0.28	67,67,67,67	0
56	MG	XA	1636	1/1	0.87	0.26	55,55,55,55	0
56	MG	YA	3461	1/1	0.87	0.09	79,79,79,79	0
56	MG	YA	3297	1/1	0.87	0.12	57,57,57,57	0
56	MG	XA	1638	1/1	0.87	0.18	61,61,61,61	0
56	MG	YA	3468	1/1	0.87	0.46	49,49,49,49	0
56	MG	XA	1643	1/1	0.87	0.18	64,64,64,64	0
56	MG	YA	3307	1/1	0.87	0.14	52,52,52,52	0
56	MG	RA	3209	1/1	0.87	0.17	51,51,51,51	0
56	MG	XA	1649	1/1	0.87	0.15	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3131	1/1	0.87	0.27	48,48,48,48	0
56	MG	RA	3329	1/1	0.87	0.08	63,63,63,63	0
56	MG	RA	3132	1/1	0.87	0.32	68,68,68,68	0
56	MG	RA	3135	1/1	0.87	0.36	56,56,56,56	0
56	MG	RA	3101	1/1	0.87	0.25	48,48,48,48	0
56	MG	RA	3052	1/1	0.87	0.16	59,59,59,59	0
56	MG	RA	3258	1/1	0.87	0.17	65,65,65,65	0
56	MG	RA	3342	1/1	0.87	0.27	64,64,64,64	0
56	MG	YA	3506	1/1	0.87	0.31	53,53,53,53	0
56	MG	YA	3173	1/1	0.87	0.29	56,56,56,56	0
56	MG	YA	3064	1/1	0.87	0.25	51,51,51,51	0
56	MG	RA	3263	1/1	0.87	0.18	50,50,50,50	0
56	MG	YA	3070	1/1	0.87	0.21	63,63,63,63	0
56	MG	RA	3169	1/1	0.87	0.34	55,55,55,55	0
56	MG	YA	3521	1/1	0.87	0.25	49,49,49,49	0
56	MG	YA	3072	1/1	0.87	0.37	65,65,65,65	0
56	MG	YA	3360	1/1	0.87	0.39	62,62,62,62	0
56	MG	YA	3527	1/1	0.87	0.49	50,50,50,50	0
56	MG	RA	3430	1/1	0.87	0.19	48,48,48,48	0
56	MG	QA	1625	1/1	0.87	0.19	60,60,60,60	0
56	MG	YA	3534	1/1	0.87	0.26	61,61,61,61	0
56	MG	RA	3276	1/1	0.87	0.31	47,47,47,47	0
56	MG	RA	3278	1/1	0.87	0.21	50,50,50,50	0
56	MG	YA	3367	1/1	0.87	0.14	56,56,56,56	0
56	MG	RO	201	1/1	0.87	0.24	53,53,53,53	0
56	MG	RA	3048	1/1	0.87	0.17	51,51,51,51	0
56	MG	RA	3092	1/1	0.87	0.41	50,50,50,50	0
56	MG	YA	3376	1/1	0.87	0.20	55,55,55,55	0
56	MG	YA	3377	1/1	0.87	0.17	68,68,68,68	0
56	MG	YA	3212	1/1	0.87	0.07	48,48,48,48	0
56	MG	Y9	101	1/1	0.87	0.10	92,92,92,92	0
56	MG	RA	3454	1/1	0.87	0.09	59,59,59,59	0
56	MG	YA	3218	1/1	0.87	0.14	65,65,65,65	0
56	MG	YA	3013	1/1	0.87	0.56	48,48,48,48	0
56	MG	YA	3391	1/1	0.87	0.07	48,48,48,48	0
56	MG	RA	3187	1/1	0.87	0.09	51,51,51,51	0
56	MG	R4	101	1/1	0.87	0.05	51,51,51,51	0
56	MG	YA	3228	1/1	0.87	0.38	63,63,63,63	0
56	MG	RA	3114	1/1	0.87	0.16	52,52,52,52	0
56	MG	YA	3098	1/1	0.87	0.18	50,50,50,50	0
56	MG	YA	3419	1/1	0.88	0.39	60,60,60,60	0
56	MG	QA	1641	1/1	0.88	0.18	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3026	1/1	0.88	0.28	53,53,53,53	0
56	MG	YA	3424	1/1	0.88	0.18	50,50,50,50	0
56	MG	QA	1643	1/1	0.88	0.10	57,57,57,57	0
56	MG	RA	3452	1/1	0.88	0.15	62,62,62,62	0
56	MG	XA	1664	1/1	0.88	0.24	65,65,65,65	0
56	MG	YA	3433	1/1	0.88	0.32	58,58,58,58	0
56	MG	QA	1609	1/1	0.88	0.25	53,53,53,53	0
56	MG	RB	206	1/1	0.88	0.22	64,64,64,64	0
56	MG	QA	1623	1/1	0.88	0.15	57,57,57,57	0
56	MG	YA	3060	1/1	0.88	0.24	66,66,66,66	0
56	MG	RA	3064	1/1	0.88	0.24	54,54,54,54	0
56	MG	YA	3311	1/1	0.88	0.21	64,64,64,64	0
56	MG	RA	3333	1/1	0.88	0.45	62,62,62,62	0
56	MG	RP	201	1/1	0.88	0.23	64,64,64,64	0
56	MG	YA	3171	1/1	0.88	0.11	53,53,53,53	0
56	MG	RA	3334	1/1	0.88	0.31	59,59,59,59	0
56	MG	YA	3319	1/1	0.88	0.25	64,64,64,64	0
56	MG	XV	102	1/1	0.88	0.22	62,62,62,62	0
56	MG	RA	3391	1/1	0.88	0.14	67,67,67,67	0
56	MG	R0	102	1/1	0.88	0.28	65,65,65,65	0
56	MG	RA	3172	1/1	0.88	0.15	58,58,58,58	0
56	MG	YA	3330	1/1	0.88	0.27	61,61,61,61	0
56	MG	RA	3287	1/1	0.88	0.14	64,64,64,64	0
56	MG	RA	3117	1/1	0.88	0.26	47,47,47,47	0
56	MG	YA	3482	1/1	0.88	0.23	49,49,49,49	0
56	MG	YA	3082	1/1	0.88	0.28	50,50,50,50	0
56	MG	YA	3343	1/1	0.88	0.26	56,56,56,56	0
56	MG	RA	3146	1/1	0.88	0.19	58,58,58,58	0
56	MG	YA	3346	1/1	0.88	0.24	60,60,60,60	0
56	MG	YA	3188	1/1	0.88	0.18	60,60,60,60	0
56	MG	RA	3302	1/1	0.88	0.21	59,59,59,59	0
56	MG	YA	3351	1/1	0.88	0.25	62,62,62,62	0
56	MG	YA	3354	1/1	0.88	0.16	64,64,64,64	0
56	MG	YA	3503	1/1	0.88	0.22	63,63,63,63	0
56	MG	YA	3505	1/1	0.88	0.07	74,74,74,74	0
56	MG	YA	3197	1/1	0.88	0.34	55,55,55,55	0
56	MG	QA	1638	1/1	0.88	0.12	63,63,63,63	0
56	MG	YA	3199	1/1	0.88	0.12	65,65,65,65	0
56	MG	RA	3409	1/1	0.88	0.28	53,53,53,53	0
56	MG	XA	1615	1/1	0.88	0.26	55,55,55,55	0
56	MG	RA	3488	1/1	0.88	0.23	58,58,58,58	0
56	MG	QV	106	1/1	0.88	0.20	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3254	1/1	0.88	0.31	48,48,48,48	0
56	MG	RA	3099	1/1	0.88	0.18	48,48,48,48	0
56	MG	RA	3068	1/1	0.88	0.23	52,52,52,52	0
56	MG	RA	3495	1/1	0.88	0.25	50,50,50,50	0
56	MG	YA	3028	1/1	0.88	0.41	53,53,53,53	0
56	MG	QA	1666	1/1	0.88	0.28	79,79,79,79	0
56	MG	RA	3357	1/1	0.88	0.16	48,48,48,48	0
56	MG	YA	3232	1/1	0.88	0.20	49,49,49,49	0
56	MG	YA	3032	1/1	0.88	0.54	57,57,57,57	0
56	MG	RA	3358	1/1	0.88	0.14	63,63,63,63	0
56	MG	YA	3034	1/1	0.88	0.16	50,50,50,50	0
56	MG	RA	3500	1/1	0.88	0.19	66,66,66,66	0
56	MG	YB	208	1/1	0.88	0.18	63,63,63,63	0
56	MG	YA	3036	1/1	0.88	0.45	58,58,58,58	0
56	MG	YA	3124	1/1	0.88	0.20	58,58,58,58	0
56	MG	XA	1641	1/1	0.88	0.19	48,48,48,48	0
56	MG	YA	3400	1/1	0.88	0.30	53,53,53,53	0
56	MG	RA	3134	1/1	0.88	0.13	62,62,62,62	0
56	MG	XA	1645	1/1	0.88	0.15	55,55,55,55	0
56	MG	YA	3041	1/1	0.88	0.29	67,67,67,67	0
56	MG	RA	3364	1/1	0.88	0.21	65,65,65,65	0
56	MG	RA	3440	1/1	0.88	0.35	65,65,65,65	0
56	MG	XA	1650	1/1	0.88	0.15	59,59,59,59	0
56	MG	YA	3261	1/1	0.88	0.20	50,50,50,50	0
56	MG	XA	1651	1/1	0.88	0.12	108,108,108,108	0
56	MG	YA	3414	1/1	0.88	0.06	62,62,62,62	0
56	MG	RA	3154	1/1	0.89	0.17	51,51,51,51	0
56	MG	YA	3015	1/1	0.89	0.34	60,60,60,60	0
56	MG	YA	3169	1/1	0.89	0.36	58,58,58,58	0
56	MG	YA	3429	1/1	0.89	0.19	63,63,63,63	0
56	MG	YA	3170	1/1	0.89	0.12	58,58,58,58	0
56	MG	YA	3302	1/1	0.89	0.23	49,49,49,49	0
56	MG	YA	3438	1/1	0.89	0.15	64,64,64,64	0
56	MG	YA	3016	1/1	0.89	0.36	62,62,62,62	0
56	MG	RA	3426	1/1	0.89	0.05	58,58,58,58	0
56	MG	RA	3023	1/1	0.89	0.14	47,47,47,47	0
56	MG	YA	3448	1/1	0.89	0.07	69,69,69,69	0
56	MG	RA	3496	1/1	0.89	0.16	65,65,65,65	0
56	MG	QA	1645	1/1	0.89	0.14	58,58,58,58	0
56	MG	XA	1631	1/1	0.89	0.13	63,63,63,63	0
56	MG	QV	101	1/1	0.89	0.35	65,65,65,65	0
56	MG	YA	3321	1/1	0.89	0.21	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1665	1/1	0.89	0.23	55,55,55,55	0
56	MG	RA	3433	1/1	0.89	0.13	56,56,56,56	0
56	MG	YA	3184	1/1	0.89	0.27	63,63,63,63	0
56	MG	RA	3268	1/1	0.89	0.33	60,60,60,60	0
56	MG	YA	3328	1/1	0.89	0.28	65,65,65,65	0
56	MG	RA	3439	1/1	0.89	0.16	58,58,58,58	0
56	MG	YA	3470	1/1	0.89	0.39	67,67,67,67	0
56	MG	YA	3475	1/1	0.89	0.25	58,58,58,58	0
56	MG	RA	3093	1/1	0.89	0.37	50,50,50,50	0
56	MG	YA	3191	1/1	0.89	0.18	51,51,51,51	0
56	MG	RA	3319	1/1	0.89	0.15	66,66,66,66	0
56	MG	RA	3271	1/1	0.89	0.20	68,68,68,68	0
56	MG	RA	3273	1/1	0.89	0.17	58,58,58,58	0
56	MG	RA	3451	1/1	0.89	0.09	55,55,55,55	0
56	MG	YA	3347	1/1	0.89	0.12	66,66,66,66	0
56	MG	RA	3126	1/1	0.89	0.23	54,54,54,54	0
56	MG	YA	3103	1/1	0.89	0.13	89,89,89,89	0
56	MG	RA	3127	1/1	0.89	0.21	56,56,56,56	0
56	MG	YA	3353	1/1	0.89	0.21	61,61,61,61	0
56	MG	YA	3105	1/1	0.89	0.25	50,50,50,50	0
56	MG	YA	3219	1/1	0.89	0.30	64,64,64,64	0
56	MG	RA	3170	1/1	0.89	0.17	63,63,63,63	0
56	MG	RA	3387	1/1	0.89	0.15	67,67,67,67	0
56	MG	YA	3110	1/1	0.89	0.22	59,59,59,59	0
56	MG	YA	3114	1/1	0.89	0.22	53,53,53,53	0
56	MG	YA	3509	1/1	0.89	0.12	61,61,61,61	0
56	MG	XA	1657	1/1	0.89	0.19	51,51,51,51	0
56	MG	XA	1658	1/1	0.89	0.07	57,57,57,57	0
56	MG	YA	3120	1/1	0.89	0.52	47,47,47,47	0
56	MG	RN	201	1/1	0.89	0.09	53,53,53,53	0
56	MG	RA	3241	1/1	0.89	0.20	48,48,48,48	0
56	MG	RA	3130	1/1	0.89	0.16	64,64,64,64	0
56	MG	RA	3464	1/1	0.89	0.31	58,58,58,58	0
56	MG	RA	3043	1/1	0.89	0.26	64,64,64,64	0
56	MG	R0	101	1/1	0.89	0.31	53,53,53,53	0
56	MG	RA	3006	1/1	0.89	0.19	61,61,61,61	0
56	MG	RA	3110	1/1	0.89	0.32	67,67,67,67	0
56	MG	RA	3343	1/1	0.89	0.10	59,59,59,59	0
56	MG	YA	3389	1/1	0.89	0.43	65,65,65,65	0
56	MG	YA	3538	1/1	0.89	0.21	105,105,105,105	0
56	MG	RA	3250	1/1	0.89	0.22	59,59,59,59	0
56	MG	YA	3542	1/1	0.89	0.23	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3251	1/1	0.89	0.27	57,57,57,57	0
56	MG	YA	3143	1/1	0.89	0.24	63,63,63,63	0
56	MG	YA	3258	1/1	0.89	0.42	55,55,55,55	0
56	MG	RA	3405	1/1	0.89	0.54	76,76,76,76	0
56	MG	YB	209	1/1	0.89	0.09	53,53,53,53	0
56	MG	RA	3347	1/1	0.89	0.18	60,60,60,60	0
56	MG	RA	3053	1/1	0.89	0.46	66,66,66,66	0
56	MG	YA	3262	1/1	0.89	0.32	66,66,66,66	0
56	MG	Y0	101	1/1	0.89	0.12	58,58,58,58	0
56	MG	XA	1607	1/1	0.89	0.13	57,57,57,57	0
56	MG	YA	3063	1/1	0.89	0.19	55,55,55,55	0
56	MG	RA	3189	1/1	0.89	0.12	61,61,61,61	0
56	MG	YA	3276	1/1	0.89	0.45	61,61,61,61	0
56	MG	RA	3253	1/1	0.89	0.23	64,64,64,64	0
56	MG	YA	3010	1/1	0.89	0.20	62,62,62,62	0
56	MG	RA	3308	1/1	0.89	0.20	53,53,53,53	0
56	MG	YA	3288	1/1	0.89	0.12	48,48,48,48	0
56	MG	YA	3289	1/1	0.89	0.12	59,59,59,59	0
56	MG	YA	3295	1/1	0.89	0.29	51,51,51,51	0
56	MG	RA	3413	1/1	0.90	0.15	52,52,52,52	0
56	MG	YA	3146	1/1	0.90	0.24	51,51,51,51	0
56	MG	RA	3211	1/1	0.90	0.15	60,60,60,60	0
56	MG	RA	3366	1/1	0.90	0.09	60,60,60,60	0
56	MG	YA	3023	1/1	0.90	0.23	61,61,61,61	0
56	MG	XA	1647	1/1	0.90	0.23	65,65,65,65	0
56	MG	YA	3467	1/1	0.90	0.16	55,55,55,55	0
56	MG	RA	3473	1/1	0.90	0.18	67,67,67,67	0
56	MG	RA	3367	1/1	0.90	0.20	57,57,57,57	0
56	MG	RA	3420	1/1	0.90	0.20	63,63,63,63	0
56	MG	YA	3162	1/1	0.90	0.27	56,56,56,56	0
56	MG	QA	1652	1/1	0.90	0.06	67,67,67,67	0
56	MG	RA	3337	1/1	0.90	0.07	65,65,65,65	0
56	MG	YA	3091	1/1	0.90	0.17	56,56,56,56	0
56	MG	RA	3485	1/1	0.90	0.11	69,69,69,69	0
56	MG	QA	1662	1/1	0.90	0.14	84,84,84,84	0
56	MG	YA	3485	1/1	0.90	0.17	65,65,65,65	0
56	MG	RA	3306	1/1	0.90	0.21	53,53,53,53	0
56	MG	YA	3372	1/1	0.90	0.15	56,56,56,56	0
56	MG	RA	3191	1/1	0.90	0.26	61,61,61,61	0
56	MG	XA	1663	1/1	0.90	0.18	64,64,64,64	0
56	MG	YA	3273	1/1	0.90	0.33	63,63,63,63	0
56	MG	RA	3195	1/1	0.90	0.09	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	R9	101	1/1	0.90	0.09	66,66,66,66	0
56	MG	RA	3493	1/1	0.90	0.53	67,67,67,67	0
56	MG	RA	3381	1/1	0.90	0.15	52,52,52,52	0
56	MG	YA	3382	1/1	0.90	0.20	66,66,66,66	0
56	MG	QA	1624	1/1	0.90	0.07	51,51,51,51	0
56	MG	RA	3221	1/1	0.90	0.09	50,50,50,50	0
56	MG	YA	3510	1/1	0.90	0.16	76,76,76,76	0
56	MG	YA	3043	1/1	0.90	0.25	65,65,65,65	0
56	MG	YA	3512	1/1	0.90	0.21	58,58,58,58	0
56	MG	YA	3514	1/1	0.90	0.13	50,50,50,50	0
56	MG	RA	3060	1/1	0.90	0.54	48,48,48,48	0
56	MG	XA	1616	1/1	0.90	0.28	54,54,54,54	0
56	MG	YA	3517	1/1	0.90	0.23	64,64,64,64	0
56	MG	RA	3390	1/1	0.90	0.23	62,62,62,62	0
56	MG	YA	3520	1/1	0.90	0.23	56,56,56,56	0
56	MG	RA	3171	1/1	0.90	0.11	48,48,48,48	0
56	MG	RA	3200	1/1	0.90	0.20	65,65,65,65	0
56	MG	RA	3010	1/1	0.90	0.16	63,63,63,63	0
56	MG	YA	3305	1/1	0.90	0.23	65,65,65,65	0
56	MG	XA	1627	1/1	0.90	0.25	57,57,57,57	0
56	MG	YA	3202	1/1	0.90	0.09	55,55,55,55	0
56	MG	YA	3532	1/1	0.90	0.24	60,60,60,60	0
56	MG	YA	3533	1/1	0.90	0.15	59,59,59,59	0
56	MG	YA	3204	1/1	0.90	0.22	64,64,64,64	0
56	MG	YA	3052	1/1	0.90	0.34	50,50,50,50	0
56	MG	YA	3314	1/1	0.90	0.30	48,48,48,48	0
56	MG	YA	3208	1/1	0.90	0.20	61,61,61,61	0
56	MG	YA	3006	1/1	0.90	0.19	50,50,50,50	0
56	MG	YA	3418	1/1	0.90	0.13	51,51,51,51	0
56	MG	YA	3213	1/1	0.90	0.16	65,65,65,65	0
56	MG	YA	3546	1/1	0.90	0.38	61,61,61,61	0
56	MG	YB	201	1/1	0.90	0.12	57,57,57,57	0
56	MG	YA	3214	1/1	0.90	0.07	65,65,65,65	0
56	MG	RA	3129	1/1	0.90	0.22	53,53,53,53	0
56	MG	YA	3055	1/1	0.90	0.45	54,54,54,54	0
56	MG	YA	3008	1/1	0.90	0.28	61,61,61,61	0
56	MG	QA	1654	1/1	0.90	0.09	61,61,61,61	0
56	MG	RA	3326	1/1	0.90	0.18	49,49,49,49	0
56	MG	YP	203	1/1	0.90	0.29	56,56,56,56	0
56	MG	YA	3430	1/1	0.90	0.28	50,50,50,50	0
56	MG	RA	3288	1/1	0.90	0.18	51,51,51,51	0
56	MG	YA	3331	1/1	0.90	0.19	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3406	1/1	0.90	0.10	53,53,53,53	0
56	MG	YA	3333	1/1	0.90	0.39	47,47,47,47	0
56	MG	YA	3334	1/1	0.90	0.16	53,53,53,53	0
56	MG	YA	3014	1/1	0.90	0.25	64,64,64,64	0
56	MG	RA	3180	1/1	0.90	0.12	49,49,49,49	0
56	MG	YA	3338	1/1	0.90	0.09	58,58,58,58	0
56	MG	YA	3340	1/1	0.90	0.24	48,48,48,48	0
56	MG	RA	3165	1/1	0.90	0.16	66,66,66,66	0
56	MG	RA	3412	1/1	0.90	0.18	61,61,61,61	0
56	MG	YA	3004	1/1	0.91	0.43	50,50,50,50	0
56	MG	YA	3472	1/1	0.91	0.12	66,66,66,66	0
56	MG	XA	1601	1/1	0.91	0.34	58,58,58,58	0
56	MG	YA	3357	1/1	0.91	0.15	53,53,53,53	0
56	MG	RA	3292	1/1	0.91	0.36	66,66,66,66	0
56	MG	YA	3154	1/1	0.91	0.14	49,49,49,49	0
56	MG	RA	3481	1/1	0.91	0.21	50,50,50,50	0
56	MG	RA	3244	1/1	0.91	0.22	50,50,50,50	0
56	MG	RA	3300	1/1	0.91	0.17	54,54,54,54	0
56	MG	RA	3109	1/1	0.91	0.33	48,48,48,48	0
56	MG	RA	3486	1/1	0.91	0.22	49,49,49,49	0
56	MG	QF	201	1/1	0.91	0.10	66,66,66,66	0
56	MG	YA	3265	1/1	0.91	0.30	63,63,63,63	0
56	MG	YA	3490	1/1	0.91	0.09	56,56,56,56	0
56	MG	YA	3495	1/1	0.91	0.21	65,65,65,65	0
56	MG	RA	3216	1/1	0.91	0.09	56,56,56,56	0
56	MG	YA	3167	1/1	0.91	0.17	56,56,56,56	0
56	MG	YA	3272	1/1	0.91	0.14	55,55,55,55	0
56	MG	RA	3218	1/1	0.91	0.16	63,63,63,63	0
56	MG	RA	3184	1/1	0.91	0.17	70,70,70,70	0
56	MG	RA	3307	1/1	0.91	0.22	65,65,65,65	0
56	MG	RA	3113	1/1	0.91	0.20	50,50,50,50	0
56	MG	RA	3310	1/1	0.91	0.39	59,59,59,59	0
56	MG	YA	3285	1/1	0.91	0.22	51,51,51,51	0
56	MG	XA	1630	1/1	0.91	0.18	61,61,61,61	0
56	MG	YA	3090	1/1	0.91	0.23	60,60,60,60	0
56	MG	QA	1601	1/1	0.91	0.24	59,59,59,59	0
56	MG	YA	3290	1/1	0.91	0.12	56,56,56,56	0
56	MG	QA	1606	1/1	0.91	0.21	66,66,66,66	0
56	MG	RA	3226	1/1	0.91	0.32	60,60,60,60	0
56	MG	RA	3194	1/1	0.91	0.08	58,58,58,58	0
56	MG	YA	3518	1/1	0.91	0.08	64,64,64,64	0
56	MG	RA	3157	1/1	0.91	0.26	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3264	1/1	0.91	0.37	57,57,57,57	0
56	MG	RA	3503	1/1	0.91	0.08	57,57,57,57	0
56	MG	YA	3523	1/1	0.91	0.45	52,52,52,52	0
56	MG	RA	3046	1/1	0.91	0.36	66,66,66,66	0
56	MG	RA	3138	1/1	0.91	0.14	59,59,59,59	0
56	MG	RA	3443	1/1	0.91	0.20	58,58,58,58	0
56	MG	RA	3508	1/1	0.91	0.22	47,47,47,47	0
56	MG	RA	3444	1/1	0.91	0.12	59,59,59,59	0
56	MG	YA	3530	1/1	0.91	0.19	54,54,54,54	0
56	MG	RA	3320	1/1	0.91	0.13	56,56,56,56	0
56	MG	RA	3231	1/1	0.91	0.30	65,65,65,65	0
56	MG	RA	3450	1/1	0.91	0.19	67,67,67,67	0
56	MG	RA	3141	1/1	0.91	0.08	63,63,63,63	0
56	MG	RA	3058	1/1	0.91	0.36	52,52,52,52	0
56	MG	RA	3275	1/1	0.91	0.29	61,61,61,61	0
56	MG	XA	1659	1/1	0.91	0.06	52,52,52,52	0
56	MG	YA	3116	1/1	0.91	0.24	54,54,54,54	0
56	MG	RA	3120	1/1	0.91	0.25	52,52,52,52	0
56	MG	RA	3456	1/1	0.91	0.10	63,63,63,63	0
56	MG	RO	202	1/1	0.91	0.22	60,60,60,60	0
56	MG	YA	3436	1/1	0.91	0.10	64,64,64,64	0
56	MG	RA	3059	1/1	0.91	0.10	48,48,48,48	0
56	MG	RQ	201	1/1	0.91	0.17	57,57,57,57	0
56	MG	YA	3441	1/1	0.91	0.15	65,65,65,65	0
56	MG	RA	3393	1/1	0.91	0.26	60,60,60,60	0
56	MG	YA	3223	1/1	0.91	0.20	51,51,51,51	0
56	MG	YD	302	1/1	0.91	0.33	55,55,55,55	0
56	MG	QA	1659	1/1	0.91	0.05	56,56,56,56	0
56	MG	YQ	201	1/1	0.91	0.19	55,55,55,55	0
56	MG	RA	3280	1/1	0.91	0.28	53,53,53,53	0
56	MG	YX	101	1/1	0.91	0.12	51,51,51,51	0
56	MG	RA	3398	1/1	0.91	0.20	62,62,62,62	0
56	MG	Y8	101	1/1	0.91	0.11	66,66,66,66	0
56	MG	RA	3089	1/1	0.91	0.29	56,56,56,56	0
56	MG	YA	3133	1/1	0.91	0.08	54,54,54,54	0
56	MG	RA	3017	1/1	0.91	0.35	50,50,50,50	0
56	MG	RA	3011	1/1	0.91	0.25	58,58,58,58	0
56	MG	YA	3141	1/1	0.91	0.15	60,60,60,60	0
56	MG	YA	3142	1/1	0.91	0.18	75,75,75,75	0
58	ZN	YY	202	1/1	0.91	0.13	189,189,189,189	0
56	MG	YA	3058	1/1	0.91	0.52	57,57,57,57	0
56	MG	QV	102	1/1	0.91	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3290	1/1	0.91	0.21	61,61,61,61	0
56	MG	YA	3247	1/1	0.91	0.23	52,52,52,52	0
56	MG	XA	1680	1/1	0.92	0.18	57,57,57,57	0
56	MG	YA	3270	1/1	0.92	0.08	52,52,52,52	0
56	MG	QA	1668	1/1	0.92	0.06	57,57,57,57	0
56	MG	RA	3294	1/1	0.92	0.19	57,57,57,57	0
56	MG	XA	1612	1/1	0.92	0.21	47,47,47,47	0
56	MG	YA	3365	1/1	0.92	0.15	47,47,47,47	0
56	MG	RA	3361	1/1	0.92	0.18	67,67,67,67	0
56	MG	YA	3277	1/1	0.92	0.24	61,61,61,61	0
56	MG	YA	3278	1/1	0.92	0.38	48,48,48,48	0
56	MG	RA	3404	1/1	0.92	0.39	60,60,60,60	0
56	MG	YA	3282	1/1	0.92	0.19	61,61,61,61	0
56	MG	XA	1618	1/1	0.92	0.20	52,52,52,52	0
56	MG	YA	3284	1/1	0.92	0.12	60,60,60,60	0
56	MG	XV	103	1/1	0.92	0.09	59,59,59,59	0
56	MG	YA	3497	1/1	0.92	0.18	67,67,67,67	0
56	MG	YA	3498	1/1	0.92	0.08	66,66,66,66	0
56	MG	YA	3189	1/1	0.92	0.10	65,65,65,65	0
56	MG	RA	3502	1/1	0.92	0.35	65,65,65,65	0
56	MG	YA	3001	1/1	0.92	0.36	60,60,60,60	0
56	MG	RA	3362	1/1	0.92	0.20	61,61,61,61	0
56	MG	YA	3385	1/1	0.92	0.18	61,61,61,61	0
56	MG	YA	3291	1/1	0.92	0.22	64,64,64,64	0
56	MG	RA	3296	1/1	0.92	0.23	58,58,58,58	0
56	MG	QA	1620	1/1	0.92	0.06	62,62,62,62	0
56	MG	YA	3395	1/1	0.92	0.27	64,64,64,64	0
56	MG	RA	3299	1/1	0.92	0.24	48,48,48,48	0
56	MG	YA	3123	1/1	0.92	0.38	67,67,67,67	0
56	MG	YA	3513	1/1	0.92	0.17	67,67,67,67	0
56	MG	YA	3398	1/1	0.92	0.12	50,50,50,50	0
56	MG	QA	1649	1/1	0.92	0.13	70,70,70,70	0
56	MG	RA	3003	1/1	0.92	0.33	49,49,49,49	0
56	MG	YA	3303	1/1	0.92	0.18	54,54,54,54	0
56	MG	RA	3004	1/1	0.92	0.30	60,60,60,60	0
56	MG	RA	3179	1/1	0.92	0.12	67,67,67,67	0
56	MG	RA	3373	1/1	0.92	0.12	69,69,69,69	0
56	MG	YA	3406	1/1	0.92	0.21	58,58,58,58	0
56	MG	YA	3522	1/1	0.92	0.32	79,79,79,79	0
56	MG	RA	3419	1/1	0.92	0.24	63,63,63,63	0
56	MG	YA	3012	1/1	0.92	0.20	62,62,62,62	0
56	MG	RA	3374	1/1	0.92	0.12	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3225	1/1	0.92	0.20	50,50,50,50	0
56	MG	YA	3134	1/1	0.92	0.19	59,59,59,59	0
56	MG	YA	3416	1/1	0.92	0.07	67,67,67,67	0
56	MG	RA	3476	1/1	0.92	0.17	57,57,57,57	0
56	MG	YA	3320	1/1	0.92	0.18	56,56,56,56	0
56	MG	YA	3421	1/1	0.92	0.14	70,70,70,70	0
56	MG	RA	3246	1/1	0.92	0.22	51,51,51,51	0
56	MG	RA	3480	1/1	0.92	0.05	57,57,57,57	0
56	MG	QA	1621	1/1	0.92	0.15	53,53,53,53	0
56	MG	YA	3019	1/1	0.92	0.35	54,54,54,54	0
56	MG	YA	3074	1/1	0.92	0.48	48,48,48,48	0
56	MG	YA	3327	1/1	0.92	0.18	61,61,61,61	0
56	MG	QA	1618	1/1	0.92	0.09	73,73,73,73	0
56	MG	YA	3233	1/1	0.92	0.06	48,48,48,48	0
56	MG	YA	3077	1/1	0.92	0.38	56,56,56,56	0
56	MG	RA	3277	1/1	0.92	0.26	53,53,53,53	0
56	MG	YB	206	1/1	0.92	0.13	49,49,49,49	0
56	MG	RT	201	1/1	0.92	0.13	62,62,62,62	0
56	MG	RU	201	1/1	0.92	0.24	65,65,65,65	0
56	MG	YA	3083	1/1	0.92	0.22	52,52,52,52	0
56	MG	YB	210	1/1	0.92	0.08	78,78,78,78	0
56	MG	YA	3084	1/1	0.92	0.24	66,66,66,66	0
56	MG	RA	3249	1/1	0.92	0.40	51,51,51,51	0
56	MG	RA	3182	1/1	0.92	0.07	77,77,77,77	0
56	MG	YO	201	1/1	0.92	0.25	65,65,65,65	0
56	MG	YA	3342	1/1	0.92	0.14	61,61,61,61	0
56	MG	RA	3436	1/1	0.92	0.11	61,61,61,61	0
56	MG	YA	3451	1/1	0.92	0.20	62,62,62,62	0
56	MG	QA	1627	1/1	0.92	0.11	59,59,59,59	0
56	MG	YX	102	1/1	0.92	0.20	63,63,63,63	0
56	MG	YA	3345	1/1	0.92	0.10	70,70,70,70	0
56	MG	RA	3210	1/1	0.92	0.21	58,58,58,58	0
56	MG	YA	3030	1/1	0.92	0.56	60,60,60,60	0
56	MG	YA	3459	1/1	0.92	0.19	58,58,58,58	0
56	MG	RA	3392	1/1	0.92	0.18	58,58,58,58	0
56	MG	QA	1639	1/1	0.92	0.12	61,61,61,61	0
56	MG	RA	3394	1/1	0.92	0.06	65,65,65,65	0
56	MG	QA	1619	1/1	0.92	0.13	48,48,48,48	0
56	MG	QA	1629	1/1	0.92	0.07	67,67,67,67	0
56	MG	XA	1668	1/1	0.92	0.08	59,59,59,59	0
56	MG	YA	3175	1/1	0.92	0.13	61,61,61,61	0
56	MG	YA	3471	1/1	0.92	0.07	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QV	105	1/1	0.92	0.23	54,54,54,54	0
56	MG	XA	1660	1/1	0.93	0.18	52,52,52,52	0
56	MG	RA	3285	1/1	0.93	0.11	58,58,58,58	0
56	MG	YA	3230	1/1	0.93	0.10	66,66,66,66	0
56	MG	RA	3205	1/1	0.93	0.30	61,61,61,61	0
56	MG	RA	3082	1/1	0.93	0.10	53,53,53,53	0
56	MG	XA	1665	1/1	0.93	0.07	60,60,60,60	0
56	MG	RA	3124	1/1	0.93	0.11	54,54,54,54	0
56	MG	RA	3479	1/1	0.93	0.18	57,57,57,57	0
56	MG	YA	3239	1/1	0.93	0.26	50,50,50,50	0
56	MG	RA	3321	1/1	0.93	0.20	57,57,57,57	0
56	MG	XA	1674	1/1	0.93	0.07	56,56,56,56	0
56	MG	XA	1676	1/1	0.93	0.10	50,50,50,50	0
56	MG	XA	1678	1/1	0.93	0.12	62,62,62,62	0
56	MG	YA	3135	1/1	0.93	0.14	55,55,55,55	0
56	MG	RA	3158	1/1	0.93	0.07	61,61,61,61	0
56	MG	XA	1681	1/1	0.93	0.10	61,61,61,61	0
56	MG	RA	3324	1/1	0.93	0.14	50,50,50,50	0
56	MG	XE	201	1/1	0.93	0.05	53,53,53,53	0
56	MG	RA	3291	1/1	0.93	0.30	54,54,54,54	0
56	MG	YA	3253	1/1	0.93	0.19	60,60,60,60	0
56	MG	YA	3366	1/1	0.93	0.04	62,62,62,62	0
56	MG	RA	3328	1/1	0.93	0.22	48,48,48,48	0
56	MG	QA	1615	1/1	0.93	0.17	57,57,57,57	0
56	MG	XA	1602	1/1	0.93	0.19	61,61,61,61	0
56	MG	RA	3330	1/1	0.93	0.13	53,53,53,53	0
56	MG	RA	3293	1/1	0.93	0.24	61,61,61,61	0
56	MG	XV	104	1/1	0.93	0.07	49,49,49,49	0
56	MG	YA	3264	1/1	0.93	0.16	51,51,51,51	0
56	MG	YA	3378	1/1	0.93	0.13	58,58,58,58	0
56	MG	XA	1606	1/1	0.93	0.30	60,60,60,60	0
56	MG	YA	3067	1/1	0.93	0.49	63,63,63,63	0
56	MG	QA	1634	1/1	0.93	0.13	52,52,52,52	0
56	MG	RA	3431	1/1	0.93	0.06	53,53,53,53	0
56	MG	RA	3163	1/1	0.93	0.16	52,52,52,52	0
56	MG	RA	3297	1/1	0.93	0.19	55,55,55,55	0
56	MG	YA	3386	1/1	0.93	0.17	66,66,66,66	0
56	MG	YA	3388	1/1	0.93	0.20	54,54,54,54	0
56	MG	YA	3073	1/1	0.93	0.11	64,64,64,64	0
56	MG	RA	3386	1/1	0.93	0.20	55,55,55,55	0
56	MG	YA	3392	1/1	0.93	0.10	66,66,66,66	0
56	MG	RA	3262	1/1	0.93	0.21	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3188	1/1	0.93	0.20	62,62,62,62	0
56	MG	RA	3389	1/1	0.93	0.18	53,53,53,53	0
56	MG	YA	3281	1/1	0.93	0.19	62,62,62,62	0
56	MG	RA	3112	1/1	0.93	0.10	55,55,55,55	0
56	MG	YA	3172	1/1	0.93	0.56	66,66,66,66	0
56	MG	YA	3081	1/1	0.93	0.48	49,49,49,49	0
56	MG	RA	3021	1/1	0.93	0.15	63,63,63,63	0
56	MG	RA	3032	1/1	0.93	0.32	51,51,51,51	0
56	MG	RA	3447	1/1	0.93	0.26	48,48,48,48	0
56	MG	RA	3217	1/1	0.93	0.11	50,50,50,50	0
56	MG	RA	3272	1/1	0.93	0.33	59,59,59,59	0
56	MG	RA	3066	1/1	0.93	0.40	57,57,57,57	0
56	MG	YA	3293	1/1	0.93	0.16	56,56,56,56	0
56	MG	RA	3396	1/1	0.93	0.20	59,59,59,59	0
56	MG	YA	3181	1/1	0.93	0.30	50,50,50,50	0
56	MG	YA	3182	1/1	0.93	0.06	51,51,51,51	0
56	MG	XA	1633	1/1	0.93	0.18	50,50,50,50	0
56	MG	YA	3417	1/1	0.93	0.23	48,48,48,48	0
56	MG	XA	1634	1/1	0.93	0.11	60,60,60,60	0
56	MG	YA	3185	1/1	0.93	0.17	66,66,66,66	0
56	MG	YA	3186	1/1	0.93	0.18	65,65,65,65	0
56	MG	QA	1605	1/1	0.93	0.31	47,47,47,47	0
56	MG	QA	1667	1/1	0.93	0.14	70,70,70,70	0
56	MG	YA	3021	1/1	0.93	0.33	47,47,47,47	0
56	MG	RB	202	1/1	0.93	0.08	49,49,49,49	0
56	MG	XA	1640	1/1	0.93	0.25	48,48,48,48	0
56	MG	RA	3309	1/1	0.93	0.17	53,53,53,53	0
56	MG	RA	3245	1/1	0.93	0.16	60,60,60,60	0
56	MG	RA	3460	1/1	0.93	0.09	47,47,47,47	0
56	MG	RA	3080	1/1	0.93	0.23	64,64,64,64	0
56	MG	RA	3223	1/1	0.93	0.41	55,55,55,55	0
56	MG	RA	3121	1/1	0.93	0.24	57,57,57,57	0
56	MG	RF	301	1/1	0.93	0.15	50,50,50,50	0
56	MG	RA	3069	1/1	0.93	0.15	61,61,61,61	0
56	MG	YA	3209	1/1	0.93	0.14	56,56,56,56	0
56	MG	XA	1652	1/1	0.93	0.17	53,53,53,53	0
56	MG	RA	3467	1/1	0.93	0.19	52,52,52,52	0
56	MG	Y7	101	1/1	0.93	0.10	63,63,63,63	0
56	MG	RA	3360	1/1	0.93	0.14	61,61,61,61	0
56	MG	YA	3216	1/1	0.93	0.15	60,60,60,60	0
56	MG	YA	3112	1/1	0.93	0.14	55,55,55,55	0
56	MG	YA	3452	1/1	0.93	0.17	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3204	1/1	0.93	0.15	61,61,61,61	0
56	MG	RA	3470	1/1	0.93	0.08	52,52,52,52	0
56	MG	YA	3037	1/1	0.93	0.33	63,63,63,63	0
56	MG	RQ	202	1/1	0.93	0.23	56,56,56,56	0
56	MG	RA	3411	1/1	0.93	0.30	53,53,53,53	0
56	MG	YA	3225	1/1	0.93	0.17	57,57,57,57	0
56	MG	YA	3121	1/1	0.93	0.14	56,56,56,56	0
56	MG	YA	3464	1/1	0.93	0.06	57,57,57,57	0
56	MG	QA	1642	1/1	0.94	0.07	54,54,54,54	0
56	MG	YA	3107	1/1	0.94	0.09	61,61,61,61	0
56	MG	RA	3421	1/1	0.94	0.15	61,61,61,61	0
56	MG	XA	1637	1/1	0.94	0.10	51,51,51,51	0
56	MG	RA	3183	1/1	0.94	0.05	59,59,59,59	0
56	MG	YA	3113	1/1	0.94	0.13	49,49,49,49	0
56	MG	XA	1639	1/1	0.94	0.04	54,54,54,54	0
56	MG	YA	3431	1/1	0.94	0.20	52,52,52,52	0
56	MG	RA	3201	1/1	0.94	0.08	62,62,62,62	0
56	MG	RA	3266	1/1	0.94	0.34	65,65,65,65	0
56	MG	YA	3117	1/1	0.94	0.23	54,54,54,54	0
56	MG	QA	1650	1/1	0.94	0.07	61,61,61,61	0
56	MG	YA	3119	1/1	0.94	0.26	66,66,66,66	0
56	MG	YA	3440	1/1	0.94	0.11	47,47,47,47	0
56	MG	QA	1614	1/1	0.94	0.14	50,50,50,50	0
56	MG	YA	3442	1/1	0.94	0.23	69,69,69,69	0
56	MG	YA	3075	1/1	0.94	0.15	48,48,48,48	0
56	MG	YA	3373	1/1	0.94	0.21	57,57,57,57	0
56	MG	YA	3241	1/1	0.94	0.28	57,57,57,57	0
56	MG	RA	3270	1/1	0.94	0.33	56,56,56,56	0
56	MG	RA	3159	1/1	0.94	0.12	58,58,58,58	0
56	MG	RA	3432	1/1	0.94	0.20	67,67,67,67	0
56	MG	RA	3506	1/1	0.94	0.08	104,104,104,104	0
56	MG	RA	3094	1/1	0.94	0.23	51,51,51,51	0
56	MG	RA	3474	1/1	0.94	0.08	61,61,61,61	0
56	MG	RA	3369	1/1	0.94	0.17	54,54,54,54	0
56	MG	RA	3370	1/1	0.94	0.17	64,64,64,64	0
56	MG	RA	3295	1/1	0.94	0.34	65,65,65,65	0
56	MG	YA	3252	1/1	0.94	0.31	59,59,59,59	0
56	MG	RA	3161	1/1	0.94	0.09	54,54,54,54	0
56	MG	YA	3387	1/1	0.94	0.29	57,57,57,57	0
56	MG	RA	3193	1/1	0.94	0.25	51,51,51,51	0
56	MG	YA	3324	1/1	0.94	0.14	61,61,61,61	0
56	MG	RA	3152	1/1	0.94	0.14	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YB	203	1/1	0.94	0.04	66,66,66,66	0
56	MG	RA	3240	1/1	0.94	0.22	51,51,51,51	0
56	MG	YA	3137	1/1	0.94	0.20	49,49,49,49	0
56	MG	XA	1661	1/1	0.94	0.12	52,52,52,52	0
56	MG	RA	3378	1/1	0.94	0.20	51,51,51,51	0
56	MG	YA	3263	1/1	0.94	0.19	67,67,67,67	0
56	MG	RA	3408	1/1	0.94	0.13	68,68,68,68	0
56	MG	XA	1623	1/1	0.94	0.07	66,66,66,66	0
56	MG	RA	3255	1/1	0.94	0.22	59,59,59,59	0
56	MG	QA	1608	1/1	0.94	0.14	52,52,52,52	0
56	MG	YE	301	1/1	0.94	0.22	62,62,62,62	0
56	MG	RA	3128	1/1	0.94	0.28	64,64,64,64	0
56	MG	YP	201	1/1	0.94	0.06	56,56,56,56	0
56	MG	YA	3271	1/1	0.94	0.23	50,50,50,50	0
56	MG	YA	3404	1/1	0.94	0.12	66,66,66,66	0
56	MG	YA	3148	1/1	0.94	0.12	54,54,54,54	0
56	MG	YA	3056	1/1	0.94	0.08	48,48,48,48	0
56	MG	RA	3490	1/1	0.94	0.17	59,59,59,59	0
56	MG	YA	3489	1/1	0.94	0.38	67,67,67,67	0
56	MG	RA	3383	1/1	0.94	0.07	52,52,52,52	0
56	MG	YA	3491	1/1	0.94	0.09	56,56,56,56	0
56	MG	YA	3494	1/1	0.94	0.12	55,55,55,55	0
56	MG	RA	3303	1/1	0.94	0.41	64,64,64,64	0
56	MG	YA	3215	1/1	0.94	0.22	51,51,51,51	0
56	MG	YA	3156	1/1	0.94	0.21	61,61,61,61	0
56	MG	YA	3415	1/1	0.94	0.06	48,48,48,48	0
56	MG	QA	1647	1/1	0.94	0.11	55,55,55,55	0
56	MG	RA	3355	1/1	0.94	0.07	59,59,59,59	0
56	MG	YA	3350	1/1	0.94	0.06	81,81,81,81	0
56	MG	YA	3159	1/1	0.94	0.10	65,65,65,65	0
56	MG	YA	3504	1/1	0.94	0.14	58,58,58,58	0
56	MG	RA	3260	1/1	0.94	0.27	64,64,64,64	0
56	MG	RA	3356	1/1	0.95	0.15	64,64,64,64	0
56	MG	XA	1667	1/1	0.95	0.10	56,56,56,56	0
56	MG	RA	3164	1/1	0.95	0.14	60,60,60,60	0
56	MG	XA	1669	1/1	0.95	0.09	50,50,50,50	0
56	MG	XA	1670	1/1	0.95	0.10	70,70,70,70	0
56	MG	XA	1672	1/1	0.95	0.06	53,53,53,53	0
56	MG	YA	3192	1/1	0.95	0.13	55,55,55,55	0
56	MG	YA	3336	1/1	0.95	0.06	52,52,52,52	0
56	MG	YA	3195	1/1	0.95	0.08	48,48,48,48	0
56	MG	RA	3203	1/1	0.95	0.09	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3327	1/1	0.95	0.21	59,59,59,59	0
56	MG	YA	3341	1/1	0.95	0.13	51,51,51,51	0
56	MG	XA	1626	1/1	0.95	0.10	65,65,65,65	0
56	MG	YA	3269	1/1	0.95	0.35	57,57,57,57	0
56	MG	YA	3138	1/1	0.95	0.20	66,66,66,66	0
56	MG	XA	1677	1/1	0.95	0.05	73,73,73,73	0
56	MG	YA	3203	1/1	0.95	0.25	61,61,61,61	0
56	MG	RE	301	1/1	0.95	0.17	59,59,59,59	0
56	MG	YA	3274	1/1	0.95	0.31	49,49,49,49	0
56	MG	YA	3205	1/1	0.95	0.14	57,57,57,57	0
56	MG	RA	3103	1/1	0.95	0.18	50,50,50,50	0
56	MG	YA	3427	1/1	0.95	0.09	57,57,57,57	0
56	MG	RA	3166	1/1	0.95	0.20	54,54,54,54	0
56	MG	YA	3352	1/1	0.95	0.08	62,62,62,62	0
56	MG	QA	1630	1/1	0.95	0.06	60,60,60,60	0
56	MG	RA	3125	1/1	0.95	0.09	56,56,56,56	0
56	MG	RA	3118	1/1	0.95	0.15	66,66,66,66	0
56	MG	YA	3434	1/1	0.95	0.09	56,56,56,56	0
56	MG	YA	3435	1/1	0.95	0.07	56,56,56,56	0
56	MG	RA	3400	1/1	0.95	0.05	52,52,52,52	0
56	MG	RA	3095	1/1	0.95	0.09	53,53,53,53	0
56	MG	YA	3358	1/1	0.95	0.28	49,49,49,49	0
56	MG	RA	3232	1/1	0.95	0.30	66,66,66,66	0
56	MG	YA	3153	1/1	0.95	0.15	59,59,59,59	0
56	MG	RA	3335	1/1	0.95	0.04	53,53,53,53	0
56	MG	RA	3190	1/1	0.95	0.07	53,53,53,53	0
56	MG	RA	3147	1/1	0.95	0.34	64,64,64,64	0
56	MG	YA	3447	1/1	0.95	0.08	55,55,55,55	0
56	MG	RA	3284	1/1	0.95	0.08	62,62,62,62	0
56	MG	RA	3192	1/1	0.95	0.15	66,66,66,66	0
56	MG	YA	3541	1/1	0.95	0.18	57,57,57,57	0
56	MG	RA	3341	1/1	0.95	0.23	58,58,58,58	0
56	MG	YA	3368	1/1	0.95	0.13	57,57,57,57	0
56	MG	YA	3369	1/1	0.95	0.10	52,52,52,52	0
56	MG	YA	3370	1/1	0.95	0.20	50,50,50,50	0
56	MG	YA	3294	1/1	0.95	0.09	55,55,55,55	0
56	MG	YB	204	1/1	0.95	0.23	58,58,58,58	0
56	MG	RA	3376	1/1	0.95	0.19	67,67,67,67	0
56	MG	RA	3047	1/1	0.95	0.12	59,59,59,59	0
56	MG	R1	102	1/1	0.95	0.23	60,60,60,60	0
56	MG	RA	3455	1/1	0.95	0.06	50,50,50,50	0
56	MG	XA	1648	1/1	0.95	0.08	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3463	1/1	0.95	0.09	55,55,55,55	0
56	MG	RA	3259	1/1	0.95	0.10	56,56,56,56	0
56	MG	RA	3174	1/1	0.95	0.10	65,65,65,65	0
56	MG	YD	301	1/1	0.95	0.24	62,62,62,62	0
56	MG	RA	3458	1/1	0.95	0.08	53,53,53,53	0
56	MG	RA	3261	1/1	0.95	0.20	56,56,56,56	0
56	MG	YA	3309	1/1	0.95	0.29	49,49,49,49	0
56	MG	YA	3310	1/1	0.95	0.38	63,63,63,63	0
56	MG	YP	202	1/1	0.95	0.27	66,66,66,66	0
56	MG	RA	3175	1/1	0.95	0.10	63,63,63,63	0
56	MG	YA	3384	1/1	0.95	0.39	61,61,61,61	0
56	MG	YQ	202	1/1	0.95	0.18	52,52,52,52	0
56	MG	YA	3473	1/1	0.95	0.14	63,63,63,63	0
56	MG	YA	3474	1/1	0.95	0.13	64,64,64,64	0
56	MG	RA	3382	1/1	0.95	0.07	59,59,59,59	0
56	MG	RA	3418	1/1	0.95	0.09	54,54,54,54	0
56	MG	QA	1613	1/1	0.95	0.10	50,50,50,50	0
56	MG	XA	1610	1/1	0.95	0.13	59,59,59,59	0
56	MG	YA	3244	1/1	0.95	0.23	51,51,51,51	0
56	MG	YA	3318	1/1	0.95	0.09	65,65,65,65	0
56	MG	RA	3384	1/1	0.95	0.05	65,65,65,65	0
56	MG	YA	3066	1/1	0.95	0.22	58,58,58,58	0
56	MG	RA	3177	1/1	0.95	0.06	59,59,59,59	0
56	MG	YA	3068	1/1	0.95	0.14	55,55,55,55	0
56	MG	XA	1614	1/1	0.95	0.18	53,53,53,53	0
56	MG	RA	3198	1/1	0.95	0.12	55,55,55,55	0
56	MG	RA	3139	1/1	0.95	0.24	60,60,60,60	0
56	MG	RA	3140	1/1	0.95	0.23	66,66,66,66	0
56	MG	RA	3115	1/1	0.95	0.14	54,54,54,54	0
56	MG	RA	3437	1/1	0.96	0.18	66,66,66,66	0
56	MG	XA	1679	1/1	0.96	0.04	58,58,58,58	0
56	MG	YA	3458	1/1	0.96	0.20	62,62,62,62	0
56	MG	RA	3465	1/1	0.96	0.16	65,65,65,65	0
56	MG	YA	3292	1/1	0.96	0.07	58,58,58,58	0
56	MG	XA	1613	1/1	0.96	0.07	51,51,51,51	0
56	MG	YA	3462	1/1	0.96	0.14	54,54,54,54	0
56	MG	QV	103	1/1	0.96	0.07	58,58,58,58	0
56	MG	RA	3111	1/1	0.96	0.09	56,56,56,56	0
56	MG	YA	3065	1/1	0.96	0.13	47,47,47,47	0
56	MG	YA	3149	1/1	0.96	0.09	63,63,63,63	0
56	MG	RA	3005	1/1	0.96	0.33	57,57,57,57	0
56	MG	XA	1617	1/1	0.96	0.09	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3152	1/1	0.96	0.07	53,53,53,53	0
56	MG	RP	202	1/1	0.96	0.06	55,55,55,55	0
56	MG	YA	3409	1/1	0.96	0.13	58,58,58,58	0
56	MG	YA	3304	1/1	0.96	0.09	65,65,65,65	0
56	MG	YA	3109	1/1	0.96	0.28	59,59,59,59	0
56	MG	RA	3289	1/1	0.96	0.27	65,65,65,65	0
56	MG	YA	3359	1/1	0.96	0.20	55,55,55,55	0
56	MG	YA	3477	1/1	0.96	0.06	65,65,65,65	0
56	MG	YA	3545	1/1	0.96	0.17	48,48,48,48	0
56	MG	YA	3308	1/1	0.96	0.10	49,49,49,49	0
56	MG	YA	3479	1/1	0.96	0.27	66,66,66,66	0
56	MG	YB	202	1/1	0.96	0.15	66,66,66,66	0
56	MG	XA	1620	1/1	0.96	0.08	63,63,63,63	0
56	MG	YA	3256	1/1	0.96	0.36	50,50,50,50	0
56	MG	RA	3083	1/1	0.96	0.19	66,66,66,66	0
56	MG	YA	3483	1/1	0.96	0.04	51,51,51,51	0
56	MG	XA	1655	1/1	0.96	0.10	60,60,60,60	0
56	MG	YA	3207	1/1	0.96	0.24	67,67,67,67	0
56	MG	XV	105	1/1	0.96	0.07	67,67,67,67	0
56	MG	RA	3471	1/1	0.96	0.17	47,47,47,47	0
56	MG	YA	3211	1/1	0.96	0.07	54,54,54,54	0
56	MG	YA	3317	1/1	0.96	0.27	56,56,56,56	0
56	MG	RA	3102	1/1	0.96	0.13	55,55,55,55	0
56	MG	RA	3375	1/1	0.96	0.04	65,65,65,65	0
56	MG	YA	3493	1/1	0.96	0.22	49,49,49,49	0
56	MG	YE	302	1/1	0.96	0.10	63,63,63,63	0
56	MG	QA	1633	1/1	0.96	0.13	64,64,64,64	0
56	MG	QA	1607	1/1	0.96	0.06	60,60,60,60	0
56	MG	QA	1648	1/1	0.96	0.04	60,60,60,60	0
56	MG	RA	3423	1/1	0.96	0.41	65,65,65,65	0
56	MG	QA	1617	1/1	0.96	0.20	57,57,57,57	0
56	MG	RA	3107	1/1	0.96	0.06	50,50,50,50	0
56	MG	QA	1655	1/1	0.96	0.12	63,63,63,63	0
56	MG	YA	3437	1/1	0.96	0.15	50,50,50,50	0
56	MG	RA	3133	1/1	0.96	0.07	56,56,56,56	0
56	MG	RA	3233	1/1	0.96	0.53	67,67,67,67	0
56	MG	YA	3329	1/1	0.96	0.16	48,48,48,48	0
56	MG	RA	3281	1/1	0.96	0.16	56,56,56,56	0
56	MG	RA	3173	1/1	0.96	0.09	57,57,57,57	0
56	MG	RA	3487	1/1	0.96	0.17	66,66,66,66	0
56	MG	XA	1671	1/1	0.96	0.05	64,64,64,64	0
56	MG	RA	3265	1/1	0.96	0.19	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1644	1/1	0.96	0.05	60,60,60,60	0
56	MG	RA	3462	1/1	0.96	0.16	50,50,50,50	0
56	MG	XA	1675	1/1	0.96	0.08	54,54,54,54	0
56	MG	RA	3323	1/1	0.96	0.20	52,52,52,52	0
56	MG	YA	3286	1/1	0.96	0.34	54,54,54,54	0
56	MG	YA	3139	1/1	0.96	0.14	60,60,60,60	0
56	MG	XA	1642	1/1	0.96	0.06	56,56,56,56	0
56	MG	XA	1625	1/1	0.97	0.07	51,51,51,51	0
56	MG	RA	3442	1/1	0.97	0.34	52,52,52,52	0
56	MG	YA	3193	1/1	0.97	0.23	52,52,52,52	0
56	MG	YA	3279	1/1	0.97	0.44	55,55,55,55	0
56	MG	YA	3194	1/1	0.97	0.09	57,57,57,57	0
56	MG	YA	3235	1/1	0.97	0.10	63,63,63,63	0
56	MG	YA	3536	1/1	0.97	0.18	77,77,77,77	0
56	MG	RA	3054	1/1	0.97	0.16	61,61,61,61	0
56	MG	YA	3238	1/1	0.97	0.19	55,55,55,55	0
56	MG	YA	3196	1/1	0.97	0.26	88,88,88,88	0
56	MG	YA	3130	1/1	0.97	0.05	51,51,51,51	0
56	MG	RA	3422	1/1	0.97	0.10	63,63,63,63	0
56	MG	YA	3543	1/1	0.97	0.17	49,49,49,49	0
56	MG	RA	3055	1/1	0.97	0.19	50,50,50,50	0
56	MG	YA	3164	1/1	0.97	0.17	67,67,67,67	0
56	MG	YA	3201	1/1	0.97	0.06	48,48,48,48	0
56	MG	YA	3165	1/1	0.97	0.09	60,60,60,60	0
56	MG	RA	3348	1/1	0.97	0.04	55,55,55,55	0
56	MG	RA	3185	1/1	0.97	0.09	66,66,66,66	0
56	MG	YA	3492	1/1	0.97	0.14	53,53,53,53	0
56	MG	RA	3449	1/1	0.97	0.04	84,84,84,84	0
56	MG	XQ	201	1/1	0.97	0.04	51,51,51,51	0
56	MG	RA	3186	1/1	0.97	0.28	67,67,67,67	0
56	MG	YA	3390	1/1	0.97	0.07	51,51,51,51	0
56	MG	XA	1608	1/1	0.97	0.08	62,62,62,62	0
56	MG	XA	1609	1/1	0.97	0.14	65,65,65,65	0
56	MG	YA	3210	1/1	0.97	0.12	57,57,57,57	0
56	MG	RA	3214	1/1	0.97	0.09	62,62,62,62	0
56	MG	YA	3301	1/1	0.97	0.29	47,47,47,47	0
56	MG	RA	3410	1/1	0.97	0.22	61,61,61,61	0
56	MG	YA	3257	1/1	0.97	0.10	58,58,58,58	0
56	MG	QA	1632	1/1	0.97	0.10	55,55,55,55	0
56	MG	RA	3267	1/1	0.97	0.18	57,57,57,57	0
56	MG	YA	3306	1/1	0.97	0.09	65,65,65,65	0
56	MG	YA	3508	1/1	0.97	0.06	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3074	1/1	0.97	0.11	49,49,49,49	0
56	MG	YA	3085	1/1	0.97	0.13	60,60,60,60	0
56	MG	RA	3314	1/1	0.97	0.25	63,63,63,63	0
56	MG	RA	3434	1/1	0.97	0.24	50,50,50,50	0
56	MG	RA	3435	1/1	0.97	0.17	57,57,57,57	0
56	MG	RA	3483	1/1	0.97	0.11	53,53,53,53	0
56	MG	YY	201	1/1	0.97	0.10	53,53,53,53	0
56	MG	YA	3266	1/1	0.97	0.02	49,49,49,49	0
56	MG	RA	3415	1/1	0.97	0.13	54,54,54,54	0
56	MG	YA	3410	1/1	0.97	0.10	55,55,55,55	0
56	MG	RA	3399	1/1	0.97	0.07	50,50,50,50	0
56	MG	YA	3412	1/1	0.97	0.15	64,64,64,64	0
56	MG	YA	3224	1/1	0.97	0.13	60,60,60,60	0
56	MG	YA	3122	1/1	0.97	0.07	57,57,57,57	0
56	MG	YA	3469	1/1	0.97	0.08	64,64,64,64	0
56	MG	QA	1640	1/1	0.97	0.09	56,56,56,56	0
56	MG	YA	3524	1/1	0.97	0.27	48,48,48,48	0
56	MG	YA	3227	1/1	0.97	0.08	56,56,56,56	0
56	MG	RA	3070	1/1	0.97	0.13	49,49,49,49	0
56	MG	RA	3077	1/1	0.97	0.16	54,54,54,54	0
56	MG	RA	3359	1/1	0.97	0.05	56,56,56,56	0
56	MG	RA	3346	1/1	0.98	0.29	59,59,59,59	0
56	MG	YA	3221	1/1	0.98	0.04	58,58,58,58	0
56	MG	RA	3459	1/1	0.98	0.09	63,63,63,63	0
56	MG	YA	3500	1/1	0.98	0.10	66,66,66,66	0
56	MG	YA	3339	1/1	0.98	0.11	82,82,82,82	0
56	MG	YA	3531	1/1	0.98	0.07	59,59,59,59	0
56	MG	RA	3283	1/1	0.98	0.26	53,53,53,53	0
56	MG	YA	3445	1/1	0.98	0.03	59,59,59,59	0
56	MG	QA	1646	1/1	0.98	0.22	48,48,48,48	0
56	MG	YA	3092	1/1	0.98	0.09	64,64,64,64	0
56	MG	YA	3393	1/1	0.98	0.07	51,51,51,51	0
56	MG	RA	3365	1/1	0.98	0.06	55,55,55,55	0
56	MG	YA	3166	1/1	0.98	0.07	48,48,48,48	0
56	MG	YA	3147	1/1	0.98	0.07	50,50,50,50	0
56	MG	YA	3111	1/1	0.98	0.08	48,48,48,48	0
56	MG	RA	3325	1/1	0.98	0.07	58,58,58,58	0
56	MG	YA	3299	1/1	0.98	0.04	58,58,58,58	0
56	MG	XA	1604	1/1	0.98	0.05	57,57,57,57	0
56	MG	YA	3457	1/1	0.98	0.12	59,59,59,59	0
56	MG	YA	3254	1/1	0.98	0.35	57,57,57,57	0
57	SF4	QD	301	8/8	0.98	0.05	61,75,124,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3079	1/1	0.98	0.09	49,49,49,49	0
56	MG	RA	3336	1/1	0.98	0.10	56,56,56,56	0
56	MG	RA	3477	1/1	0.98	0.04	59,59,59,59	0
56	MG	QA	1637	1/1	0.98	0.06	65,65,65,65	0
56	MG	YA	3236	1/1	0.98	0.10	89,89,89,89	0
56	MG	RA	3222	1/1	0.98	0.42	47,47,47,47	0
56	MG	RA	3345	1/1	0.98	0.05	55,55,55,55	0
56	MG	RA	3445	1/1	0.98	0.09	55,55,55,55	0
56	MG	R1	101	1/1	0.98	0.23	48,48,48,48	0
56	MG	RA	3425	1/1	0.98	0.08	62,62,62,62	0
56	MG	YA	3428	1/1	0.99	0.05	51,51,51,51	0
56	MG	YA	3539	1/1	0.99	0.07	58,58,58,58	0
56	MG	QY	101	1/1	0.99	0.03	50,50,50,50	0
56	MG	QA	1658	1/1	0.99	0.05	62,62,62,62	0
56	MG	YA	3420	1/1	0.99	0.03	56,56,56,56	0
58	ZN	XN	101	1/1	0.99	0.03	75,75,75,75	0
56	MG	YA	3044	1/1	0.99	0.06	66,66,66,66	0
56	MG	XA	1644	1/1	0.99	0.03	64,64,64,64	0
56	MG	YA	3446	1/1	0.99	0.05	54,54,54,54	0
57	SF4	XD	301	8/8	0.99	0.05	53,60,74,96	0
58	ZN	QN	101	1/1	0.99	0.03	115,115,115,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.