



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 04:04 AM UTC

PDB ID : 6BUW / pdb_00006buw
Title : Thermus thermophilus 70S complex containing 16S G299A ram mutation and empty A site.
Authors : Hoffer, E.D.; Maehigashi, T.; Fagan, C.E.; Dunham, C.M.
Deposited on : 2017-12-11
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

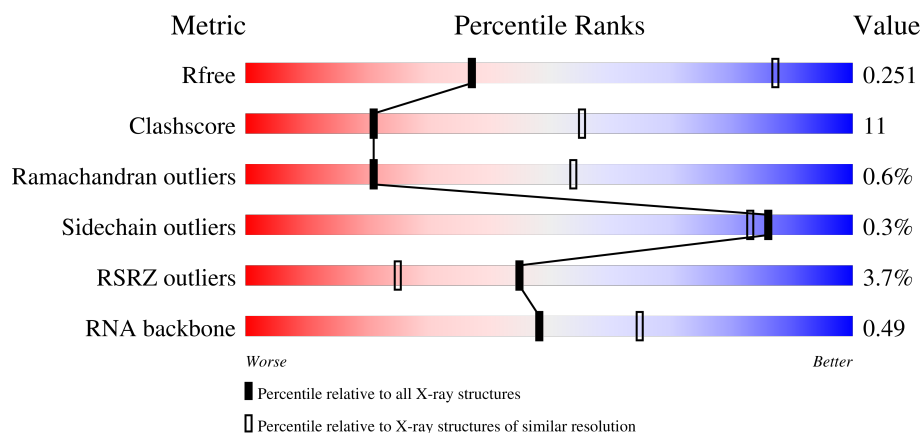
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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

Mol	Chain	Length	Quality of chain
1	QA	1508	2% 48% 43% 9%
1	XA	1508	2% 48% 42% 9%
2	QB	256	2% 58% 34% 8%
2	XB	256	2% 61% 30% 8%

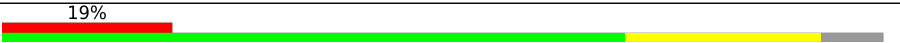
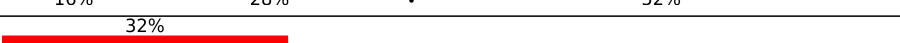
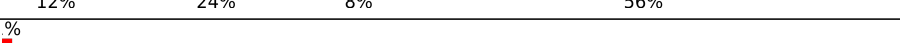
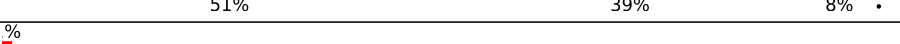
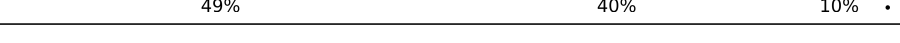
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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126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

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Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	25	
23	XX	25	
24	RA	2915	
24	YA	2915	
25	RB	122	
25	YB	122	
26	RD	276	
26	YD	276	
27	RE	206	
27	YE	206	

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Mol	Chain	Length	Quality of chain
28	RF	210	% 63% 32% .
28	YF	210	% 68% 29% .
29	RG	182	8% 58% 40% ...
29	YG	182	4% 65% 34% ..
30	RH	180	11% 61% 33% . .
30	YH	180	4% 61% 34% ..
31	RI	148	10% 67% 29% ..
31	YI	148	3% 56% 39% . .
32	RN	140	6% 77% 21% .
32	YN	140	4% 66% 31% ..
33	RO	122	2% 67% 33%
33	YO	122	79% 21%
34	RP	150	5% 67% 31% .
34	YP	150	8% 61% 37% ..
35	RQ	141	9% 60% 38% .
35	YQ	141	13% 70% 30% .
36	RR	118	2% 62% 36% ..
36	YR	118	3% 65% 34% .
37	RS	112	4% 63% 35% ..
37	YS	112	6% 68% 31% .
38	RT	146	5% 62% 32% . 6%
38	YT	146	3% 63% 29% . 6%
39	RU	118	3% 73% 23% ..
39	YU	118	5% 64% 31% ..
40	RV	101	% 71% 28% .

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Mol	Chain	Length	Quality of chain
40	YV	101	
41	RW	113	
41	YW	113	
42	RX	96	
42	YX	96	
43	RY	110	
43	YY	110	
44	RZ	206	
44	YZ	206	
45	R0	85	
45	Y0	85	
46	R1	98	
46	Y1	98	
47	R2	72	
47	Y2	72	
48	R3	60	
48	Y3	60	
49	R4	71	
49	Y4	71	
50	R5	60	
50	Y5	60	
51	R6	54	
51	Y6	54	
52	R7	49	
52	Y7	49	

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Mol	Chain	Length	Quality of chain
53	R8	65	
53	Y8	65	
54	R9	37	
54	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
55	MG	QV	106	-	-	-	X
55	MG	RA	3383	-	-	-	X
56	SF4	XD	301	-	-	X	-

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 291948 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 P-site tRNA fMet.

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

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	12	Total	C	N	O	P	0	0	0
			261	117	51	81	12			
23	XX	11	Total	C	N	O	P	0	0	0
			239	107	46	75	11			

- Molecule 24 is a RNA chain called 23S rRNA.

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

- Molecule 25 is a RNA chain called 5S rRNA.

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

- Molecule 26 is a protein called 50S ribosomal protein L2.

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

- Molecule 27 is a protein called 50S ribosomal protein L3.

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

- Molecule 28 is a protein called 50S ribosomal protein L4.

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

- Molecule 29 is a protein called 50S ribosomal protein L5.

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

- Molecule 30 is a protein called 50S ribosomal protein L6.

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

- Molecule 31 is a protein called 50S ribosomal protein L9.

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

- Molecule 32 is a protein called 50S ribosomal protein L13.

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

- Molecule 33 is a protein called 50S ribosomal protein L14.

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

- Molecule 34 is a protein called 50S ribosomal protein L15.

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

- Molecule 35 is a protein called 50S ribosomal protein L16.

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

- Molecule 36 is a protein called 50S ribosomal protein L17.

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

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

- Molecule 37 is a protein called 50S ribosomal protein L18.

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

- Molecule 38 is a protein called 50S ribosomal protein L19.

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

- Molecule 39 is a protein called 50S ribosomal protein L20.

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

- Molecule 40 is a protein called 50S ribosomal protein L21.

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

- Molecule 41 is a protein called 50S ribosomal protein L22.

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

- Molecule 42 is a protein called 50S ribosomal protein L23.

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

- Molecule 43 is a protein called 50S ribosomal protein L24.

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

- Molecule 44 is a protein called 50S ribosomal protein L25.

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

- Molecule 45 is a protein called 50S ribosomal protein L27.

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

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R1	96	Total	C	N	O	S	0	0	0
			755	475	149	130	1			
46	Y1	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			

- Molecule 47 is a protein called 50S ribosomal protein L29.

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

- Molecule 48 is a protein called 50S ribosomal protein L30.

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

- Molecule 49 is a protein called 50S ribosomal protein L31.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L33.

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

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	R7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

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

- Molecule 54 is a protein called 50S ribosomal protein L36.

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

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	180	Total	Mg	0	0
			180	180		
55	QC	1	Total	Mg	0	0
			1	1		
55	QF	1	Total	Mg	0	0
			1	1		
55	QH	1	Total	Mg	0	0
			1	1		
55	QL	1	Total	Mg	0	0
			1	1		
55	QV	6	Total	Mg	0	0
			6	6		
55	QX	2	Total	Mg	0	0
			2	2		
55	RA	493	Total	Mg	0	0
			493	493		
55	RB	10	Total	Mg	0	0
			10	10		
55	RD	1	Total	Mg	0	0
			1	1		

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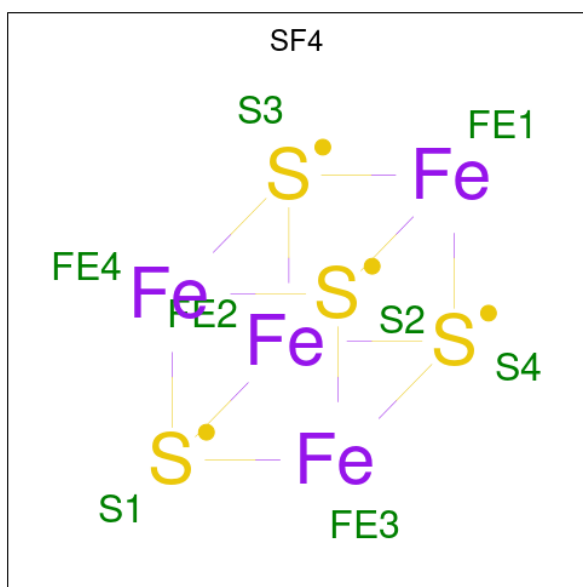
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	RE	4	Total 4	Mg 4	0	0
55	RF	1	Total 1	Mg 1	0	0
55	RI	1	Total 1	Mg 1	0	0
55	RN	1	Total 1	Mg 1	0	0
55	RO	1	Total 1	Mg 1	0	0
55	RP	3	Total 3	Mg 3	0	0
55	RQ	2	Total 2	Mg 2	0	0
55	RT	1	Total 1	Mg 1	0	0
55	RU	1	Total 1	Mg 1	0	0
55	RW	1	Total 1	Mg 1	0	0
55	RX	1	Total 1	Mg 1	0	0
55	RY	1	Total 1	Mg 1	0	0
55	R0	2	Total 2	Mg 2	0	0
55	R1	2	Total 2	Mg 2	0	0
55	R5	1	Total 1	Mg 1	0	0
55	XA	171	Total 171	Mg 171	0	0
55	XE	2	Total 2	Mg 2	0	0
55	XL	1	Total 1	Mg 1	0	0
55	XM	1	Total 1	Mg 1	0	0
55	XQ	1	Total 1	Mg 1	0	0
55	XS	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	XV	8	Total 8	Mg 8	0	0
55	YA	515	Total 515	Mg 515	0	0
55	YB	10	Total 10	Mg 10	0	0
55	YD	2	Total 2	Mg 2	0	0
55	YE	4	Total 4	Mg 4	0	0
55	YO	1	Total 1	Mg 1	0	0
55	YP	3	Total 3	Mg 3	0	0
55	YQ	3	Total 3	Mg 3	0	0
55	YU	1	Total 1	Mg 1	0	0
55	YX	2	Total 2	Mg 2	0	0
55	YY	1	Total 1	Mg 1	0	0
55	Y0	1	Total 1	Mg 1	0	0
55	Y5	1	Total 1	Mg 1	0	0
55	Y7	1	Total 1	Mg 1	0	0
55	Y8	1	Total 1	Mg 1	0	0

- Molecule 56 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

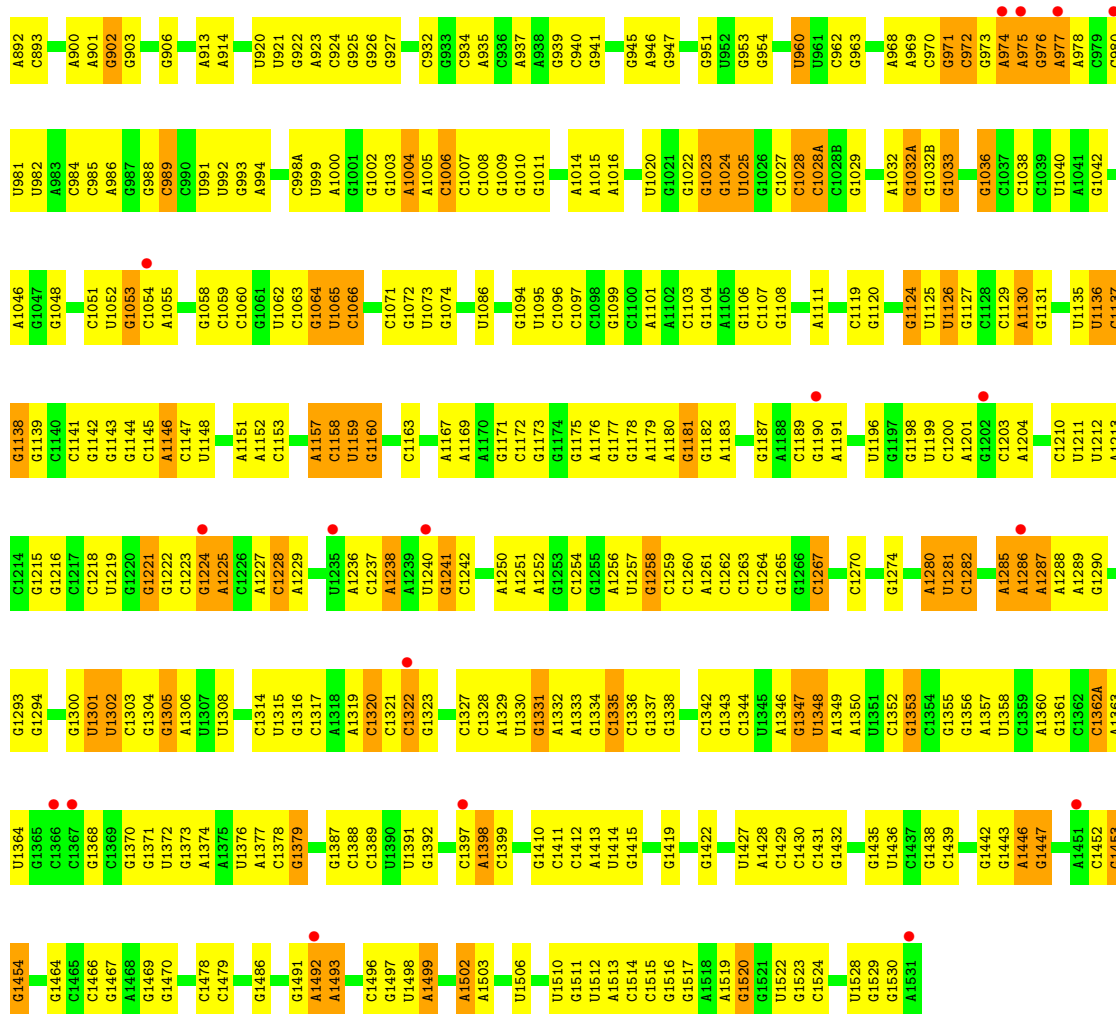
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

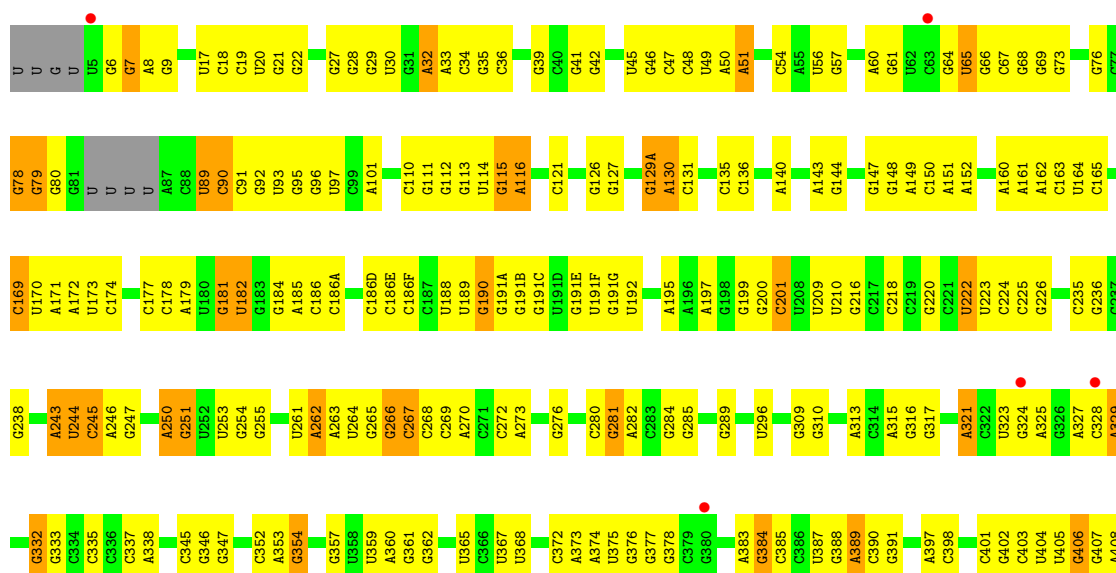
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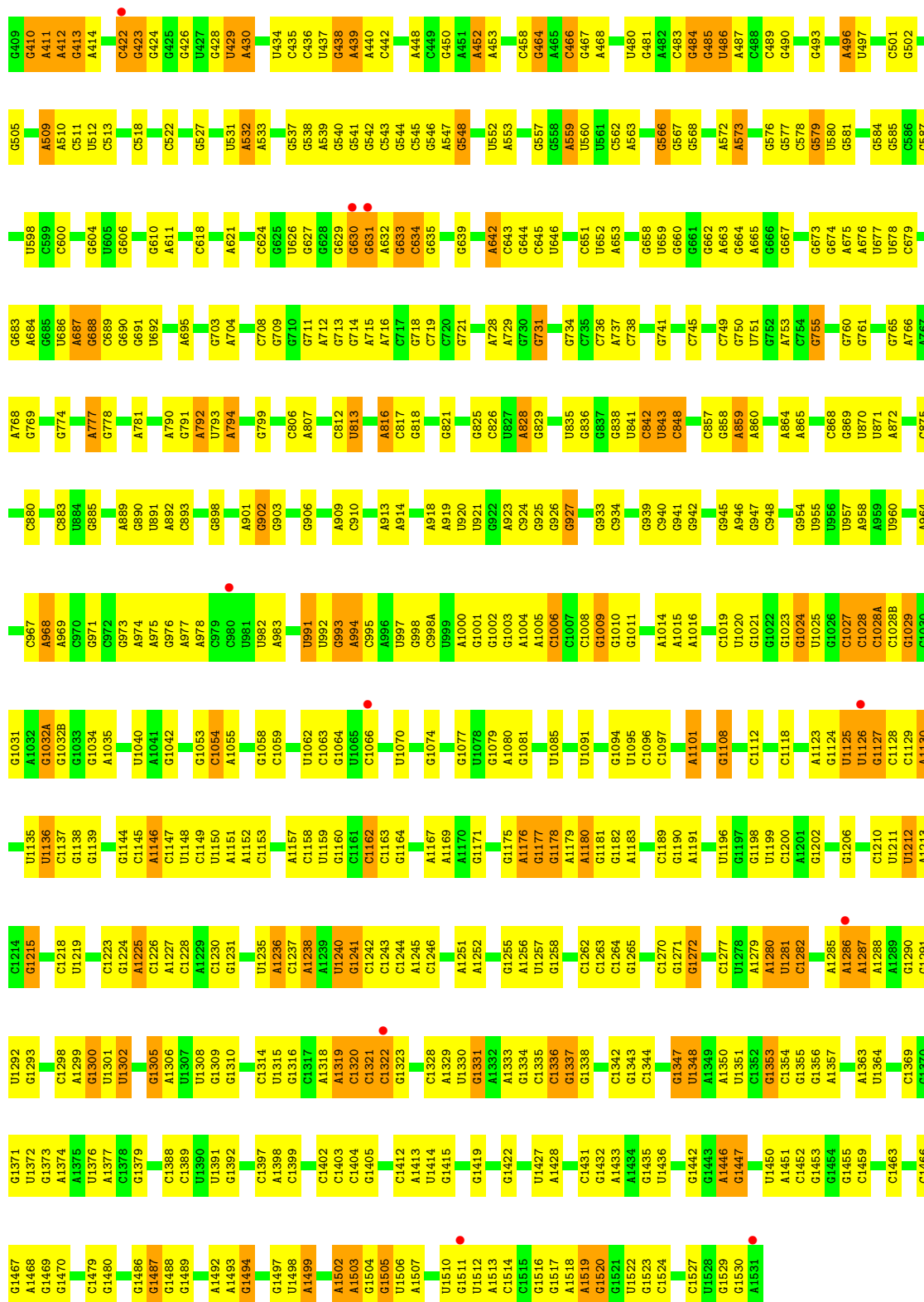
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y6	1	Total 1	Zn 1	0	0
57	Y9	1	Total 1	Zn 1	0	0



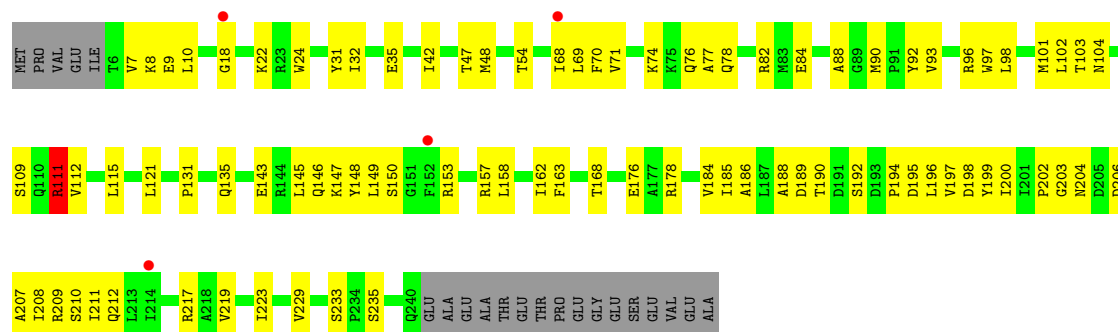
• Molecule 1: 16S rRNA



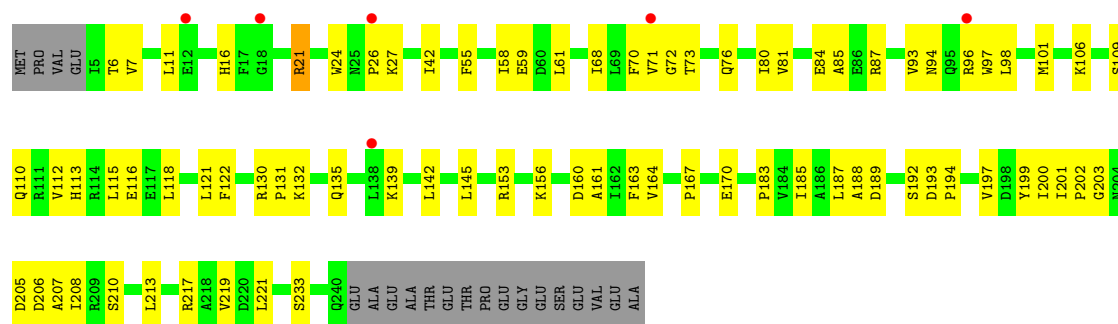


• Molecule 2: 30S ribosomal protein S2





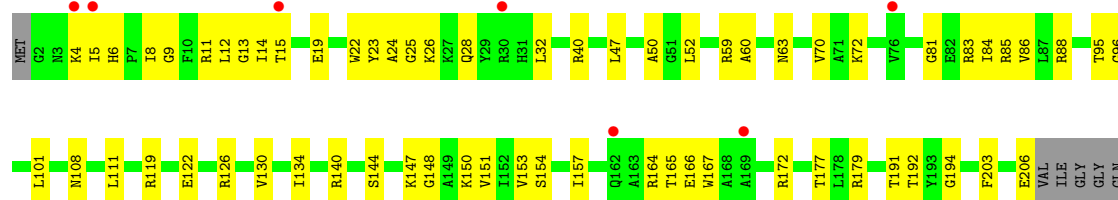
• Molecule 2: 30S ribosomal protein S2



• Molecule 3: 30S ribosomal protein S3

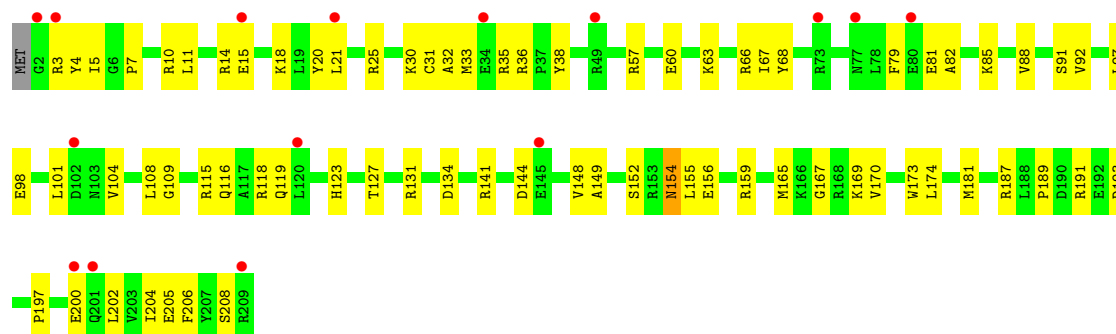


• Molecule 3: 30S ribosomal protein S3

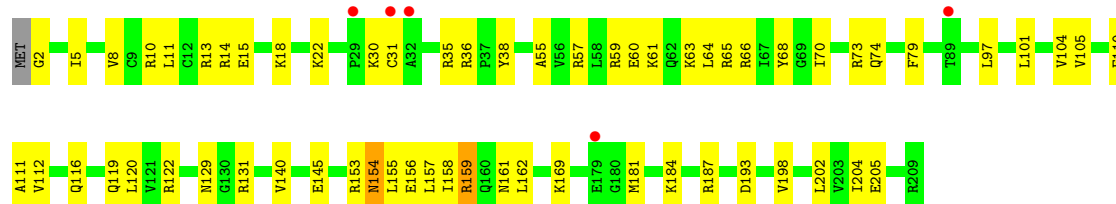
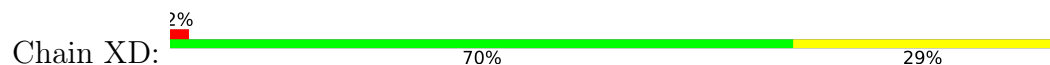


LYS
PRO
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GLU

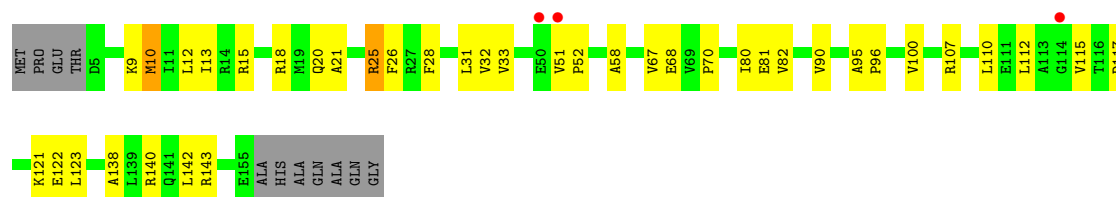
• Molecule 4: 30S ribosomal protein S4



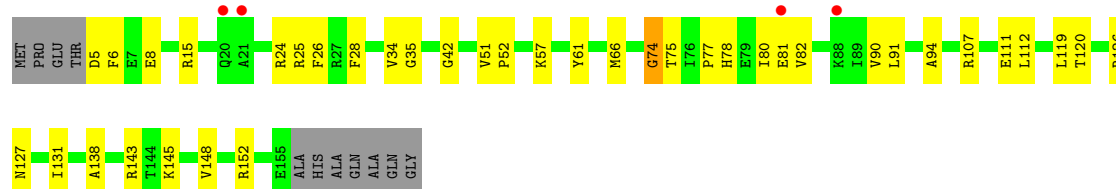
• Molecule 4: 30S ribosomal protein S4



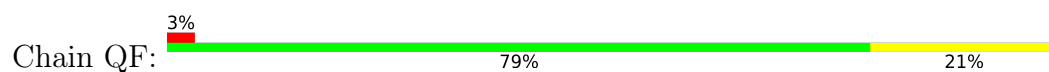
• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5



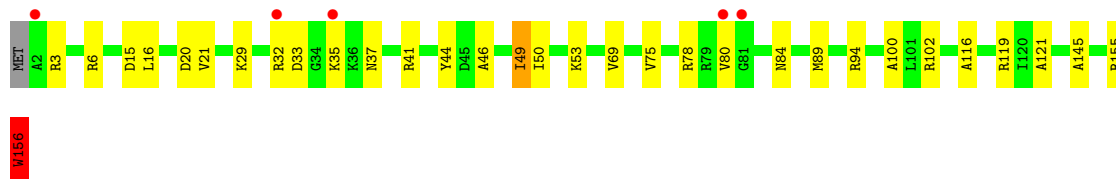
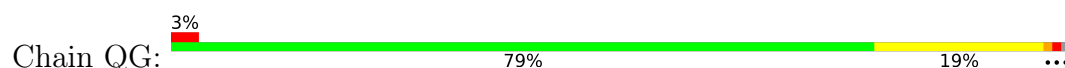
• Molecule 6: 30S ribosomal protein S6



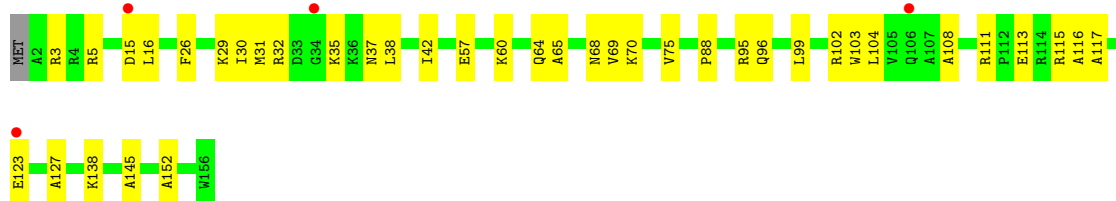
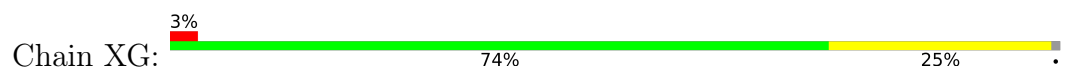
- Molecule 6: 30S ribosomal protein S6



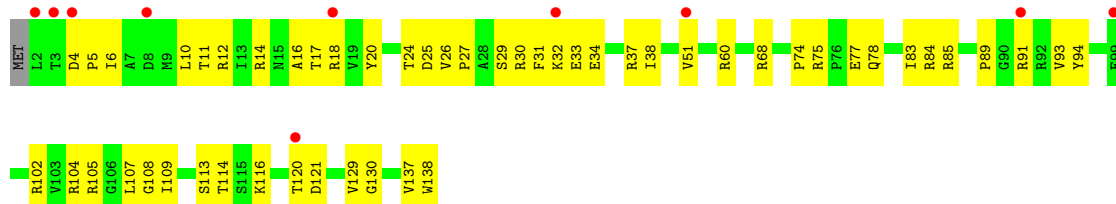
- Molecule 7: 30S ribosomal protein S7



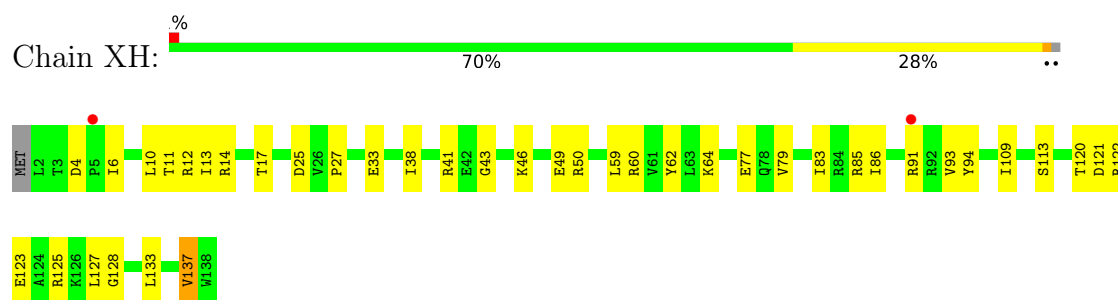
- Molecule 7: 30S ribosomal protein S7



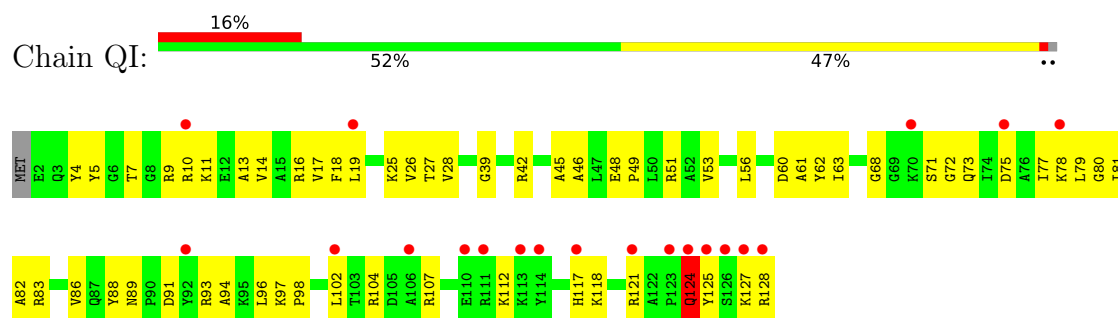
- Molecule 8: 30S ribosomal protein S8



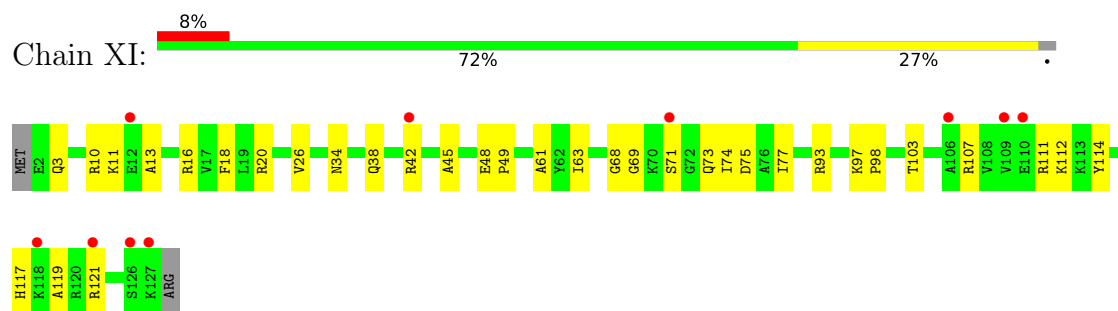
- Molecule 8: 30S ribosomal protein S8



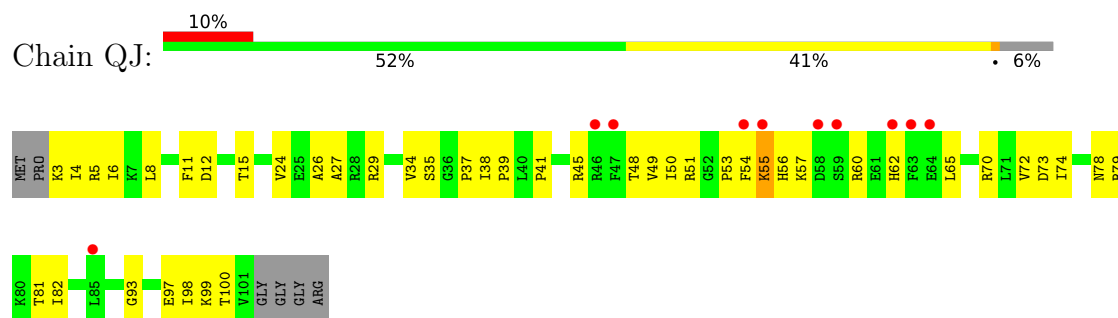
• Molecule 9: 30S ribosomal protein S9



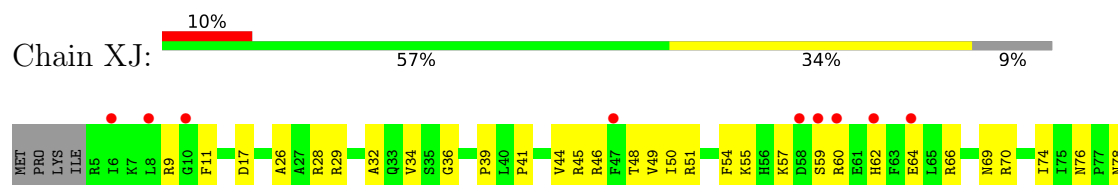
• Molecule 9: 30S ribosomal protein S9

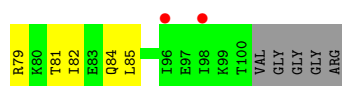


• Molecule 10: 30S ribosomal protein S10



• Molecule 10: 30S ribosomal protein S10

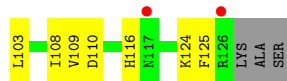




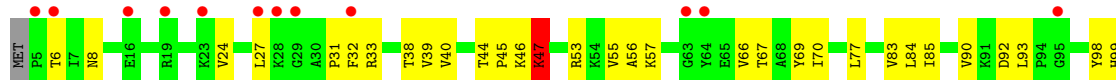
- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

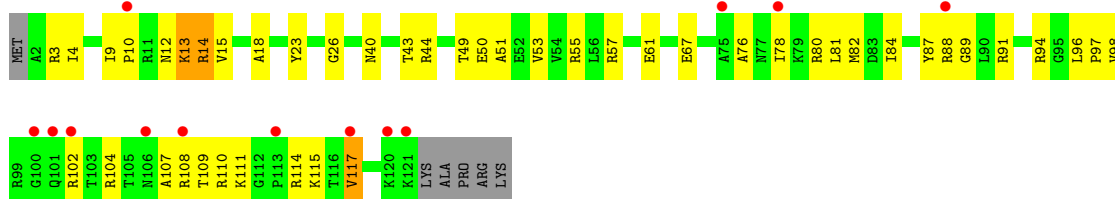


- Molecule 12: 30S ribosomal protein S12



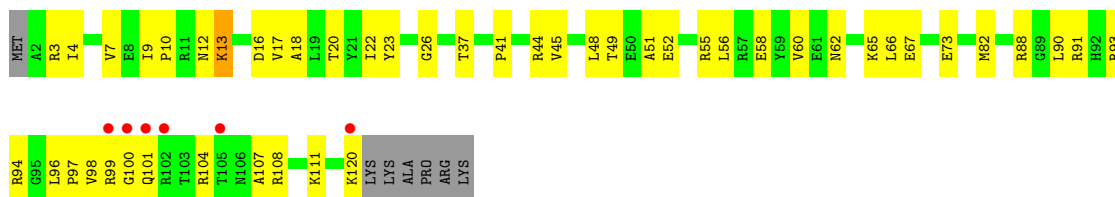
- Molecule 13: 30S ribosomal protein S13

Chain QM: 



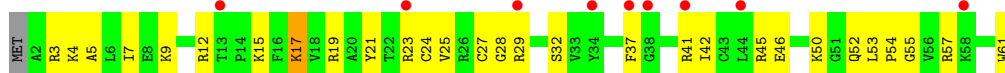
- Molecule 13: 30S ribosomal protein S13

Chain XM: 



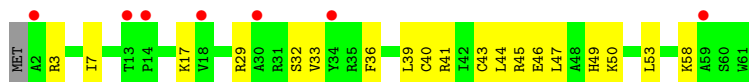
- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN: 



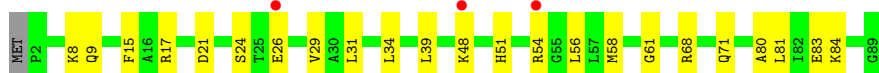
- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN: 



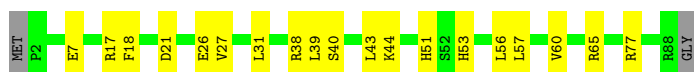
- Molecule 15: 30S ribosomal protein S15

Chain QO: 

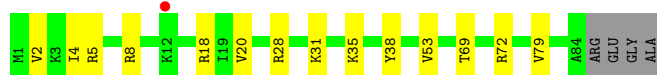
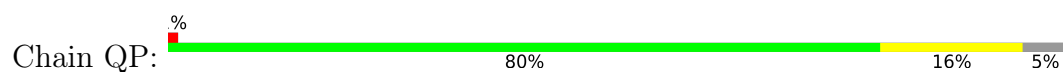


- Molecule 15: 30S ribosomal protein S15

Chain XO: 



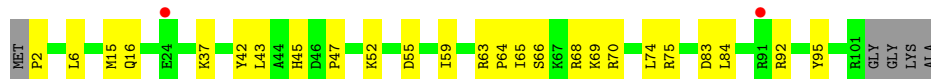
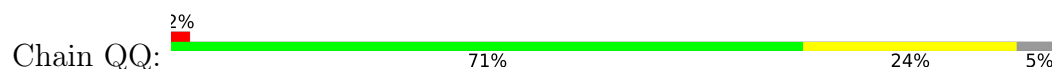
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



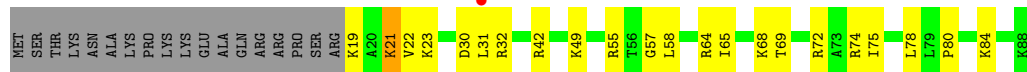
- Molecule 17: 30S ribosomal protein S17



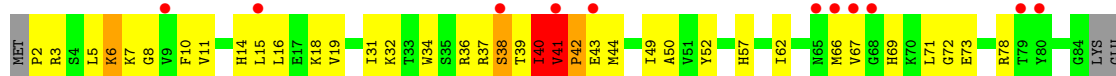
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



ALA
LYS
LYS
ALA
THR
LYS
LYS
LYS

- Molecule 19: 30S ribosomal protein S19



MET P2 F2 V9 F10 V11 L16 L16 V19 I31 K32 R36 T39 I40 V41 M44 I49 A50 K55 Q56 H57 T63 E64 R65 M66 V67 K70 L71 F74 R78 T79 Y80 R81 K85 GLU ALA LYS ALA THR LYS LYS LYS

- Molecule 20: 30S ribosomal protein S20



MET ALA GLN LYS PRO LYS R8 R9 L10 L11 A12 R22 N26 K29 K30 K34 T35 K38 K39 K54 I55 M56 R57 E60 K68 T71 L72 H73 K74 N75 A76 A77 A78 R79 R80 K81 R82 R83 L84 M85 V88 R89 A94 A97 I100 G101

G102 G103 L104 S105 A106

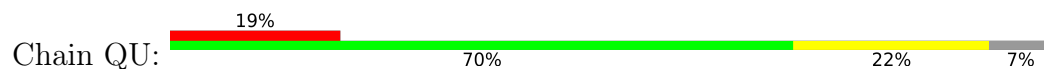
- Molecule 20: 30S ribosomal protein S20



MET ALA GLN LYS PRO LYS R8 R9 L10 L11 K14 R15 H16 R17 Q18 S19 L20 K21 R22 R23 L24 L25 R26 K27 A28 K29 K30 S31 A32 I33 K34 K38 K39 Q45 A49 I55 M56 R57 D64 K65 A66 A67 K68 G69 S70 T71 L72 H73 K74 N75 A76 R80

R83 L84 M85 R86 K87 R88 R89 Q90 L91 A94 L99 I100 G101 G102 A106

- Molecule 21: 30S ribosomal protein Thx



MET G2 R6 R7 R8 R9 R10 R15 K20 K26 LYS

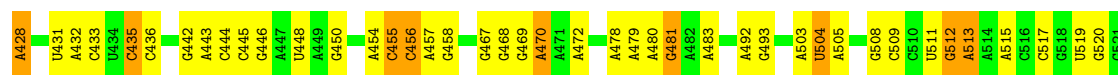
- Molecule 21: 30S ribosomal protein Thx



MET G2 R6 R10 V14 R15 G16 T17 R22 K26 LYS

- Molecule 22: P-site tRNA fMet



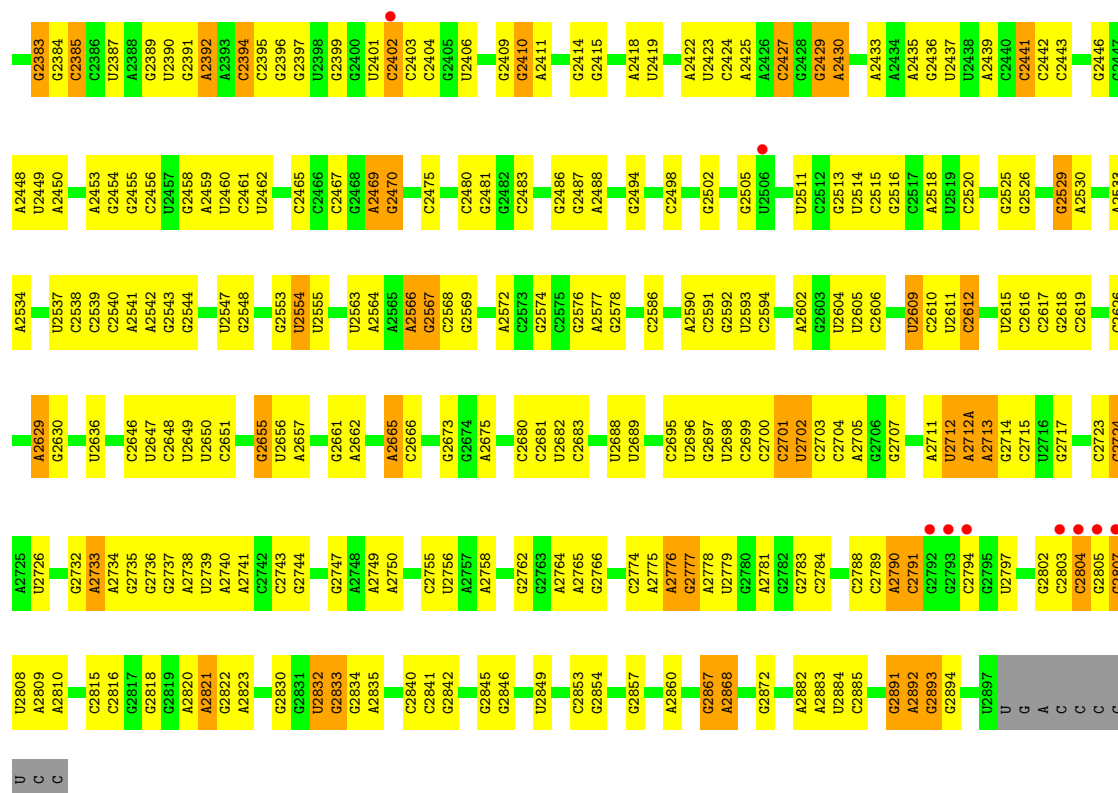


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A1586	G1418	A1336	U1255	C1166	U1078	G1002	U907	A824	A722	C	G600	C523
A1587	A1419	G1337	G1256	U1167	C1080	G1003	G1168	C825	G726	G	C901	U524
C1588	U1420	G1338	C1257	G1168	U081	A1010	A910	U826	G727	C	G602	U525
U1589	G1421	G1338	C1258	G1171	U082	U1011	A911	U827	A728	C	A603	A526
C1590	G1422	U1341	G1259	G1172	U1083	U1012	G914	U828	G729	C	G604	G527
U1591	G1423	U1341	U1263	G1173	U1084	C1013	C915	G831	G730	C	A528	A528
C1592	G1424	G1346	U1264	U1174	A1085	U1014	C915	U835	A734	G654S	A609	A529
A1593	G1425	G1347	G1265	U1175	A1086	G1015	C916	A835	A734	G656	G612	U534
C1594	G1426	G1348	G1266	U1176	A1087	G1016	A917	A836	A734	G657	U613	C535
G1595	A1427	A1348	U1267	U1177	U1088	G1017	U822	C840	A751	G658	U614	A536
A1596	G1428	A1349	G1268	U1178	A1089	G1018	U823	A841	A752	G659	G615	C537
A1597	G1429	U1352	C1270	G1179	U1090	U1019	C924	C844	A753	G660	A616	G539
C1598	C1430	A1353	G1271	G1180	U1091	A1020	U824	C845	A754	G661	G617	G540
G1599	U1431	A1354	A1272	U1181	C1092	A1021	U825	C846	A755	G662	G620	C546
U1601	U1432	A1354	G1273	U1182	U1093	G1022	A932	C847	A756	G663	A621	A547
U1516	U1433	A1359	A1274	G1186	G1094	U1023	G933	C848	A757	G664	G621	A548
U1520	G1436	A1359	A1275	U1187	A1095	G1024	G934	U847	A758	G665	G622	G549
G1521	G1436	A1365	A1276	U1188	A1096	G1025	C935	C848	A759	G666	G623	G550
G1522	G1444	A1366	G1277	U1189	U1097	U1026	U937	C849	A761	G669	G624	G551
A1600	A1444A	A1367	G1278	U1190	A1098	A1027	G938	U851	A762	A670	G625	C566
A1610	C1445	C1370	G1279	G1191	U1102	A1028	A941	C852	A763	C673	U626	G566
C1611	A1449	G1371	U1282	G1195	C1103	A1029	A941	C856	A764	C674	G627	G567
A1616	G1449A	U1372	G1283	C1196	C1104	U1033	A945	U858	A765	C675	G628	G568
C1617	U1454	A1379	A1286	G1197	U1105	G1034	G946	U859	A766	C676	G629	U569
G1627	G1455	G1380	C1287	C1201	G1107	C1040	G947	C861	A767	C677	G630	A567
G1628	A1455	A1385	U1288	G1202	C1041	G1044	G948	C862	A768	C678	A631	G563
U1629	A1460	G1385	C1289	G1203	U1111	A1045	A957	C863	A769	C679	A632	U566
C1537	G1461	G1385	G1290	A1204	G1112	U1205	U958	C864	A770	C680	A633	A567
G1538	C1464	C1389	C1291	U1206	C1116	A1046	A959	C865	A771	C681	G634	U568
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G1542	G1470	A1392	C1297	U1211	A1126	G1054	C970	C873	A775	C685	U639	C574
A1543	A1471	A1393	C1298	G1212	A1126	G1055	G974	C882	A776	C686	G640	A575
C1544	G1472	U1394	G1299	A1220	A1126	G1056	C974A	C883	A777	C687	C641	U576
A1545	U1473	A1395	C1299	C1221	G1131	A1057	G975	C884	A778	C688	G642	G577
C1648	C1474	U1397	C1301	C1222	G1136	U1058	G978	C885	A779	C689	C645	A578
G1651	C1475	C1398	A1308	G1224	U1136	G1059	C886	C886	A780	C690	A646	G579
A1652	A1476	U1400	G1309	C1225	C1140	U1060	G979	C887	A781	C691	G647	C580
C1653	U1482	G1401	G1310	A1227	U1141	U1061	A980	C888	A782	C692	G651	C581
A1654	G1483	C1402	C1311	G1226	U1141	G1062	C889	C889	A783	C693	G652	G582
G1657	G1484	C1403	U1312	G1227	U1142	G1063	A883	C890	A784	C694	A653	A586
C1658	G1485	U1405	C1313	G1235	A1142A	C1064	A884	C891	A785	C695	A654	C587
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G1667	A1490	C1408	A1317	G1238	U1148	U1066	G989	C894	A788	C698	G655	A590
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G1678	A1493	G1410	A1247	U1247	U1156	G1070	C995	C896	A790	C700	G657	G592
A1579	A1411	A1322	G1248	U1248	U1159	C1072	A896	C897	A791	C701	G658	C593
A1580	A1412	A1412	U1249	U1249	U1159	C1072	A897	A900	A792	C702	A659	G594
C1683	A1496	G1413	G1250	U1250	U1163	A1073	G997	A901	A793	C703	A660	G595
C1684	U1497	C1330	G1250	U1250	G1163	C1073	A1000	C903	A794	C704	G661	G596
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- Molecule 24: 23S rRNA

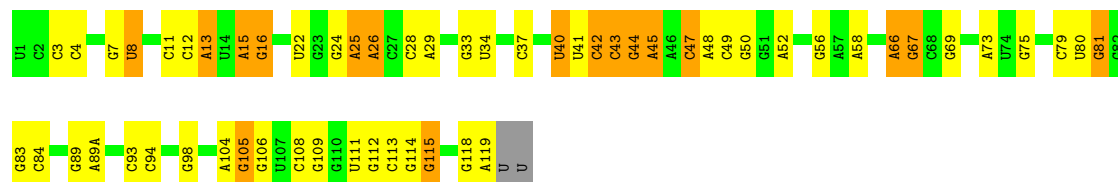


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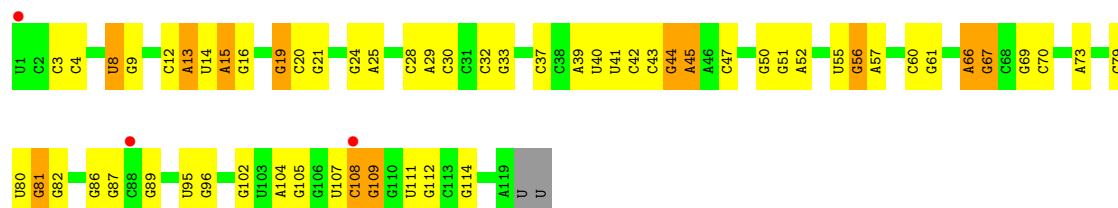
• Molecule 25: 5S rRNA

Chain RB: 51% 34% 14%



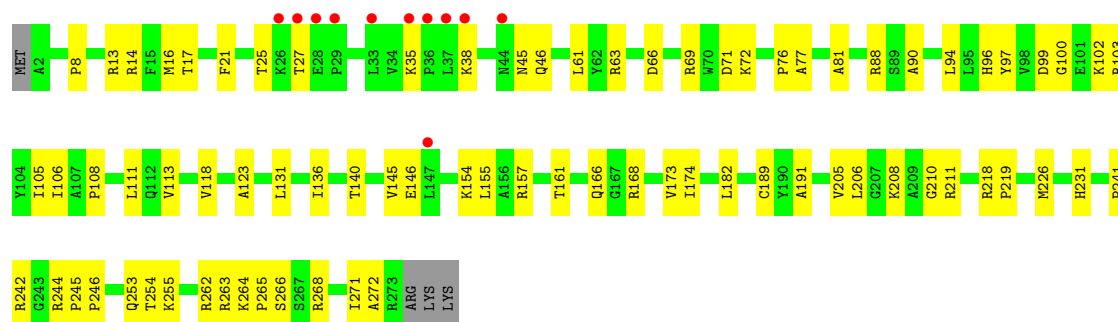
• Molecule 25: 5S rRNA

Chain YB: 50% 39% 10%

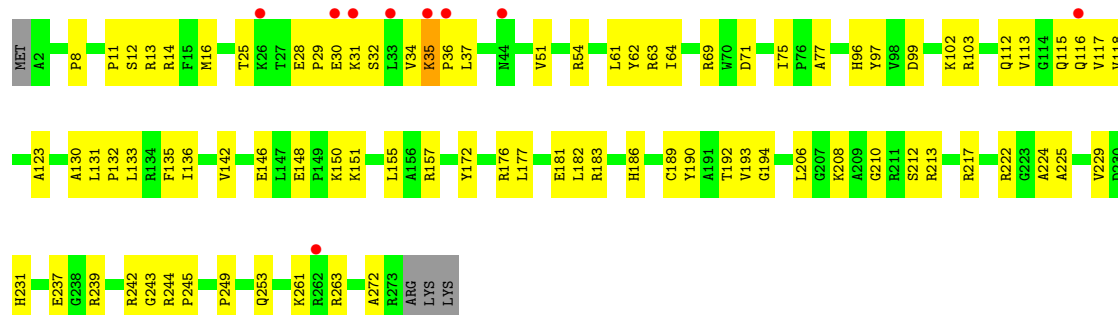


• Molecule 26: 50S ribosomal protein L2

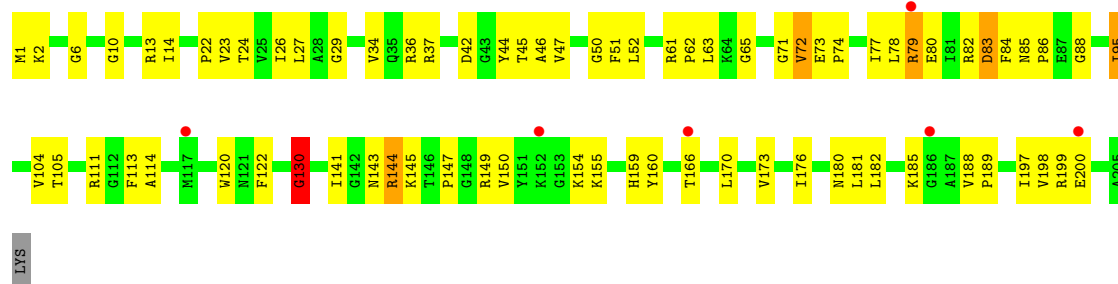
Chain RD: 70% 28% 2%



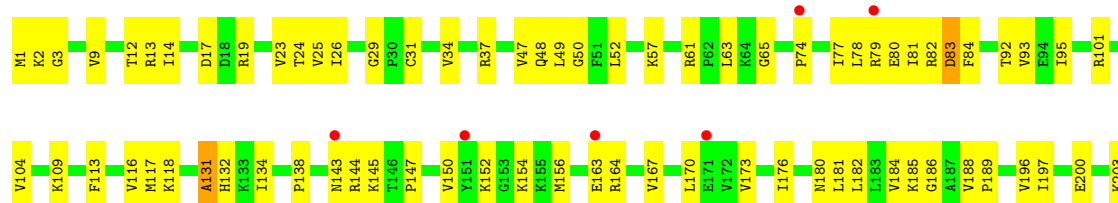
• Molecule 26: 50S ribosomal protein L2



• Molecule 27: 50S ribosomal protein L3

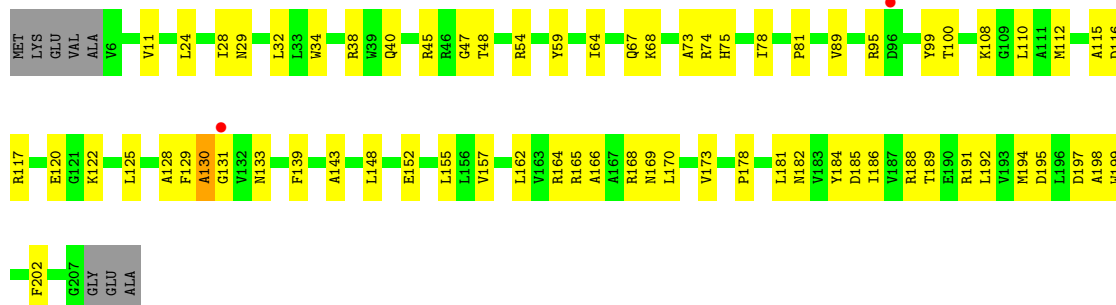


• Molecule 27: 50S ribosomal protein L3

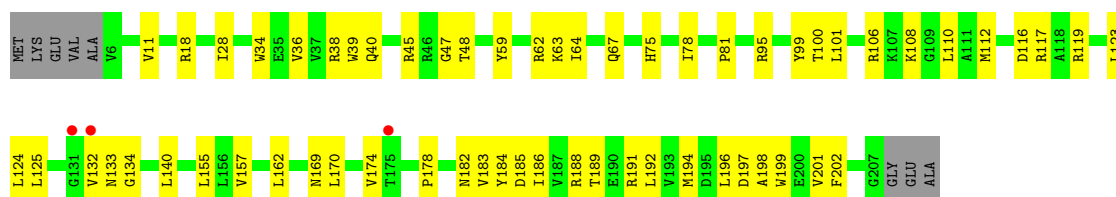




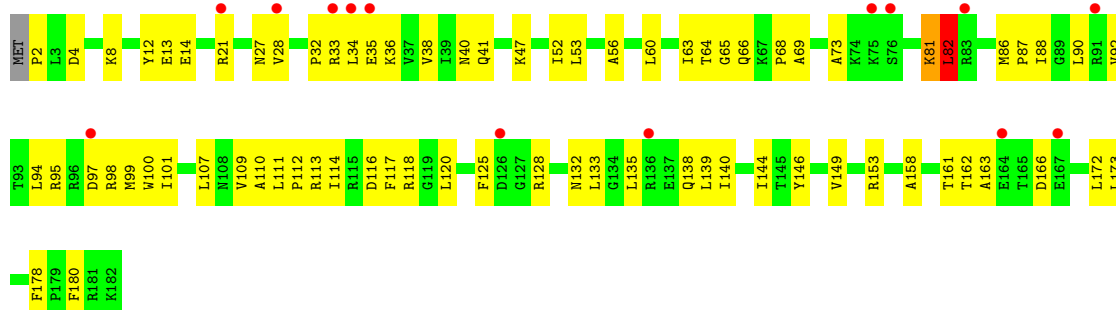
- Molecule 28: 50S ribosomal protein L4



- Molecule 28: 50S ribosomal protein L4



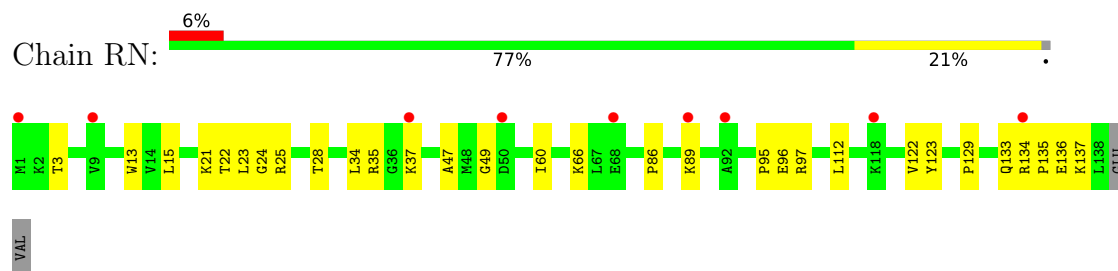
- Molecule 29: 50S ribosomal protein L5



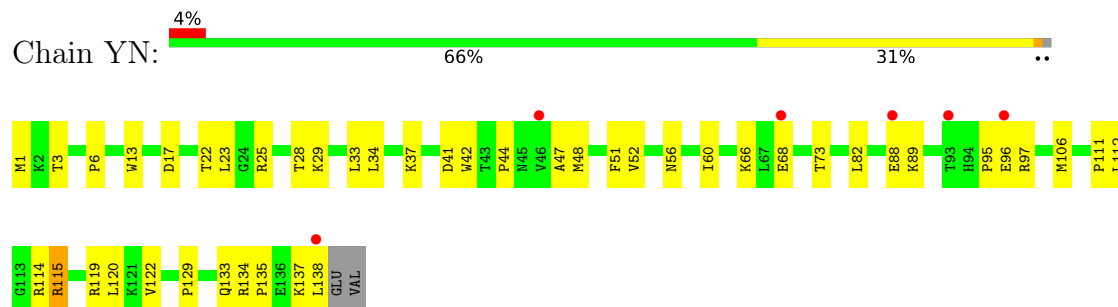
- Molecule 29: 50S ribosomal protein L5



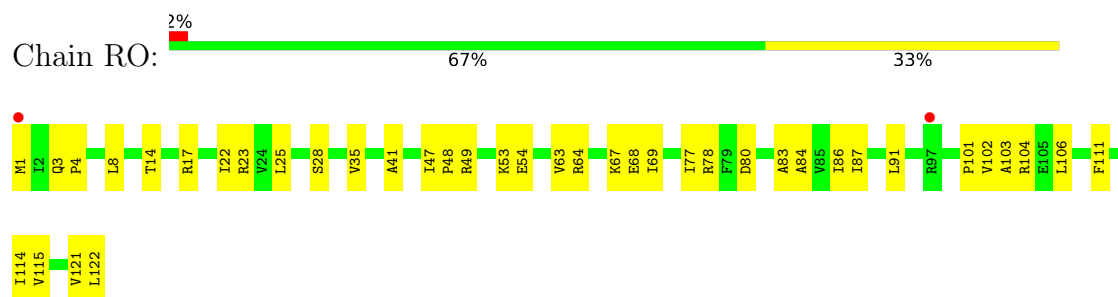
- Molecule 32: 50S ribosomal protein L13



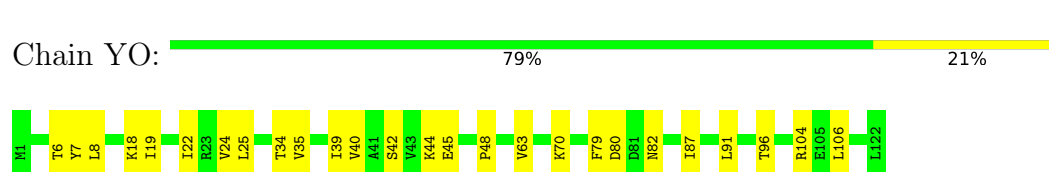
- Molecule 32: 50S ribosomal protein L13



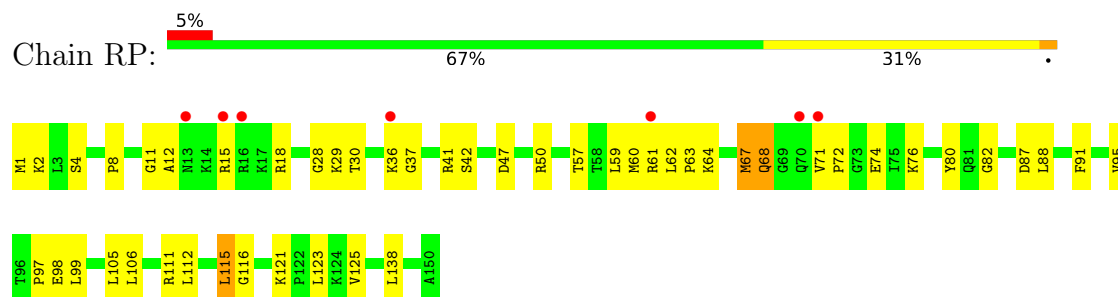
- Molecule 33: 50S ribosomal protein L14



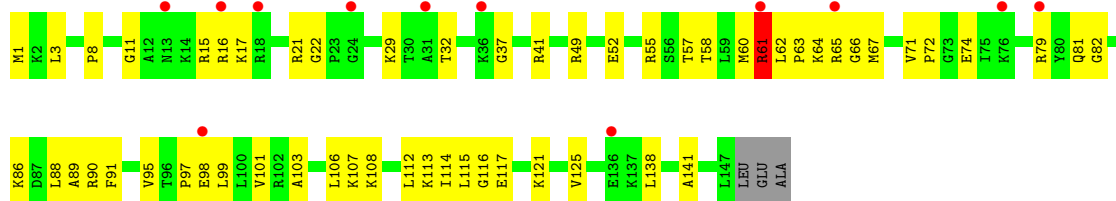
- Molecule 33: 50S ribosomal protein L14



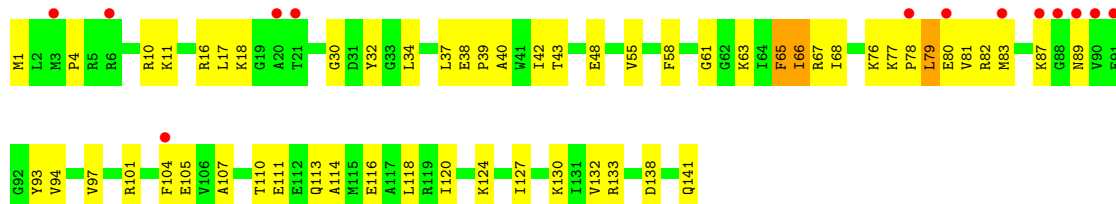
- Molecule 34: 50S ribosomal protein L15



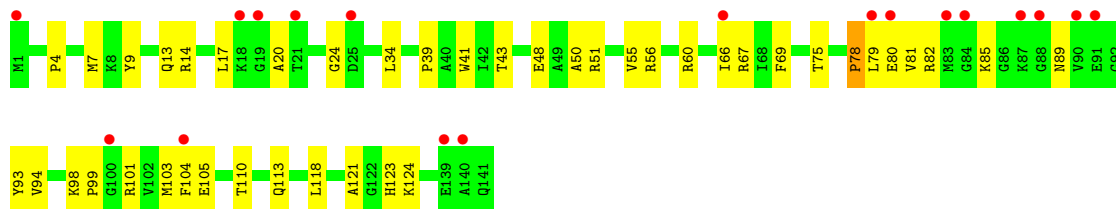
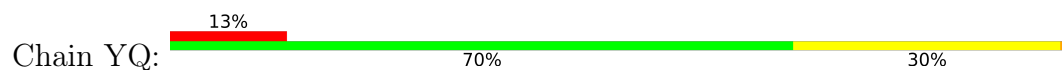
- Molecule 34: 50S ribosomal protein L15



• Molecule 35: 50S ribosomal protein L16



• Molecule 35: 50S ribosomal protein L16



• Molecule 36: 50S ribosomal protein L17



• Molecule 36: 50S ribosomal protein L17





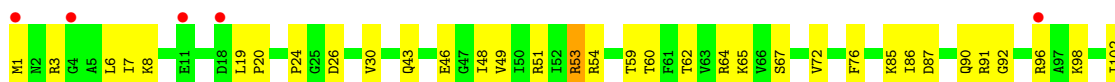
- Molecule 37: 50S ribosomal protein L18



- Molecule 37: 50S ribosomal protein L18



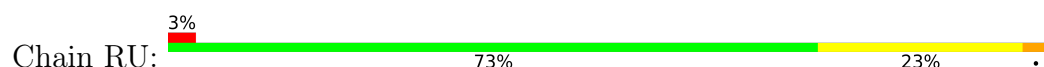
- Molecule 38: 50S ribosomal protein L19



- Molecule 38: 50S ribosomal protein L19

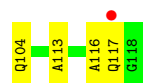
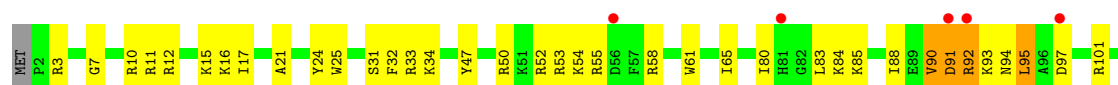


- Molecule 39: 50S ribosomal protein L20

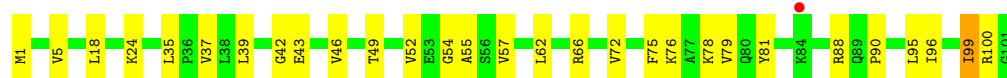
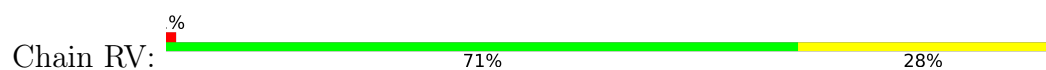




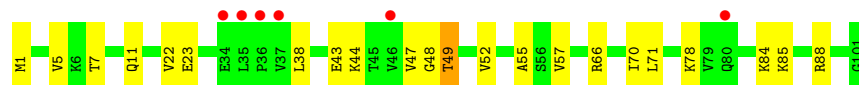
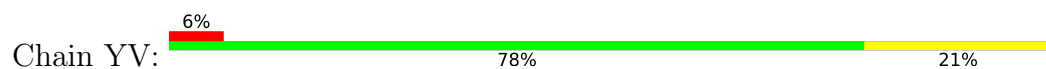
- Molecule 39: 50S ribosomal protein L20



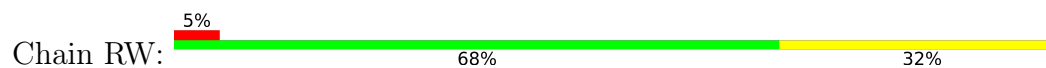
- Molecule 40: 50S ribosomal protein L21



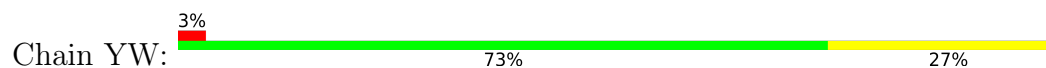
- Molecule 40: 50S ribosomal protein L21



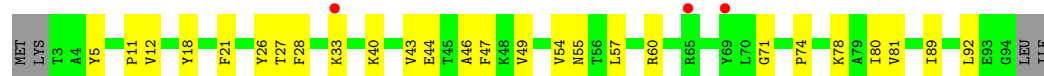
- Molecule 41: 50S ribosomal protein L22



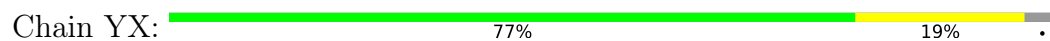
- Molecule 41: 50S ribosomal protein L22



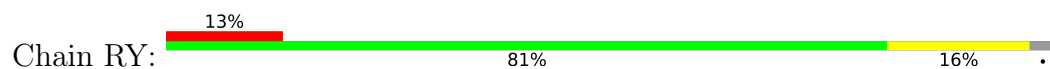
- Molecule 42: 50S ribosomal protein L23



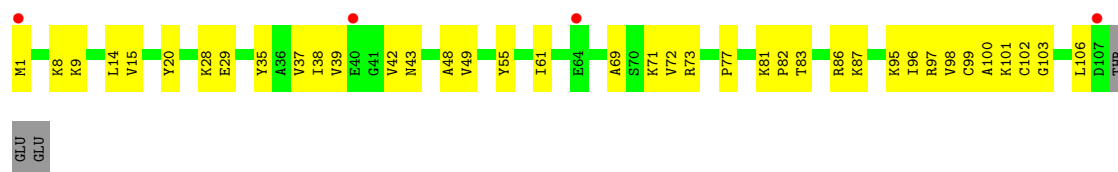
- Molecule 42: 50S ribosomal protein L23



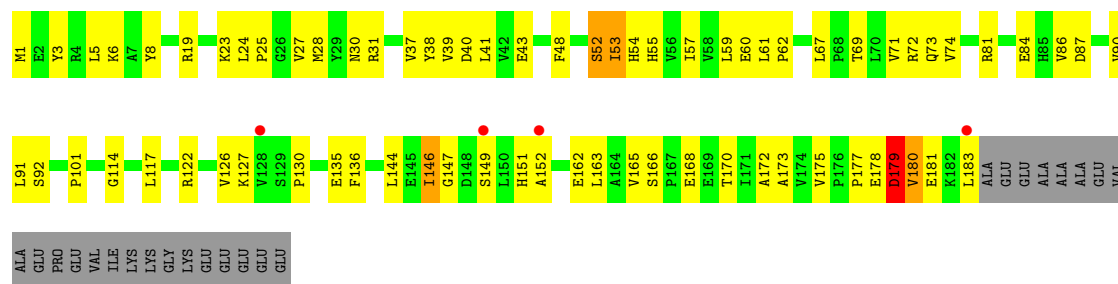
- Molecule 43: 50S ribosomal protein L24



- Molecule 43: 50S ribosomal protein L24

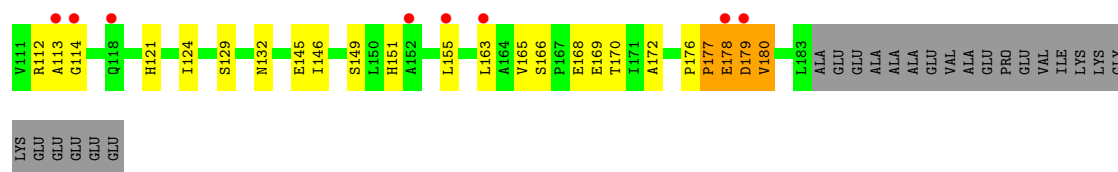


- Molecule 44: 50S ribosomal protein L25



- Molecule 44: 50S ribosomal protein L25

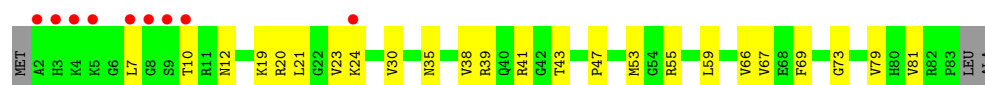




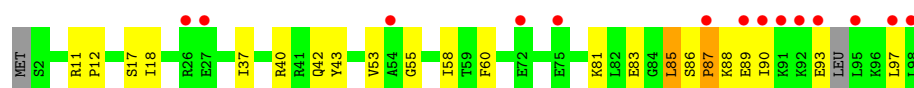
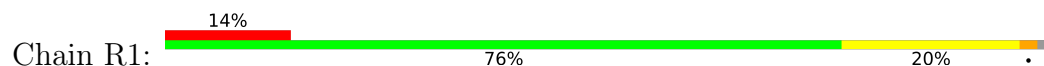
- Molecule 45: 50S ribosomal protein L27



- Molecule 45: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L28



- Molecule 46: 50S ribosomal protein L28



- Molecule 47: 50S ribosomal protein L29

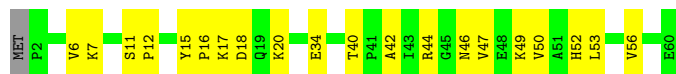


- Molecule 47: 50S ribosomal protein L29



- Molecule 48: 50S ribosomal protein L30

Chain R3:  65% 33% .



- Molecule 48: 50S ribosomal protein L30

Chain Y3:  67% 32% .



- Molecule 49: 50S ribosomal protein L31

Chain R4:  58% 30% 8% ..



- Molecule 49: 50S ribosomal protein L31

Chain Y4:  68% 23% . . .



- Molecule 50: 50S ribosomal protein L32

Chain R5:  75% 23% .



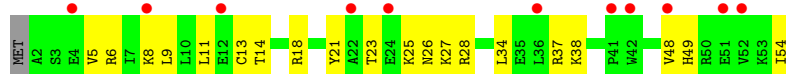
- Molecule 50: 50S ribosomal protein L32

Chain Y5:  72% 25% . .

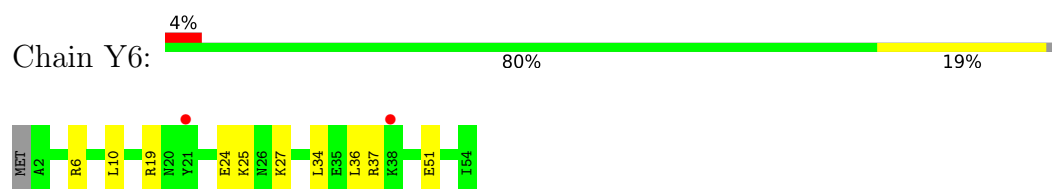


- Molecule 51: 50S ribosomal protein L33

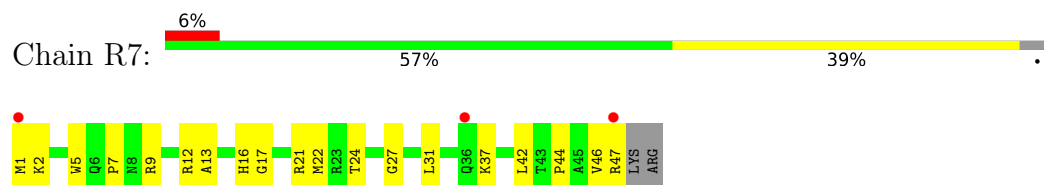
Chain R6:  61% 37% .



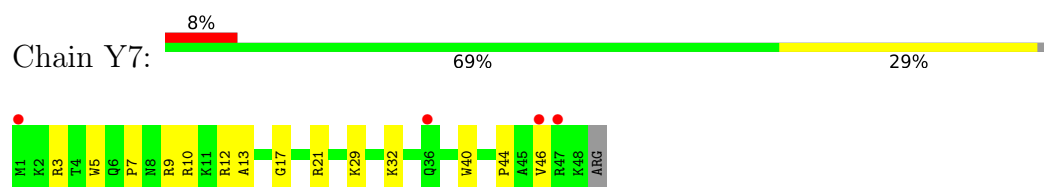
• Molecule 51: 50S ribosomal protein L33



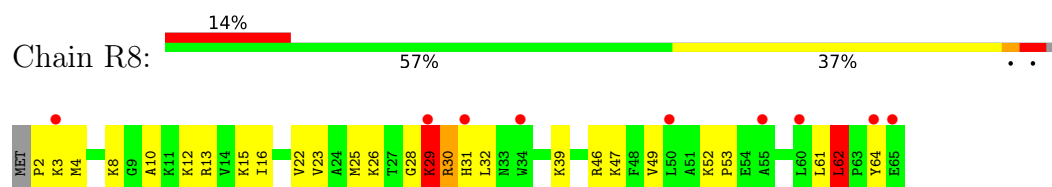
• Molecule 52: 50S ribosomal protein L34



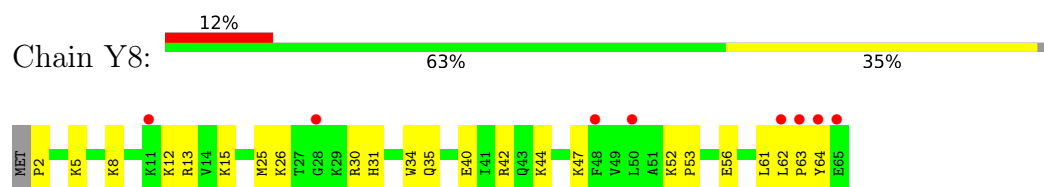
• Molecule 52: 50S ribosomal protein L34



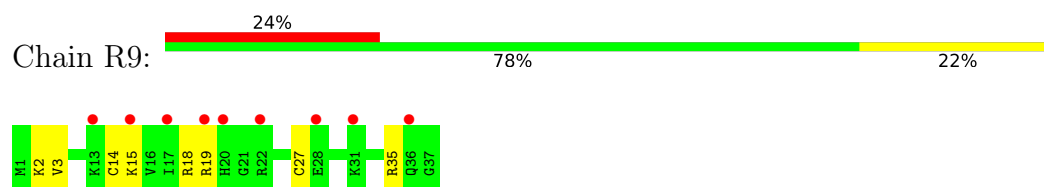
• Molecule 53: 50S ribosomal protein L35



• Molecule 53: 50S ribosomal protein L35

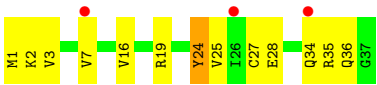


• Molecule 54: 50S ribosomal protein L36



• Molecule 54: 50S ribosomal protein L36





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.24Å 449.36Å 618.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.99 – 3.50 121.99 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.9 (121.99-3.50) 97.9 (121.99-3.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.12-2829	Depositor
R, R_{free}	0.207 , 0.250 0.208 , 0.251	Depositor DCC
R_{free} test set	38831 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	86.9	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 99.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	291948	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ZN, MG

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	0.17	0/36097	0.37	0/56339
1	XA	0.18	0/36100	0.39	0/56344
2	QB	0.18	0/1942	0.53	2/2619 (0.1%)
2	XB	0.18	0/1950	0.49	0/2630
3	QC	0.17	0/1629	0.49	0/2195
3	XC	0.16	0/1629	0.45	0/2195
4	QD	0.19	0/1733	0.54	0/2318
4	XD	0.28	1/1733 (0.1%)	0.59	2/2318 (0.1%)
5	QE	0.21	0/1171	0.50	0/1576
5	XE	0.17	0/1171	0.49	0/1576
6	QF	0.17	0/856	0.47	0/1154
6	XF	0.16	0/856	0.48	0/1154
7	QG	0.18	0/1276	0.50	1/1709 (0.1%)
7	XG	0.17	0/1276	0.46	0/1709
8	QH	0.16	0/1128	0.46	0/1517
8	XH	0.16	0/1128	0.47	0/1517
9	QI	0.26	0/1029	0.61	1/1379 (0.1%)
9	XI	0.22	0/1017	0.52	0/1365
10	QJ	0.17	0/814	0.55	0/1095
10	XJ	0.17	0/790	0.48	0/1063
11	QK	0.14	0/900	0.41	0/1213
11	XK	0.13	0/879	0.35	0/1187
12	QL	0.17	0/991	0.51	0/1327
12	XL	0.16	0/972	0.49	0/1301
13	QM	0.17	0/965	0.52	0/1292
13	XM	0.21	0/956	0.58	0/1281
14	QN	0.20	0/501	0.58	0/664
14	XN	0.18	0/501	0.55	0/664
15	QO	0.17	0/745	0.45	0/992
15	XO	0.17	0/740	0.46	0/987
16	QP	0.15	0/721	0.44	0/970
16	XP	0.16	0/721	0.48	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.17	0/847	0.48	1/1131 (0.1%)
17	XQ	0.15	0/847	0.50	0/1131
18	QR	0.17	0/579	0.44	0/768
18	XR	0.15	0/579	0.46	0/768
19	QS	0.19	0/680	0.67	3/915 (0.3%)
19	XS	0.15	0/689	0.56	0/926
20	QT	0.20	0/765	0.62	0/1007
20	XT	0.20	0/765	0.62	0/1007
21	QU	0.16	0/221	0.43	0/288
21	XU	0.37	0/221	0.60	0/288
22	QV	0.18	0/1836	0.37	0/2859
22	XV	0.19	0/1836	0.39	0/2859
23	QX	0.13	0/293	0.24	0/455
23	XX	0.13	0/268	0.25	0/416
24	RA	0.20	0/69521	0.41	1/108529 (0.0%)
24	YA	0.22	0/69543	0.43	3/108563 (0.0%)
25	RB	0.18	0/2878	0.36	0/4490
25	YB	0.19	0/2878	0.40	0/4490
26	RD	0.18	0/2165	0.50	0/2919
26	YD	0.18	0/2165	0.49	0/2919
27	RE	0.19	0/1601	0.59	0/2160
27	YE	0.61	1/1601 (0.1%)	0.61	0/2160
28	RF	0.20	0/1620	0.46	0/2194
28	YF	0.18	0/1620	0.47	0/2194
29	RG	0.24	0/1499	0.63	1/2016 (0.0%)
29	YG	0.19	0/1499	0.55	1/2016 (0.0%)
30	RH	0.20	0/1362	0.60	1/1841 (0.1%)
30	YH	0.20	0/1362	0.61	2/1841 (0.1%)
31	RI	0.22	0/1151	0.62	0/1558
31	YI	0.26	0/1151	0.67	2/1558 (0.1%)
32	RN	0.17	0/1131	0.47	0/1525
32	YN	0.17	0/1131	0.50	0/1525
33	RO	0.16	0/943	0.40	0/1269
33	YO	0.14	0/943	0.44	0/1269
34	RP	0.54	3/1162 (0.3%)	0.68	1/1544 (0.1%)
34	YP	0.22	0/1139	0.67	2/1514 (0.1%)
35	RQ	0.19	0/1143	0.58	0/1527
35	YQ	0.17	0/1143	0.51	0/1527
36	RR	0.22	0/974	0.57	0/1302
36	YR	0.34	1/974 (0.1%)	0.58	0/1302
37	RS	0.21	0/892	0.56	0/1187
37	YS	0.23	0/892	0.55	0/1187
38	RT	0.19	0/1155	0.54	0/1542

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YT	0.20	0/1155	0.58	1/1542 (0.1%)
39	RU	0.19	0/982	0.58	0/1306
39	YU	0.19	0/982	0.59	0/1306
40	RV	0.17	0/790	0.52	0/1057
40	YV	0.19	0/790	0.57	0/1057
41	RW	0.19	0/911	0.49	0/1220
41	YW	0.17	0/911	0.54	0/1220
42	RX	0.14	0/739	0.39	0/993
42	YX	0.16	0/739	0.44	0/993
43	RY	0.15	0/831	0.40	0/1108
43	YY	0.17	0/831	0.45	0/1108
44	RZ	0.21	0/1493	0.73	3/2026 (0.1%)
44	YZ	0.21	0/1493	0.70	5/2026 (0.2%)
45	R0	0.17	0/652	0.43	0/867
45	Y0	0.23	0/657	0.48	0/874
46	R1	0.19	0/761	0.47	0/1008
46	Y1	0.20	0/736	0.46	0/978
47	R2	0.19	0/583	0.54	0/771
47	Y2	0.19	0/583	0.51	0/771
48	R3	0.16	0/474	0.41	0/635
48	Y3	0.16	0/474	0.44	0/635
49	R4	0.20	0/578	0.73	0/776
49	Y4	0.20	0/578	0.66	2/776 (0.3%)
50	R5	0.14	0/473	0.40	0/639
50	Y5	0.78	2/473 (0.4%)	0.88	1/639 (0.2%)
51	R6	0.14	0/460	0.39	0/613
51	Y6	0.39	0/460	0.62	1/613 (0.2%)
52	R7	0.16	0/417	0.51	0/550
52	Y7	0.17	0/426	0.45	0/561
53	R8	0.48	1/525 (0.2%)	0.62	0/691
53	Y8	0.20	0/525	0.64	0/691
54	R9	0.14	0/310	0.43	0/407
54	Y9	0.15	0/310	0.48	0/407
All	All	0.21	9/315683 (0.0%)	0.44	37/471970 (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
2	XB	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	QC	0	1
4	QD	0	1
5	QE	0	2
5	XE	0	2
7	QG	0	1
7	XG	0	1
9	QI	0	1
12	QL	0	2
12	XL	0	2
13	QM	0	1
18	QR	0	1
18	XR	0	1
19	QS	0	5
20	QT	0	3
20	XT	0	3
26	YD	0	2
27	RE	0	3
27	YE	0	2
29	RG	0	4
29	YG	0	1
30	RH	0	7
30	YH	0	9
31	RI	0	7
31	YI	0	4
32	RN	0	2
32	YN	0	2
33	YO	0	1
34	RP	0	1
34	YP	0	2
35	RQ	0	3
35	YQ	0	2
36	RR	0	1
38	RT	0	1
38	YT	0	2
39	RU	0	1
39	YU	0	1
40	RV	0	2
40	YV	0	2
44	RZ	0	5
44	YZ	0	4
46	R1	0	1
46	Y1	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
47	R2	0	2
47	Y2	0	1
49	R4	0	4
49	Y4	0	3
53	R8	0	3
53	Y8	0	1
54	Y9	0	1
All	All	0	116

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	YE	109	LYS	C-N	22.66	1.45	1.33
50	Y5	27	PRO	CA-C	15.18	1.62	1.52
34	RP	68	GLN	CG-CD	-10.83	1.25	1.52
53	R8	62	LEU	C-O	-9.06	1.19	1.23
36	YR	38	VAL	CA-CB	-7.81	1.50	1.54

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	Y5	27	PRO	O-C-N	16.93	129.11	121.15
44	RZ	179	ASP	CA-C-N	9.08	138.31	121.97
44	RZ	179	ASP	C-N-CA	9.08	138.31	121.97
38	YT	125	ARG	N-CA-C	-8.96	104.41	114.62
4	XD	159	ARG	NE-CZ-NH2	-8.93	111.16	119.20

There are no chirality outliers.

5 of 116 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	QC	143	GLU	Peptide
4	QD	33	MET	Peptide
5	QE	10	MET	Peptide
5	QE	25	ARG	Peptide
7	QG	155	ARG	Peptide

5.2 Too-close contacts [i](#)

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	581	0
1	XA	32248	0	16279	548	2
2	QB	1907	0	1958	60	0
2	XB	1915	0	1969	58	0
3	QC	1605	0	1668	59	0
3	XC	1605	0	1668	49	0
4	QD	1703	0	1766	64	0
4	XD	1703	0	1767	53	1
5	QE	1155	0	1213	27	0
5	XE	1155	0	1213	23	0
6	QF	843	0	857	15	0
6	XF	843	0	857	29	0
7	QG	1257	0	1296	24	0
7	XG	1257	0	1296	28	0
8	QH	1108	0	1165	45	0
8	XH	1108	0	1165	37	0
9	QI	1010	0	1037	59	0
9	XI	998	0	1024	32	0
10	QJ	801	0	849	43	0
10	XJ	777	0	816	38	0
11	QK	885	0	904	26	0
11	XK	864	0	881	26	0
12	QL	975	0	1062	34	0
12	XL	956	0	1046	27	0
13	QM	955	0	1021	42	0
13	XM	946	0	1007	37	0
14	QN	492	0	529	27	0
14	XN	492	0	529	16	0
15	QO	734	0	771	20	0
15	XO	729	0	768	12	0
16	QP	705	0	725	12	0
16	XP	705	0	725	25	0
17	QQ	834	0	904	22	0
17	XQ	834	0	904	24	0
18	QR	574	0	644	16	0
18	XR	574	0	644	20	0
19	QS	665	0	686	43	0
19	XS	674	0	699	25	0
20	QT	763	0	861	25	0
20	XT	763	0	861	26	0
21	QU	217	0	234	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	XU	217	0	234	6	0
22	QV	1644	0	836	23	0
22	XV	1644	0	836	16	0
23	QX	261	0	130	2	0
23	XX	239	0	119	3	0
24	RA	62071	0	31291	867	2
24	YA	62091	0	31301	973	0
25	RB	2573	0	1306	45	0
25	YB	2573	0	1306	47	0
26	RD	2115	0	2195	57	0
26	YD	2115	0	2195	79	0
27	RE	1568	0	1634	54	0
27	YE	1568	0	1634	66	0
28	RF	1585	0	1632	55	0
28	YF	1585	0	1632	44	0
29	RG	1474	0	1535	64	0
29	YG	1474	0	1535	51	0
30	RH	1336	0	1418	40	0
30	YH	1336	0	1418	40	0
31	RI	1136	0	1223	26	2
31	YI	1136	0	1223	42	0
32	RN	1104	0	1180	18	0
32	YN	1104	0	1180	33	0
33	RO	933	0	996	27	0
33	YO	933	0	996	17	0
34	RP	1145	0	1228	46	0
34	YP	1122	0	1206	59	0
35	RQ	1122	0	1179	52	0
35	YQ	1122	0	1179	33	0
36	RR	960	0	1021	38	0
36	YR	960	0	1021	30	0
37	RS	882	0	943	33	0
37	YS	882	0	943	33	0
38	RT	1141	0	1202	40	0
38	YT	1141	0	1202	40	0
39	RU	964	0	1022	33	0
39	YU	964	0	1022	41	0
40	RV	779	0	852	24	0
40	YV	779	0	852	19	1
41	RW	900	0	964	26	0
41	YW	900	0	964	23	0
42	RX	725	0	778	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	YX	725	0	778	14	0
43	RY	818	0	911	12	0
43	YY	818	0	912	27	0
44	RZ	1461	0	1493	59	0
44	YZ	1461	0	1493	46	0
45	R0	643	0	667	19	0
45	Y0	648	0	672	24	0
46	R1	755	0	836	16	0
46	Y1	729	0	802	20	0
47	R2	581	0	629	14	0
47	Y2	581	0	629	12	1
48	R3	469	0	518	13	0
48	Y3	469	0	518	14	0
49	R4	565	0	560	31	0
49	Y4	565	0	559	20	0
50	R5	459	0	476	18	0
50	Y5	459	0	478	13	1
51	R6	453	0	475	16	0
51	Y6	453	0	474	12	0
52	R7	409	0	454	15	0
52	Y7	418	0	467	10	0
53	R8	517	0	582	26	0
53	Y8	517	0	582	24	0
54	R9	307	0	336	6	0
54	Y9	307	0	335	13	0
55	QA	180	0	0	0	0
55	QC	1	0	0	0	0
55	QF	1	0	0	0	0
55	QH	1	0	0	0	0
55	QL	1	0	0	0	0
55	QV	6	0	0	0	0
55	QX	2	0	0	0	0
55	R0	2	0	0	0	0
55	R1	2	0	0	0	0
55	R5	1	0	0	0	0
55	RA	493	0	0	0	0
55	RB	10	0	0	0	0
55	RD	1	0	0	0	0
55	RE	4	0	0	0	0
55	RF	1	0	0	0	0
55	RI	1	0	0	0	0
55	RN	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	RO	1	0	0	0	0
55	RP	3	0	0	0	0
55	RQ	2	0	0	0	0
55	RT	1	0	0	0	0
55	RU	1	0	0	0	0
55	RW	1	0	0	0	0
55	RX	1	0	0	0	0
55	RY	1	0	0	0	0
55	XA	171	0	0	0	0
55	XE	2	0	0	0	0
55	XL	1	0	0	0	0
55	XM	1	0	0	0	0
55	XQ	1	0	0	0	0
55	XS	1	0	0	0	0
55	XV	8	0	0	0	0
55	Y0	1	0	0	0	0
55	Y5	1	0	0	0	0
55	Y7	1	0	0	0	0
55	Y8	1	0	0	0	0
55	YA	515	0	0	0	0
55	YB	10	0	0	0	0
55	YD	2	0	0	0	0
55	YE	4	0	0	0	0
55	YO	1	0	0	0	0
55	YP	3	0	0	0	0
55	YQ	3	0	0	0	0
55	YU	1	0	0	0	0
55	YX	2	0	0	0	0
55	YY	1	0	0	0	0
56	QD	8	0	0	1	0
56	XD	8	0	0	2	0
57	QN	1	0	0	0	0
57	R4	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R9	1	0	0	0	0
57	RY	1	0	0	0	0
57	XN	1	0	0	0	0
57	Y4	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0
57	Y9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	YY	1	0	0	0	0
All	All	291948	0	197745	5298	5

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 11.

The worst 5 of 5298 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)
24:RA:2285:C:OP2	51:R6:6:ARG:NH2	1.85	1.08
24:RA:2068:U:H3	24:RA:2430:A:H2	1.11	0.99
24:RA:676:A:H8	24:RA:2069:G:H21	1.04	0.98
10:QJ:4:ILE:HG22	10:QJ:74:ILE:HG12	1.46	0.96
1:XA:686:U:H1'	11:XK:42:TRP:HE1	1.31	0.93

All (5) 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)
24:RA:2217:G:OP1	4:XD:159:ARG:NH2[4_555]	2.08	0.12
31:RI:89:TYR:O	1:XA:357:G:O2'[4_555]	2.11	0.09
40:YV:49:THR:OG1	50:Y5:60:VAL:O[4_445]	2.12	0.08
24:RA:310:A:OP2	47:Y2:71:ASN:ND2[3_555]	2.14	0.06
31:RI:91:SER:OG	1:XA:368:U:OP1[4_555]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	197 (84%)	35 (15%)	1 (0%)	30	62
2	XB	234/256 (91%)	203 (87%)	31 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	QC	203/239 (85%)	186 (92%)	16 (8%)	1 (0%)	24	57
3	XC	203/239 (85%)	188 (93%)	14 (7%)	1 (0%)	24	57
4	QD	206/209 (99%)	189 (92%)	16 (8%)	1 (0%)	24	57
4	XD	206/209 (99%)	196 (95%)	8 (4%)	2 (1%)	12	44
5	QE	149/162 (92%)	139 (93%)	10 (7%)	0	100	100
5	XE	149/162 (92%)	144 (97%)	4 (3%)	1 (1%)	18	51
6	QF	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	XF	99/101 (98%)	99 (100%)	0	0	100	100
7	QG	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
7	XG	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
8	QH	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
8	XH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
9	QI	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
9	XI	124/128 (97%)	114 (92%)	10 (8%)	0	100	100
10	QJ	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	12	44
10	XJ	94/105 (90%)	86 (92%)	8 (8%)	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%)	109 (89%)	12 (10%)	2 (2%)	7	36
12	XL	120/132 (91%)	104 (87%)	14 (12%)	2 (2%)	7	35
13	QM	118/126 (94%)	102 (86%)	14 (12%)	2 (2%)	7	35
13	XM	117/126 (93%)	104 (89%)	12 (10%)	1 (1%)	14	47
14	QN	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	7	35
14	XN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	7	35
15	QO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
15	XO	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
16	QP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	94 (96%)	4 (4%)	0	100	100
17	XQ	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	QR	68/88 (77%)	67 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	81/93 (87%)	66 (82%)	14 (17%)	1 (1%)	10	41
19	XS	82/93 (88%)	69 (84%)	13 (16%)	0	100	100
20	QT	97/106 (92%)	83 (86%)	11 (11%)	3 (3%)	3	25
20	XT	97/106 (92%)	86 (89%)	9 (9%)	2 (2%)	5	31
21	QU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	XU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
26	RD	270/276 (98%)	251 (93%)	19 (7%)	0	100	100
26	YD	270/276 (98%)	244 (90%)	25 (9%)	1 (0%)	30	62
27	RE	203/206 (98%)	169 (83%)	31 (15%)	3 (2%)	8	37
27	YE	203/206 (98%)	173 (85%)	29 (14%)	1 (0%)	24	57
28	RF	200/210 (95%)	183 (92%)	16 (8%)	1 (0%)	24	57
28	YF	200/210 (95%)	185 (92%)	15 (8%)	0	100	100
29	RG	179/182 (98%)	148 (83%)	30 (17%)	1 (1%)	21	54
29	YG	179/182 (98%)	157 (88%)	22 (12%)	0	100	100
30	RH	172/180 (96%)	151 (88%)	21 (12%)	0	100	100
30	YH	172/180 (96%)	145 (84%)	25 (14%)	2 (1%)	10	41
31	RI	144/148 (97%)	113 (78%)	28 (19%)	3 (2%)	5	31
31	YI	144/148 (97%)	123 (85%)	18 (12%)	3 (2%)	5	31
32	RN	136/140 (97%)	121 (89%)	15 (11%)	0	100	100
32	YN	136/140 (97%)	119 (88%)	17 (12%)	0	100	100
33	RO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
33	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
34	RP	148/150 (99%)	123 (83%)	25 (17%)	0	100	100
34	YP	145/150 (97%)	111 (77%)	34 (23%)	0	100	100
35	RQ	139/141 (99%)	115 (83%)	22 (16%)	2 (1%)	9	38
35	YQ	139/141 (99%)	118 (85%)	19 (14%)	2 (1%)	9	38
36	RR	115/118 (98%)	108 (94%)	6 (5%)	1 (1%)	14	47
36	YR	115/118 (98%)	108 (94%)	6 (5%)	1 (1%)	14	47
37	RS	109/112 (97%)	91 (84%)	18 (16%)	0	100	100
37	YS	109/112 (97%)	93 (85%)	16 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	RT	135/146 (92%)	120 (89%)	15 (11%)	0	100	100
38	YT	135/146 (92%)	115 (85%)	20 (15%)	0	100	100
39	RU	115/118 (98%)	107 (93%)	4 (4%)	4 (4%)	3	23
39	YU	115/118 (98%)	104 (90%)	8 (7%)	3 (3%)	4	27
40	RV	99/101 (98%)	84 (85%)	15 (15%)	0	100	100
40	YV	99/101 (98%)	89 (90%)	10 (10%)	0	100	100
41	RW	111/113 (98%)	101 (91%)	10 (9%)	0	100	100
41	YW	111/113 (98%)	101 (91%)	10 (9%)	0	100	100
42	RX	90/96 (94%)	85 (94%)	5 (6%)	0	100	100
42	YX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
43	RY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
43	YY	105/110 (96%)	103 (98%)	2 (2%)	0	100	100
44	RZ	181/206 (88%)	147 (81%)	30 (17%)	4 (2%)	5	30
44	YZ	181/206 (88%)	145 (80%)	32 (18%)	4 (2%)	5	30
45	R0	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
45	Y0	80/85 (94%)	76 (95%)	4 (5%)	0	100	100
46	R1	92/98 (94%)	79 (86%)	13 (14%)	0	100	100
46	Y1	91/98 (93%)	81 (89%)	10 (11%)	0	100	100
47	R2	67/72 (93%)	60 (90%)	6 (9%)	1 (2%)	8	37
47	Y2	67/72 (93%)	63 (94%)	4 (6%)	0	100	100
48	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
48	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
49	R4	67/71 (94%)	51 (76%)	11 (16%)	5 (8%)	1	9
49	Y4	67/71 (94%)	51 (76%)	12 (18%)	4 (6%)	1	12
50	R5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
50	Y5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
51	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
51	Y6	51/54 (94%)	46 (90%)	5 (10%)	0	100	100
52	R7	45/49 (92%)	45 (100%)	0	0	100	100
52	Y7	46/49 (94%)	46 (100%)	0	0	100	100
53	R8	62/65 (95%)	51 (82%)	9 (14%)	2 (3%)	3	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	Y8	62/65 (95%)	48 (77%)	14 (23%)	0	100	100
54	R9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
54	Y9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
All	All	11456/12128 (94%)	10265 (90%)	1120 (10%)	71 (1%)	21	54

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	QC	12	LEU
20	QT	74	LYS
39	RU	91	ASP
39	RU	92	ARG
44	RZ	53	ILE

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%)	202 (100%)	1 (0%)	81	80
2	XB	204/220 (93%)	203 (100%)	1 (0%)	81	80
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%)	124 (98%)	2 (2%)	55	70
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	118/119 (99%)	117 (99%)	1 (1%)	73	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	XH	118/119 (99%)	117 (99%)	1 (1%)	73	77
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%)	89 (99%)	1 (1%)	65	74
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	102 (98%)	2 (2%)	50	68
12	XL	103/109 (94%)	103 (100%)	0	100	100
13	QM	96/101 (95%)	95 (99%)	1 (1%)	68	75
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
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%)	60 (98%)	1 (2%)	55	70
19	QS	72/80 (90%)	72 (100%)	0	100	100
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
26	RD	214/218 (98%)	214 (100%)	0	100	100
26	YD	214/218 (98%)	214 (100%)	0	100	100
27	RE	165/166 (99%)	164 (99%)	1 (1%)	78	79
27	YE	165/166 (99%)	165 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	RF	161/166 (97%)	161 (100%)	0	100	100
28	YF	161/166 (97%)	161 (100%)	0	100	100
29	RG	155/156 (99%)	155 (100%)	0	100	100
29	YG	155/156 (99%)	154 (99%)	1 (1%)	78	79
30	RH	145/148 (98%)	145 (100%)	0	100	100
30	YH	145/148 (98%)	144 (99%)	1 (1%)	76	78
31	RI	122/124 (98%)	121 (99%)	1 (1%)	73	77
31	YI	122/124 (98%)	120 (98%)	2 (2%)	55	70
32	RN	117/119 (98%)	117 (100%)	0	100	100
32	YN	117/119 (98%)	116 (99%)	1 (1%)	70	76
33	RO	100/100 (100%)	100 (100%)	0	100	100
33	YO	100/100 (100%)	100 (100%)	0	100	100
34	RP	116/116 (100%)	116 (100%)	0	100	100
34	YP	114/116 (98%)	113 (99%)	1 (1%)	70	76
35	RQ	111/111 (100%)	110 (99%)	1 (1%)	70	76
35	YQ	111/111 (100%)	111 (100%)	0	100	100
36	RR	100/101 (99%)	100 (100%)	0	100	100
36	YR	100/101 (99%)	100 (100%)	0	100	100
37	RS	87/88 (99%)	86 (99%)	1 (1%)	65	74
37	YS	87/88 (99%)	87 (100%)	0	100	100
38	RT	120/127 (94%)	119 (99%)	1 (1%)	73	77
38	YT	120/127 (94%)	119 (99%)	1 (1%)	73	77
39	RU	93/94 (99%)	93 (100%)	0	100	100
39	YU	93/94 (99%)	93 (100%)	0	100	100
40	RV	82/82 (100%)	81 (99%)	1 (1%)	63	73
40	YV	82/82 (100%)	82 (100%)	0	100	100
41	RW	92/92 (100%)	92 (100%)	0	100	100
41	YW	92/92 (100%)	92 (100%)	0	100	100
42	RX	74/78 (95%)	74 (100%)	0	100	100
42	YX	74/78 (95%)	74 (100%)	0	100	100
43	RY	88/91 (97%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	YY	88/91 (97%)	88 (100%)	0	100	100
44	RZ	162/179 (90%)	162 (100%)	0	100	100
44	YZ	162/179 (90%)	162 (100%)	0	100	100
45	R0	65/67 (97%)	65 (100%)	0	100	100
45	Y0	65/67 (97%)	65 (100%)	0	100	100
46	R1	81/83 (98%)	79 (98%)	2 (2%)	42	63
46	Y1	78/83 (94%)	78 (100%)	0	100	100
47	R2	64/67 (96%)	64 (100%)	0	100	100
47	Y2	64/67 (96%)	64 (100%)	0	100	100
48	R3	51/52 (98%)	51 (100%)	0	100	100
48	Y3	51/52 (98%)	51 (100%)	0	100	100
49	R4	62/63 (98%)	62 (100%)	0	100	100
49	Y4	62/63 (98%)	62 (100%)	0	100	100
50	R5	51/52 (98%)	51 (100%)	0	100	100
50	Y5	51/52 (98%)	51 (100%)	0	100	100
51	R6	51/52 (98%)	51 (100%)	0	100	100
51	Y6	51/52 (98%)	51 (100%)	0	100	100
52	R7	40/42 (95%)	40 (100%)	0	100	100
52	Y7	41/42 (98%)	41 (100%)	0	100	100
53	R8	54/55 (98%)	54 (100%)	0	100	100
53	Y8	54/55 (98%)	54 (100%)	0	100	100
54	R9	34/34 (100%)	34 (100%)	0	100	100
54	Y9	34/34 (100%)	34 (100%)	0	100	100
All	All	9690/10066 (96%)	9664 (100%)	26 (0%)	86	83

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	R1	85	LEU
8	XH	137	VAL
34	YP	61	ARG
2	XB	21	ARG
18	XR	65	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
32	YN	130	HIS
33	YO	89	ASN
44	YZ	32	HIS
36	RR	13	HIS
34	RP	68	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1508 (99%)	263 (17%)	30 (2%)
1	XA	1498/1508 (99%)	286 (19%)	27 (1%)
22	QV	76/77 (98%)	18 (23%)	2 (2%)
22	XV	76/77 (98%)	16 (21%)	3 (3%)
23	QX	11/25 (44%)	7 (63%)	0
23	XX	10/25 (40%)	6 (60%)	0
24	RA	2879/2915 (98%)	578 (20%)	33 (1%)
24	YA	2880/2915 (98%)	571 (19%)	36 (1%)
25	RB	119/122 (97%)	24 (20%)	1 (0%)
25	YB	119/122 (97%)	23 (19%)	1 (0%)
All	All	9166/9294 (98%)	1792 (19%)	133 (1%)

5 of 1792 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 133 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	YA	1178	C
24	YA	1460	A
24	YA	2832	U
24	RA	1085	A
24	RA	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 1464 ligands modelled in this entry, 1462 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	$\# Z > 2$
56	SF4	XD	301	4	0,12,12	-	-	-		
56	SF4	QD	301	-	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
56	SF4	XD	301	4	-	-	0/6/5/5
56	SF4	QD	301	-	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	XD	301	SF4	2	0
56	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%)	0.16	21 (1%) 73 48	44, 105, 204, 408	0
1	XA	1500/1508 (99%)	-0.02	15 (1%) 79 56	32, 93, 196, 349	0
2	QB	235/256 (91%)	0.39	4 (1%) 69 43	91, 152, 223, 286	0
2	XB	236/256 (92%)	0.44	6 (2%) 58 35	58, 124, 196, 243	0
3	QC	205/239 (85%)	0.49	8 (3%) 43 23	77, 139, 196, 224	0
3	XC	205/239 (85%)	0.41	7 (3%) 48 27	56, 106, 164, 206	0
4	QD	208/209 (99%)	0.67	15 (7%) 21 14	65, 111, 168, 257	0
4	XD	208/209 (99%)	0.24	5 (2%) 59 35	49, 88, 141, 183	0
5	QE	151/162 (93%)	0.33	3 (1%) 65 39	66, 108, 158, 199	0
5	XE	151/162 (93%)	0.27	4 (2%) 57 33	50, 91, 141, 200	0
6	QF	101/101 (100%)	0.09	3 (2%) 52 30	66, 104, 149, 281	0
6	XF	101/101 (100%)	0.25	1 (0%) 79 56	51, 103, 160, 173	0
7	QG	155/156 (99%)	0.26	5 (3%) 50 29	58, 111, 165, 251	0
7	XG	155/156 (99%)	0.31	4 (2%) 57 33	71, 108, 171, 202	0
8	QH	137/138 (99%)	0.59	10 (7%) 21 13	65, 114, 158, 181	0
8	XH	137/138 (99%)	0.34	2 (1%) 72 47	55, 94, 131, 171	0
9	QI	127/128 (99%)	1.10	20 (15%) 5 5	84, 138, 188, 216	0
9	XI	126/128 (98%)	0.61	10 (7%) 18 12	68, 126, 181, 223	0
10	QJ	99/105 (94%)	0.81	10 (10%) 12 8	87, 141, 200, 247	0
10	XJ	96/105 (91%)	0.76	11 (11%) 9 6	71, 127, 181, 234	0
11	QK	119/129 (92%)	0.42	4 (3%) 48 27	58, 100, 166, 268	0
11	XK	116/129 (89%)	0.45	4 (3%) 48 27	55, 96, 163, 219	0
12	QL	125/132 (94%)	0.73	15 (12%) 9 6	51, 95, 170, 242	0
12	XL	122/132 (92%)	0.54	12 (9%) 13 9	44, 77, 136, 195	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	120/126 (95%)	0.68	13 (10%) 11 8	77, 126, 183, 244	0
13	XM	119/126 (94%)	0.43	6 (5%) 34 19	57, 107, 157, 214	0
14	QN	60/61 (98%)	1.10	9 (15%) 5 5	90, 131, 173, 228	0
14	XN	60/61 (98%)	0.93	7 (11%) 9 6	64, 101, 127, 158	0
15	QO	88/89 (98%)	0.40	3 (3%) 48 27	51, 104, 152, 205	0
15	XO	87/89 (97%)	0.10	0 100 100	54, 89, 124, 141	0
16	QP	84/88 (95%)	0.36	1 (1%) 76 52	61, 94, 134, 145	0
16	XP	84/88 (95%)	0.86	9 (10%) 11 8	62, 96, 154, 205	0
17	QQ	100/105 (95%)	0.50	2 (2%) 65 39	55, 97, 143, 167	0
17	XQ	100/105 (95%)	0.66	6 (6%) 27 16	65, 97, 148, 172	0
18	QR	70/88 (79%)	0.37	2 (2%) 53 31	57, 110, 169, 208	0
18	XR	70/88 (79%)	0.30	1 (1%) 73 48	58, 98, 158, 212	0
19	QS	83/93 (89%)	0.68	11 (13%) 7 6	98, 145, 201, 252	0
19	XS	84/93 (90%)	0.42	4 (4%) 35 19	76, 114, 176, 226	0
20	QT	99/106 (93%)	0.69	6 (6%) 27 16	55, 96, 157, 245	0
20	XT	99/106 (93%)	1.18	20 (20%) 3 3	66, 121, 178, 207	0
21	QU	25/27 (92%)	1.23	5 (20%) 3 3	66, 127, 171, 197	0
21	XU	25/27 (92%)	1.01	3 (12%) 9 6	78, 106, 135, 158	0
22	QV	77/77 (100%)	0.15	1 (1%) 75 50	57, 100, 151, 210	0
22	XV	77/77 (100%)	-0.07	2 (2%) 57 33	47, 81, 133, 192	0
23	QX	12/25 (48%)	2.25	8 (66%) 0 0	68, 195, 252, 261	0
23	XX	11/25 (44%)	2.19	8 (72%) 0 0	56, 166, 214, 246	0
24	RA	2882/2915 (98%)	-0.14	35 (1%) 76 52	28, 72, 228, 408	0
24	YA	2883/2915 (98%)	-0.23	37 (1%) 75 50	22, 64, 223, 495	0
25	RB	120/122 (98%)	0.17	0 100 100	66, 108, 153, 183	0
25	YB	120/122 (98%)	0.10	3 (2%) 58 35	59, 93, 137, 158	0
26	RD	272/276 (98%)	0.32	11 (4%) 42 23	25, 64, 109, 270	0
26	YD	272/276 (98%)	0.28	9 (3%) 49 28	23, 57, 104, 219	0
27	RE	205/206 (99%)	0.53	6 (2%) 53 31	40, 76, 146, 227	0
27	YE	205/206 (99%)	0.49	8 (3%) 43 23	26, 73, 158, 274	0
28	RF	202/210 (96%)	0.38	2 (0%) 79 56	29, 80, 144, 167	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YF	202/210 (96%)	0.12	3 (1%) 72 47	26, 65, 124, 177	0
29	RG	181/182 (99%)	0.63	14 (7%) 19 13	78, 119, 167, 219	0
29	YG	181/182 (99%)	0.50	7 (3%) 43 23	60, 103, 156, 217	0
30	RH	174/180 (96%)	0.95	19 (10%) 10 7	97, 152, 216, 254	0
30	YH	174/180 (96%)	0.35	7 (4%) 42 23	45, 91, 137, 299	0
31	RI	146/148 (98%)	0.63	15 (10%) 12 8	52, 117, 167, 219	0
31	YI	146/148 (98%)	0.39	4 (2%) 56 33	53, 116, 161, 190	0
32	RN	138/140 (98%)	0.65	9 (6%) 25 15	40, 87, 151, 183	0
32	YN	138/140 (98%)	0.53	6 (4%) 40 21	39, 77, 147, 197	0
33	RO	122/122 (100%)	0.20	2 (1%) 70 45	39, 70, 105, 146	0
33	YO	122/122 (100%)	0.19	0 100 100	21, 65, 111, 139	0
34	RP	150/150 (100%)	0.40	7 (4%) 36 20	33, 93, 155, 267	0
34	YP	147/150 (98%)	0.74	12 (8%) 17 11	27, 77, 137, 196	0
35	RQ	141/141 (100%)	0.64	13 (9%) 14 9	46, 88, 147, 238	0
35	YQ	141/141 (100%)	0.69	18 (12%) 7 6	34, 76, 141, 281	0
36	RR	117/118 (99%)	0.15	2 (1%) 69 43	40, 66, 114, 176	0
36	YR	117/118 (99%)	0.40	3 (2%) 57 33	41, 74, 113, 158	0
37	RS	111/112 (99%)	0.70	5 (4%) 38 20	55, 116, 160, 242	0
37	YS	111/112 (99%)	0.58	7 (6%) 26 15	52, 100, 160, 286	0
38	RT	137/146 (93%)	0.53	7 (5%) 33 19	38, 86, 150, 190	0
38	YT	137/146 (93%)	0.35	5 (3%) 46 25	41, 80, 160, 232	0
39	RU	117/118 (99%)	0.41	4 (3%) 48 27	38, 75, 136, 224	0
39	YU	117/118 (99%)	0.42	6 (5%) 33 19	29, 64, 115, 213	0
40	RV	101/101 (100%)	0.41	1 (0%) 79 56	43, 98, 169, 295	0
40	YV	101/101 (100%)	0.56	6 (5%) 28 16	27, 82, 147, 296	0
41	RW	113/113 (100%)	0.29	6 (5%) 32 18	33, 64, 113, 217	0
41	YW	113/113 (100%)	0.21	3 (2%) 56 33	32, 61, 125, 216	0
42	RX	92/96 (95%)	0.21	3 (3%) 49 28	38, 74, 111, 158	0
42	YX	92/96 (95%)	0.21	0 100 100	37, 60, 112, 171	0
43	RY	107/110 (97%)	0.82	14 (13%) 7 6	65, 107, 151, 224	0
43	YY	107/110 (97%)	0.62	4 (3%) 45 25	44, 85, 141, 214	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RZ	183/206 (88%)	0.44	4 (2%) 62 37	73, 120, 187, 289	0
44	YZ	183/206 (88%)	0.55	10 (5%) 30 18	48, 111, 170, 227	0
45	R0	81/85 (95%)	0.83	10 (12%) 8 6	52, 79, 161, 227	0
45	Y0	82/85 (96%)	0.74	9 (10%) 10 7	45, 78, 145, 198	0
46	R1	96/98 (97%)	0.98	14 (14%) 6 5	30, 79, 159, 297	0
46	Y1	93/98 (94%)	0.80	9 (9%) 13 9	33, 72, 138, 184	0
47	R2	69/72 (95%)	0.12	1 (1%) 73 48	53, 101, 176, 215	0
47	Y2	69/72 (95%)	0.23	4 (5%) 29 17	37, 71, 137, 222	0
48	R3	59/60 (98%)	0.47	0 100 100	44, 89, 129, 184	0
48	Y3	59/60 (98%)	0.10	1 (1%) 69 43	41, 71, 136, 221	0
49	R4	69/71 (97%)	0.18	1 (1%) 73 48	97, 152, 212, 268	0
49	Y4	69/71 (97%)	0.28	0 100 100	80, 136, 218, 265	0
50	R5	59/60 (98%)	0.41	4 (6%) 23 14	46, 77, 181, 194	0
50	Y5	59/60 (98%)	0.35	1 (1%) 69 43	37, 73, 164, 198	0
51	R6	53/54 (98%)	1.38	11 (20%) 2 3	143, 171, 235, 272	0
51	Y6	53/54 (98%)	0.50	2 (3%) 44 24	150, 181, 231, 252	0
52	R7	47/49 (95%)	0.57	3 (6%) 25 15	28, 55, 91, 161	0
52	Y7	48/49 (97%)	0.22	4 (8%) 17 11	27, 44, 88, 147	0
53	R8	64/65 (98%)	0.97	9 (14%) 6 5	38, 80, 139, 239	0
53	Y8	64/65 (98%)	0.83	8 (12%) 8 6	35, 70, 118, 268	0
54	R9	37/37 (100%)	1.50	9 (24%) 2 2	102, 146, 191, 244	0
54	Y9	37/37 (100%)	0.87	3 (8%) 18 12	88, 108, 148, 162	0
All	All	20836/21422 (97%)	0.24	766 (3%) 45 25	21, 90, 184, 495	0

The worst 5 of 766 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	QJ	62	HIS	7.5
9	XI	121	ARG	6.7
9	QI	121	ARG	6.1
26	RD	36	PRO	6.1
7	QG	32	ARG	5.9

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($\text{\AA}^2$)	Q<0.9
55	MG	RA	3419	1/1	0.01	0.17	156,156,156,156	0
55	MG	XA	1703	1/1	0.23	0.18	184,184,184,184	0
55	MG	YA	3287	1/1	0.23	0.28	115,115,115,115	0
55	MG	XV	106	1/1	0.36	0.36	140,140,140,140	0
55	MG	RA	3273	1/1	0.42	0.21	158,158,158,158	0
55	MG	RA	3411	1/1	0.47	0.18	94,94,94,94	0
55	MG	YA	3341	1/1	0.49	0.16	131,131,131,131	0
55	MG	YA	3360	1/1	0.51	0.30	80,80,80,80	0
55	MG	RB	210	1/1	0.52	0.20	99,99,99,99	0
55	MG	RA	3443	1/1	0.52	0.12	216,216,216,216	0
55	MG	QA	1779	1/1	0.53	0.15	78,78,78,78	0
55	MG	XA	1636	1/1	0.54	0.16	104,104,104,104	0
55	MG	QA	1681	1/1	0.59	0.23	122,122,122,122	0
55	MG	XA	1730	1/1	0.60	0.14	73,73,73,73	0
55	MG	YA	3478	1/1	0.60	0.31	106,106,106,106	0
55	MG	QA	1778	1/1	0.61	0.24	109,109,109,109	0
55	MG	XA	1661	1/1	0.61	0.11	80,80,80,80	0
55	MG	RA	3435	1/1	0.61	0.16	82,82,82,82	0
55	MG	QA	1757	1/1	0.63	0.20	100,100,100,100	0
55	MG	QA	1727	1/1	0.64	0.36	117,117,117,117	0
55	MG	RA	3383	1/1	0.65	0.63	105,105,105,105	0
55	MG	RA	3134	1/1	0.66	0.14	65,65,65,65	0
55	MG	QA	1765	1/1	0.68	0.22	100,100,100,100	0
57	ZN	YY	501	1/1	0.68	0.20	305,305,305,305	0
55	MG	QA	1726	1/1	0.69	0.19	35,35,35,35	0
55	MG	XA	1749	1/1	0.69	0.27	101,101,101,101	0
55	MG	RA	3201	1/1	0.70	0.30	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	QA	1717	1/1	0.70	0.10	122,122,122,122	0
55	MG	RA	3311	1/1	0.70	0.19	64,64,64,64	0
55	MG	QA	1711	1/1	0.70	0.15	60,60,60,60	0
55	MG	YA	3172	1/1	0.71	0.17	50,50,50,50	0
55	MG	RA	3468	1/1	0.71	0.28	91,91,91,91	0
55	MG	RA	3203	1/1	0.72	0.38	65,65,65,65	0
55	MG	RA	3460	1/1	0.72	0.07	54,54,54,54	0
55	MG	RA	3326	1/1	0.72	0.33	100,100,100,100	0
55	MG	RA	3135	1/1	0.72	0.23	37,37,37,37	0
55	MG	YA	3498	1/1	0.73	0.14	59,59,59,59	0
55	MG	QF	201	1/1	0.73	0.20	62,62,62,62	0
55	MG	RA	3356	1/1	0.74	0.17	65,65,65,65	0
55	MG	YA	3288	1/1	0.75	0.10	28,28,28,28	0
55	MG	XA	1648	1/1	0.75	0.14	118,118,118,118	0
55	MG	RA	3090	1/1	0.76	0.09	29,29,29,29	0
55	MG	YB	205	1/1	0.76	0.22	65,65,65,65	0
55	MG	RA	3053	1/1	0.76	0.18	24,24,24,24	0
55	MG	RA	3204	1/1	0.77	0.21	61,61,61,61	0
55	MG	RA	3316	1/1	0.77	0.10	35,35,35,35	0
55	MG	YA	3443	1/1	0.77	0.25	73,73,73,73	0
55	MG	QA	1672	1/1	0.77	0.17	61,61,61,61	0
55	MG	YA	3188	1/1	0.77	0.19	88,88,88,88	0
55	MG	RA	3448	1/1	0.77	0.19	98,98,98,98	0
55	MG	XA	1739	1/1	0.77	0.15	69,69,69,69	0
55	MG	YA	3179	1/1	0.78	0.24	26,26,26,26	0
55	MG	YA	3384	1/1	0.78	0.07	44,44,44,44	0
55	MG	QA	1728	1/1	0.78	0.28	101,101,101,101	0
55	MG	RA	3082	1/1	0.78	0.07	16,16,16,16	0
55	MG	YA	3479	1/1	0.78	0.19	100,100,100,100	0
55	MG	QV	106	1/1	0.78	0.69	71,71,71,71	0
55	MG	YA	3318	1/1	0.78	0.17	62,62,62,62	0
55	MG	RA	3120	1/1	0.78	0.24	47,47,47,47	0
55	MG	QA	1698	1/1	0.79	0.07	58,58,58,58	0
55	MG	YA	3252	1/1	0.79	0.16	28,28,28,28	0
55	MG	RA	3199	1/1	0.79	0.17	66,66,66,66	0
55	MG	XA	1664	1/1	0.79	0.07	62,62,62,62	0
55	MG	YA	3480	1/1	0.79	0.10	81,81,81,81	0
55	MG	YA	3106	1/1	0.79	0.25	54,54,54,54	0
55	MG	QA	1710	1/1	0.79	0.16	72,72,72,72	0
55	MG	YB	209	1/1	0.79	0.16	48,48,48,48	0
55	MG	QA	1612	1/1	0.79	0.30	45,45,45,45	0
55	MG	RA	3434	1/1	0.80	0.19	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3315	1/1	0.80	0.21	52,52,52,52	0
55	MG	RA	3314	1/1	0.80	0.16	50,50,50,50	0
55	MG	YA	3484	1/1	0.80	0.12	80,80,80,80	0
55	MG	QA	1644	1/1	0.80	0.26	69,69,69,69	0
55	MG	RA	3317	1/1	0.80	0.18	60,60,60,60	0
55	MG	XA	1651	1/1	0.80	0.30	99,99,99,99	0
57	ZN	R4	100	1/1	0.80	0.09	243,243,243,243	0
55	MG	QA	1768	1/1	0.80	0.21	67,67,67,67	0
55	MG	QA	1770	1/1	0.81	0.14	85,85,85,85	0
55	MG	YA	3164	1/1	0.81	0.27	96,96,96,96	0
55	MG	YA	3379	1/1	0.81	0.13	66,66,66,66	0
55	MG	QA	1712	1/1	0.81	0.10	83,83,83,83	0
55	MG	YA	3178	1/1	0.81	0.47	37,37,37,37	0
55	MG	QA	1720	1/1	0.81	0.06	52,52,52,52	0
55	MG	XA	1737	1/1	0.81	0.06	45,45,45,45	0
55	MG	RA	3151	1/1	0.81	0.12	80,80,80,80	0
55	MG	RA	3152	1/1	0.81	0.15	47,47,47,47	0
55	MG	YA	3490	1/1	0.81	0.32	100,100,100,100	0
55	MG	XA	1766	1/1	0.81	0.12	76,76,76,76	0
55	MG	YA	3304	1/1	0.81	0.17	56,56,56,56	0
55	MG	QA	1725	1/1	0.81	0.09	126,126,126,126	0
55	MG	YA	3105	1/1	0.81	0.26	23,23,23,23	0
55	MG	YA	3336	1/1	0.81	0.08	114,114,114,114	0
55	MG	XA	1705	1/1	0.82	0.23	59,59,59,59	0
55	MG	RA	3251	1/1	0.82	0.18	56,56,56,56	0
55	MG	RA	3270	1/1	0.82	0.28	53,53,53,53	0
55	MG	YA	3483	1/1	0.82	0.10	23,23,23,23	0
55	MG	QA	1756	1/1	0.82	0.22	121,121,121,121	0
55	MG	RA	3284	1/1	0.82	0.23	61,61,61,61	0
55	MG	RA	3158	1/1	0.82	0.14	47,47,47,47	0
55	MG	RX	101	1/1	0.82	0.06	63,63,63,63	0
55	MG	YA	3003	1/1	0.82	0.18	44,44,44,44	0
55	MG	YA	3279	1/1	0.82	0.21	52,52,52,52	0
55	MG	YA	3004	1/1	0.82	0.10	51,51,51,51	0
55	MG	QA	1608	1/1	0.83	0.13	85,85,85,85	0
55	MG	RA	3409	1/1	0.83	0.10	53,53,53,53	0
55	MG	RA	3447	1/1	0.83	0.48	64,64,64,64	0
55	MG	RA	3327	1/1	0.83	0.09	38,38,38,38	0
55	MG	XA	1660	1/1	0.83	0.12	33,33,33,33	0
55	MG	RA	3355	1/1	0.83	0.20	49,49,49,49	0
55	MG	XA	1663	1/1	0.83	0.19	39,39,39,39	0
55	MG	RA	3427	1/1	0.83	0.12	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RB	205	1/1	0.83	0.25	69,69,69,69	0
55	MG	YA	3123	1/1	0.83	0.34	60,60,60,60	0
55	MG	RB	206	1/1	0.83	0.20	74,74,74,74	0
55	MG	QA	1758	1/1	0.83	0.28	69,69,69,69	0
55	MG	XA	1736	1/1	0.83	0.09	67,67,67,67	0
55	MG	RA	3245	1/1	0.84	0.17	54,54,54,54	0
55	MG	YA	3193	1/1	0.84	0.07	28,28,28,28	0
55	MG	YA	3244	1/1	0.84	0.15	34,34,34,34	0
55	MG	YA	3424	1/1	0.84	0.28	64,64,64,64	0
55	MG	XA	1687	1/1	0.84	0.08	35,35,35,35	0
55	MG	YA	3262	1/1	0.84	0.15	33,33,33,33	0
55	MG	QH	201	1/1	0.84	0.31	95,95,95,95	0
55	MG	XA	1759	1/1	0.84	0.23	81,81,81,81	0
55	MG	YA	3162	1/1	0.84	0.22	49,49,49,49	0
55	MG	YA	3292	1/1	0.84	0.13	45,45,45,45	0
55	MG	QA	1721	1/1	0.84	0.19	47,47,47,47	0
55	MG	YA	3496	1/1	0.84	0.20	114,114,114,114	0
55	MG	XA	1770	1/1	0.84	0.26	79,79,79,79	0
55	MG	QA	1716	1/1	0.84	0.15	70,70,70,70	0
55	MG	YA	3334	1/1	0.84	0.12	61,61,61,61	0
55	MG	RA	3238	1/1	0.84	0.39	60,60,60,60	0
55	MG	YA	3182	1/1	0.84	0.19	119,119,119,119	0
55	MG	RA	3299	1/1	0.85	0.09	45,45,45,45	0
55	MG	QA	1697	1/1	0.85	0.19	61,61,61,61	0
55	MG	RA	3193	1/1	0.85	0.12	82,82,82,82	0
55	MG	YA	3268	1/1	0.85	0.20	65,65,65,65	0
55	MG	YA	3359	1/1	0.85	0.06	16,16,16,16	0
55	MG	QA	1731	1/1	0.85	0.07	44,44,44,44	0
55	MG	RA	3358	1/1	0.85	0.34	79,79,79,79	0
55	MG	QA	1660	1/1	0.85	0.07	98,98,98,98	0
55	MG	RA	3388	1/1	0.85	0.05	37,37,37,37	0
57	ZN	RY	501	1/1	0.85	0.14	313,313,313,313	0
55	MG	RO	201	1/1	0.85	0.27	61,61,61,61	0
55	MG	YA	3114	1/1	0.85	0.14	39,39,39,39	0
55	MG	RA	3485	1/1	0.86	0.16	44,44,44,44	0
55	MG	RA	3307	1/1	0.86	0.22	38,38,38,38	0
55	MG	QA	1741	1/1	0.86	0.12	44,44,44,44	0
55	MG	QA	1708	1/1	0.86	0.11	67,67,67,67	0
55	MG	QA	1658	1/1	0.86	0.13	68,68,68,68	0
55	MG	RA	3250	1/1	0.86	0.17	49,49,49,49	0
55	MG	YA	3387	1/1	0.86	0.11	71,71,71,71	0
55	MG	RA	3098	1/1	0.86	0.17	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3237	1/1	0.86	0.23	74,74,74,74	0
55	MG	YA	3468	1/1	0.86	0.33	91,91,91,91	0
55	MG	RA	3196	1/1	0.86	0.08	43,43,43,43	0
55	MG	RA	3338	1/1	0.86	0.11	46,46,46,46	0
55	MG	RA	3340	1/1	0.86	0.15	66,66,66,66	0
55	MG	RA	3347	1/1	0.86	0.20	66,66,66,66	0
55	MG	YA	3081	1/1	0.86	0.26	35,35,35,35	0
55	MG	YA	3089	1/1	0.86	0.11	51,51,51,51	0
55	MG	YA	3491	1/1	0.86	0.22	60,60,60,60	0
55	MG	YA	3102	1/1	0.86	0.26	37,37,37,37	0
55	MG	QA	1718	1/1	0.86	0.05	55,55,55,55	0
55	MG	QA	1653	1/1	0.86	0.10	138,138,138,138	0
55	MG	YB	206	1/1	0.86	0.08	69,69,69,69	0
55	MG	RA	3462	1/1	0.86	0.11	48,48,48,48	0
55	MG	QA	1707	1/1	0.86	0.13	67,67,67,67	0
55	MG	YA	3328	1/1	0.86	0.10	58,58,58,58	0
57	ZN	R5	101	1/1	0.86	0.16	388,388,388,388	0
55	MG	RA	3477	1/1	0.86	0.24	75,75,75,75	0
55	MG	RA	3148	1/1	0.87	0.25	27,27,27,27	0
55	MG	RA	3211	1/1	0.87	0.13	67,67,67,67	0
55	MG	RA	3070	1/1	0.87	0.20	59,59,59,59	0
55	MG	RA	3241	1/1	0.87	0.24	36,36,36,36	0
55	MG	YA	3342	1/1	0.87	0.15	68,68,68,68	0
55	MG	RA	3243	1/1	0.87	0.24	52,52,52,52	0
55	MG	YA	3135	1/1	0.87	0.10	46,46,46,46	0
55	MG	YA	3144	1/1	0.87	0.22	39,39,39,39	0
55	MG	RA	3330	1/1	0.87	0.17	70,70,70,70	0
55	MG	QA	1722	1/1	0.87	0.10	58,58,58,58	0
55	MG	YA	3408	1/1	0.87	0.20	73,73,73,73	0
55	MG	YA	3413	1/1	0.87	0.24	43,43,43,43	0
55	MG	RA	3457	1/1	0.87	0.09	59,59,59,59	0
55	MG	RA	3085	1/1	0.87	0.22	27,27,27,27	0
55	MG	XA	1729	1/1	0.87	0.14	62,62,62,62	0
55	MG	YA	3473	1/1	0.87	0.16	45,45,45,45	0
55	MG	RA	3169	1/1	0.87	0.18	91,91,91,91	0
55	MG	RA	3264	1/1	0.87	0.15	44,44,44,44	0
55	MG	RA	3179	1/1	0.87	0.25	53,53,53,53	0
55	MG	YA	3224	1/1	0.87	0.16	32,32,32,32	0
55	MG	RA	3484	1/1	0.87	0.10	54,54,54,54	0
55	MG	QA	1685	1/1	0.87	0.20	61,61,61,61	0
55	MG	XA	1755	1/1	0.87	0.18	60,60,60,60	0
55	MG	RA	3376	1/1	0.87	0.13	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	QA	1759	1/1	0.87	0.14	55,55,55,55	0
55	MG	XA	1767	1/1	0.87	0.11	87,87,87,87	0
55	MG	QA	1738	1/1	0.87	0.07	53,53,53,53	0
55	MG	RD	301	1/1	0.87	0.37	74,74,74,74	0
55	MG	RA	3407	1/1	0.87	0.10	50,50,50,50	0
55	MG	QA	1699	1/1	0.87	0.07	49,49,49,49	0
55	MG	XA	1633	1/1	0.87	0.28	43,43,43,43	0
55	MG	QA	1617	1/1	0.87	0.12	50,50,50,50	0
57	ZN	Y5	101	1/1	0.87	0.14	214,214,214,214	0
55	MG	YA	3311	1/1	0.88	0.10	63,63,63,63	0
55	MG	RA	3414	1/1	0.88	0.21	58,58,58,58	0
55	MG	YA	3317	1/1	0.88	0.18	55,55,55,55	0
55	MG	XV	107	1/1	0.88	0.23	37,37,37,37	0
55	MG	YA	3325	1/1	0.88	0.14	52,52,52,52	0
55	MG	XA	1632	1/1	0.88	0.31	33,33,33,33	0
55	MG	RA	3202	1/1	0.88	0.16	39,39,39,39	0
55	MG	QA	1652	1/1	0.88	0.09	49,49,49,49	0
55	MG	YA	3085	1/1	0.88	0.29	25,25,25,25	0
55	MG	XA	1645	1/1	0.88	0.11	87,87,87,87	0
55	MG	YA	3099	1/1	0.88	0.27	41,41,41,41	0
55	MG	QA	1661	1/1	0.88	0.23	62,62,62,62	0
55	MG	YA	3377	1/1	0.88	0.10	48,48,48,48	0
55	MG	RA	3126	1/1	0.88	0.14	89,89,89,89	0
55	MG	RA	3230	1/1	0.88	0.26	47,47,47,47	0
55	MG	QA	1615	1/1	0.88	0.14	86,86,86,86	0
55	MG	YA	3404	1/1	0.88	0.14	43,43,43,43	0
55	MG	YA	3405	1/1	0.88	0.16	65,65,65,65	0
55	MG	QA	1657	1/1	0.88	0.19	45,45,45,45	0
55	MG	RA	3452	1/1	0.88	0.33	80,80,80,80	0
55	MG	XA	1674	1/1	0.88	0.18	73,73,73,73	0
55	MG	XA	1677	1/1	0.88	0.10	32,32,32,32	0
55	MG	QX	101	1/1	0.88	0.22	72,72,72,72	0
55	MG	XA	1689	1/1	0.88	0.08	41,41,41,41	0
55	MG	YA	3474	1/1	0.88	0.12	44,44,44,44	0
55	MG	YA	3475	1/1	0.88	0.14	54,54,54,54	0
55	MG	RA	3007	1/1	0.88	0.16	55,55,55,55	0
55	MG	RA	3042	1/1	0.88	0.32	26,26,26,26	0
55	MG	XA	1725	1/1	0.88	0.11	53,53,53,53	0
55	MG	RA	3155	1/1	0.88	0.10	26,26,26,26	0
55	MG	RA	3472	1/1	0.88	0.27	78,78,78,78	0
55	MG	YA	3196	1/1	0.88	0.17	64,64,64,64	0
55	MG	QA	1651	1/1	0.88	0.08	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3054	1/1	0.88	0.19	16,16,16,16	0
55	MG	QA	1691	1/1	0.88	0.06	35,35,35,35	0
55	MG	YB	203	1/1	0.88	0.12	54,54,54,54	0
55	MG	RA	3492	1/1	0.88	0.19	76,76,76,76	0
55	MG	QA	1693	1/1	0.88	0.12	61,61,61,61	0
55	MG	RA	3389	1/1	0.88	0.06	73,73,73,73	0
55	MG	XA	1760	1/1	0.88	0.16	119,119,119,119	0
55	MG	QA	1774	1/1	0.88	0.20	78,78,78,78	0
55	MG	RA	3089	1/1	0.88	0.17	25,25,25,25	0
55	MG	QA	1750	1/1	0.88	0.11	44,44,44,44	0
55	MG	XV	103	1/1	0.88	0.15	67,67,67,67	0
55	MG	QA	1683	1/1	0.89	0.25	62,62,62,62	0
55	MG	RA	3312	1/1	0.89	0.08	27,27,27,27	0
55	MG	RA	3313	1/1	0.89	0.05	23,23,23,23	0
55	MG	YA	3337	1/1	0.89	0.26	55,55,55,55	0
55	MG	RA	3008	1/1	0.89	0.30	61,61,61,61	0
55	MG	XA	1724	1/1	0.89	0.25	66,66,66,66	0
55	MG	RA	3172	1/1	0.89	0.19	54,54,54,54	0
55	MG	RA	3107	1/1	0.89	0.19	65,65,65,65	0
55	MG	YA	3362	1/1	0.89	0.23	65,65,65,65	0
55	MG	QA	1776	1/1	0.89	0.07	40,40,40,40	0
55	MG	YA	3156	1/1	0.89	0.31	32,32,32,32	0
55	MG	XA	1735	1/1	0.89	0.09	41,41,41,41	0
55	MG	RA	3422	1/1	0.89	0.35	76,76,76,76	0
55	MG	YA	3389	1/1	0.89	0.09	39,39,39,39	0
55	MG	YA	3403	1/1	0.89	0.10	53,53,53,53	0
55	MG	RA	3425	1/1	0.89	0.09	54,54,54,54	0
55	MG	XA	1738	1/1	0.89	0.12	64,64,64,64	0
55	MG	RA	3195	1/1	0.89	0.22	48,48,48,48	0
55	MG	YA	3411	1/1	0.89	0.31	52,52,52,52	0
55	MG	YA	3412	1/1	0.89	0.20	47,47,47,47	0
55	MG	XA	1746	1/1	0.89	0.17	74,74,74,74	0
55	MG	YA	3414	1/1	0.89	0.25	49,49,49,49	0
55	MG	QA	1714	1/1	0.89	0.25	66,66,66,66	0
55	MG	YA	3191	1/1	0.89	0.09	48,48,48,48	0
55	MG	YA	3446	1/1	0.89	0.13	56,56,56,56	0
55	MG	YA	3463	1/1	0.89	0.09	56,56,56,56	0
55	MG	YA	3466	1/1	0.89	0.08	38,38,38,38	0
55	MG	XA	1752	1/1	0.89	0.13	58,58,58,58	0
55	MG	YA	3470	1/1	0.89	0.09	38,38,38,38	0
55	MG	XA	1626	1/1	0.89	0.09	49,49,49,49	0
55	MG	YA	3202	1/1	0.89	0.10	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3212	1/1	0.89	0.10	53,53,53,53	0
55	MG	XA	1757	1/1	0.89	0.11	43,43,43,43	0
55	MG	QA	1709	1/1	0.89	0.10	59,59,59,59	0
55	MG	RA	3440	1/1	0.89	0.05	50,50,50,50	0
55	MG	YA	3246	1/1	0.89	0.13	58,58,58,58	0
55	MG	QA	1736	1/1	0.89	0.08	36,36,36,36	0
55	MG	YA	3487	1/1	0.89	0.14	63,63,63,63	0
55	MG	XA	1637	1/1	0.89	0.15	28,28,28,28	0
55	MG	RA	3445	1/1	0.89	0.21	68,68,68,68	0
55	MG	YA	3495	1/1	0.89	0.09	32,32,32,32	0
55	MG	YA	3273	1/1	0.89	0.18	46,46,46,46	0
55	MG	XE	202	1/1	0.89	0.14	70,70,70,70	0
55	MG	YA	3514	1/1	0.89	0.14	84,84,84,84	0
55	MG	RA	3072	1/1	0.89	0.25	29,29,29,29	0
55	MG	RA	3353	1/1	0.89	0.11	45,45,45,45	0
55	MG	QA	1723	1/1	0.89	0.22	59,59,59,59	0
55	MG	RA	3290	1/1	0.89	0.17	50,50,50,50	0
55	MG	YB	210	1/1	0.89	0.05	51,51,51,51	0
55	MG	QA	1704	1/1	0.89	0.09	38,38,38,38	0
55	MG	YA	3016	1/1	0.89	0.28	4,4,4,4	0
55	MG	RA	3461	1/1	0.89	0.22	47,47,47,47	0
57	ZN	R9	101	1/1	0.89	0.19	174,174,174,174	0
55	MG	QA	1613	1/1	0.89	0.26	47,47,47,47	0
57	ZN	Y4	100	1/1	0.89	0.10	237,237,237,237	0
55	MG	RA	3310	1/1	0.89	0.17	49,49,49,49	0
55	MG	RA	3012	1/1	0.90	0.29	18,18,18,18	0
55	MG	YA	3305	1/1	0.90	0.17	77,77,77,77	0
55	MG	RA	3206	1/1	0.90	0.18	51,51,51,51	0
55	MG	RA	3207	1/1	0.90	0.11	61,61,61,61	0
55	MG	RA	3332	1/1	0.90	0.07	72,72,72,72	0
55	MG	RA	3208	1/1	0.90	0.23	49,49,49,49	0
55	MG	YA	3324	1/1	0.90	0.17	33,33,33,33	0
55	MG	RA	3339	1/1	0.90	0.09	29,29,29,29	0
55	MG	RA	3493	1/1	0.90	0.20	34,34,34,34	0
55	MG	RA	3209	1/1	0.90	0.18	69,69,69,69	0
55	MG	RA	3346	1/1	0.90	0.09	42,42,42,42	0
55	MG	XL	201	1/1	0.90	0.12	54,54,54,54	0
55	MG	RA	3034	1/1	0.90	0.20	27,27,27,27	0
55	MG	RA	3352	1/1	0.90	0.16	50,50,50,50	0
55	MG	RE	302	1/1	0.90	0.12	71,71,71,71	0
55	MG	RA	3217	1/1	0.90	0.06	51,51,51,51	0
55	MG	RT	201	1/1	0.90	0.13	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3015	1/1	0.90	0.32	24,24,24,24	0
55	MG	QA	1604	1/1	0.90	0.17	37,37,37,37	0
55	MG	R0	101	1/1	0.90	0.17	38,38,38,38	0
55	MG	XA	1621	1/1	0.90	0.15	43,43,43,43	0
55	MG	RA	3231	1/1	0.90	0.29	50,50,50,50	0
55	MG	YA	3093	1/1	0.90	0.25	36,36,36,36	0
55	MG	RA	3140	1/1	0.90	0.33	66,66,66,66	0
55	MG	RA	3374	1/1	0.90	0.10	17,17,17,17	0
55	MG	RA	3144	1/1	0.90	0.10	26,26,26,26	0
55	MG	RA	3145	1/1	0.90	0.19	62,62,62,62	0
55	MG	RA	3051	1/1	0.90	0.18	32,32,32,32	0
55	MG	RA	3247	1/1	0.90	0.18	54,54,54,54	0
55	MG	XA	1649	1/1	0.90	0.24	59,59,59,59	0
55	MG	YA	3420	1/1	0.90	0.15	23,23,23,23	0
55	MG	YA	3142	1/1	0.90	0.19	44,44,44,44	0
55	MG	YA	3435	1/1	0.90	0.06	32,32,32,32	0
55	MG	RA	3405	1/1	0.90	0.23	49,49,49,49	0
55	MG	RA	3406	1/1	0.90	0.14	61,61,61,61	0
55	MG	QA	1647	1/1	0.90	0.20	72,72,72,72	0
55	MG	YA	3465	1/1	0.90	0.07	73,73,73,73	0
55	MG	YA	3163	1/1	0.90	0.38	66,66,66,66	0
55	MG	QA	1619	1/1	0.90	0.21	68,68,68,68	0
55	MG	YA	3168	1/1	0.90	0.11	51,51,51,51	0
55	MG	QA	1622	1/1	0.90	0.15	42,42,42,42	0
55	MG	YA	3175	1/1	0.90	0.23	49,49,49,49	0
55	MG	QA	1734	1/1	0.90	0.18	58,58,58,58	0
55	MG	RA	3168	1/1	0.90	0.19	74,74,74,74	0
55	MG	XA	1682	1/1	0.90	0.10	44,44,44,44	0
55	MG	XA	1686	1/1	0.90	0.12	42,42,42,42	0
55	MG	RA	3077	1/1	0.90	0.31	16,16,16,16	0
55	MG	RA	3080	1/1	0.90	0.10	17,17,17,17	0
55	MG	XA	1692	1/1	0.90	0.15	31,31,31,31	0
55	MG	YA	3198	1/1	0.90	0.13	45,45,45,45	0
55	MG	RA	3291	1/1	0.90	0.20	59,59,59,59	0
55	MG	RA	3295	1/1	0.90	0.10	46,46,46,46	0
55	MG	QA	1735	1/1	0.90	0.07	36,36,36,36	0
55	MG	RA	3191	1/1	0.90	0.08	60,60,60,60	0
55	MG	YA	3509	1/1	0.90	0.05	41,41,41,41	0
55	MG	RA	3308	1/1	0.90	0.07	33,33,33,33	0
55	MG	YA	3245	1/1	0.90	0.15	40,40,40,40	0
55	MG	QV	103	1/1	0.90	0.18	65,65,65,65	0
55	MG	QA	1626	1/1	0.90	0.13	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3256	1/1	0.90	0.14	26,26,26,26	0
55	MG	QA	1677	1/1	0.90	0.11	55,55,55,55	0
55	MG	YE	303	1/1	0.90	0.06	19,19,19,19	0
55	MG	Y7	101	1/1	0.90	0.18	54,54,54,54	0
55	MG	QA	1769	1/1	0.90	0.07	35,35,35,35	0
55	MG	QA	1739	1/1	0.90	0.07	48,48,48,48	0
55	MG	RA	3010	1/1	0.90	0.20	29,29,29,29	0
55	MG	RA	3123	1/1	0.90	0.12	27,27,27,27	0
55	MG	XA	1747	1/1	0.90	0.15	49,49,49,49	0
55	MG	RA	3320	1/1	0.90	0.14	42,42,42,42	0
55	MG	YA	3297	1/1	0.90	0.12	26,26,26,26	0
55	MG	RA	3112	1/1	0.91	0.30	39,39,39,39	0
55	MG	YA	3293	1/1	0.91	0.13	50,50,50,50	0
55	MG	RA	3116	1/1	0.91	0.09	40,40,40,40	0
55	MG	YA	3001	1/1	0.91	0.15	19,19,19,19	0
55	MG	QA	1748	1/1	0.91	0.09	63,63,63,63	0
55	MG	RA	3345	1/1	0.91	0.14	72,72,72,72	0
55	MG	QV	105	1/1	0.91	0.25	39,39,39,39	0
55	MG	QA	1749	1/1	0.91	0.11	42,42,42,42	0
55	MG	YA	3041	1/1	0.91	0.27	23,23,23,23	0
55	MG	YA	3319	1/1	0.91	0.23	52,52,52,52	0
55	MG	YA	3042	1/1	0.91	0.24	18,18,18,18	0
55	MG	YA	3075	1/1	0.91	0.29	18,18,18,18	0
55	MG	YA	3327	1/1	0.91	0.12	48,48,48,48	0
55	MG	RA	3350	1/1	0.91	0.09	32,32,32,32	0
55	MG	YA	3082	1/1	0.91	0.16	40,40,40,40	0
55	MG	YA	3084	1/1	0.91	0.12	39,39,39,39	0
55	MG	RA	3455	1/1	0.91	0.06	52,52,52,52	0
55	MG	RA	3127	1/1	0.91	0.15	64,64,64,64	0
55	MG	RA	3288	1/1	0.91	0.21	28,28,28,28	0
55	MG	YA	3356	1/1	0.91	0.12	32,32,32,32	0
55	MG	XA	1678	1/1	0.91	0.06	19,19,19,19	0
55	MG	XA	1680	1/1	0.91	0.17	29,29,29,29	0
55	MG	RA	3068	1/1	0.91	0.20	48,48,48,48	0
55	MG	YA	3369	1/1	0.91	0.13	48,48,48,48	0
55	MG	YA	3374	1/1	0.91	0.34	76,76,76,76	0
55	MG	XA	1684	1/1	0.91	0.04	34,34,34,34	0
55	MG	YA	3107	1/1	0.91	0.19	26,26,26,26	0
55	MG	YA	3382	1/1	0.91	0.06	59,59,59,59	0
55	MG	YA	3109	1/1	0.91	0.17	29,29,29,29	0
55	MG	YA	3386	1/1	0.91	0.09	27,27,27,27	0
55	MG	YA	3110	1/1	0.91	0.15	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3112	1/1	0.91	0.24	35,35,35,35	0
55	MG	QA	1724	1/1	0.91	0.07	35,35,35,35	0
55	MG	YA	3119	1/1	0.91	0.16	30,30,30,30	0
55	MG	RA	3466	1/1	0.91	0.07	38,38,38,38	0
55	MG	RA	3006	1/1	0.91	0.17	32,32,32,32	0
55	MG	YA	3136	1/1	0.91	0.08	16,16,16,16	0
55	MG	YA	3137	1/1	0.91	0.19	40,40,40,40	0
55	MG	QA	1689	1/1	0.91	0.14	58,58,58,58	0
55	MG	RA	3476	1/1	0.91	0.11	33,33,33,33	0
55	MG	YA	3145	1/1	0.91	0.09	37,37,37,37	0
55	MG	YA	3146	1/1	0.91	0.23	38,38,38,38	0
55	MG	RA	3375	1/1	0.91	0.09	54,54,54,54	0
55	MG	XA	1706	1/1	0.91	0.14	38,38,38,38	0
55	MG	YA	3444	1/1	0.91	0.21	115,115,115,115	0
55	MG	XA	1707	1/1	0.91	0.11	29,29,29,29	0
55	MG	XA	1722	1/1	0.91	0.11	40,40,40,40	0
55	MG	YA	3464	1/1	0.91	0.14	44,44,44,44	0
55	MG	QA	1684	1/1	0.91	0.14	28,28,28,28	0
55	MG	YA	3169	1/1	0.91	0.15	55,55,55,55	0
55	MG	QA	1715	1/1	0.91	0.07	75,75,75,75	0
55	MG	QA	1625	1/1	0.91	0.05	52,52,52,52	0
55	MG	YA	3472	1/1	0.91	0.06	26,26,26,26	0
55	MG	RA	3210	1/1	0.91	0.15	38,38,38,38	0
55	MG	XA	1733	1/1	0.91	0.08	42,42,42,42	0
55	MG	YA	3180	1/1	0.91	0.23	32,32,32,32	0
55	MG	RA	3390	1/1	0.91	0.36	57,57,57,57	0
55	MG	RA	3087	1/1	0.91	0.15	25,25,25,25	0
55	MG	RA	3020	1/1	0.91	0.20	2,2,2,2	0
55	MG	YA	3192	1/1	0.91	0.31	72,72,72,72	0
55	MG	RA	3030	1/1	0.91	0.21	19,19,19,19	0
55	MG	YA	3194	1/1	0.91	0.07	39,39,39,39	0
55	MG	QA	1764	1/1	0.91	0.12	51,51,51,51	0
55	MG	YA	3197	1/1	0.91	0.15	44,44,44,44	0
55	MG	RA	3234	1/1	0.91	0.20	17,17,17,17	0
55	MG	RQ	202	1/1	0.91	0.15	37,37,37,37	0
55	MG	YA	3204	1/1	0.91	0.05	8,8,8,8	0
55	MG	YA	3501	1/1	0.91	0.22	38,38,38,38	0
55	MG	RA	3104	1/1	0.91	0.15	56,56,56,56	0
55	MG	RA	3416	1/1	0.91	0.08	29,29,29,29	0
55	MG	YA	3515	1/1	0.91	0.06	41,41,41,41	0
55	MG	XA	1753	1/1	0.91	0.11	76,76,76,76	0
55	MG	QA	1688	1/1	0.91	0.15	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1608	1/1	0.91	0.17	38,38,38,38	0
55	MG	RA	3175	1/1	0.91	0.13	64,64,64,64	0
55	MG	RA	3424	1/1	0.91	0.14	63,63,63,63	0
55	MG	XA	1627	1/1	0.91	0.10	33,33,33,33	0
55	MG	YO	201	1/1	0.91	0.18	40,40,40,40	0
55	MG	YQ	202	1/1	0.91	0.28	151,151,151,151	0
55	MG	YA	3260	1/1	0.91	0.13	34,34,34,34	0
55	MG	RA	3177	1/1	0.91	0.13	85,85,85,85	0
55	MG	XA	1769	1/1	0.91	0.11	70,70,70,70	0
55	MG	RA	3111	1/1	0.91	0.21	59,59,59,59	0
55	MG	XA	1635	1/1	0.91	0.06	51,51,51,51	0
55	MG	YA	3283	1/1	0.91	0.23	49,49,49,49	0
55	MG	RA	3431	1/1	0.91	0.07	32,32,32,32	0
55	MG	RA	3337	1/1	0.91	0.20	48,48,48,48	0
55	MG	YA	3326	1/1	0.92	0.21	49,49,49,49	0
55	MG	RA	3267	1/1	0.92	0.20	45,45,45,45	0
55	MG	QA	1747	1/1	0.92	0.07	47,47,47,47	0
55	MG	YA	3332	1/1	0.92	0.05	29,29,29,29	0
55	MG	RA	3197	1/1	0.92	0.16	30,30,30,30	0
55	MG	RA	3275	1/1	0.92	0.13	24,24,24,24	0
55	MG	RA	3281	1/1	0.92	0.06	25,25,25,25	0
55	MG	RA	3128	1/1	0.92	0.21	5,5,5,5	0
55	MG	RA	3357	1/1	0.92	0.18	74,74,74,74	0
55	MG	YA	3347	1/1	0.92	0.12	41,41,41,41	0
55	MG	YA	3354	1/1	0.92	0.07	26,26,26,26	0
55	MG	RA	3467	1/1	0.92	0.09	44,44,44,44	0
55	MG	RA	3129	1/1	0.92	0.20	32,32,32,32	0
55	MG	YA	3117	1/1	0.92	0.21	62,62,62,62	0
55	MG	RA	3470	1/1	0.92	0.30	63,63,63,63	0
55	MG	RA	3370	1/1	0.92	0.10	76,76,76,76	0
55	MG	YA	3373	1/1	0.92	0.15	59,59,59,59	0
55	MG	XA	1704	1/1	0.92	0.21	53,53,53,53	0
55	MG	RA	3289	1/1	0.92	0.28	49,49,49,49	0
55	MG	RA	3075	1/1	0.92	0.23	23,23,23,23	0
55	MG	RA	3482	1/1	0.92	0.10	39,39,39,39	0
55	MG	XA	1712	1/1	0.92	0.19	48,48,48,48	0
55	MG	YA	3385	1/1	0.92	0.19	60,60,60,60	0
55	MG	XA	1713	1/1	0.92	0.19	44,44,44,44	0
55	MG	XA	1714	1/1	0.92	0.18	54,54,54,54	0
55	MG	YA	3153	1/1	0.92	0.16	84,84,84,84	0
55	MG	YA	3394	1/1	0.92	0.22	23,23,23,23	0
55	MG	RA	3076	1/1	0.92	0.15	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3159	1/1	0.92	0.14	59,59,59,59	0
55	MG	QC	301	1/1	0.92	0.06	111,111,111,111	0
55	MG	RA	3387	1/1	0.92	0.05	46,46,46,46	0
55	MG	RA	3014	1/1	0.92	0.10	30,30,30,30	0
55	MG	RB	202	1/1	0.92	0.09	68,68,68,68	0
55	MG	RB	204	1/1	0.92	0.12	75,75,75,75	0
55	MG	RA	3305	1/1	0.92	0.22	46,46,46,46	0
55	MG	YA	3417	1/1	0.92	0.07	48,48,48,48	0
55	MG	QA	1687	1/1	0.92	0.10	27,27,27,27	0
55	MG	RA	3392	1/1	0.92	0.12	41,41,41,41	0
55	MG	YA	3430	1/1	0.92	0.06	33,33,33,33	0
55	MG	RA	3395	1/1	0.92	0.13	41,41,41,41	0
55	MG	YA	3437	1/1	0.92	0.14	43,43,43,43	0
55	MG	RA	3026	1/1	0.92	0.25	36,36,36,36	0
55	MG	RE	304	1/1	0.92	0.09	37,37,37,37	0
55	MG	YA	3186	1/1	0.92	0.15	50,50,50,50	0
55	MG	RA	3028	1/1	0.92	0.21	23,23,23,23	0
55	MG	QA	1614	1/1	0.92	0.08	41,41,41,41	0
55	MG	XA	1750	1/1	0.92	0.12	59,59,59,59	0
55	MG	QA	1601	1/1	0.92	0.09	19,19,19,19	0
55	MG	YA	3467	1/1	0.92	0.05	40,40,40,40	0
55	MG	QA	1664	1/1	0.92	0.21	68,68,68,68	0
55	MG	RY	502	1/1	0.92	0.34	196,196,196,196	0
55	MG	RA	3224	1/1	0.92	0.35	51,51,51,51	0
55	MG	RA	3228	1/1	0.92	0.30	63,63,63,63	0
55	MG	XA	1609	1/1	0.92	0.18	29,29,29,29	0
55	MG	XA	1617	1/1	0.92	0.12	67,67,67,67	0
55	MG	QA	1771	1/1	0.92	0.12	42,42,42,42	0
55	MG	QA	1773	1/1	0.92	0.14	48,48,48,48	0
55	MG	RA	3324	1/1	0.92	0.08	36,36,36,36	0
55	MG	XA	1630	1/1	0.92	0.17	47,47,47,47	0
55	MG	QA	1667	1/1	0.92	0.06	17,17,17,17	0
55	MG	RA	3174	1/1	0.92	0.12	30,30,30,30	0
55	MG	YA	3248	1/1	0.92	0.25	34,34,34,34	0
55	MG	RA	3429	1/1	0.92	0.08	53,53,53,53	0
55	MG	YA	3494	1/1	0.92	0.16	69,69,69,69	0
55	MG	RA	3055	1/1	0.92	0.13	53,53,53,53	0
55	MG	RA	3061	1/1	0.92	0.18	34,34,34,34	0
55	MG	XA	1643	1/1	0.92	0.21	58,58,58,58	0
55	MG	XA	1644	1/1	0.92	0.09	17,17,17,17	0
55	MG	QA	1659	1/1	0.92	0.14	89,89,89,89	0
55	MG	YA	3511	1/1	0.92	0.08	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3275	1/1	0.92	0.14	53,53,53,53	0
55	MG	YA	3277	1/1	0.92	0.15	51,51,51,51	0
55	MG	RA	3437	1/1	0.92	0.20	24,24,24,24	0
55	MG	YA	3025	1/1	0.92	0.18	17,17,17,17	0
55	MG	YA	3029	1/1	0.92	0.15	6,6,6,6	0
55	MG	YA	3034	1/1	0.92	0.18	11,11,11,11	0
55	MG	RA	3182	1/1	0.92	0.12	59,59,59,59	0
55	MG	RA	3069	1/1	0.92	0.23	37,37,37,37	0
55	MG	YE	304	1/1	0.92	0.09	87,87,87,87	0
55	MG	YA	3054	1/1	0.92	0.15	45,45,45,45	0
55	MG	YA	3061	1/1	0.92	0.06	21,21,21,21	0
55	MG	YQ	203	1/1	0.92	0.07	34,34,34,34	0
55	MG	XA	1659	1/1	0.92	0.12	47,47,47,47	0
55	MG	RA	3125	1/1	0.92	0.18	65,65,65,65	0
55	MG	RA	3258	1/1	0.92	0.12	18,18,18,18	0
55	MG	QA	1742	1/1	0.92	0.09	23,23,23,23	0
55	MG	RA	3450	1/1	0.92	0.10	55,55,55,55	0
55	MG	XA	1665	1/1	0.92	0.11	44,44,44,44	0
55	MG	YA	3091	1/1	0.92	0.20	34,34,34,34	0
55	MG	XA	1669	1/1	0.92	0.21	19,19,19,19	0
55	MG	QA	1628	1/1	0.93	0.14	66,66,66,66	0
55	MG	YA	3127	1/1	0.93	0.17	44,44,44,44	0
55	MG	RA	3058	1/1	0.93	0.20	41,41,41,41	0
55	MG	YA	3346	1/1	0.93	0.08	50,50,50,50	0
55	MG	XA	1631	1/1	0.93	0.14	36,36,36,36	0
55	MG	RA	3456	1/1	0.93	0.17	48,48,48,48	0
55	MG	YA	3138	1/1	0.93	0.25	46,46,46,46	0
55	MG	YA	3140	1/1	0.93	0.07	35,35,35,35	0
55	MG	RA	3019	1/1	0.93	0.18	16,16,16,16	0
55	MG	RA	3063	1/1	0.93	0.20	28,28,28,28	0
55	MG	XA	1740	1/1	0.93	0.05	57,57,57,57	0
55	MG	RA	3066	1/1	0.93	0.15	26,26,26,26	0
55	MG	RA	3146	1/1	0.93	0.13	39,39,39,39	0
55	MG	XA	1748	1/1	0.93	0.14	57,57,57,57	0
55	MG	YA	3158	1/1	0.93	0.17	22,22,22,22	0
55	MG	XA	1642	1/1	0.93	0.06	44,44,44,44	0
55	MG	YA	3160	1/1	0.93	0.16	42,42,42,42	0
55	MG	YA	3161	1/1	0.93	0.27	39,39,39,39	0
55	MG	RA	3465	1/1	0.93	0.13	49,49,49,49	0
55	MG	RA	3319	1/1	0.93	0.13	55,55,55,55	0
55	MG	QA	1673	1/1	0.93	0.12	34,34,34,34	0
55	MG	YA	3392	1/1	0.93	0.30	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3167	1/1	0.93	0.06	31,31,31,31	0
55	MG	YA	3395	1/1	0.93	0.15	55,55,55,55	0
55	MG	YA	3402	1/1	0.93	0.05	26,26,26,26	0
55	MG	XA	1647	1/1	0.93	0.10	32,32,32,32	0
55	MG	XA	1756	1/1	0.93	0.09	49,49,49,49	0
55	MG	RA	3321	1/1	0.93	0.19	56,56,56,56	0
55	MG	YA	3406	1/1	0.93	0.11	47,47,47,47	0
55	MG	RA	3394	1/1	0.93	0.05	37,37,37,37	0
55	MG	XA	1650	1/1	0.93	0.06	42,42,42,42	0
55	MG	RA	3110	1/1	0.93	0.30	56,56,56,56	0
55	MG	XA	1653	1/1	0.93	0.08	28,28,28,28	0
55	MG	XA	1658	1/1	0.93	0.20	47,47,47,47	0
55	MG	RA	3473	1/1	0.93	0.09	50,50,50,50	0
55	MG	RA	3404	1/1	0.93	0.18	44,44,44,44	0
55	MG	RA	3325	1/1	0.93	0.18	55,55,55,55	0
55	MG	RA	3262	1/1	0.93	0.17	47,47,47,47	0
55	MG	YA	3431	1/1	0.93	0.25	75,75,75,75	0
55	MG	RA	3021	1/1	0.93	0.18	33,33,33,33	0
55	MG	QA	1638	1/1	0.93	0.14	43,43,43,43	0
55	MG	YA	3442	1/1	0.93	0.24	100,100,100,100	0
55	MG	XA	1667	1/1	0.93	0.10	38,38,38,38	0
55	MG	RA	3205	1/1	0.93	0.27	58,58,58,58	0
55	MG	RA	3335	1/1	0.93	0.08	43,43,43,43	0
55	MG	YA	3449	1/1	0.93	0.11	28,28,28,28	0
55	MG	YA	3450	1/1	0.93	0.22	56,56,56,56	0
55	MG	YA	3453	1/1	0.93	0.20	74,74,74,74	0
55	MG	YA	3457	1/1	0.93	0.11	60,60,60,60	0
55	MG	YA	3460	1/1	0.93	0.10	27,27,27,27	0
55	MG	YA	3014	1/1	0.93	0.21	20,20,20,20	0
55	MG	RB	201	1/1	0.93	0.05	42,42,42,42	0
55	MG	RA	3071	1/1	0.93	0.18	40,40,40,40	0
55	MG	YA	3219	1/1	0.93	0.12	77,77,77,77	0
55	MG	RA	3161	1/1	0.93	0.17	37,37,37,37	0
55	MG	YA	3027	1/1	0.93	0.26	12,12,12,12	0
55	MG	RA	3119	1/1	0.93	0.17	66,66,66,66	0
55	MG	YA	3030	1/1	0.93	0.24	10,10,10,10	0
55	MG	YA	3031	1/1	0.93	0.21	11,11,11,11	0
55	MG	RA	3282	1/1	0.93	0.20	53,53,53,53	0
55	MG	RA	3002	1/1	0.93	0.11	30,30,30,30	0
55	MG	YA	3476	1/1	0.93	0.11	46,46,46,46	0
55	MG	RA	3004	1/1	0.93	0.11	15,15,15,15	0
55	MG	YA	3052	1/1	0.93	0.20	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3261	1/1	0.93	0.17	35,35,35,35	0
55	MG	QA	1690	1/1	0.93	0.12	72,72,72,72	0
55	MG	YA	3263	1/1	0.93	0.10	35,35,35,35	0
55	MG	YA	3485	1/1	0.93	0.09	32,32,32,32	0
55	MG	YA	3486	1/1	0.93	0.12	33,33,33,33	0
55	MG	RA	3348	1/1	0.93	0.10	35,35,35,35	0
55	MG	XA	1693	1/1	0.93	0.11	45,45,45,45	0
55	MG	YA	3077	1/1	0.93	0.23	27,27,27,27	0
55	MG	YA	3078	1/1	0.93	0.17	44,44,44,44	0
55	MG	RA	3433	1/1	0.93	0.12	48,48,48,48	0
55	MG	QA	1754	1/1	0.93	0.12	52,52,52,52	0
55	MG	RA	3223	1/1	0.93	0.14	59,59,59,59	0
55	MG	YA	3500	1/1	0.93	0.06	45,45,45,45	0
55	MG	RA	3176	1/1	0.93	0.05	74,74,74,74	0
55	MG	YA	3507	1/1	0.93	0.16	36,36,36,36	0
55	MG	YA	3291	1/1	0.93	0.28	28,28,28,28	0
55	MG	YA	3088	1/1	0.93	0.23	12,12,12,12	0
55	MG	QA	1702	1/1	0.93	0.05	40,40,40,40	0
55	MG	RA	3441	1/1	0.93	0.24	66,66,66,66	0
55	MG	YB	202	1/1	0.93	0.18	50,50,50,50	0
55	MG	YA	3299	1/1	0.93	0.21	55,55,55,55	0
55	MG	QA	1703	1/1	0.93	0.06	56,56,56,56	0
55	MG	QA	1678	1/1	0.93	0.20	36,36,36,36	0
55	MG	YA	3310	1/1	0.93	0.12	23,23,23,23	0
55	MG	XA	1715	1/1	0.93	0.07	44,44,44,44	0
55	MG	YA	3103	1/1	0.93	0.15	11,11,11,11	0
55	MG	XA	1716	1/1	0.93	0.23	40,40,40,40	0
55	MG	XA	1720	1/1	0.93	0.14	42,42,42,42	0
55	MG	YQ	201	1/1	0.93	0.16	33,33,33,33	0
55	MG	XA	1616	1/1	0.93	0.12	23,23,23,23	0
55	MG	XA	1723	1/1	0.93	0.06	29,29,29,29	0
55	MG	YX	102	1/1	0.93	0.14	106,106,106,106	0
55	MG	YY	502	1/1	0.93	0.14	79,79,79,79	0
55	MG	RA	3232	1/1	0.93	0.16	30,30,30,30	0
55	MG	XA	1619	1/1	0.93	0.12	65,65,65,65	0
55	MG	YA	3113	1/1	0.93	0.26	57,57,57,57	0
55	MG	RA	3367	1/1	0.93	0.10	62,62,62,62	0
55	MG	YA	3331	1/1	0.93	0.15	45,45,45,45	0
55	MG	RA	3184	1/1	0.93	0.18	43,43,43,43	0
55	MG	YA	3118	1/1	0.93	0.16	73,73,73,73	0
55	MG	XA	1732	1/1	0.93	0.12	41,41,41,41	0
57	ZN	Y6	101	1/1	0.93	0.11	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3024	1/1	0.94	0.24	25,25,25,25	0
55	MG	QA	1632	1/1	0.94	0.03	5,5,5,5	0
55	MG	RA	3086	1/1	0.94	0.20	15,15,15,15	0
55	MG	RA	3047	1/1	0.94	0.21	10,10,10,10	0
55	MG	YA	3313	1/1	0.94	0.13	49,49,49,49	0
55	MG	RA	3213	1/1	0.94	0.08	43,43,43,43	0
55	MG	YA	3316	1/1	0.94	0.08	26,26,26,26	0
55	MG	XA	1646	1/1	0.94	0.03	28,28,28,28	0
55	MG	RA	3315	1/1	0.94	0.04	34,34,34,34	0
55	MG	RA	3049	1/1	0.94	0.12	42,42,42,42	0
55	MG	YA	3320	1/1	0.94	0.12	24,24,24,24	0
55	MG	RA	3219	1/1	0.94	0.29	37,37,37,37	0
55	MG	RA	3221	1/1	0.94	0.09	20,20,20,20	0
55	MG	QA	1676	1/1	0.94	0.15	51,51,51,51	0
55	MG	RA	3157	1/1	0.94	0.07	37,37,37,37	0
55	MG	YA	3070	1/1	0.94	0.24	15,15,15,15	0
55	MG	XA	1654	1/1	0.94	0.15	34,34,34,34	0
55	MG	RA	3438	1/1	0.94	0.09	39,39,39,39	0
55	MG	RA	3227	1/1	0.94	0.19	39,39,39,39	0
55	MG	QA	1744	1/1	0.94	0.13	69,69,69,69	0
55	MG	RA	3160	1/1	0.94	0.17	45,45,45,45	0
55	MG	QA	1655	1/1	0.94	0.10	81,81,81,81	0
55	MG	RA	3166	1/1	0.94	0.06	38,38,38,38	0
55	MG	QA	1706	1/1	0.94	0.11	42,42,42,42	0
55	MG	RA	3333	1/1	0.94	0.11	26,26,26,26	0
55	MG	YA	3349	1/1	0.94	0.15	50,50,50,50	0
55	MG	RA	3451	1/1	0.94	0.06	47,47,47,47	0
55	MG	YA	3355	1/1	0.94	0.17	63,63,63,63	0
55	MG	XA	1673	1/1	0.94	0.15	30,30,30,30	0
55	MG	YA	3095	1/1	0.94	0.10	17,17,17,17	0
55	MG	RA	3334	1/1	0.94	0.12	59,59,59,59	0
55	MG	RA	3235	1/1	0.94	0.19	40,40,40,40	0
55	MG	YA	3363	1/1	0.94	0.10	47,47,47,47	0
55	MG	YA	3364	1/1	0.94	0.21	47,47,47,47	0
55	MG	YA	3366	1/1	0.94	0.09	24,24,24,24	0
55	MG	RA	3336	1/1	0.94	0.15	35,35,35,35	0
55	MG	RA	3108	1/1	0.94	0.13	13,13,13,13	0
55	MG	QA	1636	1/1	0.94	0.14	33,33,33,33	0
55	MG	XA	1683	1/1	0.94	0.10	74,74,74,74	0
55	MG	QA	1733	1/1	0.94	0.11	90,90,90,90	0
55	MG	YA	3381	1/1	0.94	0.08	31,31,31,31	0
55	MG	XA	1685	1/1	0.94	0.11	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3383	1/1	0.94	0.05	46,46,46,46	0
55	MG	RA	3062	1/1	0.94	0.14	37,37,37,37	0
55	MG	RA	3342	1/1	0.94	0.17	55,55,55,55	0
55	MG	RA	3344	1/1	0.94	0.17	49,49,49,49	0
55	MG	YA	3115	1/1	0.94	0.08	49,49,49,49	0
55	MG	YA	3388	1/1	0.94	0.10	47,47,47,47	0
55	MG	XA	1690	1/1	0.94	0.10	45,45,45,45	0
55	MG	XA	1691	1/1	0.94	0.09	58,58,58,58	0
55	MG	RA	3114	1/1	0.94	0.13	35,35,35,35	0
55	MG	QA	1751	1/1	0.94	0.08	40,40,40,40	0
55	MG	YA	3397	1/1	0.94	0.12	24,24,24,24	0
55	MG	YA	3398	1/1	0.94	0.10	21,21,21,21	0
55	MG	YA	3399	1/1	0.94	0.23	47,47,47,47	0
55	MG	YA	3400	1/1	0.94	0.17	27,27,27,27	0
55	MG	XA	1698	1/1	0.94	0.17	57,57,57,57	0
55	MG	RA	3065	1/1	0.94	0.20	16,16,16,16	0
55	MG	RA	3254	1/1	0.94	0.23	41,41,41,41	0
55	MG	RA	3181	1/1	0.94	0.16	35,35,35,35	0
55	MG	RA	3261	1/1	0.94	0.23	55,55,55,55	0
55	MG	QA	1752	1/1	0.94	0.10	52,52,52,52	0
55	MG	RA	3478	1/1	0.94	0.17	74,74,74,74	0
55	MG	YA	3143	1/1	0.94	0.18	14,14,14,14	0
55	MG	RA	3183	1/1	0.94	0.09	50,50,50,50	0
55	MG	QA	1680	1/1	0.94	0.11	41,41,41,41	0
55	MG	YA	3415	1/1	0.94	0.10	69,69,69,69	0
55	MG	RA	3185	1/1	0.94	0.08	70,70,70,70	0
55	MG	RA	3491	1/1	0.94	0.17	14,14,14,14	0
55	MG	YA	3155	1/1	0.94	0.15	16,16,16,16	0
55	MG	XA	1717	1/1	0.94	0.15	48,48,48,48	0
55	MG	RA	3188	1/1	0.94	0.11	68,68,68,68	0
55	MG	YA	3432	1/1	0.94	0.10	33,33,33,33	0
55	MG	RA	3359	1/1	0.94	0.25	42,42,42,42	0
55	MG	RA	3360	1/1	0.94	0.09	68,68,68,68	0
55	MG	RA	3366	1/1	0.94	0.23	49,49,49,49	0
55	MG	RB	203	1/1	0.94	0.20	27,27,27,27	0
55	MG	QA	1665	1/1	0.94	0.10	25,25,25,25	0
55	MG	RA	3368	1/1	0.94	0.05	25,25,25,25	0
55	MG	YA	3448	1/1	0.94	0.11	49,49,49,49	0
55	MG	YA	3165	1/1	0.94	0.07	33,33,33,33	0
55	MG	XA	1731	1/1	0.94	0.13	57,57,57,57	0
55	MG	RA	3278	1/1	0.94	0.17	64,64,64,64	0
55	MG	YA	3454	1/1	0.94	0.10	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3279	1/1	0.94	0.12	39,39,39,39	0
55	MG	YA	3459	1/1	0.94	0.11	34,34,34,34	0
55	MG	QA	1620	1/1	0.94	0.18	74,74,74,74	0
55	MG	YA	3173	1/1	0.94	0.16	29,29,29,29	0
55	MG	RE	301	1/1	0.94	0.15	29,29,29,29	0
55	MG	QA	1669	1/1	0.94	0.10	21,21,21,21	0
55	MG	RE	303	1/1	0.94	0.12	70,70,70,70	0
55	MG	QA	1640	1/1	0.94	0.07	30,30,30,30	0
55	MG	RF	301	1/1	0.94	0.07	42,42,42,42	0
55	MG	YA	3184	1/1	0.94	0.27	48,48,48,48	0
55	MG	YA	3471	1/1	0.94	0.11	54,54,54,54	0
55	MG	XA	1742	1/1	0.94	0.04	26,26,26,26	0
55	MG	XA	1743	1/1	0.94	0.09	32,32,32,32	0
55	MG	XA	1744	1/1	0.94	0.06	32,32,32,32	0
55	MG	RI	201	1/1	0.94	0.12	46,46,46,46	0
55	MG	RA	3285	1/1	0.94	0.21	41,41,41,41	0
55	MG	YA	3477	1/1	0.94	0.05	27,27,27,27	0
55	MG	RP	202	1/1	0.94	0.20	33,33,33,33	0
55	MG	YA	3195	1/1	0.94	0.17	81,81,81,81	0
55	MG	RA	3287	1/1	0.94	0.27	58,58,58,58	0
55	MG	RA	3074	1/1	0.94	0.19	24,24,24,24	0
55	MG	XA	1751	1/1	0.94	0.19	37,37,37,37	0
55	MG	RU	201	1/1	0.94	0.12	51,51,51,51	0
55	MG	RA	3027	1/1	0.94	0.18	32,32,32,32	0
55	MG	YA	3211	1/1	0.94	0.12	49,49,49,49	0
55	MG	YA	3488	1/1	0.94	0.22	43,43,43,43	0
55	MG	XA	1754	1/1	0.94	0.11	46,46,46,46	0
55	MG	YA	3213	1/1	0.94	0.07	30,30,30,30	0
55	MG	QA	1761	1/1	0.94	0.24	75,75,75,75	0
55	MG	YA	3221	1/1	0.94	0.05	20,20,20,20	0
55	MG	RA	3138	1/1	0.94	0.10	28,28,28,28	0
55	MG	YA	3497	1/1	0.94	0.09	43,43,43,43	0
55	MG	YA	3228	1/1	0.94	0.06	14,14,14,14	0
55	MG	RA	3293	1/1	0.94	0.20	30,30,30,30	0
55	MG	YA	3239	1/1	0.94	0.12	31,31,31,31	0
55	MG	RA	3397	1/1	0.94	0.15	43,43,43,43	0
55	MG	XA	1610	1/1	0.94	0.14	28,28,28,28	0
55	MG	XA	1761	1/1	0.94	0.07	36,36,36,36	0
55	MG	RA	3403	1/1	0.94	0.17	35,35,35,35	0
55	MG	YA	3251	1/1	0.94	0.18	20,20,20,20	0
55	MG	QV	104	1/1	0.94	0.11	81,81,81,81	0
55	MG	YA	3255	1/1	0.94	0.13	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3141	1/1	0.94	0.19	42,42,42,42	0
55	MG	RA	3303	1/1	0.94	0.10	41,41,41,41	0
55	MG	XA	1625	1/1	0.94	0.06	27,27,27,27	0
55	MG	RA	3304	1/1	0.94	0.11	48,48,48,48	0
55	MG	XS	101	1/1	0.94	0.04	53,53,53,53	0
55	MG	RA	3142	1/1	0.94	0.10	7,7,7,7	0
55	MG	XV	104	1/1	0.94	0.07	48,48,48,48	0
55	MG	XA	1628	1/1	0.94	0.08	34,34,34,34	0
55	MG	RA	3410	1/1	0.94	0.05	70,70,70,70	0
55	MG	RA	3143	1/1	0.94	0.13	29,29,29,29	0
55	MG	YA	3282	1/1	0.94	0.17	34,34,34,34	0
55	MG	RA	3412	1/1	0.94	0.14	57,57,57,57	0
55	MG	YA	3284	1/1	0.94	0.18	37,37,37,37	0
55	MG	Y8	101	1/1	0.94	0.07	40,40,40,40	0
55	MG	RA	3031	1/1	0.94	0.14	16,16,16,16	0
55	MG	YA	3008	1/1	0.94	0.18	25,25,25,25	0
55	MG	YA	3010	1/1	0.94	0.19	26,26,26,26	0
55	MG	YA	3012	1/1	0.94	0.24	23,23,23,23	0
55	MG	RA	3309	1/1	0.94	0.06	23,23,23,23	0
55	MG	YA	3294	1/1	0.94	0.18	38,38,38,38	0
55	MG	RA	3417	1/1	0.94	0.13	33,33,33,33	0
55	MG	QA	1762	1/1	0.94	0.07	50,50,50,50	0
57	ZN	Y9	101	1/1	0.94	0.14	181,181,181,181	0
55	MG	YA	3321	1/1	0.95	0.04	25,25,25,25	0
55	MG	YA	3096	1/1	0.95	0.15	47,47,47,47	0
55	MG	YA	3098	1/1	0.95	0.19	62,62,62,62	0
55	MG	XA	1709	1/1	0.95	0.07	57,57,57,57	0
55	MG	YA	3100	1/1	0.95	0.20	33,33,33,33	0
55	MG	XA	1711	1/1	0.95	0.11	50,50,50,50	0
55	MG	YA	3329	1/1	0.95	0.04	36,36,36,36	0
55	MG	YA	3330	1/1	0.95	0.11	65,65,65,65	0
55	MG	QA	1645	1/1	0.95	0.09	73,73,73,73	0
55	MG	RA	3426	1/1	0.95	0.08	37,37,37,37	0
55	MG	RW	201	1/1	0.95	0.23	136,136,136,136	0
55	MG	YA	3335	1/1	0.95	0.19	52,52,52,52	0
55	MG	RA	3192	1/1	0.95	0.12	43,43,43,43	0
55	MG	RA	3018	1/1	0.95	0.17	1,1,1,1	0
55	MG	YA	3339	1/1	0.95	0.15	49,49,49,49	0
55	MG	RA	3268	1/1	0.95	0.17	25,25,25,25	0
55	MG	XA	1718	1/1	0.95	0.04	29,29,29,29	0
55	MG	YA	3345	1/1	0.95	0.09	35,35,35,35	0
55	MG	R0	102	1/1	0.95	0.05	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	R1	102	1/1	0.95	0.50	112,112,112,112	0
55	MG	XA	1601	1/1	0.95	0.14	27,27,27,27	0
55	MG	YA	3353	1/1	0.95	0.11	43,43,43,43	0
55	MG	YA	3116	1/1	0.95	0.08	41,41,41,41	0
55	MG	XA	1602	1/1	0.95	0.17	28,28,28,28	0
55	MG	XA	1606	1/1	0.95	0.07	21,21,21,21	0
55	MG	YA	3357	1/1	0.95	0.07	43,43,43,43	0
55	MG	XA	1726	1/1	0.95	0.05	32,32,32,32	0
55	MG	YA	3120	1/1	0.95	0.16	34,34,34,34	0
55	MG	RA	3432	1/1	0.95	0.08	43,43,43,43	0
55	MG	YA	3126	1/1	0.95	0.13	61,61,61,61	0
55	MG	RA	3269	1/1	0.95	0.10	31,31,31,31	0
55	MG	YA	3132	1/1	0.95	0.07	62,62,62,62	0
55	MG	YA	3368	1/1	0.95	0.17	36,36,36,36	0
55	MG	YA	3133	1/1	0.95	0.07	56,56,56,56	0
55	MG	YA	3372	1/1	0.95	0.09	39,39,39,39	0
55	MG	YA	3134	1/1	0.95	0.14	11,11,11,11	0
55	MG	QA	1646	1/1	0.95	0.15	44,44,44,44	0
55	MG	YA	3376	1/1	0.95	0.23	45,45,45,45	0
55	MG	XA	1612	1/1	0.95	0.17	12,12,12,12	0
55	MG	RA	3272	1/1	0.95	0.09	29,29,29,29	0
55	MG	XA	1734	1/1	0.95	0.12	70,70,70,70	0
55	MG	RA	3343	1/1	0.95	0.06	33,33,33,33	0
55	MG	XA	1618	1/1	0.95	0.18	24,24,24,24	0
55	MG	QA	1746	1/1	0.95	0.18	56,56,56,56	0
55	MG	RA	3274	1/1	0.95	0.10	20,20,20,20	0
55	MG	QA	1705	1/1	0.95	0.04	28,28,28,28	0
55	MG	RA	3024	1/1	0.95	0.16	31,31,31,31	0
55	MG	YA	3150	1/1	0.95	0.07	34,34,34,34	0
55	MG	YA	3151	1/1	0.95	0.22	19,19,19,19	0
55	MG	YA	3391	1/1	0.95	0.13	42,42,42,42	0
55	MG	RA	3025	1/1	0.95	0.21	44,44,44,44	0
55	MG	YA	3154	1/1	0.95	0.10	37,37,37,37	0
55	MG	RA	3280	1/1	0.95	0.10	55,55,55,55	0
55	MG	YA	3396	1/1	0.95	0.10	43,43,43,43	0
55	MG	RA	3078	1/1	0.95	0.15	7,7,7,7	0
55	MG	XA	1745	1/1	0.95	0.07	22,22,22,22	0
55	MG	QA	1610	1/1	0.95	0.19	29,29,29,29	0
55	MG	QA	1777	1/1	0.95	0.04	39,39,39,39	0
55	MG	RA	3084	1/1	0.95	0.21	14,14,14,14	0
55	MG	QA	1648	1/1	0.95	0.09	32,32,32,32	0
55	MG	QA	1650	1/1	0.95	0.09	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	QA	1637	1/1	0.95	0.07	72,72,72,72	0
55	MG	XA	1638	1/1	0.95	0.19	48,48,48,48	0
55	MG	XA	1641	1/1	0.95	0.11	53,53,53,53	0
55	MG	YA	3410	1/1	0.95	0.04	16,16,16,16	0
55	MG	QA	1671	1/1	0.95	0.22	53,53,53,53	0
55	MG	RA	3154	1/1	0.95	0.05	32,32,32,32	0
55	MG	RA	3038	1/1	0.95	0.19	10,10,10,10	0
55	MG	RA	3096	1/1	0.95	0.18	86,86,86,86	0
55	MG	QA	1730	1/1	0.95	0.05	44,44,44,44	0
55	MG	RA	3372	1/1	0.95	0.26	62,62,62,62	0
55	MG	RA	3218	1/1	0.95	0.18	23,23,23,23	0
55	MG	XA	1762	1/1	0.95	0.19	60,60,60,60	0
55	MG	YA	3426	1/1	0.95	0.05	47,47,47,47	0
55	MG	RA	3469	1/1	0.95	0.05	64,64,64,64	0
55	MG	RA	3159	1/1	0.95	0.07	32,32,32,32	0
55	MG	RA	3220	1/1	0.95	0.10	43,43,43,43	0
55	MG	YA	3187	1/1	0.95	0.24	38,38,38,38	0
55	MG	RA	3102	1/1	0.95	0.20	21,21,21,21	0
55	MG	RA	3474	1/1	0.95	0.05	37,37,37,37	0
55	MG	XA	1655	1/1	0.95	0.14	38,38,38,38	0
55	MG	XM	201	1/1	0.95	0.07	45,45,45,45	0
55	MG	XA	1656	1/1	0.95	0.12	36,36,36,36	0
55	MG	YA	3447	1/1	0.95	0.06	32,32,32,32	0
55	MG	QV	102	1/1	0.95	0.13	75,75,75,75	0
55	MG	QA	1616	1/1	0.95	0.11	31,31,31,31	0
55	MG	XV	105	1/1	0.95	0.14	42,42,42,42	0
55	MG	QA	1623	1/1	0.95	0.20	37,37,37,37	0
55	MG	YA	3199	1/1	0.95	0.17	64,64,64,64	0
55	MG	YA	3200	1/1	0.95	0.18	33,33,33,33	0
55	MG	RA	3480	1/1	0.95	0.15	37,37,37,37	0
55	MG	XV	108	1/1	0.95	0.11	34,34,34,34	0
55	MG	YA	3462	1/1	0.95	0.10	33,33,33,33	0
55	MG	YA	3209	1/1	0.95	0.17	43,43,43,43	0
55	MG	RA	3481	1/1	0.95	0.18	31,31,31,31	0
55	MG	YA	3002	1/1	0.95	0.08	30,30,30,30	0
55	MG	QA	1692	1/1	0.95	0.18	44,44,44,44	0
55	MG	YA	3215	1/1	0.95	0.08	52,52,52,52	0
55	MG	RA	3229	1/1	0.95	0.26	23,23,23,23	0
55	MG	YA	3469	1/1	0.95	0.12	56,56,56,56	0
55	MG	YA	3007	1/1	0.95	0.14	27,27,27,27	0
55	MG	YA	3222	1/1	0.95	0.17	38,38,38,38	0
55	MG	QA	1674	1/1	0.95	0.11	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1668	1/1	0.95	0.15	16,16,16,16	0
55	MG	YA	3233	1/1	0.95	0.15	10,10,10,10	0
55	MG	YA	3236	1/1	0.95	0.47	57,57,57,57	0
55	MG	RA	3487	1/1	0.95	0.18	43,43,43,43	0
55	MG	XA	1670	1/1	0.95	0.14	17,17,17,17	0
55	MG	YA	3242	1/1	0.95	0.15	25,25,25,25	0
55	MG	YA	3243	1/1	0.95	0.15	17,17,17,17	0
55	MG	XA	1671	1/1	0.95	0.07	20,20,20,20	0
55	MG	QA	1760	1/1	0.95	0.10	38,38,38,38	0
55	MG	RA	3396	1/1	0.95	0.08	40,40,40,40	0
55	MG	QX	102	1/1	0.95	0.08	34,34,34,34	0
55	MG	RA	3398	1/1	0.95	0.19	54,54,54,54	0
55	MG	YA	3028	1/1	0.95	0.17	24,24,24,24	0
55	MG	YA	3254	1/1	0.95	0.21	28,28,28,28	0
55	MG	QA	1641	1/1	0.95	0.11	45,45,45,45	0
55	MG	RA	3118	1/1	0.95	0.13	58,58,58,58	0
55	MG	YA	3258	1/1	0.95	0.17	26,26,26,26	0
55	MG	RA	3178	1/1	0.95	0.08	31,31,31,31	0
55	MG	QA	1737	1/1	0.95	0.18	47,47,47,47	0
55	MG	YA	3035	1/1	0.95	0.14	19,19,19,19	0
55	MG	QA	1642	1/1	0.95	0.17	49,49,49,49	0
55	MG	YA	3265	1/1	0.95	0.12	35,35,35,35	0
55	MG	RB	208	1/1	0.95	0.11	75,75,75,75	0
55	MG	YA	3502	1/1	0.95	0.20	13,13,13,13	0
55	MG	YA	3272	1/1	0.95	0.16	24,24,24,24	0
55	MG	YA	3049	1/1	0.95	0.15	37,37,37,37	0
55	MG	YA	3050	1/1	0.95	0.13	13,13,13,13	0
55	MG	YA	3276	1/1	0.95	0.07	2,2,2,2	0
55	MG	YA	3051	1/1	0.95	0.20	33,33,33,33	0
55	MG	YB	201	1/1	0.95	0.05	47,47,47,47	0
55	MG	RB	209	1/1	0.95	0.05	77,77,77,77	0
55	MG	RA	3323	1/1	0.95	0.03	13,13,13,13	0
55	MG	YB	204	1/1	0.95	0.07	20,20,20,20	0
55	MG	RA	3121	1/1	0.95	0.07	35,35,35,35	0
55	MG	YA	3062	1/1	0.95	0.11	48,48,48,48	0
55	MG	YB	207	1/1	0.95	0.10	40,40,40,40	0
55	MG	YB	208	1/1	0.95	0.13	53,53,53,53	0
55	MG	YA	3063	1/1	0.95	0.12	9,9,9,9	0
55	MG	YA	3065	1/1	0.95	0.17	13,13,13,13	0
55	MG	YA	3067	1/1	0.95	0.23	21,21,21,21	0
55	MG	QA	1643	1/1	0.95	0.13	39,39,39,39	0
55	MG	QA	1766	1/1	0.95	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	QA	1740	1/1	0.95	0.14	75,75,75,75	0
55	MG	XA	1694	1/1	0.95	0.08	35,35,35,35	0
55	MG	YA	3080	1/1	0.95	0.16	22,22,22,22	0
55	MG	YA	3303	1/1	0.95	0.05	24,24,24,24	0
55	MG	XA	1696	1/1	0.95	0.10	39,39,39,39	0
55	MG	RA	3329	1/1	0.95	0.14	20,20,20,20	0
55	MG	XA	1699	1/1	0.95	0.06	28,28,28,28	0
55	MG	RA	3186	1/1	0.95	0.17	48,48,48,48	0
55	MG	YA	3086	1/1	0.95	0.27	19,19,19,19	0
55	MG	YA	3314	1/1	0.95	0.18	32,32,32,32	0
55	MG	RA	3187	1/1	0.95	0.04	70,70,70,70	0
55	MG	RA	3420	1/1	0.95	0.11	39,39,39,39	0
55	MG	RA	3260	1/1	0.95	0.09	27,27,27,27	0
55	MG	QA	1624	1/1	0.95	0.11	42,42,42,42	0
55	MG	YA	3094	1/1	0.95	0.10	17,17,17,17	0
55	MG	XA	1708	1/1	0.95	0.10	59,59,59,59	0
55	MG	RA	3150	1/1	0.96	0.18	14,14,14,14	0
55	MG	RA	3105	1/1	0.96	0.14	47,47,47,47	0
55	MG	YA	3338	1/1	0.96	0.09	18,18,18,18	0
55	MG	XA	1634	1/1	0.96	0.15	54,54,54,54	0
55	MG	RA	3449	1/1	0.96	0.07	37,37,37,37	0
55	MG	QA	1775	1/1	0.96	0.04	54,54,54,54	0
55	MG	RA	3277	1/1	0.96	0.19	34,34,34,34	0
55	MG	RA	3064	1/1	0.96	0.14	23,23,23,23	0
55	MG	YA	3139	1/1	0.96	0.11	19,19,19,19	0
55	MG	RA	3349	1/1	0.96	0.16	47,47,47,47	0
55	MG	YA	3351	1/1	0.96	0.17	42,42,42,42	0
55	MG	YA	3352	1/1	0.96	0.05	37,37,37,37	0
55	MG	YA	3141	1/1	0.96	0.13	16,16,16,16	0
55	MG	QA	1656	1/1	0.96	0.05	17,17,17,17	0
55	MG	RA	3351	1/1	0.96	0.11	57,57,57,57	0
55	MG	RA	3459	1/1	0.96	0.09	35,35,35,35	0
55	MG	QA	1621	1/1	0.96	0.08	42,42,42,42	0
55	MG	XA	1758	1/1	0.96	0.17	71,71,71,71	0
55	MG	RA	3029	1/1	0.96	0.16	2,2,2,2	0
55	MG	RA	3113	1/1	0.96	0.13	15,15,15,15	0
55	MG	RA	3283	1/1	0.96	0.09	26,26,26,26	0
55	MG	QA	1763	1/1	0.96	0.12	85,85,85,85	0
55	MG	XA	1763	1/1	0.96	0.05	65,65,65,65	0
55	MG	YA	3367	1/1	0.96	0.09	31,31,31,31	0
55	MG	RA	3115	1/1	0.96	0.16	22,22,22,22	0
55	MG	RA	3286	1/1	0.96	0.07	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3370	1/1	0.96	0.07	55,55,55,55	0
55	MG	YA	3371	1/1	0.96	0.03	19,19,19,19	0
55	MG	XA	1652	1/1	0.96	0.17	33,33,33,33	0
55	MG	RA	3214	1/1	0.96	0.16	25,25,25,25	0
55	MG	RA	3363	1/1	0.96	0.11	31,31,31,31	0
55	MG	YA	3375	1/1	0.96	0.05	28,28,28,28	0
55	MG	RA	3215	1/1	0.96	0.10	6,6,6,6	0
55	MG	RA	3163	1/1	0.96	0.05	27,27,27,27	0
55	MG	RA	3164	1/1	0.96	0.18	32,32,32,32	0
55	MG	YA	3380	1/1	0.96	0.12	20,20,20,20	0
55	MG	XV	101	1/1	0.96	0.19	31,31,31,31	0
55	MG	RA	3475	1/1	0.96	0.26	55,55,55,55	0
55	MG	RA	3165	1/1	0.96	0.15	55,55,55,55	0
55	MG	QA	1629	1/1	0.96	0.04	31,31,31,31	0
55	MG	YA	3170	1/1	0.96	0.08	19,19,19,19	0
55	MG	RA	3294	1/1	0.96	0.11	39,39,39,39	0
55	MG	RA	3167	1/1	0.96	0.11	55,55,55,55	0
55	MG	YA	3174	1/1	0.96	0.09	45,45,45,45	0
55	MG	RA	3298	1/1	0.96	0.06	30,30,30,30	0
55	MG	YA	3390	1/1	0.96	0.14	28,28,28,28	0
55	MG	YA	3177	1/1	0.96	0.10	57,57,57,57	0
55	MG	XA	1666	1/1	0.96	0.09	59,59,59,59	0
55	MG	YA	3393	1/1	0.96	0.11	22,22,22,22	0
55	MG	RA	3377	1/1	0.96	0.08	39,39,39,39	0
55	MG	RA	3483	1/1	0.96	0.18	21,21,21,21	0
55	MG	YA	3181	1/1	0.96	0.04	42,42,42,42	0
55	MG	RA	3378	1/1	0.96	0.10	31,31,31,31	0
55	MG	YA	3006	1/1	0.96	0.21	9,9,9,9	0
55	MG	RA	3381	1/1	0.96	0.10	31,31,31,31	0
55	MG	RA	3382	1/1	0.96	0.13	41,41,41,41	0
55	MG	RA	3490	1/1	0.96	0.17	32,32,32,32	0
55	MG	YA	3011	1/1	0.96	0.19	26,26,26,26	0
55	MG	RA	3032	1/1	0.96	0.14	21,21,21,21	0
55	MG	RA	3384	1/1	0.96	0.12	44,44,44,44	0
55	MG	RA	3300	1/1	0.96	0.14	26,26,26,26	0
55	MG	QA	1609	1/1	0.96	0.07	52,52,52,52	0
55	MG	YA	3018	1/1	0.96	0.13	39,39,39,39	0
55	MG	YA	3019	1/1	0.96	0.14	26,26,26,26	0
55	MG	YA	3020	1/1	0.96	0.25	22,22,22,22	0
55	MG	YA	3022	1/1	0.96	0.20	22,22,22,22	0
55	MG	YA	3023	1/1	0.96	0.19	13,13,13,13	0
55	MG	XA	1681	1/1	0.96	0.14	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3226	1/1	0.96	0.08	1,1,1,1	0
55	MG	YA	3418	1/1	0.96	0.10	23,23,23,23	0
55	MG	YA	3419	1/1	0.96	0.18	43,43,43,43	0
55	MG	YA	3206	1/1	0.96	0.16	36,36,36,36	0
55	MG	RA	3170	1/1	0.96	0.08	17,17,17,17	0
55	MG	RA	3306	1/1	0.96	0.17	30,30,30,30	0
55	MG	YA	3428	1/1	0.96	0.12	32,32,32,32	0
55	MG	RA	3035	1/1	0.96	0.15	12,12,12,12	0
55	MG	RA	3037	1/1	0.96	0.09	10,10,10,10	0
55	MG	RA	3122	1/1	0.96	0.14	16,16,16,16	0
55	MG	QA	1753	1/1	0.96	0.10	37,37,37,37	0
55	MG	YA	3220	1/1	0.96	0.24	74,74,74,74	0
55	MG	YA	3438	1/1	0.96	0.04	32,32,32,32	0
55	MG	YA	3441	1/1	0.96	0.09	47,47,47,47	0
55	MG	RA	3041	1/1	0.96	0.16	24,24,24,24	0
55	MG	RA	3233	1/1	0.96	0.18	49,49,49,49	0
55	MG	QA	1767	1/1	0.96	0.07	39,39,39,39	0
55	MG	YA	3445	1/1	0.96	0.03	42,42,42,42	0
55	MG	YA	3227	1/1	0.96	0.07	39,39,39,39	0
55	MG	YA	3045	1/1	0.96	0.04	13,13,13,13	0
55	MG	YA	3231	1/1	0.96	0.10	33,33,33,33	0
55	MG	YA	3046	1/1	0.96	0.12	13,13,13,13	0
55	MG	YA	3235	1/1	0.96	0.20	19,19,19,19	0
55	MG	YA	3452	1/1	0.96	0.11	52,52,52,52	0
55	MG	RA	3045	1/1	0.96	0.21	51,51,51,51	0
55	MG	QV	101	1/1	0.96	0.10	22,22,22,22	0
55	MG	YA	3238	1/1	0.96	0.10	13,13,13,13	0
55	MG	YA	3458	1/1	0.96	0.17	52,52,52,52	0
55	MG	XA	1695	1/1	0.96	0.06	42,42,42,42	0
55	MG	YA	3241	1/1	0.96	0.07	8,8,8,8	0
55	MG	RA	3239	1/1	0.96	0.13	29,29,29,29	0
55	MG	RA	3016	1/1	0.96	0.20	23,23,23,23	0
55	MG	YA	3057	1/1	0.96	0.15	31,31,31,31	0
55	MG	YA	3058	1/1	0.96	0.18	12,12,12,12	0
55	MG	YA	3059	1/1	0.96	0.15	40,40,40,40	0
55	MG	YA	3247	1/1	0.96	0.15	30,30,30,30	0
55	MG	YA	3060	1/1	0.96	0.08	42,42,42,42	0
55	MG	YA	3250	1/1	0.96	0.14	32,32,32,32	0
55	MG	RA	3318	1/1	0.96	0.09	41,41,41,41	0
55	MG	XA	1701	1/1	0.96	0.07	28,28,28,28	0
55	MG	XA	1702	1/1	0.96	0.07	29,29,29,29	0
55	MG	RA	3130	1/1	0.96	0.12	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3244	1/1	0.96	0.14	19,19,19,19	0
55	MG	YA	3069	1/1	0.96	0.20	3,3,3,3	0
55	MG	RP	203	1/1	0.96	0.08	86,86,86,86	0
55	MG	YA	3074	1/1	0.96	0.17	21,21,21,21	0
55	MG	RQ	201	1/1	0.96	0.18	56,56,56,56	0
55	MG	RA	3132	1/1	0.96	0.12	20,20,20,20	0
55	MG	RA	3415	1/1	0.96	0.12	45,45,45,45	0
55	MG	YA	3267	1/1	0.96	0.14	20,20,20,20	0
55	MG	YA	3079	1/1	0.96	0.17	43,43,43,43	0
55	MG	YA	3269	1/1	0.96	0.09	23,23,23,23	0
55	MG	YA	3270	1/1	0.96	0.14	43,43,43,43	0
55	MG	RA	3322	1/1	0.96	0.05	15,15,15,15	0
55	MG	XA	1710	1/1	0.96	0.11	35,35,35,35	0
55	MG	RA	3017	1/1	0.96	0.19	20,20,20,20	0
55	MG	YA	3083	1/1	0.96	0.17	20,20,20,20	0
55	MG	RA	3418	1/1	0.96	0.13	77,77,77,77	0
55	MG	RA	3248	1/1	0.96	0.15	51,51,51,51	0
55	MG	RA	3249	1/1	0.96	0.17	41,41,41,41	0
55	MG	RA	3052	1/1	0.96	0.10	36,36,36,36	0
55	MG	RA	3137	1/1	0.96	0.05	26,26,26,26	0
55	MG	YA	3499	1/1	0.96	0.14	36,36,36,36	0
55	MG	YA	3286	1/1	0.96	0.04	22,22,22,22	0
55	MG	R5	102	1/1	0.96	0.10	32,32,32,32	0
55	MG	RA	3328	1/1	0.96	0.11	22,22,22,22	0
55	MG	YA	3505	1/1	0.96	0.29	78,78,78,78	0
55	MG	XA	1719	1/1	0.96	0.27	63,63,63,63	0
55	MG	QA	1695	1/1	0.96	0.20	57,57,57,57	0
55	MG	XA	1721	1/1	0.96	0.15	33,33,33,33	0
55	MG	YA	3513	1/1	0.96	0.13	22,22,22,22	0
55	MG	XA	1604	1/1	0.96	0.21	30,30,30,30	0
55	MG	RA	3257	1/1	0.96	0.19	38,38,38,38	0
55	MG	YA	3298	1/1	0.96	0.18	28,28,28,28	0
55	MG	XA	1607	1/1	0.96	0.08	84,84,84,84	0
55	MG	YA	3302	1/1	0.96	0.06	17,17,17,17	0
55	MG	YA	3101	1/1	0.96	0.16	43,43,43,43	0
55	MG	RA	3331	1/1	0.96	0.07	37,37,37,37	0
55	MG	RA	3430	1/1	0.96	0.14	64,64,64,64	0
55	MG	YA	3307	1/1	0.96	0.23	53,53,53,53	0
55	MG	YA	3104	1/1	0.96	0.14	29,29,29,29	0
55	MG	XA	1728	1/1	0.96	0.10	42,42,42,42	0
55	MG	RA	3190	1/1	0.96	0.17	27,27,27,27	0
55	MG	YD	302	1/1	0.96	0.12	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YE	302	1/1	0.96	0.15	38,38,38,38	0
55	MG	RA	3139	1/1	0.96	0.06	49,49,49,49	0
55	MG	YA	3108	1/1	0.96	0.17	1,1,1,1	0
55	MG	XA	1615	1/1	0.96	0.14	8,8,8,8	0
55	MG	YP	203	1/1	0.96	0.21	58,58,58,58	0
55	MG	QA	1686	1/1	0.96	0.10	25,25,25,25	0
55	MG	YA	3111	1/1	0.96	0.18	38,38,38,38	0
55	MG	QA	1654	1/1	0.96	0.06	48,48,48,48	0
55	MG	QA	1679	1/1	0.96	0.14	23,23,23,23	0
55	MG	RA	3097	1/1	0.96	0.15	14,14,14,14	0
55	MG	Y0	101	1/1	0.96	0.19	25,25,25,25	0
55	MG	Y5	102	1/1	0.96	0.10	39,39,39,39	0
55	MG	RA	3059	1/1	0.96	0.12	18,18,18,18	0
55	MG	XA	1622	1/1	0.96	0.10	59,59,59,59	0
56	SF4	XD	301	8/8	0.96	0.09	75,80,85,91	0
55	MG	XA	1623	1/1	0.96	0.11	45,45,45,45	0
55	MG	RA	3439	1/1	0.96	0.16	59,59,59,59	0
55	MG	RA	3099	1/1	0.96	0.18	31,31,31,31	0
57	ZN	R6	101	1/1	0.96	0.11	152,152,152,152	0
55	MG	QA	1700	1/1	0.96	0.14	50,50,50,50	0
55	MG	RA	3442	1/1	0.96	0.07	39,39,39,39	0
55	MG	RA	3271	1/1	0.96	0.14	36,36,36,36	0
55	MG	QA	1603	1/1	0.96	0.13	24,24,24,24	0
55	MG	YA	3128	1/1	0.96	0.13	69,69,69,69	0
55	MG	YA	3129	1/1	0.96	0.16	27,27,27,27	0
55	MG	QA	1602	1/1	0.97	0.09	28,28,28,28	0
55	MG	RA	3486	1/1	0.97	0.21	56,56,56,56	0
55	MG	RA	3237	1/1	0.97	0.17	34,34,34,34	0
55	MG	YA	3021	1/1	0.97	0.21	7,7,7,7	0
55	MG	XA	1639	1/1	0.97	0.06	15,15,15,15	0
55	MG	RA	3488	1/1	0.97	0.10	29,29,29,29	0
55	MG	QA	1701	1/1	0.97	0.05	33,33,33,33	0
55	MG	RA	3050	1/1	0.97	0.23	23,23,23,23	0
55	MG	RA	3240	1/1	0.97	0.11	26,26,26,26	0
55	MG	RA	3117	1/1	0.97	0.13	5,5,5,5	0
55	MG	YA	3274	1/1	0.97	0.06	38,38,38,38	0
55	MG	RA	3242	1/1	0.97	0.18	9,9,9,9	0
55	MG	RA	3421	1/1	0.97	0.08	41,41,41,41	0
55	MG	RA	3022	1/1	0.97	0.16	19,19,19,19	0
55	MG	YA	3278	1/1	0.97	0.15	36,36,36,36	0
55	MG	YA	3033	1/1	0.97	0.16	18,18,18,18	0
55	MG	YA	3281	1/1	0.97	0.08	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3081	1/1	0.97	0.17	18,18,18,18	0
55	MG	YA	3422	1/1	0.97	0.05	24,24,24,24	0
55	MG	YA	3149	1/1	0.97	0.15	42,42,42,42	0
55	MG	RA	3301	1/1	0.97	0.11	16,16,16,16	0
55	MG	YA	3285	1/1	0.97	0.14	32,32,32,32	0
55	MG	YA	3429	1/1	0.97	0.08	54,54,54,54	0
55	MG	YA	3037	1/1	0.97	0.25	24,24,24,24	0
55	MG	YA	3038	1/1	0.97	0.16	0,0,0,0	0
55	MG	RA	3302	1/1	0.97	0.17	37,37,37,37	0
55	MG	YA	3433	1/1	0.97	0.12	32,32,32,32	0
55	MG	YA	3434	1/1	0.97	0.04	24,24,24,24	0
55	MG	YA	3289	1/1	0.97	0.13	37,37,37,37	0
55	MG	RB	207	1/1	0.97	0.12	32,32,32,32	0
55	MG	RA	3354	1/1	0.97	0.03	34,34,34,34	0
55	MG	QA	1772	1/1	0.97	0.05	40,40,40,40	0
55	MG	YA	3048	1/1	0.97	0.09	2,2,2,2	0
55	MG	YA	3295	1/1	0.97	0.15	31,31,31,31	0
55	MG	YA	3296	1/1	0.97	0.14	30,30,30,30	0
55	MG	RA	3246	1/1	0.97	0.14	28,28,28,28	0
55	MG	RA	3200	1/1	0.97	0.15	36,36,36,36	0
55	MG	XA	1657	1/1	0.97	0.04	37,37,37,37	0
55	MG	YA	3300	1/1	0.97	0.17	50,50,50,50	0
55	MG	YA	3301	1/1	0.97	0.05	25,25,25,25	0
55	MG	RA	3083	1/1	0.97	0.10	15,15,15,15	0
55	MG	YA	3053	1/1	0.97	0.17	26,26,26,26	0
55	MG	QA	1713	1/1	0.97	0.05	22,22,22,22	0
55	MG	YA	3055	1/1	0.97	0.04	13,13,13,13	0
55	MG	YA	3456	1/1	0.97	0.08	33,33,33,33	0
55	MG	YA	3056	1/1	0.97	0.13	11,11,11,11	0
55	MG	RA	3162	1/1	0.97	0.14	24,24,24,24	0
55	MG	QA	1668	1/1	0.97	0.18	46,46,46,46	0
55	MG	XA	1662	1/1	0.97	0.12	31,31,31,31	0
55	MG	RA	3365	1/1	0.97	0.15	54,54,54,54	0
55	MG	RA	3124	1/1	0.97	0.12	16,16,16,16	0
55	MG	RA	3256	1/1	0.97	0.10	16,16,16,16	0
55	MG	YA	3176	1/1	0.97	0.10	44,44,44,44	0
55	MG	QA	1743	1/1	0.97	0.04	47,47,47,47	0
55	MG	QA	1630	1/1	0.97	0.04	56,56,56,56	0
55	MG	RA	3371	1/1	0.97	0.17	32,32,32,32	0
55	MG	RA	3259	1/1	0.97	0.19	31,31,31,31	0
55	MG	YA	3323	1/1	0.97	0.16	16,16,16,16	0
55	MG	RA	3444	1/1	0.97	0.09	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3072	1/1	0.97	0.12	34,34,34,34	0
55	MG	RA	3373	1/1	0.97	0.15	36,36,36,36	0
55	MG	QA	1745	1/1	0.97	0.12	54,54,54,54	0
55	MG	YA	3076	1/1	0.97	0.15	25,25,25,25	0
55	MG	QA	1670	1/1	0.97	0.18	33,33,33,33	0
55	MG	YA	3189	1/1	0.97	0.27	28,28,28,28	0
55	MG	YA	3190	1/1	0.97	0.09	14,14,14,14	0
55	MG	XA	1675	1/1	0.97	0.12	20,20,20,20	0
55	MG	YA	3333	1/1	0.97	0.09	26,26,26,26	0
55	MG	YA	3482	1/1	0.97	0.07	54,54,54,54	0
55	MG	RA	3095	1/1	0.97	0.09	32,32,32,32	0
55	MG	QA	1606	1/1	0.97	0.13	36,36,36,36	0
55	MG	RA	3265	1/1	0.97	0.09	26,26,26,26	0
55	MG	RA	3171	1/1	0.97	0.15	36,36,36,36	0
55	MG	RA	3454	1/1	0.97	0.04	50,50,50,50	0
55	MG	RA	3009	1/1	0.97	0.15	8,8,8,8	0
55	MG	YA	3340	1/1	0.97	0.23	60,60,60,60	0
55	MG	QA	1634	1/1	0.97	0.12	69,69,69,69	0
55	MG	YA	3493	1/1	0.97	0.11	51,51,51,51	0
55	MG	QA	1719	1/1	0.97	0.06	35,35,35,35	0
55	MG	YA	3087	1/1	0.97	0.13	3,3,3,3	0
55	MG	XA	1764	1/1	0.97	0.14	10,10,10,10	0
55	MG	YA	3203	1/1	0.97	0.06	23,23,23,23	0
55	MG	YA	3348	1/1	0.97	0.08	37,37,37,37	0
55	MG	RA	3136	1/1	0.97	0.06	7,7,7,7	0
55	MG	YA	3350	1/1	0.97	0.12	32,32,32,32	0
55	MG	YA	3090	1/1	0.97	0.14	1,1,1,1	0
55	MG	YA	3207	1/1	0.97	0.11	37,37,37,37	0
55	MG	YA	3504	1/1	0.97	0.15	19,19,19,19	0
55	MG	YA	3208	1/1	0.97	0.04	23,23,23,23	0
55	MG	RA	3100	1/1	0.97	0.10	56,56,56,56	0
55	MG	YA	3508	1/1	0.97	0.13	50,50,50,50	0
55	MG	RA	3101	1/1	0.97	0.07	30,30,30,30	0
55	MG	QA	1663	1/1	0.97	0.14	8,8,8,8	0
55	MG	YA	3512	1/1	0.97	0.06	46,46,46,46	0
55	MG	XA	1771	1/1	0.97	0.06	45,45,45,45	0
55	MG	XE	201	1/1	0.97	0.11	27,27,27,27	0
55	MG	YA	3216	1/1	0.97	0.13	27,27,27,27	0
55	MG	RA	3464	1/1	0.97	0.05	37,37,37,37	0
55	MG	RA	3222	1/1	0.97	0.13	19,19,19,19	0
55	MG	XA	1613	1/1	0.97	0.13	19,19,19,19	0
55	MG	YA	3365	1/1	0.97	0.07	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1614	1/1	0.97	0.09	18,18,18,18	0
55	MG	RA	3276	1/1	0.97	0.12	19,19,19,19	0
55	MG	YA	3225	1/1	0.97	0.05	15,15,15,15	0
55	MG	XV	102	1/1	0.97	0.07	47,47,47,47	0
55	MG	RA	3180	1/1	0.97	0.03	29,29,29,29	0
55	MG	YA	3229	1/1	0.97	0.14	34,34,34,34	0
55	MG	YD	301	1/1	0.97	0.04	13,13,13,13	0
55	MG	RA	3067	1/1	0.97	0.14	19,19,19,19	0
55	MG	YE	301	1/1	0.97	0.13	27,27,27,27	0
55	MG	RA	3225	1/1	0.97	0.17	28,28,28,28	0
55	MG	YA	3234	1/1	0.97	0.15	1,1,1,1	0
55	MG	XA	1700	1/1	0.97	0.04	38,38,38,38	0
55	MG	QL	2601	1/1	0.97	0.11	38,38,38,38	0
55	MG	YP	202	1/1	0.97	0.06	14,14,14,14	0
55	MG	XA	1620	1/1	0.97	0.05	15,15,15,15	0
55	MG	RA	3399	1/1	0.97	0.07	34,34,34,34	0
55	MG	RA	3402	1/1	0.97	0.08	47,47,47,47	0
55	MG	RA	3039	1/1	0.97	0.15	24,24,24,24	0
55	MG	YU	201	1/1	0.97	0.11	26,26,26,26	0
55	MG	YX	101	1/1	0.97	0.09	45,45,45,45	0
55	MG	RA	3040	1/1	0.97	0.18	15,15,15,15	0
55	MG	YA	3005	1/1	0.97	0.03	15,15,15,15	0
55	MG	RA	3109	1/1	0.97	0.10	14,14,14,14	0
55	MG	QA	1627	1/1	0.97	0.11	33,33,33,33	0
55	MG	QA	1675	1/1	0.97	0.09	26,26,26,26	0
55	MG	YA	3009	1/1	0.97	0.15	23,23,23,23	0
56	SF4	QD	301	8/8	0.97	0.07	95,98,100,103	0
55	MG	RA	3479	1/1	0.97	0.10	53,53,53,53	0
55	MG	RA	3408	1/1	0.97	0.05	30,30,30,30	0
55	MG	YA	3122	1/1	0.97	0.08	26,26,26,26	0
55	MG	QA	1607	1/1	0.97	0.06	36,36,36,36	0
55	MG	YA	3013	1/1	0.97	0.15	16,16,16,16	0
55	MG	RA	3189	1/1	0.97	0.14	36,36,36,36	0
55	MG	RA	3341	1/1	0.97	0.13	38,38,38,38	0
55	MG	YA	3257	1/1	0.97	0.08	11,11,11,11	0
55	MG	RA	3046	1/1	0.97	0.12	24,24,24,24	0
55	MG	YA	3259	1/1	0.97	0.26	26,26,26,26	0
55	MG	YA	3131	1/1	0.97	0.12	26,26,26,26	0
55	MG	YA	3423	1/1	0.98	0.12	25,25,25,25	0
55	MG	RA	3048	1/1	0.98	0.10	15,15,15,15	0
55	MG	YA	3425	1/1	0.98	0.06	46,46,46,46	0
55	MG	RA	3296	1/1	0.98	0.11	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3427	1/1	0.98	0.03	57,57,57,57	0
55	MG	RA	3297	1/1	0.98	0.10	18,18,18,18	0
55	MG	YA	3092	1/1	0.98	0.15	6,6,6,6	0
55	MG	RA	3156	1/1	0.98	0.07	16,16,16,16	0
55	MG	YA	3306	1/1	0.98	0.07	15,15,15,15	0
55	MG	XA	1640	1/1	0.98	0.11	28,28,28,28	0
55	MG	YA	3308	1/1	0.98	0.11	16,16,16,16	0
55	MG	YA	3309	1/1	0.98	0.09	30,30,30,30	0
55	MG	RA	3385	1/1	0.98	0.03	33,33,33,33	0
55	MG	YA	3436	1/1	0.98	0.08	34,34,34,34	0
55	MG	RA	3386	1/1	0.98	0.16	32,32,32,32	0
55	MG	YA	3312	1/1	0.98	0.23	23,23,23,23	0
55	MG	YA	3439	1/1	0.98	0.09	31,31,31,31	0
55	MG	YA	3440	1/1	0.98	0.11	35,35,35,35	0
55	MG	RA	3011	1/1	0.98	0.17	29,29,29,29	0
55	MG	QA	1755	1/1	0.98	0.07	74,74,74,74	0
55	MG	QA	1666	1/1	0.98	0.26	40,40,40,40	0
55	MG	QA	1694	1/1	0.98	0.09	40,40,40,40	0
55	MG	RA	3446	1/1	0.98	0.04	35,35,35,35	0
55	MG	YA	3201	1/1	0.98	0.11	30,30,30,30	0
55	MG	RA	3391	1/1	0.98	0.10	37,37,37,37	0
55	MG	RA	3263	1/1	0.98	0.24	36,36,36,36	0
55	MG	RA	3393	1/1	0.98	0.04	24,24,24,24	0
55	MG	YA	3322	1/1	0.98	0.06	29,29,29,29	0
55	MG	YA	3205	1/1	0.98	0.14	2,2,2,2	0
55	MG	RA	3103	1/1	0.98	0.07	22,22,22,22	0
55	MG	RN	201	1/1	0.98	0.16	42,42,42,42	0
55	MG	YA	3455	1/1	0.98	0.05	29,29,29,29	0
55	MG	YA	3017	1/1	0.98	0.18	0,0,0,0	0
55	MG	QA	1682	1/1	0.98	0.07	36,36,36,36	0
55	MG	YA	3210	1/1	0.98	0.05	18,18,18,18	0
55	MG	RP	201	1/1	0.98	0.06	21,21,21,21	0
55	MG	XA	1727	1/1	0.98	0.03	48,48,48,48	0
55	MG	RA	3266	1/1	0.98	0.18	36,36,36,36	0
55	MG	YA	3214	1/1	0.98	0.07	20,20,20,20	0
55	MG	RA	3453	1/1	0.98	0.05	28,28,28,28	0
55	MG	RA	3194	1/1	0.98	0.05	49,49,49,49	0
55	MG	RA	3001	1/1	0.98	0.05	3,3,3,3	0
55	MG	RA	3133	1/1	0.98	0.10	38,38,38,38	0
55	MG	RA	3400	1/1	0.98	0.07	27,27,27,27	0
55	MG	RA	3458	1/1	0.98	0.08	37,37,37,37	0
55	MG	YA	3223	1/1	0.98	0.25	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3401	1/1	0.98	0.07	13,13,13,13	0
55	MG	RA	3106	1/1	0.98	0.09	35,35,35,35	0
55	MG	YA	3226	1/1	0.98	0.11	2,2,2,2	0
55	MG	YA	3343	1/1	0.98	0.13	38,38,38,38	0
55	MG	YA	3344	1/1	0.98	0.15	57,57,57,57	0
55	MG	RA	3036	1/1	0.98	0.14	10,10,10,10	0
55	MG	YA	3032	1/1	0.98	0.07	6,6,6,6	0
55	MG	YA	3124	1/1	0.98	0.18	50,50,50,50	0
55	MG	YA	3125	1/1	0.98	0.09	26,26,26,26	0
55	MG	YA	3232	1/1	0.98	0.14	14,14,14,14	0
55	MG	RA	3079	1/1	0.98	0.11	3,3,3,3	0
55	MG	R1	101	1/1	0.98	0.11	28,28,28,28	0
55	MG	RA	3056	1/1	0.98	0.11	16,16,16,16	0
55	MG	YA	3036	1/1	0.98	0.13	15,15,15,15	0
55	MG	RA	3236	1/1	0.98	0.17	27,27,27,27	0
55	MG	RA	3057	1/1	0.98	0.13	18,18,18,18	0
55	MG	YA	3039	1/1	0.98	0.12	8,8,8,8	0
55	MG	YA	3240	1/1	0.98	0.17	11,11,11,11	0
55	MG	YA	3040	1/1	0.98	0.12	21,21,21,21	0
55	MG	YA	3492	1/1	0.98	0.06	23,23,23,23	0
55	MG	QA	1696	1/1	0.98	0.11	25,25,25,25	0
55	MG	YA	3361	1/1	0.98	0.06	37,37,37,37	0
55	MG	XA	1603	1/1	0.98	0.17	1,1,1,1	0
55	MG	YA	3043	1/1	0.98	0.09	8,8,8,8	0
55	MG	YA	3044	1/1	0.98	0.13	0,0,0,0	0
55	MG	XA	1672	1/1	0.98	0.14	26,26,26,26	0
55	MG	RA	3003	1/1	0.98	0.18	13,13,13,13	0
55	MG	XA	1605	1/1	0.98	0.16	20,20,20,20	0
55	MG	YA	3249	1/1	0.98	0.13	8,8,8,8	0
55	MG	QA	1729	1/1	0.98	0.06	17,17,17,17	0
55	MG	YA	3503	1/1	0.98	0.13	20,20,20,20	0
55	MG	XA	1676	1/1	0.98	0.12	9,9,9,9	0
55	MG	RA	3173	1/1	0.98	0.05	46,46,46,46	0
55	MG	RA	3471	1/1	0.98	0.05	56,56,56,56	0
55	MG	XA	1679	1/1	0.98	0.13	19,19,19,19	0
55	MG	YA	3147	1/1	0.98	0.05	19,19,19,19	0
55	MG	YA	3510	1/1	0.98	0.09	81,81,81,81	0
55	MG	YA	3148	1/1	0.98	0.03	16,16,16,16	0
55	MG	RA	3005	1/1	0.98	0.14	3,3,3,3	0
55	MG	RA	3413	1/1	0.98	0.10	39,39,39,39	0
55	MG	YA	3378	1/1	0.98	0.08	17,17,17,17	0
55	MG	RA	3361	1/1	0.98	0.06	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3152	1/1	0.98	0.08	60,60,60,60	0
55	MG	RA	3362	1/1	0.98	0.10	30,30,30,30	0
55	MG	QA	1635	1/1	0.98	0.15	26,26,26,26	0
55	MG	YA	3264	1/1	0.98	0.12	10,10,10,10	0
55	MG	QA	1605	1/1	0.98	0.13	8,8,8,8	0
55	MG	RA	3088	1/1	0.98	0.04	11,11,11,11	0
55	MG	YA	3157	1/1	0.98	0.10	43,43,43,43	0
55	MG	RA	3043	1/1	0.98	0.05	5,5,5,5	0
55	MG	XA	1688	1/1	0.98	0.07	12,12,12,12	0
55	MG	YA	3271	1/1	0.98	0.10	8,8,8,8	0
55	MG	RA	3147	1/1	0.98	0.11	23,23,23,23	0
55	MG	RA	3369	1/1	0.98	0.07	38,38,38,38	0
55	MG	XA	1765	1/1	0.98	0.13	17,17,17,17	0
55	MG	YA	3068	1/1	0.98	0.11	17,17,17,17	0
55	MG	RA	3044	1/1	0.98	0.08	7,7,7,7	0
55	MG	RA	3423	1/1	0.98	0.21	59,59,59,59	0
55	MG	YA	3071	1/1	0.98	0.11	19,19,19,19	0
55	MG	YP	201	1/1	0.98	0.19	90,90,90,90	0
55	MG	XA	1768	1/1	0.98	0.04	39,39,39,39	0
55	MG	YA	3280	1/1	0.98	0.10	29,29,29,29	0
55	MG	YA	3073	1/1	0.98	0.06	11,11,11,11	0
55	MG	RA	3149	1/1	0.98	0.02	26,26,26,26	0
55	MG	YA	3401	1/1	0.98	0.04	36,36,36,36	0
55	MG	YA	3171	1/1	0.98	0.09	22,22,22,22	0
55	MG	RA	3091	1/1	0.98	0.09	34,34,34,34	0
55	MG	XA	1624	1/1	0.98	0.09	24,24,24,24	0
55	MG	QA	1732	1/1	0.98	0.10	21,21,21,21	0
55	MG	XA	1697	1/1	0.98	0.04	42,42,42,42	0
55	MG	YA	3407	1/1	0.98	0.18	30,30,30,30	0
55	MG	RA	3253	1/1	0.98	0.04	11,11,11,11	0
55	MG	YA	3409	1/1	0.98	0.05	67,67,67,67	0
55	MG	RA	3428	1/1	0.98	0.12	33,33,33,33	0
55	MG	RA	3489	1/1	0.98	0.29	32,32,32,32	0
57	ZN	QN	101	1/1	0.98	0.04	107,107,107,107	0
55	MG	XA	1629	1/1	0.98	0.12	21,21,21,21	0
55	MG	QA	1633	1/1	0.98	0.07	45,45,45,45	0
55	MG	RA	3292	1/1	0.98	0.10	6,6,6,6	0
55	MG	RA	3255	1/1	0.98	0.16	25,25,25,25	0
55	MG	YA	3183	1/1	0.98	0.06	16,16,16,16	0
55	MG	QA	1618	1/1	0.98	0.06	31,31,31,31	0
55	MG	YA	3185	1/1	0.98	0.16	31,31,31,31	0
55	MG	RA	3379	1/1	0.98	0.09	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3421	1/1	0.98	0.04	14,14,14,14	0
55	MG	RA	3380	1/1	0.98	0.23	29,29,29,29	0
55	MG	RA	3153	1/1	0.99	0.10	28,28,28,28	0
55	MG	RA	3463	1/1	0.99	0.04	34,34,34,34	0
55	MG	YA	3121	1/1	0.99	0.06	21,21,21,21	0
55	MG	QA	1662	1/1	0.99	0.17	37,37,37,37	0
55	MG	RA	3092	1/1	0.99	0.10	11,11,11,11	0
55	MG	XA	1611	1/1	0.99	0.03	16,16,16,16	0
55	MG	YA	3266	1/1	0.99	0.14	26,26,26,26	0
55	MG	RA	3093	1/1	0.99	0.09	26,26,26,26	0
55	MG	RA	3094	1/1	0.99	0.03	4,4,4,4	0
55	MG	YA	3230	1/1	0.99	0.21	1,1,1,1	0
55	MG	YA	3064	1/1	0.99	0.09	11,11,11,11	0
55	MG	QA	1631	1/1	0.99	0.06	76,76,76,76	0
55	MG	YA	3097	1/1	0.99	0.04	17,17,17,17	0
55	MG	YA	3130	1/1	0.99	0.13	38,38,38,38	0
55	MG	YA	3481	1/1	0.99	0.25	54,54,54,54	0
55	MG	QA	1611	1/1	0.99	0.08	12,12,12,12	0
55	MG	XA	1741	1/1	0.99	0.03	38,38,38,38	0
55	MG	YA	3166	1/1	0.99	0.03	10,10,10,10	0
55	MG	RA	3252	1/1	0.99	0.07	40,40,40,40	0
55	MG	YA	3358	1/1	0.99	0.09	34,34,34,34	0
55	MG	RA	3212	1/1	0.99	0.04	40,40,40,40	0
55	MG	QA	1780	1/1	0.99	0.03	53,53,53,53	0
55	MG	YA	3489	1/1	0.99	0.08	29,29,29,29	0
55	MG	RA	3060	1/1	0.99	0.11	8,8,8,8	0
55	MG	RA	3013	1/1	0.99	0.08	7,7,7,7	0
55	MG	RA	3216	1/1	0.99	0.13	7,7,7,7	0
55	MG	RA	3073	1/1	0.99	0.08	6,6,6,6	0
55	MG	RA	3364	1/1	0.99	0.10	27,27,27,27	0
55	MG	XQ	201	1/1	0.99	0.04	65,65,65,65	0
55	MG	YA	3047	1/1	0.99	0.18	12,12,12,12	0
55	MG	YA	3451	1/1	0.99	0.14	34,34,34,34	0
55	MG	RA	3198	1/1	0.99	0.04	14,14,14,14	0
55	MG	RA	3131	1/1	0.99	0.05	16,16,16,16	0
55	MG	QA	1639	1/1	0.99	0.08	49,49,49,49	0
55	MG	YA	3290	1/1	0.99	0.08	14,14,14,14	0
55	MG	RA	3023	1/1	0.99	0.03	3,3,3,3	0
55	MG	RA	3033	1/1	0.99	0.10	9,9,9,9	0
55	MG	YA	3253	1/1	0.99	0.10	9,9,9,9	0
55	MG	YA	3416	1/1	0.99	0.14	42,42,42,42	0
55	MG	RA	3436	1/1	0.99	0.20	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3461	1/1	0.99	0.06	29,29,29,29	0
57	ZN	XN	101	1/1	0.99	0.03	70,70,70,70	0
55	MG	YA	3217	1/1	0.99	0.10	24,24,24,24	0
55	MG	YA	3218	1/1	0.99	0.06	43,43,43,43	0
55	MG	RA	3015	1/1	0.99	0.11	35,35,35,35	0
55	MG	YA	3026	1/1	0.99	0.06	0,0,0,0	0
55	MG	QA	1649	1/1	0.99	0.04	26,26,26,26	0
55	MG	YA	3066	1/1	1.00	0.16	1,1,1,1	0
55	MG	YA	3506	1/1	1.00	0.02	4,4,4,4	0

6.5 Other polymers [i](#)

There are no such residues in this entry.