



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 10:07 AM UTC

PDB ID : 5D8B / pdb\_00005d8b  
Title : Crystal structure of T. thermophilus ribosome containing a P-site wobble mismatch  
Authors : Svidritskiy, E.; Korostelev, A.A.  
Deposited on : 2015-08-17  
Resolution : 3.63 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

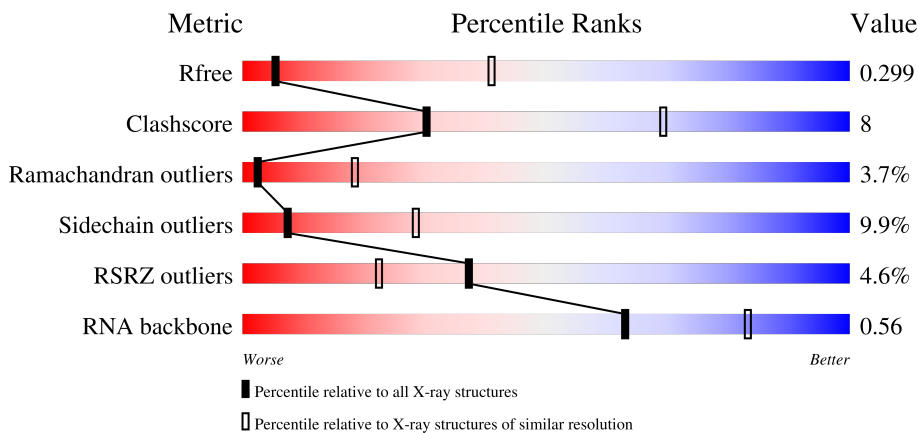
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.63 Å.

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





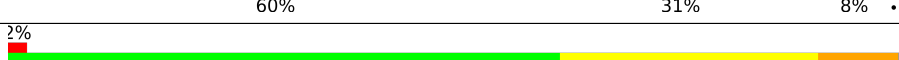
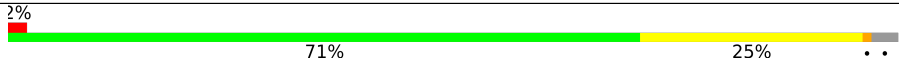
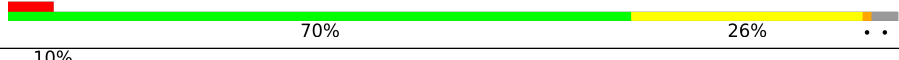

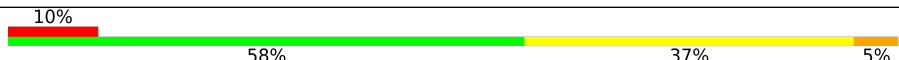
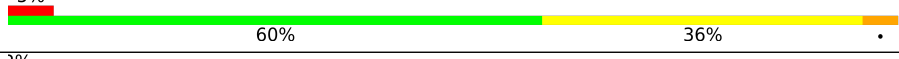

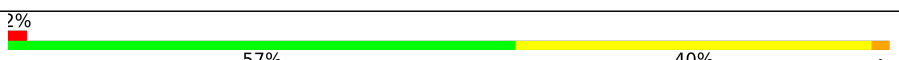
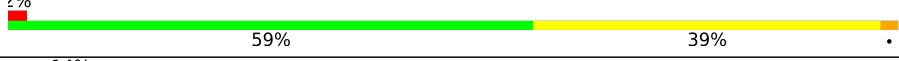
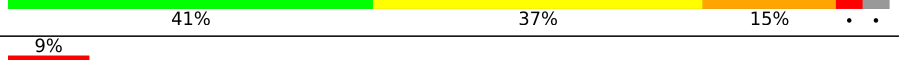
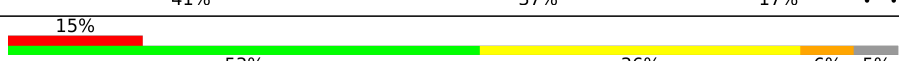


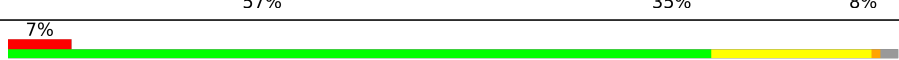






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1132 (3.76-3.52)
Clashscore	190562	1014 (3.74-3.54)
Ramachandran outliers	187476	1123 (3.76-3.52)
Sidechain outliers	187428	1121 (3.76-3.52)
RSRZ outliers	180081	1130 (3.76-3.52)
RNA backbone	3983	1026 (4.22-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	271	 5% 63% 31% 6%
1	WA	271	 5% 62% 32% 6%
2	B	206	 2% 66% 26% 7%
2	XA	206	 3% 67% 26% 6%

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Mol	Chain	Length	Quality of chain
3	C	205	 %
3	YA	205	 %
4	D	182	 %
4	ZA	182	 %
5	AB	180	 %
5	E	180	 %
6	BB	148	 %
6	F	148	 %
7	CB	147	 %
7	G	147	 %
8	DB	140	 %
8	H	140	 %
9	EB	122	 %
9	I	122	 %
10	FB	150	 %
10	J	150	 %
11	GB	141	 %
11	K	141	 %
12	HB	118	 %
12	L	118	 %
13	IB	112	 %
13	M	112	 %
14	JB	146	%
14	N	146	%
15	KB	118	%

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Mol	Chain	Length	Quality of chain
15	O	118	5% 67% 27% 5%
16	LB	101	3% 60% 34% 6%
16	P	101	3% 60% 34% 6%
17	MB	113	% 64% 34% ..
17	Q	113	2% 64% 33% ..
18	NB	96	3% 71% 24% ..
18	R	96	4% 71% 24% ..
19	OB	110	9% 51% 30% 9% . 9%
19	S	110	19% 51% 31% 8% . 9%
20	PB	206	% 65% 24% . 9%
20	T	206	2% 63% 25% . 9%
21	QB	85	5% 53% 29% 7% 11%
21	U	85	4% 53% 31% 6% 11%
22	RB	98	17% 41% 38% 11% 10%
22	V	98	18% 44% 38% 8% 10%
23	SB	72	7% 42% 35% 10% 14%
23	W	72	4% 43% 35% 8% 14%
24	TB	60	5% 73% 22% ..
24	X	60	2% 73% 22% ..
25	UB	60	12% 57% 27% .. 13%
25	Y	60	12% 55% 30% . 13%
26	VB	54	9% 39% 35% 7% 19%
26	Z	54	13% 39% 35% 7% 19%
27	AA	49	6% 63% 33% ..
27	WB	49	8% 63% 33% ..

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Mol	Chain	Length	Quality of chain
28	BA	65	17% 52% 37% 6% . .
28	XB	65	20% 52% 37% 6% . .
29	CA	256	2% 61% 25% 5% 9%
29	YB	256	2% 62% 25% 5% 9%
30	DA	239	2% 56% 27% . 14%
30	ZB	239	4% 55% 28% . 14%
31	AC	209	6% 67% 31% .
31	EA	209	5% 66% 30% .
32	BC	162	4% 61% 30% . 7%
32	FA	162	3% 59% 33% . 7%
33	CC	101	69% 27% .
33	GA	101	% 69% 27% .
34	DC	156	% 79% 19% ..
34	HA	156	3% 79% 20% ..
35	EC	138	3% 72% 25% ..
35	IA	138	3% 74% 23% ..
36	FC	128	14% 63% 31% 5% .
36	JA	128	16% 64% 31% . .
37	GC	105	18% 57% 29% 8% 7%
37	KA	105	11% 57% 28% 9% 7%
38	HC	129	5% 57% 27% 5% 12%
38	LA	129	5% 57% 26% 5% 12%
39	IC	132	11% 66% 22% 5% 8%
39	MA	132	6% 62% 26% 5% 8%
40	JC	126	5% 57% 32% . . 7%

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Mol	Chain	Length	Quality of chain
40	NA	126	4% 58% 31% 7%
41	KC	61	10% 70% 26%
41	OA	61	8% 64% 28% 7%
42	LC	89	3% 66% 24% 9%
42	PA	89	3% 69% 21% 9%
43	MC	88	26% 65% 30% 6%
43	QA	88	14% 68% 26% 6%
44	NC	105	11% 64% 28% 6%
44	RA	105	3% 65% 28% 6%
45	OC	88	59% 19% 20%
45	SA	88	59% 17% 20%
46	PC	93	2% 44% 34% 5% 16%
46	TA	93	5% 44% 33% 6% 16%
47	QC	106	21% 68% 23% 7%
47	UA	106	13% 65% 25% 7%
48	RC	27	33% 63% 26% 11%
48	VA	27	22% 70% 19% 11%
49	SC	71	27% 14% 58%
49	TC	71	27% 13% 58%
50	UC	1509	2% 62% 33% 5%
50	YC	1509	3% 61% 34% 5%
51	VC	2893	3% 61% 33% 6%
51	ZC	2893	2% 61% 33% 6%
52	AD	121	3% 69% 24% 5%
52	WC	121	2% 71% 22% 5%

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Mol	Chain	Length	Quality of chain
53	BD	77	
53	ED	77	
53	FD	77	
53	XC	77	
54	GD	27	
54	HD	27	

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	P	201	-	-	-	X
55	MG	UA	201	-	-	-	X
55	MG	VC	3011	-	-	-	X
55	MG	VC	3031	-	-	-	X
55	MG	VC	3040	-	-	-	X
55	MG	VC	3046	-	-	-	X
55	MG	VC	3083	-	-	-	X
55	MG	VC	3156	-	-	-	X
55	MG	VC	3695	-	-	-	X
55	MG	YC	1607	-	-	-	X
55	MG	YC	1672	-	-	-	X
55	MG	ZC	3025	-	-	-	X
55	MG	ZC	3052	-	-	-	X
55	MG	ZC	3169	-	-	-	X
55	MG	ZC	3238	-	-	-	X
55	MG	ZC	3264	-	-	-	X
55	MG	ZC	3760	-	-	-	X
55	MG	ZC	3769	-	-	-	X

## 2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 295576 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 protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	271	2105	1329	416	357	3	0	0	0
1	WA	271	2105	1329	416	357	3	0	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	204	1563	988	299	270	6	0	0	0
2	XA	204	1563	988	299	270	6	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	202	1586	1011	297	275	3	0	0	0
3	YA	202	1586	1011	297	275	3	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	181	1475	943	268	260	4	0	0	0
4	ZA	181	1475	943	268	260	4	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
5	AB	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	145	Total	C	N	O	S	0	0	0
			1132	724	200	207	1			
6	BB	145	Total	C	N	O	S	0	0	0
			1132	724	200	207	1			

- Molecule 7 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	147	Total	C	N	O	S	0	0	0
			1088	692	191	199	6			
7	CB	147	Total	C	N	O	S	0	0	0
			1088	692	191	199	6			

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			
8	DB	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			
9	EB	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	FB	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	134	Total	C	N	O	S	0	0	0
			1064	680	201	178	5			
11	GB	134	Total	C	N	O	S	0	0	0
			1064	680	201	178	5			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	L	117	Total	C	N	O	0	0	0
			960	599	202	159			
12	HB	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	110	Total	C	N	O	0	0	0
			877	553	175	149			
13	IB	110	Total	C	N	O	0	0	0
			877	553	175	149			

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			
14	JB	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
15	KB	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
16	LB	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			
17	MB	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	92	Total	C	N	O	0	0	0
			725	471	131	123			
18	NB	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			
19	OB	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	187	Total	C	N	O	S	0	0	0
			1482	945	264	271	2			
20	PB	187	Total	C	N	O	S	0	0	0
			1482	945	264	271	2			

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			
21	QB	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	88	Total	C	N	O	S	0	0	0
			694	435	141	118				
22	RB	88	Total	C	N	O	S	0	0	0
			694	435	141	118				

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	62	Total	C	N	O	S	0	0	0
			520	325	102	91	2			
23	SB	62	Total	C	N	O	S	0	0	0
			520	325	102	91	2			

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			
24	TB	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	52	Total	C	N	O	S	0	0	0
			404	255	79	65	5			
25	UB	52	Total	C	N	O	S	0	0	0
			404	255	79	65	5			

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	44	Total	C	N	O	S	0	0	0
			380	235	77	64	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	VB	44	Total	C	N	O	S	0	0	0
			380	235	77	64	4			

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	AA	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
27	WB	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BA	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			
28	XB	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

- Molecule 29 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	CA	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			
29	YB	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	DA	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
30	ZB	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 31 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	EA	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
31	AC	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 32 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	FA	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
32	BC	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 33 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	GA	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
33	CC	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 34 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	HA	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
34	DC	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 35 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	IA	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
35	EC	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 36 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	JA	127	Total	C	N	O	0	0	0
			1011	639	198	174			
36	FC	127	Total	C	N	O	0	0	0
			1011	639	198	174			

- Molecule 37 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	KA	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			
37	GC	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 38 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	LA	114	Total	C	N	O	S	0	0	0
			842	522	159	158	3			
38	HC	114	Total	C	N	O	S	0	0	0
			842	522	159	158	3			

- Molecule 39 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	MA	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			
39	IC	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			

- Molecule 40 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	NA	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			
40	JC	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

- Molecule 41 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	OA	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
41	KC	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 42 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	PA	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	LC	88	734	459	147	126	2	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	QA	83	700	443	139	117	1	0	0	0
43	MC	83	700	443	139	117	1	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	RA	99	823	528	152	141	2	0	0	0
44	NC	99	823	528	152	141	2	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
45	SA	70	574	367	112	95	0	0	0
45	OC	70	574	367	112	95	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	TA	78	629	403	114	110	2	0	0	0
46	PC	78	629	403	114	110	2	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	UA	99	762	469	162	129	2	0	0	0
47	QC	99	762	469	162	129	2	0	0	0

- Molecule 48 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
48	VA	24	208	128	50	30	0	0	0
48	RC	24	208	128	50	30	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	SC	30	225	142	36	43	4	0	0	0
49	TC	30	225	142	36	43	4	0	0	0

- Molecule 50 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
50	UC	1504	32332	14391	5994	10444	1503	0	0	0
50	YC	1504	32332	14391	5994	10444	1503	0	0	0

- Molecule 51 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
51	VC	2879	62000	27595	11586	19941	2878	0	0	0
51	ZC	2879	62000	27595	11586	19941	2878	0	0	0

- Molecule 52 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
52	WC	119	2551	1136	471	826	118	0	0	0
52	AD	119	2551	1136	471	826	118	0	0	0

- Molecule 53 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	XC	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
53	BD	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
53	ED	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
53	FD	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	GD	8	Total	C	N	O	P	0	0	0
			170	77	32	53	8			
54	HD	8	Total	C	N	O	P	0	0	0
			170	77	32	53	8			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	A	5	Total	Mg	0	0
			5	5		
55	B	2	Total	Mg	0	0
			2	2		
55	C	3	Total	Mg	0	0
			3	3		
55	D	3	Total	Mg	0	0
			3	3		
55	H	2	Total	Mg	0	0
			2	2		
55	I	1	Total	Mg	0	0
			1	1		
55	J	3	Total	Mg	0	0
			3	3		
55	L	1	Total	Mg	0	0
			1	1		
55	N	1	Total	Mg	0	0
			1	1		
55	O	2	Total	Mg	0	0
			2	2		
55	P	2	Total	Mg	0	0
			2	2		
55	Q	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	V	1	Total Mg 1 1	0	0
55	X	1	Total Mg 1 1	0	0
55	Y	1	Total Mg 1 1	0	0
55	AA	1	Total Mg 1 1	0	0
55	BA	2	Total Mg 2 2	0	0
55	EA	1	Total Mg 1 1	0	0
55	FA	1	Total Mg 1 1	0	0
55	HA	2	Total Mg 2 2	0	0
55	LA	4	Total Mg 4 4	0	0
55	OA	2	Total Mg 2 2	0	0
55	PA	2	Total Mg 2 2	0	0
55	QA	1	Total Mg 1 1	0	0
55	RA	1	Total Mg 1 1	0	0
55	UA	2	Total Mg 2 2	0	0
55	WA	5	Total Mg 5 5	0	0
55	XA	3	Total Mg 3 3	0	0
55	YA	8	Total Mg 8 8	0	0
55	BB	2	Total Mg 2 2	0	0
55	CB	1	Total Mg 1 1	0	0
55	DB	1	Total Mg 1 1	0	0
55	EB	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	FB	4	Total Mg 4 4	0	0
55	GB	1	Total Mg 1 1	0	0
55	HB	2	Total Mg 2 2	0	0
55	IB	1	Total Mg 1 1	0	0
55	JB	1	Total Mg 1 1	0	0
55	MB	1	Total Mg 1 1	0	0
55	NB	1	Total Mg 1 1	0	0
55	OB	1	Total Mg 1 1	0	0
55	QB	2	Total Mg 2 2	0	0
55	SB	1	Total Mg 1 1	0	0
55	WB	2	Total Mg 2 2	0	0
55	AC	1	Total Mg 1 1	0	0
55	BC	3	Total Mg 3 3	0	0
55	DC	1	Total Mg 1 1	0	0
55	FC	1	Total Mg 1 1	0	0
55	IC	1	Total Mg 1 1	0	0
55	LC	1	Total Mg 1 1	0	0
55	RC	1	Total Mg 1 1	0	0
55	UC	264	Total Mg 264 264	0	0
55	VC	707	Total Mg 707 707	0	0
55	WC	29	Total Mg 29 29	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	XC	5	Total Mg 5 5	0	0
55	YC	271	Total Mg 271 271	0	0
55	ZC	774	Total Mg 774 774	0	0
55	AD	30	Total Mg 30 30	0	0
55	BD	8	Total Mg 8 8	0	0
55	ED	16	Total Mg 16 16	0	0
55	FD	16	Total Mg 16 16	0	0
55	HD	1	Total Mg 1 1	0	0

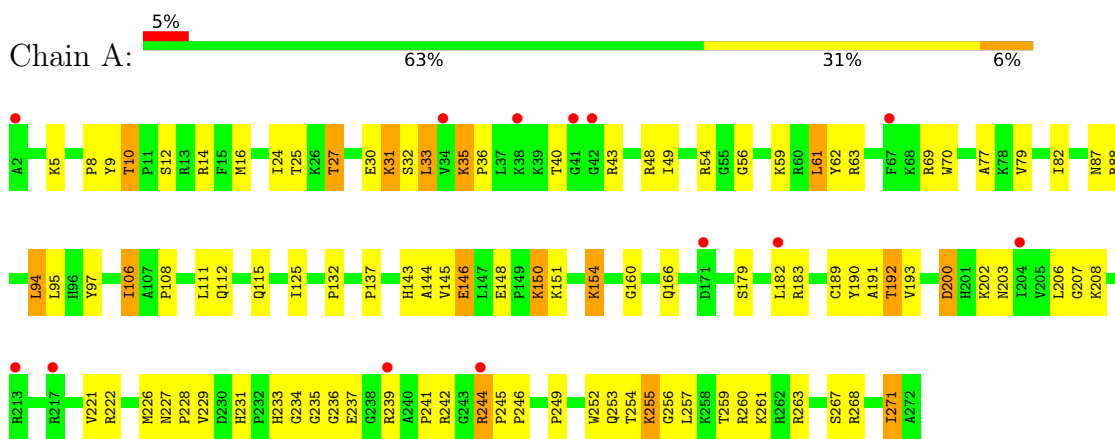
- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	EA	1	Total Zn 1 1	0	0
56	OA	1	Total Zn 1 1	0	0
56	AC	1	Total Zn 1 1	0	0
56	KC	1	Total Zn 1 1	0	0

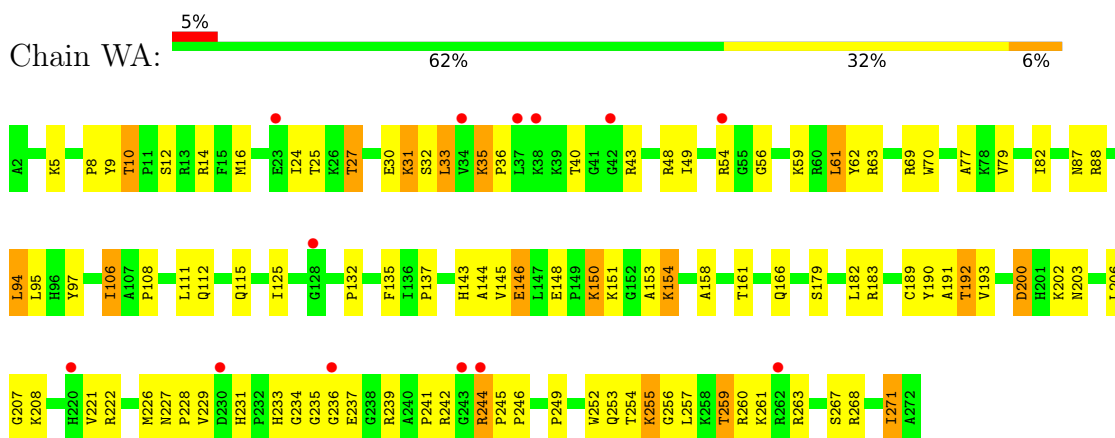
### 3 Residue-property plots [i](#)

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

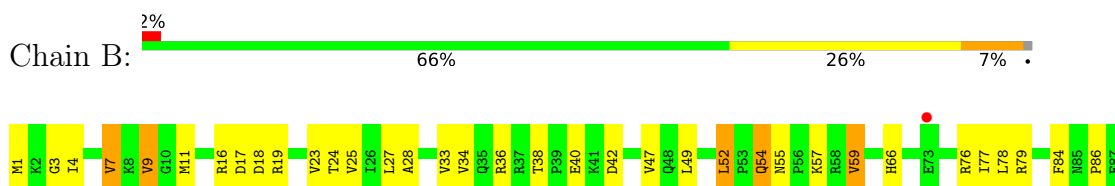
- Molecule 1: 50S ribosomal protein L2



- Molecule 1: 50S ribosomal protein L2

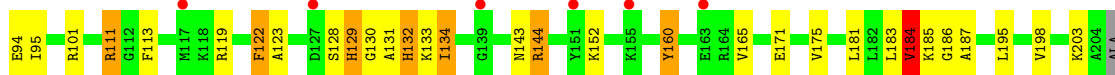
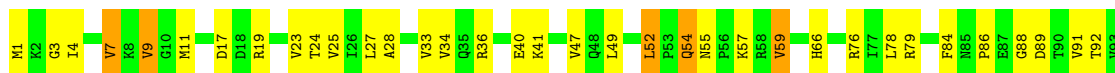


- Molecule 2: 50S ribosomal protein L3



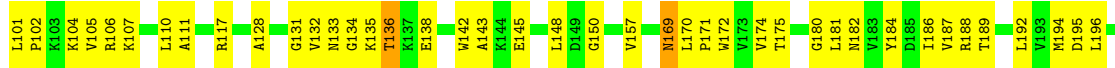


• Molecule 2: 50S ribosomal protein L3



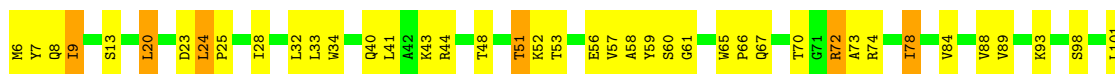
LYS

• Molecule 3: 50S ribosomal protein L4



W199  
I206  
G207  
GLY  
GLU  
ALA

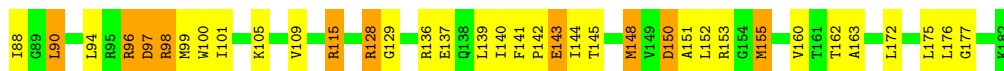
• Molecule 3: 50S ribosomal protein L4



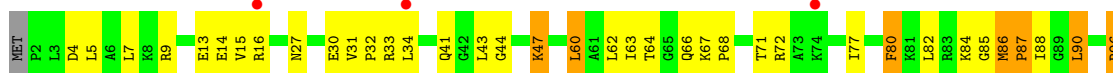
I206  
G207  
GLY  
GLU  
ALA

• Molecule 4: 50S ribosomal protein L5

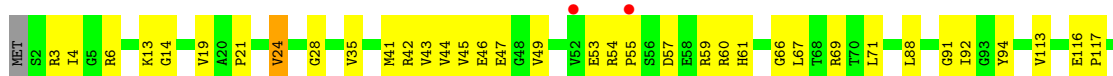




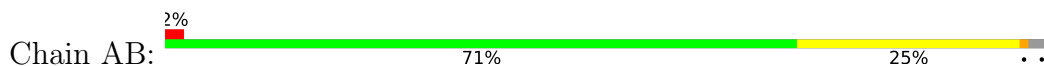
- Molecule 4: 50S ribosomal protein L5



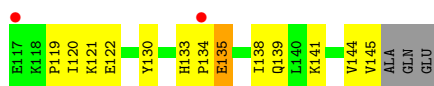
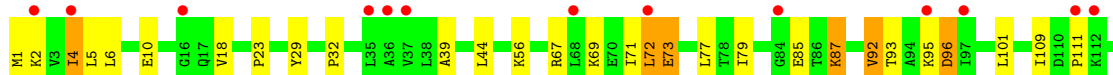
- Molecule 5: 50S ribosomal protein L6



- Molecule 5: 50S ribosomal protein L6

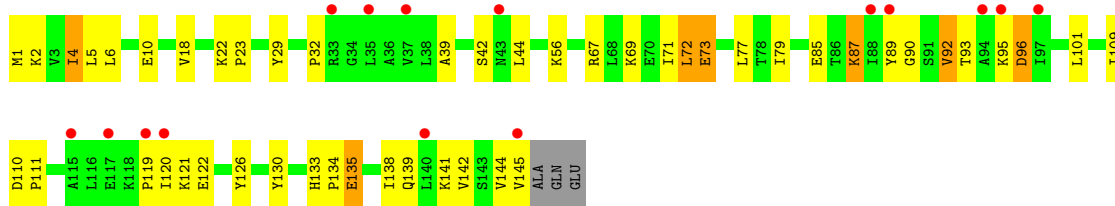


- Molecule 6: 50S ribosomal protein L9

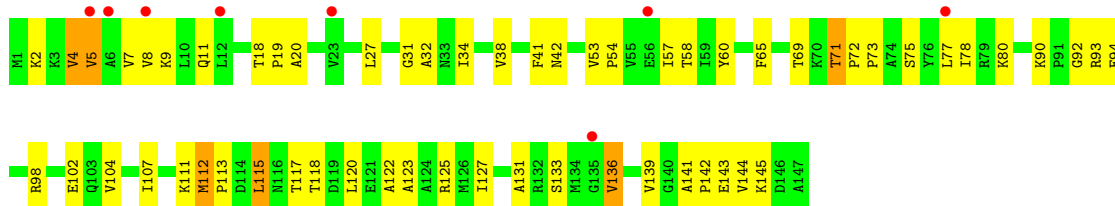


- Molecule 6: 50S ribosomal protein L9

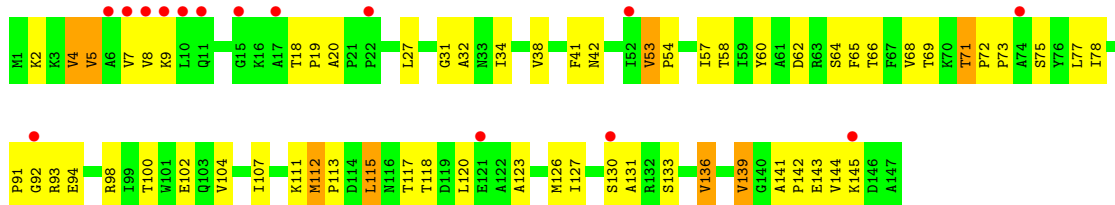




• Molecule 7: 50S ribosomal protein L11



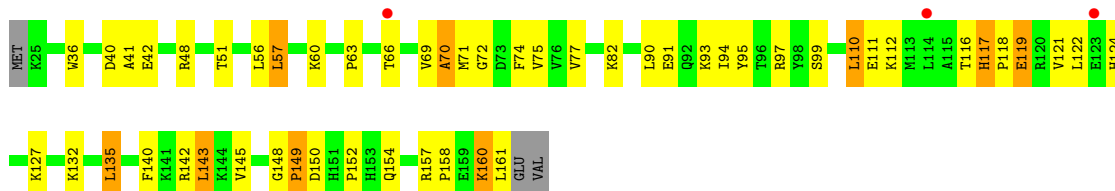
• Molecule 7: 50S ribosomal protein L11



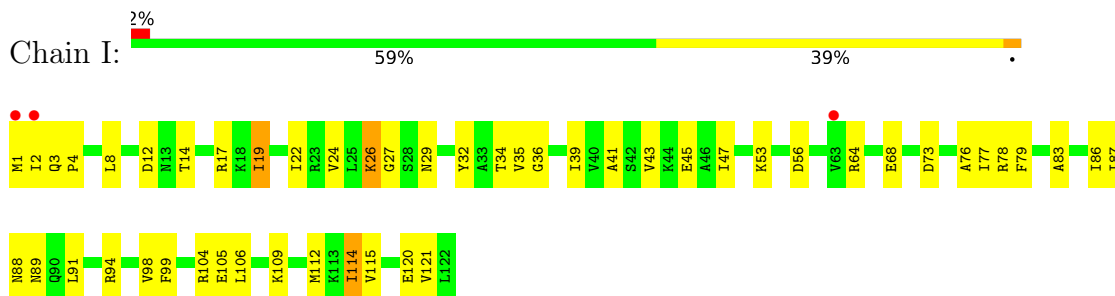
• Molecule 8: 50S ribosomal protein L13



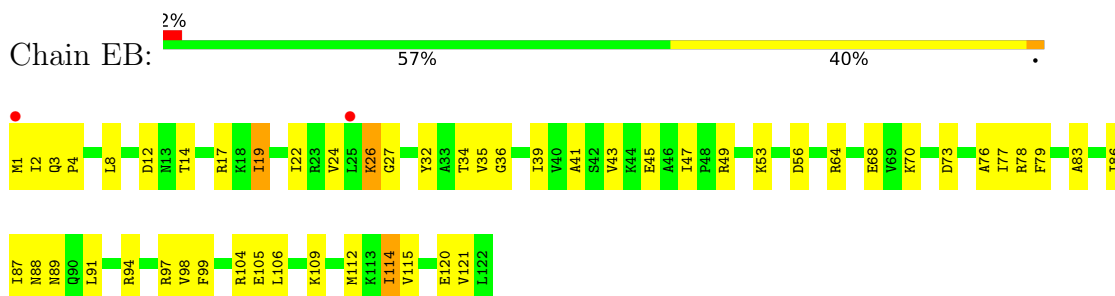
• Molecule 8: 50S ribosomal protein L13



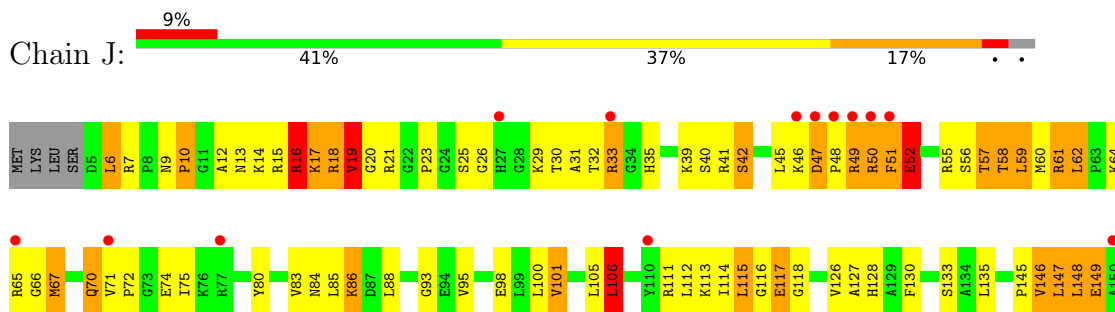
- Molecule 9: 50S ribosomal protein L14



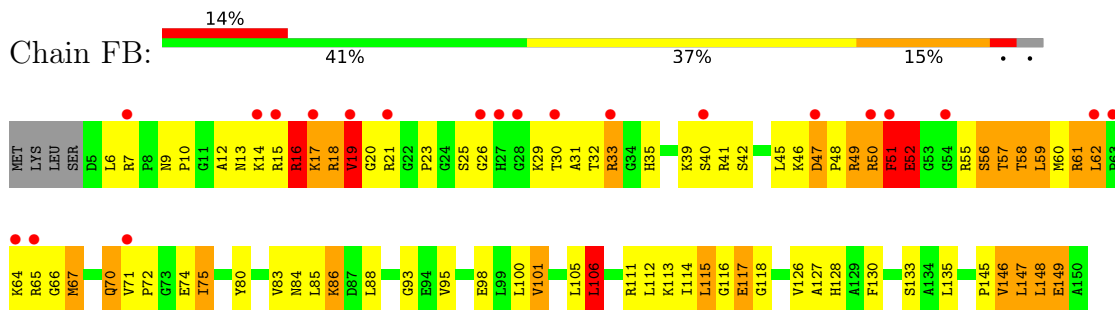
- Molecule 9: 50S ribosomal protein L14



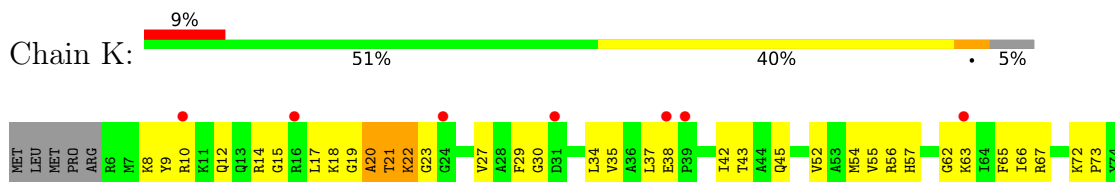
- Molecule 10: 50S ribosomal protein L15



- Molecule 10: 50S ribosomal protein L15

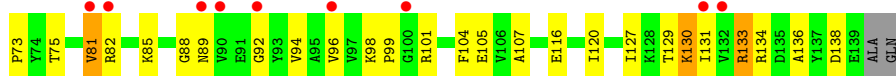
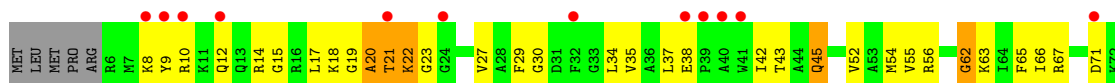


- Molecule 11: 50S ribosomal protein L16





• Molecule 11: 50S ribosomal protein L16



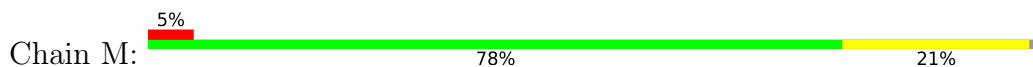
• Molecule 12: 50S ribosomal protein L17



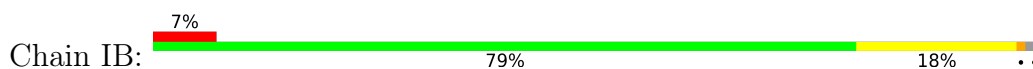
• Molecule 12: 50S ribosomal protein L17



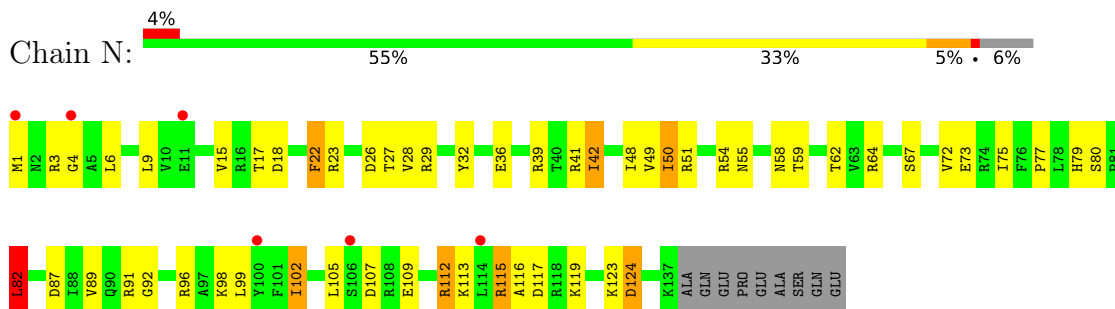
• Molecule 13: 50S ribosomal protein L18



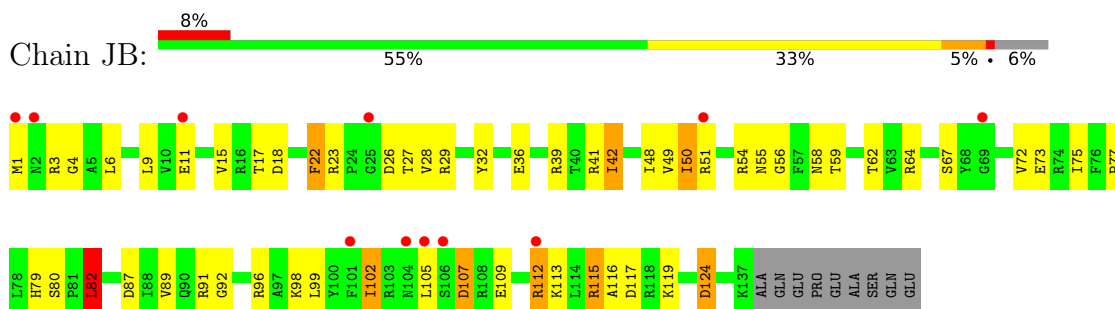
• Molecule 13: 50S ribosomal protein L18



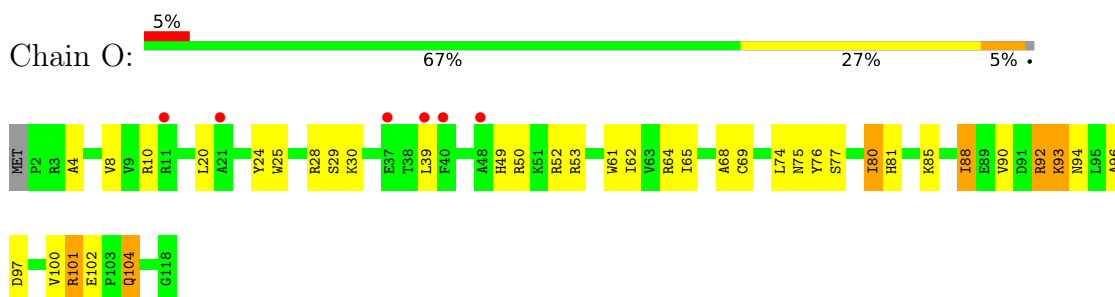
- Molecule 14: 50S ribosomal protein L19



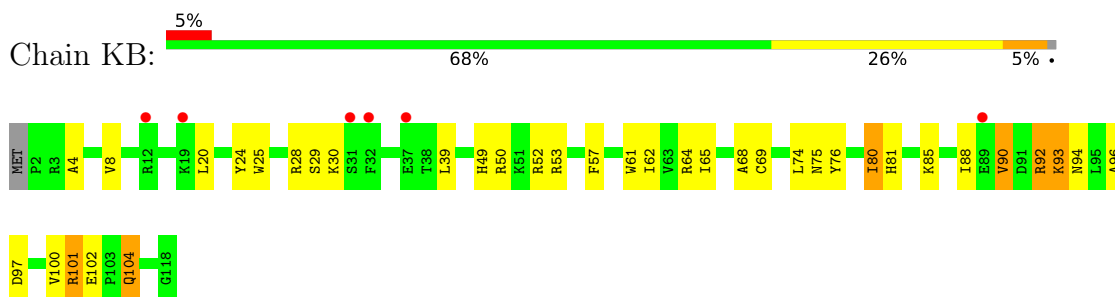
- Molecule 14: 50S ribosomal protein L19



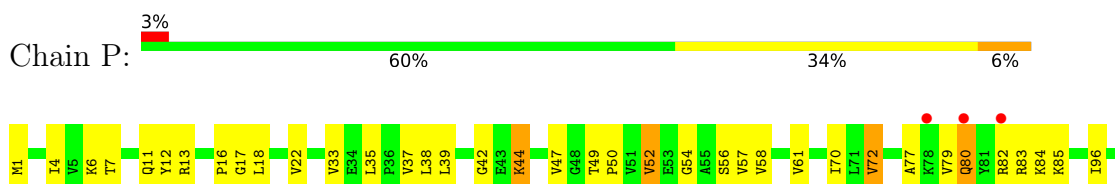
- Molecule 15: 50S ribosomal protein L20



- Molecule 15: 50S ribosomal protein L20



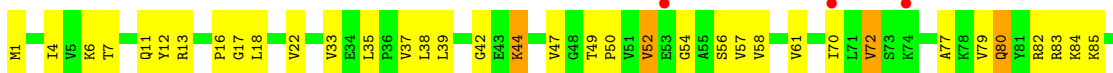
- Molecule 16: 50S ribosomal protein L21



I99  
R100  
G101

- Molecule 16: 50S ribosomal protein L21

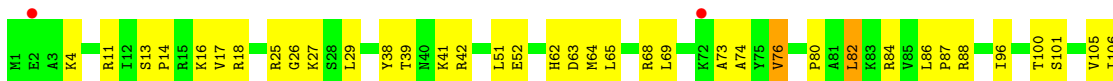
Chain LB: 3% 60% 34% 6%



I96  
I99  
R100  
G101

- Molecule 17: 50S ribosomal protein L22

Chain Q: 2% 64% 33% ..



L107  
K110  
H111  
G112  
LYS

- Molecule 17: 50S ribosomal protein L22

Chain MB: 64% 34% ..



T104  
Y105  
L106  
L107  
K110  
H111  
G112  
LYS

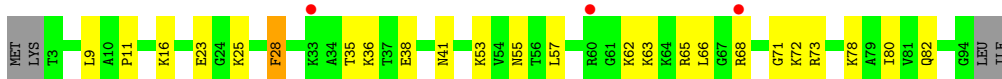
- Molecule 18: 50S ribosomal protein L23

Chain R: 4% 71% 24% ..

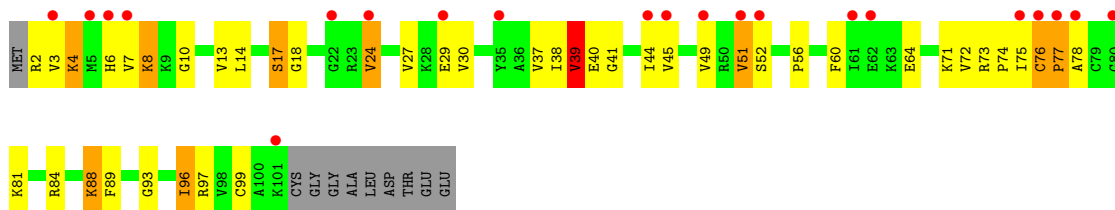


- Molecule 18: 50S ribosomal protein L23

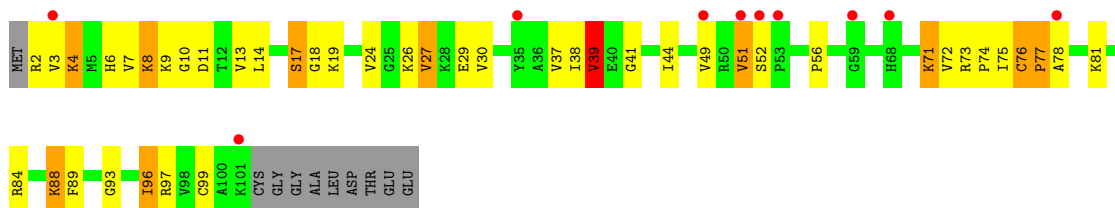
Chain NB: 3% 71% 24% ..



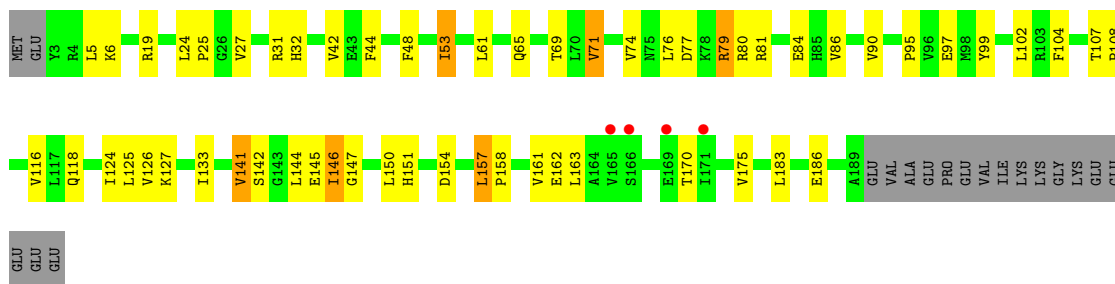
- Molecule 19: 50S ribosomal protein L24



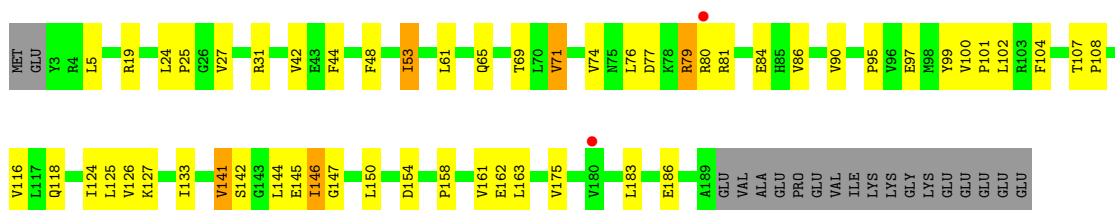
• Molecule 19: 50S ribosomal protein L24



• Molecule 20: 50S ribosomal protein L25

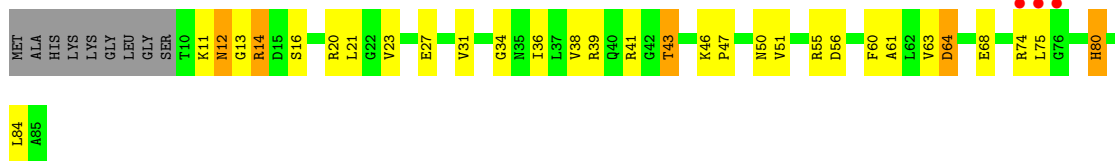


• Molecule 20: 50S ribosomal protein L25

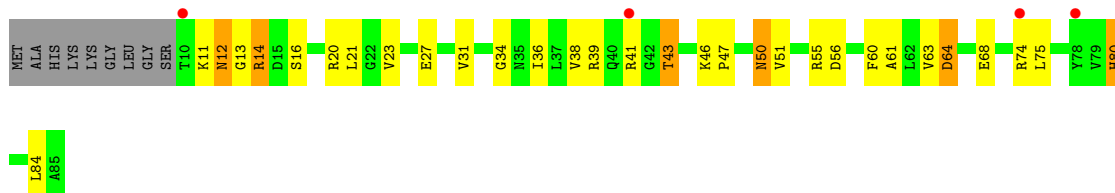


• Molecule 21: 50S ribosomal protein L27

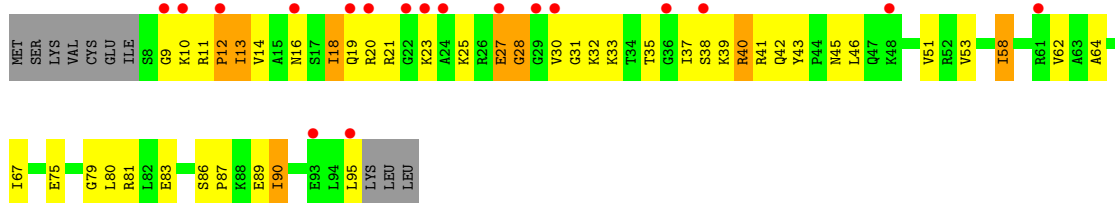
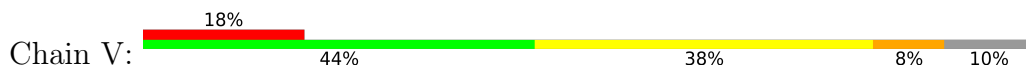




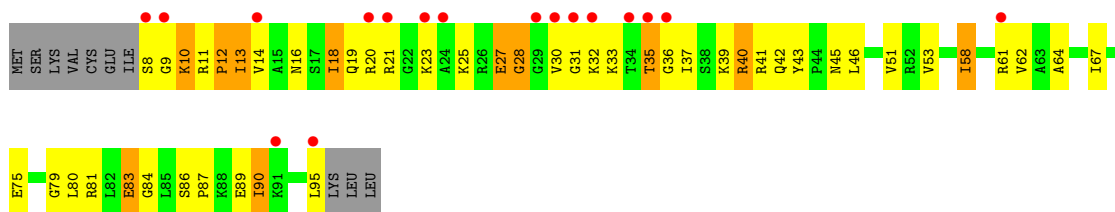
• Molecule 21: 50S ribosomal protein L27



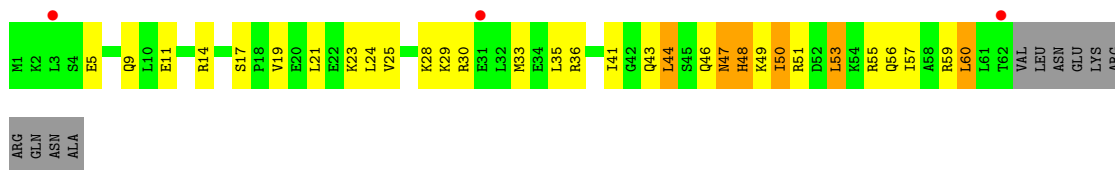
• Molecule 22: 50S ribosomal protein L28



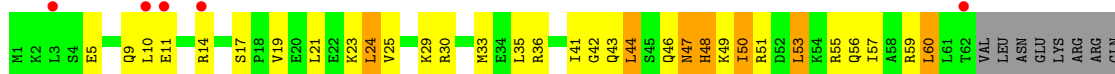
• Molecule 22: 50S ribosomal protein L28



• Molecule 23: 50S ribosomal protein L29

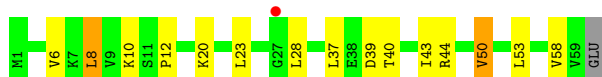
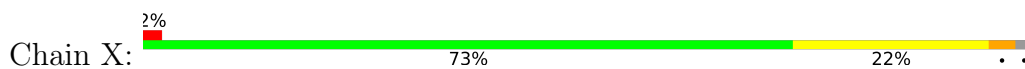


• Molecule 23: 50S ribosomal protein L29

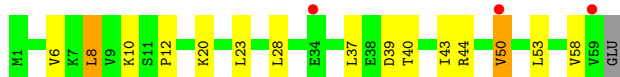
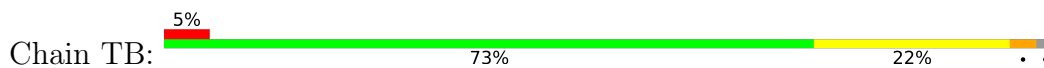


ASN  
ALA

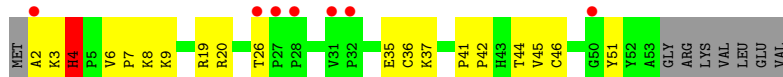
- Molecule 24: 50S ribosomal protein L30



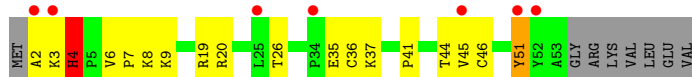
- Molecule 24: 50S ribosomal protein L30



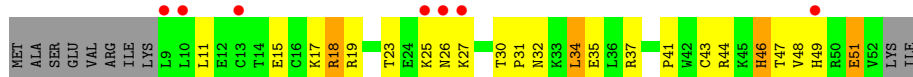
- Molecule 25: 50S ribosomal protein L32



- Molecule 25: 50S ribosomal protein L32

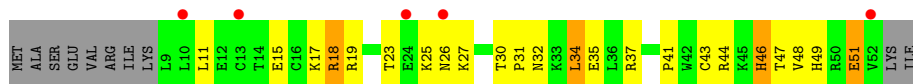


- Molecule 26: 50S ribosomal protein L33



- Molecule 26: 50S ribosomal protein L33

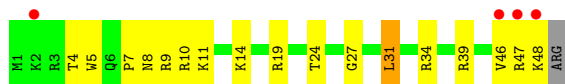




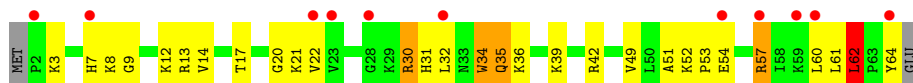
• Molecule 27: 50S ribosomal protein L34



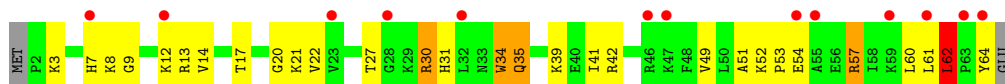
• Molecule 27: 50S ribosomal protein L34



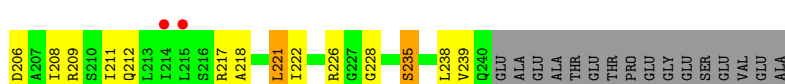
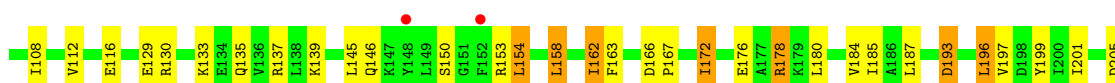
• Molecule 28: 50S ribosomal protein L35



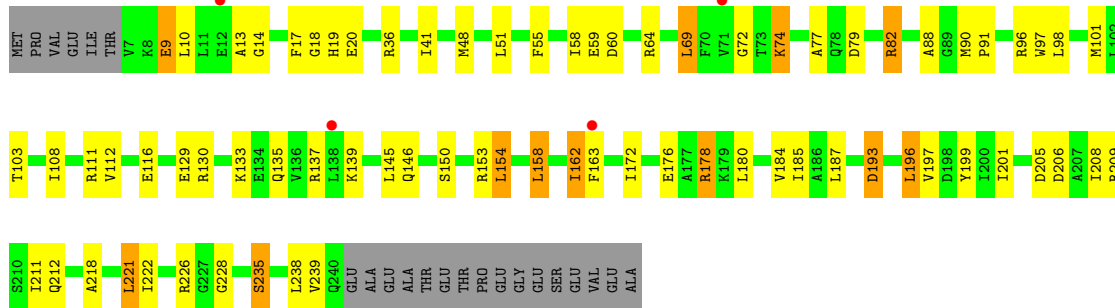
• Molecule 28: 50S ribosomal protein L35



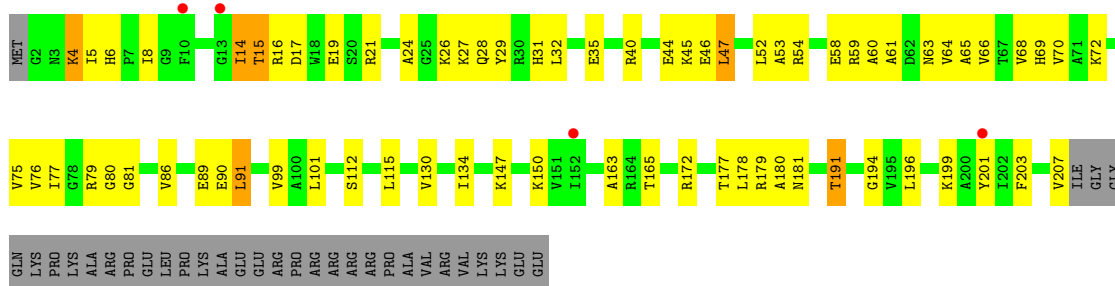
• Molecule 29: 30S ribosomal protein S2



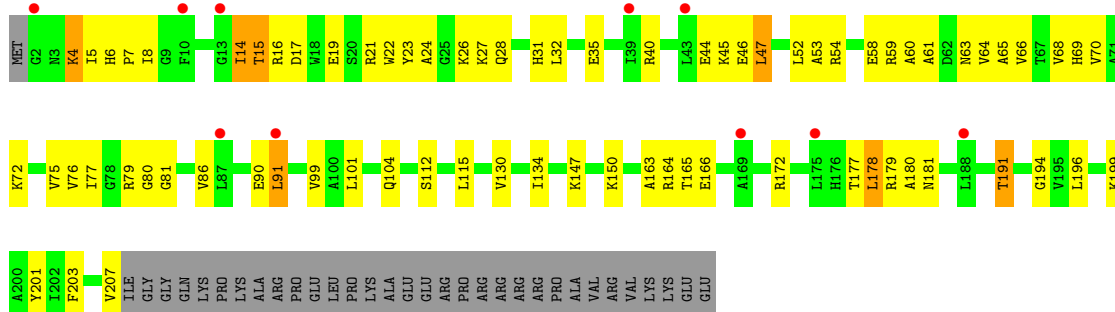
• Molecule 29: 30S ribosomal protein S2



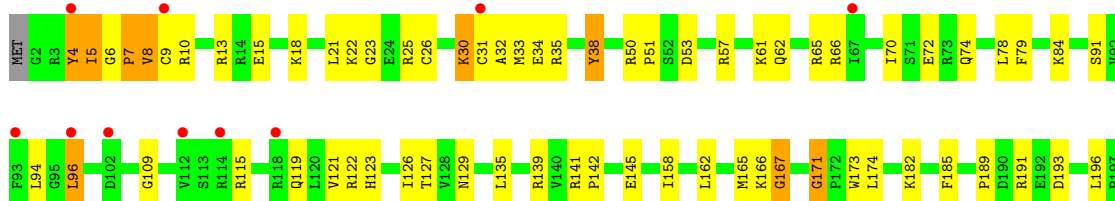
• Molecule 30: 30S ribosomal protein S3

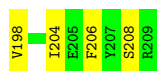


• Molecule 30: 30S ribosomal protein S3

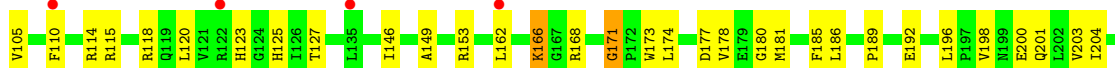
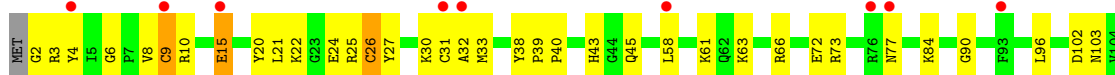


• Molecule 31: 30S ribosomal protein S4

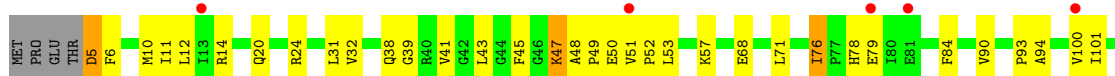




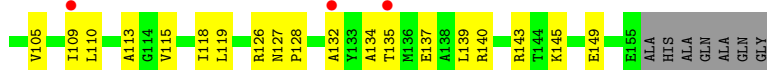
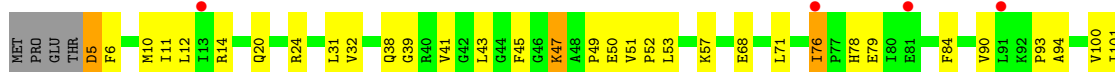
- Molecule 31: 30S ribosomal protein S4



- Molecule 32: 30S ribosomal protein S5



- Molecule 32: 30S ribosomal protein S5



- Molecule 33: 30S ribosomal protein S6

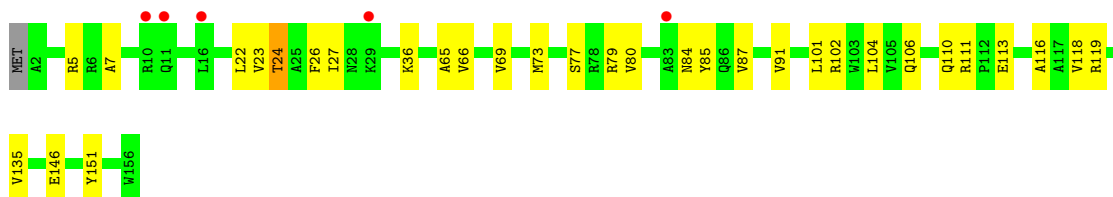
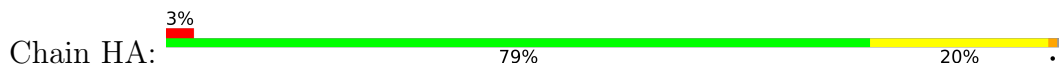


- Molecule 33: 30S ribosomal protein S6

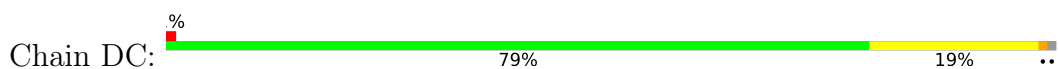




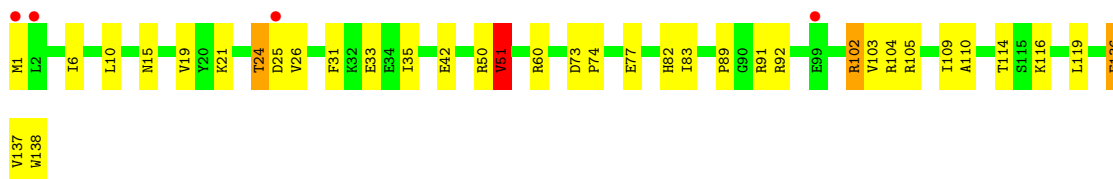
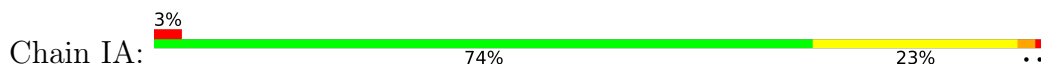
- Molecule 34: 30S ribosomal protein S7



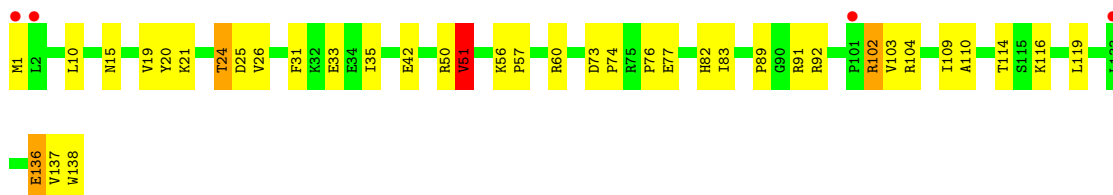
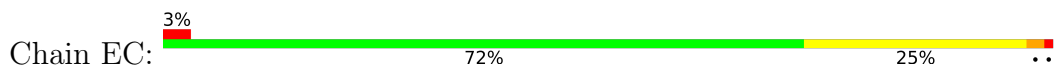
- Molecule 34: 30S ribosomal protein S7



- Molecule 35: 30S ribosomal protein S8

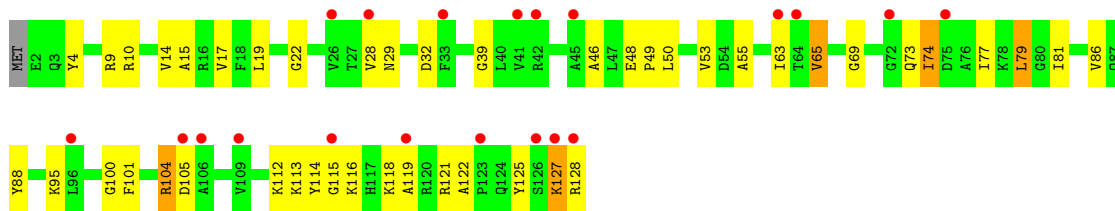


- Molecule 35: 30S ribosomal protein S8

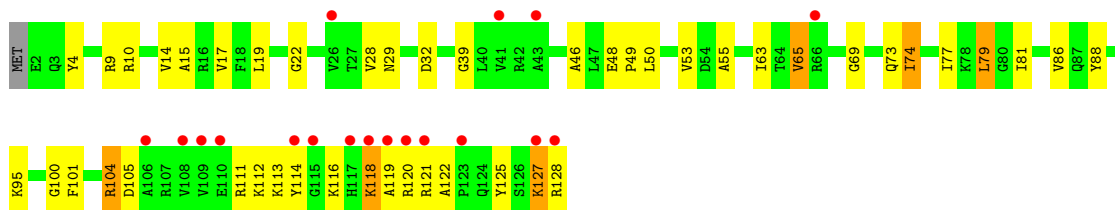


- Molecule 36: 30S ribosomal protein S9

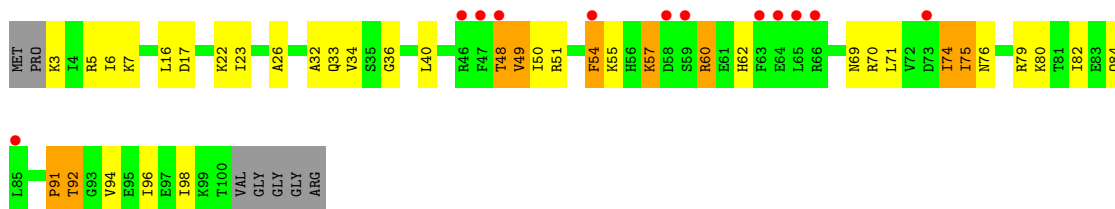




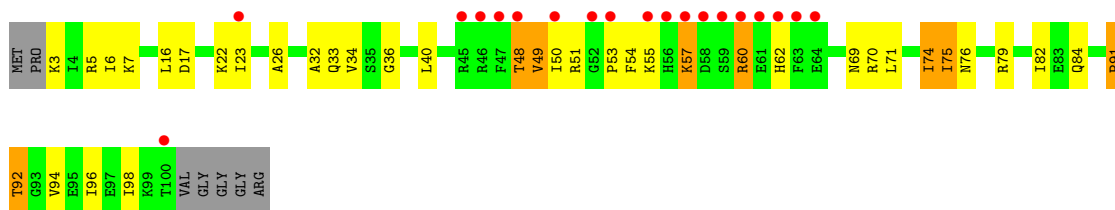
• Molecule 36: 30S ribosomal protein S9



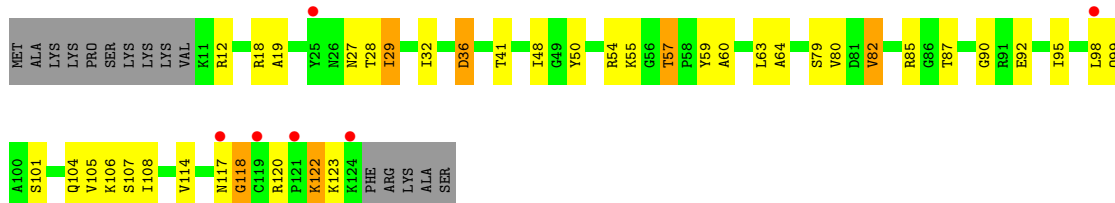
• Molecule 37: 30S ribosomal protein S10



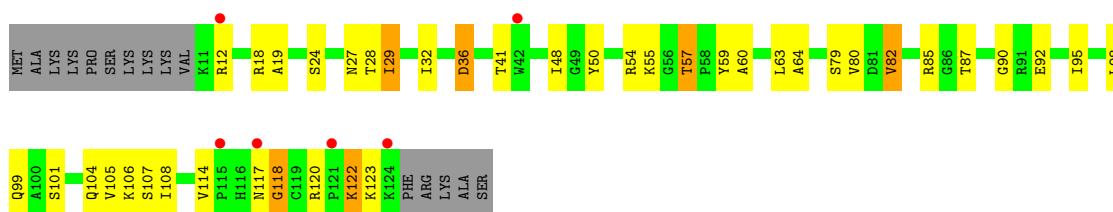
• Molecule 37: 30S ribosomal protein S10



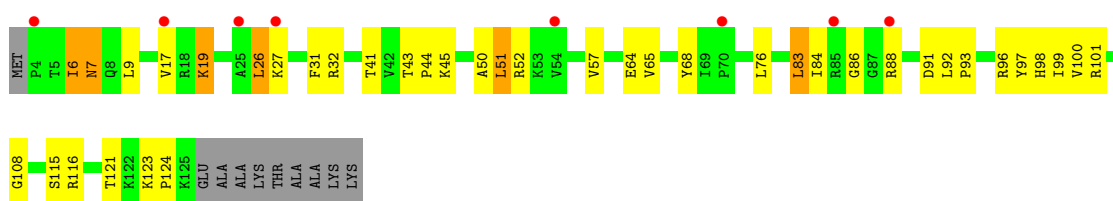
• Molecule 38: 30S ribosomal protein S11



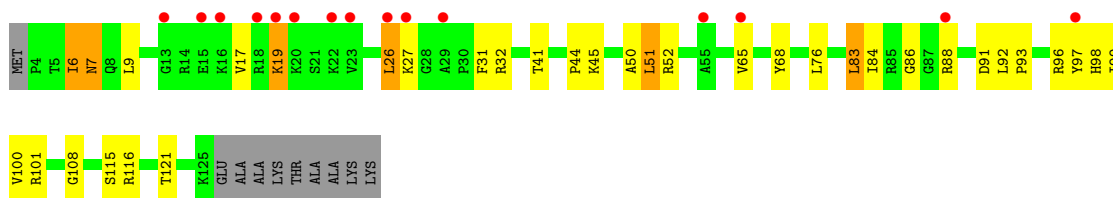
- Molecule 38: 30S ribosomal protein S11



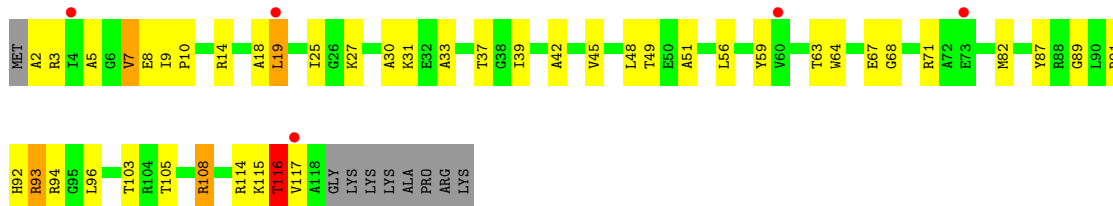
- Molecule 39: 30S ribosomal protein S12



- Molecule 39: 30S ribosomal protein S12

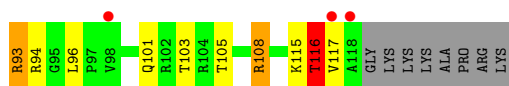


- Molecule 40: 30S ribosomal protein S13



- Molecule 40: 30S ribosomal protein S13





- Molecule 41: 30S ribosomal protein S14



- Molecule 41: 30S ribosomal protein S14



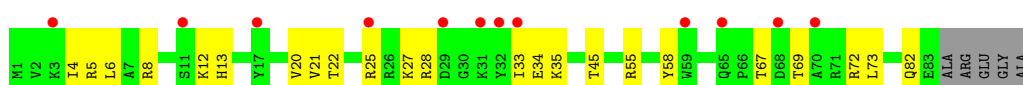
- Molecule 42: 30S ribosomal protein S15



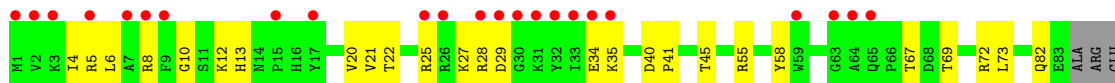
- Molecule 42: 30S ribosomal protein S15



- Molecule 43: 30S ribosomal protein S16



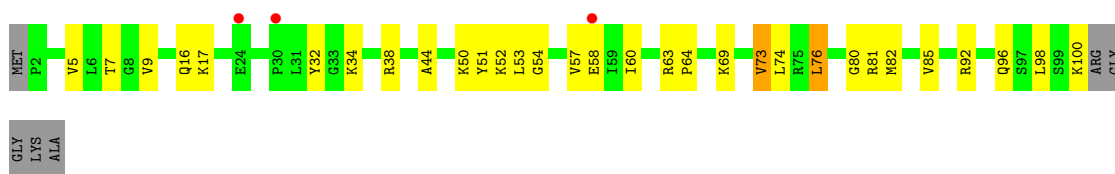
- Molecule 43: 30S ribosomal protein S16



GLY  
ALA

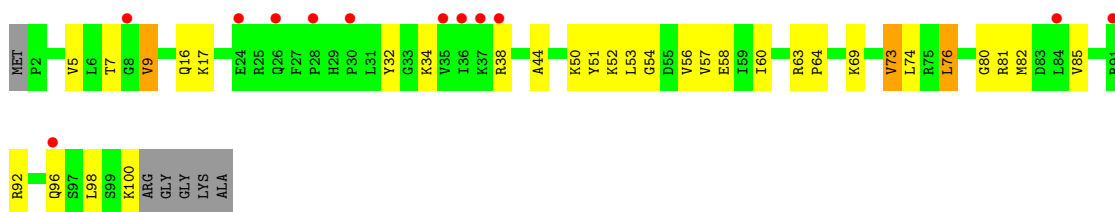
- Molecule 44: 30S ribosomal protein S17

Chain RA: 3% 65% 28% 6%



- Molecule 44: 30S ribosomal protein S17

Chain NC: 11% 64% 28% 6%



- Molecule 45: 30S ribosomal protein S18

Chain SA: 59% 17% 20%



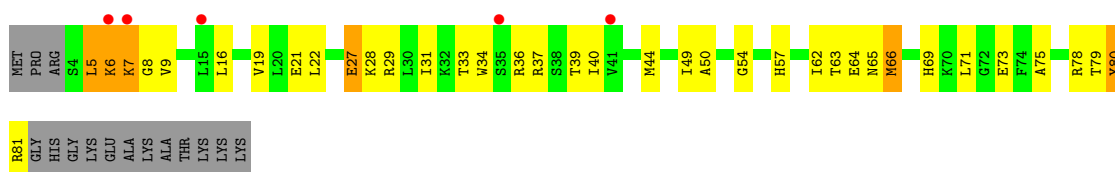
- Molecule 45: 30S ribosomal protein S18

Chain OC: 59% 19% 20%



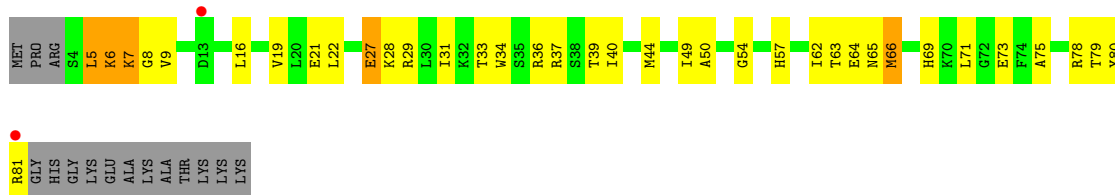
- Molecule 46: 30S ribosomal protein S19

Chain TA: 5% 44% 33% 6% 16%



- Molecule 46: 30S ribosomal protein S19

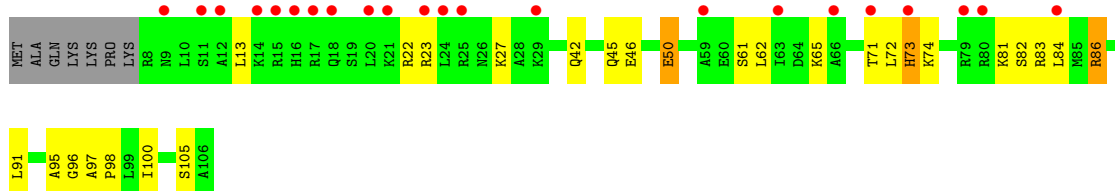
Chain PC: 2% 44% 34% 5% 16%



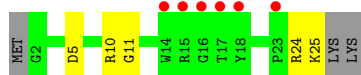
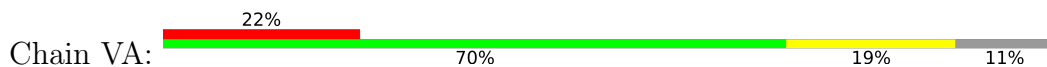
- Molecule 47: 30S ribosomal protein S20



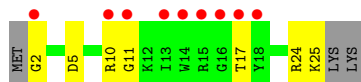
- Molecule 47: 30S ribosomal protein S20



- Molecule 48: 30S ribosomal protein Thx



- Molecule 48: 30S ribosomal protein Thx

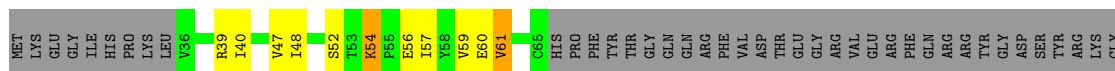


- Molecule 49: 50S ribosomal protein L31



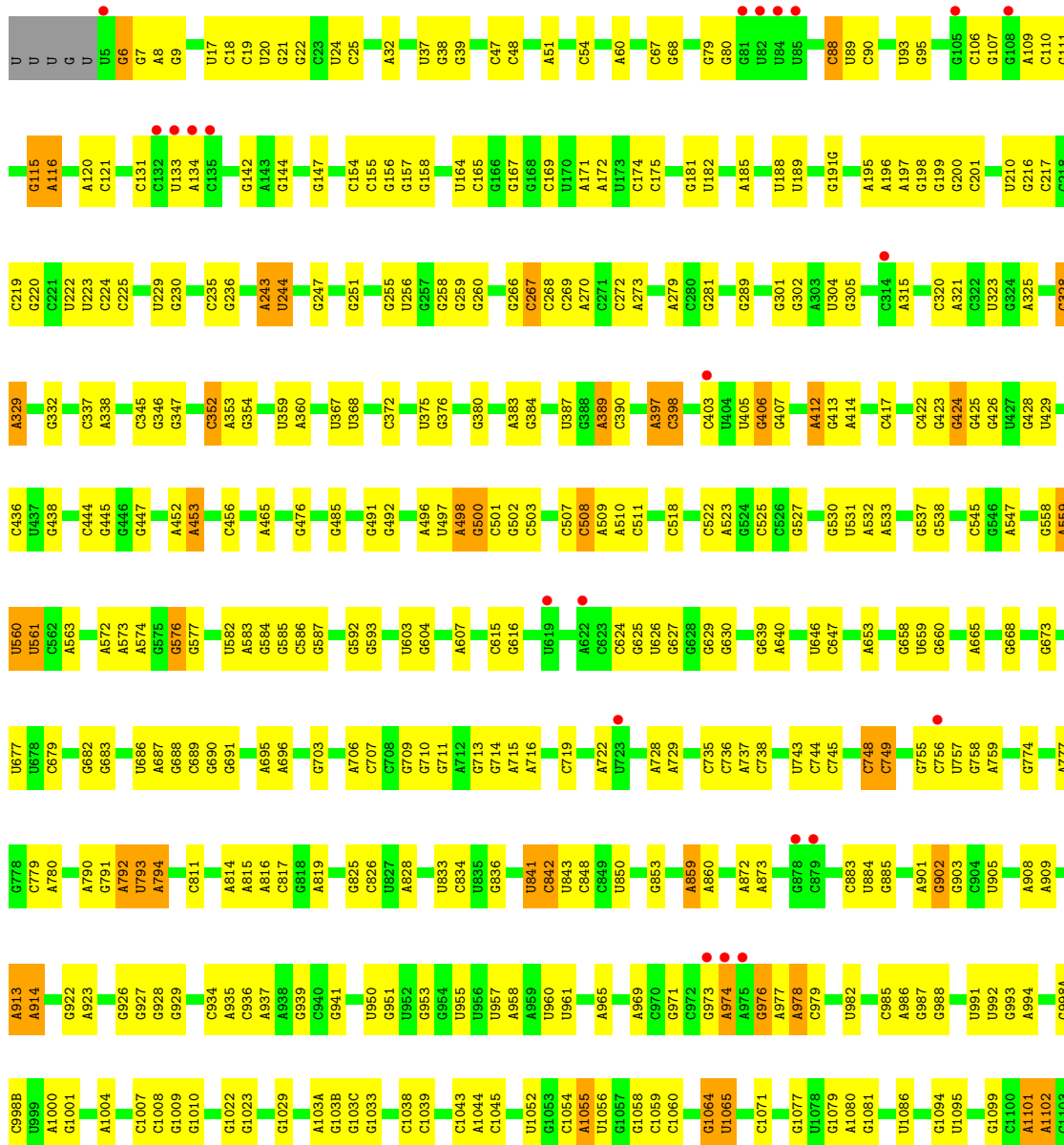
ARG

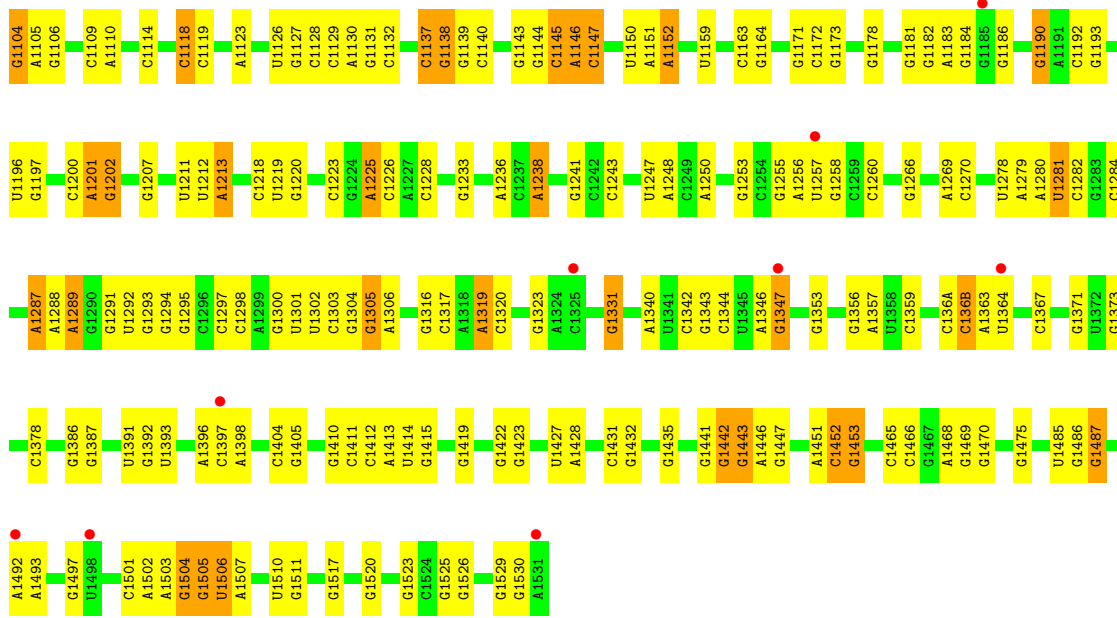
## ● Molecule 49: 50S ribosomal protein L31

Chain TC:  27% 13% 58%

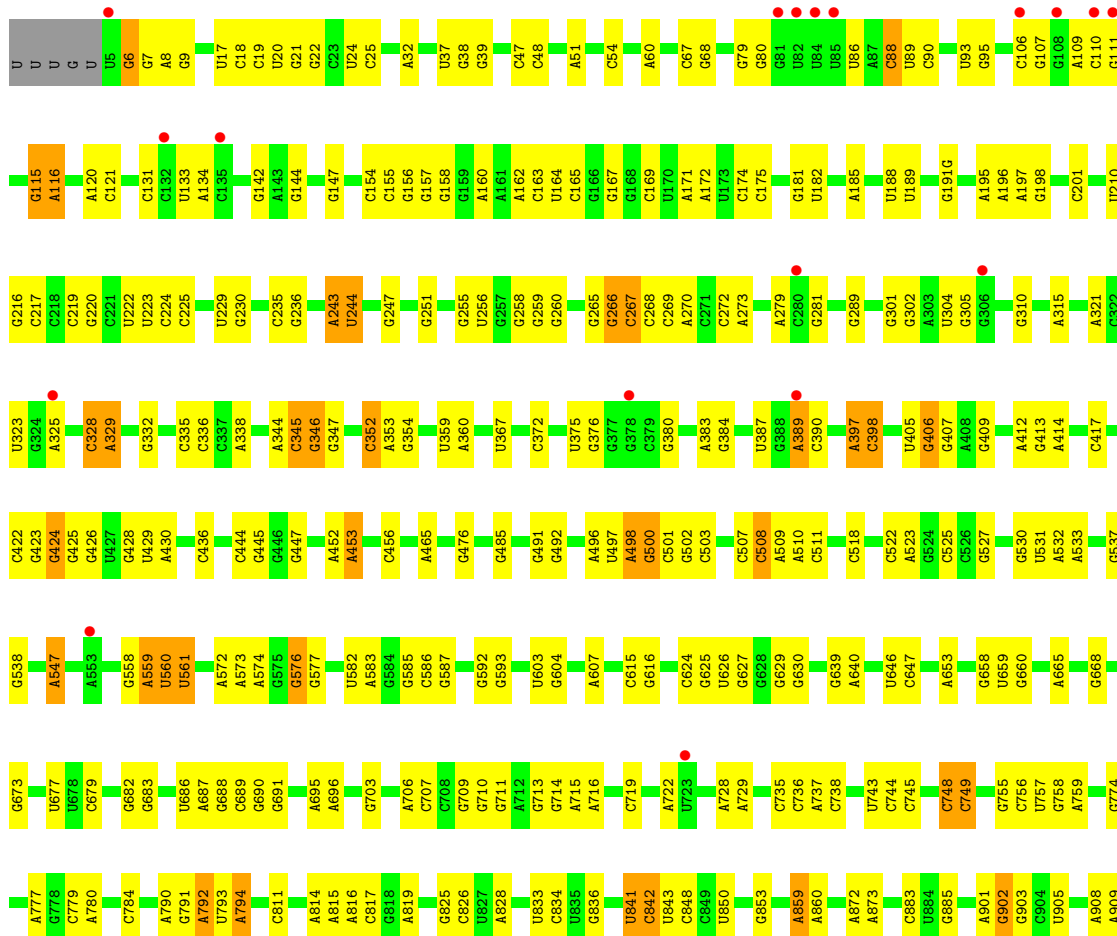
ARG

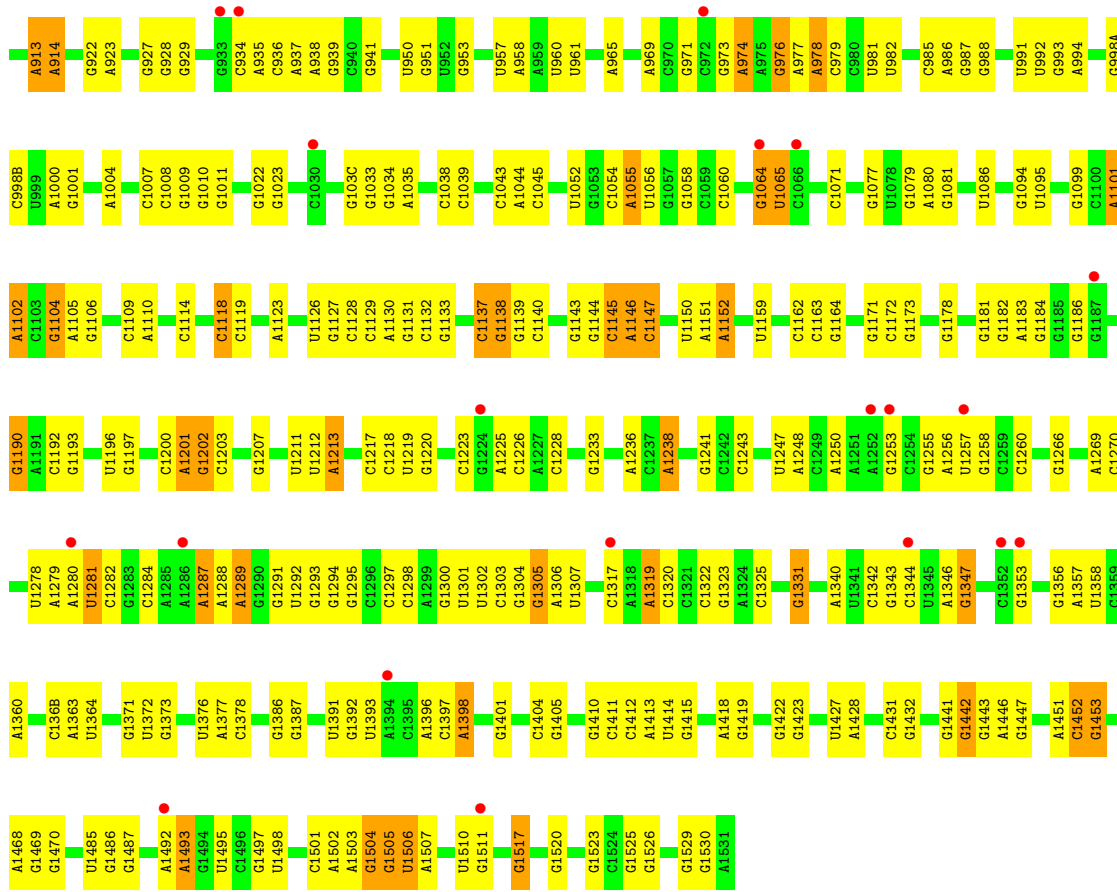
## ● Molecule 50: 16S ribosomal RNA

Chain UC:  2% 62% 33% 5%

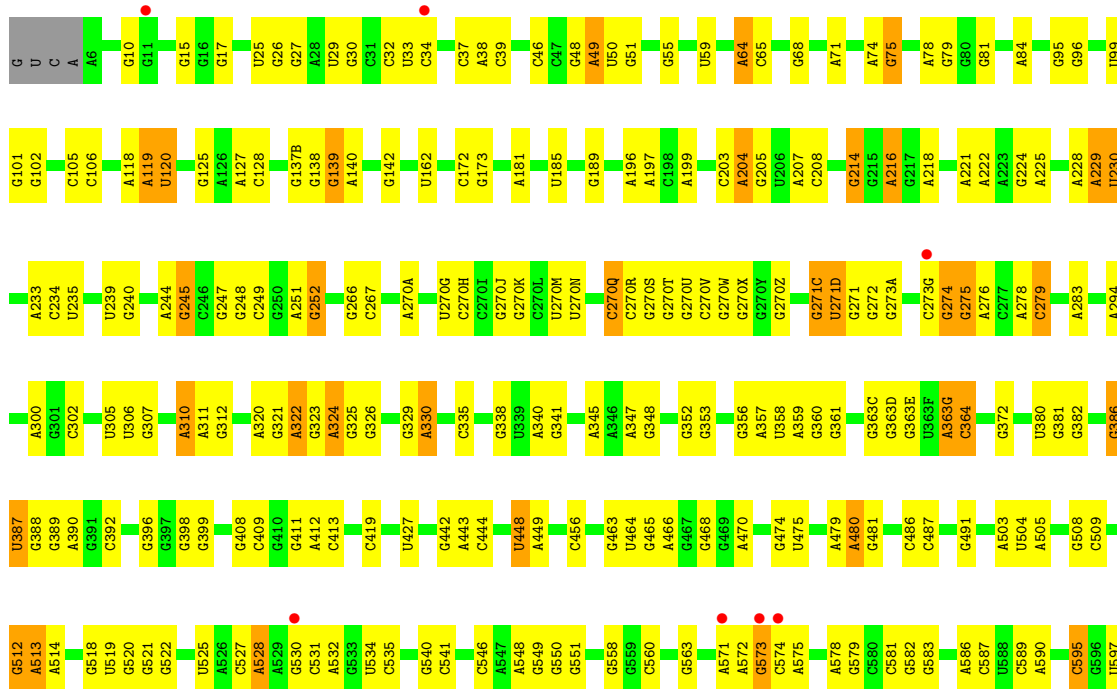


● Molecule 50: 16S ribosomal RNA

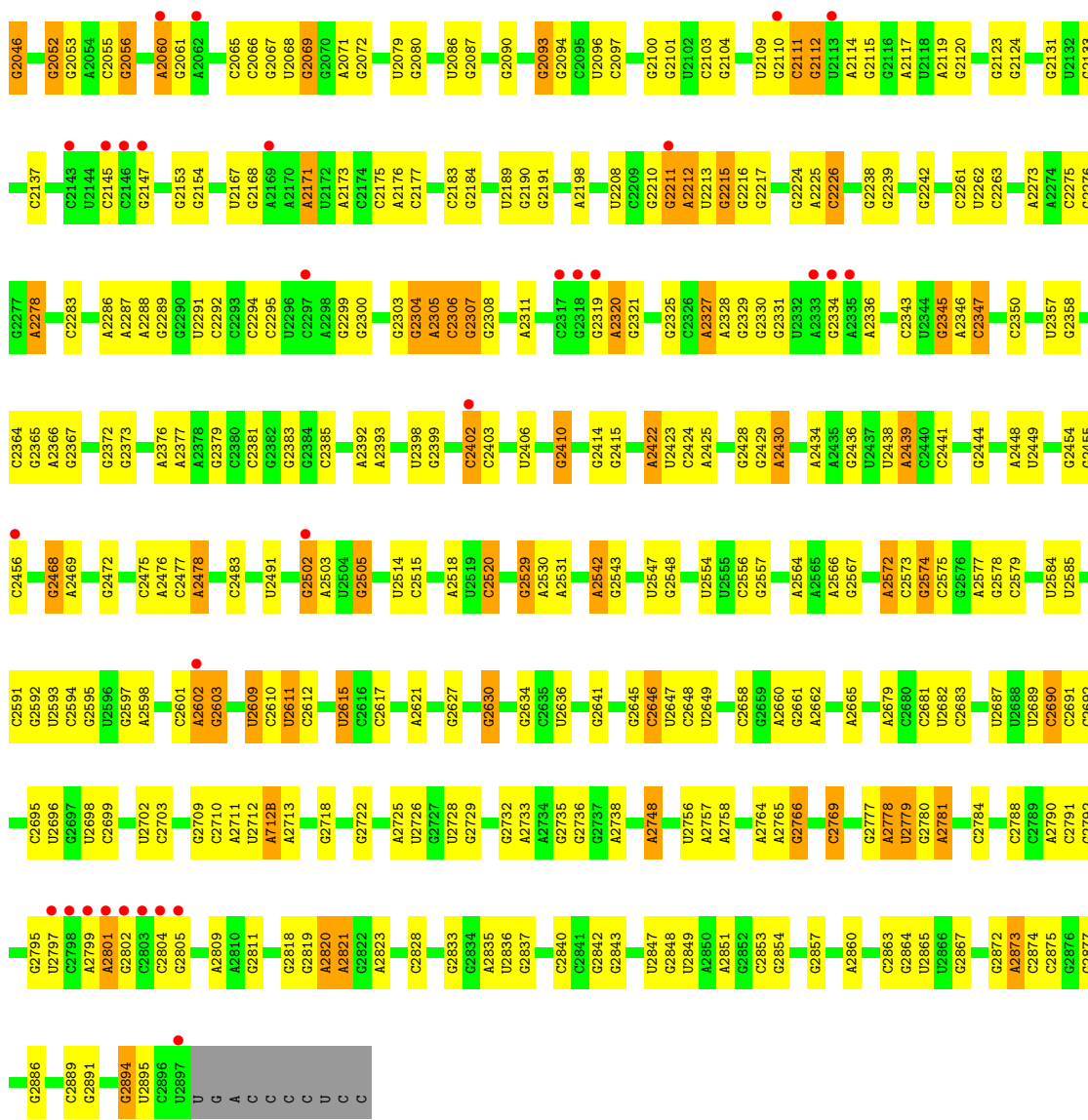


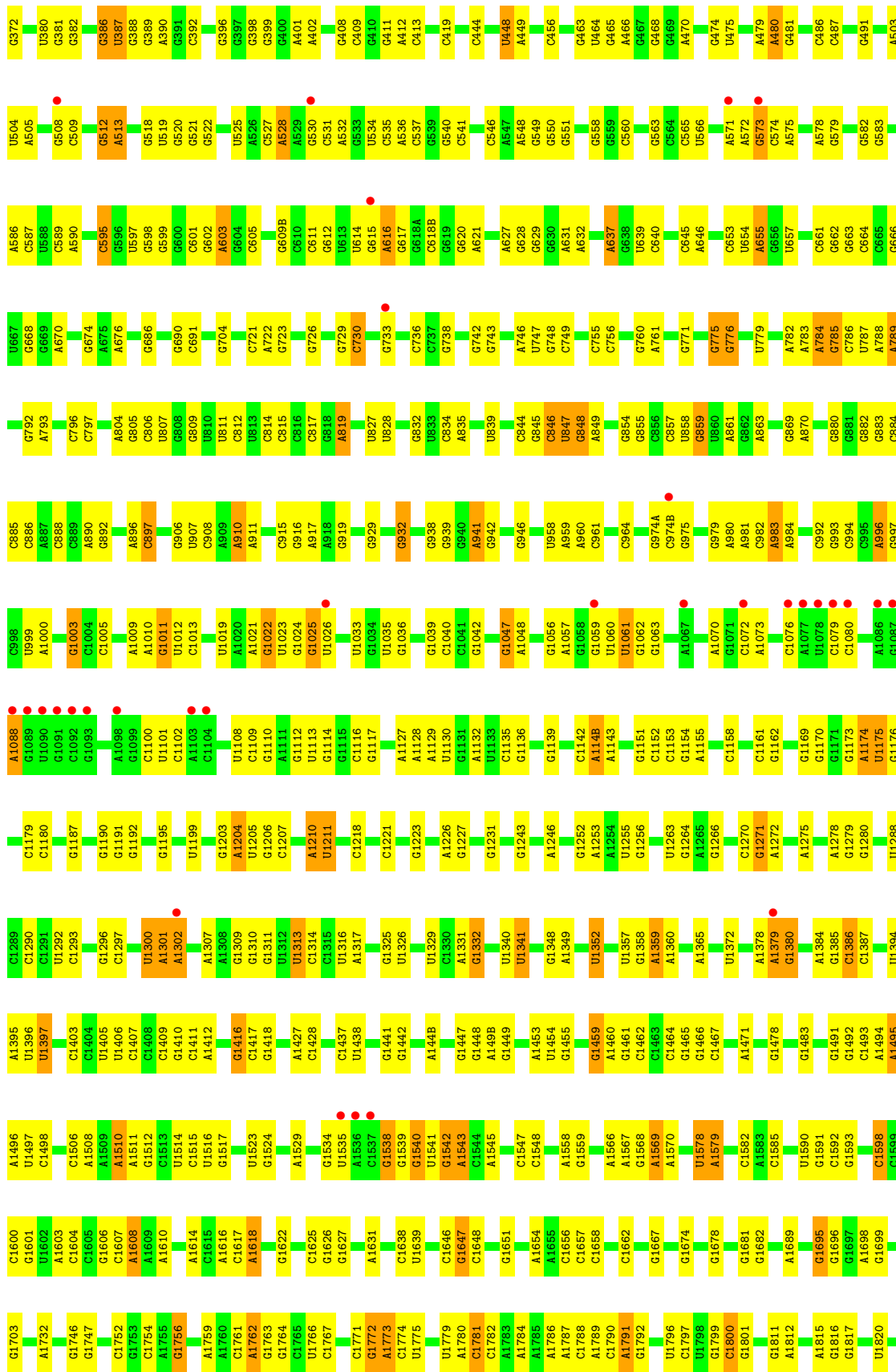


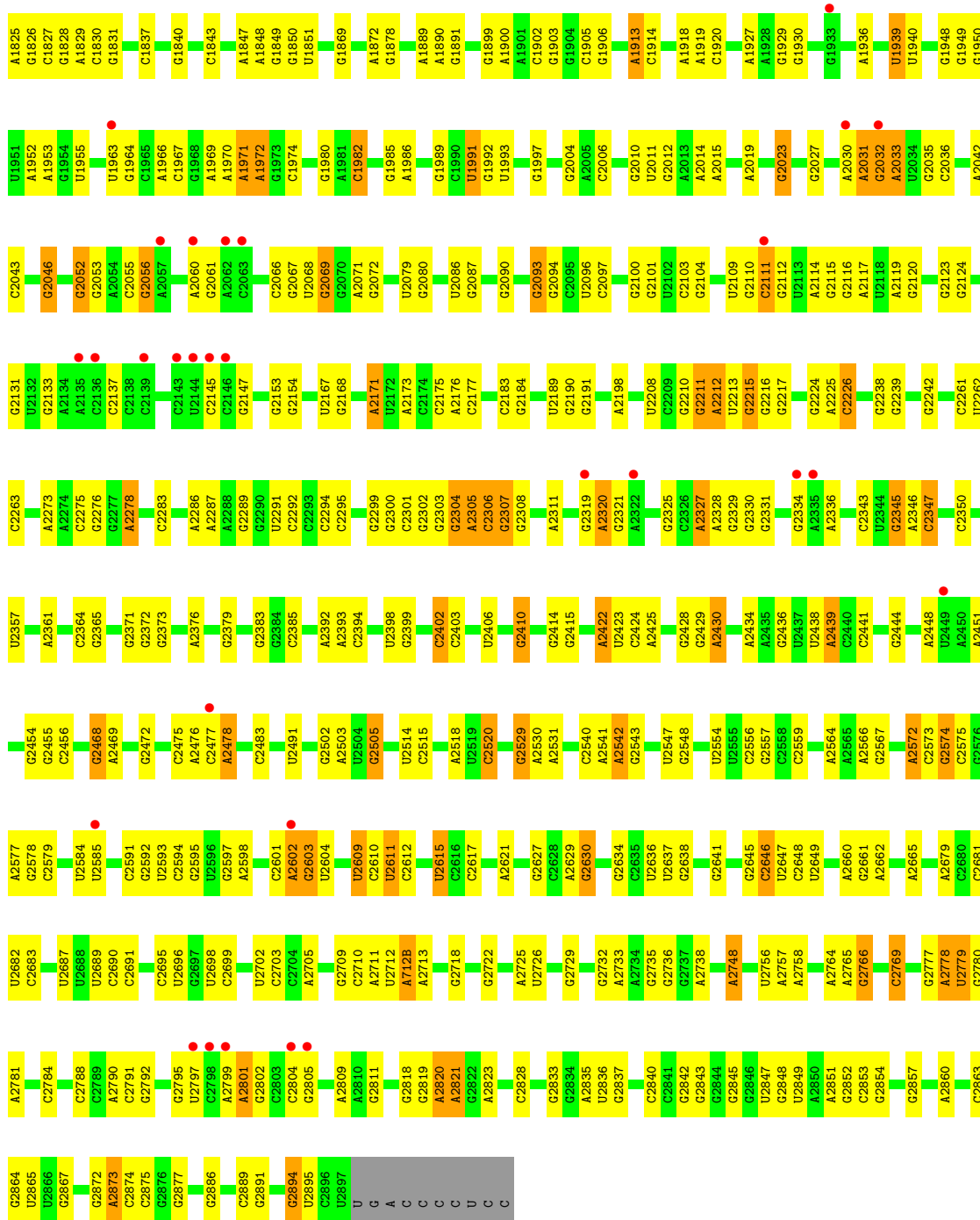
• Molecule 51: 23S ribosomal RNA



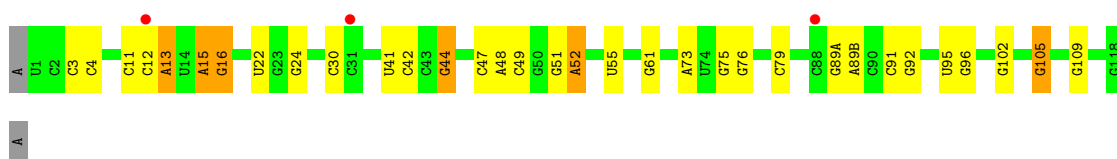
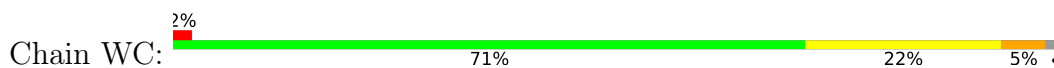
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A685	G686	G690	G691	G704	G721	G722	G723	G726	G729	G730	G732	G733	G736	G746	G747	G755	G756	G760	G761	G775	G776	G779	G782	G783	G784	G785	G786	G787	G788	G789	G792	G793	G804	G805	G806	G807	G808	G809	G810	G811	G812	G813	G814	G815	G816	G817	G818	G819	G820	G821	G827	G828	G829	G830	G831	G837	G838	G839	G840	G845	G846	G853	G854	G855	G856	G857	G858	G859	G860	G861	G862	G863	G869	G870	G874	G875	G880	G881	G882	G883	G884	G885	G886	G887	G888	G889	G890	G892	G896																																																									
C897	G906	G907	G908	G909	G910	G911	G915	G916	G917	G918	G919	G929	G932	G938	G939	G940	G941	G942	G945	G946	G949	G958	G959	G960	G961	G964	G974A	G974B	G975	G979	G980	G981	G982	G983	G985	G986	G987	G988	G989	G992	G993	G994	G995	G996	G999	G1000	G1003	G1004	G1005	G1006	G1009	G1010	G1011	G1012	G1013	G1019	G1020	G1021	G1022	G1023	G1024	G1025	G1026	G1033	G1034	G1035	G1036	G1039	G1040	G1042	G1047	G1048	G1056	G1057	G1060	G1061	G1062	G1063	G1064	G1065	G1066	G1067	G1070	G1071	G1072	G1073	G1074	G1075	G1076	G1077	G1078	G1079	G1080	G1081	G1082	G1083	G1084																																																	
A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1100	A1101	A1102	A1103	A1105	A1106	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1129	A1130	A1131	A1132	A1133	A1135	A1136	A1139	A1142	A1143	A1144	A1151	A1152	A1153	A1154	A1155	A1161	A1162	A1163	A1169	A1170	A1171	A1172	A1173	A1174	A1176	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1100	A1101	A1102	A1103	A1105	A1106	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1129	A1130	A1131	A1132	A1133	A1135	A1136	A1139	A1142	A1143	A1144	A1151	A1152	A1153	A1154	A1155	A1161	A1162	A1163	A1169	A1170	A1171	A1172	A1173	A1174	A1176																																															
C1179	C1180	G1187	G1188	G1189	G1190	G1191	G1192	G1195	G1199	G1203	G1204	G1205	G1210	G1218	G1221	G1223	A1226	G1227	G1231	G1243	A1246	G1252	A1253	A1254	G1256	G1263	G1264	A1265	G1266	G1271	A1272	A1275	A1278	G1279	G1280	U1288	C1289	C1291	U1292	C1293	G1296	U1300	A1301	A1302	A1307	A1308	G1309	G1310	G1311	U1312	U1313	G1314	G1315	U1316	A1317	G1325	U1329	G1332	U1340	U1341	G1348	A1349	U1352	U1357	A1358	A1359	A1360	A1365	U1372	A1378	A1379	G1380	G1381	G1382	C1383	A1384	G1385	G1386	C1387	U1394	A1395	U1396	U1397																																																															
C1403	C1404	U1406	C1407	C1409	C1410	C1411	C1412	G1416	G1417	G1418	A1419	G1423	G1424	G1425	G1426	A1427	C1428	C1437	U1438	G1441	G1442	A1443	G1447	G1448	G1449	A1453	U1454	G1455	G1459	A1460	A1461	A1462	C1463	C1464	G1465	G1466	C1467	A1471	G1478	G1483	G1491	G1492	A1494	A1495	U1497	C1498	U1506	A1508	A1509	A1510	A1511	A1512	A1513	A1514	C1515	U1516	G1517	U1523	G1524	A1529	G1534	U1535	G1538	G1539	U1541	G1542	A1543	C1544	C1547	C1548	A1558	G1559	A1566	A1567	G1568	A1569	A1570	A1571	G1572	G1573	C1574	U1578	A1579	C1582	A1583	C1585	U1590	G1591	C1592																																																									
G1593	C1598	C1599	C1600	G1601	U1602	A1603	C1604	C1605	C1606	C1607	A1608	A1610	A1614	A1615	A1616	C1617	A1618	G1622	G1625	G1626	G1627	A1631	G1638	U1639	C1646	C1647	C1648	G1651	A1654	A1655	C1656	C1657	C1658	C1662	G1674	G1678	G1681	G1682	A1689	U1693	C1694	G1695	G1696	G1697	G1703	G1704	G1705	G1706	G1707	G1708	G1709	G1710	G1711	G1712	G1713	G1714	G1715	G1716	G1717	G1718	G1719	G1720	G1721	G1722	G1723	G1724	G1725	G1726	G1727	G1728	G1729	G1730	G1731	G1732	G1733	G1734	G1735	G1736	G1737	G1738	G1739	G1740	G1741	G1742	G1743	G1744	G1745	G1746	G1747	G1748	G1749	G1750	G1751	G1752	G1753	G1754	G1755	G1756	A1759	A1760	C1761	A1762	G1763	G1764	G1765	G1766	C1767	C1771	A1772	A1773	C1774	U1779	A1780	C1781	C1782	A1783	A1784	A1785	A1786	C1787	A1788	A1789	C1790	A1791	G1792	U1796	C1797	U1798	G1799	G1800	G1801	U1802	A1803	G1804	G1805	G1806	G1807	G1808	G1809	G1810	G1811	G1812	G1813	G1814	A1815	C1816
G1817	U1820	A1825	G1826	C1827	G1828	A1829	G1830	G1831	C1837	G1840	A1847	G1848	G1849	G1850	U1851	G1869	A1872	G1878	A1889	A1890	G1891	G1897	A1900	A1901	A1902	G1903	G1904	C1905	G1906	A1913	C1914	A1918	A1919	C1920	A1927	G1928	G1929	G1930	G1935	A1936	U1939	U1940	G1949	G1950	U1955	U1963	G1964	C1965	C1967	A1970	A1971	A1972	C1973	G1974	G1979	G1980	A1981	C1982	G1985	A1986	G1989	C1990	U1991	G1992	U1993	G1997	G2004	A2005	C2006	G2010	U2011	G2012	A2015	A2019	G2023	G2027	A2030	A2031	G2032	A2033	U2034	G2035	C2036	A2042	C2043																																																													



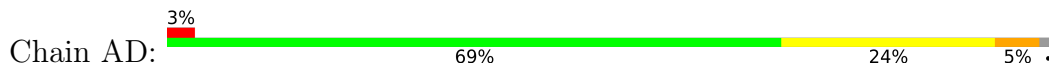




• Molecule 52: 5S ribosomal RNA

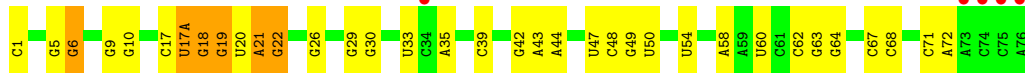


• Molecule 52: 5S ribosomal RNA

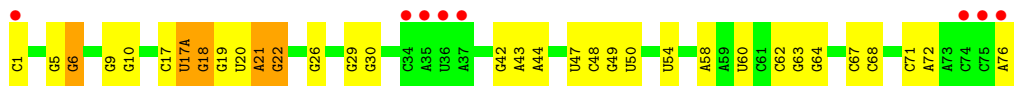


A

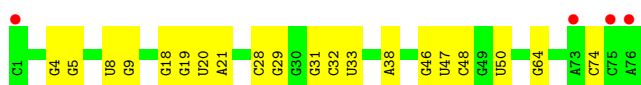
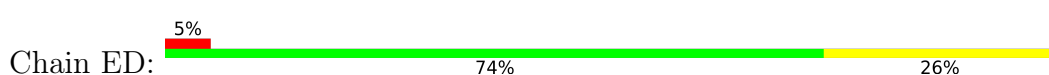
• Molecule 53: tRNA



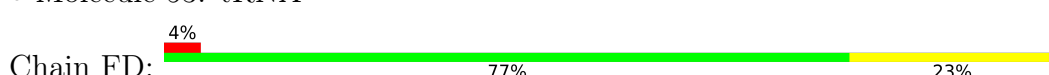
• Molecule 53: tRNA



• Molecule 53: tRNA



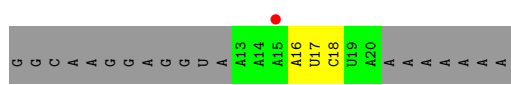
• Molecule 53: tRNA



• Molecule 54: mRNA



• Molecule 54: mRNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.98Å 453.75Å 620.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 3.63 60.00 – 3.63	Depositor EDS
% Data completeness (in resolution range)	99.3 (60.00-3.63) 99.1 (60.00-3.63)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 3.67Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.268 , 0.287 0.281 , 0.299	Depositor DCC
$R_{free}$ test set	6615 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	115.3	Xtrriage
Anisotropy	0.262	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 61.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	295576	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	147.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.34	0/2155	0.75	0/2905
1	WA	0.34	0/2155	0.75	0/2905
2	B	0.32	0/1596	0.78	0/2153
2	XA	0.32	0/1596	0.78	0/2153
3	C	0.31	0/1621	0.78	2/2194 (0.1%)
3	YA	0.33	0/1621	0.79	2/2194 (0.1%)
4	D	0.30	0/1500	0.74	0/2017
4	ZA	0.30	0/1500	0.74	0/2017
5	AB	0.28	0/1356	0.78	2/1834 (0.1%)
5	E	0.28	0/1356	0.78	2/1834 (0.1%)
6	BB	0.30	0/1147	0.72	0/1552
6	F	0.29	0/1147	0.73	0/1552
7	CB	0.35	0/1108	0.84	3/1500 (0.2%)
7	G	0.35	0/1108	0.84	3/1500 (0.2%)
8	DB	0.30	0/1123	0.73	0/1515
8	H	0.29	0/1123	0.74	2/1515 (0.1%)
9	EB	0.32	0/942	0.75	0/1268
9	I	0.31	0/942	0.75	0/1268
10	FB	0.35	0/1131	0.92	2/1504 (0.1%)
10	J	0.34	0/1131	0.92	2/1504 (0.1%)
11	GB	0.29	0/1084	0.73	0/1449
11	K	0.29	0/1084	0.72	0/1449
12	HB	0.32	0/974	0.74	1/1302 (0.1%)
12	L	0.32	0/974	0.74	1/1302 (0.1%)
13	IB	0.27	0/887	0.68	0/1180
13	M	0.26	0/887	0.68	0/1180
14	JB	0.34	0/1157	0.72	0/1544
14	N	0.34	0/1157	0.72	0/1544
15	KB	0.33	0/982	0.74	0/1306
15	O	0.34	0/982	0.74	0/1306
16	LB	0.33	0/790	0.75	2/1057 (0.2%)
16	P	0.31	0/790	0.75	2/1057 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	MB	0.34	0/901	0.78	0/1209
17	Q	0.34	0/901	0.77	0/1209
18	NB	0.32	0/739	0.72	0/993
18	R	0.31	0/739	0.72	0/993
19	OB	0.37	0/788	0.88	2/1051 (0.2%)
19	S	0.36	0/788	0.88	2/1051 (0.2%)
20	PB	0.29	0/1514	0.74	0/2056
20	T	0.29	0/1514	0.74	2/2056 (0.1%)
21	QB	0.31	0/613	0.74	0/816
21	U	0.29	0/613	0.74	0/816
22	RB	0.36	0/701	0.88	2/932 (0.2%)
22	V	0.35	0/701	0.87	2/932 (0.2%)
23	SB	0.35	0/522	0.82	1/690 (0.1%)
23	W	0.34	0/522	0.82	1/690 (0.1%)
24	TB	0.28	0/472	0.81	0/634
24	X	0.28	0/472	0.80	0/634
25	UB	0.36	0/418	0.95	2/567 (0.4%)
25	Y	0.36	0/418	0.95	2/567 (0.4%)
26	VB	0.29	0/387	0.68	0/518
26	Z	0.30	0/387	0.71	0/518
27	AA	0.33	0/426	0.81	2/561 (0.4%)
27	WB	0.36	0/426	0.81	0/561
28	BA	0.33	0/515	0.86	2/679 (0.3%)
28	XB	0.34	0/515	0.85	2/679 (0.3%)
29	CA	0.28	0/1935	0.75	4/2609 (0.2%)
29	YB	0.28	0/1935	0.75	4/2609 (0.2%)
30	DA	0.30	0/1636	0.71	0/2205
30	ZB	0.30	0/1636	0.71	0/2205
31	AC	0.28	0/1733	0.79	5/2318 (0.2%)
31	EA	0.29	0/1733	0.77	3/2318 (0.1%)
32	BC	0.30	0/1171	0.77	0/1576
32	FA	0.31	0/1171	0.78	0/1576
33	CC	0.28	0/856	0.71	0/1154
33	GA	0.28	0/856	0.71	0/1154
34	DC	0.27	0/1276	0.71	0/1709
34	HA	0.28	0/1276	0.71	0/1709
35	EC	0.28	0/1136	0.73	0/1527
35	IA	0.28	0/1136	0.73	0/1527
36	FC	0.30	0/1029	0.71	0/1378
36	JA	0.30	0/1029	0.70	0/1378
37	GC	0.27	0/807	0.73	0/1085
37	KA	0.28	0/807	0.73	0/1085
38	HC	0.29	0/856	0.75	0/1157

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	LA	0.31	0/856	0.74	0/1157
39	IC	0.30	0/972	0.78	0/1301
39	MA	0.30	0/972	0.78	0/1301
40	JC	0.29	0/943	0.76	1/1265 (0.1%)
40	NA	0.29	0/943	0.76	1/1265 (0.1%)
41	KC	0.27	0/501	0.65	0/664
41	OA	0.26	0/501	0.64	0/664
42	LC	0.33	0/745	0.68	0/992
42	PA	0.33	0/745	0.67	0/992
43	MC	0.26	0/716	0.70	0/963
43	QA	0.27	0/716	0.71	0/963
44	NC	0.24	0/836	0.70	0/1117
44	RA	0.24	0/836	0.70	0/1117
45	OC	0.28	0/579	0.69	0/768
45	SA	0.28	0/579	0.70	0/768
46	PC	0.28	0/642	0.72	0/865
46	TA	0.28	0/642	0.73	0/865
47	QC	0.28	0/764	0.73	0/1006
47	UA	0.28	0/764	0.73	0/1006
48	RC	0.25	0/212	0.66	0/277
48	VA	0.25	0/212	0.65	0/277
49	SC	0.33	0/228	0.85	2/309 (0.6%)
49	TC	0.33	0/228	0.85	2/309 (0.6%)
50	UC	0.10	0/36194	0.22	0/56493
50	YC	0.10	0/36194	0.22	0/56493
51	VC	0.13	1/69441 (0.0%)	0.25	0/108408
51	ZC	0.14	1/69441 (0.0%)	0.26	0/108408
52	AD	0.11	0/2853	0.23	0/4451
52	WC	0.10	0/2853	0.22	0/4451
53	BD	0.10	0/1832	0.25	0/2855
53	ED	0.09	0/1832	0.18	0/2855
53	FD	0.09	0/1832	0.18	0/2855
53	XC	0.10	0/1832	0.24	0/2855
54	GD	0.08	0/190	0.13	0/293
54	HD	0.08	0/190	0.13	0/293
All	All	0.20	2/318928 (0.0%)	0.44	70/477172 (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
10	FB	0	2
10	J	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	ZC	1142	C	O3'-P	9.63	1.75	1.61
51	VC	1142	C	O3'-P	9.42	1.75	1.61

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	35	THR	N-CA-C	9.04	119.85	108.19
22	RB	35	THR	N-CA-C	9.01	119.81	108.19
28	BA	62	LEU	CA-C-N	-8.89	110.58	119.56
28	BA	62	LEU	C-N-CA	-8.89	110.58	119.56
28	XB	62	LEU	CA-C-N	-8.63	110.84	119.56

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	FB	51	PHE	Peptide
10	FB	9	ASN	Peptide
10	J	51	PHE	Peptide
10	J	9	ASN	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	A	2105	0	2182	67	0
1	WA	2105	0	2182	68	0
2	B	1563	0	1629	37	0
2	XA	1563	0	1629	35	0
3	C	1586	0	1632	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	YA	1586	0	1632	43	0
4	D	1475	0	1537	45	0
4	ZA	1475	0	1537	46	0
5	AB	1330	0	1407	22	0
5	E	1330	0	1407	22	1
6	BB	1132	0	1220	28	0
6	F	1132	0	1220	20	0
7	CB	1088	0	1138	37	0
7	G	1088	0	1138	35	0
8	DB	1096	0	1168	30	0
8	H	1096	0	1168	28	0
9	EB	932	0	994	31	0
9	I	932	0	994	28	0
10	FB	1114	0	1187	87	0
10	J	1114	0	1187	84	0
11	GB	1064	0	1114	33	0
11	K	1064	0	1114	32	0
12	HB	960	0	1021	33	0
12	L	960	0	1021	33	0
13	IB	877	0	938	12	0
13	M	877	0	938	13	0
14	JB	1143	0	1211	38	0
14	N	1143	0	1211	36	0
15	KB	964	0	1022	36	0
15	O	964	0	1022	39	0
16	LB	779	0	852	22	0
16	P	779	0	852	23	0
17	MB	890	0	951	20	0
17	Q	890	0	951	22	0
18	NB	725	0	778	17	0
18	R	725	0	778	16	0
19	OB	775	0	870	27	0
19	S	775	0	870	24	0
20	PB	1482	0	1507	27	0
20	T	1482	0	1507	29	0
21	QB	605	0	628	21	0
21	U	605	0	628	19	0
22	RB	694	0	764	31	0
22	V	694	0	764	26	0
23	SB	520	0	575	21	0
23	W	520	0	575	20	0
24	TB	467	0	523	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	X	467	0	523	7	0
25	UB	404	0	420	12	0
25	Y	404	0	420	12	0
26	VB	380	0	391	14	0
26	Z	380	0	391	12	0
27	AA	418	0	467	12	0
27	WB	418	0	467	13	0
28	BA	507	0	576	17	0
28	XB	507	0	576	20	0
29	CA	1900	0	1951	38	0
29	YB	1900	0	1951	36	0
30	DA	1612	0	1677	41	0
30	ZB	1612	0	1677	41	0
31	AC	1703	0	1765	41	0
31	EA	1703	0	1764	40	0
32	BC	1155	0	1213	28	0
32	FA	1155	0	1213	30	0
33	CC	843	0	857	20	0
33	GA	843	0	857	20	0
34	DC	1257	0	1296	17	0
34	HA	1257	0	1296	17	0
35	EC	1116	0	1177	22	0
35	IA	1116	0	1177	23	0
36	FC	1011	0	1043	24	0
36	JA	1011	0	1043	23	0
37	GC	794	0	840	22	0
37	KA	794	0	840	23	0
38	HC	842	0	859	23	0
38	LA	842	0	859	22	0
39	IC	956	0	1046	27	0
39	MA	956	0	1046	30	0
40	JC	933	0	992	29	0
40	NA	933	0	992	26	0
41	KC	492	0	531	17	0
41	OA	492	0	529	14	0
42	LC	734	0	771	18	0
42	PA	734	0	771	17	0
43	MC	700	0	720	17	0
43	QA	700	0	720	14	0
44	NC	823	0	893	20	0
44	RA	823	0	893	19	0
45	OC	574	0	644	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	SA	574	0	644	14	0
46	PC	629	0	652	26	0
46	TA	629	0	652	25	0
47	QC	762	0	859	13	0
47	UA	762	0	859	14	0
48	RC	208	0	221	5	0
48	VA	208	0	221	3	0
49	SC	225	0	229	6	0
49	TC	225	0	229	9	0
50	UC	32332	0	16315	330	0
50	YC	32332	0	16314	339	1
51	VC	62000	0	31247	661	0
51	ZC	62000	0	31244	664	0
52	AD	2551	0	1295	22	0
52	WC	2551	0	1295	20	0
53	BD	1640	0	837	21	0
53	ED	1640	0	837	9	0
53	FD	1640	0	837	8	0
53	XC	1640	0	837	22	0
54	GD	170	0	87	1	0
54	HD	170	0	87	2	0
55	A	5	0	0	0	0
55	AA	1	0	0	0	0
55	AC	1	0	0	0	0
55	AD	30	0	0	0	0
55	B	2	0	0	0	0
55	BA	2	0	0	0	0
55	BB	2	0	0	0	0
55	BC	3	0	0	0	0
55	BD	8	0	0	0	0
55	C	3	0	0	0	0
55	CB	1	0	0	0	0
55	D	3	0	0	0	0
55	DB	1	0	0	0	0
55	DC	1	0	0	0	0
55	EA	1	0	0	0	0
55	EB	3	0	0	0	0
55	ED	16	0	0	0	0
55	FA	1	0	0	0	0
55	FB	4	0	0	0	0
55	FC	1	0	0	0	0
55	FD	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	GB	1	0	0	0	0
55	H	2	0	0	0	0
55	HA	2	0	0	0	0
55	HB	2	0	0	0	0
55	HD	1	0	0	0	0
55	I	1	0	0	0	0
55	IB	1	0	0	0	0
55	IC	1	0	0	0	0
55	J	3	0	0	0	0
55	JB	1	0	0	0	0
55	L	1	0	0	0	0
55	LA	4	0	0	0	0
55	LC	1	0	0	0	0
55	MB	1	0	0	0	0
55	N	1	0	0	0	0
55	NB	1	0	0	0	0
55	O	2	0	0	0	0
55	OA	2	0	0	0	0
55	OB	1	0	0	0	0
55	P	2	0	0	0	0
55	PA	2	0	0	0	0
55	Q	1	0	0	0	0
55	QA	1	0	0	0	0
55	QB	2	0	0	0	0
55	RA	1	0	0	0	0
55	RC	1	0	0	0	0
55	SB	1	0	0	0	0
55	UA	2	0	0	0	0
55	UC	264	0	0	0	0
55	V	1	0	0	0	0
55	VC	707	0	0	0	0
55	WA	5	0	0	0	0
55	WB	2	0	0	0	0
55	WC	29	0	0	0	0
55	X	1	0	0	0	0
55	XA	3	0	0	0	0
55	XC	5	0	0	0	0
55	Y	1	0	0	0	0
55	YA	8	0	0	0	0
55	YC	271	0	0	0	0
55	ZC	774	0	0	0	0
56	AC	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	EA	1	0	0	0	0
56	KC	1	0	0	0	0
56	OA	1	0	0	0	0
All	All	295576	0	199105	4009	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 4009 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)
30:ZB:6:HIS:HD2	30:ZB:7:PRO:HD2	1.24	1.00
7:CB:75:SER:HB3	51:ZC:1063:G:H5''	1.55	0.89
32:FA:41:VAL:HG21	32:FA:113:ALA:HA	1.55	0.87
35:IA:102:ARG:HE	35:IA:102:ARG:H	1.23	0.86
35:EC:102:ARG:H	35:EC:102:ARG:HE	1.24	0.86

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:126:PRO:O	50:YC:86:U:O2'[2_455]	2.11	0.09

## 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
1	A	269/271 (99%)	227 (84%)	31 (12%)	11 (4%)	<b>2</b> <b>17</b>
1	WA	269/271 (99%)	228 (85%)	30 (11%)	11 (4%)	<b>2</b> <b>17</b>
2	B	202/206 (98%)	173 (86%)	20 (10%)	9 (4%)	<b>2</b> <b>15</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	XA	202/206 (98%)	173 (86%)	20 (10%)	9 (4%)	2	15
3	C	200/205 (98%)	174 (87%)	19 (10%)	7 (4%)	3	20
3	YA	200/205 (98%)	174 (87%)	19 (10%)	7 (4%)	3	20
4	D	179/182 (98%)	148 (83%)	26 (14%)	5 (3%)	4	22
4	ZA	179/182 (98%)	148 (83%)	26 (14%)	5 (3%)	4	22
5	AB	172/180 (96%)	161 (94%)	10 (6%)	1 (1%)	21	51
5	E	172/180 (96%)	161 (94%)	9 (5%)	2 (1%)	10	38
6	BB	143/148 (97%)	127 (89%)	14 (10%)	2 (1%)	9	34
6	F	143/148 (97%)	127 (89%)	14 (10%)	2 (1%)	9	34
7	CB	145/147 (99%)	113 (78%)	22 (15%)	10 (7%)	1	9
7	G	145/147 (99%)	113 (78%)	22 (15%)	10 (7%)	1	9
8	DB	135/140 (96%)	112 (83%)	20 (15%)	3 (2%)	5	27
8	H	135/140 (96%)	112 (83%)	20 (15%)	3 (2%)	5	27
9	EB	120/122 (98%)	104 (87%)	14 (12%)	2 (2%)	7	31
9	I	120/122 (98%)	104 (87%)	13 (11%)	3 (2%)	4	24
10	FB	144/150 (96%)	93 (65%)	34 (24%)	17 (12%)	0	3
10	J	144/150 (96%)	94 (65%)	34 (24%)	16 (11%)	0	3
11	GB	132/141 (94%)	99 (75%)	24 (18%)	9 (7%)	1	9
11	K	132/141 (94%)	99 (75%)	23 (17%)	10 (8%)	1	7
12	HB	115/118 (98%)	94 (82%)	17 (15%)	4 (4%)	3	20
12	L	115/118 (98%)	95 (83%)	16 (14%)	4 (4%)	3	20
13	IB	108/112 (96%)	99 (92%)	9 (8%)	0	100	100
13	M	108/112 (96%)	99 (92%)	9 (8%)	0	100	100
14	JB	135/146 (92%)	109 (81%)	20 (15%)	6 (4%)	2	15
14	N	135/146 (92%)	109 (81%)	20 (15%)	6 (4%)	2	15
15	KB	115/118 (98%)	105 (91%)	7 (6%)	3 (3%)	4	23
15	O	115/118 (98%)	105 (91%)	8 (7%)	2 (2%)	7	31
16	LB	99/101 (98%)	76 (77%)	18 (18%)	5 (5%)	1	13
16	P	99/101 (98%)	77 (78%)	17 (17%)	5 (5%)	1	13
17	MB	110/113 (97%)	100 (91%)	8 (7%)	2 (2%)	6	30
17	Q	110/113 (97%)	100 (91%)	9 (8%)	1 (1%)	14	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	NB	90/96 (94%)	82 (91%)	8 (9%)	0	100	100
18	R	90/96 (94%)	82 (91%)	8 (9%)	0	100	100
19	OB	98/110 (89%)	69 (70%)	17 (17%)	12 (12%)	0	3
19	S	98/110 (89%)	69 (70%)	17 (17%)	12 (12%)	0	3
20	PB	185/206 (90%)	159 (86%)	21 (11%)	5 (3%)	4	23
20	T	185/206 (90%)	159 (86%)	21 (11%)	5 (3%)	4	23
21	QB	74/85 (87%)	63 (85%)	8 (11%)	3 (4%)	2	17
21	U	74/85 (87%)	63 (85%)	8 (11%)	3 (4%)	2	17
22	RB	86/98 (88%)	62 (72%)	16 (19%)	8 (9%)	0	5
22	V	86/98 (88%)	63 (73%)	15 (17%)	8 (9%)	0	5
23	SB	60/72 (83%)	50 (83%)	7 (12%)	3 (5%)	1	14
23	W	60/72 (83%)	50 (83%)	7 (12%)	3 (5%)	1	14
24	TB	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	6	30
24	X	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	6	30
25	UB	50/60 (83%)	45 (90%)	3 (6%)	2 (4%)	2	17
25	Y	50/60 (83%)	45 (90%)	3 (6%)	2 (4%)	2	17
26	VB	42/54 (78%)	31 (74%)	7 (17%)	4 (10%)	0	5
26	Z	42/54 (78%)	31 (74%)	7 (17%)	4 (10%)	0	5
27	AA	46/49 (94%)	42 (91%)	4 (9%)	0	100	100
27	WB	46/49 (94%)	42 (91%)	4 (9%)	0	100	100
28	BA	61/65 (94%)	47 (77%)	6 (10%)	8 (13%)	0	2
28	XB	61/65 (94%)	47 (77%)	6 (10%)	8 (13%)	0	2
29	CA	232/256 (91%)	195 (84%)	27 (12%)	10 (4%)	2	15
29	YB	232/256 (91%)	195 (84%)	27 (12%)	10 (4%)	2	15
30	DA	204/239 (85%)	172 (84%)	21 (10%)	11 (5%)	1	13
30	ZB	204/239 (85%)	171 (84%)	22 (11%)	11 (5%)	1	13
31	AC	206/209 (99%)	185 (90%)	17 (8%)	4 (2%)	6	29
31	EA	206/209 (99%)	182 (88%)	17 (8%)	7 (3%)	3	20
32	BC	149/162 (92%)	130 (87%)	16 (11%)	3 (2%)	6	28
32	FA	149/162 (92%)	130 (87%)	16 (11%)	3 (2%)	6	28
33	CC	99/101 (98%)	88 (89%)	9 (9%)	2 (2%)	6	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	GA	99/101 (98%)	88 (89%)	9 (9%)	2 (2%)	6	28
34	DC	153/156 (98%)	142 (93%)	9 (6%)	2 (1%)	9	36
34	HA	153/156 (98%)	142 (93%)	10 (6%)	1 (1%)	18	48
35	EC	136/138 (99%)	121 (89%)	13 (10%)	2 (2%)	8	33
35	IA	136/138 (99%)	122 (90%)	12 (9%)	2 (2%)	8	33
36	FC	125/128 (98%)	102 (82%)	20 (16%)	3 (2%)	4	25
36	JA	125/128 (98%)	102 (82%)	20 (16%)	3 (2%)	4	25
37	GC	96/105 (91%)	78 (81%)	15 (16%)	3 (3%)	3	21
37	KA	96/105 (91%)	78 (81%)	15 (16%)	3 (3%)	3	21
38	HC	112/129 (87%)	98 (88%)	8 (7%)	6 (5%)	1	13
38	LA	112/129 (87%)	98 (88%)	8 (7%)	6 (5%)	1	13
39	IC	120/132 (91%)	106 (88%)	12 (10%)	2 (2%)	7	31
39	MA	120/132 (91%)	106 (88%)	12 (10%)	2 (2%)	7	31
40	JC	115/126 (91%)	105 (91%)	9 (8%)	1 (1%)	14	43
40	NA	115/126 (91%)	105 (91%)	9 (8%)	1 (1%)	14	43
41	KC	58/61 (95%)	46 (79%)	12 (21%)	0	100	100
41	OA	58/61 (95%)	49 (84%)	4 (7%)	5 (9%)	0	6
42	LC	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	5	26
42	PA	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	5	26
43	MC	81/88 (92%)	75 (93%)	6 (7%)	0	100	100
43	QA	81/88 (92%)	75 (93%)	6 (7%)	0	100	100
44	NC	97/105 (92%)	84 (87%)	13 (13%)	0	100	100
44	RA	97/105 (92%)	84 (87%)	13 (13%)	0	100	100
45	OC	68/88 (77%)	58 (85%)	8 (12%)	2 (3%)	3	22
45	SA	68/88 (77%)	59 (87%)	7 (10%)	2 (3%)	3	22
46	PC	76/93 (82%)	58 (76%)	14 (18%)	4 (5%)	1	13
46	TA	76/93 (82%)	58 (76%)	13 (17%)	5 (7%)	1	10
47	QC	97/106 (92%)	82 (84%)	10 (10%)	5 (5%)	1	13
47	UA	97/106 (92%)	82 (84%)	8 (8%)	7 (7%)	1	8
48	RC	22/27 (82%)	17 (77%)	5 (23%)	0	100	100
48	VA	22/27 (82%)	17 (77%)	5 (23%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	SC	28/71 (39%)	20 (71%)	4 (14%)	4 (14%)	0	2
49	TC	28/71 (39%)	20 (71%)	4 (14%)	4 (14%)	0	2
All	All	11464/12328 (93%)	9726 (85%)	1312 (11%)	426 (4%)	2	18

5 of 426 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	17	ASP
2	B	129	HIS
3	C	73	ALA
4	D	84	LYS
8	H	149	PRO

### 5.3.2 Protein sidechains [i](#)

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	
1	A	213/213 (100%)	190 (89%)	23 (11%)	6	25
1	WA	213/213 (100%)	190 (89%)	23 (11%)	6	25
2	B	165/166 (99%)	145 (88%)	20 (12%)	5	21
2	XA	165/166 (99%)	145 (88%)	20 (12%)	5	21
3	C	161/162 (99%)	143 (89%)	18 (11%)	6	24
3	YA	161/162 (99%)	143 (89%)	18 (11%)	6	24
4	D	155/156 (99%)	133 (86%)	22 (14%)	3	16
4	ZA	155/156 (99%)	133 (86%)	22 (14%)	3	16
5	AB	144/148 (97%)	134 (93%)	10 (7%)	14	39
5	E	144/148 (97%)	134 (93%)	10 (7%)	14	39
6	BB	122/124 (98%)	107 (88%)	15 (12%)	4	20
6	F	122/124 (98%)	107 (88%)	15 (12%)	4	20
7	CB	111/111 (100%)	100 (90%)	11 (10%)	7	28
7	G	111/111 (100%)	100 (90%)	11 (10%)	7	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	DB	116/119 (98%)	100 (86%)	16 (14%)	3	17
8	H	116/119 (98%)	100 (86%)	16 (14%)	3	17
9	EB	100/100 (100%)	92 (92%)	8 (8%)	11	34
9	I	100/100 (100%)	92 (92%)	8 (8%)	11	34
10	FB	112/116 (97%)	88 (79%)	24 (21%)	1	7
10	J	112/116 (97%)	88 (79%)	24 (21%)	1	7
11	GB	105/111 (95%)	93 (89%)	12 (11%)	5	23
11	K	105/111 (95%)	93 (89%)	12 (11%)	5	23
12	HB	100/101 (99%)	90 (90%)	10 (10%)	7	28
12	L	100/101 (99%)	90 (90%)	10 (10%)	7	28
13	IB	87/88 (99%)	83 (95%)	4 (5%)	24	47
13	M	87/88 (99%)	83 (95%)	4 (5%)	24	47
14	JB	121/128 (94%)	106 (88%)	15 (12%)	4	20
14	N	121/128 (94%)	107 (88%)	14 (12%)	5	22
15	KB	93/94 (99%)	86 (92%)	7 (8%)	12	36
15	O	93/94 (99%)	86 (92%)	7 (8%)	12	36
16	LB	82/82 (100%)	70 (85%)	12 (15%)	3	15
16	P	82/82 (100%)	70 (85%)	12 (15%)	3	15
17	MB	91/92 (99%)	82 (90%)	9 (10%)	7	28
17	Q	91/92 (99%)	82 (90%)	9 (10%)	7	28
18	NB	74/78 (95%)	70 (95%)	4 (5%)	20	44
18	R	74/78 (95%)	70 (95%)	4 (5%)	20	44
19	OB	84/91 (92%)	74 (88%)	10 (12%)	5	21
19	S	84/91 (92%)	74 (88%)	10 (12%)	5	21
20	PB	162/179 (90%)	149 (92%)	13 (8%)	11	34
20	T	162/179 (90%)	149 (92%)	13 (8%)	11	34
21	QB	61/67 (91%)	51 (84%)	10 (16%)	2	13
21	U	61/67 (91%)	52 (85%)	9 (15%)	3	15
22	RB	73/83 (88%)	63 (86%)	10 (14%)	3	17
22	V	73/83 (88%)	63 (86%)	10 (14%)	3	17
23	SB	58/67 (87%)	50 (86%)	8 (14%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	W	58/67 (87%)	50 (86%)	8 (14%)	3	17
24	TB	51/52 (98%)	47 (92%)	4 (8%)	11	35
24	X	51/52 (98%)	47 (92%)	4 (8%)	11	35
25	UB	45/52 (86%)	40 (89%)	5 (11%)	6	24
25	Y	45/52 (86%)	40 (89%)	5 (11%)	6	24
26	VB	43/52 (83%)	37 (86%)	6 (14%)	3	17
26	Z	43/52 (83%)	37 (86%)	6 (14%)	3	17
27	AA	41/42 (98%)	38 (93%)	3 (7%)	13	37
27	WB	41/42 (98%)	38 (93%)	3 (7%)	13	37
28	BA	53/55 (96%)	48 (91%)	5 (9%)	8	30
28	XB	53/55 (96%)	48 (91%)	5 (9%)	8	30
29	CA	202/220 (92%)	185 (92%)	17 (8%)	10	32
29	YB	202/220 (92%)	185 (92%)	17 (8%)	10	32
30	DA	160/188 (85%)	153 (96%)	7 (4%)	25	48
30	ZB	160/188 (85%)	152 (95%)	8 (5%)	22	46
31	AC	180/181 (99%)	170 (94%)	10 (6%)	19	43
31	EA	180/181 (99%)	165 (92%)	15 (8%)	10	33
32	BC	116/123 (94%)	106 (91%)	10 (9%)	10	32
32	FA	116/123 (94%)	106 (91%)	10 (9%)	10	32
33	CC	90/90 (100%)	85 (94%)	5 (6%)	19	43
33	GA	90/90 (100%)	85 (94%)	5 (6%)	19	43
34	DC	126/127 (99%)	120 (95%)	6 (5%)	23	46
34	HA	126/127 (99%)	120 (95%)	6 (5%)	23	46
35	EC	119/119 (100%)	111 (93%)	8 (7%)	15	40
35	IA	119/119 (100%)	111 (93%)	8 (7%)	15	40
36	FC	98/99 (99%)	85 (87%)	13 (13%)	4	18
36	JA	98/99 (99%)	85 (87%)	13 (13%)	4	18
37	GC	88/92 (96%)	78 (89%)	10 (11%)	5	23
37	KA	88/92 (96%)	78 (89%)	10 (11%)	5	23
38	HC	86/99 (87%)	75 (87%)	11 (13%)	4	19
38	LA	86/99 (87%)	75 (87%)	11 (13%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	IC	103/109 (94%)	93 (90%)	10 (10%)	8	29
39	MA	103/109 (94%)	93 (90%)	10 (10%)	8	29
40	JC	94/101 (93%)	85 (90%)	9 (10%)	8	29
40	NA	94/101 (93%)	85 (90%)	9 (10%)	8	29
41	KC	49/50 (98%)	48 (98%)	1 (2%)	48	63
41	OA	49/50 (98%)	46 (94%)	3 (6%)	17	41
42	LC	79/80 (99%)	67 (85%)	12 (15%)	3	14
42	PA	79/80 (99%)	67 (85%)	12 (15%)	3	14
43	MC	72/74 (97%)	68 (94%)	4 (6%)	19	43
43	QA	72/74 (97%)	68 (94%)	4 (6%)	19	43
44	NC	94/97 (97%)	86 (92%)	8 (8%)	10	32
44	RA	94/97 (97%)	86 (92%)	8 (8%)	10	32
45	OC	61/77 (79%)	55 (90%)	6 (10%)	7	29
45	SA	61/77 (79%)	55 (90%)	6 (10%)	7	29
46	PC	69/80 (86%)	62 (90%)	7 (10%)	7	27
46	TA	69/80 (86%)	62 (90%)	7 (10%)	7	27
47	QC	76/82 (93%)	70 (92%)	6 (8%)	11	35
47	UA	76/82 (93%)	70 (92%)	6 (8%)	11	35
48	RC	19/22 (86%)	19 (100%)	0	100	100
48	VA	19/22 (86%)	19 (100%)	0	100	100
49	SC	27/63 (43%)	26 (96%)	1 (4%)	30	52
49	TC	27/63 (43%)	26 (96%)	1 (4%)	30	52
All	All	9662/10204 (95%)	8706 (90%)	956 (10%)	7	28

5 of 956 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	SA	84	LYS
38	HC	80	VAL
6	BB	4	ILE
37	GC	75	ILE
46	PC	39	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
26	VB	46	HIS
42	LC	53	HIS
30	ZB	6	HIS
32	BC	141	GLN
47	QC	75	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	UC	1503/1509 (99%)	205 (13%)	15 (0%)
50	YC	1503/1509 (99%)	205 (13%)	15 (0%)
51	VC	2878/2893 (99%)	449 (15%)	18 (0%)
51	ZC	2878/2893 (99%)	448 (15%)	17 (0%)
52	AD	118/121 (97%)	11 (9%)	0
52	WC	118/121 (97%)	11 (9%)	0
53	BD	76/77 (98%)	12 (15%)	3 (3%)
53	ED	76/77 (98%)	8 (10%)	0
53	FD	76/77 (98%)	8 (10%)	0
53	XC	76/77 (98%)	12 (15%)	3 (3%)
54	GD	7/27 (25%)	1 (14%)	0
54	HD	7/27 (25%)	1 (14%)	0
All	All	9316/9408 (99%)	1371 (14%)	71 (0%)

5 of 1371 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	UC	6	G
50	UC	8	A
50	UC	9	G
50	UC	32	A
50	UC	39	G

5 of 71 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
51	ZC	775	G
51	ZC	1022	G
51	ZC	2225	A
51	VC	1210	A
51	VC	1022	G

## 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 2222 ligands modelled in this entry, 2222 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
51	ZC	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	ZC	1142:C	O3'	114(B):A	P	1.75

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	271/271 (100%)	0.45	13 (4%) 35 22	77, 103, 124, 137	0
1	WA	271/271 (100%)	0.44	13 (4%) 35 22	65, 91, 109, 116	0
2	B	204/206 (99%)	0.31	5 (2%) 58 35	89, 129, 158, 168	0
2	XA	204/206 (99%)	0.35	6 (2%) 53 31	78, 109, 136, 144	0
3	C	202/205 (98%)	0.15	2 (0%) 79 54	80, 116, 144, 151	0
3	YA	202/205 (98%)	0.07	0 100 100	66, 100, 127, 140	0
4	D	181/182 (99%)	0.34	6 (3%) 49 29	174, 191, 207, 214	0
4	ZA	181/182 (99%)	0.15	4 (2%) 62 37	144, 163, 186, 199	0
5	AB	174/180 (96%)	0.15	3 (1%) 69 42	113, 134, 153, 164	0
5	E	174/180 (96%)	0.33	9 (5%) 33 20	198, 228, 258, 267	0
6	BB	145/148 (97%)	0.52	15 (10%) 12 11	101, 174, 197, 202	0
6	F	145/148 (97%)	0.73	15 (10%) 12 11	128, 191, 205, 209	0
7	CB	147/147 (100%)	0.89	15 (10%) 12 11	303, 345, 363, 370	0
7	G	147/147 (100%)	0.59	8 (5%) 31 19	327, 363, 391, 395	0
8	DB	137/140 (97%)	0.38	3 (2%) 62 37	89, 108, 131, 136	0
8	H	137/140 (97%)	0.44	4 (2%) 53 31	111, 132, 150, 154	0
9	EB	122/122 (100%)	0.41	2 (1%) 70 44	86, 105, 120, 131	0
9	I	122/122 (100%)	0.33	3 (2%) 58 35	97, 117, 131, 135	0
10	FB	146/150 (97%)	0.88	21 (14%) 6 6	72, 119, 149, 159	0
10	J	146/150 (97%)	0.69	13 (8%) 15 12	92, 141, 171, 179	0
11	GB	134/141 (95%)	1.09	21 (15%) 5 5	126, 143, 167, 205	0
11	K	134/141 (95%)	0.67	12 (8%) 15 11	134, 163, 188, 227	0
12	HB	117/118 (99%)	0.53	5 (4%) 40 23	81, 100, 124, 130	0
12	L	117/118 (99%)	0.66	6 (5%) 33 21	96, 115, 132, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	IB	110/112 (98%)	0.58	8 (7%) 21 15	135, 150, 160, 170	0
13	M	110/112 (98%)	0.40	6 (5%) 30 19	157, 177, 190, 195	0
14	JB	137/146 (93%)	0.42	11 (8%) 18 13	104, 124, 183, 205	0
14	N	137/146 (93%)	0.29	6 (4%) 39 23	118, 134, 176, 189	0
15	KB	117/118 (99%)	0.44	6 (5%) 33 21	75, 95, 118, 126	0
15	O	117/118 (99%)	0.41	6 (5%) 33 21	94, 121, 150, 164	0
16	LB	101/101 (100%)	0.37	3 (2%) 52 31	79, 119, 140, 154	0
16	P	101/101 (100%)	0.03	3 (2%) 52 31	96, 137, 157, 170	0
17	MB	112/113 (99%)	0.23	1 (0%) 81 57	72, 87, 126, 157	0
17	Q	112/113 (99%)	0.24	2 (1%) 67 41	85, 98, 133, 160	0
18	NB	92/96 (95%)	0.27	3 (3%) 49 29	78, 91, 116, 126	0
18	R	92/96 (95%)	0.44	4 (4%) 40 23	107, 118, 137, 142	0
19	OB	100/110 (90%)	0.77	10 (10%) 12 11	94, 108, 172, 189	0
19	S	100/110 (90%)	1.23	21 (21%) 2 3	109, 127, 180, 189	0
20	PB	187/206 (90%)	0.14	2 (1%) 78 53	133, 167, 208, 246	0
20	T	187/206 (90%)	0.08	4 (2%) 63 38	157, 196, 230, 264	0
21	QB	76/85 (89%)	0.75	4 (5%) 32 20	100, 108, 134, 147	0
21	U	76/85 (89%)	0.48	3 (3%) 43 26	122, 135, 155, 182	0
22	RB	88/98 (89%)	1.10	17 (19%) 3 3	80, 103, 135, 148	0
22	V	88/98 (89%)	1.12	18 (20%) 2 3	93, 116, 154, 164	0
23	SB	62/72 (86%)	0.42	5 (8%) 18 13	87, 107, 126, 135	0
23	W	62/72 (86%)	0.55	3 (4%) 35 22	120, 138, 156, 172	0
24	TB	59/60 (98%)	0.56	3 (5%) 33 21	90, 108, 140, 148	0
24	X	59/60 (98%)	0.52	1 (1%) 69 42	106, 123, 144, 154	0
25	UB	52/60 (86%)	0.68	7 (13%) 7 7	77, 98, 141, 152	0
25	Y	52/60 (86%)	0.72	7 (13%) 7 7	91, 117, 148, 156	0
26	VB	44/54 (81%)	0.76	5 (11%) 10 9	245, 251, 259, 267	0
26	Z	44/54 (81%)	1.08	7 (15%) 5 5	238, 256, 273, 278	0
27	AA	48/49 (97%)	0.64	3 (6%) 26 17	80, 86, 105, 120	0
27	WB	48/49 (97%)	0.61	4 (8%) 17 12	68, 72, 91, 103	0
28	BA	63/65 (96%)	1.29	11 (17%) 4 4	102, 115, 155, 169	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	XB	63/65 (96%)	1.21	13 (20%) 2 3	92, 102, 143, 159	0
29	CA	234/256 (91%)	0.18	5 (2%) 63 38	163, 189, 211, 222	0
29	YB	234/256 (91%)	0.14	4 (1%) 69 42	186, 215, 233, 245	0
30	DA	206/239 (86%)	0.13	4 (1%) 66 40	162, 177, 204, 208	0
30	ZB	206/239 (86%)	0.24	10 (4%) 35 21	174, 199, 226, 235	0
31	AC	208/209 (99%)	0.63	13 (6%) 26 17	165, 187, 203, 211	0
31	EA	208/209 (99%)	0.44	10 (4%) 35 22	130, 146, 157, 167	0
32	BC	151/162 (93%)	0.44	7 (4%) 37 22	151, 172, 185, 197	0
32	FA	151/162 (93%)	0.27	5 (3%) 49 29	127, 144, 158, 185	0
33	CC	101/101 (100%)	0.12	0 100 100	141, 153, 167, 190	0
33	GA	101/101 (100%)	0.03	1 (0%) 79 54	144, 159, 172, 186	0
34	DC	155/156 (99%)	0.15	1 (0%) 85 65	174, 190, 201, 204	0
34	HA	155/156 (99%)	0.15	5 (3%) 50 30	167, 180, 192, 199	0
35	EC	138/138 (100%)	0.40	4 (2%) 53 31	149, 174, 191, 195	0
35	IA	138/138 (100%)	0.25	4 (2%) 53 31	126, 150, 168, 172	0
36	FC	127/128 (99%)	0.79	18 (14%) 6 6	167, 221, 232, 239	0
36	JA	127/128 (99%)	0.88	20 (15%) 5 5	165, 212, 230, 235	0
37	GC	98/105 (93%)	0.98	19 (19%) 3 3	184, 239, 262, 265	0
37	KA	98/105 (93%)	0.86	12 (12%) 8 8	178, 206, 216, 220	0
38	HC	114/129 (88%)	0.38	6 (5%) 32 20	127, 148, 161, 168	0
38	LA	114/129 (88%)	0.38	6 (5%) 32 20	124, 146, 157, 168	0
39	IC	122/132 (92%)	0.94	15 (12%) 8 8	134, 150, 167, 178	0
39	MA	122/132 (92%)	0.42	8 (6%) 24 16	119, 133, 142, 165	0
40	JC	117/126 (92%)	0.39	6 (5%) 33 21	163, 202, 219, 224	0
40	NA	117/126 (92%)	0.50	5 (4%) 40 23	175, 213, 231, 234	0
41	KC	60/61 (98%)	0.90	6 (10%) 12 11	182, 196, 206, 211	0
41	OA	60/61 (98%)	0.92	5 (8%) 17 12	173, 184, 204, 207	0
42	LC	88/89 (98%)	0.48	3 (3%) 48 28	124, 150, 169, 176	0
42	PA	88/89 (98%)	0.44	3 (3%) 48 28	125, 143, 159, 165	0
43	MC	83/88 (94%)	1.52	23 (27%) 1 1	174, 199, 220, 244	0
43	QA	83/88 (94%)	0.99	12 (14%) 6 6	128, 136, 157, 186	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	NC	99/105 (94%)	0.82	12 (12%) 8 8	124, 150, 162, 168	0
44	RA	99/105 (94%)	0.26	3 (3%) 52 31	115, 130, 137, 143	0
45	OC	70/88 (79%)	-0.06	0 100 100	146, 161, 181, 183	0
45	SA	70/88 (79%)	0.16	0 100 100	142, 159, 180, 183	0
46	PC	78/93 (83%)	0.26	2 (2%) 57 34	188, 203, 212, 213	0
46	TA	78/93 (83%)	0.38	5 (6%) 25 17	197, 218, 226, 228	0
47	QC	99/106 (93%)	1.16	22 (22%) 2 2	167, 185, 204, 207	0
47	UA	99/106 (93%)	0.75	14 (14%) 6 6	128, 144, 164, 166	0
48	RC	24/27 (88%)	1.52	9 (37%) 1 1	191, 201, 218, 233	0
48	VA	24/27 (88%)	1.30	6 (25%) 2 2	191, 197, 210, 222	0
49	SC	30/71 (42%)	-0.05	0 100 100	228, 232, 244, 245	0
49	TC	30/71 (42%)	-0.03	0 100 100	260, 274, 286, 287	0
50	UC	1504/1509 (99%)	0.09	31 (2%) 63 38	95, 145, 230, 315	0
50	YC	1504/1509 (99%)	0.24	38 (2%) 58 35	101, 175, 259, 344	0
51	VC	2879/2893 (99%)	0.01	74 (2%) 57 34	76, 116, 271, 416	0
51	ZC	2879/2893 (99%)	-0.05	66 (2%) 61 37	57, 98, 250, 374	0
52	AD	119/121 (98%)	-0.03	4 (3%) 48 28	111, 143, 163, 192	0
52	WC	119/121 (98%)	0.16	3 (2%) 58 35	124, 181, 214, 219	0
53	BD	77/77 (100%)	0.28	8 (10%) 11 11	232, 277, 322, 329	0
53	ED	77/77 (100%)	-0.03	4 (5%) 33 20	147, 184, 203, 257	0
53	FD	77/77 (100%)	0.03	3 (3%) 43 26	143, 173, 192, 240	0
53	XC	77/77 (100%)	0.25	5 (6%) 25 16	207, 268, 290, 301	0
54	GD	8/27 (29%)	1.01	0 100 100	138, 198, 252, 253	0
54	HD	8/27 (29%)	0.92	1 (12%) 8 8	144, 202, 243, 244	0
All	All	20988/21736 (96%)	0.28	961 (4%) 37 22	57, 140, 248, 416	0

The worst 5 of 961 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	NC	37	LYS	12.1
4	D	74	LYS	8.7
11	GB	10	ARG	8.1
51	ZC	1077	A	7.9
10	J	50	ARG	7.6

## 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, 95<sup>th</sup> 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	UC	1731	1/1	-0.59	0.30	200,200,200,200	0
55	MG	VC	3096	1/1	-0.53	0.27	207,207,207,207	0
55	MG	YC	1652	1/1	-0.50	0.22	196,196,196,196	0
55	MG	YC	1646	1/1	-0.44	0.18	177,177,177,177	0
55	MG	WC	205	1/1	-0.44	0.21	185,185,185,185	0
55	MG	VC	3376	1/1	-0.41	0.11	200,200,200,200	0
55	MG	BD	103	1/1	-0.37	0.10	218,218,218,218	0
55	MG	UC	1695	1/1	-0.26	0.20	197,197,197,197	0
55	MG	CB	201	1/1	-0.23	0.13	222,222,222,222	0
55	MG	UC	1760	1/1	-0.23	0.35	146,146,146,146	0
55	MG	YC	1741	1/1	-0.23	0.16	219,219,219,219	0
55	MG	UC	1783	1/1	-0.23	0.15	242,242,242,242	0
55	MG	YC	1773	1/1	-0.22	0.17	232,232,232,232	0
55	MG	ZC	3224	1/1	-0.22	0.19	222,222,222,222	0
55	MG	ZC	3349	1/1	-0.22	0.16	270,270,270,270	0
55	MG	UC	1754	1/1	-0.22	0.14	275,275,275,275	0
55	MG	BD	105	1/1	-0.21	0.17	223,223,223,223	0
55	MG	YC	1617	1/1	-0.18	0.33	175,175,175,175	0
55	MG	YC	1625	1/1	-0.16	0.39	121,121,121,121	0
55	MG	FD	102	1/1	-0.14	0.30	169,169,169,169	0
55	MG	ZC	3384	1/1	-0.13	0.22	136,136,136,136	0
55	MG	UC	1712	1/1	-0.12	0.17	212,212,212,212	0
55	MG	VC	3132	1/1	-0.11	0.13	181,181,181,181	0
55	MG	YC	1640	1/1	-0.09	0.25	155,155,155,155	0
55	MG	YC	1692	1/1	-0.08	0.26	178,178,178,178	0
55	MG	YC	1620	1/1	-0.07	0.21	153,153,153,153	0
55	MG	VC	3489	1/1	-0.06	0.15	238,238,238,238	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	ZC	3680	1/1	-0.05	0.23	123,123,123,123	0
55	MG	UC	1773	1/1	-0.05	0.40	158,158,158,158	0
55	MG	BD	104	1/1	-0.04	0.12	253,253,253,253	0
55	MG	UC	1696	1/1	-0.04	0.28	159,159,159,159	0
55	MG	OA	103	1/1	-0.04	0.37	169,169,169,169	0
55	MG	VC	3440	1/1	-0.03	0.18	287,287,287,287	0
55	MG	UC	1643	1/1	-0.03	0.21	170,170,170,170	0
55	MG	UC	1737	1/1	-0.02	0.12	211,211,211,211	0
55	MG	ZC	3360	1/1	-0.02	0.25	193,193,193,193	0
55	MG	D	201	1/1	-0.01	0.17	178,178,178,178	0
55	MG	BD	101	1/1	-0.01	0.18	244,244,244,244	0
55	MG	UC	1676	1/1	-0.01	0.27	128,128,128,128	0
55	MG	YC	1659	1/1	0.00	0.19	194,194,194,194	0
55	MG	UC	1846	1/1	0.00	0.07	227,227,227,227	0
55	MG	YC	1738	1/1	-0.00	0.15	144,144,144,144	0
55	MG	VC	3480	1/1	0.01	0.21	151,151,151,151	0
55	MG	VC	3190	1/1	0.01	0.18	159,159,159,159	0
55	MG	YC	1769	1/1	0.03	0.23	159,159,159,159	0
55	MG	XC	104	1/1	0.03	0.16	251,251,251,251	0
55	MG	ZC	3761	1/1	0.05	0.10	197,197,197,197	0
55	MG	VC	3231	1/1	0.05	0.29	119,119,119,119	0
55	MG	UC	1604	1/1	0.05	0.34	151,151,151,151	0
55	MG	VC	3381	1/1	0.06	0.08	130,130,130,130	0
55	MG	YC	1762	1/1	0.07	0.18	192,192,192,192	0
55	MG	ED	109	1/1	0.07	0.13	177,177,177,177	0
55	MG	UC	1697	1/1	0.07	0.28	136,136,136,136	0
55	MG	FD	108	1/1	0.07	0.19	153,153,153,153	0
55	MG	ZC	3737	1/1	0.08	0.13	204,204,204,204	0
55	MG	YC	1680	1/1	0.08	0.25	148,148,148,148	0
55	MG	YC	1657	1/1	0.08	0.13	179,179,179,179	0
55	MG	ZC	3218	1/1	0.09	0.23	136,136,136,136	0
55	MG	YC	1737	1/1	0.09	0.20	180,180,180,180	0
55	MG	VC	3606	1/1	0.09	0.08	243,243,243,243	0
55	MG	ED	116	1/1	0.10	0.13	167,167,167,167	0
55	MG	UC	1785	1/1	0.10	0.16	190,190,190,190	0
55	MG	BD	102	1/1	0.10	0.14	270,270,270,270	0
55	MG	UC	1779	1/1	0.11	0.29	161,161,161,161	0
55	MG	BD	106	1/1	0.11	0.15	192,192,192,192	0
55	MG	ED	101	1/1	0.11	0.16	182,182,182,182	0
55	MG	ED	104	1/1	0.11	0.18	159,159,159,159	0
55	MG	UC	1699	1/1	0.12	0.11	197,197,197,197	0
55	MG	YC	1721	1/1	0.12	0.21	145,145,145,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	UC	1609	1/1	0.12	0.17	144,144,144,144	0
55	MG	VC	3066	1/1	0.12	0.35	102,102,102,102	0
55	MG	UC	1669	1/1	0.12	0.17	189,189,189,189	0
55	MG	ZC	3341	1/1	0.12	0.23	110,110,110,110	0
55	MG	UC	1807	1/1	0.13	0.24	113,113,113,113	0
55	MG	WC	218	1/1	0.14	0.21	136,136,136,136	0
55	MG	YC	1664	1/1	0.14	0.11	199,199,199,199	0
55	MG	UC	1651	1/1	0.14	0.23	147,147,147,147	0
55	MG	ZC	3197	1/1	0.14	0.31	152,152,152,152	0
55	MG	VC	3595	1/1	0.14	0.09	301,301,301,301	0
55	MG	XC	103	1/1	0.15	0.14	217,217,217,217	0
55	MG	ZC	3310	1/1	0.15	0.22	124,124,124,124	0
55	MG	ZC	3061	1/1	0.15	0.25	103,103,103,103	0
55	MG	ZC	3502	1/1	0.16	0.25	171,171,171,171	0
55	MG	YC	1691	1/1	0.16	0.19	193,193,193,193	0
55	MG	UC	1657	1/1	0.17	0.17	175,175,175,175	0
55	MG	VC	3441	1/1	0.17	0.11	201,201,201,201	0
55	MG	YC	1789	1/1	0.18	0.14	279,279,279,279	0
55	MG	YC	1843	1/1	0.18	0.34	138,138,138,138	0
55	MG	ZC	3657	1/1	0.18	0.14	108,108,108,108	0
55	MG	ZC	3133	1/1	0.19	0.22	124,124,124,124	0
55	MG	UC	1710	1/1	0.19	0.21	142,142,142,142	0
55	MG	VC	3289	1/1	0.19	0.14	224,224,224,224	0
55	MG	ZC	3344	1/1	0.19	0.17	124,124,124,124	0
55	MG	VC	3102	1/1	0.20	0.32	124,124,124,124	0
55	MG	UC	1647	1/1	0.20	0.28	143,143,143,143	0
55	MG	YC	1700	1/1	0.20	0.17	208,208,208,208	0
55	MG	WC	209	1/1	0.20	0.20	182,182,182,182	0
55	MG	UC	1667	1/1	0.20	0.13	145,145,145,145	0
55	MG	YC	1720	1/1	0.21	0.24	165,165,165,165	0
55	MG	YC	1609	1/1	0.21	0.28	193,193,193,193	0
55	MG	VC	3114	1/1	0.22	0.23	134,134,134,134	0
55	MG	WC	210	1/1	0.22	0.24	169,169,169,169	0
55	MG	UC	1815	1/1	0.22	0.24	134,134,134,134	0
55	MG	ZC	3289	1/1	0.23	0.19	130,130,130,130	0
55	MG	BC	201	1/1	0.23	0.28	128,128,128,128	0
55	MG	YC	1730	1/1	0.23	0.15	225,225,225,225	0
55	MG	VC	3498	1/1	0.23	0.39	95,95,95,95	0
55	MG	YC	1668	1/1	0.23	0.15	143,143,143,143	0
55	MG	UC	1646	1/1	0.23	0.14	184,184,184,184	0
55	MG	VC	3122	1/1	0.24	0.35	82,82,82,82	0
55	MG	WC	207	1/1	0.24	0.19	164,164,164,164	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	ED	114	1/1	0.24	0.17	158,158,158,158	0
55	MG	VC	3145	1/1	0.24	0.29	123,123,123,123	0
55	MG	YC	1627	1/1	0.24	0.35	157,157,157,157	0
55	MG	VC	3157	1/1	0.24	0.22	125,125,125,125	0
55	MG	UC	1654	1/1	0.25	0.25	117,117,117,117	0
55	MG	YC	1619	1/1	0.25	0.19	186,186,186,186	0
55	MG	ZC	3262	1/1	0.25	0.34	115,115,115,115	0
55	MG	YC	1676	1/1	0.25	0.13	147,147,147,147	0
55	MG	OA	102	1/1	0.26	0.16	180,180,180,180	0
55	MG	ZC	3388	1/1	0.26	0.32	97,97,97,97	0
55	MG	D	203	1/1	0.26	0.16	188,188,188,188	0
55	MG	P	202	1/1	0.26	0.10	131,131,131,131	0
55	MG	VC	3487	1/1	0.26	0.19	126,126,126,126	0
55	MG	UC	1763	1/1	0.27	0.26	159,159,159,159	0
55	MG	YC	1675	1/1	0.27	0.12	232,232,232,232	0
55	MG	YC	1679	1/1	0.28	0.17	281,281,281,281	0
55	MG	YC	1757	1/1	0.28	0.12	171,171,171,171	0
55	MG	UC	1732	1/1	0.28	0.21	148,148,148,148	0
55	MG	VC	3368	1/1	0.29	0.12	160,160,160,160	0
55	MG	ZC	3635	1/1	0.29	0.11	216,216,216,216	0
55	MG	ED	105	1/1	0.29	0.21	153,153,153,153	0
55	MG	YC	1749	1/1	0.29	0.22	164,164,164,164	0
55	MG	YC	1651	1/1	0.30	0.12	197,197,197,197	0
55	MG	UC	1709	1/1	0.30	0.35	109,109,109,109	0
55	MG	UC	1653	1/1	0.30	0.22	204,204,204,204	0
55	MG	VC	3023	1/1	0.30	0.34	118,118,118,118	0
55	MG	ED	106	1/1	0.30	0.16	148,148,148,148	0
55	MG	WC	220	1/1	0.30	0.10	205,205,205,205	0
55	MG	YC	1641	1/1	0.30	0.29	118,118,118,118	0
55	MG	YC	1717	1/1	0.30	0.22	210,210,210,210	0
55	MG	YC	1670	1/1	0.30	0.39	132,132,132,132	0
55	MG	XC	101	1/1	0.30	0.13	190,190,190,190	0
55	MG	VC	3194	1/1	0.31	0.20	101,101,101,101	0
55	MG	YC	1710	1/1	0.31	0.14	185,185,185,185	0
55	MG	ZC	3724	1/1	0.31	0.23	165,165,165,165	0
55	MG	YC	1677	1/1	0.31	0.19	136,136,136,136	0
55	MG	YC	1615	1/1	0.31	0.37	150,150,150,150	0
55	MG	JB	201	1/1	0.32	0.10	145,145,145,145	0
55	MG	VC	3514	1/1	0.32	0.18	138,138,138,138	0
55	MG	UC	1718	1/1	0.32	0.20	120,120,120,120	0
55	MG	VC	3447	1/1	0.32	0.09	121,121,121,121	0
55	MG	BB	202	1/1	0.32	0.11	153,153,153,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	UC	1854	1/1	0.32	0.24	146,146,146,146	0
55	MG	ZC	3457	1/1	0.32	0.20	97,97,97,97	0
55	MG	ZC	3500	1/1	0.32	0.24	115,115,115,115	0
55	MG	YC	1633	1/1	0.32	0.20	141,141,141,141	0
55	MG	VC	3420	1/1	0.32	0.12	192,192,192,192	0
55	MG	ZC	3163	1/1	0.33	0.33	130,130,130,130	0
55	MG	VC	3164	1/1	0.33	0.20	134,134,134,134	0
55	MG	VC	3184	1/1	0.33	0.25	109,109,109,109	0
55	MG	UC	1774	1/1	0.33	0.19	149,149,149,149	0
55	MG	UC	1617	1/1	0.33	0.11	151,151,151,151	0
55	MG	ZC	3718	1/1	0.33	0.14	124,124,124,124	0
55	MG	VC	3150	1/1	0.33	0.11	139,139,139,139	0
55	MG	VC	3006	1/1	0.33	0.17	147,147,147,147	0
55	MG	VC	3472	1/1	0.34	0.22	154,154,154,154	0
55	MG	YC	1743	1/1	0.34	0.14	224,224,224,224	0
55	MG	YC	1690	1/1	0.34	0.19	215,215,215,215	0
55	MG	UC	1622	1/1	0.34	0.18	121,121,121,121	0
55	MG	LA	201	1/1	0.34	0.22	142,142,142,142	0
55	MG	VC	3168	1/1	0.34	0.27	108,108,108,108	0
55	MG	YC	1630	1/1	0.34	0.21	136,136,136,136	0
55	MG	VC	3608	1/1	0.35	0.12	219,219,219,219	0
55	MG	VC	3666	1/1	0.35	0.24	131,131,131,131	0
55	MG	AD	216	1/1	0.35	0.24	134,134,134,134	0
55	MG	VC	3682	1/1	0.35	0.17	123,123,123,123	0
55	MG	ZC	3247	1/1	0.35	0.24	136,136,136,136	0
55	MG	ED	113	1/1	0.35	0.31	170,170,170,170	0
55	MG	WC	204	1/1	0.35	0.20	153,153,153,153	0
55	MG	ZC	3706	1/1	0.35	0.14	95,95,95,95	0
55	MG	D	202	1/1	0.35	0.22	152,152,152,152	0
55	MG	VC	3276	1/1	0.35	0.07	138,138,138,138	0
55	MG	EB	201	1/1	0.36	0.15	128,128,128,128	0
55	MG	ZC	3331	1/1	0.36	0.10	71,71,71,71	0
55	MG	VC	3410	1/1	0.36	0.16	117,117,117,117	0
55	MG	UC	1803	1/1	0.37	0.21	147,147,147,147	0
55	MG	UC	1603	1/1	0.37	0.28	106,106,106,106	0
55	MG	HA	202	1/1	0.37	0.33	171,171,171,171	0
55	MG	VC	3098	1/1	0.37	0.27	114,114,114,114	0
55	MG	YC	1682	1/1	0.37	0.23	121,121,121,121	0
55	MG	YC	1711	1/1	0.37	0.17	174,174,174,174	0
55	MG	WC	212	1/1	0.38	0.27	118,118,118,118	0
55	MG	YC	1689	1/1	0.38	0.27	117,117,117,117	0
55	MG	UC	1607	1/1	0.38	0.29	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	UC	1829	1/1	0.38	0.12	145,145,145,145	0
55	MG	UC	1746	1/1	0.38	0.21	155,155,155,155	0
55	MG	YC	1726	1/1	0.38	0.38	162,162,162,162	0
55	MG	UC	1724	1/1	0.38	0.30	150,150,150,150	0
55	MG	VC	3596	1/1	0.39	0.09	173,173,173,173	0
55	MG	VC	3216	1/1	0.39	0.13	200,200,200,200	0
55	MG	VC	3109	1/1	0.39	0.37	92,92,92,92	0
55	MG	AD	227	1/1	0.39	0.17	136,136,136,136	0
55	MG	YC	1653	1/1	0.39	0.27	140,140,140,140	0
55	MG	WC	214	1/1	0.39	0.20	166,166,166,166	0
55	MG	YC	1739	1/1	0.39	0.13	206,206,206,206	0
55	MG	VC	3322	1/1	0.39	0.32	114,114,114,114	0
55	MG	YC	1790	1/1	0.39	0.17	209,209,209,209	0
55	MG	YC	1805	1/1	0.39	0.21	115,115,115,115	0
55	MG	YC	1821	1/1	0.40	0.17	204,204,204,204	0
55	MG	UC	1658	1/1	0.40	0.26	169,169,169,169	0
55	MG	YC	1858	1/1	0.40	0.20	132,132,132,132	0
55	MG	VC	3437	1/1	0.40	0.15	199,199,199,199	0
55	MG	VC	3188	1/1	0.40	0.19	152,152,152,152	0
55	MG	VC	3044	1/1	0.40	0.16	243,243,243,243	0
55	MG	GB	201	1/1	0.40	0.29	126,126,126,126	0
55	MG	AD	215	1/1	0.40	0.16	120,120,120,120	0
55	MG	VC	3215	1/1	0.40	0.08	168,168,168,168	0
55	MG	UC	1626	1/1	0.40	0.18	129,129,129,129	0
55	MG	FB	202	1/1	0.40	0.14	118,118,118,118	0
55	MG	YC	1808	1/1	0.40	0.21	167,167,167,167	0
55	MG	YC	1814	1/1	0.40	0.13	224,224,224,224	0
55	MG	VC	3692	1/1	0.41	0.23	119,119,119,119	0
55	MG	YC	1622	1/1	0.41	0.08	159,159,159,159	0
55	MG	VC	3479	1/1	0.41	0.19	133,133,133,133	0
55	MG	BC	202	1/1	0.41	0.27	127,127,127,127	0
55	MG	XC	102	1/1	0.41	0.09	217,217,217,217	0
55	MG	YC	1632	1/1	0.41	0.25	112,112,112,112	0
55	MG	ZC	3119	1/1	0.41	0.15	182,182,182,182	0
55	MG	ED	115	1/1	0.41	0.13	171,171,171,171	0
55	MG	UC	1629	1/1	0.41	0.18	134,134,134,134	0
55	MG	ZC	3319	1/1	0.41	0.11	117,117,117,117	0
55	MG	BD	108	1/1	0.41	0.20	109,109,109,109	0
55	MG	UC	1819	1/1	0.42	0.12	142,142,142,142	0
55	MG	VC	3548	1/1	0.42	0.12	135,135,135,135	0
55	MG	YC	1794	1/1	0.42	0.10	192,192,192,192	0
55	MG	WC	202	1/1	0.42	0.26	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	VC	3603	1/1	0.42	0.15	166,166,166,166	0
55	MG	XC	105	1/1	0.42	0.17	164,164,164,164	0
55	MG	UC	1744	1/1	0.43	0.25	130,130,130,130	0
55	MG	ZC	3392	1/1	0.43	0.28	137,137,137,137	0
55	MG	ZC	3094	1/1	0.43	0.33	62,62,62,62	0
55	MG	ZC	3498	1/1	0.43	0.18	109,109,109,109	0
55	MG	VC	3380	1/1	0.43	0.18	82,82,82,82	0
55	MG	YA	303	1/1	0.43	0.33	67,67,67,67	0
55	MG	ZC	3159	1/1	0.43	0.32	103,103,103,103	0
55	MG	UC	1642	1/1	0.44	0.22	123,123,123,123	0
55	MG	ZC	3086	1/1	0.44	0.29	124,124,124,124	0
55	MG	UC	1790	1/1	0.44	0.18	144,144,144,144	0
55	MG	UC	1674	1/1	0.44	0.30	110,110,110,110	0
55	MG	LC	101	1/1	0.44	0.10	135,135,135,135	0
55	MG	VC	3248	1/1	0.44	0.15	128,128,128,128	0
55	MG	YC	1854	1/1	0.44	0.09	166,166,166,166	0
55	MG	UC	1849	1/1	0.44	0.09	149,149,149,149	0
55	MG	VC	3421	1/1	0.45	0.15	145,145,145,145	0
55	MG	BB	201	1/1	0.45	0.29	143,143,143,143	0
55	MG	VC	3247	1/1	0.45	0.14	140,140,140,140	0
55	MG	VC	3163	1/1	0.45	0.14	99,99,99,99	0
55	MG	YC	1656	1/1	0.45	0.15	206,206,206,206	0
55	MG	VC	3446	1/1	0.45	0.10	109,109,109,109	0
55	MG	YC	1764	1/1	0.45	0.14	146,146,146,146	0
55	MG	IC	201	1/1	0.45	0.16	155,155,155,155	0
55	MG	YC	1771	1/1	0.45	0.15	229,229,229,229	0
55	MG	VC	3076	1/1	0.45	0.20	103,103,103,103	0
55	MG	UC	1689	1/1	0.45	0.10	153,153,153,153	0
55	MG	ZC	3098	1/1	0.45	0.24	87,87,87,87	0
55	MG	WC	221	1/1	0.45	0.11	179,179,179,179	0
55	MG	VC	3196	1/1	0.46	0.27	87,87,87,87	0
55	MG	ZC	3110	1/1	0.46	0.29	99,99,99,99	0
55	MG	VC	3630	1/1	0.46	0.15	126,126,126,126	0
55	MG	YC	1639	1/1	0.46	0.11	176,176,176,176	0
55	MG	VC	3511	1/1	0.46	0.12	182,182,182,182	0
55	MG	YC	1815	1/1	0.46	0.14	155,155,155,155	0
55	MG	VC	3208	1/1	0.46	0.13	137,137,137,137	0
55	MG	WC	208	1/1	0.46	0.25	133,133,133,133	0
55	MG	AD	208	1/1	0.46	0.19	135,135,135,135	0
55	MG	YC	1607	1/1	0.46	0.42	101,101,101,101	0
55	MG	ZC	3418	1/1	0.46	0.17	115,115,115,115	0
55	MG	YC	1696	1/1	0.46	0.22	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	UC	1634	1/1	0.46	0.28	142,142,142,142	0
55	MG	YC	1613	1/1	0.46	0.15	145,145,145,145	0
55	MG	YC	1793	1/1	0.46	0.17	141,141,141,141	0
55	MG	VC	3040	1/1	0.47	0.41	99,99,99,99	0
55	MG	YC	1864	1/1	0.47	0.13	105,105,105,105	0
55	MG	ZC	3288	1/1	0.47	0.32	95,95,95,95	0
55	MG	ZC	3055	1/1	0.47	0.20	89,89,89,89	0
55	MG	YC	1732	1/1	0.47	0.24	137,137,137,137	0
55	MG	UC	1625	1/1	0.47	0.26	109,109,109,109	0
55	MG	VC	3285	1/1	0.47	0.13	135,135,135,135	0
55	MG	UC	1766	1/1	0.47	0.21	130,130,130,130	0
55	MG	UC	1782	1/1	0.47	0.18	116,116,116,116	0
55	MG	VC	3095	1/1	0.47	0.21	105,105,105,105	0
55	MG	ZC	3741	1/1	0.47	0.16	203,203,203,203	0
55	MG	VC	3226	1/1	0.47	0.17	133,133,133,133	0
55	MG	VC	3011	1/1	0.47	0.43	88,88,88,88	0
55	MG	WC	216	1/1	0.47	0.12	160,160,160,160	0
55	MG	YC	1686	1/1	0.47	0.28	136,136,136,136	0
55	MG	YC	1766	1/1	0.47	0.38	130,130,130,130	0
55	MG	UC	1708	1/1	0.47	0.18	146,146,146,146	0
55	MG	VC	3228	1/1	0.48	0.09	120,120,120,120	0
55	MG	VC	3173	1/1	0.48	0.24	93,93,93,93	0
55	MG	ZC	3519	1/1	0.48	0.15	114,114,114,114	0
55	MG	ZC	3527	1/1	0.48	0.17	92,92,92,92	0
55	MG	YC	1650	1/1	0.48	0.17	99,99,99,99	0
55	MG	YC	1838	1/1	0.48	0.19	154,154,154,154	0
55	MG	ZC	3142	1/1	0.48	0.30	70,70,70,70	0
55	MG	YC	1693	1/1	0.48	0.20	148,148,148,148	0
55	MG	YC	1604	1/1	0.48	0.12	136,136,136,136	0
55	MG	VC	3347	1/1	0.48	0.13	99,99,99,99	0
55	MG	UC	1792	1/1	0.48	0.17	151,151,151,151	0
55	MG	WC	224	1/1	0.48	0.14	161,161,161,161	0
55	MG	ZC	3233	1/1	0.48	0.16	141,141,141,141	0
55	MG	VC	3138	1/1	0.48	0.23	162,162,162,162	0
55	MG	AD	209	1/1	0.48	0.16	115,115,115,115	0
55	MG	UC	1802	1/1	0.48	0.27	110,110,110,110	0
55	MG	ZC	3470	1/1	0.48	0.09	89,89,89,89	0
55	MG	UC	1649	1/1	0.48	0.13	261,261,261,261	0
55	MG	UC	1817	1/1	0.49	0.15	156,156,156,156	0
55	MG	UC	1778	1/1	0.49	0.14	153,153,153,153	0
55	MG	VC	3038	1/1	0.49	0.24	115,115,115,115	0
55	MG	UC	1847	1/1	0.49	0.20	157,157,157,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	ED	110	1/1	0.49	0.21	139,139,139,139	0
55	MG	ZC	3558	1/1	0.49	0.17	168,168,168,168	0
55	MG	ZC	3571	1/1	0.49	0.10	131,131,131,131	0
55	MG	ZC	3626	1/1	0.49	0.14	110,110,110,110	0
55	MG	YC	1841	1/1	0.49	0.23	185,185,185,185	0
55	MG	ZC	3651	1/1	0.49	0.15	104,104,104,104	0
55	MG	YC	1685	1/1	0.49	0.13	113,113,113,113	0
55	MG	FD	111	1/1	0.49	0.19	130,130,130,130	0
55	MG	YC	1837	1/1	0.50	0.21	145,145,145,145	0
55	MG	ZC	3758	1/1	0.50	0.28	128,128,128,128	0
55	MG	WC	201	1/1	0.50	0.15	178,178,178,178	0
55	MG	AD	201	1/1	0.50	0.20	105,105,105,105	0
55	MG	AD	206	1/1	0.50	0.23	128,128,128,128	0
55	MG	YC	1665	1/1	0.50	0.31	115,115,115,115	0
55	MG	VC	3317	1/1	0.50	0.10	122,122,122,122	0
55	MG	ZC	3275	1/1	0.50	0.20	98,98,98,98	0
55	MG	ZC	3132	1/1	0.50	0.19	107,107,107,107	0
55	MG	VC	3010	1/1	0.50	0.23	121,121,121,121	0
55	MG	UC	1612	1/1	0.50	0.22	114,114,114,114	0
55	MG	YC	1602	1/1	0.50	0.14	157,157,157,157	0
55	MG	YC	1697	1/1	0.50	0.15	143,143,143,143	0
55	MG	YC	1746	1/1	0.50	0.18	106,106,106,106	0
55	MG	YC	1775	1/1	0.50	0.12	132,132,132,132	0
55	MG	FD	116	1/1	0.50	0.15	136,136,136,136	0
55	MG	UC	1828	1/1	0.51	0.16	199,199,199,199	0
55	MG	YC	1851	1/1	0.51	0.12	183,183,183,183	0
55	MG	VC	3144	1/1	0.51	0.20	124,124,124,124	0
55	MG	AD	226	1/1	0.51	0.12	157,157,157,157	0
55	MG	ZC	3162	1/1	0.51	0.24	89,89,89,89	0
55	MG	ZC	3728	1/1	0.51	0.08	94,94,94,94	0
55	MG	VC	3261	1/1	0.51	0.18	102,102,102,102	0
55	MG	YC	1631	1/1	0.51	0.24	96,96,96,96	0
55	MG	ZC	3593	1/1	0.51	0.19	97,97,97,97	0
55	MG	ZC	3314	1/1	0.51	0.12	97,97,97,97	0
55	MG	ZC	3021	1/1	0.51	0.18	88,88,88,88	0
55	MG	ZC	3036	1/1	0.51	0.31	95,95,95,95	0
55	MG	ZC	3038	1/1	0.51	0.14	110,110,110,110	0
55	MG	UC	1825	1/1	0.52	0.16	104,104,104,104	0
55	MG	VC	3358	1/1	0.52	0.20	120,120,120,120	0
55	MG	VC	3524	1/1	0.52	0.23	187,187,187,187	0
55	MG	YC	1802	1/1	0.52	0.10	134,134,134,134	0
55	MG	J	202	1/1	0.52	0.18	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	ZC	3366	1/1	0.52	0.29	83,83,83,83	0
55	MG	ZC	3383	1/1	0.52	0.14	110,110,110,110	0
55	MG	UC	1638	1/1	0.52	0.23	109,109,109,109	0
55	MG	C	303	1/1	0.52	0.36	68,68,68,68	0
55	MG	VC	3345	1/1	0.52	0.15	111,111,111,111	0
55	MG	ZC	3630	1/1	0.52	0.09	99,99,99,99	0
55	MG	ZC	3317	1/1	0.52	0.25	126,126,126,126	0
55	MG	VC	3392	1/1	0.52	0.22	85,85,85,85	0
55	MG	VC	3198	1/1	0.53	0.33	88,88,88,88	0
55	MG	UC	1786	1/1	0.53	0.37	96,96,96,96	0
55	MG	YC	1809	1/1	0.53	0.11	174,174,174,174	0
55	MG	ZC	3485	1/1	0.53	0.20	101,101,101,101	0
55	MG	VC	3013	1/1	0.53	0.32	86,86,86,86	0
55	MG	BD	107	1/1	0.53	0.13	249,249,249,249	0
55	MG	ZC	3330	1/1	0.53	0.25	93,93,93,93	0
55	MG	ZC	3739	1/1	0.53	0.10	115,115,115,115	0
55	MG	YC	1683	1/1	0.53	0.27	155,155,155,155	0
55	MG	YC	1704	1/1	0.53	0.26	85,85,85,85	0
55	MG	YC	1667	1/1	0.53	0.11	149,149,149,149	0
55	MG	ZC	3347	1/1	0.53	0.29	92,92,92,92	0
55	MG	YC	1785	1/1	0.53	0.31	106,106,106,106	0
55	MG	UC	1688	1/1	0.53	0.11	202,202,202,202	0
55	MG	ZC	3610	1/1	0.53	0.31	96,96,96,96	0
55	MG	VC	3156	1/1	0.53	0.41	94,94,94,94	0
55	MG	VC	3031	1/1	0.53	0.44	79,79,79,79	0
55	MG	AD	225	1/1	0.53	0.23	133,133,133,133	0
55	MG	UC	1640	1/1	0.53	0.11	136,136,136,136	0
55	MG	UC	1811	1/1	0.53	0.11	131,131,131,131	0
55	MG	FD	114	1/1	0.53	0.15	132,132,132,132	0
55	MG	ZC	3304	1/1	0.53	0.24	100,100,100,100	0
55	MG	UC	1698	1/1	0.54	0.16	114,114,114,114	0
55	MG	UC	1693	1/1	0.54	0.16	141,141,141,141	0
55	MG	ZC	3506	1/1	0.54	0.14	77,77,77,77	0
55	MG	ZC	3146	1/1	0.54	0.18	125,125,125,125	0
55	MG	ZC	3300	1/1	0.54	0.32	83,83,83,83	0
55	MG	UC	1605	1/1	0.54	0.26	132,132,132,132	0
55	MG	UC	1624	1/1	0.54	0.21	119,119,119,119	0
55	MG	WC	203	1/1	0.54	0.21	162,162,162,162	0
55	MG	YC	1842	1/1	0.54	0.12	140,140,140,140	0
55	MG	UC	1665	1/1	0.54	0.13	142,142,142,142	0
55	MG	YC	1624	1/1	0.54	0.15	138,138,138,138	0
55	MG	VC	3318	1/1	0.54	0.15	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	VC	3201	1/1	0.54	0.09	139,139,139,139	0
55	MG	UC	1826	1/1	0.54	0.14	163,163,163,163	0
55	MG	YC	1681	1/1	0.55	0.15	193,193,193,193	0
55	MG	ZC	3082	1/1	0.55	0.26	105,105,105,105	0
55	MG	AD	203	1/1	0.55	0.13	137,137,137,137	0
55	MG	ED	103	1/1	0.55	0.09	183,183,183,183	0
55	MG	ZC	3180	1/1	0.55	0.36	86,86,86,86	0
55	MG	VC	3051	1/1	0.55	0.20	117,117,117,117	0
55	MG	ZC	3199	1/1	0.55	0.24	103,103,103,103	0
55	MG	VC	3459	1/1	0.55	0.18	146,146,146,146	0
55	MG	ZC	3664	1/1	0.55	0.19	142,142,142,142	0
55	MG	VC	3287	1/1	0.55	0.12	125,125,125,125	0
55	MG	UC	1608	1/1	0.55	0.18	127,127,127,127	0
55	MG	VC	3210	1/1	0.55	0.08	111,111,111,111	0
55	MG	ZC	3260	1/1	0.55	0.25	87,87,87,87	0
55	MG	VC	3578	1/1	0.55	0.28	72,72,72,72	0
55	MG	YC	1784	1/1	0.55	0.23	139,139,139,139	0
55	MG	YA	305	1/1	0.55	0.20	88,88,88,88	0
55	MG	VC	3419	1/1	0.55	0.14	146,146,146,146	0
55	MG	YC	1642	1/1	0.55	0.14	150,150,150,150	0
55	MG	VC	3046	1/1	0.56	0.48	101,101,101,101	0
55	MG	ZC	3551	1/1	0.56	0.12	83,83,83,83	0
55	MG	YC	1723	1/1	0.56	0.15	188,188,188,188	0
55	MG	VC	3219	1/1	0.56	0.17	128,128,128,128	0
55	MG	VC	3700	1/1	0.56	0.14	91,91,91,91	0
55	MG	YC	1806	1/1	0.56	0.07	145,145,145,145	0
55	MG	ZC	3460	1/1	0.56	0.13	117,117,117,117	0
55	MG	ZC	3343	1/1	0.56	0.21	111,111,111,111	0
55	MG	YC	1845	1/1	0.56	0.20	127,127,127,127	0
55	MG	YC	1781	1/1	0.56	0.10	146,146,146,146	0
55	MG	VC	3075	1/1	0.56	0.12	149,149,149,149	0
55	MG	YC	1672	1/1	0.56	0.45	137,137,137,137	0
55	MG	VC	3331	1/1	0.56	0.12	134,134,134,134	0
55	MG	VC	3131	1/1	0.56	0.20	142,142,142,142	0
55	MG	YC	1849	1/1	0.57	0.28	154,154,154,154	0
55	MG	AD	207	1/1	0.57	0.16	109,109,109,109	0
55	MG	YC	1616	1/1	0.57	0.27	93,93,93,93	0
55	MG	UC	1759	1/1	0.57	0.15	162,162,162,162	0
55	MG	WC	215	1/1	0.57	0.11	180,180,180,180	0
55	MG	VC	3386	1/1	0.57	0.20	134,134,134,134	0
55	MG	VC	3187	1/1	0.57	0.13	152,152,152,152	0
55	MG	YC	1635	1/1	0.57	0.26	150,150,150,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	VC	3560	1/1	0.57	0.09	144,144,144,144	0
55	MG	VC	3008	1/1	0.57	0.27	92,92,92,92	0
55	MG	ZC	3134	1/1	0.57	0.29	74,74,74,74	0
55	MG	FC	201	1/1	0.58	0.32	181,181,181,181	0
55	MG	ZC	3521	1/1	0.58	0.25	109,109,109,109	0
55	MG	VC	3360	1/1	0.58	0.19	153,153,153,153	0
55	MG	YC	1643	1/1	0.58	0.19	112,112,112,112	0
55	MG	VC	3366	1/1	0.58	0.17	111,111,111,111	0
55	MG	ZC	3282	1/1	0.58	0.10	82,82,82,82	0
55	MG	ZC	3284	1/1	0.58	0.15	105,105,105,105	0
55	MG	YC	1647	1/1	0.58	0.23	161,161,161,161	0
55	MG	UC	1808	1/1	0.58	0.16	126,126,126,126	0
55	MG	VC	3492	1/1	0.58	0.12	113,113,113,113	0
55	MG	UC	1787	1/1	0.58	0.09	150,150,150,150	0
55	MG	VC	3609	1/1	0.58	0.07	134,134,134,134	0
55	MG	UC	1672	1/1	0.58	0.27	108,108,108,108	0
55	MG	ZC	3659	1/1	0.58	0.21	99,99,99,99	0
55	MG	VC	3651	1/1	0.58	0.26	94,94,94,94	0
55	MG	UC	1749	1/1	0.58	0.22	134,134,134,134	0
55	MG	VC	3332	1/1	0.58	0.12	121,121,121,121	0
55	MG	UC	1684	1/1	0.58	0.16	110,110,110,110	0
55	MG	VC	3559	1/1	0.58	0.18	97,97,97,97	0
55	MG	UC	1673	1/1	0.58	0.27	114,114,114,114	0
55	MG	ZC	3270	1/1	0.59	0.21	87,87,87,87	0
55	MG	ZC	3648	1/1	0.59	0.07	116,116,116,116	0
55	MG	ZC	3100	1/1	0.59	0.25	105,105,105,105	0
55	MG	VC	3099	1/1	0.59	0.16	171,171,171,171	0
55	MG	VC	3644	1/1	0.59	0.12	167,167,167,167	0
55	MG	ZC	3428	1/1	0.59	0.26	91,91,91,91	0
55	MG	BA	101	1/1	0.59	0.17	130,130,130,130	0
55	MG	VC	3396	1/1	0.59	0.24	112,112,112,112	0
55	MG	YC	1648	1/1	0.59	0.09	112,112,112,112	0
55	MG	VC	3677	1/1	0.59	0.20	111,111,111,111	0
55	MG	YC	1601	1/1	0.59	0.09	209,209,209,209	0
55	MG	VC	3678	1/1	0.59	0.14	76,76,76,76	0
55	MG	VC	3580	1/1	0.59	0.13	113,113,113,113	0
55	MG	YC	1758	1/1	0.59	0.15	127,127,127,127	0
55	MG	YC	1759	1/1	0.59	0.24	141,141,141,141	0
55	MG	VC	3402	1/1	0.59	0.29	100,100,100,100	0
55	MG	ZC	3052	1/1	0.59	0.48	89,89,89,89	0
55	MG	AD	202	1/1	0.59	0.26	125,125,125,125	0
55	MG	ZC	3204	1/1	0.59	0.21	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	VC	3093	1/1	0.59	0.16	152,152,152,152	0
55	MG	VC	3451	1/1	0.59	0.31	90,90,90,90	0
55	MG	VC	3055	1/1	0.59	0.11	103,103,103,103	0
55	MG	FD	101	1/1	0.59	0.17	132,132,132,132	0
55	MG	VC	3012	1/1	0.59	0.35	107,107,107,107	0
55	MG	FD	104	1/1	0.59	0.09	167,167,167,167	0
55	MG	YC	1772	1/1	0.59	0.11	131,131,131,131	0
55	MG	UC	1758	1/1	0.59	0.10	120,120,120,120	0
55	MG	AD	217	1/1	0.59	0.12	106,106,106,106	0
55	MG	AD	223	1/1	0.59	0.13	151,151,151,151	0
55	MG	UC	1611	1/1	0.60	0.20	113,113,113,113	0
55	MG	ZC	3708	1/1	0.60	0.19	74,74,74,74	0
55	MG	VC	3344	1/1	0.60	0.19	101,101,101,101	0
55	MG	VC	3171	1/1	0.60	0.13	115,115,115,115	0
55	MG	UC	1725	1/1	0.60	0.19	145,145,145,145	0
55	MG	YC	1791	1/1	0.60	0.08	170,170,170,170	0
55	MG	ZC	3490	1/1	0.60	0.15	100,100,100,100	0
55	MG	YC	1792	1/1	0.60	0.19	124,124,124,124	0
55	MG	VC	3238	1/1	0.60	0.26	92,92,92,92	0
55	MG	UC	1736	1/1	0.60	0.19	139,139,139,139	0
55	MG	ZC	3774	1/1	0.60	0.11	132,132,132,132	0
55	MG	UC	1838	1/1	0.60	0.11	150,150,150,150	0
55	MG	VC	3255	1/1	0.60	0.18	107,107,107,107	0
55	MG	VC	3199	1/1	0.60	0.13	103,103,103,103	0
55	MG	VC	3535	1/1	0.60	0.23	114,114,114,114	0
55	MG	ZC	3669	1/1	0.60	0.12	126,126,126,126	0
55	MG	ZC	3545	1/1	0.60	0.18	140,140,140,140	0
55	MG	UC	1728	1/1	0.61	0.15	119,119,119,119	0
55	MG	UC	1797	1/1	0.61	0.10	130,130,130,130	0
55	MG	VC	3125	1/1	0.61	0.23	122,122,122,122	0
55	MG	UC	1836	1/1	0.61	0.14	138,138,138,138	0
55	MG	YC	1829	1/1	0.61	0.12	146,146,146,146	0
55	MG	VC	3246	1/1	0.61	0.23	106,106,106,106	0
55	MG	YC	1716	1/1	0.61	0.12	249,249,249,249	0
55	MG	YC	1645	1/1	0.61	0.10	184,184,184,184	0
55	MG	VC	3382	1/1	0.61	0.15	104,104,104,104	0
55	MG	VC	3564	1/1	0.61	0.07	151,151,151,151	0
55	MG	ZC	3152	1/1	0.61	0.32	83,83,83,83	0
55	MG	YC	1844	1/1	0.61	0.19	133,133,133,133	0
55	MG	UC	1863	1/1	0.61	0.15	106,106,106,106	0
55	MG	VC	3705	1/1	0.61	0.18	100,100,100,100	0
55	MG	VC	3387	1/1	0.61	0.13	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	DC	201	1/1	0.61	0.13	175,175,175,175	0
55	MG	ZC	3371	1/1	0.61	0.15	91,91,91,91	0
55	MG	ZC	3375	1/1	0.61	0.10	101,101,101,101	0
55	MG	YC	1735	1/1	0.61	0.18	159,159,159,159	0
55	MG	YC	1862	1/1	0.61	0.10	169,169,169,169	0
55	MG	VC	3336	1/1	0.61	0.14	119,119,119,119	0
55	MG	YC	1688	1/1	0.61	0.17	189,189,189,189	0
55	MG	ZC	3399	1/1	0.61	0.15	101,101,101,101	0
55	MG	YC	1629	1/1	0.61	0.17	152,152,152,152	0
55	MG	ZC	3239	1/1	0.61	0.22	82,82,82,82	0
55	MG	ZC	3037	1/1	0.61	0.25	59,59,59,59	0
55	MG	VC	3026	1/1	0.61	0.20	97,97,97,97	0
55	MG	VC	3256	1/1	0.61	0.16	101,101,101,101	0
55	MG	ZC	3269	1/1	0.61	0.13	112,112,112,112	0
55	MG	VC	3061	1/1	0.61	0.16	101,101,101,101	0
55	MG	FD	103	1/1	0.61	0.12	155,155,155,155	0
55	MG	VC	3062	1/1	0.61	0.24	91,91,91,91	0
55	MG	ZC	3070	1/1	0.61	0.25	91,91,91,91	0
55	MG	YC	1752	1/1	0.61	0.24	129,129,129,129	0
55	MG	YA	308	1/1	0.61	0.34	59,59,59,59	0
55	MG	ZC	3507	1/1	0.61	0.15	99,99,99,99	0
55	MG	ZC	3699	1/1	0.62	0.09	124,124,124,124	0
55	MG	ZC	3497	1/1	0.62	0.20	102,102,102,102	0
55	MG	VC	3423	1/1	0.62	0.17	136,136,136,136	0
55	MG	ZC	3050	1/1	0.62	0.28	82,82,82,82	0
55	MG	YC	1824	1/1	0.62	0.11	138,138,138,138	0
55	MG	ZC	3201	1/1	0.62	0.10	88,88,88,88	0
55	MG	ZC	3732	1/1	0.62	0.26	91,91,91,91	0
55	MG	UC	1714	1/1	0.62	0.22	154,154,154,154	0
55	MG	YC	1831	1/1	0.62	0.14	208,208,208,208	0
55	MG	UC	1627	1/1	0.62	0.10	149,149,149,149	0
55	MG	ZC	3076	1/1	0.62	0.24	105,105,105,105	0
55	MG	VC	3165	1/1	0.62	0.29	87,87,87,87	0
55	MG	YC	1706	1/1	0.62	0.15	122,122,122,122	0
55	MG	VC	3043	1/1	0.62	0.20	118,118,118,118	0
55	MG	YC	1747	1/1	0.62	0.16	319,319,319,319	0
55	MG	UC	1730	1/1	0.62	0.11	198,198,198,198	0
55	MG	UC	1663	1/1	0.62	0.15	140,140,140,140	0
55	MG	YC	1846	1/1	0.62	0.10	100,100,100,100	0
55	MG	YC	1660	1/1	0.62	0.15	171,171,171,171	0
55	MG	VC	3407	1/1	0.62	0.11	97,97,97,97	0
55	MG	VC	3149	1/1	0.62	0.17	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	VC	3081	1/1	0.62	0.31	93,93,93,93	0
55	MG	VC	3662	1/1	0.62	0.26	85,85,85,85	0
55	MG	YC	1728	1/1	0.62	0.12	179,179,179,179	0
55	MG	VC	3009	1/1	0.62	0.28	70,70,70,70	0
55	MG	UC	1831	1/1	0.62	0.14	113,113,113,113	0
55	MG	VC	3579	1/1	0.62	0.16	105,105,105,105	0
55	MG	ZC	3467	1/1	0.63	0.14	114,114,114,114	0
55	MG	VC	3549	1/1	0.63	0.11	90,90,90,90	0
55	MG	YC	1699	1/1	0.63	0.18	97,97,97,97	0
55	MG	ZC	3184	1/1	0.63	0.21	121,121,121,121	0
55	MG	UC	1816	1/1	0.63	0.17	126,126,126,126	0
55	MG	ZC	3069	1/1	0.63	0.27	85,85,85,85	0
55	MG	VC	3321	1/1	0.63	0.13	124,124,124,124	0
55	MG	VC	3039	1/1	0.63	0.17	135,135,135,135	0
55	MG	ZC	3217	1/1	0.63	0.27	86,86,86,86	0
55	MG	VC	3577	1/1	0.63	0.12	135,135,135,135	0
55	MG	PA	102	1/1	0.63	0.24	118,118,118,118	0
55	MG	UC	1705	1/1	0.63	0.14	110,110,110,110	0
55	MG	YC	1634	1/1	0.63	0.16	132,132,132,132	0
55	MG	ZC	3352	1/1	0.63	0.20	84,84,84,84	0
55	MG	UC	1747	1/1	0.63	0.20	95,95,95,95	0
55	MG	VC	3342	1/1	0.63	0.26	109,109,109,109	0
55	MG	YC	1687	1/1	0.63	0.14	113,113,113,113	0
55	MG	UC	1727	1/1	0.63	0.16	164,164,164,164	0
55	MG	ZC	3596	1/1	0.63	0.24	102,102,102,102	0
55	MG	YC	1863	1/1	0.63	0.11	128,128,128,128	0
55	MG	ZC	3271	1/1	0.63	0.19	99,99,99,99	0
55	MG	VC	3239	1/1	0.63	0.08	171,171,171,171	0
55	MG	VC	3048	1/1	0.63	0.33	89,89,89,89	0
55	MG	VC	3311	1/1	0.63	0.10	119,119,119,119	0
55	MG	YC	1669	1/1	0.63	0.36	154,154,154,154	0
55	MG	VC	3540	1/1	0.63	0.17	139,139,139,139	0
55	MG	VC	3139	1/1	0.63	0.31	96,96,96,96	0
55	MG	ZC	3303	1/1	0.63	0.26	101,101,101,101	0
55	MG	YC	1855	1/1	0.64	0.24	124,124,124,124	0
55	MG	UC	1861	1/1	0.64	0.26	113,113,113,113	0
55	MG	ZC	3705	1/1	0.64	0.19	225,225,225,225	0
55	MG	YC	1811	1/1	0.64	0.13	167,167,167,167	0
55	MG	VC	3092	1/1	0.64	0.20	123,123,123,123	0
55	MG	VC	3325	1/1	0.64	0.12	82,82,82,82	0
55	MG	YC	1871	1/1	0.64	0.09	153,153,153,153	0
55	MG	YC	1776	1/1	0.64	0.28	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	YC	1778	1/1	0.64	0.10	238,238,238,238	0
55	MG	UC	1835	1/1	0.64	0.12	137,137,137,137	0
55	MG	VC	3004	1/1	0.64	0.12	101,101,101,101	0
55	MG	A	303	1/1	0.64	0.08	101,101,101,101	0
55	MG	UC	1685	1/1	0.64	0.15	103,103,103,103	0
55	MG	YC	1754	1/1	0.64	0.20	112,112,112,112	0
55	MG	VC	3575	1/1	0.64	0.24	94,94,94,94	0
55	MG	VC	3436	1/1	0.64	0.13	111,111,111,111	0
55	MG	ZC	3412	1/1	0.64	0.25	83,83,83,83	0
55	MG	ZC	3415	1/1	0.64	0.06	157,157,157,157	0
55	MG	ZC	3616	1/1	0.64	0.10	90,90,90,90	0
55	MG	ZC	3416	1/1	0.64	0.12	87,87,87,87	0
55	MG	QB	101	1/1	0.64	0.32	83,83,83,83	0
55	MG	UC	1798	1/1	0.64	0.18	168,168,168,168	0
55	MG	PA	101	1/1	0.64	0.16	120,120,120,120	0
55	MG	VC	3591	1/1	0.64	0.11	114,114,114,114	0
55	MG	VC	3444	1/1	0.64	0.17	113,113,113,113	0
55	MG	C	301	1/1	0.64	0.13	118,118,118,118	0
55	MG	ZC	3226	1/1	0.64	0.15	114,114,114,114	0
55	MG	ZC	3489	1/1	0.64	0.17	119,119,119,119	0
55	MG	VC	3639	1/1	0.65	0.24	116,116,116,116	0
55	MG	ZC	3575	1/1	0.65	0.08	105,105,105,105	0
55	MG	HA	201	1/1	0.65	0.09	147,147,147,147	0
55	MG	ZC	3117	1/1	0.65	0.18	87,87,87,87	0
55	MG	UC	1827	1/1	0.65	0.14	93,93,93,93	0
55	MG	ZC	3615	1/1	0.65	0.17	176,176,176,176	0
55	MG	VC	3658	1/1	0.65	0.13	138,138,138,138	0
55	MG	VC	3290	1/1	0.65	0.19	107,107,107,107	0
55	MG	ZC	3627	1/1	0.65	0.17	92,92,92,92	0
55	MG	YC	1859	1/1	0.65	0.16	125,125,125,125	0
55	MG	UC	1635	1/1	0.65	0.25	93,93,93,93	0
55	MG	VC	3398	1/1	0.65	0.11	128,128,128,128	0
55	MG	VC	3455	1/1	0.65	0.21	93,93,93,93	0
55	MG	VC	3315	1/1	0.65	0.16	119,119,119,119	0
55	MG	VC	3352	1/1	0.65	0.16	122,122,122,122	0
55	MG	VC	3153	1/1	0.65	0.12	106,106,106,106	0
55	MG	UC	1837	1/1	0.65	0.21	115,115,115,115	0
55	MG	ZC	3472	1/1	0.65	0.13	98,98,98,98	0
55	MG	ZC	3475	1/1	0.65	0.14	96,96,96,96	0
55	MG	VC	3707	1/1	0.65	0.21	106,106,106,106	0
55	MG	ZC	3187	1/1	0.65	0.20	103,103,103,103	0
55	MG	VC	3482	1/1	0.65	0.09	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	VC	3067	1/1	0.65	0.15	135,135,135,135	0
55	MG	VC	3585	1/1	0.65	0.09	121,121,121,121	0
55	MG	ZC	3726	1/1	0.65	0.24	115,115,115,115	0
55	MG	VC	3160	1/1	0.65	0.20	108,108,108,108	0
55	MG	ZC	3210	1/1	0.65	0.23	108,108,108,108	0
55	MG	VC	3422	1/1	0.65	0.11	112,112,112,112	0
55	MG	VC	3497	1/1	0.65	0.36	95,95,95,95	0
55	MG	VC	3281	1/1	0.65	0.17	126,126,126,126	0
55	MG	VC	3326	1/1	0.65	0.19	152,152,152,152	0
55	MG	VC	3283	1/1	0.65	0.21	104,104,104,104	0
55	MG	ZC	3528	1/1	0.65	0.12	97,97,97,97	0
55	MG	UC	1670	1/1	0.65	0.22	115,115,115,115	0
55	MG	VC	3533	1/1	0.65	0.22	106,106,106,106	0
55	MG	ZC	3554	1/1	0.65	0.12	122,122,122,122	0
55	MG	FD	115	1/1	0.65	0.10	150,150,150,150	0
55	MG	ZC	3248	1/1	0.65	0.24	94,94,94,94	0
55	MG	VC	3557	1/1	0.66	0.07	155,155,155,155	0
55	MG	VC	3687	1/1	0.66	0.28	88,88,88,88	0
55	MG	UC	1610	1/1	0.66	0.27	110,110,110,110	0
55	MG	YC	1801	1/1	0.66	0.11	148,148,148,148	0
55	MG	ZC	3054	1/1	0.66	0.19	103,103,103,103	0
55	MG	UC	1733	1/1	0.66	0.15	129,129,129,129	0
55	MG	VC	3330	1/1	0.66	0.18	105,105,105,105	0
55	MG	VC	3024	1/1	0.66	0.35	91,91,91,91	0
55	MG	ZC	3487	1/1	0.66	0.16	83,83,83,83	0
55	MG	VC	3460	1/1	0.66	0.33	97,97,97,97	0
55	MG	ZC	3749	1/1	0.66	0.32	110,110,110,110	0
55	MG	ZC	3277	1/1	0.66	0.31	86,86,86,86	0
55	MG	VC	3364	1/1	0.66	0.07	124,124,124,124	0
55	MG	ZC	3629	1/1	0.66	0.19	91,91,91,91	0
55	MG	YC	1663	1/1	0.66	0.20	118,118,118,118	0
55	MG	VC	3193	1/1	0.66	0.27	80,80,80,80	0
55	MG	ZC	3646	1/1	0.66	0.14	127,127,127,127	0
55	MG	UC	1644	1/1	0.66	0.10	112,112,112,112	0
55	MG	ZC	3649	1/1	0.66	0.29	90,90,90,90	0
55	MG	YC	1783	1/1	0.66	0.22	102,102,102,102	0
55	MG	ZC	3656	1/1	0.66	0.12	105,105,105,105	0
55	MG	VC	3161	1/1	0.66	0.19	122,122,122,122	0
55	MG	WC	206	1/1	0.66	0.16	120,120,120,120	0
55	MG	VC	3543	1/1	0.66	0.07	107,107,107,107	0
55	MG	UC	1800	1/1	0.66	0.17	126,126,126,126	0
55	MG	ZC	3029	1/1	0.66	0.35	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	ZC	3538	1/1	0.66	0.15	121,121,121,121	0
55	MG	VC	3221	1/1	0.66	0.15	94,94,94,94	0
55	MG	ZC	3505	1/1	0.67	0.32	68,68,68,68	0
55	MG	ZC	3279	1/1	0.67	0.15	121,121,121,121	0
55	MG	YC	1765	1/1	0.67	0.12	108,108,108,108	0
55	MG	VC	3626	1/1	0.67	0.16	110,110,110,110	0
55	MG	VC	3517	1/1	0.67	0.13	75,75,75,75	0
55	MG	ZC	3389	1/1	0.67	0.20	86,86,86,86	0
55	MG	UC	1613	1/1	0.67	0.40	115,115,115,115	0
55	MG	ZC	3529	1/1	0.67	0.06	124,124,124,124	0
55	MG	VC	3035	1/1	0.67	0.29	76,76,76,76	0
55	MG	UC	1615	1/1	0.67	0.21	139,139,139,139	0
55	MG	YC	1740	1/1	0.67	0.18	146,146,146,146	0
55	MG	ZC	3307	1/1	0.67	0.22	117,117,117,117	0
55	MG	UC	1833	1/1	0.67	0.22	117,117,117,117	0
55	MG	YC	1777	1/1	0.67	0.22	97,97,97,97	0
55	MG	ZC	3439	1/1	0.67	0.18	91,91,91,91	0
55	MG	ZC	3577	1/1	0.67	0.10	126,126,126,126	0
55	MG	ZC	3115	1/1	0.67	0.27	98,98,98,98	0
55	MG	UC	1768	1/1	0.67	0.16	116,116,116,116	0
55	MG	VC	3586	1/1	0.67	0.14	99,99,99,99	0
55	MG	VC	3263	1/1	0.67	0.11	125,125,125,125	0
55	MG	ZC	3760	1/1	0.67	0.60	117,117,117,117	0
55	MG	VC	3271	1/1	0.67	0.23	101,101,101,101	0
55	MG	VC	3428	1/1	0.67	0.29	93,93,93,93	0
55	MG	VC	3501	1/1	0.67	0.07	122,122,122,122	0
55	MG	YC	1840	1/1	0.67	0.31	145,145,145,145	0
55	MG	VC	3401	1/1	0.67	0.16	114,114,114,114	0
55	MG	VC	3607	1/1	0.67	0.15	137,137,137,137	0
55	MG	ZC	3636	1/1	0.67	0.20	132,132,132,132	0
55	MG	ZC	3356	1/1	0.67	0.31	50,50,50,50	0
55	MG	VC	3562	1/1	0.67	0.09	110,110,110,110	0
55	MG	AD	214	1/1	0.67	0.18	103,103,103,103	0
55	MG	VC	3292	1/1	0.67	0.33	93,93,93,93	0
55	MG	VC	3612	1/1	0.67	0.18	90,90,90,90	0
55	MG	FA	201	1/1	0.68	0.28	98,98,98,98	0
55	MG	VC	3632	1/1	0.68	0.10	121,121,121,121	0
55	MG	AD	210	1/1	0.68	0.10	112,112,112,112	0
55	MG	VC	3633	1/1	0.68	0.08	115,115,115,115	0
55	MG	UC	1679	1/1	0.68	0.14	131,131,131,131	0
55	MG	ZC	3071	1/1	0.68	0.21	96,96,96,96	0
55	MG	ZC	3213	1/1	0.68	0.10	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AD	222	1/1	0.68	0.27	115,115,115,115	0
55	MG	ZC	3486	1/1	0.68	0.09	83,83,83,83	0
55	MG	VC	3483	1/1	0.68	0.13	181,181,181,181	0
55	MG	UC	1682	1/1	0.68	0.10	145,145,145,145	0
55	MG	UC	1703	1/1	0.68	0.10	136,136,136,136	0
55	MG	VC	3435	1/1	0.68	0.17	105,105,105,105	0
55	MG	UC	1856	1/1	0.68	0.09	102,102,102,102	0
55	MG	VC	3667	1/1	0.68	0.11	96,96,96,96	0
55	MG	EB	203	1/1	0.68	0.11	106,106,106,106	0
55	MG	UA	201	1/1	0.68	0.53	124,124,124,124	0
55	MG	ZC	3363	1/1	0.68	0.16	74,74,74,74	0
55	MG	WC	228	1/1	0.68	0.09	178,178,178,178	0
55	MG	VC	3505	1/1	0.68	0.09	116,116,116,116	0
55	MG	ZC	3128	1/1	0.68	0.23	87,87,87,87	0
55	MG	ZC	3382	1/1	0.68	0.09	80,80,80,80	0
55	MG	VC	3107	1/1	0.68	0.17	118,118,118,118	0
55	MG	UC	1639	1/1	0.68	0.22	128,128,128,128	0
55	MG	ZC	3536	1/1	0.68	0.08	116,116,116,116	0
55	MG	LA	203	1/1	0.68	0.11	99,99,99,99	0
55	MG	LA	204	1/1	0.68	0.24	123,123,123,123	0
55	MG	VC	3450	1/1	0.68	0.13	116,116,116,116	0
55	MG	ZC	3151	1/1	0.68	0.14	80,80,80,80	0
55	MG	ZC	3403	1/1	0.68	0.26	76,76,76,76	0
55	MG	ZC	3565	1/1	0.68	0.06	102,102,102,102	0
55	MG	ZC	3408	1/1	0.68	0.17	123,123,123,123	0
55	MG	UC	1630	1/1	0.68	0.13	146,146,146,146	0
55	MG	VC	3355	1/1	0.68	0.16	131,131,131,131	0
55	MG	UC	1633	1/1	0.68	0.17	125,125,125,125	0
55	MG	VC	3091	1/1	0.68	0.14	107,107,107,107	0
55	MG	VC	3362	1/1	0.68	0.23	88,88,88,88	0
55	MG	YC	1834	1/1	0.68	0.14	160,160,160,160	0
55	MG	VC	3166	1/1	0.68	0.20	80,80,80,80	0
55	MG	ZC	3620	1/1	0.68	0.11	86,86,86,86	0
55	MG	BC	203	1/1	0.69	0.20	115,115,115,115	0
55	MG	VC	3527	1/1	0.69	0.12	96,96,96,96	0
55	MG	ZC	3123	1/1	0.69	0.27	93,93,93,93	0
55	MG	VC	3180	1/1	0.69	0.10	126,126,126,126	0
55	MG	UC	1864	1/1	0.69	0.12	138,138,138,138	0
55	MG	ZC	3365	1/1	0.69	0.19	104,104,104,104	0
55	MG	ZC	3268	1/1	0.69	0.12	104,104,104,104	0
55	MG	ZC	3654	1/1	0.69	0.12	115,115,115,115	0
55	MG	UC	1734	1/1	0.69	0.14	153,153,153,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	VC	3158	1/1	0.69	0.14	132,132,132,132	0
55	MG	UC	1645	1/1	0.69	0.23	116,116,116,116	0
55	MG	AD	229	1/1	0.69	0.16	106,106,106,106	0
55	MG	YC	1678	1/1	0.69	0.12	146,146,146,146	0
55	MG	VC	3369	1/1	0.69	0.15	81,81,81,81	0
55	MG	ZC	3385	1/1	0.69	0.10	103,103,103,103	0
55	MG	VC	3551	1/1	0.69	0.12	109,109,109,109	0
55	MG	ZC	3153	1/1	0.69	0.22	74,74,74,74	0
55	MG	VC	3097	1/1	0.69	0.30	79,79,79,79	0
55	MG	ZC	3393	1/1	0.69	0.20	105,105,105,105	0
55	MG	UC	1720	1/1	0.69	0.10	125,125,125,125	0
55	MG	ZC	3400	1/1	0.69	0.08	106,106,106,106	0
55	MG	VC	3431	1/1	0.69	0.12	97,97,97,97	0
55	MG	ZC	3407	1/1	0.69	0.22	92,92,92,92	0
55	MG	VC	3488	1/1	0.69	0.07	92,92,92,92	0
55	MG	VC	3288	1/1	0.69	0.18	107,107,107,107	0
55	MG	UC	1738	1/1	0.69	0.33	118,118,118,118	0
55	MG	VC	3101	1/1	0.69	0.19	86,86,86,86	0
55	MG	UC	1704	1/1	0.69	0.10	128,128,128,128	0
55	MG	ZC	3750	1/1	0.69	0.13	89,89,89,89	0
55	MG	VC	3390	1/1	0.69	0.21	116,116,116,116	0
55	MG	ZC	3759	1/1	0.69	0.13	140,140,140,140	0
55	MG	ZC	3078	1/1	0.69	0.23	99,99,99,99	0
55	MG	ZC	3598	1/1	0.69	0.12	99,99,99,99	0
55	MG	YC	1623	1/1	0.69	0.18	104,104,104,104	0
55	MG	VC	3082	1/1	0.69	0.20	96,96,96,96	0
55	MG	VC	3170	1/1	0.69	0.27	89,89,89,89	0
55	MG	FD	110	1/1	0.69	0.20	148,148,148,148	0
55	MG	WA	301	1/1	0.69	0.34	78,78,78,78	0
55	MG	VC	3357	1/1	0.69	0.16	118,118,118,118	0
55	MG	WC	222	1/1	0.69	0.13	157,157,157,157	0
55	MG	VC	3685	1/1	0.69	0.33	81,81,81,81	0
55	MG	HD	101	1/1	0.69	0.19	156,156,156,156	0
55	MG	ZC	3764	1/1	0.70	0.07	105,105,105,105	0
55	MG	UC	1830	1/1	0.70	0.07	118,118,118,118	0
55	MG	WC	226	1/1	0.70	0.08	175,175,175,175	0
55	MG	UC	1767	1/1	0.70	0.11	134,134,134,134	0
55	MG	VC	3506	1/1	0.70	0.17	136,136,136,136	0
55	MG	ZC	3068	1/1	0.70	0.31	61,61,61,61	0
55	MG	VC	3604	1/1	0.70	0.11	125,125,125,125	0
55	MG	UC	1706	1/1	0.70	0.15	98,98,98,98	0
55	MG	YC	1774	1/1	0.70	0.19	143,143,143,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	VC	3018	1/1	0.70	0.25	116,116,116,116	0
55	MG	ZC	3410	1/1	0.70	0.10	134,134,134,134	0
55	MG	ZC	3504	1/1	0.70	0.14	99,99,99,99	0
55	MG	VC	3047	1/1	0.70	0.26	78,78,78,78	0
55	MG	ZC	3362	1/1	0.70	0.15	88,88,88,88	0
55	MG	VC	3556	1/1	0.70	0.13	129,129,129,129	0
55	MG	ZC	3508	1/1	0.70	0.18	190,190,190,190	0
55	MG	VC	3137	1/1	0.70	0.17	127,127,127,127	0
55	MG	VC	3614	1/1	0.70	0.15	99,99,99,99	0
55	MG	VC	3021	1/1	0.70	0.29	88,88,88,88	0
55	MG	ZC	3456	1/1	0.70	0.14	77,77,77,77	0
55	MG	ZC	3240	1/1	0.70	0.19	63,63,63,63	0
55	MG	YC	1666	1/1	0.70	0.14	134,134,134,134	0
55	MG	UC	1750	1/1	0.70	0.20	100,100,100,100	0
55	MG	ZC	3176	1/1	0.70	0.26	77,77,77,77	0
55	MG	ZC	3112	1/1	0.70	0.26	87,87,87,87	0
55	MG	ZC	3537	1/1	0.71	0.10	105,105,105,105	0
55	MG	VC	3116	1/1	0.71	0.30	92,92,92,92	0
55	MG	VC	3641	1/1	0.71	0.08	114,114,114,114	0
55	MG	UC	1675	1/1	0.71	0.37	103,103,103,103	0
55	MG	VC	3412	1/1	0.71	0.19	98,98,98,98	0
55	MG	ZC	3555	1/1	0.71	0.08	131,131,131,131	0
55	MG	ZC	3396	1/1	0.71	0.13	114,114,114,114	0
55	MG	YC	1787	1/1	0.71	0.27	198,198,198,198	0
55	MG	UC	1691	1/1	0.71	0.10	103,103,103,103	0
55	MG	VC	3224	1/1	0.71	0.09	129,129,129,129	0
55	MG	YC	1638	1/1	0.71	0.21	135,135,135,135	0
55	MG	VC	3568	1/1	0.71	0.19	102,102,102,102	0
55	MG	ZC	3287	1/1	0.71	0.13	85,85,85,85	0
55	MG	AD	213	1/1	0.71	0.14	121,121,121,121	0
55	MG	UC	1692	1/1	0.71	0.32	94,94,94,94	0
55	MG	ZC	3602	1/1	0.71	0.13	95,95,95,95	0
55	MG	YC	1867	1/1	0.71	0.10	198,198,198,198	0
55	MG	ZC	3291	1/1	0.71	0.14	167,167,167,167	0
55	MG	VC	3669	1/1	0.71	0.13	133,133,133,133	0
55	MG	ZC	3427	1/1	0.71	0.11	95,95,95,95	0
55	MG	VC	3671	1/1	0.71	0.33	92,92,92,92	0
55	MG	ZC	3161	1/1	0.71	0.14	96,96,96,96	0
55	MG	VC	3085	1/1	0.71	0.17	77,77,77,77	0
55	MG	UC	1614	1/1	0.71	0.19	130,130,130,130	0
55	MG	AD	230	1/1	0.71	0.17	104,104,104,104	0
55	MG	ZC	3171	1/1	0.71	0.20	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	ZC	3463	1/1	0.71	0.14	103,103,103,103	0
55	MG	UC	1606	1/1	0.71	0.30	104,104,104,104	0
55	MG	UC	1729	1/1	0.71	0.26	92,92,92,92	0
55	MG	UC	1844	1/1	0.71	0.12	117,117,117,117	0
55	MG	VC	3374	1/1	0.71	0.22	96,96,96,96	0
55	MG	ZC	3652	1/1	0.71	0.33	86,86,86,86	0
55	MG	ZC	3482	1/1	0.71	0.18	100,100,100,100	0
55	MG	VC	3510	1/1	0.71	0.13	77,77,77,77	0
55	MG	ZC	3342	1/1	0.71	0.30	78,78,78,78	0
55	MG	UC	1824	1/1	0.71	0.15	120,120,120,120	0
55	MG	AC	302	1/1	0.71	0.22	164,164,164,164	0
55	MG	EB	202	1/1	0.71	0.25	89,89,89,89	0
55	MG	ZC	3674	1/1	0.71	0.09	74,74,74,74	0
55	MG	YC	1828	1/1	0.71	0.14	186,186,186,186	0
55	MG	UC	1852	1/1	0.71	0.17	207,207,207,207	0
55	MG	UC	1664	1/1	0.71	0.08	183,183,183,183	0
55	MG	UC	1601	1/1	0.71	0.24	163,163,163,163	0
55	MG	ZC	3220	1/1	0.71	0.13	73,73,73,73	0
55	MG	YC	1836	1/1	0.71	0.10	106,106,106,106	0
55	MG	VC	3389	1/1	0.71	0.15	83,83,83,83	0
55	MG	VC	3334	1/1	0.71	0.26	91,91,91,91	0
55	MG	VC	3103	1/1	0.71	0.24	85,85,85,85	0
55	MG	ZC	3510	1/1	0.71	0.14	84,84,84,84	0
55	MG	ZC	3372	1/1	0.71	0.12	132,132,132,132	0
55	MG	UC	1806	1/1	0.71	0.07	102,102,102,102	0
55	MG	VC	3027	1/1	0.71	0.26	82,82,82,82	0
55	MG	VC	3112	1/1	0.71	0.27	81,81,81,81	0
55	MG	VC	3555	1/1	0.71	0.24	82,82,82,82	0
55	MG	UC	1702	1/1	0.71	0.17	151,151,151,151	0
55	MG	ZC	3334	1/1	0.72	0.21	68,68,68,68	0
55	MG	VC	3373	1/1	0.72	0.08	101,101,101,101	0
55	MG	VC	3185	1/1	0.72	0.22	97,97,97,97	0
55	MG	ZC	3125	1/1	0.72	0.18	89,89,89,89	0
55	MG	YC	1722	1/1	0.72	0.24	131,131,131,131	0
55	MG	AD	228	1/1	0.72	0.07	91,91,91,91	0
55	MG	ZC	3002	1/1	0.72	0.21	82,82,82,82	0
55	MG	UC	1680	1/1	0.72	0.27	107,107,107,107	0
55	MG	WC	219	1/1	0.72	0.20	131,131,131,131	0
55	MG	VC	3304	1/1	0.72	0.20	91,91,91,91	0
55	MG	VC	3146	1/1	0.72	0.19	79,79,79,79	0
55	MG	VC	3561	1/1	0.72	0.19	92,92,92,92	0
55	MG	FB	203	1/1	0.72	0.14	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	Y	101	1/1	0.72	0.20	124,124,124,124	0
55	MG	ZC	3154	1/1	0.72	0.28	95,95,95,95	0
55	MG	ZC	3273	1/1	0.72	0.14	72,72,72,72	0
55	MG	UC	1661	1/1	0.72	0.07	127,127,127,127	0
55	MG	VC	3274	1/1	0.72	0.16	100,100,100,100	0
55	MG	VC	3526	1/1	0.72	0.19	97,97,97,97	0
55	MG	UC	1784	1/1	0.72	0.09	138,138,138,138	0
55	MG	UC	1770	1/1	0.72	0.09	130,130,130,130	0
55	MG	VC	3485	1/1	0.72	0.09	107,107,107,107	0
55	MG	VC	3537	1/1	0.72	0.13	119,119,119,119	0
55	MG	ZC	3182	1/1	0.72	0.20	72,72,72,72	0
55	MG	ZC	3632	1/1	0.72	0.10	97,97,97,97	0
55	MG	YC	1748	1/1	0.72	0.12	160,160,160,160	0
55	MG	VC	3654	1/1	0.72	0.24	98,98,98,98	0
55	MG	VC	3232	1/1	0.72	0.12	164,164,164,164	0
55	MG	ZC	3398	1/1	0.72	0.25	93,93,93,93	0
55	MG	VC	3172	1/1	0.72	0.14	81,81,81,81	0
55	MG	YC	1674	1/1	0.72	0.09	138,138,138,138	0
55	MG	VC	3664	1/1	0.72	0.09	180,180,180,180	0
55	MG	AD	212	1/1	0.72	0.14	118,118,118,118	0
55	MG	UC	1602	1/1	0.72	0.11	124,124,124,124	0
55	MG	YC	1712	1/1	0.72	0.08	153,153,153,153	0
55	MG	YC	1861	1/1	0.72	0.16	136,136,136,136	0
55	MG	UC	1821	1/1	0.72	0.10	103,103,103,103	0
55	MG	HB	202	1/1	0.72	0.10	82,82,82,82	0
55	MG	ZC	3395	1/1	0.73	0.14	105,105,105,105	0
55	MG	UC	1795	1/1	0.73	0.12	97,97,97,97	0
55	MG	UC	1678	1/1	0.73	0.25	106,106,106,106	0
55	MG	H	201	1/1	0.73	0.22	117,117,117,117	0
55	MG	ZC	3099	1/1	0.73	0.25	72,72,72,72	0
55	MG	ZC	3512	1/1	0.73	0.18	84,84,84,84	0
55	MG	VC	3474	1/1	0.73	0.16	100,100,100,100	0
55	MG	VC	3478	1/1	0.73	0.10	94,94,94,94	0
55	MG	ZC	3524	1/1	0.73	0.15	94,94,94,94	0
55	MG	VC	3359	1/1	0.73	0.21	102,102,102,102	0
55	MG	YC	1761	1/1	0.73	0.11	163,163,163,163	0
55	MG	UC	1715	1/1	0.73	0.28	120,120,120,120	0
55	MG	VC	3433	1/1	0.73	0.15	114,114,114,114	0
55	MG	VC	3017	1/1	0.73	0.31	97,97,97,97	0
55	MG	UC	1762	1/1	0.73	0.19	105,105,105,105	0
55	MG	ZC	3541	1/1	0.73	0.07	249,249,249,249	0
55	MG	YC	1813	1/1	0.73	0.17	231,231,231,231	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	YC	1767	1/1	0.73	0.16	116,116,116,116	0
55	MG	ZC	3552	1/1	0.73	0.12	190,190,190,190	0
55	MG	ZC	3245	1/1	0.73	0.16	71,71,71,71	0
55	MG	ZC	3440	1/1	0.73	0.23	95,95,95,95	0
55	MG	ZC	3007	1/1	0.73	0.13	72,72,72,72	0
55	MG	YC	1768	1/1	0.73	0.12	168,168,168,168	0
55	MG	VC	3539	1/1	0.73	0.13	109,109,109,109	0
55	MG	VC	3333	1/1	0.73	0.27	105,105,105,105	0
55	MG	ZC	3147	1/1	0.73	0.31	85,85,85,85	0
55	MG	YC	1661	1/1	0.73	0.12	142,142,142,142	0
55	MG	YC	1731	1/1	0.73	0.08	170,170,170,170	0
55	MG	ZC	3473	1/1	0.73	0.17	87,87,87,87	0
55	MG	YC	1662	1/1	0.73	0.17	118,118,118,118	0
55	MG	UC	1751	1/1	0.73	0.16	129,129,129,129	0
55	MG	YC	1736	1/1	0.73	0.17	137,137,137,137	0
55	MG	ZC	3769	1/1	0.73	0.47	115,115,115,115	0
55	MG	VC	3592	1/1	0.73	0.07	95,95,95,95	0
55	MG	VC	3307	1/1	0.73	0.21	98,98,98,98	0
55	MG	VC	3404	1/1	0.73	0.09	161,161,161,161	0
55	MG	VC	3068	1/1	0.73	0.17	128,128,128,128	0
55	MG	AD	205	1/1	0.73	0.29	117,117,117,117	0
55	MG	UC	1753	1/1	0.73	0.08	94,94,94,94	0
55	MG	UC	1832	1/1	0.73	0.06	108,108,108,108	0
55	MG	UC	1652	1/1	0.73	0.08	140,140,140,140	0
55	MG	VC	3133	1/1	0.73	0.33	86,86,86,86	0
55	MG	YC	1673	1/1	0.73	0.10	119,119,119,119	0
55	MG	AD	211	1/1	0.73	0.17	105,105,105,105	0
55	MG	VC	3094	1/1	0.74	0.12	130,130,130,130	0
55	MG	VC	3270	1/1	0.74	0.07	81,81,81,81	0
55	MG	YC	1763	1/1	0.74	0.23	161,161,161,161	0
55	MG	VC	3425	1/1	0.74	0.14	95,95,95,95	0
55	MG	YC	1725	1/1	0.74	0.24	126,126,126,126	0
55	MG	ZC	3113	1/1	0.74	0.16	93,93,93,93	0
55	MG	UC	1794	1/1	0.74	0.07	105,105,105,105	0
55	MG	ZC	3325	1/1	0.74	0.26	93,93,93,93	0
55	MG	P	201	1/1	0.74	0.43	96,96,96,96	0
55	MG	YC	1868	1/1	0.74	0.11	179,179,179,179	0
55	MG	VC	3147	1/1	0.74	0.12	129,129,129,129	0
55	MG	ZC	3679	1/1	0.74	0.12	84,84,84,84	0
55	MG	ZC	3426	1/1	0.74	0.11	85,85,85,85	0
55	MG	UC	1761	1/1	0.74	0.17	113,113,113,113	0
55	MG	ZC	3237	1/1	0.74	0.11	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	VC	3528	1/1	0.74	0.11	121,121,121,121	0
55	MG	YC	1733	1/1	0.74	0.12	69,69,69,69	0
55	MG	ZC	3446	1/1	0.74	0.15	121,121,121,121	0
55	MG	UC	1857	1/1	0.74	0.09	107,107,107,107	0
55	MG	VC	3029	1/1	0.74	0.16	93,93,93,93	0
55	MG	VC	3241	1/1	0.74	0.07	124,124,124,124	0
55	MG	ZC	3257	1/1	0.74	0.13	104,104,104,104	0
55	MG	VC	3638	1/1	0.74	0.21	112,112,112,112	0
55	MG	UC	1842	1/1	0.74	0.15	103,103,103,103	0
55	MG	VC	3583	1/1	0.74	0.17	130,130,130,130	0
55	MG	UC	1660	1/1	0.74	0.24	76,76,76,76	0
55	MG	UC	1623	1/1	0.74	0.32	119,119,119,119	0
55	MG	ZC	3059	1/1	0.74	0.33	79,79,79,79	0
55	MG	ZC	3483	1/1	0.74	0.10	96,96,96,96	0
55	MG	VC	3653	1/1	0.74	0.10	116,116,116,116	0
55	MG	VC	3590	1/1	0.74	0.12	140,140,140,140	0
55	MG	VC	3291	1/1	0.74	0.16	102,102,102,102	0
55	MG	ZC	3766	1/1	0.74	0.12	82,82,82,82	0
55	MG	UC	1801	1/1	0.74	0.23	107,107,107,107	0
55	MG	ZC	3773	1/1	0.74	0.08	112,112,112,112	0
55	MG	ZC	3625	1/1	0.74	0.13	117,117,117,117	0
55	MG	YC	1611	1/1	0.74	0.19	110,110,110,110	0
55	MG	ZC	3072	1/1	0.74	0.27	91,91,91,91	0
55	MG	YC	1753	1/1	0.74	0.32	169,169,169,169	0
55	MG	UC	1719	1/1	0.74	0.17	89,89,89,89	0
55	MG	VC	3142	1/1	0.74	0.25	84,84,84,84	0
55	MG	ZC	3634	1/1	0.74	0.15	95,95,95,95	0
55	MG	WC	213	1/1	0.74	0.17	110,110,110,110	0
55	MG	ZC	3297	1/1	0.74	0.11	100,100,100,100	0
55	MG	VC	3309	1/1	0.74	0.20	94,94,94,94	0
55	MG	ZC	3120	1/1	0.75	0.25	78,78,78,78	0
55	MG	VC	3015	1/1	0.75	0.14	81,81,81,81	0
55	MG	UC	1745	1/1	0.75	0.23	106,106,106,106	0
55	MG	VC	3647	1/1	0.75	0.32	87,87,87,87	0
55	MG	YC	1707	1/1	0.75	0.14	131,131,131,131	0
55	MG	UC	1713	1/1	0.75	0.19	109,109,109,109	0
55	MG	ZC	3520	1/1	0.75	0.17	82,82,82,82	0
55	MG	VC	3104	1/1	0.75	0.09	142,142,142,142	0
55	MG	ZC	3242	1/1	0.75	0.18	90,90,90,90	0
55	MG	ZC	3417	1/1	0.75	0.11	86,86,86,86	0
55	MG	ZC	3660	1/1	0.75	0.16	111,111,111,111	0
55	MG	ZC	3662	1/1	0.75	0.13	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	UC	1641	1/1	0.75	0.17	98,98,98,98	0
55	MG	UC	1853	1/1	0.75	0.17	108,108,108,108	0
55	MG	VC	3141	1/1	0.75	0.17	92,92,92,92	0
55	MG	ZC	3251	1/1	0.75	0.13	85,85,85,85	0
55	MG	ZC	3431	1/1	0.75	0.33	130,130,130,130	0
55	MG	ZC	3694	1/1	0.75	0.11	120,120,120,120	0
55	MG	ZC	3436	1/1	0.75	0.19	109,109,109,109	0
55	MG	UC	1755	1/1	0.75	0.14	129,129,129,129	0
55	MG	YC	1649	1/1	0.75	0.12	116,116,116,116	0
55	MG	ZC	3445	1/1	0.75	0.14	106,106,106,106	0
55	MG	ZC	3355	1/1	0.75	0.09	78,78,78,78	0
55	MG	VC	3257	1/1	0.75	0.12	101,101,101,101	0
55	MG	VC	3298	1/1	0.75	0.28	60,60,60,60	0
55	MG	ZC	3564	1/1	0.75	0.10	105,105,105,105	0
55	MG	ZC	3155	1/1	0.75	0.22	69,69,69,69	0
55	MG	YC	1853	1/1	0.75	0.16	137,137,137,137	0
55	MG	VC	3340	1/1	0.75	0.11	128,128,128,128	0
55	MG	ZC	3075	1/1	0.75	0.29	94,94,94,94	0
55	MG	ZC	3582	1/1	0.75	0.10	95,95,95,95	0
55	MG	UC	1764	1/1	0.75	0.09	151,151,151,151	0
55	MG	UC	1765	1/1	0.75	0.23	107,107,107,107	0
55	MG	ZC	3373	1/1	0.75	0.16	72,72,72,72	0
55	MG	VC	3471	1/1	0.75	0.10	142,142,142,142	0
55	MG	VC	3515	1/1	0.75	0.10	134,134,134,134	0
55	MG	VC	3563	1/1	0.75	0.19	89,89,89,89	0
55	MG	O	202	1/1	0.75	0.25	113,113,113,113	0
55	MG	UC	1662	1/1	0.75	0.16	92,92,92,92	0
55	MG	VC	3128	1/1	0.75	0.29	71,71,71,71	0
55	MG	ZC	3107	1/1	0.75	0.27	65,65,65,65	0
55	MG	VC	3576	1/1	0.75	0.09	122,122,122,122	0
55	MG	VC	3429	1/1	0.75	0.11	117,117,117,117	0
55	MG	VC	3634	1/1	0.75	0.12	115,115,115,115	0
55	MG	AD	204	1/1	0.75	0.25	110,110,110,110	0
55	MG	VC	3233	1/1	0.75	0.11	165,165,165,165	0
55	MG	ZC	3020	1/1	0.75	0.10	71,71,71,71	0
55	MG	VC	3277	1/1	0.75	0.21	75,75,75,75	0
55	MG	ZC	3263	1/1	0.76	0.18	76,76,76,76	0
55	MG	ZC	3264	1/1	0.76	0.63	121,121,121,121	0
55	MG	ZC	3141	1/1	0.76	0.19	100,100,100,100	0
55	MG	ZC	3380	1/1	0.76	0.13	108,108,108,108	0
55	MG	VC	3262	1/1	0.76	0.20	82,82,82,82	0
55	MG	ZC	3041	1/1	0.76	0.21	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	VC	3635	1/1	0.76	0.14	108,108,108,108	0
55	MG	YC	1770	1/1	0.76	0.05	149,149,149,149	0
55	MG	VC	3148	1/1	0.76	0.07	137,137,137,137	0
55	MG	YC	1605	1/1	0.76	0.13	114,114,114,114	0
55	MG	YC	1606	1/1	0.76	0.19	131,131,131,131	0
55	MG	VC	3365	1/1	0.76	0.19	101,101,101,101	0
55	MG	VC	3400	1/1	0.76	0.15	120,120,120,120	0
55	MG	YC	1734	1/1	0.76	0.12	170,170,170,170	0
55	MG	VC	3438	1/1	0.76	0.24	112,112,112,112	0
55	MG	BA	102	1/1	0.76	0.21	87,87,87,87	0
55	MG	ZC	3513	1/1	0.76	0.10	86,86,86,86	0
55	MG	VC	3587	1/1	0.76	0.15	92,92,92,92	0
55	MG	UC	1843	1/1	0.76	0.12	156,156,156,156	0
55	MG	VC	3237	1/1	0.76	0.20	109,109,109,109	0
55	MG	ZC	3302	1/1	0.76	0.24	69,69,69,69	0
55	MG	YC	1618	1/1	0.76	0.06	132,132,132,132	0
55	MG	VC	3372	1/1	0.76	0.18	107,107,107,107	0
55	MG	ZC	3084	1/1	0.76	0.23	81,81,81,81	0
55	MG	UC	1772	1/1	0.76	0.12	85,85,85,85	0
55	MG	ZC	3090	1/1	0.76	0.20	70,70,70,70	0
55	MG	VC	3105	1/1	0.76	0.26	102,102,102,102	0
55	MG	ZC	3096	1/1	0.76	0.17	93,93,93,93	0
55	MG	VC	3598	1/1	0.76	0.17	84,84,84,84	0
55	MG	ZC	3547	1/1	0.76	0.09	126,126,126,126	0
55	MG	ZC	3715	1/1	0.76	0.13	112,112,112,112	0
55	MG	VC	3375	1/1	0.76	0.06	125,125,125,125	0
55	MG	YA	302	1/1	0.76	0.23	91,91,91,91	0
55	MG	ZC	3433	1/1	0.76	0.10	93,93,93,93	0
55	MG	ZC	3104	1/1	0.76	0.20	67,67,67,67	0
55	MG	VC	3458	1/1	0.76	0.15	80,80,80,80	0
55	MG	ZC	3561	1/1	0.76	0.07	103,103,103,103	0
55	MG	YC	1797	1/1	0.76	0.19	130,130,130,130	0
55	MG	UC	1628	1/1	0.76	0.12	107,107,107,107	0
55	MG	ZC	3746	1/1	0.76	0.15	81,81,81,81	0
55	MG	J	201	1/1	0.76	0.24	117,117,117,117	0
55	MG	VC	3470	1/1	0.76	0.29	83,83,83,83	0
55	MG	VC	3022	1/1	0.76	0.15	91,91,91,91	0
55	MG	WC	227	1/1	0.76	0.10	89,89,89,89	0
55	MG	ZC	3584	1/1	0.76	0.17	115,115,115,115	0
55	MG	FB	204	1/1	0.76	0.16	56,56,56,56	0
55	MG	VC	3569	1/1	0.76	0.14	116,116,116,116	0
55	MG	FD	109	1/1	0.76	0.12	145,145,145,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	ZC	3124	1/1	0.76	0.28	77,77,77,77	0
55	MG	YC	1718	1/1	0.76	0.10	156,156,156,156	0
55	MG	RA	201	1/1	0.76	0.16	105,105,105,105	0
55	MG	VC	3631	1/1	0.76	0.19	82,82,82,82	0
55	MG	UC	1701	1/1	0.76	0.17	99,99,99,99	0
55	MG	V	101	1/1	0.76	0.35	90,90,90,90	0
55	MG	UC	1810	1/1	0.77	0.11	104,104,104,104	0
55	MG	ZC	3522	1/1	0.77	0.16	78,78,78,78	0
55	MG	ZC	3073	1/1	0.77	0.32	52,52,52,52	0
55	MG	YC	1796	1/1	0.77	0.20	166,166,166,166	0
55	MG	WA	302	1/1	0.77	0.11	83,83,83,83	0
55	MG	UC	1789	1/1	0.77	0.11	88,88,88,88	0
55	MG	ZC	3358	1/1	0.77	0.17	91,91,91,91	0
55	MG	VC	3542	1/1	0.77	0.14	171,171,171,171	0
55	MG	VC	3424	1/1	0.77	0.22	95,95,95,95	0
55	MG	ZC	3443	1/1	0.77	0.19	76,76,76,76	0
55	MG	ZC	3543	1/1	0.77	0.08	80,80,80,80	0
55	MG	ZC	3085	1/1	0.77	0.19	112,112,112,112	0
55	MG	VC	3258	1/1	0.77	0.31	102,102,102,102	0
55	MG	AD	220	1/1	0.77	0.18	121,121,121,121	0
55	MG	ZC	3448	1/1	0.77	0.09	98,98,98,98	0
55	MG	VC	3115	1/1	0.77	0.29	91,91,91,91	0
55	MG	ZC	3681	1/1	0.77	0.13	89,89,89,89	0
55	MG	VC	3395	1/1	0.77	0.15	101,101,101,101	0
55	MG	YC	1810	1/1	0.77	0.13	126,126,126,126	0
55	MG	ZC	3701	1/1	0.77	0.11	90,90,90,90	0
55	MG	ZC	3556	1/1	0.77	0.13	89,89,89,89	0
55	MG	VC	3553	1/1	0.77	0.13	88,88,88,88	0
55	MG	YC	1694	1/1	0.77	0.08	179,179,179,179	0
55	MG	VC	3509	1/1	0.77	0.16	118,118,118,118	0
55	MG	ZC	3717	1/1	0.77	0.05	91,91,91,91	0
55	MG	VC	3078	1/1	0.77	0.14	141,141,141,141	0
55	MG	ZC	3198	1/1	0.77	0.12	116,116,116,116	0
55	MG	YC	1816	1/1	0.77	0.13	106,106,106,106	0
55	MG	VC	3118	1/1	0.77	0.23	78,78,78,78	0
55	MG	ZC	3386	1/1	0.77	0.06	79,79,79,79	0
55	MG	VC	3079	1/1	0.77	0.21	78,78,78,78	0
55	MG	VC	3652	1/1	0.77	0.13	125,125,125,125	0
55	MG	ZC	3212	1/1	0.77	0.24	77,77,77,77	0
55	MG	VC	3054	1/1	0.77	0.17	83,83,83,83	0
55	MG	ZC	3748	1/1	0.77	0.06	117,117,117,117	0
55	MG	YC	1830	1/1	0.77	0.12	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	VC	3599	1/1	0.77	0.27	84,84,84,84	0
55	MG	YC	1833	1/1	0.77	0.12	97,97,97,97	0
55	MG	WA	305	1/1	0.77	0.08	86,86,86,86	0
55	MG	VC	3519	1/1	0.77	0.10	72,72,72,72	0
55	MG	VC	3042	1/1	0.77	0.32	74,74,74,74	0
55	MG	ZC	3762	1/1	0.77	0.17	85,85,85,85	0
55	MG	VC	3090	1/1	0.77	0.18	121,121,121,121	0
55	MG	ZC	3765	1/1	0.77	0.30	74,74,74,74	0
55	MG	YC	1786	1/1	0.77	0.20	85,85,85,85	0
55	MG	ZC	3767	1/1	0.77	0.12	85,85,85,85	0
55	MG	VC	3242	1/1	0.77	0.23	94,94,94,94	0
55	MG	EA	302	1/1	0.77	0.09	134,134,134,134	0
55	MG	RC	101	1/1	0.77	0.25	162,162,162,162	0
55	MG	VC	3676	1/1	0.77	0.14	127,127,127,127	0
55	MG	VC	3033	1/1	0.77	0.28	78,78,78,78	0
55	MG	VC	3620	1/1	0.77	0.17	103,103,103,103	0
55	MG	ZC	3420	1/1	0.77	0.14	83,83,83,83	0
55	MG	UC	1620	1/1	0.78	0.16	158,158,158,158	0
55	MG	ZC	3106	1/1	0.78	0.22	77,77,77,77	0
55	MG	YC	1742	1/1	0.78	0.29	106,106,106,106	0
55	MG	VC	3053	1/1	0.78	0.27	79,79,79,79	0
55	MG	ZC	3553	1/1	0.78	0.15	151,151,151,151	0
55	MG	VC	3594	1/1	0.78	0.11	85,85,85,85	0
55	MG	ZC	3683	1/1	0.78	0.09	87,87,87,87	0
55	MG	ZC	3684	1/1	0.78	0.17	79,79,79,79	0
55	MG	ZC	3690	1/1	0.78	0.14	98,98,98,98	0
55	MG	AD	219	1/1	0.78	0.13	106,106,106,106	0
55	MG	ZC	3378	1/1	0.78	0.29	82,82,82,82	0
55	MG	VC	3439	1/1	0.78	0.15	77,77,77,77	0
55	MG	UC	1632	1/1	0.78	0.20	118,118,118,118	0
55	MG	VC	3297	1/1	0.78	0.15	117,117,117,117	0
55	MG	ZC	3290	1/1	0.78	0.21	102,102,102,102	0
55	MG	UC	1659	1/1	0.78	0.13	106,106,106,106	0
55	MG	VC	3060	1/1	0.78	0.27	71,71,71,71	0
55	MG	VC	3279	1/1	0.78	0.11	115,115,115,115	0
55	MG	C	302	1/1	0.78	0.08	108,108,108,108	0
55	MG	UC	1780	1/1	0.78	0.15	112,112,112,112	0
55	MG	VC	3572	1/1	0.78	0.09	131,131,131,131	0
55	MG	ZC	3305	1/1	0.78	0.23	71,71,71,71	0
55	MG	VC	3494	1/1	0.78	0.13	89,89,89,89	0
55	MG	VC	3339	1/1	0.78	0.12	102,102,102,102	0
55	MG	ZC	3599	1/1	0.78	0.22	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	ZC	3313	1/1	0.78	0.09	128,128,128,128	0
55	MG	YC	1800	1/1	0.78	0.18	173,173,173,173	0
55	MG	VC	3119	1/1	0.78	0.22	92,92,92,92	0
55	MG	VC	3616	1/1	0.78	0.32	92,92,92,92	0
55	MG	VC	3673	1/1	0.78	0.17	82,82,82,82	0
55	MG	WC	217	1/1	0.78	0.10	155,155,155,155	0
55	MG	ZC	3148	1/1	0.78	0.38	56,56,56,56	0
55	MG	ZC	3246	1/1	0.78	0.14	105,105,105,105	0
55	MG	ZC	3340	1/1	0.78	0.15	91,91,91,91	0
55	MG	ED	111	1/1	0.78	0.11	170,170,170,170	0
55	MG	VC	3152	1/1	0.78	0.17	132,132,132,132	0
55	MG	ZC	3514	1/1	0.78	0.23	106,106,106,106	0
55	MG	VC	3504	1/1	0.78	0.10	202,202,202,202	0
55	MG	YC	1860	1/1	0.78	0.14	104,104,104,104	0
55	MG	VC	3430	1/1	0.78	0.10	96,96,96,96	0
55	MG	VC	3189	1/1	0.78	0.11	60,60,60,60	0
55	MG	VC	3683	1/1	0.78	0.08	84,84,84,84	0
55	MG	VC	3550	1/1	0.78	0.16	127,127,127,127	0
55	MG	FD	107	1/1	0.78	0.11	123,123,123,123	0
55	MG	VC	3320	1/1	0.78	0.09	113,113,113,113	0
55	MG	ZC	3265	1/1	0.78	0.18	78,78,78,78	0
55	MG	ZC	3530	1/1	0.78	0.10	87,87,87,87	0
55	MG	UC	1619	1/1	0.78	0.09	127,127,127,127	0
55	MG	ZC	3169	1/1	0.78	0.41	78,78,78,78	0
55	MG	VC	3695	1/1	0.78	0.41	83,83,83,83	0
55	MG	VC	3351	1/1	0.78	0.16	84,84,84,84	0
55	MG	YC	1698	1/1	0.78	0.09	140,140,140,140	0
55	MG	VC	3260	1/1	0.79	0.21	77,77,77,77	0
55	MG	ZC	3222	1/1	0.79	0.10	69,69,69,69	0
55	MG	VC	3605	1/1	0.79	0.15	112,112,112,112	0
55	MG	VC	3028	1/1	0.79	0.23	76,76,76,76	0
55	MG	ZC	3228	1/1	0.79	0.12	89,89,89,89	0
55	MG	ZC	3116	1/1	0.79	0.18	80,80,80,80	0
55	MG	ZC	3608	1/1	0.79	0.08	134,134,134,134	0
55	MG	ZC	3354	1/1	0.79	0.08	109,109,109,109	0
55	MG	ZC	3612	1/1	0.79	0.08	85,85,85,85	0
55	MG	YC	1719	1/1	0.79	0.15	118,118,118,118	0
55	MG	UC	1851	1/1	0.79	0.16	113,113,113,113	0
55	MG	ZC	3478	1/1	0.79	0.12	88,88,88,88	0
55	MG	ZC	3016	1/1	0.79	0.29	71,71,71,71	0
55	MG	ZC	3121	1/1	0.79	0.22	89,89,89,89	0
55	MG	VC	3566	1/1	0.79	0.08	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	VC	3175	1/1	0.79	0.23	81,81,81,81	0
55	MG	VC	3294	1/1	0.79	0.30	73,73,73,73	0
55	MG	ZC	3127	1/1	0.79	0.21	73,73,73,73	0
55	MG	VC	3570	1/1	0.79	0.08	105,105,105,105	0
55	MG	VC	3399	1/1	0.79	0.11	109,109,109,109	0
55	MG	VC	3573	1/1	0.79	0.09	143,143,143,143	0
55	MG	VC	3624	1/1	0.79	0.07	104,104,104,104	0
55	MG	ZC	3135	1/1	0.79	0.12	77,77,77,77	0
55	MG	VC	3204	1/1	0.79	0.22	80,80,80,80	0
55	MG	ZC	3051	1/1	0.79	0.11	79,79,79,79	0
55	MG	UC	1711	1/1	0.79	0.11	150,150,150,150	0
55	MG	VC	3300	1/1	0.79	0.29	83,83,83,83	0
55	MG	VC	3338	1/1	0.79	0.17	80,80,80,80	0
55	MG	ZC	3150	1/1	0.79	0.17	81,81,81,81	0
55	MG	UC	1814	1/1	0.79	0.08	107,107,107,107	0
55	MG	OB	201	1/1	0.79	0.09	94,94,94,94	0
55	MG	ZC	3390	1/1	0.79	0.09	105,105,105,105	0
55	MG	YC	1780	1/1	0.79	0.12	142,142,142,142	0
55	MG	VC	3581	1/1	0.79	0.21	90,90,90,90	0
55	MG	UC	1855	1/1	0.79	0.13	121,121,121,121	0
55	MG	ZC	3157	1/1	0.79	0.30	51,51,51,51	0
55	MG	VC	3343	1/1	0.79	0.08	115,115,115,115	0
55	MG	VC	3496	1/1	0.79	0.13	140,140,140,140	0
55	MG	YC	1614	1/1	0.79	0.28	90,90,90,90	0
55	MG	VC	3448	1/1	0.79	0.28	100,100,100,100	0
55	MG	ZC	3685	1/1	0.79	0.08	94,94,94,94	0
55	MG	VC	3278	1/1	0.79	0.12	117,117,117,117	0
55	MG	ZC	3292	1/1	0.79	0.13	64,64,64,64	0
55	MG	ZC	3696	1/1	0.79	0.10	145,145,145,145	0
55	MG	YC	1847	1/1	0.79	0.20	122,122,122,122	0
55	MG	YC	1848	1/1	0.79	0.10	153,153,153,153	0
55	MG	YC	1744	1/1	0.79	0.15	121,121,121,121	0
55	MG	UC	1650	1/1	0.79	0.17	111,111,111,111	0
55	MG	VC	3452	1/1	0.79	0.21	83,83,83,83	0
55	MG	ZC	3711	1/1	0.79	0.12	309,309,309,309	0
55	MG	ED	108	1/1	0.79	0.08	161,161,161,161	0
55	MG	ZC	3713	1/1	0.79	0.08	94,94,94,94	0
55	MG	ZC	3087	1/1	0.79	0.22	83,83,83,83	0
55	MG	ZC	3189	1/1	0.79	0.18	58,58,58,58	0
55	MG	UC	1637	1/1	0.79	0.20	99,99,99,99	0
55	MG	ZC	3723	1/1	0.79	0.11	85,85,85,85	0
55	MG	VC	3110	1/1	0.79	0.34	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	YC	1857	1/1	0.79	0.18	111,111,111,111	0
55	MG	YC	1750	1/1	0.79	0.20	138,138,138,138	0
55	MG	UC	1621	1/1	0.79	0.13	120,120,120,120	0
55	MG	VC	3113	1/1	0.79	0.17	100,100,100,100	0
55	MG	ZC	3211	1/1	0.79	0.34	75,75,75,75	0
55	MG	VC	3663	1/1	0.79	0.10	124,124,124,124	0
55	MG	ZC	3744	1/1	0.79	0.08	99,99,99,99	0
55	MG	VC	3465	1/1	0.79	0.12	95,95,95,95	0
55	MG	ZC	3747	1/1	0.79	0.22	101,101,101,101	0
55	MG	ZC	3568	1/1	0.79	0.21	70,70,70,70	0
55	MG	ZC	3339	1/1	0.79	0.12	90,90,90,90	0
55	MG	VC	3602	1/1	0.79	0.16	113,113,113,113	0
55	MG	UC	1820	1/1	0.79	0.09	114,114,114,114	0
55	MG	ZC	3449	1/1	0.79	0.05	92,92,92,92	0
55	MG	YC	1626	1/1	0.80	0.23	103,103,103,103	0
55	MG	UC	1781	1/1	0.80	0.16	116,116,116,116	0
55	MG	VC	3367	1/1	0.80	0.09	125,125,125,125	0
55	MG	ZC	3655	1/1	0.80	0.18	70,70,70,70	0
55	MG	ZC	3249	1/1	0.80	0.11	105,105,105,105	0
55	MG	ZC	3532	1/1	0.80	0.10	106,106,106,106	0
55	MG	VC	3162	1/1	0.80	0.21	97,97,97,97	0
55	MG	WC	223	1/1	0.80	0.06	172,172,172,172	0
55	MG	UC	1793	1/1	0.80	0.25	129,129,129,129	0
55	MG	UC	1671	1/1	0.80	0.11	138,138,138,138	0
55	MG	VC	3295	1/1	0.80	0.16	104,104,104,104	0
55	MG	VC	3191	1/1	0.80	0.26	107,107,107,107	0
55	MG	VC	3622	1/1	0.80	0.16	102,102,102,102	0
55	MG	ZC	3548	1/1	0.80	0.09	86,86,86,86	0
55	MG	ZC	3267	1/1	0.80	0.10	71,71,71,71	0
55	MG	UC	1707	1/1	0.80	0.28	116,116,116,116	0
55	MG	ZC	3451	1/1	0.80	0.11	85,85,85,85	0
55	MG	ZC	3165	1/1	0.80	0.26	85,85,85,85	0
55	MG	VC	3268	1/1	0.80	0.23	96,96,96,96	0
55	MG	ZC	3692	1/1	0.80	0.06	106,106,106,106	0
55	MG	ZC	3458	1/1	0.80	0.07	98,98,98,98	0
55	MG	VC	3379	1/1	0.80	0.18	88,88,88,88	0
55	MG	ZC	3697	1/1	0.80	0.06	71,71,71,71	0
55	MG	ZC	3559	1/1	0.80	0.17	111,111,111,111	0
55	MG	YA	301	1/1	0.80	0.30	64,64,64,64	0
55	MG	ZC	3001	1/1	0.80	0.38	64,64,64,64	0
55	MG	YC	1817	1/1	0.80	0.15	143,143,143,143	0
55	MG	VC	3235	1/1	0.80	0.24	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	VC	3308	1/1	0.80	0.26	64,64,64,64	0
55	MG	ZC	3574	1/1	0.80	0.34	61,61,61,61	0
55	MG	VC	3167	1/1	0.80	0.08	126,126,126,126	0
55	MG	ZC	3190	1/1	0.80	0.27	62,62,62,62	0
55	MG	VC	3432	1/1	0.80	0.13	112,112,112,112	0
55	MG	ZC	3025	1/1	0.80	0.50	95,95,95,95	0
55	MG	VC	3083	1/1	0.80	0.40	65,65,65,65	0
55	MG	VC	3016	1/1	0.80	0.33	95,95,95,95	0
55	MG	UC	1813	1/1	0.80	0.07	186,186,186,186	0
55	MG	UC	1686	1/1	0.80	0.10	115,115,115,115	0
55	MG	ZC	3601	1/1	0.80	0.07	104,104,104,104	0
55	MG	VC	3394	1/1	0.80	0.34	92,92,92,92	0
55	MG	ZC	3044	1/1	0.80	0.17	70,70,70,70	0
55	MG	VC	3356	1/1	0.80	0.10	102,102,102,102	0
55	MG	VC	3493	1/1	0.80	0.20	84,84,84,84	0
55	MG	H	202	1/1	0.80	0.13	89,89,89,89	0
55	MG	VC	3495	1/1	0.80	0.20	106,106,106,106	0
55	MG	UC	1636	1/1	0.80	0.21	111,111,111,111	0
55	MG	VC	3442	1/1	0.80	0.15	105,105,105,105	0
55	MG	ZC	3755	1/1	0.80	0.09	91,91,91,91	0
55	MG	UC	1723	1/1	0.80	0.08	101,101,101,101	0
55	MG	ZC	3316	1/1	0.80	0.31	68,68,68,68	0
55	MG	VC	3323	1/1	0.80	0.12	79,79,79,79	0
55	MG	ZC	3137	1/1	0.80	0.23	83,83,83,83	0
55	MG	YC	1701	1/1	0.80	0.07	137,137,137,137	0
55	MG	ZC	3238	1/1	0.80	0.49	74,74,74,74	0
55	MG	YC	1702	1/1	0.80	0.13	164,164,164,164	0
55	MG	VC	3251	1/1	0.80	0.19	72,72,72,72	0
55	MG	UC	1818	1/1	0.80	0.17	111,111,111,111	0
55	MG	FD	112	1/1	0.80	0.07	170,170,170,170	0
55	MG	FD	113	1/1	0.80	0.13	145,145,145,145	0
55	MG	ZC	3647	1/1	0.80	0.10	93,93,93,93	0
55	MG	ZC	3772	1/1	0.80	0.10	96,96,96,96	0
55	MG	IB	201	1/1	0.80	0.39	140,140,140,140	0
55	MG	ZC	3423	1/1	0.80	0.17	95,95,95,95	0
55	MG	VC	3155	1/1	0.81	0.21	102,102,102,102	0
55	MG	ZC	3254	1/1	0.81	0.20	76,76,76,76	0
55	MG	YC	1788	1/1	0.81	0.14	126,126,126,126	0
55	MG	ZC	3186	1/1	0.81	0.26	90,90,90,90	0
55	MG	ZC	3461	1/1	0.81	0.19	111,111,111,111	0
55	MG	ZC	3391	1/1	0.81	0.07	105,105,105,105	0
55	MG	VC	3378	1/1	0.81	0.10	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	ZC	3733	1/1	0.81	0.10	127,127,127,127	0
55	MG	ZC	3544	1/1	0.81	0.37	76,76,76,76	0
55	MG	ZC	3130	1/1	0.81	0.20	84,84,84,84	0
55	MG	VC	3182	1/1	0.81	0.26	73,73,73,73	0
55	MG	ZC	3742	1/1	0.81	0.17	72,72,72,72	0
55	MG	ZC	3337	1/1	0.81	0.14	78,78,78,78	0
55	MG	YC	1603	1/1	0.81	0.08	126,126,126,126	0
55	MG	VC	3405	1/1	0.81	0.18	94,94,94,94	0
55	MG	VC	3406	1/1	0.81	0.13	115,115,115,115	0
55	MG	VC	3502	1/1	0.81	0.15	100,100,100,100	0
55	MG	ZC	3405	1/1	0.81	0.38	81,81,81,81	0
55	MG	UC	1700	1/1	0.81	0.17	114,114,114,114	0
55	MG	VC	3070	1/1	0.81	0.26	68,68,68,68	0
55	MG	VC	3211	1/1	0.81	0.12	92,92,92,92	0
55	MG	YC	1612	1/1	0.81	0.22	110,110,110,110	0
55	MG	VC	3341	1/1	0.81	0.07	131,131,131,131	0
55	MG	VC	3195	1/1	0.81	0.23	94,94,94,94	0
55	MG	VC	3249	1/1	0.81	0.27	87,87,87,87	0
55	MG	ED	107	1/1	0.81	0.13	128,128,128,128	0
55	MG	ZC	3671	1/1	0.81	0.08	155,155,155,155	0
55	MG	ZC	3501	1/1	0.81	0.15	86,86,86,86	0
55	MG	YC	1705	1/1	0.81	0.21	99,99,99,99	0
55	MG	VC	3696	1/1	0.81	0.10	126,126,126,126	0
55	MG	ZC	3771	1/1	0.81	0.42	119,119,119,119	0
55	MG	UC	1656	1/1	0.81	0.15	90,90,90,90	0
55	MG	YC	1852	1/1	0.81	0.15	111,111,111,111	0
55	MG	VC	3252	1/1	0.81	0.19	88,88,88,88	0
55	MG	ZC	3586	1/1	0.81	0.19	67,67,67,67	0
55	MG	ZC	3232	1/1	0.81	0.36	73,73,73,73	0
55	MG	UC	1687	1/1	0.81	0.24	107,107,107,107	0
55	MG	VC	3348	1/1	0.81	0.16	107,107,107,107	0
55	MG	YC	1621	1/1	0.81	0.13	178,178,178,178	0
55	MG	ZC	3438	1/1	0.81	0.09	85,85,85,85	0
55	MG	VC	3310	1/1	0.81	0.10	132,132,132,132	0
55	MG	ZC	3700	1/1	0.81	0.06	179,179,179,179	0
55	MG	VC	3618	1/1	0.81	0.15	136,136,136,136	0
55	MG	UC	1742	1/1	0.81	0.11	92,92,92,92	0
55	MG	ZC	3170	1/1	0.81	0.16	82,82,82,82	0
55	MG	VC	3621	1/1	0.81	0.17	101,101,101,101	0
55	MG	VC	3353	1/1	0.81	0.10	72,72,72,72	0
55	MG	ZC	3178	1/1	0.81	0.14	103,103,103,103	0
55	MG	VC	3314	1/1	0.81	0.16	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	VC	3074	1/1	0.82	0.13	104,104,104,104	0
55	MG	ZC	3164	1/1	0.82	0.18	73,73,73,73	0
55	MG	UC	1839	1/1	0.82	0.14	130,130,130,130	0
55	MG	VC	3385	1/1	0.82	0.12	113,113,113,113	0
55	MG	VC	3084	1/1	0.82	0.26	90,90,90,90	0
55	MG	VC	3030	1/1	0.82	0.20	90,90,90,90	0
55	MG	ZC	3308	1/1	0.82	0.17	78,78,78,78	0
55	MG	ZC	3172	1/1	0.82	0.18	68,68,68,68	0
55	MG	ZC	3312	1/1	0.82	0.15	64,64,64,64	0
55	MG	AD	224	1/1	0.82	0.07	155,155,155,155	0
55	MG	ZC	3725	1/1	0.82	0.10	88,88,88,88	0
55	MG	VC	3301	1/1	0.82	0.16	134,134,134,134	0
55	MG	VC	3691	1/1	0.82	0.24	95,95,95,95	0
55	MG	VC	3346	1/1	0.82	0.17	94,94,94,94	0
55	MG	VC	3650	1/1	0.82	0.13	112,112,112,112	0
55	MG	ZC	3734	1/1	0.82	0.11	135,135,135,135	0
55	MG	ZC	3468	1/1	0.82	0.08	74,74,74,74	0
55	MG	VC	3206	1/1	0.82	0.14	65,65,65,65	0
55	MG	ZC	3322	1/1	0.82	0.20	94,94,94,94	0
55	MG	VC	3284	1/1	0.82	0.27	113,113,113,113	0
55	MG	VC	3371	1/1	0.82	0.22	93,93,93,93	0
55	MG	YC	1798	1/1	0.82	0.13	134,134,134,134	0
55	MG	VC	3484	1/1	0.82	0.11	136,136,136,136	0
55	MG	ZC	3335	1/1	0.82	0.17	87,87,87,87	0
55	MG	ZC	3008	1/1	0.82	0.04	104,104,104,104	0
55	MG	ZC	3009	1/1	0.82	0.17	72,72,72,72	0
55	MG	VC	3177	1/1	0.82	0.20	94,94,94,94	0
55	MG	VC	3661	1/1	0.82	0.20	73,73,73,73	0
55	MG	YC	1803	1/1	0.82	0.12	137,137,137,137	0
55	MG	ZC	3661	1/1	0.82	0.14	80,80,80,80	0
55	MG	ZC	3143	1/1	0.82	0.20	84,84,84,84	0
55	MG	ZC	3091	1/1	0.82	0.20	81,81,81,81	0
55	MG	ZC	3567	1/1	0.82	0.14	86,86,86,86	0
55	MG	ZC	3093	1/1	0.82	0.25	76,76,76,76	0
55	MG	ED	112	1/1	0.82	0.11	156,156,156,156	0
55	MG	ZC	3673	1/1	0.82	0.15	95,95,95,95	0
55	MG	VC	3449	1/1	0.82	0.15	90,90,90,90	0
55	MG	VC	3086	1/1	0.82	0.07	116,116,116,116	0
55	MG	UC	1823	1/1	0.82	0.10	162,162,162,162	0
55	MG	VC	3665	1/1	0.82	0.10	78,78,78,78	0
55	MG	ZC	3580	1/1	0.82	0.09	143,143,143,143	0
55	MG	UC	1791	1/1	0.82	0.07	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	VC	3453	1/1	0.82	0.23	77,77,77,77	0
55	MG	ZC	3688	1/1	0.82	0.10	90,90,90,90	0
55	MG	VC	3236	1/1	0.82	0.11	93,93,93,93	0
55	MG	ZC	3591	1/1	0.82	0.12	71,71,71,71	0
55	MG	ZC	3049	1/1	0.82	0.12	102,102,102,102	0
55	MG	VC	3253	1/1	0.82	0.13	117,117,117,117	0
55	MG	VC	3275	1/1	0.82	0.16	91,91,91,91	0
55	MG	ZC	3296	1/1	0.82	0.20	95,95,95,95	0
55	MG	ZC	3518	1/1	0.82	0.07	96,96,96,96	0
55	MG	UC	1822	1/1	0.82	0.13	96,96,96,96	0
55	MG	ZC	3703	1/1	0.82	0.19	90,90,90,90	0
55	MG	ZC	3299	1/1	0.82	0.19	90,90,90,90	0
55	MG	VC	3213	1/1	0.83	0.14	79,79,79,79	0
55	MG	ZC	3645	1/1	0.83	0.07	98,98,98,98	0
55	MG	VC	3675	1/1	0.83	0.23	110,110,110,110	0
55	MG	VC	3259	1/1	0.83	0.13	113,113,113,113	0
55	MG	ZC	3730	1/1	0.83	0.25	71,71,71,71	0
55	MG	ZC	3731	1/1	0.83	0.17	90,90,90,90	0
55	MG	VC	3154	1/1	0.83	0.19	81,81,81,81	0
55	MG	ZC	3010	1/1	0.83	0.20	59,59,59,59	0
55	MG	UC	1804	1/1	0.83	0.20	93,93,93,93	0
55	MG	VC	3681	1/1	0.83	0.33	89,89,89,89	0
55	MG	VC	3637	1/1	0.83	0.20	105,105,105,105	0
55	MG	VC	3217	1/1	0.83	0.18	99,99,99,99	0
55	MG	HB	201	1/1	0.83	0.17	65,65,65,65	0
55	MG	VC	3461	1/1	0.83	0.18	93,93,93,93	0
55	MG	VC	3045	1/1	0.83	0.17	94,94,94,94	0
55	MG	VC	3466	1/1	0.83	0.15	104,104,104,104	0
55	MG	VC	3649	1/1	0.83	0.11	96,96,96,96	0
55	MG	ZC	3221	1/1	0.83	0.17	78,78,78,78	0
55	MG	ZC	3351	1/1	0.83	0.09	90,90,90,90	0
55	MG	ZC	3665	1/1	0.83	0.10	70,70,70,70	0
55	MG	UC	1777	1/1	0.83	0.07	107,107,107,107	0
55	MG	VC	3361	1/1	0.83	0.20	84,84,84,84	0
55	MG	VC	3383	1/1	0.83	0.09	80,80,80,80	0
55	MG	VC	3611	1/1	0.83	0.12	111,111,111,111	0
55	MG	ZC	3229	1/1	0.83	0.10	70,70,70,70	0
55	MG	VC	3200	1/1	0.83	0.27	70,70,70,70	0
55	MG	UC	1860	1/1	0.83	0.17	97,97,97,97	0
55	MG	ZC	3235	1/1	0.83	0.17	72,72,72,72	0
55	MG	VC	3230	1/1	0.83	0.08	134,134,134,134	0
55	MG	VC	3584	1/1	0.83	0.24	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	ZC	3301	1/1	0.83	0.18	89,89,89,89	0
55	MG	ZC	3118	1/1	0.83	0.14	66,66,66,66	0
55	MG	ZC	3442	1/1	0.83	0.19	75,75,75,75	0
55	MG	UC	1757	1/1	0.83	0.15	127,127,127,127	0
55	MG	ZC	3374	1/1	0.83	0.29	88,88,88,88	0
55	MG	VC	3140	1/1	0.83	0.20	98,98,98,98	0
55	MG	A	304	1/1	0.83	0.14	87,87,87,87	0
55	MG	ZC	3613	1/1	0.83	0.39	90,90,90,90	0
55	MG	VC	3192	1/1	0.83	0.21	114,114,114,114	0
55	MG	VC	3329	1/1	0.83	0.17	68,68,68,68	0
55	MG	ZC	3454	1/1	0.83	0.12	83,83,83,83	0
55	MG	VC	3427	1/1	0.83	0.30	75,75,75,75	0
55	MG	YC	1608	1/1	0.83	0.11	148,148,148,148	0
55	MG	WC	211	1/1	0.83	0.16	110,110,110,110	0
55	MG	YC	1751	1/1	0.83	0.10	92,92,92,92	0
55	MG	ZC	3714	1/1	0.83	0.17	83,83,83,83	0
55	MG	ZC	3255	1/1	0.83	0.26	77,77,77,77	0
55	MG	ZC	3131	1/1	0.83	0.18	93,93,93,93	0
55	MG	UC	1690	1/1	0.83	0.09	133,133,133,133	0
55	MG	ZC	3321	1/1	0.83	0.18	67,67,67,67	0
55	MG	YC	1832	1/1	0.84	0.14	135,135,135,135	0
55	MG	ZC	3691	1/1	0.84	0.09	65,65,65,65	0
55	MG	VC	3354	1/1	0.84	0.13	105,105,105,105	0
55	MG	ZC	3324	1/1	0.84	0.20	58,58,58,58	0
55	MG	ZC	3585	1/1	0.84	0.07	116,116,116,116	0
55	MG	VC	3019	1/1	0.84	0.19	91,91,91,91	0
55	MG	VC	3020	1/1	0.84	0.26	77,77,77,77	0
55	MG	ZC	3032	1/1	0.84	0.14	91,91,91,91	0
55	MG	ZC	3594	1/1	0.84	0.28	94,94,94,94	0
55	MG	VC	3473	1/1	0.84	0.11	125,125,125,125	0
55	MG	ZC	3411	1/1	0.84	0.12	95,95,95,95	0
55	MG	AD	218	1/1	0.84	0.17	96,96,96,96	0
55	MG	VC	3613	1/1	0.84	0.07	158,158,158,158	0
55	MG	ZC	3414	1/1	0.84	0.11	65,65,65,65	0
55	MG	VC	3002	1/1	0.84	0.15	132,132,132,132	0
55	MG	VC	3069	1/1	0.84	0.19	86,86,86,86	0
55	MG	ZC	3511	1/1	0.84	0.18	78,78,78,78	0
55	MG	UC	1616	1/1	0.84	0.26	87,87,87,87	0
55	MG	LA	202	1/1	0.84	0.15	130,130,130,130	0
55	MG	UC	1631	1/1	0.84	0.12	105,105,105,105	0
55	MG	VC	3025	1/1	0.84	0.29	69,69,69,69	0
55	MG	VC	3135	1/1	0.84	0.08	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	ZC	3623	1/1	0.84	0.12	77,77,77,77	0
55	MG	UC	1769	1/1	0.84	0.09	119,119,119,119	0
55	MG	VC	3229	1/1	0.84	0.25	55,55,55,55	0
55	MG	ZC	3274	1/1	0.84	0.17	94,94,94,94	0
55	MG	VC	3335	1/1	0.84	0.26	115,115,115,115	0
55	MG	B	302	1/1	0.84	0.10	132,132,132,132	0
55	MG	VC	3547	1/1	0.84	0.16	89,89,89,89	0
55	MG	ZC	3280	1/1	0.84	0.14	60,60,60,60	0
55	MG	VC	3049	1/1	0.84	0.23	90,90,90,90	0
55	MG	ZC	3531	1/1	0.84	0.10	71,71,71,71	0
55	MG	UC	1655	1/1	0.84	0.25	113,113,113,113	0
55	MG	VC	3267	1/1	0.84	0.24	84,84,84,84	0
55	MG	X	101	1/1	0.84	0.23	91,91,91,91	0
55	MG	ZC	3136	1/1	0.84	0.10	88,88,88,88	0
55	MG	VC	3411	1/1	0.84	0.42	77,77,77,77	0
55	MG	ZC	3138	1/1	0.84	0.18	73,73,73,73	0
55	MG	VC	3269	1/1	0.84	0.33	81,81,81,81	0
55	MG	ZC	3293	1/1	0.84	0.15	92,92,92,92	0
55	MG	VC	3643	1/1	0.84	0.17	109,109,109,109	0
55	MG	VC	3108	1/1	0.84	0.10	125,125,125,125	0
55	MG	ZC	3081	1/1	0.84	0.23	143,143,143,143	0
55	MG	ZC	3379	1/1	0.84	0.15	96,96,96,96	0
55	MG	VC	3645	1/1	0.84	0.16	104,104,104,104	0
55	MG	VC	3646	1/1	0.84	0.06	122,122,122,122	0
55	MG	UC	1859	1/1	0.84	0.13	156,156,156,156	0
55	MG	YC	1866	1/1	0.84	0.12	112,112,112,112	0
55	MG	YA	307	1/1	0.84	0.10	98,98,98,98	0
55	MG	UC	1775	1/1	0.84	0.14	88,88,88,88	0
55	MG	ZC	3670	1/1	0.84	0.09	83,83,83,83	0
55	MG	YC	1820	1/1	0.84	0.11	152,152,152,152	0
55	MG	VC	3089	1/1	0.84	0.20	97,97,97,97	0
55	MG	YC	1822	1/1	0.84	0.08	145,145,145,145	0
55	MG	UA	202	1/1	0.84	0.13	132,132,132,132	0
55	MG	ZC	3244	1/1	0.84	0.14	74,74,74,74	0
55	MG	YC	1610	1/1	0.84	0.13	112,112,112,112	0
55	MG	UC	1834	1/1	0.84	0.10	222,222,222,222	0
55	MG	VC	3209	1/1	0.84	0.26	79,79,79,79	0
55	MG	VC	3063	1/1	0.84	0.08	98,98,98,98	0
55	MG	ZC	3578	1/1	0.84	0.17	78,78,78,78	0
55	MG	YC	1869	1/1	0.85	0.19	157,157,157,157	0
55	MG	VC	3303	1/1	0.85	0.15	120,120,120,120	0
55	MG	ZC	3668	1/1	0.85	0.07	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	ZC	3592	1/1	0.85	0.10	71,71,71,71	0
55	MG	ZC	3236	1/1	0.85	0.13	71,71,71,71	0
55	MG	AA	101	1/1	0.85	0.21	60,60,60,60	0
55	MG	YC	1636	1/1	0.85	0.17	174,174,174,174	0
55	MG	VC	3306	1/1	0.85	0.28	67,67,67,67	0
55	MG	YC	1703	1/1	0.85	0.17	136,136,136,136	0
55	MG	ZC	3241	1/1	0.85	0.17	89,89,89,89	0
55	MG	ZC	3067	1/1	0.85	0.22	67,67,67,67	0
55	MG	ZC	3402	1/1	0.85	0.10	113,113,113,113	0
55	MG	ZC	3140	1/1	0.85	0.28	76,76,76,76	0
55	MG	ZC	3105	1/1	0.85	0.28	55,55,55,55	0
55	MG	VC	3080	1/1	0.85	0.17	64,64,64,64	0
55	MG	UC	1716	1/1	0.85	0.21	106,106,106,106	0
55	MG	ZC	3477	1/1	0.85	0.11	85,85,85,85	0
55	MG	ZC	3144	1/1	0.85	0.09	92,92,92,92	0
55	MG	ZC	3108	1/1	0.85	0.14	65,65,65,65	0
55	MG	UC	1726	1/1	0.85	0.21	111,111,111,111	0
55	MG	VC	3202	1/1	0.85	0.19	80,80,80,80	0
55	MG	UC	1694	1/1	0.85	0.15	104,104,104,104	0
55	MG	ZC	3206	1/1	0.85	0.07	74,74,74,74	0
55	MG	ZC	3306	1/1	0.85	0.16	73,73,73,73	0
55	MG	ZC	3258	1/1	0.85	0.24	76,76,76,76	0
55	MG	ZC	3493	1/1	0.85	0.09	87,87,87,87	0
55	MG	VC	3220	1/1	0.85	0.24	108,108,108,108	0
55	MG	ZC	3707	1/1	0.85	0.12	63,63,63,63	0
55	MG	ZC	3074	1/1	0.85	0.28	76,76,76,76	0
55	MG	ZC	3642	1/1	0.85	0.05	105,105,105,105	0
55	MG	VC	3183	1/1	0.85	0.11	93,93,93,93	0
55	MG	VC	3513	1/1	0.85	0.11	98,98,98,98	0
55	MG	ZC	3215	1/1	0.85	0.10	117,117,117,117	0
55	MG	ZC	3376	1/1	0.85	0.09	101,101,101,101	0
55	MG	UC	1841	1/1	0.85	0.13	129,129,129,129	0
55	MG	VC	3134	1/1	0.85	0.34	76,76,76,76	0
55	MG	VC	3443	1/1	0.85	0.16	116,116,116,116	0
55	MG	VC	3468	1/1	0.85	0.10	131,131,131,131	0
55	MG	ZC	3042	1/1	0.85	0.18	58,58,58,58	0
55	MG	ZC	3043	1/1	0.85	0.42	102,102,102,102	0
55	MG	VC	3403	1/1	0.85	0.11	97,97,97,97	0
55	MG	VC	3319	1/1	0.85	0.29	72,72,72,72	0
55	MG	ZC	3387	1/1	0.85	0.11	89,89,89,89	0
55	MG	VC	3005	1/1	0.85	0.23	79,79,79,79	0
55	MG	ZC	3092	1/1	0.85	0.12	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	ZC	3735	1/1	0.85	0.10	85,85,85,85	0
55	MG	ZC	3409	1/1	0.86	0.09	66,66,66,66	0
55	MG	VC	3197	1/1	0.86	0.14	144,144,144,144	0
55	MG	VC	3525	1/1	0.86	0.18	79,79,79,79	0
55	MG	YC	1819	1/1	0.86	0.28	160,160,160,160	0
55	MG	ZC	3689	1/1	0.86	0.15	94,94,94,94	0
55	MG	VC	3266	1/1	0.86	0.14	89,89,89,89	0
55	MG	ZC	3203	1/1	0.86	0.07	84,84,84,84	0
55	MG	VC	3058	1/1	0.86	0.16	105,105,105,105	0
55	MG	VC	3218	1/1	0.86	0.17	99,99,99,99	0
55	MG	ZC	3595	1/1	0.86	0.09	75,75,75,75	0
55	MG	VC	3151	1/1	0.86	0.12	98,98,98,98	0
55	MG	YC	1870	1/1	0.86	0.12	164,164,164,164	0
55	MG	VC	3036	1/1	0.86	0.38	72,72,72,72	0
55	MG	VC	3120	1/1	0.86	0.16	98,98,98,98	0
55	MG	ZC	3702	1/1	0.86	0.25	92,92,92,92	0
55	MG	VC	3538	1/1	0.86	0.10	82,82,82,82	0
55	MG	ZC	3704	1/1	0.86	0.05	102,102,102,102	0
55	MG	VC	3690	1/1	0.86	0.18	77,77,77,77	0
55	MG	WC	225	1/1	0.86	0.16	180,180,180,180	0
55	MG	VC	3464	1/1	0.86	0.24	79,79,79,79	0
55	MG	VC	3003	1/1	0.86	0.28	96,96,96,96	0
55	MG	ZC	3088	1/1	0.86	0.23	71,71,71,71	0
55	MG	ZC	3012	1/1	0.86	0.27	53,53,53,53	0
55	MG	YC	1628	1/1	0.86	0.17	97,97,97,97	0
55	MG	ZC	3622	1/1	0.86	0.19	105,105,105,105	0
55	MG	VC	3694	1/1	0.86	0.07	105,105,105,105	0
55	MG	VC	3328	1/1	0.86	0.17	81,81,81,81	0
55	MG	VC	3250	1/1	0.86	0.17	77,77,77,77	0
55	MG	UC	1681	1/1	0.86	0.10	254,254,254,254	0
55	MG	VC	3205	1/1	0.86	0.18	87,87,87,87	0
55	MG	ZC	3034	1/1	0.86	0.17	75,75,75,75	0
55	MG	ZC	3631	1/1	0.86	0.08	80,80,80,80	0
55	MG	VC	3087	1/1	0.86	0.07	87,87,87,87	0
55	MG	VC	3207	1/1	0.86	0.14	140,140,140,140	0
55	MG	VC	3129	1/1	0.86	0.17	79,79,79,79	0
55	MG	YC	1799	1/1	0.86	0.07	182,182,182,182	0
55	MG	ZC	3542	1/1	0.86	0.23	114,114,114,114	0
55	MG	VC	3657	1/1	0.86	0.12	85,85,85,85	0
55	MG	VC	3619	1/1	0.86	0.10	119,119,119,119	0
55	MG	A	302	1/1	0.86	0.19	81,81,81,81	0
55	MG	ZC	3311	1/1	0.86	0.20	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	ZC	3465	1/1	0.86	0.05	80,80,80,80	0
55	MG	ZC	3549	1/1	0.86	0.14	98,98,98,98	0
55	MG	ZC	3466	1/1	0.86	0.16	70,70,70,70	0
55	MG	UC	1809	1/1	0.86	0.08	106,106,106,106	0
55	MG	VC	3032	1/1	0.86	0.14	90,90,90,90	0
55	MG	ZC	3114	1/1	0.86	0.06	113,113,113,113	0
55	MG	VC	3589	1/1	0.86	0.17	97,97,97,97	0
55	MG	ZC	3658	1/1	0.86	0.09	87,87,87,87	0
55	MG	YC	1644	1/1	0.86	0.21	103,103,103,103	0
55	MG	ZC	3053	1/1	0.86	0.11	73,73,73,73	0
55	MG	ZC	3177	1/1	0.86	0.11	95,95,95,95	0
55	MG	VC	3625	1/1	0.86	0.20	105,105,105,105	0
55	MG	VC	3212	1/1	0.86	0.35	85,85,85,85	0
55	MG	VC	3627	1/1	0.86	0.11	114,114,114,114	0
55	MG	ZC	3060	1/1	0.86	0.17	65,65,65,65	0
55	MG	ZC	3185	1/1	0.86	0.20	70,70,70,70	0
55	MG	ZC	3122	1/1	0.86	0.27	49,49,49,49	0
55	MG	ZC	3404	1/1	0.86	0.12	118,118,118,118	0
55	MG	VC	3007	1/1	0.86	0.11	102,102,102,102	0
55	MG	ZC	3491	1/1	0.86	0.11	90,90,90,90	0
55	MG	ZC	3676	1/1	0.86	0.21	114,114,114,114	0
55	MG	VC	3316	1/1	0.86	0.12	73,73,73,73	0
55	MG	QB	102	1/1	0.86	0.17	92,92,92,92	0
55	MG	ZC	3581	1/1	0.86	0.36	75,75,75,75	0
55	MG	ZC	3517	1/1	0.87	0.07	120,120,120,120	0
55	MG	VC	3672	1/1	0.87	0.14	111,111,111,111	0
55	MG	ZC	3430	1/1	0.87	0.18	66,66,66,66	0
55	MG	YC	1760	1/1	0.87	0.20	111,111,111,111	0
55	MG	ZC	3359	1/1	0.87	0.09	103,103,103,103	0
55	MG	VC	3462	1/1	0.87	0.12	89,89,89,89	0
55	MG	SB	101	1/1	0.87	0.15	60,60,60,60	0
55	MG	VC	3179	1/1	0.87	0.24	106,106,106,106	0
55	MG	FB	201	1/1	0.87	0.57	64,64,64,64	0
55	MG	VC	3159	1/1	0.87	0.09	136,136,136,136	0
55	MG	VC	3416	1/1	0.87	0.16	107,107,107,107	0
55	MG	VC	3642	1/1	0.87	0.07	101,101,101,101	0
55	MG	ZC	3046	1/1	0.87	0.12	97,97,97,97	0
55	MG	ZC	3298	1/1	0.87	0.15	89,89,89,89	0
55	MG	AD	221	1/1	0.87	0.11	140,140,140,140	0
55	MG	ZC	3047	1/1	0.87	0.14	69,69,69,69	0
55	MG	UC	1862	1/1	0.87	0.06	143,143,143,143	0
55	MG	VC	3072	1/1	0.87	0.20	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	VC	3123	1/1	0.87	0.17	76,76,76,76	0
55	MG	VC	3056	1/1	0.87	0.18	89,89,89,89	0
55	MG	VC	3106	1/1	0.87	0.19	77,77,77,77	0
55	MG	ZC	3166	1/1	0.87	0.16	60,60,60,60	0
55	MG	VC	3254	1/1	0.87	0.20	63,63,63,63	0
55	MG	ZC	3729	1/1	0.87	0.12	92,92,92,92	0
55	MG	UC	1722	1/1	0.87	0.14	107,107,107,107	0
55	MG	VC	3512	1/1	0.87	0.08	73,73,73,73	0
55	MG	VC	3350	1/1	0.87	0.18	104,104,104,104	0
55	MG	YC	1818	1/1	0.87	0.15	122,122,122,122	0
55	MG	ZC	3065	1/1	0.87	0.32	58,58,58,58	0
55	MG	ZC	3653	1/1	0.87	0.08	84,84,84,84	0
55	MG	VC	3059	1/1	0.87	0.15	98,98,98,98	0
55	MG	VC	3702	1/1	0.87	0.30	95,95,95,95	0
55	MG	ZC	3315	1/1	0.87	0.29	80,80,80,80	0
55	MG	ZC	3250	1/1	0.87	0.10	105,105,105,105	0
55	MG	YC	1779	1/1	0.87	0.11	180,180,180,180	0
55	MG	ZC	3183	1/1	0.87	0.56	68,68,68,68	0
55	MG	A	301	1/1	0.87	0.09	70,70,70,70	0
55	MG	UC	1845	1/1	0.87	0.10	124,124,124,124	0
55	MG	YC	1826	1/1	0.87	0.14	146,146,146,146	0
55	MG	VC	3623	1/1	0.87	0.14	87,87,87,87	0
55	MG	ZC	3752	1/1	0.87	0.09	167,167,167,167	0
55	MG	ZC	3329	1/1	0.87	0.14	90,90,90,90	0
55	MG	ZC	3261	1/1	0.87	0.19	80,80,80,80	0
55	MG	YC	1745	1/1	0.87	0.10	144,144,144,144	0
55	MG	ZC	3406	1/1	0.87	0.09	70,70,70,70	0
55	MG	VC	3486	1/1	0.87	0.16	117,117,117,117	0
55	MG	ZC	3495	1/1	0.87	0.11	95,95,95,95	0
55	MG	ZC	3194	1/1	0.87	0.10	68,68,68,68	0
55	MG	ZC	3006	1/1	0.87	0.15	76,76,76,76	0
55	MG	UC	1618	1/1	0.87	0.12	102,102,102,102	0
55	MG	ZC	3080	1/1	0.87	0.21	148,148,148,148	0
55	MG	YC	1671	1/1	0.87	0.11	99,99,99,99	0
55	MG	QA	101	1/1	0.87	0.08	104,104,104,104	0
55	MG	VC	3065	1/1	0.87	0.21	67,67,67,67	0
55	MG	ZC	3205	1/1	0.87	0.09	107,107,107,107	0
55	MG	VC	3628	1/1	0.87	0.17	63,63,63,63	0
55	MG	UC	1858	1/1	0.87	0.14	149,149,149,149	0
55	MG	UC	1666	1/1	0.87	0.14	149,149,149,149	0
55	MG	VC	3668	1/1	0.87	0.09	109,109,109,109	0
55	MG	ZC	3424	1/1	0.87	0.24	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	VC	3530	1/1	0.87	0.09	96,96,96,96	0
55	MG	VC	3601	1/1	0.87	0.17	66,66,66,66	0
55	MG	UC	1756	1/1	0.88	0.12	112,112,112,112	0
55	MG	VC	3546	1/1	0.88	0.18	112,112,112,112	0
55	MG	VC	3434	1/1	0.88	0.05	79,79,79,79	0
55	MG	YC	1812	1/1	0.88	0.25	179,179,179,179	0
55	MG	ZC	3318	1/1	0.88	0.05	126,126,126,126	0
55	MG	VC	3574	1/1	0.88	0.18	126,126,126,126	0
55	MG	VC	3684	1/1	0.88	0.37	80,80,80,80	0
55	MG	VC	3600	1/1	0.88	0.18	98,98,98,98	0
55	MG	ZC	3095	1/1	0.88	0.24	52,52,52,52	0
55	MG	ZC	3569	1/1	0.88	0.11	106,106,106,106	0
55	MG	ZC	3145	1/1	0.88	0.21	73,73,73,73	0
55	MG	ZC	3572	1/1	0.88	0.12	73,73,73,73	0
55	MG	ZC	3327	1/1	0.88	0.14	50,50,50,50	0
55	MG	ZC	3328	1/1	0.88	0.10	117,117,117,117	0
55	MG	WB	101	1/1	0.88	0.19	62,62,62,62	0
55	MG	ZC	3687	1/1	0.88	0.11	87,87,87,87	0
55	MG	ZC	3488	1/1	0.88	0.09	126,126,126,126	0
55	MG	VC	3111	1/1	0.88	0.15	60,60,60,60	0
55	MG	YC	1708	1/1	0.88	0.07	110,110,110,110	0
55	MG	ZC	3332	1/1	0.88	0.12	95,95,95,95	0
55	MG	VC	3521	1/1	0.88	0.12	78,78,78,78	0
55	MG	YC	1782	1/1	0.88	0.13	130,130,130,130	0
55	MG	VC	3660	1/1	0.88	0.11	95,95,95,95	0
55	MG	ZC	3589	1/1	0.88	0.13	66,66,66,66	0
55	MG	ZC	3338	1/1	0.88	0.15	85,85,85,85	0
55	MG	ZC	3216	1/1	0.88	0.09	77,77,77,77	0
55	MG	XA	301	1/1	0.88	0.19	115,115,115,115	0
55	MG	YC	1715	1/1	0.88	0.11	107,107,107,107	0
55	MG	ZC	3413	1/1	0.88	0.11	89,89,89,89	0
55	MG	ZC	3276	1/1	0.88	0.19	78,78,78,78	0
55	MG	VC	3477	1/1	0.88	0.18	93,93,93,93	0
55	MG	ZC	3056	1/1	0.88	0.11	104,104,104,104	0
55	MG	ZC	3346	1/1	0.88	0.20	77,77,77,77	0
55	MG	VC	3454	1/1	0.88	0.06	96,96,96,96	0
55	MG	ZC	3710	1/1	0.88	0.19	119,119,119,119	0
55	MG	ZC	3223	1/1	0.88	0.12	82,82,82,82	0
55	MG	ZC	3421	1/1	0.88	0.19	76,76,76,76	0
55	MG	ZC	3611	1/1	0.88	0.10	88,88,88,88	0
55	MG	ZC	3283	1/1	0.88	0.30	61,61,61,61	0
55	MG	VC	3699	1/1	0.88	0.27	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	ZC	3425	1/1	0.88	0.15	71,71,71,71	0
55	MG	ZC	3721	1/1	0.88	0.07	114,114,114,114	0
55	MG	ZC	3353	1/1	0.88	0.24	62,62,62,62	0
55	MG	ZC	3225	1/1	0.88	0.38	79,79,79,79	0
55	MG	VC	3293	1/1	0.88	0.14	79,79,79,79	0
55	MG	ZC	3062	1/1	0.88	0.12	67,67,67,67	0
55	MG	YC	1755	1/1	0.88	0.13	113,113,113,113	0
55	MG	VC	3701	1/1	0.88	0.22	102,102,102,102	0
55	MG	ZC	3525	1/1	0.88	0.22	85,85,85,85	0
55	MG	VC	3169	1/1	0.88	0.10	83,83,83,83	0
55	MG	ZC	3234	1/1	0.88	0.14	89,89,89,89	0
55	MG	ZC	3167	1/1	0.88	0.17	72,72,72,72	0
55	MG	ZC	3004	1/1	0.88	0.12	95,95,95,95	0
55	MG	VC	3704	1/1	0.88	0.08	100,100,100,100	0
55	MG	ZC	3367	1/1	0.88	0.18	85,85,85,85	0
55	MG	ZC	3534	1/1	0.88	0.13	82,82,82,82	0
55	MG	ZC	3535	1/1	0.88	0.14	90,90,90,90	0
55	MG	YC	1655	1/1	0.88	0.09	106,106,106,106	0
55	MG	VC	3223	1/1	0.88	0.13	130,130,130,130	0
55	MG	VC	3531	1/1	0.88	0.17	84,84,84,84	0
55	MG	ZC	3540	1/1	0.88	0.07	93,93,93,93	0
55	MG	UC	1771	1/1	0.88	0.07	75,75,75,75	0
55	MG	UC	1683	1/1	0.88	0.11	121,121,121,121	0
55	MG	FD	106	1/1	0.88	0.10	155,155,155,155	0
55	MG	VC	3670	1/1	0.88	0.13	89,89,89,89	0
55	MG	VC	3588	1/1	0.88	0.15	119,119,119,119	0
55	MG	VC	3227	1/1	0.88	0.07	80,80,80,80	0
55	MG	ZC	3546	1/1	0.88	0.09	95,95,95,95	0
55	MG	B	301	1/1	0.88	0.15	96,96,96,96	0
55	MG	ZC	3459	1/1	0.88	0.17	83,83,83,83	0
55	MG	ZC	3026	1/1	0.88	0.09	98,98,98,98	0
55	MG	UC	1743	1/1	0.88	0.30	129,129,129,129	0
55	MG	VC	3244	1/1	0.88	0.15	91,91,91,91	0
55	MG	VC	3415	1/1	0.88	0.14	82,82,82,82	0
55	MG	ZC	3252	1/1	0.88	0.18	69,69,69,69	0
55	MG	VC	3571	1/1	0.89	0.17	85,85,85,85	0
55	MG	ZC	3231	1/1	0.89	0.07	99,99,99,99	0
55	MG	VC	3136	1/1	0.89	0.15	76,76,76,76	0
55	MG	ZC	3727	1/1	0.89	0.13	81,81,81,81	0
55	MG	ZC	3587	1/1	0.89	0.21	80,80,80,80	0
55	MG	ZC	3022	1/1	0.89	0.22	82,82,82,82	0
55	MG	ZC	3024	1/1	0.89	0.06	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	ZC	3533	1/1	0.89	0.09	102,102,102,102	0
55	MG	ZC	3320	1/1	0.89	0.17	84,84,84,84	0
55	MG	VC	3014	1/1	0.89	0.12	96,96,96,96	0
55	MG	ZC	3667	1/1	0.89	0.07	81,81,81,81	0
55	MG	N	201	1/1	0.89	0.09	132,132,132,132	0
55	MG	ZC	3736	1/1	0.89	0.22	82,82,82,82	0
55	MG	VC	3052	1/1	0.89	0.17	83,83,83,83	0
55	MG	VC	3273	1/1	0.89	0.07	80,80,80,80	0
55	MG	ZC	3422	1/1	0.89	0.08	80,80,80,80	0
55	MG	VC	3457	1/1	0.89	0.07	101,101,101,101	0
55	MG	ZC	3743	1/1	0.89	0.09	92,92,92,92	0
55	MG	VC	3127	1/1	0.89	0.17	88,88,88,88	0
55	MG	ZC	3605	1/1	0.89	0.23	82,82,82,82	0
55	MG	YC	1724	1/1	0.89	0.26	161,161,161,161	0
55	MG	ZC	3149	1/1	0.89	0.20	70,70,70,70	0
55	MG	VC	3181	1/1	0.89	0.32	75,75,75,75	0
55	MG	UC	1735	1/1	0.89	0.34	116,116,116,116	0
55	MG	ZC	3333	1/1	0.89	0.23	79,79,79,79	0
55	MG	ED	102	1/1	0.89	0.08	50,50,50,50	0
55	MG	YC	1807	1/1	0.89	0.16	122,122,122,122	0
55	MG	VC	3532	1/1	0.89	0.21	66,66,66,66	0
55	MG	MB	201	1/1	0.89	0.20	84,84,84,84	0
55	MG	ZC	3295	1/1	0.89	0.12	124,124,124,124	0
55	MG	VC	3117	1/1	0.89	0.27	102,102,102,102	0
55	MG	ZC	3624	1/1	0.89	0.09	96,96,96,96	0
55	MG	VC	3001	1/1	0.89	0.10	133,133,133,133	0
55	MG	VC	3214	1/1	0.89	0.24	76,76,76,76	0
55	MG	VC	3034	1/1	0.89	0.41	79,79,79,79	0
55	MG	ZC	3628	1/1	0.89	0.15	93,93,93,93	0
55	MG	ZC	3768	1/1	0.89	0.16	107,107,107,107	0
55	MG	VC	3659	1/1	0.89	0.12	138,138,138,138	0
55	MG	ZC	3089	1/1	0.89	0.18	71,71,71,71	0
55	MG	VC	3057	1/1	0.89	0.34	73,73,73,73	0
55	MG	VC	3491	1/1	0.89	0.14	90,90,90,90	0
55	MG	ZC	3129	1/1	0.89	0.13	43,43,43,43	0
55	MG	ZC	3566	1/1	0.89	0.17	75,75,75,75	0
55	MG	ZC	3452	1/1	0.89	0.10	76,76,76,76	0
55	MG	FD	105	1/1	0.89	0.13	161,161,161,161	0
55	MG	ZC	3638	1/1	0.89	0.14	288,288,288,288	0
55	MG	WC	229	1/1	0.89	0.05	115,115,115,115	0
55	MG	ZC	3168	1/1	0.89	0.06	101,101,101,101	0
55	MG	VC	3121	1/1	0.89	0.10	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	YC	1713	1/1	0.89	0.06	150,150,150,150	0
55	MG	YC	1714	1/1	0.89	0.11	221,221,221,221	0
55	MG	VC	3393	1/1	0.89	0.07	82,82,82,82	0
55	MG	ZC	3357	1/1	0.89	0.10	86,86,86,86	0
55	MG	ZC	3462	1/1	0.89	0.15	88,88,88,88	0
55	MG	ZC	3175	1/1	0.89	0.25	74,74,74,74	0
55	MG	ZC	3097	1/1	0.89	0.21	78,78,78,78	0
55	MG	ZC	3019	1/1	0.89	0.13	57,57,57,57	0
55	MG	ZC	3716	1/1	0.90	0.15	90,90,90,90	0
55	MG	VC	3413	1/1	0.90	0.08	121,121,121,121	0
55	MG	VC	3414	1/1	0.90	0.09	105,105,105,105	0
55	MG	ZC	3719	1/1	0.90	0.09	96,96,96,96	0
55	MG	ZC	3720	1/1	0.90	0.07	90,90,90,90	0
55	MG	ZC	3401	1/1	0.90	0.10	78,78,78,78	0
55	MG	ZC	3523	1/1	0.90	0.12	58,58,58,58	0
55	MG	ZC	3259	1/1	0.90	0.07	98,98,98,98	0
55	MG	YA	306	1/1	0.90	0.25	94,94,94,94	0
55	MG	VC	3693	1/1	0.90	0.28	96,96,96,96	0
55	MG	VC	3234	1/1	0.90	0.26	63,63,63,63	0
55	MG	ZC	3064	1/1	0.90	0.35	81,81,81,81	0
55	MG	ZC	3309	1/1	0.90	0.13	74,74,74,74	0
55	MG	VC	3418	1/1	0.90	0.08	91,91,91,91	0
55	MG	ZC	3139	1/1	0.90	0.21	69,69,69,69	0
55	MG	VC	3130	1/1	0.90	0.21	76,76,76,76	0
55	MG	ZC	3179	1/1	0.90	0.14	69,69,69,69	0
55	MG	ZC	3361	1/1	0.90	0.21	78,78,78,78	0
55	MG	VC	3286	1/1	0.90	0.25	105,105,105,105	0
55	MG	YC	1827	1/1	0.90	0.08	103,103,103,103	0
55	MG	VC	3222	1/1	0.90	0.09	94,94,94,94	0
55	MG	ZC	3030	1/1	0.90	0.11	78,78,78,78	0
55	MG	ZC	3603	1/1	0.90	0.15	75,75,75,75	0
55	MG	ZC	3031	1/1	0.90	0.26	47,47,47,47	0
55	MG	ZC	3675	1/1	0.90	0.17	96,96,96,96	0
55	MG	ZC	3368	1/1	0.90	0.23	76,76,76,76	0
55	MG	ZC	3677	1/1	0.90	0.16	66,66,66,66	0
55	MG	ZC	3678	1/1	0.90	0.06	89,89,89,89	0
55	MG	VC	3037	1/1	0.90	0.25	74,74,74,74	0
55	MG	A	305	1/1	0.90	0.08	115,115,115,115	0
55	MG	VC	3225	1/1	0.90	0.10	78,78,78,78	0
55	MG	ZC	3751	1/1	0.90	0.27	78,78,78,78	0
55	MG	VC	3529	1/1	0.90	0.16	79,79,79,79	0
55	MG	UC	1721	1/1	0.90	0.14	155,155,155,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	ZC	3281	1/1	0.90	0.13	71,71,71,71	0
55	MG	ZC	3617	1/1	0.90	0.21	81,81,81,81	0
55	MG	ZC	3079	1/1	0.90	0.27	89,89,89,89	0
55	MG	YC	1804	1/1	0.90	0.09	177,177,177,177	0
55	MG	VC	3500	1/1	0.90	0.10	134,134,134,134	0
55	MG	ZC	3286	1/1	0.90	0.11	87,87,87,87	0
55	MG	ZC	3243	1/1	0.90	0.15	68,68,68,68	0
55	MG	VC	3203	1/1	0.90	0.15	76,76,76,76	0
55	MG	ZC	3434	1/1	0.90	0.12	70,70,70,70	0
55	MG	VC	3363	1/1	0.90	0.13	100,100,100,100	0
55	MG	ZC	3698	1/1	0.90	0.14	76,76,76,76	0
55	MG	VC	3503	1/1	0.90	0.11	94,94,94,94	0
55	MG	VC	3071	1/1	0.90	0.26	68,68,68,68	0
55	MG	YC	1729	1/1	0.90	0.07	169,169,169,169	0
55	MG	UC	1788	1/1	0.90	0.14	148,148,148,148	0
55	MG	VC	3349	1/1	0.90	0.08	77,77,77,77	0
55	MG	WA	303	1/1	0.90	0.23	80,80,80,80	0
55	MG	VC	3388	1/1	0.90	0.16	78,78,78,78	0
55	MG	ZC	3447	1/1	0.90	0.17	87,87,87,87	0
55	MG	ZC	3640	1/1	0.90	0.10	83,83,83,83	0
55	MG	ZC	3570	1/1	0.90	0.29	78,78,78,78	0
55	MG	ZC	3253	1/1	0.90	0.22	52,52,52,52	0
55	MG	ZC	3394	1/1	0.90	0.07	92,92,92,92	0
55	MG	VC	3186	1/1	0.90	0.20	69,69,69,69	0
55	MG	UC	1741	1/1	0.90	0.16	71,71,71,71	0
55	MG	ZC	3256	1/1	0.90	0.14	78,78,78,78	0
55	MG	ZC	3693	1/1	0.91	0.09	80,80,80,80	0
55	MG	VC	3302	1/1	0.91	0.09	82,82,82,82	0
55	MG	VC	3088	1/1	0.91	0.21	79,79,79,79	0
55	MG	ZC	3494	1/1	0.91	0.11	65,65,65,65	0
55	MG	NB	101	1/1	0.91	0.18	76,76,76,76	0
55	MG	VC	3617	1/1	0.91	0.09	115,115,115,115	0
55	MG	ZC	3077	1/1	0.91	0.07	68,68,68,68	0
55	MG	ZC	3499	1/1	0.91	0.12	76,76,76,76	0
55	MG	VC	3516	1/1	0.91	0.09	92,92,92,92	0
55	MG	ZC	3757	1/1	0.91	0.16	81,81,81,81	0
55	MG	ZC	3109	1/1	0.91	0.33	61,61,61,61	0
55	MG	YC	1856	1/1	0.91	0.13	170,170,170,170	0
55	MG	ZC	3600	1/1	0.91	0.09	121,121,121,121	0
55	MG	VC	3176	1/1	0.91	0.09	83,83,83,83	0
55	MG	VC	3143	1/1	0.91	0.14	98,98,98,98	0
55	MG	ZC	3763	1/1	0.91	0.18	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	YC	1695	1/1	0.91	0.20	94,94,94,94	0
55	MG	ZC	3709	1/1	0.91	0.19	69,69,69,69	0
55	MG	ZC	3174	1/1	0.91	0.26	75,75,75,75	0
55	MG	ZC	3606	1/1	0.91	0.24	63,63,63,63	0
55	MG	VC	3041	1/1	0.91	0.11	86,86,86,86	0
55	MG	ZC	3345	1/1	0.91	0.10	71,71,71,71	0
55	MG	ZC	3770	1/1	0.91	0.34	92,92,92,92	0
55	MG	VC	3686	1/1	0.91	0.14	90,90,90,90	0
55	MG	UC	1812	1/1	0.91	0.08	114,114,114,114	0
55	MG	YC	1654	1/1	0.91	0.11	157,157,157,157	0
55	MG	VC	3064	1/1	0.91	0.12	79,79,79,79	0
55	MG	ZC	3515	1/1	0.91	0.07	111,111,111,111	0
55	MG	ZC	3285	1/1	0.91	0.10	80,80,80,80	0
55	MG	ZC	3672	1/1	0.91	0.09	80,80,80,80	0
55	MG	VC	3567	1/1	0.91	0.09	152,152,152,152	0
55	MG	VC	3124	1/1	0.91	0.21	91,91,91,91	0
55	MG	ZC	3063	1/1	0.91	0.27	36,36,36,36	0
55	MG	VC	3426	1/1	0.91	0.05	104,104,104,104	0
55	MG	ZC	3429	1/1	0.91	0.11	80,80,80,80	0
55	MG	ZC	3476	1/1	0.91	0.08	74,74,74,74	0
55	MG	VC	3648	1/1	0.91	0.14	116,116,116,116	0
55	MG	VC	3507	1/1	0.91	0.09	99,99,99,99	0
55	MG	ZC	3479	1/1	0.91	0.27	87,87,87,87	0
55	MG	VC	3397	1/1	0.91	0.13	107,107,107,107	0
55	MG	ZC	3188	1/1	0.91	0.17	63,63,63,63	0
55	MG	ZC	3484	1/1	0.91	0.25	81,81,81,81	0
55	MG	ZC	3686	1/1	0.91	0.06	76,76,76,76	0
55	MG	ZC	3326	1/1	0.91	0.13	71,71,71,71	0
55	MG	VC	3384	1/1	0.91	0.14	79,79,79,79	0
55	MG	VC	3312	1/1	0.91	0.12	105,105,105,105	0
55	MG	ZC	3364	1/1	0.91	0.18	86,86,86,86	0
55	MG	ZC	3003	1/1	0.91	0.14	74,74,74,74	0
55	MG	UC	1848	1/1	0.91	0.18	111,111,111,111	0
55	MG	YC	1727	1/1	0.92	0.14	71,71,71,71	0
55	MG	VC	3610	1/1	0.92	0.13	104,104,104,104	0
55	MG	YC	1637	1/1	0.92	0.27	75,75,75,75	0
55	MG	ZC	3083	1/1	0.92	0.45	58,58,58,58	0
55	MG	ZC	3419	1/1	0.92	0.07	71,71,71,71	0
55	MG	VC	3305	1/1	0.92	0.14	88,88,88,88	0
55	MG	ZC	3381	1/1	0.92	0.54	83,83,83,83	0
55	MG	VC	3240	1/1	0.92	0.29	78,78,78,78	0
55	MG	VC	3391	1/1	0.92	0.17	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	ZC	3474	1/1	0.92	0.07	112,112,112,112	0
55	MG	UC	1850	1/1	0.92	0.08	156,156,156,156	0
55	MG	ZC	3576	1/1	0.92	0.13	84,84,84,84	0
55	MG	VC	3073	1/1	0.92	0.25	81,81,81,81	0
55	MG	VC	3698	1/1	0.92	0.14	81,81,81,81	0
55	MG	ZC	3637	1/1	0.92	0.17	93,93,93,93	0
55	MG	VC	3674	1/1	0.92	0.15	78,78,78,78	0
55	MG	UC	1748	1/1	0.92	0.06	162,162,162,162	0
55	MG	YC	1835	1/1	0.92	0.15	116,116,116,116	0
55	MG	ZC	3643	1/1	0.92	0.09	67,67,67,67	0
55	MG	ZC	3350	1/1	0.92	0.07	70,70,70,70	0
55	MG	VC	3544	1/1	0.92	0.14	81,81,81,81	0
55	MG	ZC	3028	1/1	0.92	0.10	60,60,60,60	0
55	MG	VC	3490	1/1	0.92	0.08	101,101,101,101	0
55	MG	ZC	3588	1/1	0.92	0.08	89,89,89,89	0
55	MG	ZC	3435	1/1	0.92	0.19	71,71,71,71	0
55	MG	ZC	3590	1/1	0.92	0.21	63,63,63,63	0
55	MG	VC	3296	1/1	0.92	0.12	84,84,84,84	0
55	MG	VC	3640	1/1	0.92	0.10	141,141,141,141	0
55	MG	ZC	3207	1/1	0.92	0.24	71,71,71,71	0
55	MG	ZC	3209	1/1	0.92	0.17	67,67,67,67	0
55	MG	VC	3706	1/1	0.92	0.14	112,112,112,112	0
55	MG	VC	3272	1/1	0.92	0.20	78,78,78,78	0
55	MG	ZC	3597	1/1	0.92	0.26	77,77,77,77	0
55	MG	ZC	3035	1/1	0.92	0.13	85,85,85,85	0
55	MG	ZC	3103	1/1	0.92	0.17	87,87,87,87	0
55	MG	ZC	3214	1/1	0.92	0.07	77,77,77,77	0
55	MG	ZC	3663	1/1	0.92	0.12	81,81,81,81	0
55	MG	VC	3100	1/1	0.92	0.25	71,71,71,71	0
55	MG	UC	1776	1/1	0.92	0.10	117,117,117,117	0
55	MG	VC	3264	1/1	0.92	0.12	76,76,76,76	0
55	MG	VC	3265	1/1	0.92	0.32	84,84,84,84	0
55	MG	YC	1795	1/1	0.92	0.25	172,172,172,172	0
55	MG	ZC	3455	1/1	0.92	0.11	80,80,80,80	0
55	MG	ZC	3294	1/1	0.92	0.08	66,66,66,66	0
55	MG	ZC	3370	1/1	0.92	0.06	64,64,64,64	0
55	MG	UC	1840	1/1	0.92	0.15	134,134,134,134	0
55	MG	ZC	3509	1/1	0.92	0.07	77,77,77,77	0
55	MG	ZC	3557	1/1	0.92	0.12	98,98,98,98	0
55	MG	ZC	3005	1/1	0.92	0.14	110,110,110,110	0
55	MG	ZC	3045	1/1	0.92	0.20	60,60,60,60	0
55	MG	DB	201	1/1	0.92	0.08	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	ZC	3621	1/1	0.92	0.25	80,80,80,80	0
55	MG	ZC	3191	1/1	0.93	0.11	53,53,53,53	0
55	MG	ZC	3023	1/1	0.93	0.08	71,71,71,71	0
55	MG	ZC	3480	1/1	0.93	0.08	64,64,64,64	0
55	MG	ZC	3579	1/1	0.93	0.17	61,61,61,61	0
55	MG	ZC	3481	1/1	0.93	0.16	67,67,67,67	0
55	MG	ZC	3432	1/1	0.93	0.05	68,68,68,68	0
55	MG	ZC	3272	1/1	0.93	0.17	66,66,66,66	0
55	MG	ZC	3196	1/1	0.93	0.27	69,69,69,69	0
55	MG	VC	3545	1/1	0.93	0.22	88,88,88,88	0
55	MG	ZC	3641	1/1	0.93	0.12	69,69,69,69	0
55	MG	ZC	3126	1/1	0.93	0.10	66,66,66,66	0
55	MG	ZC	3754	1/1	0.93	0.10	54,54,54,54	0
55	MG	VC	3370	1/1	0.93	0.11	75,75,75,75	0
55	MG	ZC	3200	1/1	0.93	0.19	92,92,92,92	0
55	MG	ZC	3278	1/1	0.93	0.12	160,160,160,160	0
55	MG	J	203	1/1	0.93	0.21	83,83,83,83	0
55	MG	WA	304	1/1	0.93	0.07	77,77,77,77	0
55	MG	ZC	3492	1/1	0.93	0.06	68,68,68,68	0
55	MG	VC	3126	1/1	0.93	0.15	51,51,51,51	0
55	MG	VC	3593	1/1	0.93	0.08	109,109,109,109	0
55	MG	YC	1865	1/1	0.93	0.17	115,115,115,115	0
55	MG	VC	3688	1/1	0.93	0.16	97,97,97,97	0
55	MG	UC	1717	1/1	0.93	0.19	110,110,110,110	0
55	MG	ZC	3450	1/1	0.93	0.10	87,87,87,87	0
55	MG	YC	1839	1/1	0.93	0.08	173,173,173,173	0
55	MG	VC	3077	1/1	0.93	0.12	75,75,75,75	0
55	MG	ZC	3550	1/1	0.93	0.04	86,86,86,86	0
55	MG	VC	3552	1/1	0.93	0.21	139,139,139,139	0
55	MG	VC	3050	1/1	0.93	0.06	101,101,101,101	0
55	MG	UC	1677	1/1	0.93	0.22	113,113,113,113	0
55	MG	VC	3280	1/1	0.93	0.21	88,88,88,88	0
55	MG	VC	3476	1/1	0.93	0.17	75,75,75,75	0
55	MG	YC	1658	1/1	0.93	0.10	87,87,87,87	0
55	MG	VC	3456	1/1	0.93	0.12	76,76,76,76	0
55	MG	VC	3409	1/1	0.93	0.12	103,103,103,103	0
55	MG	VC	3243	1/1	0.93	0.18	75,75,75,75	0
55	MG	YC	1850	1/1	0.93	0.12	179,179,179,179	0
55	MG	UC	1752	1/1	0.93	0.10	116,116,116,116	0
55	MG	UC	1739	1/1	0.93	0.04	111,111,111,111	0
55	MG	ZC	3618	1/1	0.93	0.20	65,65,65,65	0
55	MG	ZC	3619	1/1	0.93	0.07	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	UC	1805	1/1	0.93	0.06	122,122,122,122	0
55	MG	VC	3565	1/1	0.93	0.14	76,76,76,76	0
55	MG	ZC	3227	1/1	0.93	0.12	80,80,80,80	0
55	MG	XA	302	1/1	0.93	0.11	79,79,79,79	0
55	MG	VC	3655	1/1	0.93	0.15	84,84,84,84	0
55	MG	ZC	3230	1/1	0.93	0.09	57,57,57,57	0
55	MG	VC	3679	1/1	0.93	0.12	73,73,73,73	0
55	MG	ZC	3573	1/1	0.93	0.08	85,85,85,85	0
55	MG	VC	3656	1/1	0.93	0.08	95,95,95,95	0
55	MG	ZC	3348	1/1	0.93	0.21	59,59,59,59	0
55	MG	ZC	3560	1/1	0.94	0.08	71,71,71,71	0
55	MG	ZC	3607	1/1	0.94	0.11	94,94,94,94	0
55	MG	VC	3469	1/1	0.94	0.14	84,84,84,84	0
55	MG	ZC	3192	1/1	0.94	0.13	92,92,92,92	0
55	MG	ZC	3017	1/1	0.94	0.08	68,68,68,68	0
55	MG	ZC	3195	1/1	0.94	0.15	89,89,89,89	0
55	MG	ZC	3437	1/1	0.94	0.06	99,99,99,99	0
55	MG	ZC	3018	1/1	0.94	0.09	86,86,86,86	0
55	MG	L	201	1/1	0.94	0.09	81,81,81,81	0
55	MG	ZC	3712	1/1	0.94	0.23	81,81,81,81	0
55	MG	VC	3417	1/1	0.94	0.05	101,101,101,101	0
55	MG	ZC	3441	1/1	0.94	0.07	94,94,94,94	0
55	MG	VC	3680	1/1	0.94	0.15	90,90,90,90	0
55	MG	VC	3299	1/1	0.94	0.08	88,88,88,88	0
55	MG	ZC	3444	1/1	0.94	0.06	102,102,102,102	0
55	MG	ZC	3336	1/1	0.94	0.18	73,73,73,73	0
55	MG	YC	1756	1/1	0.94	0.11	98,98,98,98	0
55	MG	ZC	3202	1/1	0.94	0.08	64,64,64,64	0
55	MG	VC	3629	1/1	0.94	0.04	95,95,95,95	0
55	MG	I	201	1/1	0.94	0.25	80,80,80,80	0
55	MG	VC	3178	1/1	0.94	0.14	91,91,91,91	0
55	MG	ZC	3377	1/1	0.94	0.16	58,58,58,58	0
55	MG	YC	1823	1/1	0.94	0.14	102,102,102,102	0
55	MG	ZC	3583	1/1	0.94	0.07	92,92,92,92	0
55	MG	ZC	3173	1/1	0.94	0.24	75,75,75,75	0
55	MG	ZC	3208	1/1	0.94	0.18	68,68,68,68	0
55	MG	VC	3534	1/1	0.94	0.12	110,110,110,110	0
55	MG	YC	1825	1/1	0.94	0.06	116,116,116,116	0
55	MG	VC	3582	1/1	0.94	0.09	75,75,75,75	0
55	MG	VC	3475	1/1	0.94	0.07	117,117,117,117	0
55	MG	XA	303	1/1	0.94	0.15	78,78,78,78	0
55	MG	ZC	3503	1/1	0.94	0.12	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	VC	3689	1/1	0.94	0.23	130,130,130,130	0
55	MG	VC	3463	1/1	0.94	0.08	94,94,94,94	0
55	MG	VC	3554	1/1	0.94	0.05	151,151,151,151	0
55	MG	ZC	3740	1/1	0.94	0.14	63,63,63,63	0
55	MG	ZC	3464	1/1	0.94	0.19	102,102,102,102	0
55	MG	UC	1740	1/1	0.94	0.07	105,105,105,105	0
55	MG	ZC	3039	1/1	0.94	0.10	73,73,73,73	0
55	MG	VC	3327	1/1	0.94	0.10	93,93,93,93	0
55	MG	VC	3377	1/1	0.94	0.09	76,76,76,76	0
55	MG	YC	1709	1/1	0.94	0.07	109,109,109,109	0
55	MG	O	201	1/1	0.94	0.24	67,67,67,67	0
55	MG	ZC	3101	1/1	0.94	0.25	58,58,58,58	0
55	MG	ZC	3160	1/1	0.94	0.14	75,75,75,75	0
55	MG	ZC	3516	1/1	0.94	0.08	85,85,85,85	0
55	MG	UC	1648	1/1	0.95	0.13	97,97,97,97	0
55	MG	ZC	3753	1/1	0.95	0.10	88,88,88,88	0
55	MG	VC	3508	1/1	0.95	0.16	97,97,97,97	0
55	MG	VC	3467	1/1	0.95	0.09	100,100,100,100	0
55	MG	ZC	3397	1/1	0.95	0.17	73,73,73,73	0
55	MG	VC	3518	1/1	0.95	0.10	69,69,69,69	0
55	MG	ZC	3469	1/1	0.95	0.14	67,67,67,67	0
55	MG	ZC	3219	1/1	0.95	0.08	69,69,69,69	0
55	MG	ZC	3471	1/1	0.95	0.11	92,92,92,92	0
55	MG	ZC	3040	1/1	0.95	0.44	61,61,61,61	0
55	MG	VC	3324	1/1	0.95	0.11	98,98,98,98	0
55	MG	ZC	3156	1/1	0.95	0.09	63,63,63,63	0
55	MG	ZC	3639	1/1	0.95	0.06	86,86,86,86	0
55	MG	ZC	3609	1/1	0.95	0.11	78,78,78,78	0
55	MG	ZC	3526	1/1	0.95	0.12	53,53,53,53	0
55	MG	VC	3520	1/1	0.95	0.12	126,126,126,126	0
55	MG	ZC	3158	1/1	0.95	0.07	68,68,68,68	0
55	MG	VC	3481	1/1	0.95	0.08	87,87,87,87	0
55	MG	ZC	3738	1/1	0.95	0.22	82,82,82,82	0
55	MG	VC	3522	1/1	0.95	0.08	94,94,94,94	0
55	MG	VC	3523	1/1	0.95	0.08	99,99,99,99	0
55	MG	ZC	3102	1/1	0.95	0.14	75,75,75,75	0
55	MG	ZC	3066	1/1	0.95	0.22	48,48,48,48	0
55	MG	VC	3697	1/1	0.95	0.46	137,137,137,137	0
55	MG	ZC	3563	1/1	0.95	0.09	98,98,98,98	0
55	MG	VC	3536	1/1	0.95	0.34	97,97,97,97	0
55	MG	ZC	3011	1/1	0.95	0.05	94,94,94,94	0
55	MG	VC	3174	1/1	0.95	0.26	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	ZC	3015	1/1	0.95	0.09	77,77,77,77	0
55	MG	VC	3282	1/1	0.95	0.12	81,81,81,81	0
55	MG	VC	3445	1/1	0.95	0.09	92,92,92,92	0
56	ZN	AC	301	1/1	0.95	0.30	151,151,151,151	0
55	MG	UC	1668	1/1	0.96	0.14	94,94,94,94	0
55	MG	YA	304	1/1	0.96	0.10	53,53,53,53	0
55	MG	VC	3703	1/1	0.96	0.10	87,87,87,87	0
55	MG	UC	1796	1/1	0.96	0.09	109,109,109,109	0
55	MG	ZC	3756	1/1	0.96	0.14	88,88,88,88	0
55	MG	ZC	3266	1/1	0.96	0.09	70,70,70,70	0
55	MG	YC	1684	1/1	0.96	0.08	127,127,127,127	0
55	MG	ZC	3644	1/1	0.96	0.05	76,76,76,76	0
55	MG	ZC	3033	1/1	0.96	0.11	80,80,80,80	0
55	MG	VC	3597	1/1	0.96	0.10	74,74,74,74	0
55	MG	VC	3313	1/1	0.96	0.08	97,97,97,97	0
55	MG	ZC	3614	1/1	0.96	0.08	88,88,88,88	0
55	MG	ZC	3057	1/1	0.96	0.09	115,115,115,115	0
55	MG	ZC	3058	1/1	0.96	0.23	37,37,37,37	0
55	MG	ZC	3633	1/1	0.96	0.07	92,92,92,92	0
55	MG	VC	3636	1/1	0.96	0.04	97,97,97,97	0
55	MG	ZC	3181	1/1	0.96	0.20	61,61,61,61	0
55	MG	VC	3558	1/1	0.96	0.04	104,104,104,104	0
55	MG	ZC	3604	1/1	0.96	0.15	82,82,82,82	0
55	MG	ZC	3722	1/1	0.97	0.09	82,82,82,82	0
55	MG	VC	3541	1/1	0.97	0.24	95,95,95,95	0
55	MG	VC	3337	1/1	0.97	0.06	77,77,77,77	0
55	MG	ZC	3048	1/1	0.97	0.07	69,69,69,69	0
55	MG	ZC	3496	1/1	0.97	0.09	93,93,93,93	0
55	MG	VC	3245	1/1	0.97	0.10	94,94,94,94	0
55	MG	ZC	3745	1/1	0.97	0.05	74,74,74,74	0
55	MG	ZC	3695	1/1	0.97	0.08	70,70,70,70	0
55	MG	ZC	3650	1/1	0.97	0.05	96,96,96,96	0
55	MG	ZC	3453	1/1	0.97	0.05	91,91,91,91	0
55	MG	ZC	3666	1/1	0.97	0.04	94,94,94,94	0
55	MG	VC	3499	1/1	0.97	0.17	111,111,111,111	0
55	MG	ZC	3323	1/1	0.97	0.11	64,64,64,64	0
55	MG	ZC	3562	1/1	0.97	0.05	116,116,116,116	0
55	MG	VC	3615	1/1	0.97	0.10	88,88,88,88	0
55	MG	ZC	3027	1/1	0.97	0.05	94,94,94,94	0
55	MG	WB	102	1/1	0.97	0.08	59,59,59,59	0
55	MG	ZC	3013	1/1	0.97	0.11	70,70,70,70	0
56	ZN	KC	101	1/1	0.97	0.06	189,189,189,189	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	ZC	3111	1/1	0.98	0.12	72,72,72,72	0
55	MG	VC	3408	1/1	0.98	0.05	85,85,85,85	0
55	MG	ZC	3193	1/1	0.98	0.12	95,95,95,95	0
55	MG	Q	201	1/1	0.98	0.10	88,88,88,88	0
55	MG	ZC	3369	1/1	0.98	0.07	100,100,100,100	0
55	MG	ZC	3682	1/1	0.98	0.12	76,76,76,76	0
55	MG	UC	1799	1/1	0.98	0.05	101,101,101,101	0
56	ZN	EA	301	1/1	0.98	0.23	97,97,97,97	0
55	MG	ZC	3539	1/1	0.98	0.07	64,64,64,64	0
55	MG	ZC	3014	1/1	0.98	0.05	90,90,90,90	0
56	ZN	OA	101	1/1	0.99	0.11	157,157,157,157	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.