



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 30, 2024 – 02:11 PM EDT

PDB ID : 4V8E  
Title : Crystal structure analysis of ribosomal decoding (near-cognate tRNA-tyr complex).  
Authors : Jenner, L.; Demeshkina, N.; Yusupov, M.; Yusupova, G.  
Deposited on : 2011-12-07  
Resolution : 3.30 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

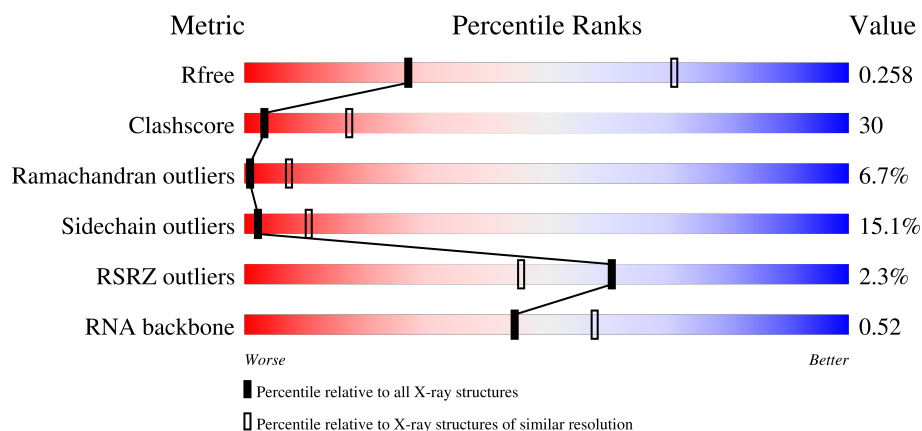
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)
RNA backbone	3690	1014 (3.64-2.96)

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	AA	2912	
1	CA	2912	
2	AB	122	
2	CB	122	

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Mol	Chain	Length	Quality of chain
3	AD	276	
3	CD	276	
4	AE	206	
4	CE	206	
5	AF	210	
5	CF	210	
6	AG	182	
6	CG	182	
7	AH	180	
7	CH	180	
8	AK	148	
8	CK	148	
9	AM	140	
9	CM	140	
10	AN	122	
10	CN	122	
11	AO	150	
11	CO	150	
12	AP	141	
12	CP	141	
13	A0	118	
13	C0	118	
14	AQ	112	
14	CQ	112	
15	AR	146	

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Mol	Chain	Length	Quality of chain
15	CR	146	
16	A1	118	
16	C1	118	
17	A2	101	
17	C2	101	
18	AS	113	
18	CS	113	
19	AT	96	
19	CT	96	
20	AU	110	
20	CU	110	
21	AV	206	
21	CV	206	
22	A3	85	
22	C3	85	
23	AZ	98	
23	CZ	98	
24	AW	72	
24	CW	72	
25	AX	60	
25	CX	60	
26	A4	71	
26	C4	71	
27	A5	60	
27	C5	60	

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Mol	Chain	Length	Quality of chain
28	A6	54	
28	C6	54	
29	A7	49	
29	C7	49	
30	A8	65	
30	C8	65	
31	BA	1506	
31	DA	1506	
32	BE	256	
32	DE	256	
33	BF	239	
33	DF	239	
34	BG	208	
34	DG	208	
35	BH	162	
35	DH	162	
36	BI	101	
36	DI	101	
37	BJ	156	
37	DJ	156	
38	BK	138	
38	DK	138	
39	BL	128	
39	DL	128	
40	BM	105	



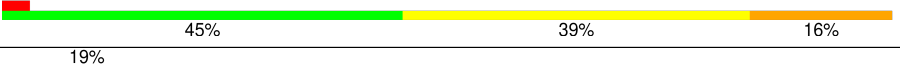
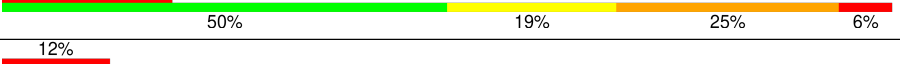
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Mol	Chain	Length	Quality of chain
40	DM	105	
41	BN	129	
41	DN	129	
42	BO	132	
42	DO	132	
43	BP	126	
43	DP	126	
44	BQ	61	
44	DQ	61	
45	BR	89	
45	DR	89	
46	BS	88	
46	DS	88	
47	BT	105	
47	DT	105	
48	BU	88	
48	DU	88	
49	BV	93	
49	DV	93	
50	BW	106	
50	DW	106	
51	BX	27	
51	DX	27	
52	BB	85	
52	BD	85	

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Mol	Chain	Length	Quality of chain
52	DB	85	
52	DD	85	
53	BC	77	
53	DC	77	
54	B1	16	
54	D1	16	

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	AA	3144	-	-	-	X
55	MG	BA	1745	-	-	-	X
55	MG	BB	104	-	-	-	X
55	MG	BC	105	-	-	-	X
55	MG	BQ	101	-	-	-	X
55	MG	CA	3045	-	-	-	X
55	MG	CA	3145	-	-	-	X
55	MG	CA	3264	-	-	-	X
55	MG	CA	3455	-	-	-	X
56	OHX	AA	3568	-	-	X	-
56	OHX	BA	1673	-	-	X	-
56	OHX	BA	1684	-	-	X	-
56	OHX	C6	101	-	-	X	-
56	OHX	DA	1731	-	-	X	-
56	OHX	DA	1760	-	-	X	-
56	OHX	DA	1767	-	-	X	-
56	OHX	DC	107	-	-	X	-

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 303952 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called RNA (2912-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
1	CA	2907	Total	C	N	O	P	0	0	0
			62607	27866	11712	20123	2906			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	161	U	-	insertion	GB AP008226.1
AA	654A	A	G	conflict	GB AP008226.1
AA	654E	C	G	conflict	GB AP008226.1
AA	654P	G	C	conflict	GB AP008226.1
AA	654T	A	C	conflict	GB AP008226.1
AA	1058	U	G	conflict	GB AP008226.1
AA	1080	A	C	conflict	GB AP008226.1
CA	156	U	-	insertion	GB AP008226.1
CA	681	A	G	conflict	GB AP008226.1
CA	685	C	G	conflict	GB AP008226.1
CA	696	G	C	conflict	GB AP008226.1
CA	700	A	C	conflict	GB AP008226.1
CA	1105	U	G	conflict	GB AP008226.1
CA	1127	A	C	conflict	GB AP008226.1

- Molecule 2 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
2	CB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
3	CD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
4	CE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
5	CF	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
6	CG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			
7	CH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	CK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
9	CM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
10	CN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
11	CO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	CP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	A0	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	C0	117	Total	C	N	O	S	0	0	0
			960	599	202	159				

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AQ	111	Total	C	N	O	0	0	0
			882	556	176	150			
14	CQ	111	Total	C	N	O	0	0	0
			882	556	176	150			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
15	CR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	A1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
16	C1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	A2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
17	C2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
18	CS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	AT	92	Total	C	N	O	0	0	0
			725	471	131	123			
19	CT	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
20	CU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AV	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			
21	CV	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	A3	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
22	C3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
23	CZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	CW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AX	59	Total	C	N	O		0	0	0
			469	298	90	81				
25	CX	59	Total	C	N	O		0	0	0
			469	298	90	81				

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A4	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
26	C4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	C5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
28	C6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A7	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			
29	C7	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A8	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			
30	C8	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BA	1502	Total	C	N	O	P	0	0	0
			32284	14370	5982	10431	1501			
31	DA	1502	Total	C	N	O	P	0	0	0
			32287	14370	5982	10433	1502			

- Molecule 32 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
32	DE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- Molecule 33 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BF	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
33	DF	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 34 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
34	DG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 35 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
35	DH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 36 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
36	DI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 37 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
37	DJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 38 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
38	DK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 39 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BL	127	Total	C	N	O		0	0	0
			1010	639	197	174				
39	DL	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- Molecule 40 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	DM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 41 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
41	DN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 42 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
42	DO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 43 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BP	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
43	DP	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

- Molecule 44 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BQ	58	Total	C	N	O	S	0	0	0
			476	303	99	70	4			
44	DQ	58	Total	C	N	O	S	0	0	0
			476	303	99	70	4			

- Molecule 45 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
45	DR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 46 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
46	DS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 47 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
47	DT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 48 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	BU	72	Total	C	N	O	0	0	0
			591	376	117	98			
48	DU	72	Total	C	N	O	0	0	0
			591	376	117	98			

- Molecule 49 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			
49	DV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

- Molecule 50 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
50	DW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 51 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	BX	25	Total	C	N	O	0	0	0
			217	134	52	31			
51	DX	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 52 is a RNA chain called TRNA-TYR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
52	BB	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			
52	BD	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			
52	DB	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			
52	DD	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			

- Molecule 53 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
53	DC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	18	C	U	conflict	GB AP012306.1
DC	18	C	U	conflict	GB AP012306.1

- Molecule 54 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B1	16	Total	C	N	O	P	0	0	0
			347	156	69	106	16			
54	D1	16	Total	C	N	O	P	0	0	0
			347	156	69	106	16			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

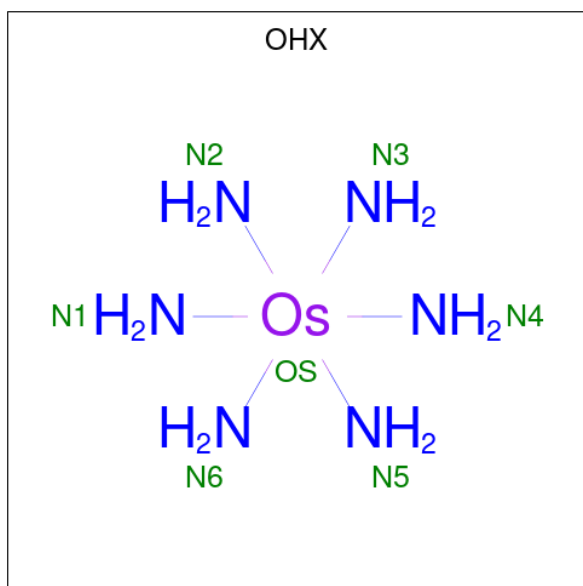
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	AA	331	Total Mg 331 331	0	0
55	AB	6	Total Mg 6 6	0	0
55	AE	3	Total Mg 3 3	0	0
55	AF	2	Total Mg 2 2	0	0
55	AO	3	Total Mg 3 3	0	0
55	A0	1	Total Mg 1 1	0	0
55	A1	1	Total Mg 1 1	0	0
55	A3	1	Total Mg 1 1	0	0
55	A5	1	Total Mg 1 1	0	0
55	BA	115	Total Mg 115 115	0	0
55	BN	1	Total Mg 1 1	0	0
55	BQ	1	Total Mg 1 1	0	0
55	BS	1	Total Mg 1 1	0	0
55	BB	5	Total Mg 5 5	0	0
55	BC	5	Total Mg 5 5	0	0
55	BD	1	Total Mg 1 1	0	0
55	B1	1	Total Mg 1 1	0	0
55	CA	274	Total Mg 274 274	0	0
55	CB	7	Total Mg 7 7	0	0
55	CE	1	Total Mg 1 1	0	0
55	C0	1	Total Mg 1 1	0	0
55	C5	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	C7	1	Total 1	Mg 1	0	0
55	DA	119	Total 119	Mg 119	0	0
55	DL	1	Total 1	Mg 1	0	0
55	DN	1	Total 1	Mg 1	0	0
55	DB	2	Total 2	Mg 2	0	0
55	DC	6	Total 6	Mg 6	0	0
55	D1	1	Total 1	Mg 1	0	0

- Molecule 56 is osmium (III) hexammine (three-letter code: OHX) (formula:  $\text{H}_{12}\text{N}_6\text{Os}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total 7	N 6	Os 1	0	0
56	AA	1	Total 7	N 6	Os 1	0	0
56	AA	1	Total 7	N 6	Os 1	0	0
56	AA	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AE	1	Total	N	Os	0	0
			7	6	1		
56	AF	1	Total	N	Os	0	0
			7	6	1		
56	AO	1	Total	N	Os	0	0
			7	6	1		
56	AO	1	Total	N	Os	0	0
			7	6	1		
56	A1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	A1	1	Total	N	Os	0	0
			7	6	1		
56	A3	1	Total	N	Os	0	0
			7	6	1		
56	AW	1	Total	N	Os	0	0
			7	6	1		
56	A6	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	BG	1	Total	N	Os	0	0
			7	6	1		
56	BR	1	Total	N	Os	0	0
			7	6	1		
56	BB	1	Total	N	Os	0	0
			7	6	1		
56	BB	1	Total	N	Os	0	0
			7	6	1		
56	BC	1	Total	N	Os	0	0
			7	6	1		
56	BC	1	Total	N	Os	0	0
			7	6	1		
56	BD	1	Total	N	Os	0	0
			7	6	1		
56	BD	1	Total	N	Os	0	0
			7	6	1		
56	BD	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
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56	CA	1	Total	N	Os	0	0
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			7	6	1		
56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
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			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
			7	6	1		
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56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CF	1	Total	N	Os	0	0
			7	6	1		
56	CO	1	Total	N	Os	0	0
			7	6	1		
56	C1	1	Total	N	Os	0	0
			7	6	1		
56	C3	1	Total	N	Os	0	0
			7	6	1		
56	C5	1	Total	N	Os	0	0
			7	6	1		
56	C6	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DG	1	Total	N	Os	0	0
			7	6	1		
56	DK	1	Total	N	Os	0	0
			7	6	1		
56	DR	1	Total	N	Os	0	0
			7	6	1		
56	DV	1	Total	N	Os	0	0
			7	6	1		
56	DB	1	Total	N	Os	0	0
			7	6	1		
56	DB	1	Total	N	Os	0	0
			7	6	1		
56	DB	1	Total	N	Os	0	0
			7	6	1		
56	DC	1	Total	N	Os	0	0
			7	6	1		
56	DC	1	Total	N	Os	0	0
			7	6	1		
56	DC	1	Total	N	Os	0	0
			7	6	1		
56	DC	1	Total	N	Os	0	0
			7	6	1		
56	DD	1	Total	N	Os	0	0
			7	6	1		

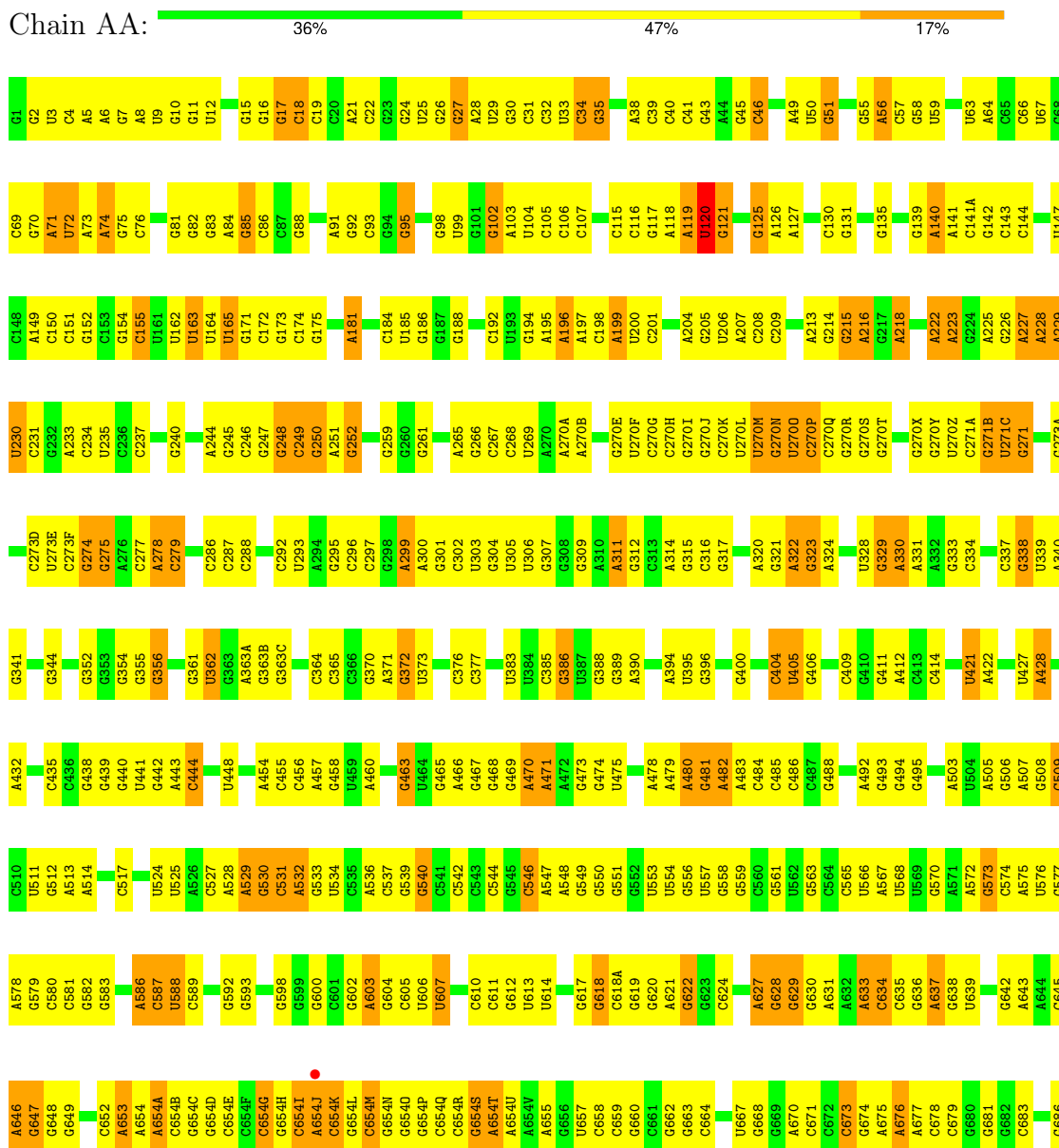
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BG	1	Total	Zn	0	0
			1	1		
57	BQ	1	Total	Zn	0	0
			1	1		
57	DG	1	Total	Zn	0	0
			1	1		
57	DQ	1	Total	Zn	0	0
			1	1		

### 3 Residue-property plots

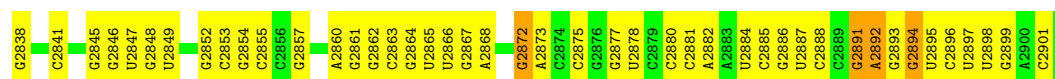
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: RNA (2912-MER)



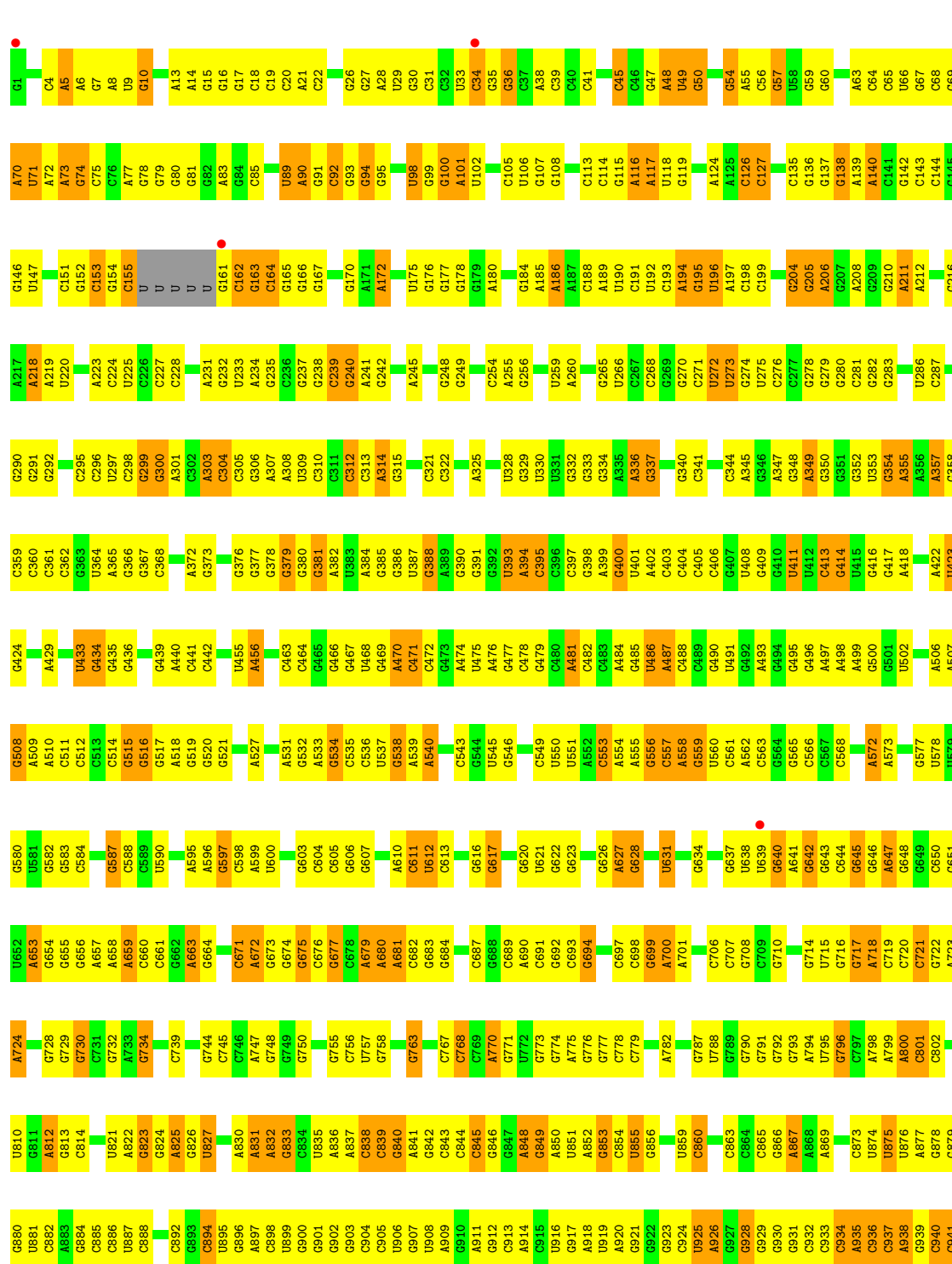
C1663	C1583	U1516	A1449	G1369	U1294	A1214	C1152	U1080	U1014	G946	C867	C791	G680
G1667	C1585	G1517	G1449A	U1372	C1295	G1215	C1153	U1081	G1015	G947	U868	G792	G691
A1668	A1586	G1518	C1450	A1373	G1296	G1216	G1297	U1082	G1016	G948	G869	A793	
A1669	A1587	U1520	C1451	G1374	C1297			U1083	G1017		G870	A794	
			U1454	G1374	C1298	G1219	A1155	U1084	C1018	C951	U871	C795	A705
			G1454	U1299	G1299	A1220	A1156	A1085	U1019	A952	G872	C796	
			G1455	U1300	C1221	C1221		U1086	A1020	A953	G873	C797	G717
				A1301	C1222			G1087	A1021	G954		G798	
				G1379	A1302			A1088	G1022	C955	U877		G723
				G1380	G1303	C1230	C1161	U1089	G1023	G956	A878	A802	U724
				G1381		C1231	G1162	U1090	G1024	A957	G879		U725
				G1382		G1230	G1163	G1091	G1025	U958	G880	C805	G726
				G1383		G1235	G1164	C1092	U1026	U959	G881	C806	A727
				A1384		G1236	U1165	G1093	A1027	A960	G882	U807	G728
				G1385			C1166	U1094	U1033	C961	G883	G808	
				G1386			U1167	A1095		G962	G884	G809	C730
				G1387		G1239	G1168	A1096	G1036		C967	U810	C731
				G1388		U1240	G1169	U1097	C1043		G885	U811	C732
				G1389		A1241	G1170	U1098	G1044		G886	C812	G733
							G1171	G1099	C1038		G887	U813	
						G1244	G1172	C1100	G1039		C970	C814	G741
							G1173	C1101			A890		G742
						A1247	A1174	U1101	G1042		G892	C817	
						G1248	U1175	C1102	C1043		C893	G818	G745
						U1249	G1176	A1103	G1044		G894	A746	
						G1250	A1177	C1104	A1045		U895	A819	U747
							C1178	U1105	A1046		G896	A820	G748
						A1253	C1179	G1106	G1047		C897	A821	G749
						U1254	G1180	U1107	A1048		G898	U827	A750
						G1255	C1181	U1108	C1049		A899	U828	A751
						U1256	A1182	C1109	A1050		A900	A752	
						C1257		G1110	A1051		A901	G753	
							C1185	A1111	C1052		G902	G831	C754
						C1261	G1186	C1112	C1053		C903	G832	C755
						U1262	U1187	U1113	A1054		G904	U833	C756
						G1263	A1188	C1114	G1055		U905	C834	
						G1264	A1189		G1056		G906	A835	G760
						U1265	G1190	G1122	A1057		U907	G836	A761
						G1266	G1191		U1058		C908	C837	U762
						U1267	G1192	G1125	U1059		A990	G838	G763
						A1268	G1193	U1126	U1060		C991	A764	
						C1269	A1194	A1127	U1061		C992	U839	
						U1270	G1195		G1062		G993	G845	C766
						G1271	C1196	U1130	G1063		A917	C846	
						A1272	G1197	G1131	C1064		A918	U847	U773
						U1273	U1198	A1132	G1065		G919	A774	
						A1274	U1199	U1133	U1066		G997	G848	A775
						U1275	C1200	C1135	U1067		C998	A849	G776
						A1276	C1201	G1136	A1067		G928	C850	
						G1277	C1202	G1137	G1068		G929	U851	
						U1278	G1203	G1138	A1069		A1000	G857	G780
						G1279	A1204	G1139	A1070		G932	A761	
						G1280	U1205	C1140	G1071		A933	A762	
						G1281	G1206	U1141	C1072		G1003	A783	
							C1207	U1142	G1073		G938	U860	A784
						A1287	C1208	A1143	G1074		C1005	G785	
						U1288	G1209	A1143	C1075		C1006	C786	
							A1210	G1144	G1076		G942	U787	
						C1291	U1211	C1145	A1077		U943	A788	
						U1292	G1212		U1078		G944	A789	
						C1293	A1213	G1149	C1079		A945	C850	C790

C2755	C2681	G2597	C2297	C2226	G2151	G2087	G2012	G1930	C1832	C1761
U2756	U2682	A2598	A2298	C2231	G2152	U2092	A2013	U1931	U1833	A1762
A2757	C2683	G2599	G2299	U2232	G2153	G2092	A2014	A1932	U1834	G1763
	U2684	A2433	G2300	G2366	G2154	G2093	A2015	G1933	G1835	G1764
	A2435	A2435	C2301	G2367	G2155	G2094	U2016		C1836	
	G2685	C2601	G2302	G2368	G2156	C2095	U2017	A1937		G1769
	U2687	A2602	G2303	G2369	G2157	U2096	G2018	A1938	A1847	G1770
	U2688	U2605		A2370	G2158	C2097	A2019	A1848	A1848	
	U2689	C2606	G2307	G2238	G2159	C2098	A2020			G1771
	C2690	G2517	G2308	G2239	G2160	U2099	A2021	G1945	G1772	G1772
	C2691	A2518	A2309	G2242	G2161	G2100	U2022		A1854	C1773
	G2692		G2310	U2243	G2162	G2101	G2023	G1950	C1774	C1774
	A2693	G2629	A2311	G2374	G2163	G2102	G2024	U1951	U1775	U1775
	G2694	U2629	U2312	G2375	G2164	G2103	C2025	A1952	G1776	G1776
			G2313	A2376	G2165	C2104	G2026	A1953	U1777	U1777
			C2314	A2246	G2166	C2105		G1954	U1778	U1778
			G2315	G2247	G2167	G2106	G2029	U1955	U1779	U1779
			G2316	G2250	U2167	C2107	A2030	U1956		A1780
			C2317	G2251	A2169	C2108	A2031		C1781	C1781
			G2318	G2252	A2170	U2109	G2032		C1782	C1782
			G2319	G2253	A2171	G2110	A2033		A1783	A1783
			A2320	G2254	U2172	G2111	U2034	C1962		A1784
			G2321	G2255	A2173	G2112	G2035	U1963	A1871	A1785
			A2322	G2256	C2174	U2113	G2036	G1965	A1872	A1786
				U2257	G2175	U2114	G2037	A1966	G1878	A1787
				C2258	A2176	G2115	G2038	C1967		C1790
			G2325	G2259	C2177	G2116	C2039	C1968		G1791
			A2326	C2260		A2117		A1969	G1792	G1792
			A2328	G2261	G2181	U2118	C2043	G1970	C1793	C1793
				U2262	G2182	A2119		A1971	U1794	U1794
			G2331		G2183	G2120	G2053	C1972	C1795	C1795
				A2266	G2184	G2121	A2054	A1973	U1796	U1796
				A2267	C2185	U2122	C2055	C1974		C1797
				G2270	G2187	G2123	A2056	A1889		U1798
				U2271	G2188	G2124	G2057	G1799		G1799
				G2272	G2190	G2125	A2058	C1893		C1800
				U2273	G2191	A2126	A2059	G1894	G1801	G1801
				A2274	G2192	G2127	A2060	C1895	A1802	A1802
				C2275	G2193	C2128	G2061	G1896	A1803	A1803
				G2276	G2194		A2062	G1985	C1804	C1804
				G2277		G2131	G2063	U1805	U1805	U1805
				G2278	U2197	U2132	C2064		A1812	A1812
				A2278	A2198	G2133	C2065		G1813	G1813
					A2199	A2135	G2067			
					G2200	C2136	U2068		G1816	G1816
					C2201	C2137	G2069		G1817	G1817
					G2202	C2138	U2070		U1818	U1818
					U2212	C2139	G2070		A1819	A1819
					G2215	C2140			U1820	U1820
					G2216	G2141	U2075		A1912	A1912
					G2219	G2142	U2076		A1913	A1913
					G2224	C2143	A2077		G1914	G1914
					A2225	U2144	G2078		U1915	U1915
						G2145	U2079		A1825	A1825
						C2146	G2080		G1826	G1826
						G2147	C2081		C1827	C1827
						G2148	A2082		G1828	G1828
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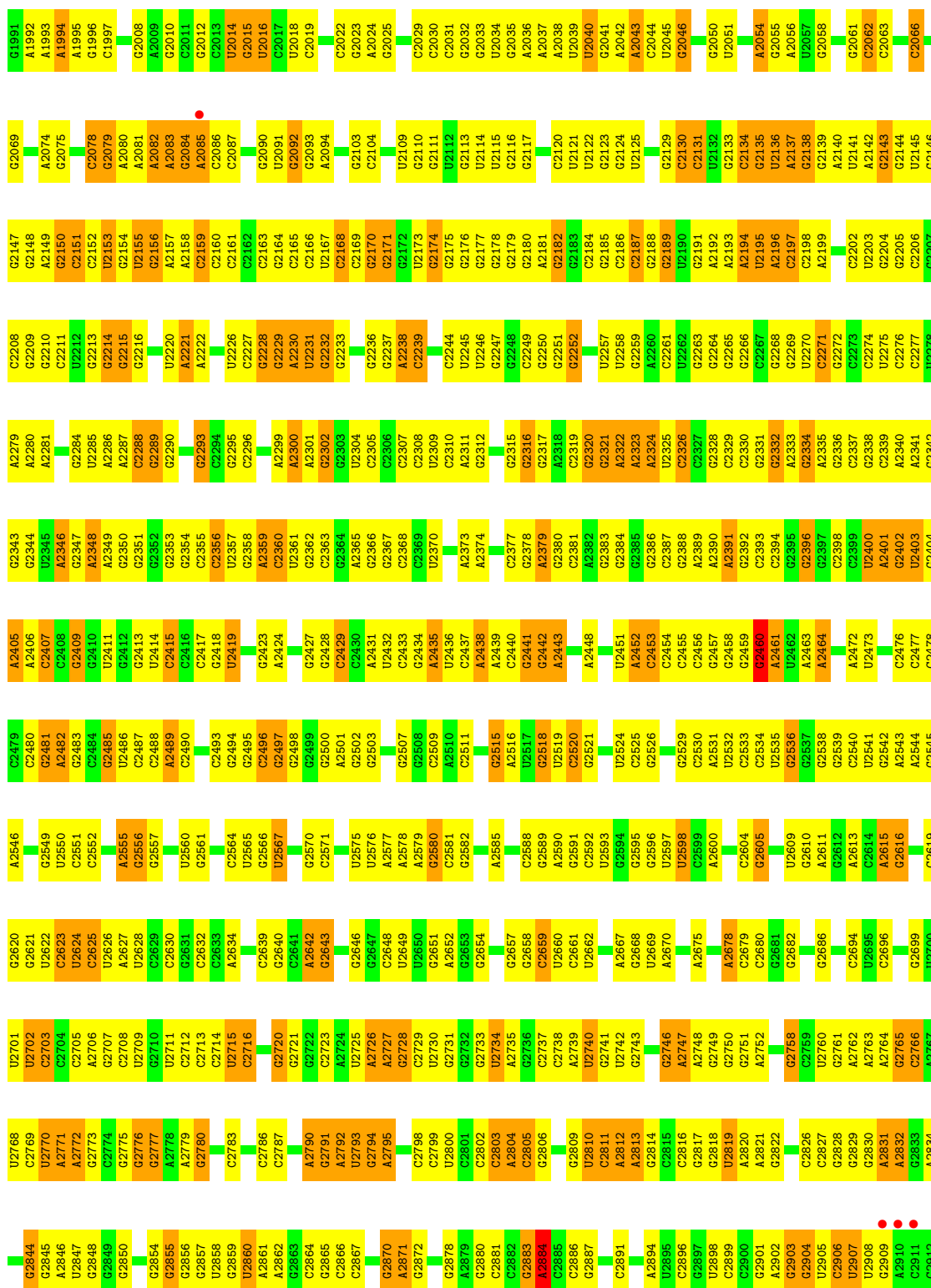


● Molecule 1: RNA (2912-MER)

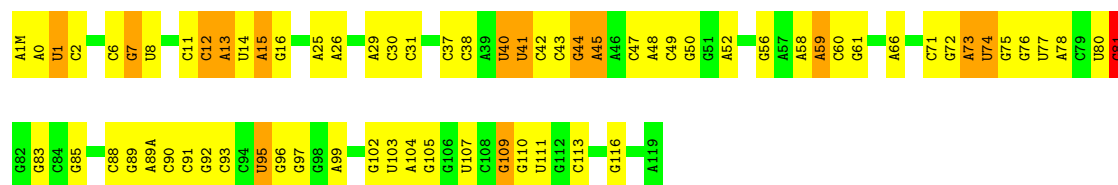
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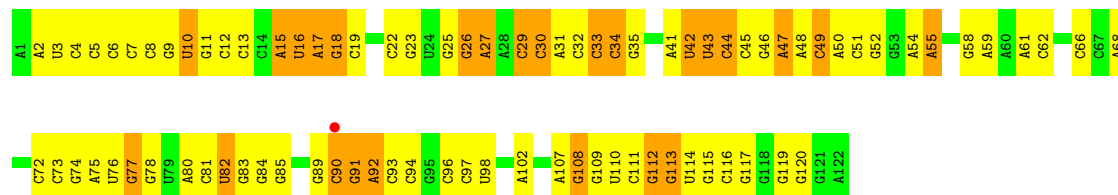
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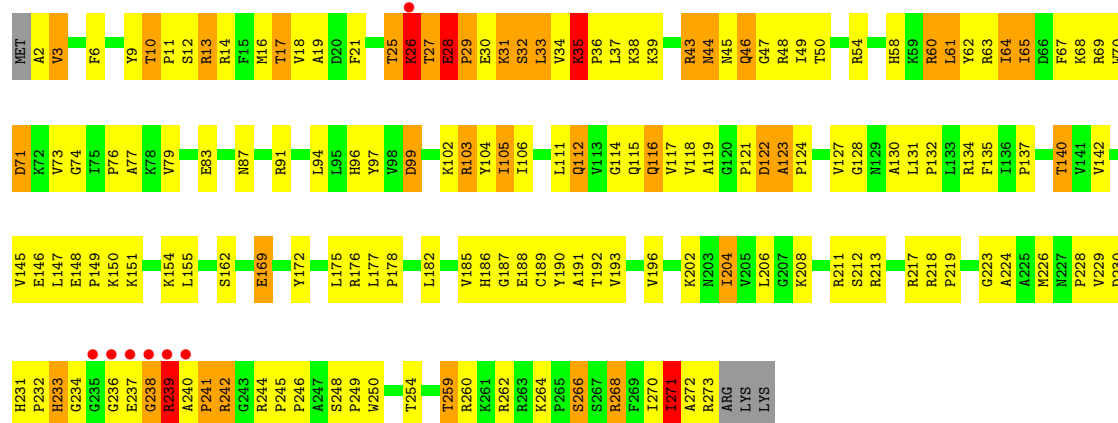
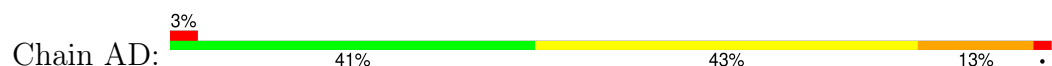
• Molecule 2: 5S RIBOSOMAL RNA



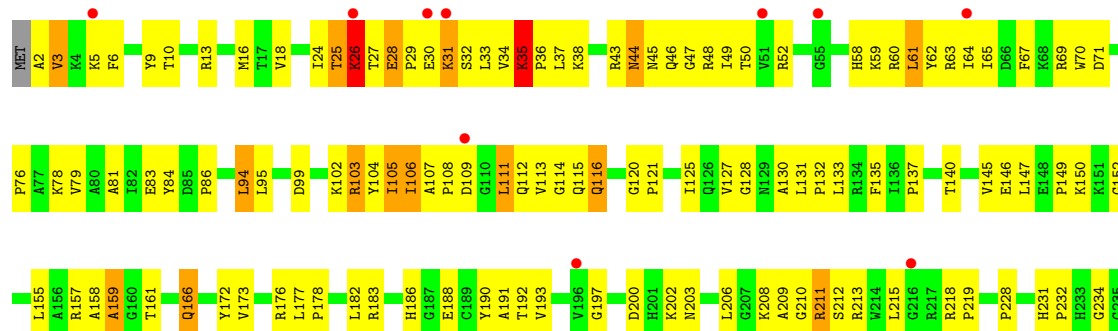
### • Molecule 2: 5S RIBOSOMAL RNA

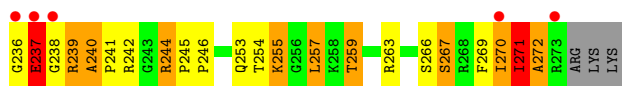


### • Molecule 3: 50S ribosomal protein L2

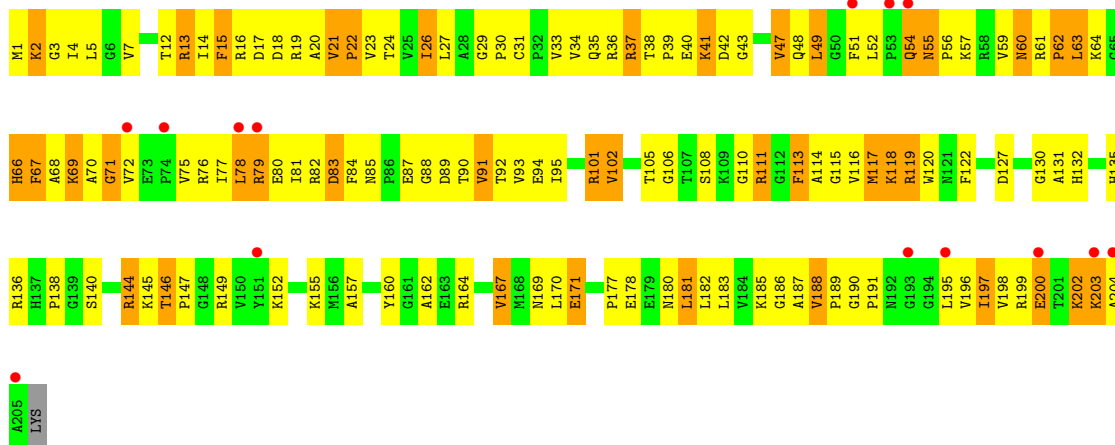


### • Molecule 3: 50S ribosomal protein L2

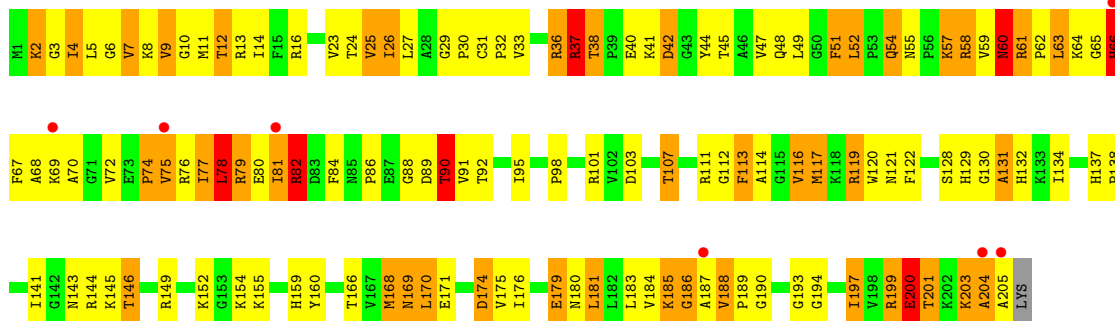




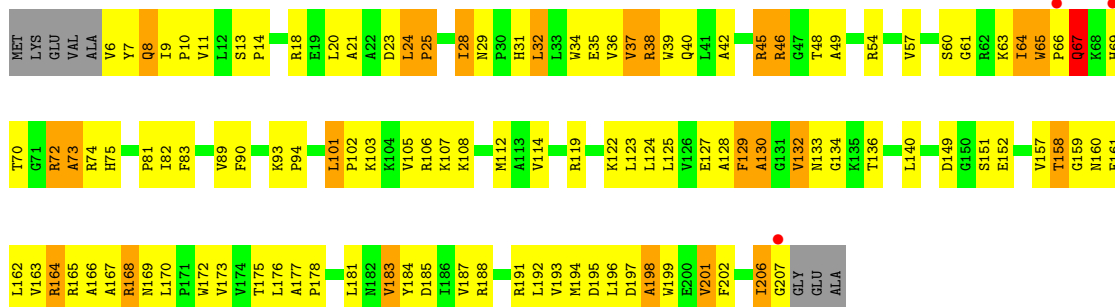
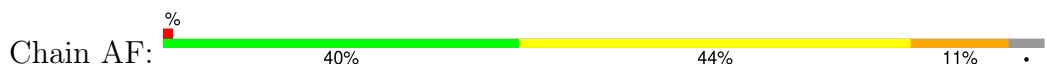
• Molecule 4: 50S ribosomal protein L3



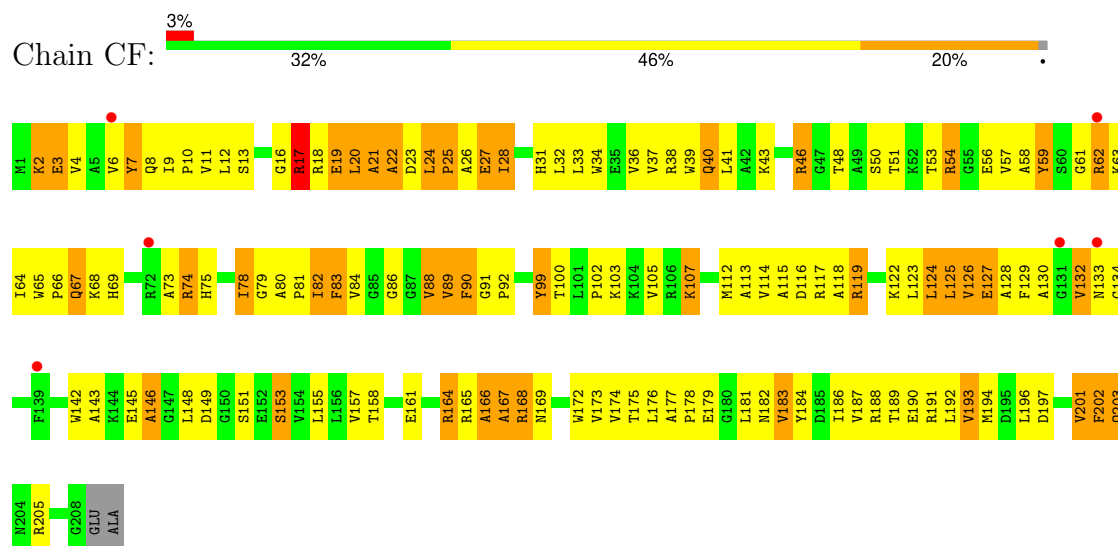
• Molecule 4: 50S ribosomal protein L3



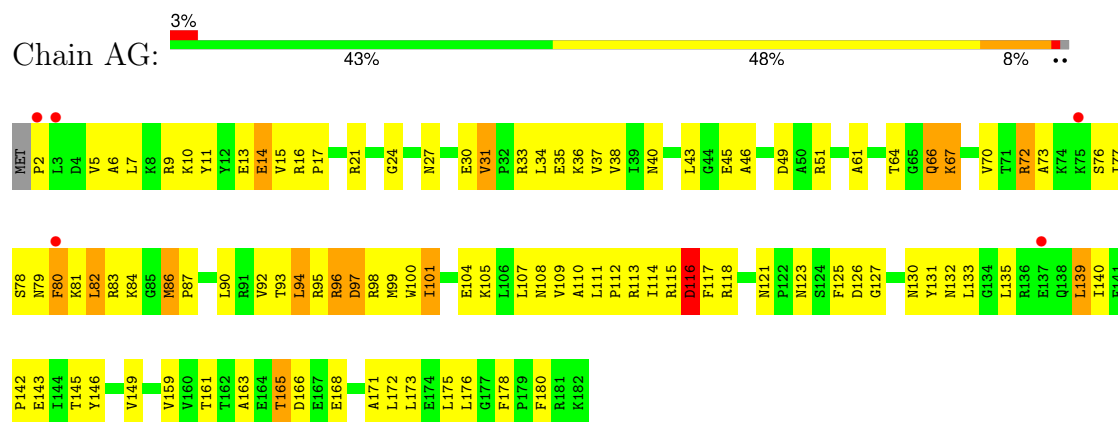
• Molecule 5: 50S ribosomal protein L4



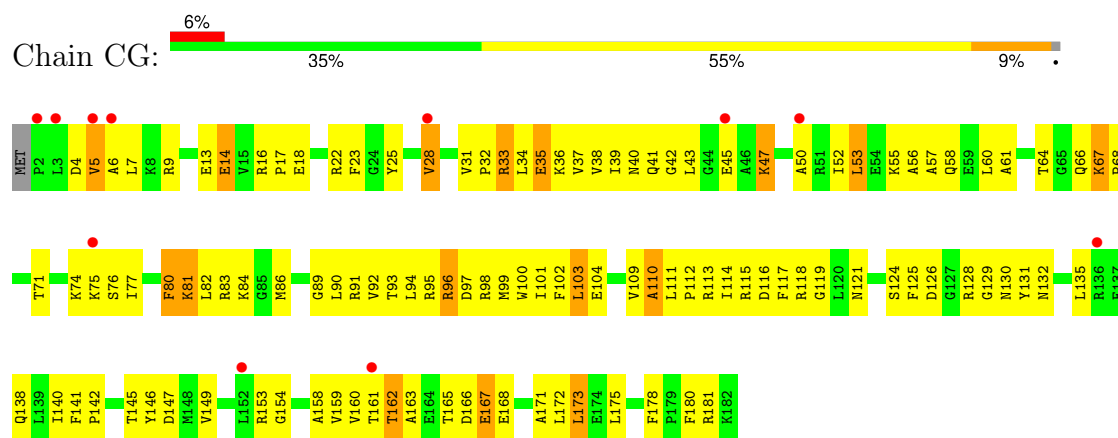
- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5

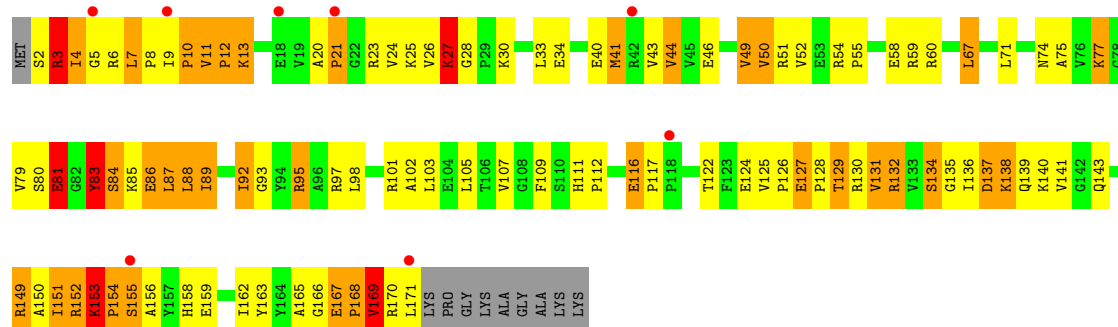


- Molecule 6: 50S ribosomal protein L5

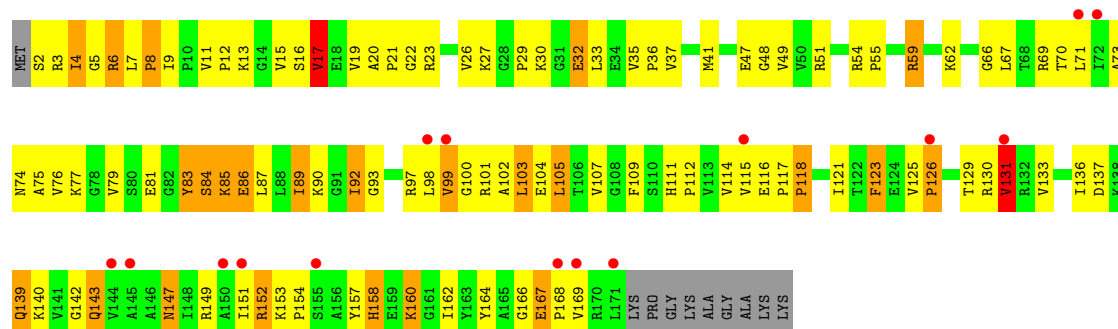


- Molecule 7: 50S ribosomal protein L6

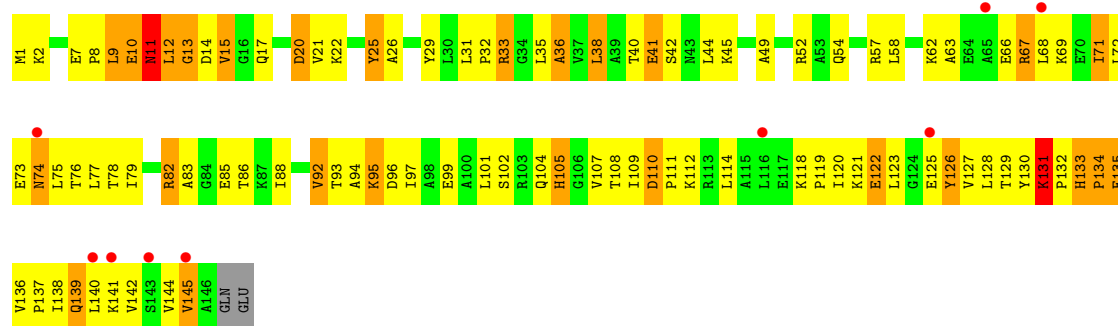




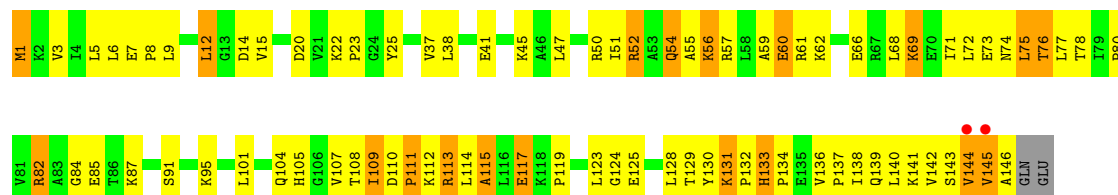
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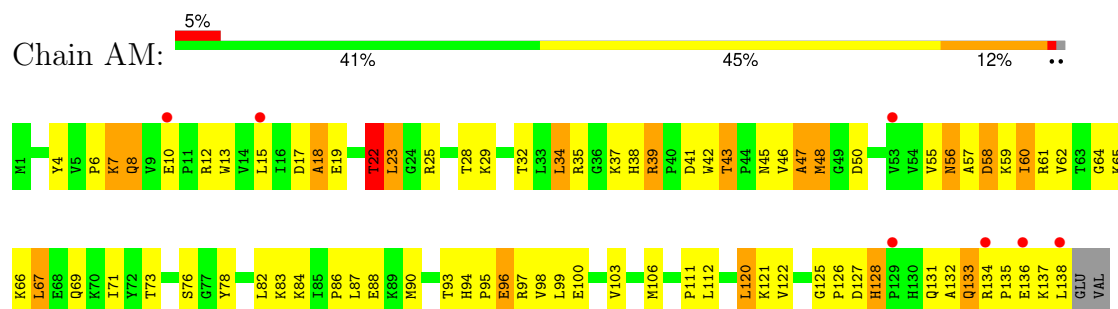
• Molecule 8: 50S ribosomal protein L9



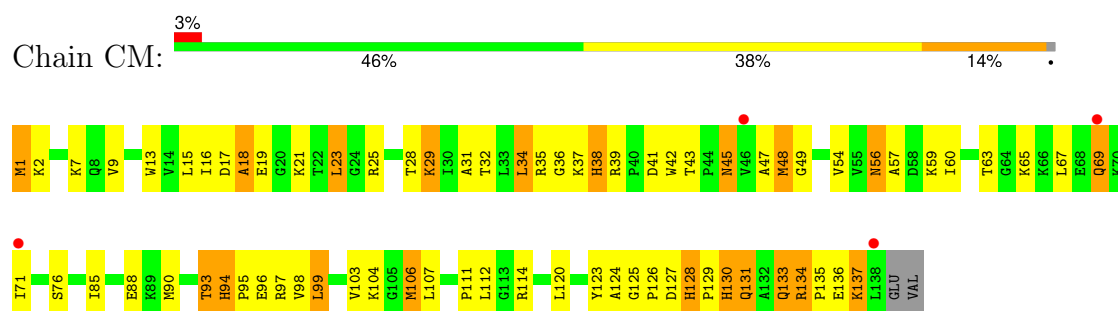
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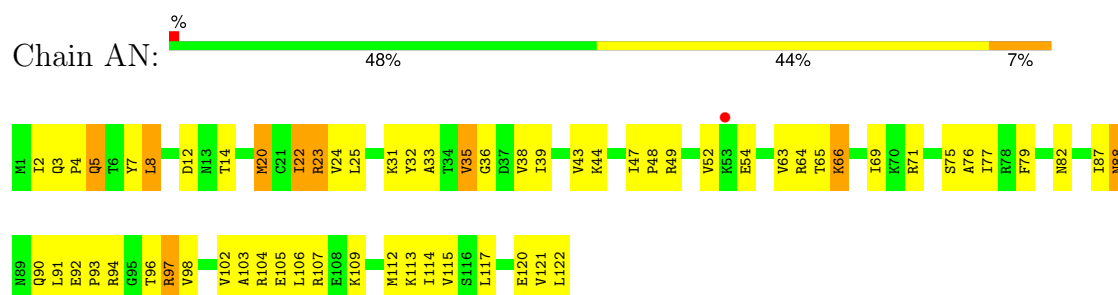
- Molecule 9: 50S ribosomal protein L13



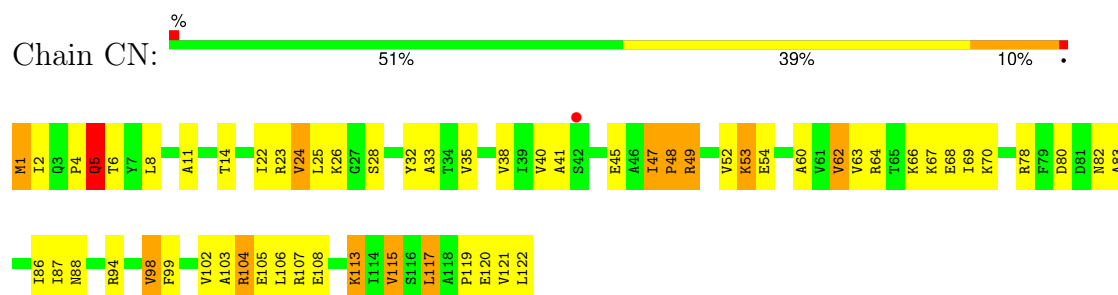
- Molecule 9: 50S ribosomal protein L13



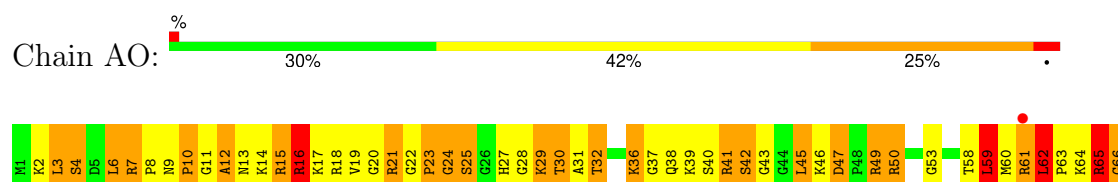
- Molecule 10: 50S ribosomal protein L14

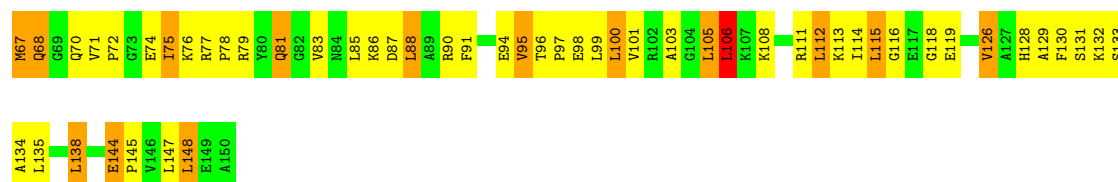


- Molecule 10: 50S ribosomal protein L14

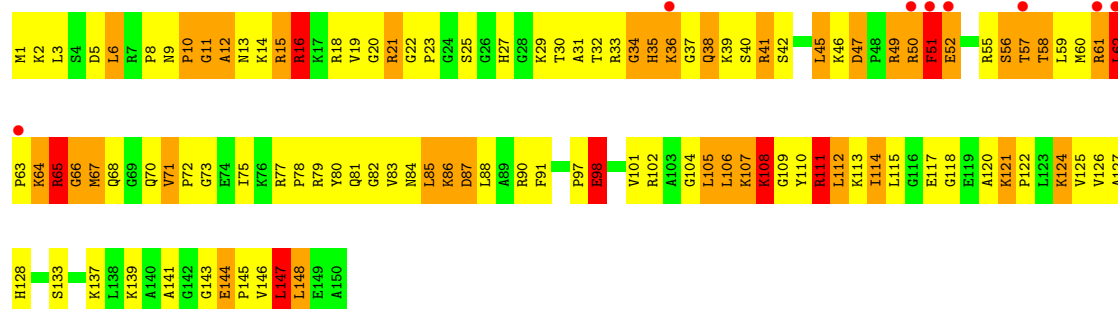


- Molecule 11: 50S ribosomal protein L15

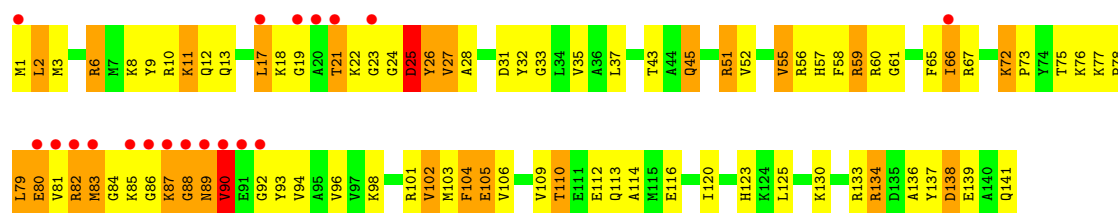
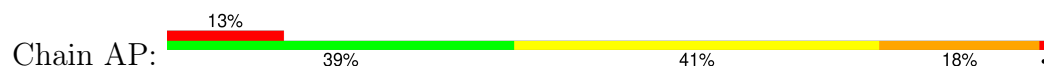




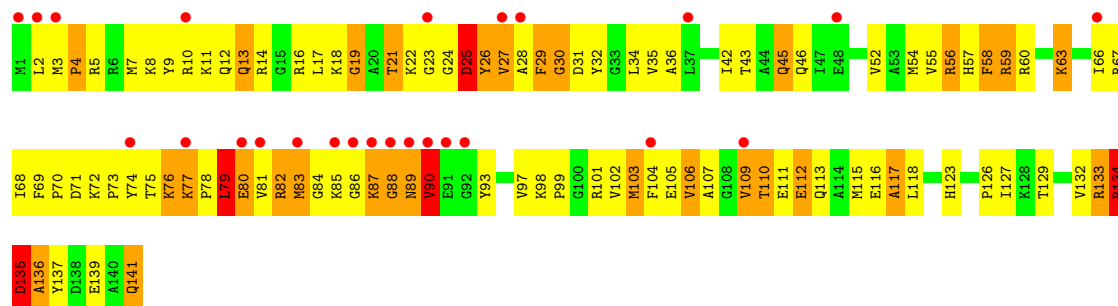
• Molecule 11: 50S ribosomal protein L15



• Molecule 12: 50S ribosomal protein L16

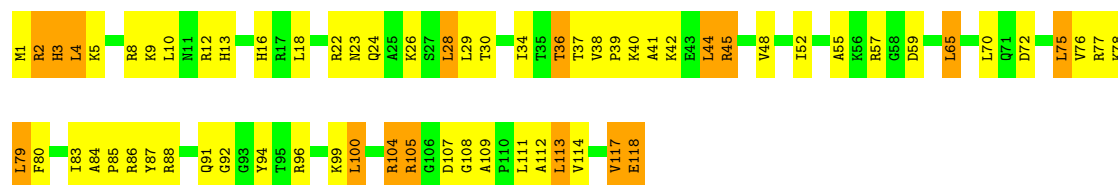


• Molecule 12: 50S ribosomal protein L16

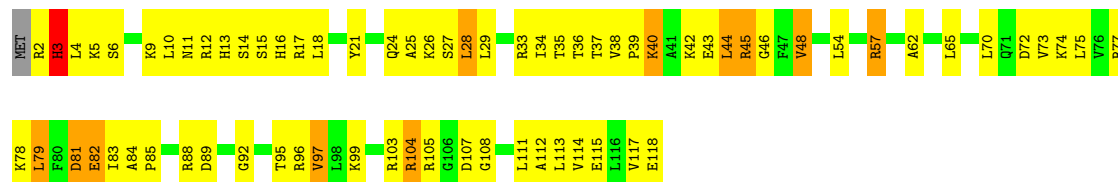


• Molecule 13: 50S ribosomal protein L17

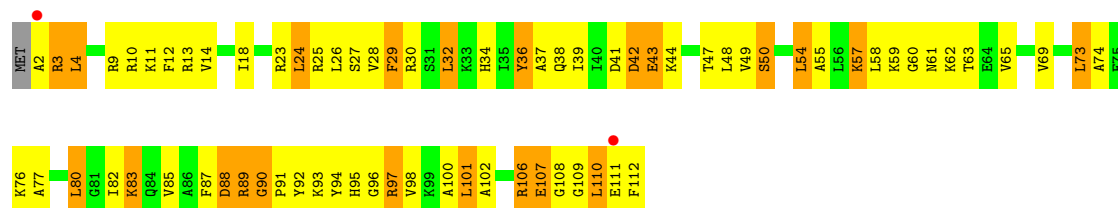




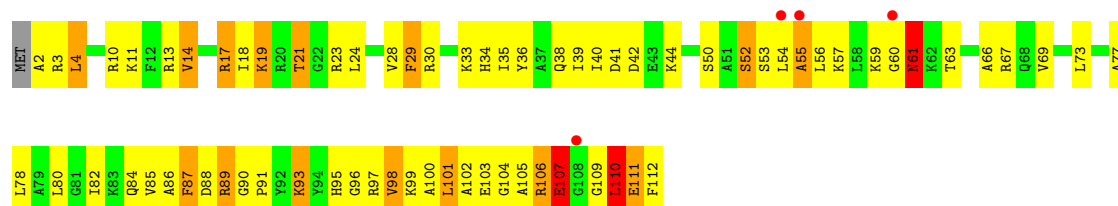
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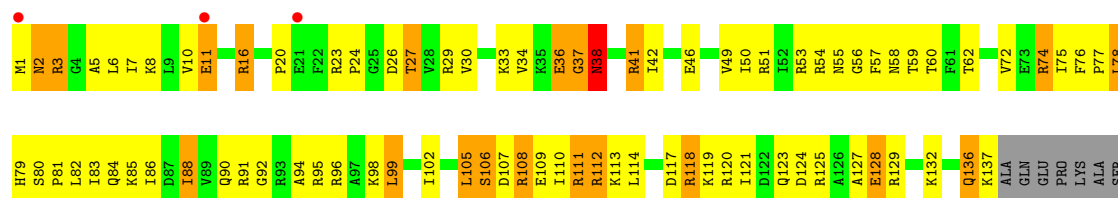
• Molecule 14: 50S ribosomal protein L18



• Molecule 14: 50S ribosomal protein L18

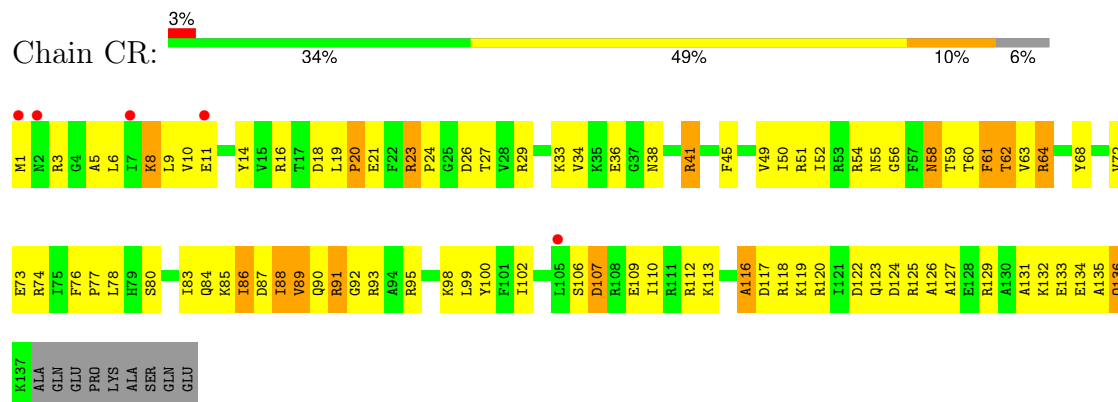


• Molecule 15: 50S ribosomal protein L19

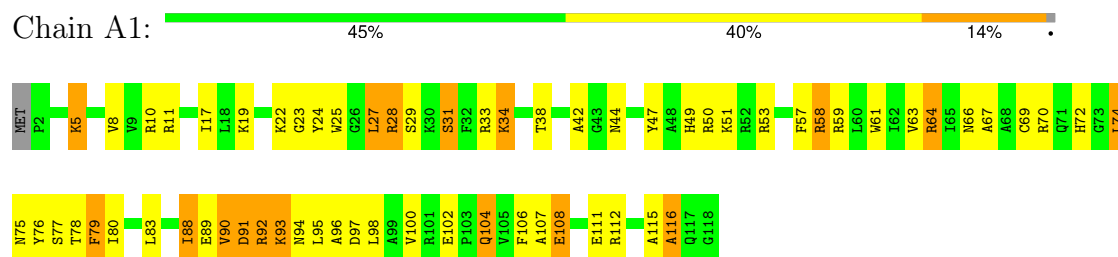


GLN  
GLU

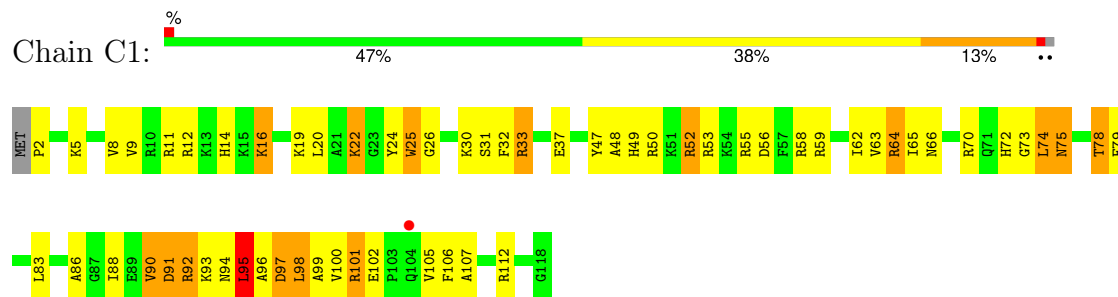
- Molecule 15: 50S ribosomal protein L19



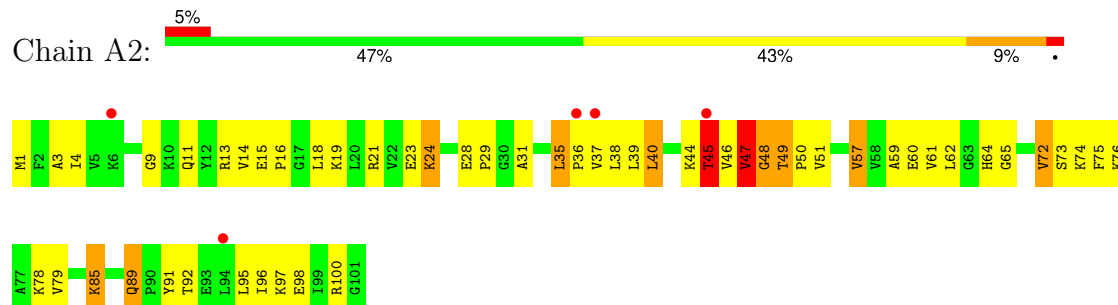
- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



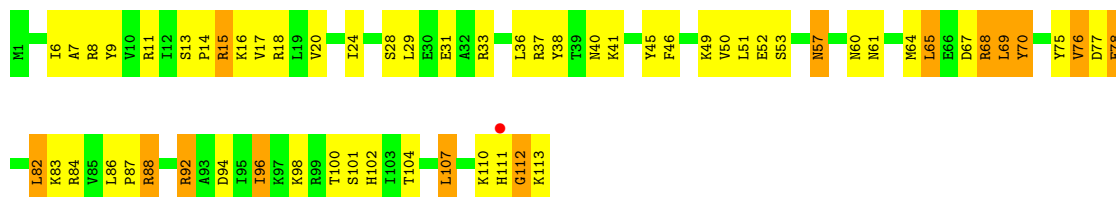
- Molecule 17: 50S ribosomal protein L21



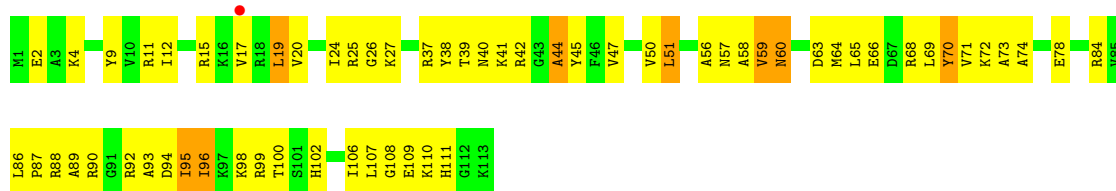
- Molecule 17: 50S ribosomal protein L21



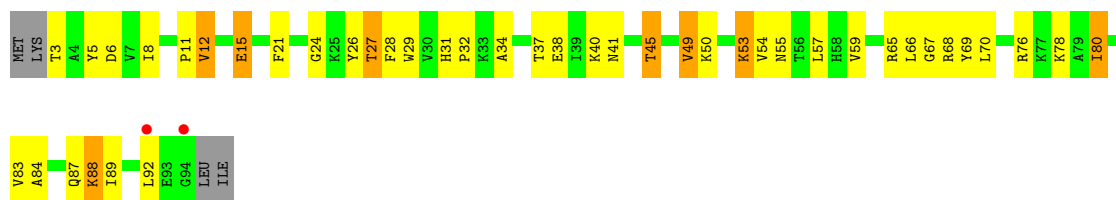
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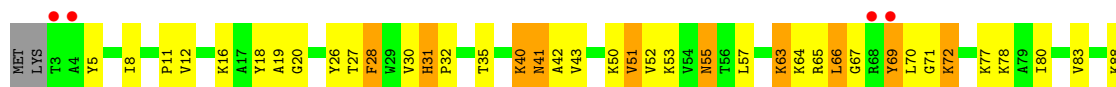
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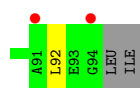


• Molecule 19: 50S ribosomal protein L23



• Molecule 19: 50S ribosomal protein L23

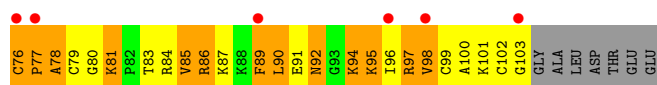
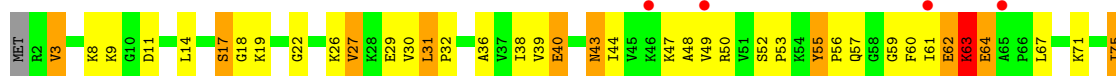




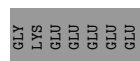
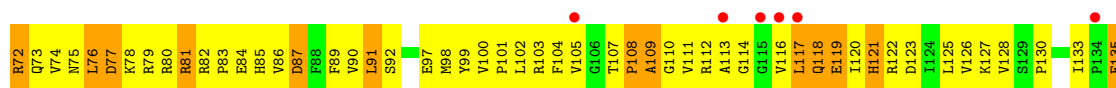
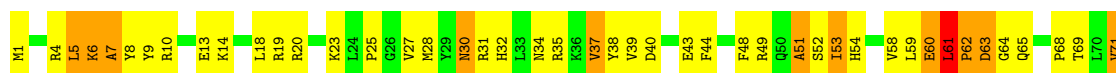
- Molecule 20: 50S ribosomal protein L24



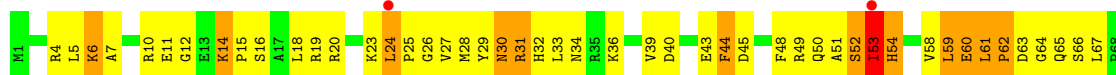
- Molecule 20: 50S ribosomal protein L24

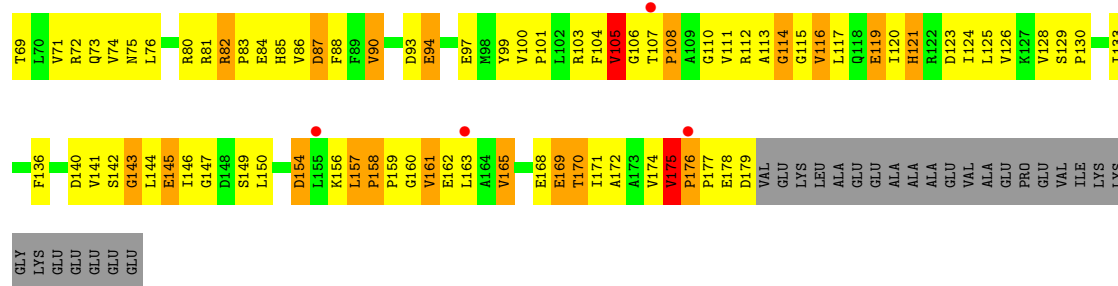


- Molecule 21: 50S ribosomal protein L25

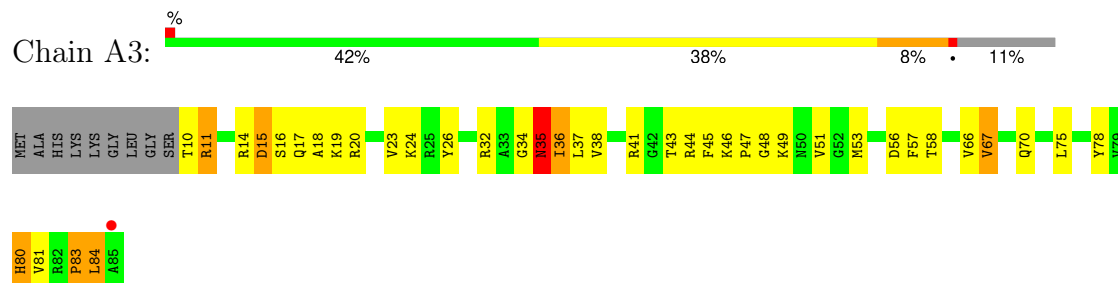


- Molecule 21: 50S ribosomal protein L25

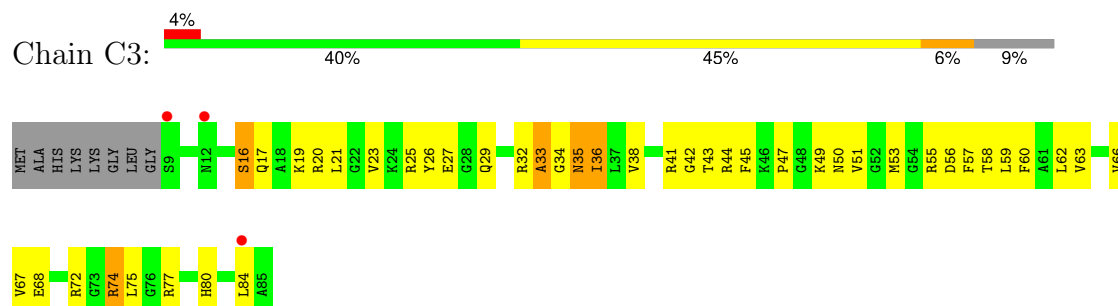




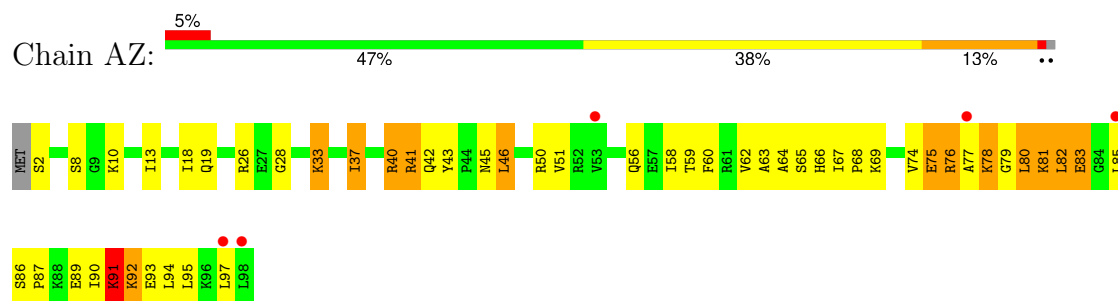
- Molecule 22: 50S ribosomal protein L27



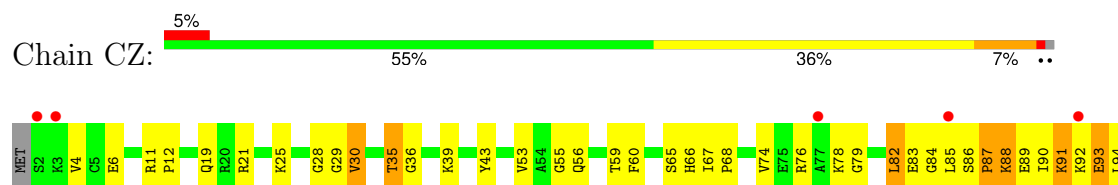
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28

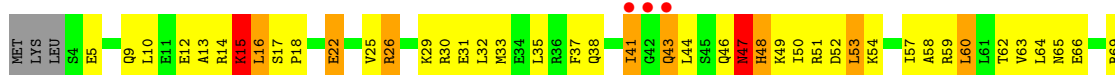




• Molecule 24: 50S ribosomal protein L29



• Molecule 24: 50S ribosomal protein L29



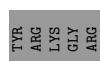
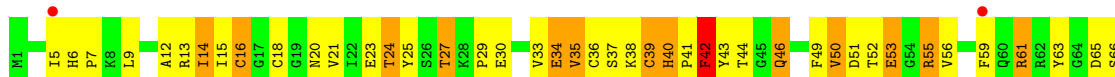
• Molecule 25: 50S ribosomal protein L30



• Molecule 25: 50S ribosomal protein L30

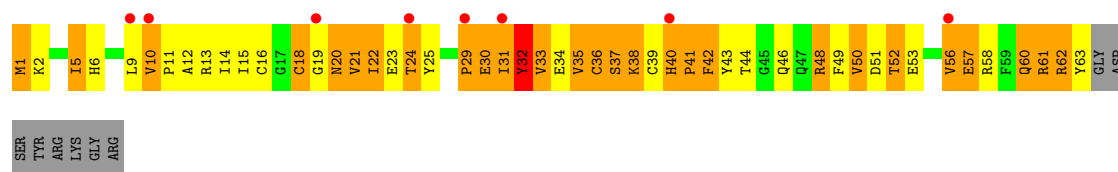


• Molecule 26: 50S ribosomal protein L31

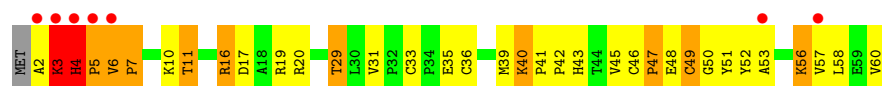


• Molecule 26: 50S ribosomal protein L31





- Molecule 27: 50S ribosomal protein L32



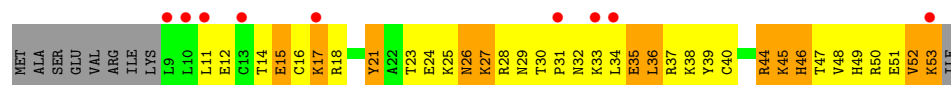
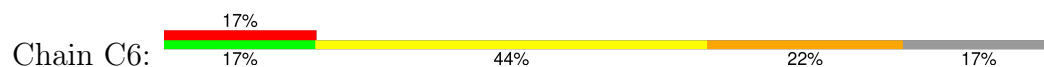
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



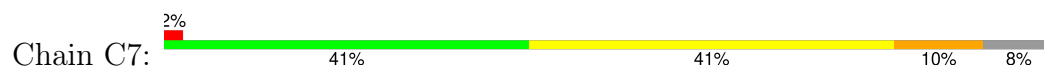
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34




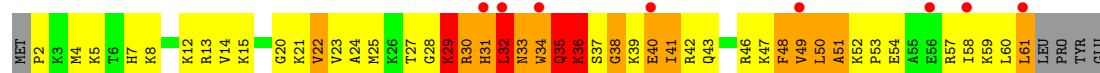
- Molecule 30: 50S ribosomal protein L35

Chain A8: 



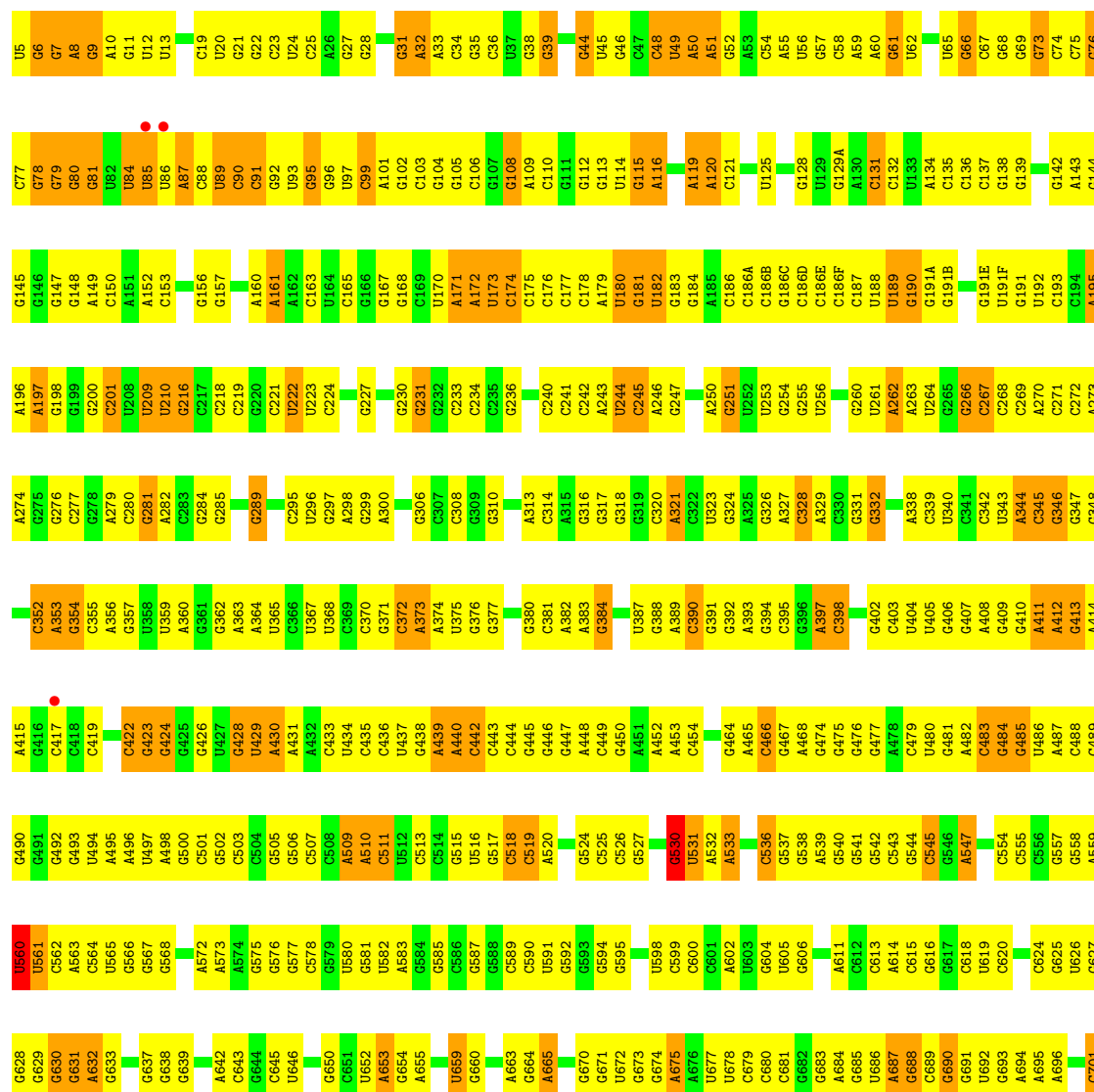
- Molecule 30: 50S ribosomal protein L35

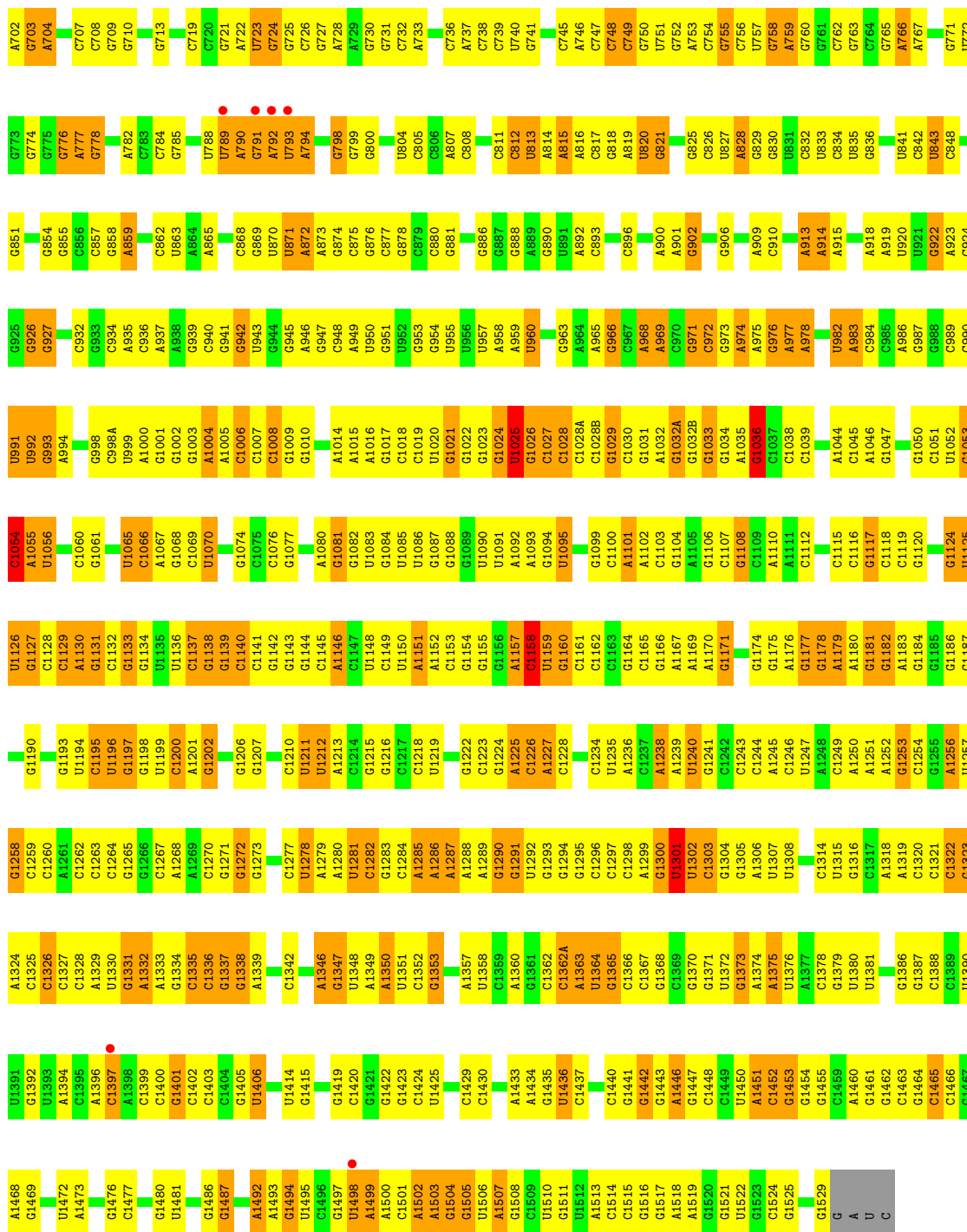
Chain C8: 



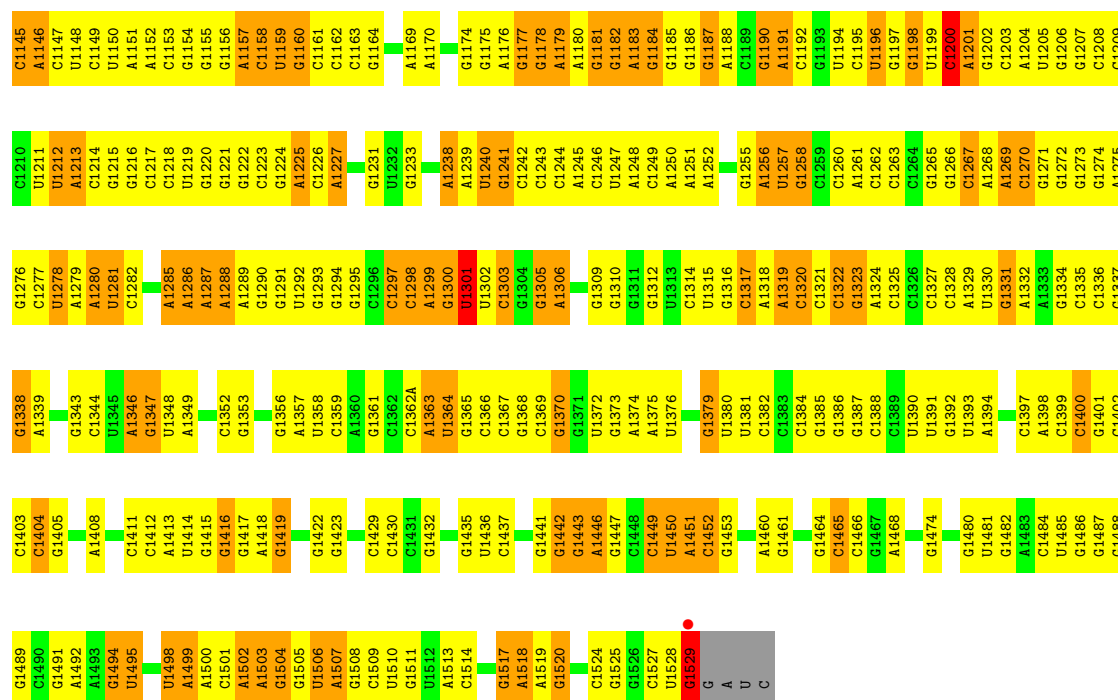
- Molecule 31: 16S ribosomal RNA

Chain BA: 

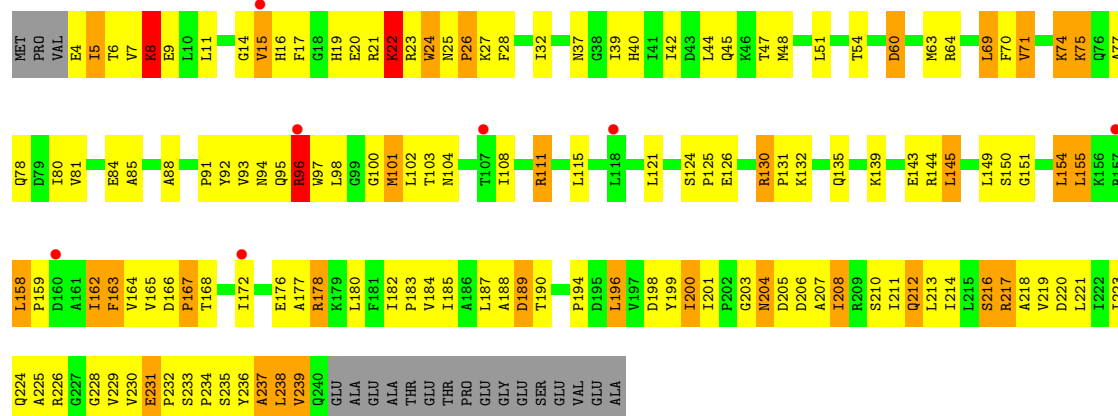




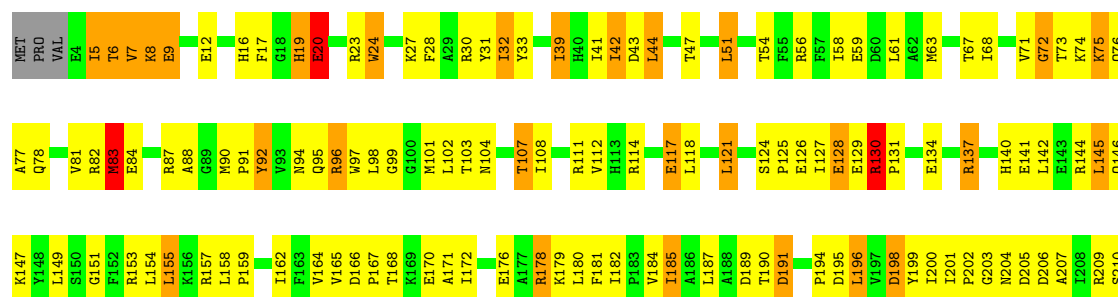
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G1081	G1023	C962	C812	G741	U677	G604	U534	A453	A303	C154	U62
G1082	G1024	G963	U813	G742	U678	U605	A535	C454	U304	G155	U84
U1083	U1025	A964	U814	G743	U679	U606	C536	C455	G305	G156	U85
G1084	G1026	U891	A815	C744	G680	A607	G537	C456	G306	G157	U86
U1085	C1027	G966	A816	G745	C681		G538	C457	C225	C224	A87
U1086	C1028	C967	A817	G746	U682		A539	C458	C312	A160	C88
U1087	U1028A	A968	C817	G749	G683	C615	G540	G464	A313	A161	U89
	C1028B	A969	G818	G750	U684	G616	G541	A465	G316	G165	C90
A1092	G1029	C970	U819	G751	U685	G617	G542	C466	G231	C166	C91
U1093	C1030	C899	U820	G752	C618	C543	G544	C467	C235	G167	G92
G1094	G1031	A900	G821	A753	U686	U619	G545	A468	A321	G168	U93
U1095	A1032	A901		G754	A687	C620	G546	G474	C322	G169	G95
U1096	G1033	G902	C826	G755	G688	A621	A547	G475	U323	U170	G96
C1097	U1032B		U827	G756	C689	A622	G548	G476	A243		U97
C1098	G1033	A907	A828	U757	G690	G623	G549	G477	C398		C99
U1099	G1034	A908	U830	G758	G691	C624	C550	A478	U173	U174	A101
G1100	A1035	A909	U833	A759	U692	G625	C551	C479	C245	C174	G102
C1101	G1036	C910	C834	G760	U693	U626	U551	U480	C328	C175	C103
A1102	C1037		U835	G769	C699	G627	U552		A329	G247	
	U1038	U981	C842	A694	A695	G628	A553	G484	U405	C177	G108
A1105	C1038	A913	U836	G763	A696	G629	G554	G485	G332	C178	A109
G1106	U1039	A914	C837	G764	A697	G630	C555	U486	G333	C179	C110
C1107	U1040	A915	U838	G765	U697	G631	C556		G334	U180	G111
G1108	A1041		U841		C698	G632	G557	G491	C337	G181	
C1109	C1043	U918	U843	G773	C699	G633	G558	G492	A338	G182	G113
A1110	A1044	A919	C848	G774	A702	G634	A559	G493	C339	G183	U114
G1111	U1045	U920	C849	G775	G703	G635	U560	U494	U340	G186	
C1112	A1046	U921	U850	G776	A704	U636	U561	A495	C341		A116
C1113	G1047	A922	C851	G777	U705	G637	C562	A496	A262		
C1114	C990	A923	C852	A777	A706		A563	U497	A263	G186C	C121
U1048	U1048	G924	G853	G778	C707	C643	C564	A498	U264	C186D	C122
G993	G1050	G925	C854	G779	C708	G644	G500	C501	G265	C186E	
A994	C1051	G927	G855	A780	U709	U646	U571	C502	C266	C186F	G127
C995	U1052		C856	G781	G710	C647	A572	C503	C267	C187	G128
	G1053	C934	G858	A782	A715		A573	C504	C268	U188	U129
G998	A1055	A935	A859	G783	G716	C651	A574	G505	C269	U189	G129A
	U1056		A860	G784	A717	U652	G575		A270	G190	
A1000	G1057	G939	C861	G785	C717	A653	G576	C508	C271	G191A	A130
G1001	G1058	C940	C862	G786	G718	G654	U577	A509	C272	G191B	C131
G1002	C1059	G941	A865	A787	C719	A655	G577	A510	A273	G191C	C132
U1004	U1060	U943	U866	U788	C720	A656		U429	C355	U191D	U133
A1005		C944	G867	U789	G721	C656	U580	A430	C277	U191E	U134
C1006	G1064	G945	C868	A790	G657	G658	G581	A431	G278	C135	
C1007	U1065	G946	C869	G791	G724	G659	U582	A432	A279	C136	
G1008	C1066	U947	U870	A792	G725	U659	A583	C433	G191F	C137	
U1009	A1067	G948	U871	G793	G726	G660	G584	U434	U192	G193	G138
G1010	G1068	A949	C872	A794	G727	G661	G585	C435	C281	C194	G139
G1011	C1069	U950	A873	C795	A728	G662	C586	A520	A282	G195	A140
U1012	U1070	G951	C874	G796	G729	A663	G587	G521	C283	A196	A141
G1013	C1071	U952	C875	G797	G730	G664	G588	C522	G284	A197	G142
U1014	G1072	G953	C879	G798	G731	A665	G592	A523	G285	G198	A143
A1015	U1073	G954	G880	G799	C732	G666		A440	G289	G199	G144
G1016	G1074	U955	G881	G800	G733	G667	G595	C442	U296	C201	G145
U1017	C1075	U956	C882	G803	G734	U668	C596	A374	G297	G208	G146
C1018	U1076	U957	C883	U804	C735	U669	G597	U375	A298	U209	G148
C1019	G1077	A958	U884	C805	G736	G670	G598	G376	G299	U210	A149
U1020	U1078	A959	C885	C806	A737	U671	U599	G449	A300	G216	
G1021	G1079	U960		A807	C738	G672	C600	A451	G301	C217	A152

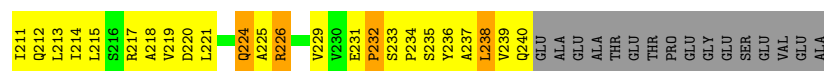


### • Molecule 32: 30S RIBOSOMAL PROTEIN S2

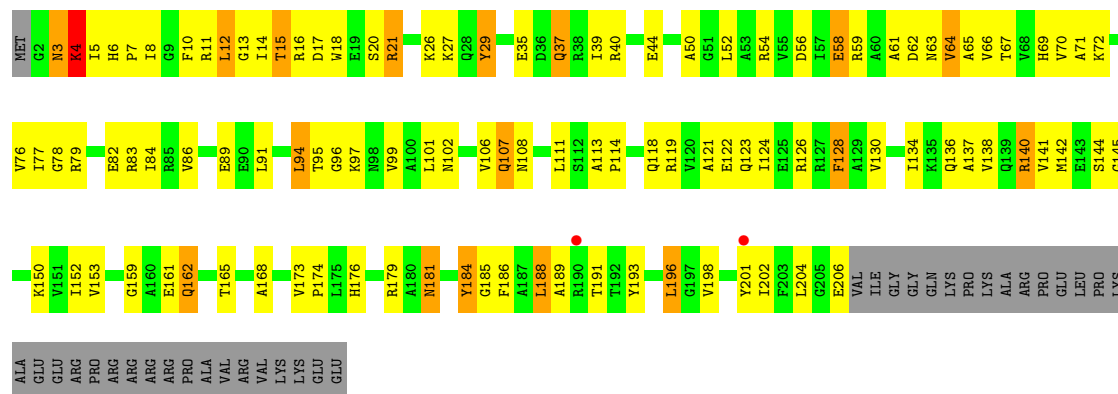
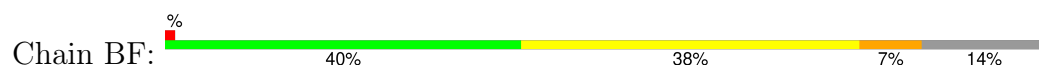


### • Molecule 32: 30S RIBOSOMAL PROTEIN S2

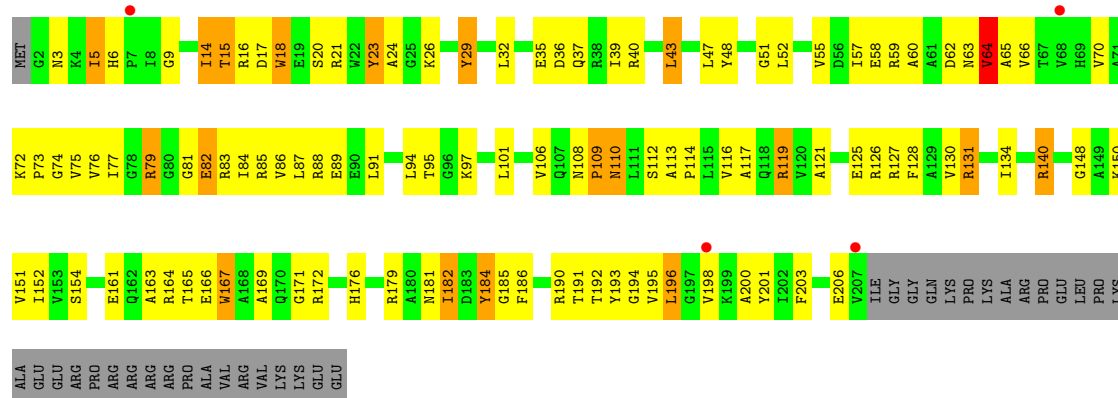




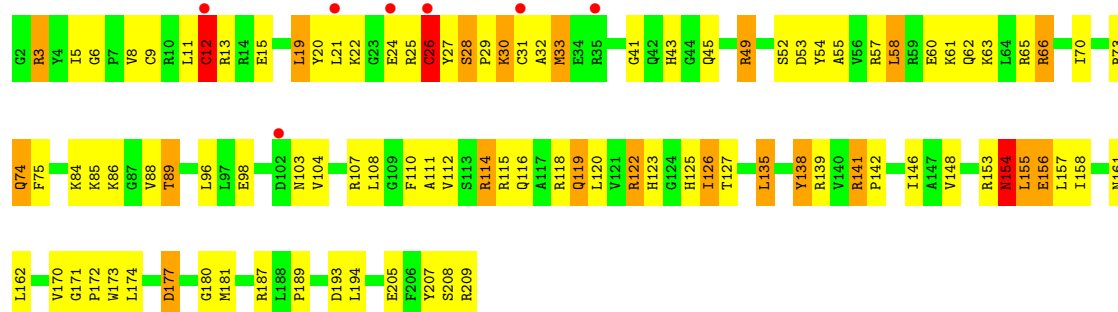
• Molecule 33: 30S RIBOSOMAL PROTEIN S3



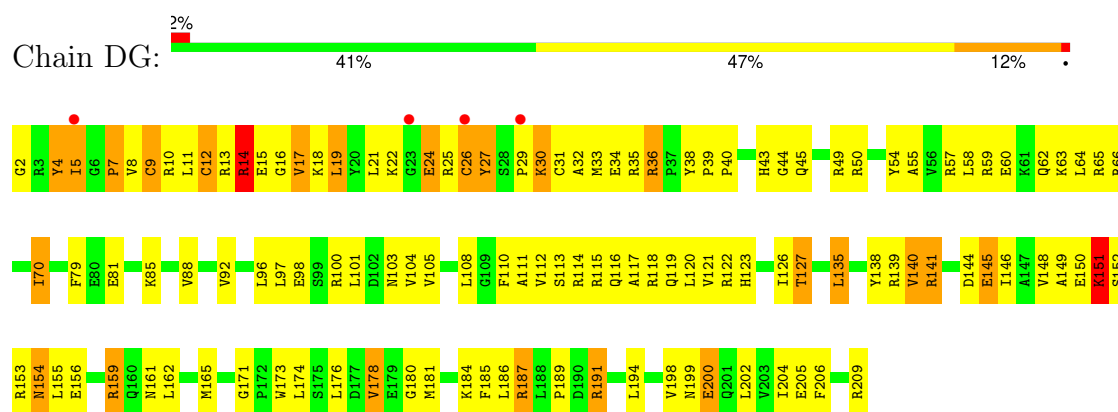
• Molecule 33: 30S RIBOSOMAL PROTEIN S3



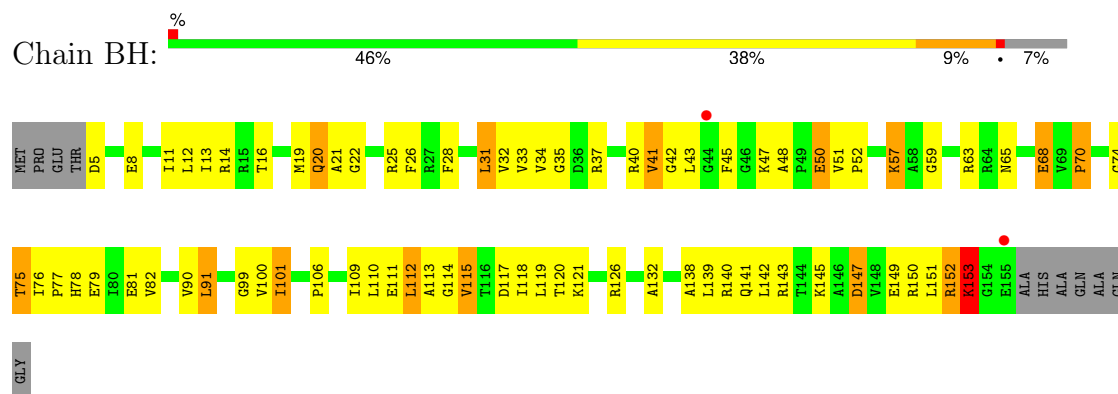
• Molecule 34: 30S RIBOSOMAL PROTEIN S4



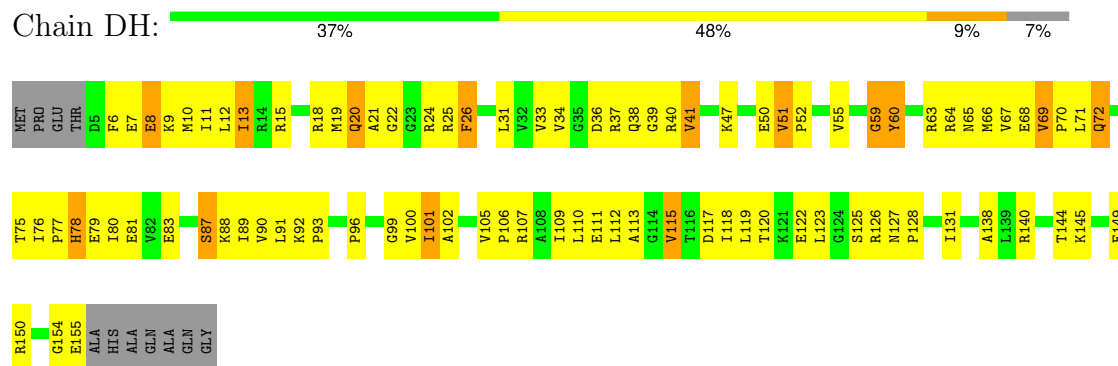
• Molecule 34: 30S RIBOSOMAL PROTEIN S4



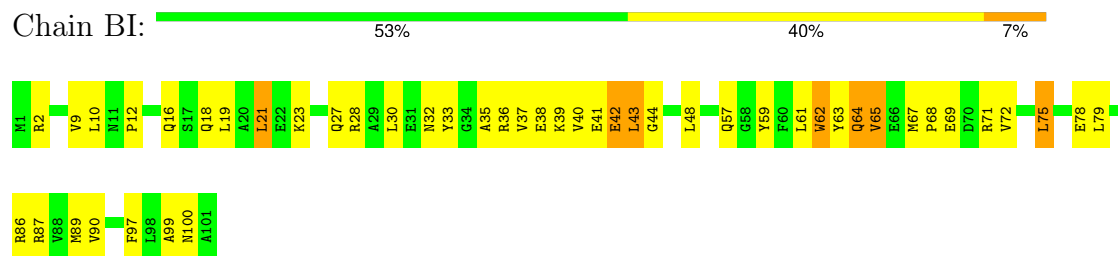
• Molecule 35: 30S RIBOSOMAL PROTEIN S5



• Molecule 35: 30S RIBOSOMAL PROTEIN S5

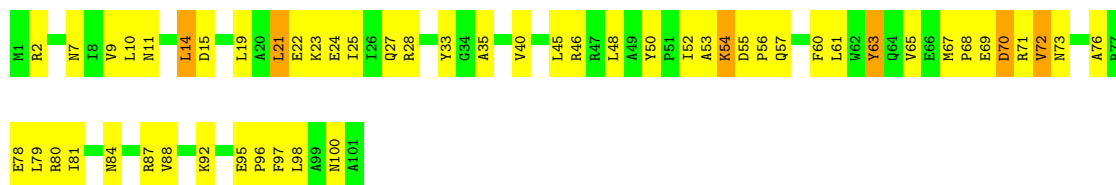


• Molecule 36: 30S RIBOSOMAL PROTEIN S6



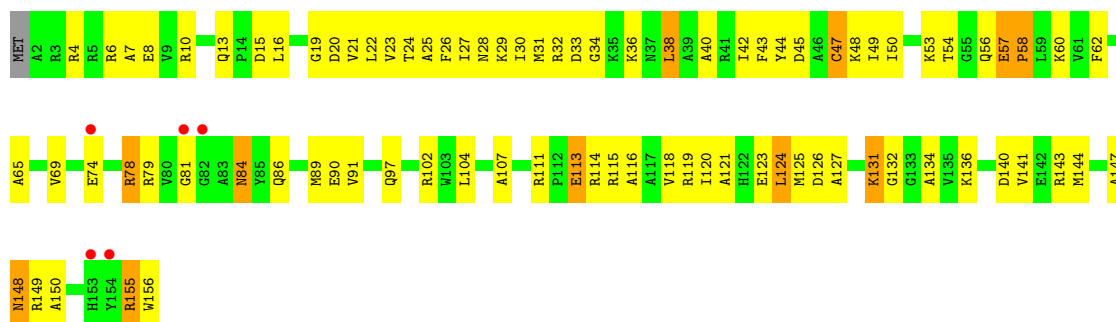
• Molecule 36: 30S RIBOSOMAL PROTEIN S6

Chain DI: 



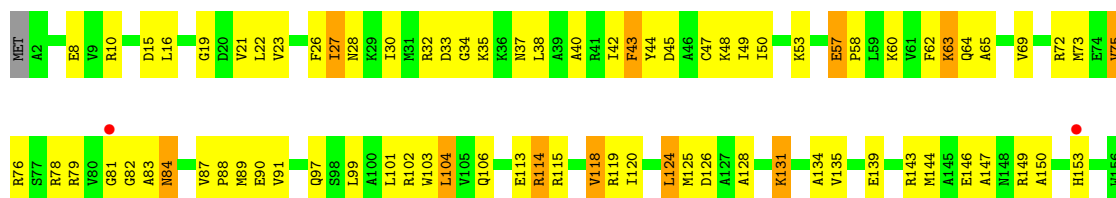
• Molecule 37: 30S RIBOSOMAL PROTEIN S7

Chain BJ: 



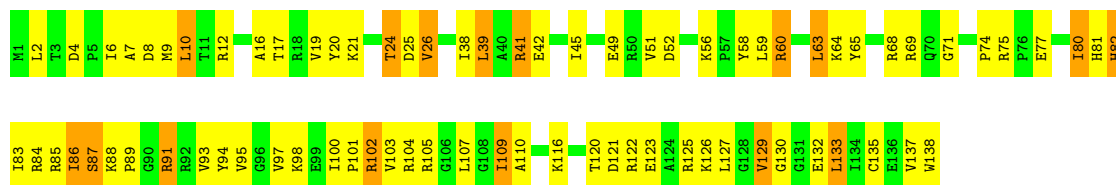
• Molecule 37: 30S RIBOSOMAL PROTEIN S7

Chain DJ: 



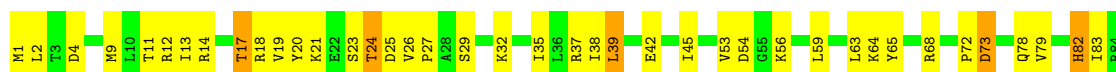
• Molecule 38: 30S RIBOSOMAL PROTEIN S8

Chain BK: 



• Molecule 38: 30S RIBOSOMAL PROTEIN S8

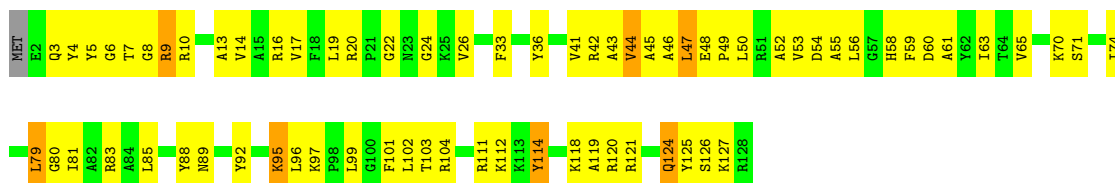
Chain DK: 





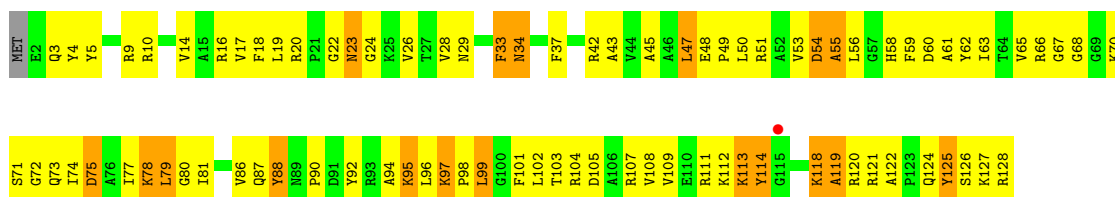
• Molecule 39: 30S RIBOSOMAL PROTEIN S9

Chain BL: 45% 49% 5% .



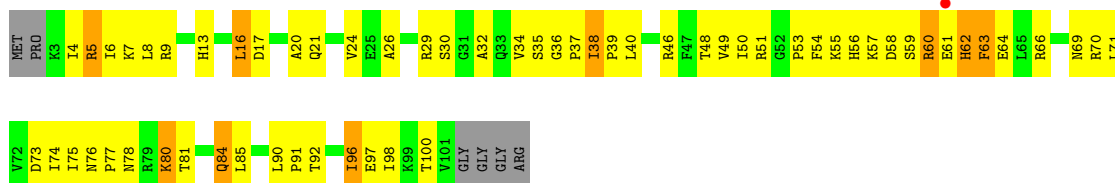
• Molecule 39: 30S RIBOSOMAL PROTEIN S9

Chain DL: 32% 53% 14% .



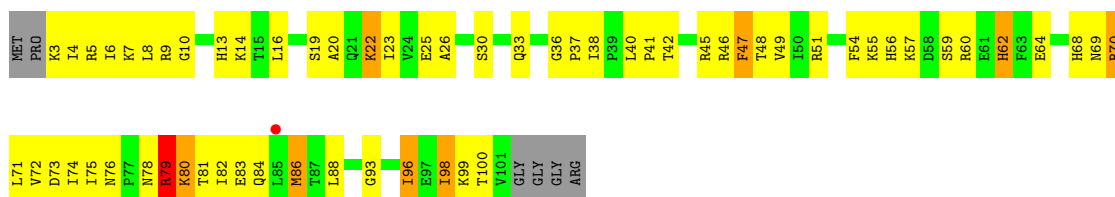
• Molecule 40: 30S RIBOSOMAL PROTEIN S10

Chain BM: 36% 50% 9% 6% .



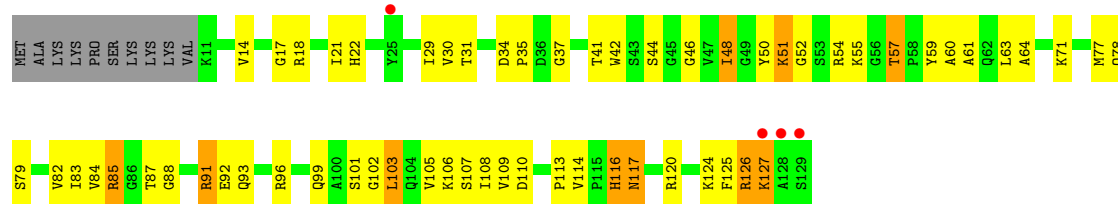
• Molecule 40: 30S RIBOSOMAL PROTEIN S10

Chain DM: 35% 50% 8% 6% .

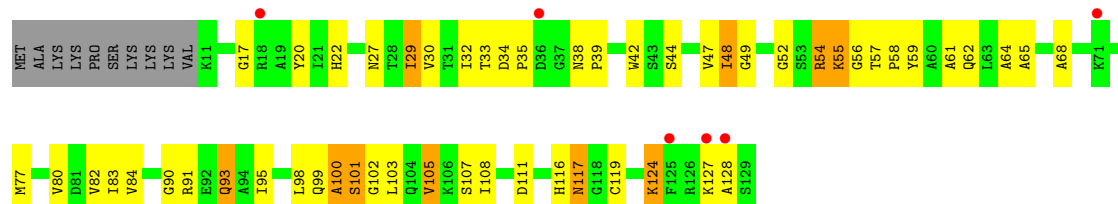


• Molecule 41: 30S RIBOSOMAL PROTEIN S11

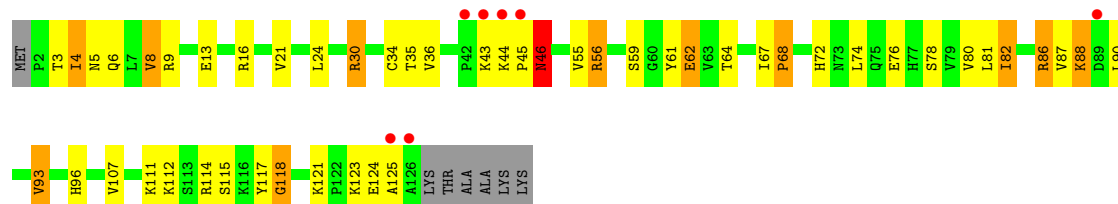
Chain BN: 3% 46% 39% 8% 8% .



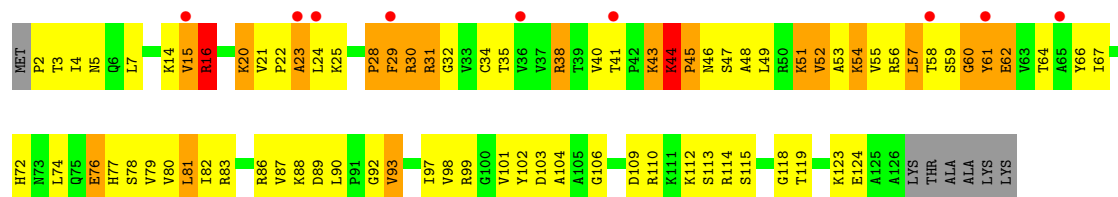
• Molecule 41: 30S RIBOSOMAL PROTEIN S11



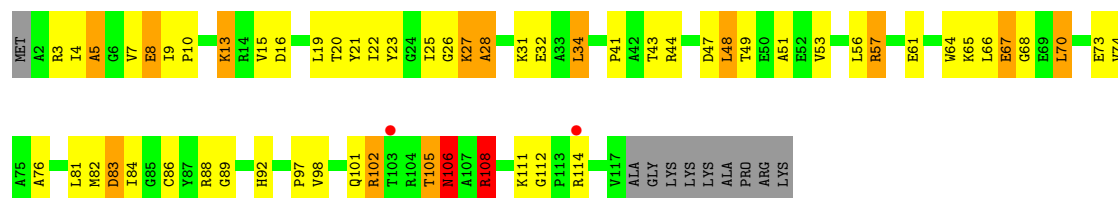
• Molecule 42: 30S RIBOSOMAL PROTEIN S12



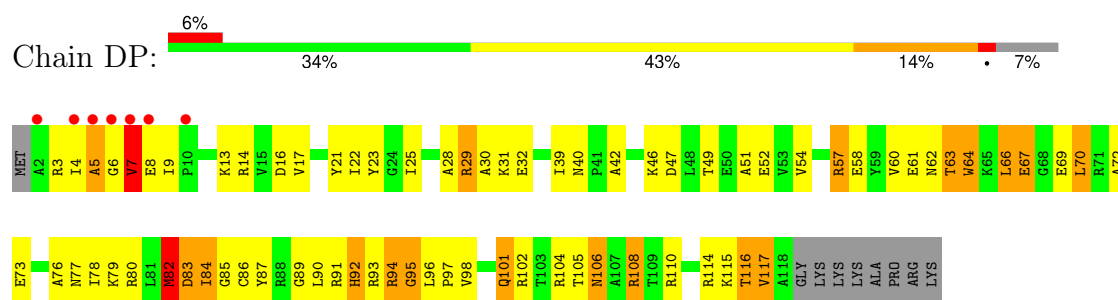
• Molecule 42: 30S RIBOSOMAL PROTEIN S12



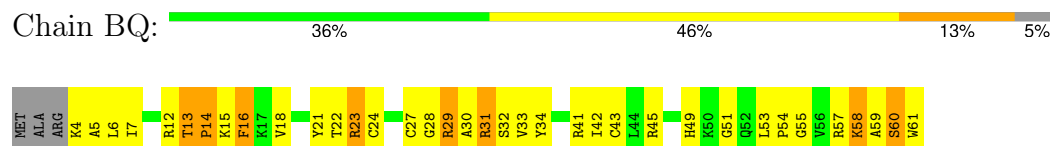
• Molecule 43: 30S RIBOSOMAL PROTEIN S13



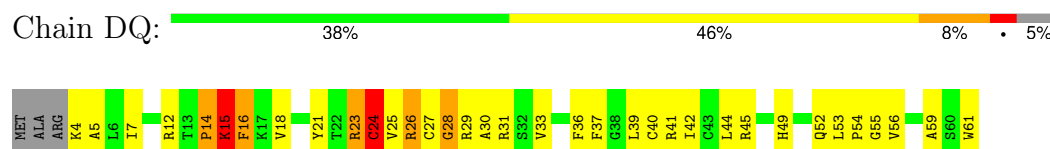
• Molecule 43: 30S RIBOSOMAL PROTEIN S13



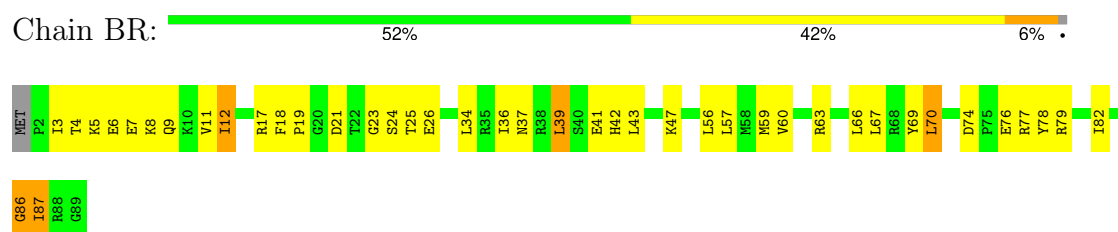
• Molecule 44: 30S RIBOSOMAL PROTEIN S14



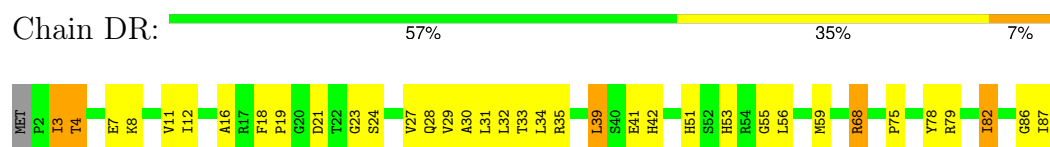
• Molecule 44: 30S RIBOSOMAL PROTEIN S14



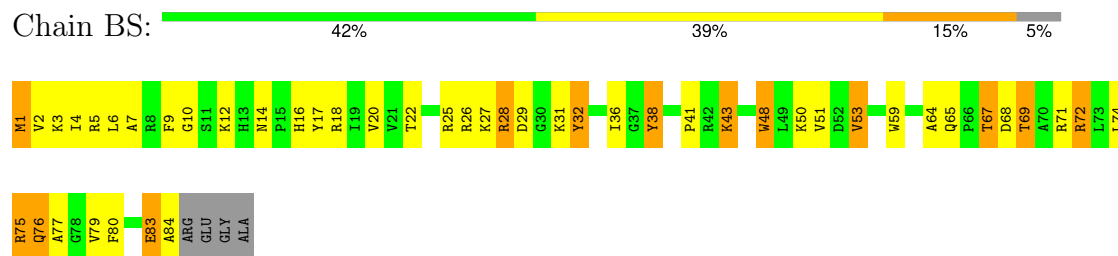
• Molecule 45: 30S RIBOSOMAL PROTEIN S15



• Molecule 45: 30S RIBOSOMAL PROTEIN S15

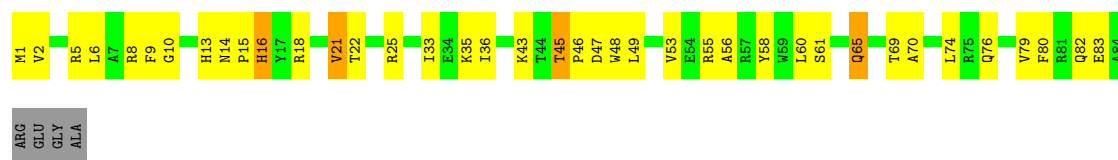


• Molecule 46: 30S RIBOSOMAL PROTEIN S16




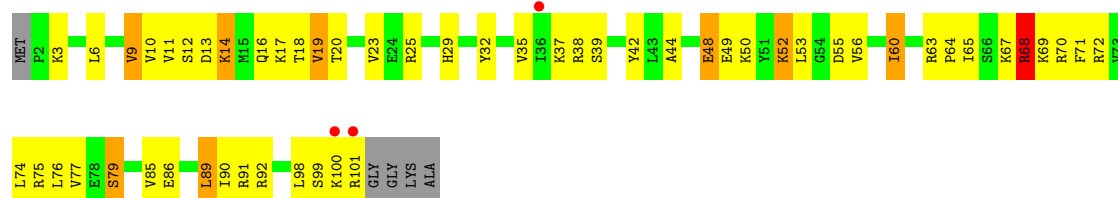
• Molecule 46: 30S RIBOSOMAL PROTEIN S16

Chain DS: 



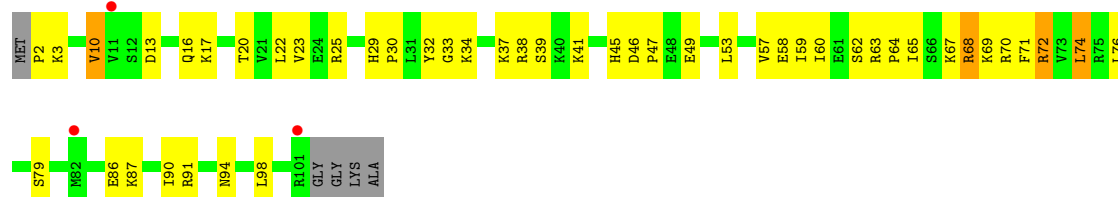
• Molecule 47: 30S RIBOSOMAL PROTEIN S17

Chain BT: 



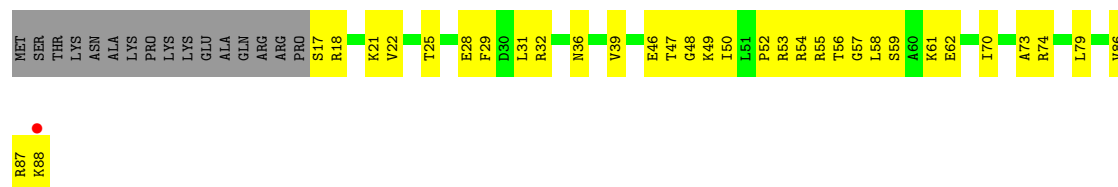
• Molecule 47: 30S RIBOSOMAL PROTEIN S17

Chain DT: 



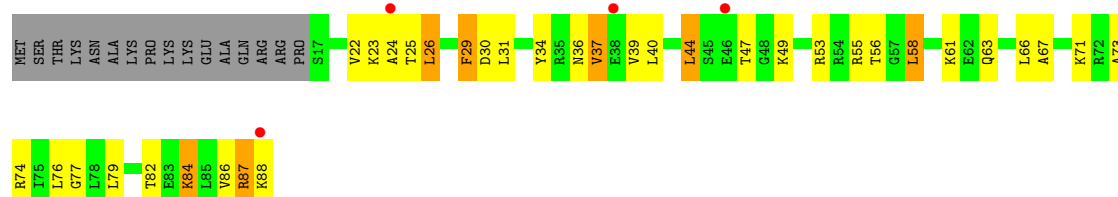
• Molecule 48: 30S RIBOSOMAL PROTEIN S18

Chain BU: 

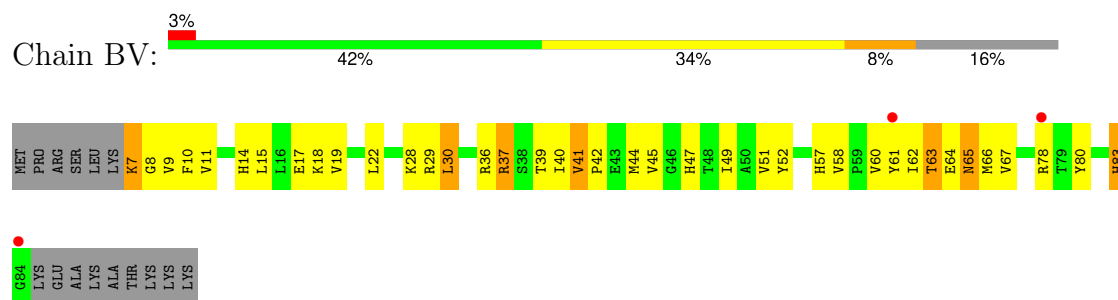


• Molecule 48: 30S RIBOSOMAL PROTEIN S18

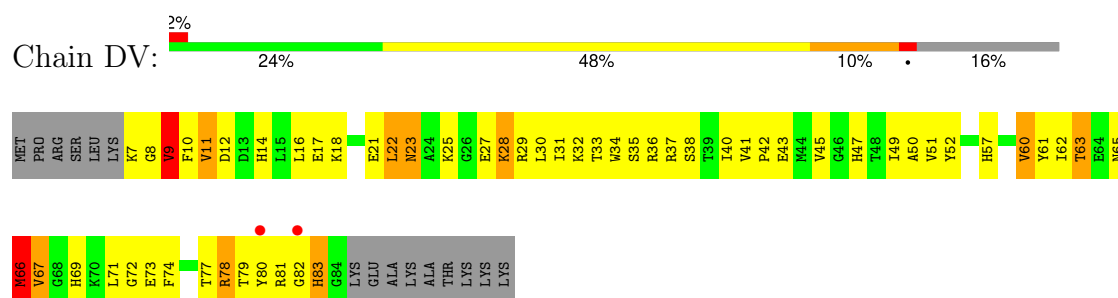
Chain DU: 



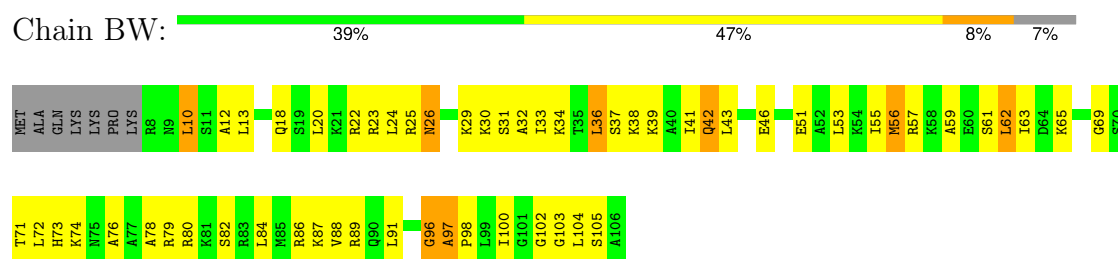
- Molecule 49: 30S RIBOSOMAL PROTEIN S19



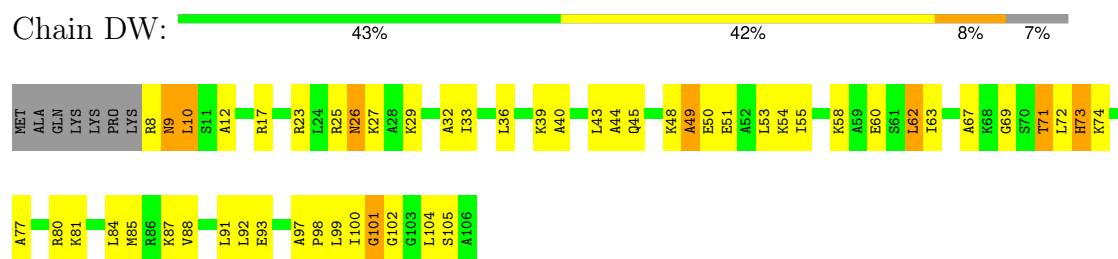
- Molecule 49: 30S RIBOSOMAL PROTEIN S19



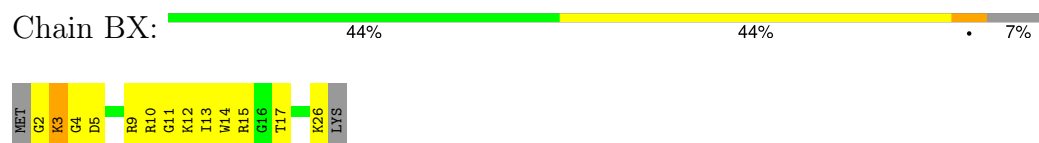
- Molecule 50: 30S RIBOSOMAL PROTEIN S20



- Molecule 50: 30S RIBOSOMAL PROTEIN S20



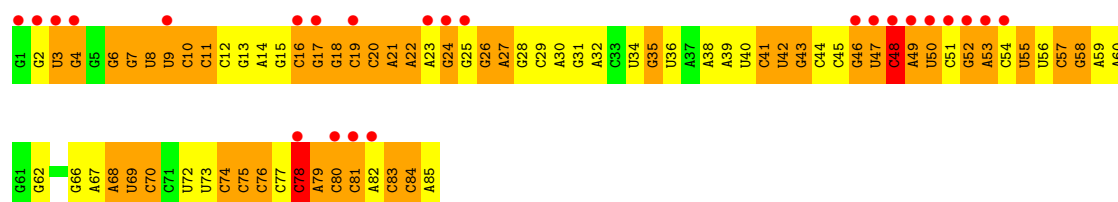
- Molecule 51: 30S RIBOSOMAL PROTEIN THX



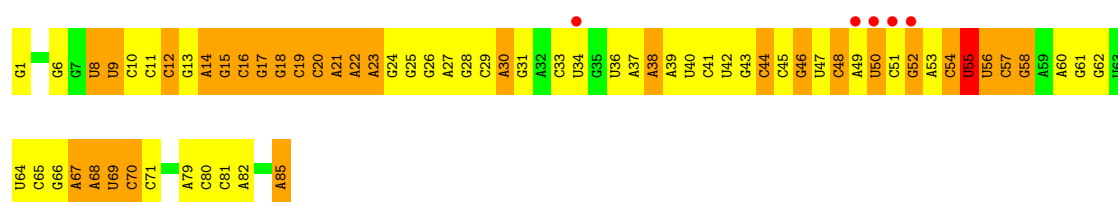
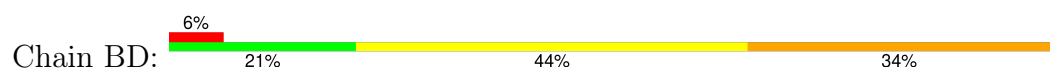
- Molecule 51: 30S RIBOSOMAL PROTEIN THX



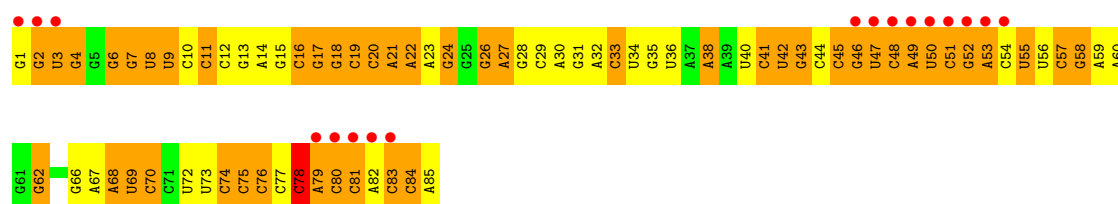
• Molecule 52: TRNA-TYR



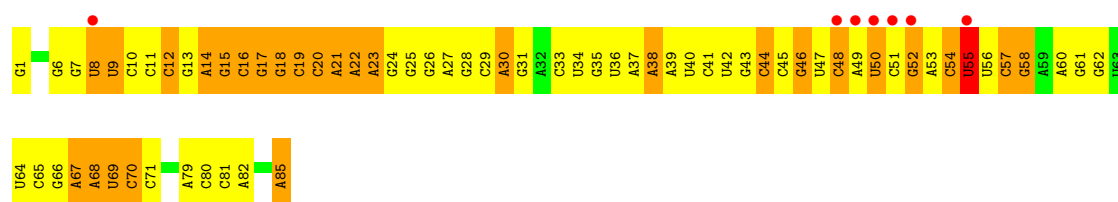
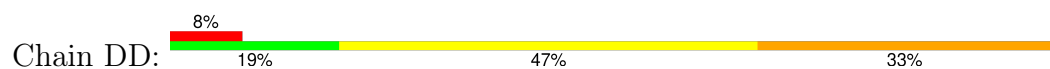
• Molecule 52: TRNA-TYR



• Molecule 52: TRNA-TYR

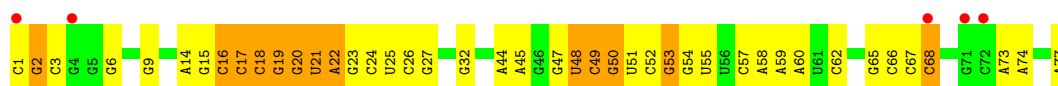


• Molecule 52: TRNA-TYR



• Molecule 53: TRNA-FMET

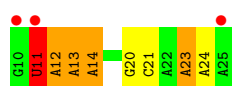




• Molecule 53: TRNA-FMET



• 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, $\alpha$ , $\beta$ , $\gamma$	210.25Å 450.87Å 622.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	256.19 – 3.30 256.19 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (256.19-3.30) 94.2 (256.19-3.30)	Depositor EDS
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 3.19Å)	Xtriage
Refinement program	PHENIX dev_810	Depositor
R, $R_{free}$	0.206 , 0.259 0.206 , 0.258	Depositor DCC
$R_{free}$ test set	1826 reflections (0.21%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	90.6	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 72.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	303952	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	AA	0.34	0/70233	0.73	38/109643 (0.0%)
1	CA	0.30	1/70122 (0.0%)	0.70	35/109469 (0.0%)
2	AB	0.32	0/2928	0.79	11/4568 (0.2%)
2	CB	0.27	0/2928	0.70	1/4568 (0.0%)
3	AD	0.30	0/2165	0.56	0/2919
3	CD	0.28	0/2165	0.50	0/2919
4	AE	0.27	0/1601	0.53	0/2160
4	CE	0.26	0/1601	0.51	0/2160
5	AF	0.27	0/1620	0.49	0/2194
5	CF	0.25	0/1662	0.54	0/2249
6	AG	0.23	0/1499	0.45	0/2016
6	CG	0.21	0/1499	0.42	0/2016
7	AH	0.27	0/1332	0.51	0/1802
7	CH	0.23	0/1332	0.47	0/1802
8	AK	0.24	0/1151	0.50	0/1558
8	CK	0.22	0/1151	0.50	0/1558
9	AM	0.26	0/1131	0.48	0/1525
9	CM	0.23	0/1131	0.45	0/1525
10	AN	0.26	0/943	0.47	0/1269
10	CN	0.25	0/943	0.45	0/1269
11	AO	0.27	0/1162	0.60	1/1544 (0.1%)
11	CO	0.24	0/1162	0.47	0/1544
12	AP	0.27	0/1143	0.45	0/1527
12	CP	0.23	0/1143	0.43	0/1527
13	A0	0.25	0/982	0.48	0/1312
13	C0	0.24	0/974	0.44	0/1302
14	AQ	0.25	0/892	0.47	0/1187
14	CQ	0.24	0/892	0.47	0/1187
15	AR	0.27	0/1155	0.50	0/1542
15	CR	0.24	0/1155	0.44	0/1542
16	A1	0.27	0/982	0.50	0/1306
16	C1	0.24	0/982	0.41	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	A2	0.26	0/790	0.50	0/1057
17	C2	0.26	0/790	0.53	0/1057
18	AS	0.26	0/911	0.46	0/1220
18	CS	0.25	0/911	0.46	0/1220
19	AT	0.31	0/739	0.49	0/993
19	CT	0.28	0/739	0.47	0/993
20	AU	0.27	0/798	0.49	0/1064
20	CU	0.25	0/798	0.48	0/1064
21	AV	0.25	0/1427	0.50	1/1935 (0.1%)
21	CV	0.22	0/1460	0.45	0/1982
22	A3	0.27	0/615	0.50	0/819
22	C3	0.25	0/621	0.48	0/827
23	AZ	0.26	0/770	0.50	0/1022
23	CZ	0.26	0/770	0.51	0/1022
24	AW	0.29	0/560	0.54	0/741
24	CW	0.24	0/560	0.45	0/741
25	AX	0.24	0/474	0.40	0/635
25	CX	0.21	0/474	0.40	0/635
26	A4	0.25	0/545	0.58	0/733
26	C4	0.26	0/527	0.55	0/709
27	A5	0.24	0/473	0.49	0/639
27	C5	0.25	0/473	0.51	0/639
28	A6	0.28	0/396	0.54	0/529
28	C6	0.25	0/396	0.58	0/529
29	A7	0.31	0/399	0.48	0/526
29	C7	0.25	0/399	0.45	0/526
30	A8	0.34	0/486	0.61	0/638
30	C8	0.27	0/486	0.51	0/638
31	BA	0.28	0/36139	0.68	22/56406 (0.0%)
31	DA	0.26	0/36142	0.65	20/56410 (0.0%)
32	BE	0.22	0/1959	0.43	0/2642
32	DE	0.22	0/1959	0.43	0/2642
33	BF	0.23	0/1629	0.41	0/2195
33	DF	0.21	0/1636	0.40	0/2205
34	BG	0.26	0/1733	0.45	0/2318
34	DG	0.24	0/1733	0.45	0/2318
35	BH	0.24	0/1171	0.44	0/1576
35	DH	0.22	0/1171	0.43	0/1576
36	BI	0.24	0/856	0.43	0/1154
36	DI	0.23	0/856	0.44	0/1154
37	BJ	0.23	0/1276	0.38	0/1709
37	DJ	0.21	0/1276	0.37	0/1709
38	BK	0.23	0/1136	0.47	0/1527

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DK	0.21	0/1136	0.42	0/1527
39	BL	0.22	0/1029	0.41	0/1379
39	DL	0.23	0/1029	0.44	0/1379
40	BM	0.22	0/814	0.45	0/1095
40	DM	0.21	0/814	0.44	0/1095
41	BN	0.24	0/900	0.47	0/1213
41	DN	0.23	0/900	0.45	0/1213
42	BO	0.26	0/991	0.47	0/1327
42	DO	0.24	0/991	0.47	0/1327
43	BP	0.22	0/938	0.47	0/1258
43	DP	0.21	0/943	0.43	0/1265
44	BQ	0.26	0/485	0.45	0/643
44	DQ	0.23	0/485	0.46	0/643
45	BR	0.24	0/745	0.41	0/992
45	DR	0.22	0/745	0.40	0/992
46	BS	0.22	0/721	0.43	0/970
46	DS	0.22	0/721	0.43	0/970
47	BT	0.24	0/847	0.41	0/1131
47	DT	0.23	0/847	0.40	0/1131
48	BU	0.24	0/596	0.45	0/790
48	DU	0.24	0/596	0.43	0/790
49	BV	0.22	0/638	0.44	0/860
49	DV	0.23	0/638	0.46	0/860
50	BW	0.22	0/765	0.42	0/1007
50	DW	0.23	0/765	0.47	0/1007
51	BX	0.22	0/221	0.39	0/288
51	DX	0.21	0/221	0.41	0/288
52	BB	0.35	0/1992	0.71	2/3099 (0.1%)
52	BD	0.32	0/1992	0.66	2/3099 (0.1%)
52	DB	0.35	0/1992	0.68	1/3099 (0.0%)
52	DD	0.32	0/1992	0.64	2/3099 (0.1%)
53	BC	0.26	0/1835	0.61	0/2859
53	DC	0.24	0/1835	0.56	0/2859
54	B1	0.33	0/390	0.59	1/606 (0.2%)
54	D1	0.34	0/390	0.63	1/606 (0.2%)
All	All	0.29	1/324159 (0.0%)	0.65	138/485455 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	2884	A	N7-C5	-5.57	1.35	1.39

The worst 5 of 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BA	1495	U	N1-C2-O2	9.65	129.55	122.80
1	AA	673	C	C2-N3-C4	-8.89	115.45	119.90
2	AB	81	G	C5-C6-O6	-8.73	123.36	128.60
1	CA	979	A	C4-N9-C1'	8.38	141.38	126.30
1	CA	1922	G	N3-C4-N9	-8.15	121.11	126.00

There are no chirality outliers.

There are no planarity outliers.

## 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	AA	62707	0	31613	2349	0
1	CA	62607	0	31564	2395	0
2	AB	2617	0	1328	88	0
2	CB	2617	0	1328	126	0
3	AD	2115	0	2195	232	0
3	CD	2115	0	2195	198	0
4	AE	1568	0	1634	155	0
4	CE	1568	0	1634	162	0
5	AF	1585	0	1632	122	0
5	CF	1627	0	1680	182	0
6	AG	1474	0	1535	112	0
6	CG	1474	0	1535	112	0
7	AH	1307	0	1382	129	0
7	CH	1307	0	1382	110	1
8	AK	1136	0	1223	92	0
8	CK	1136	0	1223	77	0
9	AM	1104	0	1180	81	0
9	CM	1104	0	1180	64	0
10	AN	933	0	996	64	0
10	CN	933	0	996	53	0
11	AO	1145	0	1228	178	0
11	CO	1145	0	1228	265	0
12	AP	1122	0	1179	168	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	CP	1122	0	1179	189	0
13	A0	968	0	1033	74	0
13	C0	960	0	1021	70	0
14	AQ	882	0	943	83	0
14	CQ	882	0	943	89	0
15	AR	1141	0	1202	107	0
15	CR	1141	0	1202	94	0
16	A1	964	0	1022	87	0
16	C1	964	0	1022	83	0
17	A2	779	0	852	63	0
17	C2	779	0	852	99	0
18	AS	900	0	964	55	0
18	CS	900	0	964	54	0
19	AT	725	0	778	43	0
19	CT	725	0	778	39	0
20	AU	785	0	878	75	0
20	CU	785	0	878	80	0
21	AV	1397	0	1430	140	0
21	CV	1428	0	1454	149	0
22	A3	607	0	628	42	0
22	C3	613	0	633	47	0
23	AZ	763	0	848	49	0
23	CZ	763	0	848	44	0
24	AW	558	0	610	45	0
24	CW	558	0	610	51	0
25	AX	469	0	518	28	0
25	CX	469	0	518	27	0
26	A4	533	0	522	72	0
26	C4	515	0	510	96	0
27	A5	459	0	480	88	0
27	C5	459	0	478	33	0
28	A6	389	0	404	59	0
28	C6	389	0	404	51	0
29	A7	391	0	432	21	0
29	C7	391	0	432	33	0
30	A8	480	0	549	67	0
30	C8	480	0	549	114	0
31	BA	32284	0	16296	1465	1
31	DA	32287	0	16295	1435	0
32	BE	1924	0	1975	137	0
32	DE	1924	0	1975	162	0
33	BF	1605	0	1668	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	DF	1612	0	1677	110	0
34	BG	1703	0	1763	120	0
34	DG	1703	0	1763	129	0
35	BH	1155	0	1213	71	0
35	DH	1155	0	1213	79	0
36	BI	843	0	857	36	0
36	DI	843	0	857	46	0
37	BJ	1257	0	1296	70	0
37	DJ	1257	0	1296	91	0
38	BK	1116	0	1177	83	0
38	DK	1116	0	1177	56	0
39	BL	1010	0	1037	72	0
39	DL	1010	0	1037	112	0
40	BM	801	0	849	79	0
40	DM	801	0	849	87	0
41	BN	885	0	904	54	0
41	DN	885	0	904	58	0
42	BO	975	0	1062	53	0
42	DO	975	0	1062	89	0
43	BP	928	0	987	74	0
43	DP	933	0	992	81	0
44	BQ	476	0	511	43	0
44	DQ	476	0	511	53	0
45	BR	734	0	771	34	0
45	DR	734	0	771	38	0
46	BS	705	0	725	54	0
46	DS	705	0	725	35	0
47	BT	834	0	904	53	0
47	DT	834	0	904	41	0
48	BU	591	0	662	38	0
48	DU	591	0	662	40	0
49	BV	624	0	636	50	0
49	DV	624	0	636	77	0
50	BW	763	0	861	59	0
50	DW	763	0	861	48	0
51	BX	217	0	234	12	0
51	DX	217	0	234	21	0
52	BB	1814	0	932	159	0
52	BD	1814	0	932	154	0
52	DB	1814	0	932	174	0
52	DD	1814	0	932	173	0
53	BC	1643	0	837	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	DC	1643	0	837	51	0
54	B1	347	0	174	24	0
54	D1	347	0	174	25	0
55	A0	1	0	0	0	0
55	A1	1	0	0	0	0
55	A3	1	0	0	0	0
55	A5	1	0	0	0	0
55	AA	331	0	0	0	0
55	AB	6	0	0	0	0
55	AE	3	0	0	0	0
55	AF	2	0	0	0	0
55	AO	3	0	0	0	0
55	B1	1	0	0	0	0
55	BA	115	0	0	0	0
55	BB	5	0	0	0	0
55	BC	5	0	0	0	0
55	BD	1	0	0	0	0
55	BN	1	0	0	0	0
55	BQ	1	0	0	0	0
55	BS	1	0	0	0	0
55	C0	1	0	0	0	0
55	C5	1	0	0	0	0
55	C7	1	0	0	0	0
55	CA	274	0	0	0	0
55	CB	7	0	0	0	0
55	CE	1	0	0	0	0
55	D1	1	0	0	0	0
55	DA	119	0	0	0	0
55	DB	2	0	0	0	0
55	DC	6	0	0	0	0
55	DL	1	0	0	0	0
55	DN	1	0	0	0	0
56	A1	14	0	0	0	0
56	A3	7	0	0	0	0
56	A6	7	0	0	3	0
56	AA	1666	0	0	98	0
56	AB	91	0	0	4	0
56	AE	7	0	0	0	0
56	AF	7	0	0	1	0
56	AO	14	0	0	1	0
56	AW	7	0	0	0	0
56	BA	707	0	0	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BB	14	0	0	1	0
56	BC	14	0	0	2	0
56	BD	21	0	0	1	0
56	BG	7	0	0	2	0
56	BR	7	0	0	0	0
56	C1	7	0	0	0	0
56	C3	7	0	0	0	0
56	C5	7	0	0	1	0
56	C6	7	0	0	4	0
56	CA	1526	0	0	72	0
56	CB	91	0	0	4	0
56	CF	7	0	0	0	0
56	CO	7	0	0	0	0
56	DA	651	0	0	55	0
56	DB	21	0	0	1	0
56	DC	28	0	0	10	0
56	DD	7	0	0	1	0
56	DG	7	0	0	2	0
56	DK	7	0	0	1	0
56	DR	7	0	0	0	0
56	DV	7	0	0	1	0
57	BG	1	0	0	0	0
57	BQ	1	0	0	0	0
57	DG	1	0	0	0	0
57	DQ	1	0	0	0	0
All	All	303952	0	200977	14995	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 30.

The worst 5 of 14995 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)
1:CA:2320:G:C8	1:CA:2324:A:C2	1.85	1.64
1:CA:216:G:N2	1:CA:218:A:H61	1.09	1.47
1:AA:2308:G:N1	1:AA:2311:A:N1	1.63	1.43
1:CA:216:G:H21	1:CA:218:A:N6	0.92	1.42
1:AA:2308:G:N2	1:AA:2311:A:H2	1.02	1.42

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)
31:BA:85:U:O2'	7:CH:100:GLY:O[3_555]	1.93	0.27

## 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	
3	AD	270/276 (98%)	218 (81%)	35 (13%)	17 (6%)	1	8
3	CD	270/276 (98%)	218 (81%)	40 (15%)	12 (4%)	2	14
4	AE	203/206 (98%)	141 (70%)	39 (19%)	23 (11%)	0	2
4	CE	203/206 (98%)	131 (64%)	46 (23%)	26 (13%)	0	1
5	AF	200/210 (95%)	168 (84%)	23 (12%)	9 (4%)	2	13
5	CF	206/210 (98%)	144 (70%)	35 (17%)	27 (13%)	0	1
6	AG	179/182 (98%)	147 (82%)	25 (14%)	7 (4%)	2	16
6	CG	179/182 (98%)	144 (80%)	27 (15%)	8 (4%)	2	13
7	AH	168/180 (93%)	123 (73%)	20 (12%)	25 (15%)	0	1
7	CH	168/180 (93%)	111 (66%)	41 (24%)	16 (10%)	0	3
8	AK	144/148 (97%)	99 (69%)	31 (22%)	14 (10%)	0	3
8	CK	144/148 (97%)	104 (72%)	32 (22%)	8 (6%)	1	10
9	AM	136/140 (97%)	108 (79%)	17 (12%)	11 (8%)	1	5
9	CM	136/140 (97%)	106 (78%)	23 (17%)	7 (5%)	1	11
10	AN	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	7	31
10	CN	120/122 (98%)	107 (89%)	9 (8%)	4 (3%)	3	19
11	AO	148/150 (99%)	93 (63%)	35 (24%)	20 (14%)	0	1
11	CO	148/150 (99%)	91 (62%)	32 (22%)	25 (17%)	0	1
12	AP	139/141 (99%)	101 (73%)	21 (15%)	17 (12%)	0	1
12	CP	139/141 (99%)	95 (68%)	24 (17%)	20 (14%)	0	1
13	A0	116/118 (98%)	96 (83%)	15 (13%)	5 (4%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	C0	115/118 (98%)	97 (84%)	12 (10%)	6 (5%)	1	11
14	AQ	109/112 (97%)	86 (79%)	14 (13%)	9 (8%)	0	5
14	CQ	109/112 (97%)	72 (66%)	24 (22%)	13 (12%)	0	1
15	AR	135/146 (92%)	107 (79%)	22 (16%)	6 (4%)	2	14
15	CR	135/146 (92%)	112 (83%)	15 (11%)	8 (6%)	1	9
16	A1	115/118 (98%)	96 (84%)	13 (11%)	6 (5%)	1	11
16	C1	115/118 (98%)	89 (77%)	16 (14%)	10 (9%)	0	4
17	A2	99/101 (98%)	85 (86%)	9 (9%)	5 (5%)	1	11
17	C2	99/101 (98%)	73 (74%)	14 (14%)	12 (12%)	0	1
18	AS	111/113 (98%)	97 (87%)	13 (12%)	1 (1%)	14	44
18	CS	111/113 (98%)	99 (89%)	9 (8%)	3 (3%)	4	22
19	AT	90/96 (94%)	84 (93%)	5 (6%)	1 (1%)	12	40
19	CT	90/96 (94%)	73 (81%)	14 (16%)	3 (3%)	3	19
20	AU	100/110 (91%)	76 (76%)	13 (13%)	11 (11%)	0	2
20	CU	100/110 (91%)	62 (62%)	27 (27%)	11 (11%)	0	2
21	AV	173/206 (84%)	113 (65%)	40 (23%)	20 (12%)	0	2
21	CV	177/206 (86%)	112 (63%)	40 (23%)	25 (14%)	0	1
22	A3	74/85 (87%)	62 (84%)	7 (10%)	5 (7%)	1	7
22	C3	75/85 (88%)	59 (79%)	13 (17%)	3 (4%)	2	16
23	AZ	95/98 (97%)	76 (80%)	13 (14%)	6 (6%)	1	8
23	CZ	95/98 (97%)	76 (80%)	9 (10%)	10 (10%)	0	2
24	AW	64/72 (89%)	57 (89%)	4 (6%)	3 (5%)	2	13
24	CW	64/72 (89%)	52 (81%)	7 (11%)	5 (8%)	1	5
25	AX	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
25	CX	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
26	A4	64/71 (90%)	39 (61%)	13 (20%)	12 (19%)	0	0
26	C4	61/71 (86%)	23 (38%)	20 (33%)	18 (30%)	0	0
27	A5	57/60 (95%)	42 (74%)	9 (16%)	6 (10%)	0	2
27	C5	57/60 (95%)	47 (82%)	8 (14%)	2 (4%)	3	19
28	A6	43/54 (80%)	23 (54%)	13 (30%)	7 (16%)	0	1
28	C6	43/54 (80%)	23 (54%)	11 (26%)	9 (21%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	A7	43/49 (88%)	41 (95%)	2 (5%)	0	100	100
29	C7	43/49 (88%)	40 (93%)	3 (7%)	0	100	100
30	A8	58/65 (89%)	47 (81%)	8 (14%)	3 (5%)	1	11
30	C8	58/65 (89%)	41 (71%)	6 (10%)	11 (19%)	0	0
32	BE	235/256 (92%)	181 (77%)	38 (16%)	16 (7%)	1	7
32	DE	235/256 (92%)	177 (75%)	40 (17%)	18 (8%)	1	5
33	BF	203/239 (85%)	161 (79%)	36 (18%)	6 (3%)	3	21
33	DF	204/239 (85%)	163 (80%)	35 (17%)	6 (3%)	3	22
34	BG	206/208 (99%)	179 (87%)	19 (9%)	8 (4%)	2	16
34	DG	206/208 (99%)	159 (77%)	35 (17%)	12 (6%)	1	9
35	BH	149/162 (92%)	127 (85%)	16 (11%)	6 (4%)	2	16
35	DH	149/162 (92%)	132 (89%)	15 (10%)	2 (1%)	10	36
36	BI	99/101 (98%)	89 (90%)	7 (7%)	3 (3%)	3	21
36	DI	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	6	28
37	BJ	153/156 (98%)	128 (84%)	21 (14%)	4 (3%)	4	23
37	DJ	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	10	36
38	BK	136/138 (99%)	116 (85%)	16 (12%)	4 (3%)	3	22
38	DK	136/138 (99%)	116 (85%)	15 (11%)	5 (4%)	2	17
39	BL	125/128 (98%)	95 (76%)	25 (20%)	5 (4%)	2	16
39	DL	125/128 (98%)	97 (78%)	21 (17%)	7 (6%)	1	10
40	BM	97/105 (92%)	83 (86%)	13 (13%)	1 (1%)	13	42
40	DM	97/105 (92%)	82 (84%)	14 (14%)	1 (1%)	13	42
41	BN	117/129 (91%)	99 (85%)	12 (10%)	6 (5%)	1	11
41	DN	117/129 (91%)	103 (88%)	8 (7%)	6 (5%)	1	11
42	BO	123/132 (93%)	100 (81%)	17 (14%)	6 (5%)	2	12
42	DO	123/132 (93%)	94 (76%)	17 (14%)	12 (10%)	0	3
43	BP	114/126 (90%)	82 (72%)	22 (19%)	10 (9%)	0	4
43	DP	115/126 (91%)	85 (74%)	18 (16%)	12 (10%)	0	2
44	BQ	56/61 (92%)	40 (71%)	10 (18%)	6 (11%)	0	2
44	DQ	56/61 (92%)	41 (73%)	8 (14%)	7 (12%)	0	1
45	BR	86/89 (97%)	76 (88%)	8 (9%)	2 (2%)	5	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	DR	86/89 (97%)	77 (90%)	8 (9%)	1 (1%)	11	38
46	BS	82/88 (93%)	60 (73%)	20 (24%)	2 (2%)	5	25
46	DS	82/88 (93%)	70 (85%)	11 (13%)	1 (1%)	11	38
47	BT	98/105 (93%)	82 (84%)	13 (13%)	3 (3%)	3	21
47	DT	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	6	28
48	BU	70/88 (80%)	59 (84%)	10 (14%)	1 (1%)	9	34
48	DU	70/88 (80%)	57 (81%)	12 (17%)	1 (1%)	9	34
49	BV	76/93 (82%)	59 (78%)	14 (18%)	3 (4%)	2	16
49	DV	76/93 (82%)	55 (72%)	17 (22%)	4 (5%)	1	10
50	BW	97/106 (92%)	78 (80%)	16 (16%)	3 (3%)	3	21
50	DW	97/106 (92%)	82 (84%)	9 (9%)	6 (6%)	1	9
51	BX	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	2	14
51	DX	23/27 (85%)	21 (91%)	0	2 (9%)	0	4
All	All	11319/12052 (94%)	8877 (78%)	1684 (15%)	758 (7%)	1	7

5 of 758 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AD	28	GLU
3	AD	32	SER
3	AD	122	ASP
3	AD	123	ALA
3	AD	238	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AD	214/218 (98%)	172 (80%)	42 (20%)	1	5
3	CD	214/218 (98%)	187 (87%)	27 (13%)	3	16
4	AE	165/166 (99%)	137 (83%)	28 (17%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CE	165/166 (99%)	125 (76%)	40 (24%)	0	2
5	AF	161/166 (97%)	137 (85%)	24 (15%)	2	11
5	CF	165/166 (99%)	137 (83%)	28 (17%)	1	8
6	AG	155/156 (99%)	136 (88%)	19 (12%)	4	16
6	CG	155/156 (99%)	139 (90%)	16 (10%)	6	22
7	AH	142/148 (96%)	112 (79%)	30 (21%)	1	4
7	CH	142/148 (96%)	123 (87%)	19 (13%)	3	14
8	AK	122/124 (98%)	98 (80%)	24 (20%)	1	5
8	CK	122/124 (98%)	104 (85%)	18 (15%)	2	11
9	AM	117/119 (98%)	98 (84%)	19 (16%)	2	9
9	CM	117/119 (98%)	95 (81%)	22 (19%)	1	6
10	AN	100/100 (100%)	92 (92%)	8 (8%)	10	32
10	CN	100/100 (100%)	88 (88%)	12 (12%)	4	17
11	AO	116/116 (100%)	84 (72%)	32 (28%)	0	1
11	CO	116/116 (100%)	84 (72%)	32 (28%)	0	1
12	AP	111/111 (100%)	91 (82%)	20 (18%)	1	7
12	CP	111/111 (100%)	88 (79%)	23 (21%)	1	4
13	A0	101/101 (100%)	83 (82%)	18 (18%)	1	7
13	C0	100/101 (99%)	84 (84%)	16 (16%)	2	9
14	AQ	87/88 (99%)	70 (80%)	17 (20%)	1	5
14	CQ	87/88 (99%)	72 (83%)	15 (17%)	1	8
15	AR	120/127 (94%)	103 (86%)	17 (14%)	2	13
15	CR	120/127 (94%)	105 (88%)	15 (12%)	3	16
16	A1	93/94 (99%)	79 (85%)	14 (15%)	2	10
16	C1	93/94 (99%)	80 (86%)	13 (14%)	3	13
17	A2	82/82 (100%)	69 (84%)	13 (16%)	2	9
17	C2	82/82 (100%)	62 (76%)	20 (24%)	0	2
18	AS	92/92 (100%)	73 (79%)	19 (21%)	1	4
18	CS	92/92 (100%)	80 (87%)	12 (13%)	3	14
19	AT	74/78 (95%)	65 (88%)	9 (12%)	4	16
19	CT	74/78 (95%)	64 (86%)	10 (14%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AU	85/91 (93%)	72 (85%)	13 (15%)	2	10
20	CU	85/91 (93%)	65 (76%)	20 (24%)	0	3
21	AV	154/179 (86%)	130 (84%)	24 (16%)	2	10
21	CV	158/179 (88%)	137 (87%)	21 (13%)	3	14
22	A3	61/67 (91%)	55 (90%)	6 (10%)	6	24
22	C3	62/67 (92%)	58 (94%)	4 (6%)	14	40
23	AZ	82/83 (99%)	70 (85%)	12 (15%)	2	12
23	CZ	82/83 (99%)	73 (89%)	9 (11%)	5	20
24	AW	62/67 (92%)	49 (79%)	13 (21%)	1	4
24	CW	62/67 (92%)	52 (84%)	10 (16%)	2	9
25	AX	51/52 (98%)	43 (84%)	8 (16%)	2	10
25	CX	51/52 (98%)	46 (90%)	5 (10%)	6	24
26	A4	59/63 (94%)	52 (88%)	7 (12%)	4	17
26	C4	57/63 (90%)	45 (79%)	12 (21%)	1	4
27	A5	51/52 (98%)	41 (80%)	10 (20%)	1	5
27	C5	51/52 (98%)	44 (86%)	7 (14%)	3	13
28	A6	44/52 (85%)	30 (68%)	14 (32%)	0	1
28	C6	44/52 (85%)	38 (86%)	6 (14%)	3	14
29	A7	38/42 (90%)	33 (87%)	5 (13%)	3	14
29	C7	38/42 (90%)	31 (82%)	7 (18%)	1	6
30	A8	50/55 (91%)	39 (78%)	11 (22%)	1	3
30	C8	50/55 (91%)	37 (74%)	13 (26%)	0	2
32	BE	205/220 (93%)	172 (84%)	33 (16%)	2	9
32	DE	205/220 (93%)	177 (86%)	28 (14%)	3	13
33	BF	159/188 (85%)	134 (84%)	25 (16%)	2	10
33	DF	160/188 (85%)	141 (88%)	19 (12%)	4	17
34	BG	180/180 (100%)	158 (88%)	22 (12%)	4	16
34	DG	180/180 (100%)	156 (87%)	24 (13%)	3	14
35	BH	116/123 (94%)	100 (86%)	16 (14%)	3	13
35	DH	116/123 (94%)	95 (82%)	21 (18%)	1	6
36	BI	90/90 (100%)	82 (91%)	8 (9%)	8	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	DI	90/90 (100%)	80 (89%)	10 (11%)	5	19
37	BJ	126/127 (99%)	106 (84%)	20 (16%)	2	9
37	DJ	126/127 (99%)	109 (86%)	17 (14%)	3	14
38	BK	119/119 (100%)	99 (83%)	20 (17%)	1	8
38	DK	119/119 (100%)	105 (88%)	14 (12%)	4	17
39	BL	98/99 (99%)	85 (87%)	13 (13%)	3	14
39	DL	98/99 (99%)	82 (84%)	16 (16%)	2	9
40	BM	89/92 (97%)	76 (85%)	13 (15%)	2	12
40	DM	89/92 (97%)	80 (90%)	9 (10%)	6	23
41	BN	90/99 (91%)	78 (87%)	12 (13%)	3	14
41	DN	90/99 (91%)	83 (92%)	7 (8%)	10	33
42	BO	104/109 (95%)	92 (88%)	12 (12%)	4	18
42	DO	104/109 (95%)	85 (82%)	19 (18%)	1	6
43	BP	94/101 (93%)	80 (85%)	14 (15%)	2	11
43	DP	94/101 (93%)	82 (87%)	12 (13%)	3	15
44	BQ	48/50 (96%)	42 (88%)	6 (12%)	3	16
44	DQ	48/50 (96%)	44 (92%)	4 (8%)	9	31
45	BR	79/80 (99%)	74 (94%)	5 (6%)	15	41
45	DR	79/80 (99%)	72 (91%)	7 (9%)	8	28
46	BS	72/74 (97%)	60 (83%)	12 (17%)	2	8
46	DS	72/74 (97%)	66 (92%)	6 (8%)	9	31
47	BT	95/97 (98%)	84 (88%)	11 (12%)	4	18
47	DT	95/97 (98%)	88 (93%)	7 (7%)	11	34
48	BU	63/77 (82%)	61 (97%)	2 (3%)	34	61
48	DU	63/77 (82%)	54 (86%)	9 (14%)	2	12
49	BV	67/80 (84%)	55 (82%)	12 (18%)	1	7
49	DV	67/80 (84%)	55 (82%)	12 (18%)	1	7
50	BW	76/82 (93%)	68 (90%)	8 (10%)	5	21
50	DW	76/82 (93%)	68 (90%)	8 (10%)	5	21
51	BX	20/22 (91%)	19 (95%)	1 (5%)	20	48
51	DX	20/22 (91%)	19 (95%)	1 (5%)	20	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9565/9996 (96%)	8122 (85%)	1443 (15%)	<b>2</b> <b>10</b>

5 of 1443 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	CO	21	ARG
25	CX	37	LEU
11	CO	147	LEU
11	CO	16	ARG
17	C2	35	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 281 such sidechains are listed below:

Mol	Chain	Res	Type
33	DF	28	GLN
34	DG	119	GLN
41	DN	99	GLN
33	BF	181	ASN
33	BF	162	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2911/2912 (99%)	616 (21%)	54 (1%)
1	CA	2905/2912 (99%)	632 (21%)	51 (1%)
2	AB	121/122 (99%)	16 (13%)	0
2	CB	121/122 (99%)	29 (23%)	2 (1%)
31	BA	1501/1506 (99%)	318 (21%)	42 (2%)
31	DA	1501/1506 (99%)	325 (21%)	46 (3%)
52	BB	83/85 (97%)	47 (56%)	10 (12%)
52	BD	83/85 (97%)	32 (38%)	5 (6%)
52	DB	83/85 (97%)	49 (59%)	9 (10%)
52	DD	83/85 (97%)	31 (37%)	5 (6%)
53	BC	76/77 (98%)	16 (21%)	2 (2%)
53	DC	76/77 (98%)	15 (19%)	2 (2%)
54	B1	15/16 (93%)	5 (33%)	3 (20%)
54	D1	15/16 (93%)	5 (33%)	3 (20%)
All	All	9574/9606 (99%)	2136 (22%)	234 (2%)

5 of 2136 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	U
1	AA	12	U
1	AA	17	G
1	AA	18	C
1	AA	27	G

5 of 234 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	B1	13	A
52	DB	57	C
1	CA	1606	A
52	DB	19	C
31	DA	1049	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
52	MIA	DD	38	52	24,31,32	2.09	3 (12%)	22,44,47	2.37	7 (31%)
52	MIA	BB	38	52	24,31,32	2.07	3 (12%)	22,44,47	2.23	7 (31%)
52	MIA	BD	38	52	24,31,32	2.05	3 (12%)	22,44,47	2.75	7 (31%)
52	MIA	DB	38	52	24,31,32	2.16	3 (12%)	22,44,47	2.57	8 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	MIA	DD	38	52	-	7/11/33/34	0/3/3/3
52	MIA	BB	38	52	-	3/11/33/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	MIA	BD	38	52	-	8/11/33/34	0/3/3/3
52	MIA	DB	38	52	-	4/11/33/34	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	DB	38	MIA	C6-N6	7.29	1.46	1.34
52	BB	38	MIA	C6-N6	7.02	1.46	1.34
52	DD	38	MIA	C6-N6	6.98	1.45	1.34
52	BD	38	MIA	C6-N6	6.85	1.45	1.34
52	DB	38	MIA	C13-C14	6.06	1.50	1.32

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	BD	38	MIA	C11-S10-C2	9.55	109.41	102.25
52	DB	38	MIA	C11-S10-C2	9.07	109.06	102.25
52	DD	38	MIA	C11-S10-C2	7.40	107.80	102.25
52	BB	38	MIA	C11-S10-C2	6.23	106.93	102.25
52	BD	38	MIA	C12-C13-C14	-5.72	116.73	127.01

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	BB	38	MIA	N1-C2-S10-C11
52	BB	38	MIA	N3-C2-S10-C11
52	BB	38	MIA	C12-C13-C14-C16
52	BD	38	MIA	N1-C2-S10-C11
52	BD	38	MIA	N3-C2-S10-C11

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	DD	38	MIA	4	0
52	BD	38	MIA	3	0
52	DB	38	MIA	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1610 ligands modelled in this entry, 898 are monoatomic - leaving 712 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
56	OHX	AA	3438	-	0,6,6	-	-	-		
56	OHX	DA	1771	-	0,6,6	-	-	-		
56	OHX	CA	3307	-	0,6,6	-	-	-		
56	OHX	AA	3474	-	0,6,6	-	-	-		
56	OHX	BA	1770	-	0,6,6	-	-	-		
56	OHX	AA	3568	-	0,6,6	-	-	-		
56	OHX	BA	1763	-	0,6,6	-	-	-		
56	OHX	BA	1671	-	0,6,6	-	-	-		
56	OHX	AA	3424	-	0,6,6	-	-	-		
56	OHX	DA	1809	-	0,6,6	-	-	-		
56	OHX	CA	3437	-	0,6,6	-	-	-		
56	OHX	DA	1733	-	0,6,6	-	-	-		
56	OHX	CA	3282	-	0,6,6	-	-	-		
56	OHX	DA	1751	-	0,6,6	-	-	-		
56	OHX	CA	3394	-	0,6,6	-	-	-		
56	OHX	BA	1787	-	0,6,6	-	-	-		
56	OHX	BC	107	-	0,6,6	-	-	-		
56	OHX	CA	3237	-	0,6,6	-	-	-		
56	OHX	CA	3406	-	0,6,6	-	-	-		
56	OHX	CA	3488	-	0,6,6	-	-	-		
56	OHX	CA	3272	-	0,6,6	-	-	-		
56	OHX	AA	3371	-	0,6,6	-	-	-		
56	OHX	AA	3500	-	0,6,6	-	-	-		
56	OHX	CA	3434	-	0,6,6	-	-	-		
56	OHX	CA	3309	-	0,6,6	-	-	-		
56	OHX	BA	1788	-	0,6,6	-	-	-		
56	OHX	BA	1663	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	DB	103	-	0,6,6	-	-	-		
56	OHX	AA	3327	-	0,6,6	-	-	-		
56	OHX	AA	3426	-	0,6,6	-	-	-		
56	OHX	BA	1672	-	0,6,6	-	-	-		
56	OHX	BA	1760	-	0,6,6	-	-	-		
56	OHX	CA	3300	-	0,6,6	-	-	-		
56	OHX	BA	1762	-	0,6,6	-	-	-		
56	OHX	DA	1727	-	0,6,6	-	-	-		
56	OHX	DA	1728	-	0,6,6	-	-	-		
56	OHX	CA	3293	-	0,6,6	-	-	-		
56	OHX	CA	3280	-	0,6,6	-	-	-		
56	OHX	BA	1677	-	0,6,6	-	-	-		
56	OHX	CA	3466	-	0,6,6	-	-	-		
56	OHX	AA	3516	-	0,6,6	-	-	-		
56	OHX	CA	3288	-	0,6,6	-	-	-		
56	OHX	AA	3511	-	0,6,6	-	-	-		
56	OHX	DA	1755	-	0,6,6	-	-	-		
56	OHX	DA	1796	-	0,6,6	-	-	-		
56	OHX	BA	1789	-	0,6,6	-	-	-		
56	OHX	CA	3290	-	0,6,6	-	-	-		
56	OHX	AA	3430	-	0,6,6	-	-	-		
56	OHX	CA	3450	-	0,6,6	-	-	-		
56	OHX	AA	3444	-	0,6,6	-	-	-		
56	OHX	CA	3366	-	0,6,6	-	-	-		
56	OHX	AA	3407	-	0,6,6	-	-	-		
56	OHX	AA	3456	-	0,6,6	-	-	-		
56	OHX	AA	3503	-	0,6,6	-	-	-		
56	OHX	AA	3542	-	0,6,6	-	-	-		
56	OHX	CA	3249	-	0,6,6	-	-	-		
56	OHX	BA	1779	-	0,6,6	-	-	-		
56	OHX	CA	3284	-	0,6,6	-	-	-		
56	OHX	AA	3558	-	0,6,6	-	-	-		
56	OHX	DA	1753	-	0,6,6	-	-	-		
56	OHX	BA	1784	-	0,6,6	-	-	-		
56	OHX	CA	3362	-	0,6,6	-	-	-		
56	OHX	AA	3404	-	0,6,6	-	-	-		
56	OHX	AA	3147	-	0,6,6	-	-	-		
56	OHX	AA	3361	-	0,6,6	-	-	-		
56	OHX	CA	3289	-	0,6,6	-	-	-		
56	OHX	CA	3376	-	0,6,6	-	-	-		
56	OHX	CA	3279	-	0,6,6	-	-	-		
56	OHX	AA	3494	-	0,6,6	-	-	-		
56	OHX	AA	3523	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	AB	219	-	0,6,6	-	-	-		
56	OHX	CA	3239	-	0,6,6	-	-	-		
56	OHX	AA	3447	-	0,6,6	-	-	-		
56	OHX	CA	3254	-	0,6,6	-	-	-		
56	OHX	CA	3328	-	0,6,6	-	-	-		
56	OHX	DA	1787	-	0,6,6	-	-	-		
56	OHX	CA	3465	-	0,6,6	-	-	-		
56	OHX	BA	1801	-	0,6,6	-	-	-		
56	OHX	CB	219	-	0,6,6	-	-	-		
56	OHX	DA	1745	-	0,6,6	-	-	-		
56	OHX	AA	3307	-	0,6,6	-	-	-		
56	OHX	A3	102	-	0,6,6	-	-	-		
56	OHX	CA	3364	-	0,6,6	-	-	-		
56	OHX	CA	3346	-	0,6,6	-	-	-		
56	OHX	DA	1721	-	0,6,6	-	-	-		
56	OHX	AA	3421	-	0,6,6	-	-	-		
56	OHX	CA	3313	-	0,6,6	-	-	-		
56	OHX	AA	3443	-	0,6,6	-	-	-		
56	OHX	CA	3250	-	0,6,6	-	-	-		
56	OHX	CA	3271	-	0,6,6	-	-	-		
56	OHX	AA	3304	-	0,6,6	-	-	-		
56	OHX	CA	3481	-	0,6,6	-	-	-		
56	OHX	AA	3337	-	0,6,6	-	-	-		
56	OHX	BA	1809	-	0,6,6	-	-	-		
56	OHX	CA	3486	-	0,6,6	-	-	-		
56	OHX	AA	3369	-	0,6,6	-	-	-		
56	OHX	CA	3369	-	0,6,6	-	-	-		
56	OHX	BA	1755	-	0,6,6	-	-	-		
56	OHX	AA	3493	-	0,6,6	-	-	-		
56	OHX	DA	1763	-	0,6,6	-	-	-		
56	OHX	AA	3326	-	0,6,6	-	-	-		
56	OHX	AA	3569	-	0,6,6	-	-	-		
56	OHX	DA	1804	-	0,6,6	-	-	-		
56	OHX	AA	3328	-	0,6,6	-	-	-		
56	OHX	AA	3342	-	0,6,6	-	-	-		
56	OHX	CA	3367	-	0,6,6	-	-	-		
56	OHX	AA	3332	-	0,6,6	-	-	-		
56	OHX	BA	1814	-	0,6,6	-	-	-		
56	OHX	CA	3389	-	0,6,6	-	-	-		
56	OHX	AA	3289	-	0,6,6	-	-	-		
56	OHX	AA	3462	-	0,6,6	-	-	-		
56	OHX	AA	3567	-	0,6,6	-	-	-		
56	OHX	AA	3402	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	CA	3350	-	0,6,6	-	-	-		
56	OHX	DA	1794	-	0,6,6	-	-	-		
56	OHX	BA	1766	-	0,6,6	-	-	-		
56	OHX	CA	3344	-	0,6,6	-	-	-		
56	OHX	CA	3256	-	0,6,6	-	-	-		
56	OHX	AA	3287	-	0,6,6	-	-	-		
56	OHX	CA	3319	-	0,6,6	-	-	-		
56	OHX	CA	3338	-	0,6,6	-	-	-		
56	OHX	CA	3236	-	0,6,6	-	-	-		
56	OHX	DA	1722	-	0,6,6	-	-	-		
56	OHX	AA	3467	-	0,6,6	-	-	-		
56	OHX	AA	3566	-	0,6,6	-	-	-		
56	OHX	CA	3414	-	0,6,6	-	-	-		
56	OHX	AA	3160	-	0,6,6	-	-	-		
56	OHX	AA	3314	-	0,6,6	-	-	-		
56	OHX	CA	3353	-	0,6,6	-	-	-		
56	OHX	DA	1760	-	0,6,6	-	-	-		
56	OHX	CA	3438	-	0,6,6	-	-	-		
56	OHX	CA	3407	-	0,6,6	-	-	-		
56	OHX	AA	3491	-	0,6,6	-	-	-		
56	OHX	AA	3481	-	0,6,6	-	-	-		
56	OHX	DA	1774	-	0,6,6	-	-	-		
56	OHX	BA	1775	-	0,6,6	-	-	-		
56	OHX	CA	3429	-	0,6,6	-	-	-		
56	OHX	AA	3497	-	0,6,6	-	-	-		
56	OHX	AA	3451	-	0,6,6	-	-	-		
56	OHX	AA	3439	-	0,6,6	-	-	-		
56	OHX	DA	1801	-	0,6,6	-	-	-		
56	OHX	AA	3154	-	0,6,6	-	-	-		
56	OHX	DA	1764	-	0,6,6	-	-	-		
56	OHX	BA	1813	-	0,6,6	-	-	-		
56	OHX	CA	3352	-	0,6,6	-	-	-		
56	OHX	BA	1804	-	0,6,6	-	-	-		
56	OHX	BA	1676	-	0,6,6	-	-	-		
56	OHX	BR	101	-	0,6,6	-	-	-		
56	OHX	AA	3532	-	0,6,6	-	-	-		
56	OHX	CA	3233	-	0,6,6	-	-	-		
56	OHX	DA	1779	-	0,6,6	-	-	-		
56	OHX	DA	1775	-	0,6,6	-	-	-		
56	OHX	DA	1765	-	0,6,6	-	-	-		
56	OHX	DA	1761	-	0,6,6	-	-	-		
56	OHX	BA	1806	-	0,6,6	-	-	-		
56	OHX	AA	3539	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	CA	3377	-	0,6,6	-	-	-		
56	OHX	BA	1668	-	0,6,6	-	-	-		
56	OHX	BA	1757	-	0,6,6	-	-	-		
56	OHX	CB	215	-	0,6,6	-	-	-		
56	OHX	AA	3556	-	0,6,6	-	-	-		
56	OHX	AA	3338	-	0,6,6	-	-	-		
56	OHX	BA	1797	-	0,6,6	-	-	-		
56	OHX	CA	3383	-	0,6,6	-	-	-		
56	OHX	CA	3283	-	0,6,6	-	-	-		
56	OHX	DA	1742	-	0,6,6	-	-	-		
56	OHX	CA	3351	-	0,6,6	-	-	-		
56	OHX	AA	3291	-	0,6,6	-	-	-		
56	OHX	AA	3433	-	0,6,6	-	-	-		
56	OHX	BA	1811	-	0,6,6	-	-	-		
56	OHX	CA	3339	-	0,6,6	-	-	-		
56	OHX	BA	1669	-	0,6,6	-	-	-		
56	OHX	CA	3321	-	0,6,6	-	-	-		
56	OHX	DA	1766	-	0,6,6	-	-	-		
56	OHX	CA	3413	-	0,6,6	-	-	-		
56	OHX	CA	3341	-	0,6,6	-	-	-		
56	OHX	CA	3417	-	0,6,6	-	-	-		
56	OHX	DA	1740	-	0,6,6	-	-	-		
56	OHX	BA	1769	-	0,6,6	-	-	-		
56	OHX	A1	203	-	0,6,6	-	-	-		
56	OHX	AA	3550	-	0,6,6	-	-	-		
56	OHX	BA	1661	-	0,6,6	-	-	-		
56	OHX	DB	105	-	0,6,6	-	-	-		
56	OHX	CA	3317	-	0,6,6	-	-	-		
56	OHX	CB	209	-	0,6,6	-	-	-		
56	OHX	DA	1770	-	0,6,6	-	-	-		
56	OHX	CA	3365	-	0,6,6	-	-	-		
56	OHX	AA	3513	-	0,6,6	-	-	-		
56	OHX	AA	3471	-	0,6,6	-	-	-		
56	OHX	CA	3234	-	0,6,6	-	-	-		
56	OHX	AA	3535	-	0,6,6	-	-	-		
56	OHX	CB	208	-	0,6,6	-	-	-		
56	OHX	CA	3400	-	0,6,6	-	-	-		
56	OHX	AA	3315	-	0,6,6	-	-	-		
56	OHX	AA	3324	-	0,6,6	-	-	-		
56	OHX	AA	3333	-	0,6,6	-	-	-		
56	OHX	AA	3499	-	0,6,6	-	-	-		
56	OHX	BA	1678	-	0,6,6	-	-	-		
56	OHX	AA	3360	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	AA	3509	-	0,6,6	-	-	-		
56	OHX	AA	3296	-	0,6,6	-	-	-		
56	OHX	AA	3525	-	0,6,6	-	-	-		
56	OHX	BA	1674	-	0,6,6	-	-	-		
56	OHX	CA	3463	-	0,6,6	-	-	-		
56	OHX	CA	3303	-	0,6,6	-	-	-		
56	OHX	BA	1812	-	0,6,6	-	-	-		
56	OHX	CA	3421	-	0,6,6	-	-	-		
56	OHX	AA	3440	-	0,6,6	-	-	-		
56	OHX	CA	3397	-	0,6,6	-	-	-		
56	OHX	AA	3453	-	0,6,6	-	-	-		
56	OHX	CA	3427	-	0,6,6	-	-	-		
56	OHX	BA	1683	-	0,6,6	-	-	-		
56	OHX	AW	101	-	0,6,6	-	-	-		
56	OHX	CA	3428	-	0,6,6	-	-	-		
56	OHX	CA	3431	-	0,6,6	-	-	-		
56	OHX	CA	3232	-	0,6,6	-	-	-		
56	OHX	BB	106	-	0,6,6	-	-	-		
56	OHX	DA	1797	-	0,6,6	-	-	-		
56	OHX	CA	3244	-	0,6,6	-	-	-		
56	OHX	CB	210	-	0,6,6	-	-	-		
56	OHX	CA	3415	-	0,6,6	-	-	-		
56	OHX	BA	1662	-	0,6,6	-	-	-		
56	OHX	AA	3529	-	0,6,6	-	-	-		
56	OHX	C1	201	-	0,6,6	-	-	-		
56	OHX	AA	3496	-	0,6,6	-	-	-		
56	OHX	AA	3476	-	0,6,6	-	-	-		
56	OHX	CA	3318	-	0,6,6	-	-	-		
56	OHX	BA	1808	-	0,6,6	-	-	-		
56	OHX	AA	3487	-	0,6,6	-	-	-		
56	OHX	AA	3448	-	0,6,6	-	-	-		
56	OHX	AA	3311	-	0,6,6	-	-	-		
56	OHX	AA	3400	-	0,6,6	-	-	-		
56	OHX	BA	1689	-	0,6,6	-	-	-		
56	OHX	BA	1778	-	0,6,6	-	-	-		
56	OHX	CA	3340	-	0,6,6	-	-	-		
56	OHX	CA	3468	-	0,6,6	-	-	-		
56	OHX	AB	212	-	0,6,6	-	-	-		
56	OHX	BA	1800	-	0,6,6	-	-	-		
56	OHX	CA	3312	-	0,6,6	-	-	-		
56	OHX	AA	3541	-	0,6,6	-	-	-		
56	OHX	BA	1695	-	0,6,6	-	-	-		
56	OHX	DA	1731	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	CA	3359	-	0,6,6	-	-	-		
56	OHX	CA	3387	-	0,6,6	-	-	-		
56	OHX	AA	3465	-	0,6,6	-	-	-		
56	OHX	BA	1691	-	0,6,6	-	-	-		
56	OHX	AA	3484	-	0,6,6	-	-	-		
56	OHX	AA	3368	-	0,6,6	-	-	-		
56	OHX	AA	3543	-	0,6,6	-	-	-		
56	OHX	AA	3524	-	0,6,6	-	-	-		
56	OHX	BA	1786	-	0,6,6	-	-	-		
56	OHX	DD	101	-	0,6,6	-	-	-		
56	OHX	AA	3547	-	0,6,6	-	-	-		
56	OHX	CA	3485	-	0,6,6	-	-	-		
56	OHX	DA	1795	-	0,6,6	-	-	-		
56	OHX	AA	3298	-	0,6,6	-	-	-		
56	OHX	AB	211	-	0,6,6	-	-	-		
56	OHX	CA	3420	-	0,6,6	-	-	-		
56	OHX	AA	3515	-	0,6,6	-	-	-		
56	OHX	AA	3504	-	0,6,6	-	-	-		
56	OHX	DA	1767	-	0,6,6	-	-	-		
56	OHX	DA	1769	-	0,6,6	-	-	-		
56	OHX	CA	3235	-	0,6,6	-	-	-		
56	OHX	BD	104	-	0,6,6	-	-	-		
56	OHX	AA	3428	-	0,6,6	-	-	-		
56	OHX	AA	3432	-	0,6,6	-	-	-		
56	OHX	CA	3326	-	0,6,6	-	-	-		
56	OHX	DA	1738	-	0,6,6	-	-	-		
56	OHX	DA	1746	-	0,6,6	-	-	-		
56	OHX	CA	3306	-	0,6,6	-	-	-		
56	OHX	CA	3368	-	0,6,6	-	-	-		
56	OHX	CA	3490	-	0,6,6	-	-	-		
56	OHX	AA	3489	-	0,6,6	-	-	-		
56	OHX	BA	1798	-	0,6,6	-	-	-		
56	OHX	CA	3416	-	0,6,6	-	-	-		
56	OHX	DA	1800	-	0,6,6	-	-	-		
56	OHX	BA	1792	-	0,6,6	-	-	-		
56	OHX	CA	3393	-	0,6,6	-	-	-		
56	OHX	CA	3294	-	0,6,6	-	-	-		
56	OHX	AA	3498	-	0,6,6	-	-	-		
56	OHX	CA	3299	-	0,6,6	-	-	-		
56	OHX	CA	3324	-	0,6,6	-	-	-		
56	OHX	CA	3245	-	0,6,6	-	-	-		
56	OHX	AA	3544	-	0,6,6	-	-	-		
56	OHX	AA	3373	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	CA	3483	-	0,6,6	-	-	-		
56	OHX	AA	3527	-	0,6,6	-	-	-		
56	OHX	AA	3301	-	0,6,6	-	-	-		
56	OHX	AA	3319	-	0,6,6	-	-	-		
56	OHX	BA	1685	-	0,6,6	-	-	-		
56	OHX	AA	3417	-	0,6,6	-	-	-		
56	OHX	AA	3322	-	0,6,6	-	-	-		
56	OHX	AA	3530	-	0,6,6	-	-	-		
56	OHX	AA	3521	-	0,6,6	-	-	-		
56	OHX	AA	3559	-	0,6,6	-	-	-		
56	OHX	DA	1790	-	0,6,6	-	-	-		
56	OHX	DA	1786	-	0,6,6	-	-	-		
56	OHX	AA	3418	-	0,6,6	-	-	-		
56	OHX	AA	3533	-	0,6,6	-	-	-		
56	OHX	CA	3361	-	0,6,6	-	-	-		
56	OHX	CA	3315	-	0,6,6	-	-	-		
56	OHX	BA	1693	-	0,6,6	-	-	-		
56	OHX	CA	3333	-	0,6,6	-	-	-		
56	OHX	BA	1667	-	0,6,6	-	-	-		
56	OHX	BA	1799	-	0,6,6	-	-	-		
56	OHX	AA	3562	-	0,6,6	-	-	-		
56	OHX	AA	3329	-	0,6,6	-	-	-		
56	OHX	CA	3484	-	0,6,6	-	-	-		
56	OHX	AA	3288	-	0,6,6	-	-	-		
56	OHX	AA	3446	-	0,6,6	-	-	-		
56	OHX	DA	1756	-	0,6,6	-	-	-		
56	OHX	CA	3404	-	0,6,6	-	-	-		
56	OHX	AA	3406	-	0,6,6	-	-	-		
56	OHX	AA	3299	-	0,6,6	-	-	-		
56	OHX	BA	1776	-	0,6,6	-	-	-		
56	OHX	CA	3355	-	0,6,6	-	-	-		
56	OHX	DA	1808	-	0,6,6	-	-	-		
56	OHX	BD	103	-	0,6,6	-	-	-		
56	OHX	AA	3429	-	0,6,6	-	-	-		
56	OHX	CA	3412	-	0,6,6	-	-	-		
56	OHX	CA	3343	-	0,6,6	-	-	-		
56	OHX	CA	3386	-	0,6,6	-	-	-		
56	OHX	AA	3425	-	0,6,6	-	-	-		
56	OHX	CA	3491	-	0,6,6	-	-	-		
56	OHX	CB	217	-	0,6,6	-	-	-		
56	OHX	BA	1761	-	0,6,6	-	-	-		
56	OHX	AA	3302	-	0,6,6	-	-	-		
56	OHX	DA	1750	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	AA	3470	-	0,6,6	-	-	-		
56	OHX	AO	204	-	0,6,6	-	-	-		
56	OHX	CA	3295	-	0,6,6	-	-	-		
56	OHX	DA	1741	-	0,6,6	-	-	-		
56	OHX	DA	1789	-	0,6,6	-	-	-		
56	OHX	BA	1692	-	0,6,6	-	-	-		
56	OHX	CA	3380	-	0,6,6	-	-	-		
56	OHX	BA	1790	-	0,6,6	-	-	-		
56	OHX	DA	1743	-	0,6,6	-	-	-		
56	OHX	CA	3370	-	0,6,6	-	-	-		
56	OHX	AA	3506	-	0,6,6	-	-	-		
56	OHX	CA	3277	-	0,6,6	-	-	-		
56	OHX	CA	3247	-	0,6,6	-	-	-		
56	OHX	DA	1735	-	0,6,6	-	-	-		
56	OHX	AA	3420	-	0,6,6	-	-	-		
56	OHX	DA	1759	-	0,6,6	-	-	-		
56	OHX	CA	3402	-	0,6,6	-	-	-		
56	OHX	DA	1788	-	0,6,6	-	-	-		
56	OHX	AA	3459	-	0,6,6	-	-	-		
56	OHX	CA	3379	-	0,6,6	-	-	-		
56	OHX	AA	3341	-	0,6,6	-	-	-		
56	OHX	AA	3477	-	0,6,6	-	-	-		
56	OHX	CA	3335	-	0,6,6	-	-	-		
56	OHX	AA	3340	-	0,6,6	-	-	-		
56	OHX	CA	3273	-	0,6,6	-	-	-		
56	OHX	CA	3390	-	0,6,6	-	-	-		
56	OHX	BA	1767	-	0,6,6	-	-	-		
56	OHX	AA	3423	-	0,6,6	-	-	-		
56	OHX	AA	3313	-	0,6,6	-	-	-		
56	OHX	AA	3366	-	0,6,6	-	-	-		
56	OHX	AB	214	-	0,6,6	-	-	-		
56	OHX	CA	3251	-	0,6,6	-	-	-		
56	OHX	AA	3436	-	0,6,6	-	-	-		
56	OHX	AA	3372	-	0,6,6	-	-	-		
56	OHX	CA	3347	-	0,6,6	-	-	-		
56	OHX	AA	3565	-	0,6,6	-	-	-		
56	OHX	CA	3316	-	0,6,6	-	-	-		
56	OHX	AA	3534	-	0,6,6	-	-	-		
56	OHX	CA	3467	-	0,6,6	-	-	-		
56	OHX	CA	3371	-	0,6,6	-	-	-		
56	OHX	CA	3248	-	0,6,6	-	-	-		
56	OHX	AA	3422	-	0,6,6	-	-	-		
56	OHX	BA	1682	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	CA	3381	-	0,6,6	-	-	-		
56	OHX	DA	1778	-	0,6,6	-	-	-		
56	OHX	AA	3501	-	0,6,6	-	-	-		
56	OHX	CB	220	-	0,6,6	-	-	-		
56	OHX	CA	3349	-	0,6,6	-	-	-		
56	OHX	AA	3335	-	0,6,6	-	-	-		
56	OHX	DA	1736	-	0,6,6	-	-	-		
56	OHX	DA	1752	-	0,6,6	-	-	-		
56	OHX	DC	110	-	0,6,6	-	-	-		
56	OHX	AB	215	-	0,6,6	-	-	-		
56	OHX	DA	1762	-	0,6,6	-	-	-		
56	OHX	AA	3419	-	0,6,6	-	-	-		
56	OHX	AA	3478	-	0,6,6	-	-	-		
56	OHX	CA	3482	-	0,6,6	-	-	-		
56	OHX	DA	1784	-	0,6,6	-	-	-		
56	OHX	CA	3461	-	0,6,6	-	-	-		
56	OHX	AA	3309	-	0,6,6	-	-	-		
56	OHX	DV	101	-	0,6,6	-	-	-		
56	OHX	AA	3555	-	0,6,6	-	-	-		
56	OHX	CB	216	-	0,6,6	-	-	-		
56	OHX	AA	3138	-	0,6,6	-	-	-		
56	OHX	AA	3323	-	0,6,6	-	-	-		
56	OHX	AB	209	-	0,6,6	-	-	-		
56	OHX	AA	3363	-	0,6,6	-	-	-		
56	OHX	CA	3360	-	0,6,6	-	-	-		
56	OHX	CA	3411	-	0,6,6	-	-	-		
56	OHX	BB	107	-	0,6,6	-	-	-		
56	OHX	CA	3358	-	0,6,6	-	-	-		
56	OHX	BA	1783	-	0,6,6	-	-	-		
56	OHX	AA	3461	-	0,6,6	-	-	-		
56	OHX	AA	3537	-	0,6,6	-	-	-		
56	OHX	CA	3243	-	0,6,6	-	-	-		
56	OHX	AA	3367	-	0,6,6	-	-	-		
56	OHX	BA	1807	-	0,6,6	-	-	-		
56	OHX	CA	3322	-	0,6,6	-	-	-		
56	OHX	CA	3433	-	0,6,6	-	-	-		
56	OHX	CA	3336	-	0,6,6	-	-	-		
56	OHX	CA	3409	-	0,6,6	-	-	-		
56	OHX	DG	302	-	0,6,6	-	-	-		
56	OHX	BA	1681	-	0,6,6	-	-	-		
56	OHX	AA	3464	-	0,6,6	-	-	-		
56	OHX	CO	201	-	0,6,6	-	-	-		
56	OHX	C6	101	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	CA	3418	-	0,6,6	-	-	-		
56	OHX	AA	3517	-	0,6,6	-	-	-		
56	OHX	AA	3548	-	0,6,6	-	-	-		
56	OHX	CA	3398	-	0,6,6	-	-	-		
56	OHX	DA	1807	-	0,6,6	-	-	-		
56	OHX	CA	3323	-	0,6,6	-	-	-		
56	OHX	AA	3362	-	0,6,6	-	-	-		
56	OHX	DA	1732	-	0,6,6	-	-	-		
56	OHX	AA	3482	-	0,6,6	-	-	-		
56	OHX	AF	303	-	0,6,6	-	-	-		
56	OHX	CA	3395	-	0,6,6	-	-	-		
56	OHX	CA	3426	-	0,6,6	-	-	-		
56	OHX	CF	301	-	0,6,6	-	-	-		
56	OHX	CA	3281	-	0,6,6	-	-	-		
56	OHX	DA	1798	-	0,6,6	-	-	-		
56	OHX	AB	210	-	0,6,6	-	-	-		
56	OHX	AA	3554	-	0,6,6	-	-	-		
56	OHX	DA	1724	-	0,6,6	-	-	-		
56	OHX	CA	3487	-	0,6,6	-	-	-		
56	OHX	CA	3374	-	0,6,6	-	-	-		
56	OHX	CA	3285	-	0,6,6	-	-	-		
56	OHX	BA	1686	-	0,6,6	-	-	-		
56	OHX	AA	3475	-	0,6,6	-	-	-		
56	OHX	BA	1656	-	0,6,6	-	-	-		
56	OHX	CA	3356	-	0,6,6	-	-	-		
56	OHX	C5	102	-	0,6,6	-	-	-		
56	OHX	CA	3425	-	0,6,6	-	-	-		
56	OHX	CA	3246	-	0,6,6	-	-	-		
56	OHX	AA	3263	-	0,6,6	-	-	-		
56	OHX	CA	3240	-	0,6,6	-	-	-		
56	OHX	BA	1772	-	0,6,6	-	-	-		
56	OHX	BA	1688	-	0,6,6	-	-	-		
56	OHX	BA	1815	-	0,6,6	-	-	-		
56	OHX	DA	1718	-	0,6,6	-	-	-		
56	OHX	CA	3325	-	0,6,6	-	-	-		
56	OHX	CA	3348	-	0,6,6	-	-	-		
56	OHX	DC	108	-	0,6,6	-	-	-		
56	OHX	AA	3502	-	0,6,6	-	-	-		
56	OHX	BA	1795	-	0,6,6	-	-	-		
56	OHX	CA	3363	-	0,6,6	-	-	-		
56	OHX	BA	1687	-	0,6,6	-	-	-		
56	OHX	AA	3553	-	0,6,6	-	-	-		
56	OHX	BA	1816	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	AA	3452	-	0,6,6	-	-	-		
56	OHX	DB	104	-	0,6,6	-	-	-		
56	OHX	CA	3275	-	0,6,6	-	-	-		
56	OHX	BA	1696	-	0,6,6	-	-	-		
56	OHX	DA	1805	-	0,6,6	-	-	-		
56	OHX	AA	3561	-	0,6,6	-	-	-		
56	OHX	BA	1802	-	0,6,6	-	-	-		
56	OHX	CA	3435	-	0,6,6	-	-	-		
56	OHX	AA	3512	-	0,6,6	-	-	-		
56	OHX	CB	218	-	0,6,6	-	-	-		
56	OHX	DA	1792	-	0,6,6	-	-	-		
56	OHX	BA	1803	-	0,6,6	-	-	-		
56	OHX	BA	1758	-	0,6,6	-	-	-		
56	OHX	DA	1806	-	0,6,6	-	-	-		
56	OHX	BD	102	-	0,6,6	-	-	-		
56	OHX	BA	1796	-	0,6,6	-	-	-		
56	OHX	CA	3311	-	0,6,6	-	-	-		
56	OHX	DA	1812	-	0,6,6	-	-	-		
56	OHX	CA	3375	-	0,6,6	-	-	-		
56	OHX	AA	3457	-	0,6,6	-	-	-		
56	OHX	DA	1719	-	0,6,6	-	-	-		
56	OHX	BA	1666	-	0,6,6	-	-	-		
56	OHX	AA	3318	-	0,6,6	-	-	-		
56	OHX	AA	3531	-	0,6,6	-	-	-		
56	OHX	AA	3522	-	0,6,6	-	-	-		
56	OHX	CA	3301	-	0,6,6	-	-	-		
56	OHX	AA	3434	-	0,6,6	-	-	-		
56	OHX	AA	3557	-	0,6,6	-	-	-		
56	OHX	CB	213	-	0,6,6	-	-	-		
56	OHX	DA	1723	-	0,6,6	-	-	-		
56	OHX	CA	3304	-	0,6,6	-	-	-		
56	OHX	DA	1776	-	0,6,6	-	-	-		
56	OHX	CA	3403	-	0,6,6	-	-	-		
56	OHX	AA	3331	-	0,6,6	-	-	-		
56	OHX	CA	3330	-	0,6,6	-	-	-		
56	OHX	AA	3297	-	0,6,6	-	-	-		
56	OHX	CA	3310	-	0,6,6	-	-	-		
56	OHX	CA	3297	-	0,6,6	-	-	-		
56	OHX	AA	3449	-	0,6,6	-	-	-		
56	OHX	CA	3241	-	0,6,6	-	-	-		
56	OHX	DA	1748	-	0,6,6	-	-	-		
56	OHX	BA	1781	-	0,6,6	-	-	-		
56	OHX	DA	1749	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	BA	1774	-	0,6,6	-	-	-		
56	OHX	AA	3460	-	0,6,6	-	-	-		
56	OHX	AA	3437	-	0,6,6	-	-	-		
56	OHX	CA	3419	-	0,6,6	-	-	-		
56	OHX	CA	3430	-	0,6,6	-	-	-		
56	OHX	DA	1780	-	0,6,6	-	-	-		
56	OHX	AA	3469	-	0,6,6	-	-	-		
56	OHX	BA	1684	-	0,6,6	-	-	-		
56	OHX	CA	3334	-	0,6,6	-	-	-		
56	OHX	AA	3472	-	0,6,6	-	-	-		
56	OHX	AA	3290	-	0,6,6	-	-	-		
56	OHX	AA	3480	-	0,6,6	-	-	-		
56	OHX	CA	3432	-	0,6,6	-	-	-		
56	OHX	CA	3396	-	0,6,6	-	-	-		
56	OHX	CA	3255	-	0,6,6	-	-	-		
56	OHX	CA	3342	-	0,6,6	-	-	-		
56	OHX	AA	3445	-	0,6,6	-	-	-		
56	OHX	CA	3399	-	0,6,6	-	-	-		
56	OHX	AA	3303	-	0,6,6	-	-	-		
56	OHX	CA	3292	-	0,6,6	-	-	-		
56	OHX	DA	1739	-	0,6,6	-	-	-		
56	OHX	BA	1768	-	0,6,6	-	-	-		
56	OHX	AA	3458	-	0,6,6	-	-	-		
56	OHX	DA	1777	-	0,6,6	-	-	-		
56	OHX	AA	3518	-	0,6,6	-	-	-		
56	OHX	AA	3495	-	0,6,6	-	-	-		
56	OHX	CA	3424	-	0,6,6	-	-	-		
56	OHX	AA	3538	-	0,6,6	-	-	-		
56	OHX	AA	3293	-	0,6,6	-	-	-		
56	OHX	AA	3560	-	0,6,6	-	-	-		
56	OHX	CA	3329	-	0,6,6	-	-	-		
56	OHX	AA	3520	-	0,6,6	-	-	-		
56	OHX	DA	1758	-	0,6,6	-	-	-		
56	OHX	BA	1794	-	0,6,6	-	-	-		
56	OHX	DA	1793	-	0,6,6	-	-	-		
56	OHX	AA	3551	-	0,6,6	-	-	-		
56	OHX	CA	3373	-	0,6,6	-	-	-		
56	OHX	AA	3454	-	0,6,6	-	-	-		
56	OHX	CA	3378	-	0,6,6	-	-	-		
56	OHX	AA	3514	-	0,6,6	-	-	-		
56	OHX	BA	1773	-	0,6,6	-	-	-		
56	OHX	CA	3492	-	0,6,6	-	-	-		
56	OHX	CA	3470	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	AA	3312	-	0,6,6	-	-	-		
56	OHX	AB	217	-	0,6,6	-	-	-		
56	OHX	AB	208	-	0,6,6	-	-	-		
56	OHX	DA	1802	-	0,6,6	-	-	-		
56	OHX	AA	3359	-	0,6,6	-	-	-		
56	OHX	CA	3238	-	0,6,6	-	-	-		
56	OHX	AA	3463	-	0,6,6	-	-	-		
56	OHX	AA	3294	-	0,6,6	-	-	-		
56	OHX	AA	3399	-	0,6,6	-	-	-		
56	OHX	AA	3473	-	0,6,6	-	-	-		
56	OHX	CA	3382	-	0,6,6	-	-	-		
56	OHX	AA	3292	-	0,6,6	-	-	-		
56	OHX	A1	202	-	0,6,6	-	-	-		
56	OHX	BA	1694	-	0,6,6	-	-	-		
56	OHX	AA	3549	-	0,6,6	-	-	-		
56	OHX	BA	1764	-	0,6,6	-	-	-		
56	OHX	CA	3305	-	0,6,6	-	-	-		
56	OHX	DA	1730	-	0,6,6	-	-	-		
56	OHX	AA	3505	-	0,6,6	-	-	-		
56	OHX	BA	1665	-	0,6,6	-	-	-		
56	OHX	CA	3422	-	0,6,6	-	-	-		
56	OHX	AA	3295	-	0,6,6	-	-	-		
56	OHX	CA	3410	-	0,6,6	-	-	-		
56	OHX	DA	1783	-	0,6,6	-	-	-		
56	OHX	CA	3392	-	0,6,6	-	-	-		
56	OHX	BA	1777	-	0,6,6	-	-	-		
56	OHX	DC	107	-	0,6,6	-	-	-		
56	OHX	AA	3492	-	0,6,6	-	-	-		
56	OHX	AA	3540	-	0,6,6	-	-	-		
56	OHX	BA	1759	-	0,6,6	-	-	-		
56	OHX	AB	218	-	0,6,6	-	-	-		
56	OHX	CA	3308	-	0,6,6	-	-	-		
56	OHX	CA	3302	-	0,6,6	-	-	-		
56	OHX	AA	3490	-	0,6,6	-	-	-		
56	OHX	DA	1773	-	0,6,6	-	-	-		
56	OHX	A6	101	-	0,6,6	-	-	-		
56	OHX	AA	3450	-	0,6,6	-	-	-		
56	OHX	BA	1785	-	0,6,6	-	-	-		
56	OHX	BA	1670	-	0,6,6	-	-	-		
56	OHX	CA	3423	-	0,6,6	-	-	-		
56	OHX	DA	1768	-	0,6,6	-	-	-		
56	OHX	DA	1729	-	0,6,6	-	-	-		
56	OHX	DA	1757	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	BA	1791	-	0,6,6	-	-	-		
56	OHX	CA	3270	-	0,6,6	-	-	-		
56	OHX	DA	1772	-	0,6,6	-	-	-		
56	OHX	AA	3486	-	0,6,6	-	-	-		
56	OHX	BC	106	-	0,6,6	-	-	-		
56	OHX	CA	3278	-	0,6,6	-	-	-		
56	OHX	BA	1780	-	0,6,6	-	-	-		
56	OHX	CA	3296	-	0,6,6	-	-	-		
56	OHX	AA	3441	-	0,6,6	-	-	-		
56	OHX	CA	3384	-	0,6,6	-	-	-		
56	OHX	CB	211	-	0,6,6	-	-	-		
56	OHX	DA	1811	-	0,6,6	-	-	-		
56	OHX	BG	302	-	0,6,6	-	-	-		
56	OHX	CA	3408	-	0,6,6	-	-	-		
56	OHX	AA	3488	-	0,6,6	-	-	-		
56	OHX	AA	3564	-	0,6,6	-	-	-		
56	OHX	BA	1680	-	0,6,6	-	-	-		
56	OHX	AA	3483	-	0,6,6	-	-	-		
56	OHX	BA	1805	-	0,6,6	-	-	-		
56	OHX	AO	205	-	0,6,6	-	-	-		
56	OHX	DA	1781	-	0,6,6	-	-	-		
56	OHX	DA	1799	-	0,6,6	-	-	-		
56	OHX	CA	3253	-	0,6,6	-	-	-		
56	OHX	BA	1771	-	0,6,6	-	-	-		
56	OHX	AA	3507	-	0,6,6	-	-	-		
56	OHX	BA	1675	-	0,6,6	-	-	-		
56	OHX	AA	3435	-	0,6,6	-	-	-		
56	OHX	CA	3269	-	0,6,6	-	-	-		
56	OHX	C3	101	-	0,6,6	-	-	-		
56	OHX	BA	1756	-	0,6,6	-	-	-		
56	OHX	BA	1679	-	0,6,6	-	-	-		
56	OHX	AA	3442	-	0,6,6	-	-	-		
56	OHX	CA	3372	-	0,6,6	-	-	-		
56	OHX	CA	3436	-	0,6,6	-	-	-		
56	OHX	CA	3327	-	0,6,6	-	-	-		
56	OHX	AA	3563	-	0,6,6	-	-	-		
56	OHX	CA	3291	-	0,6,6	-	-	-		
56	OHX	AA	3508	-	0,6,6	-	-	-		
56	OHX	BA	1690	-	0,6,6	-	-	-		
56	OHX	DR	101	-	0,6,6	-	-	-		
56	OHX	AA	3364	-	0,6,6	-	-	-		
56	OHX	AA	3316	-	0,6,6	-	-	-		
56	OHX	BA	1664	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	AA	3308	-	0,6,6	-	-	-		
56	OHX	CA	3391	-	0,6,6	-	-	-		
56	OHX	AA	3403	-	0,6,6	-	-	-		
56	OHX	DA	1737	-	0,6,6	-	-	-		
56	OHX	AA	3310	-	0,6,6	-	-	-		
56	OHX	BA	1765	-	0,6,6	-	-	-		
56	OHX	CA	3320	-	0,6,6	-	-	-		
56	OHX	AA	3321	-	0,6,6	-	-	-		
56	OHX	DC	109	-	0,6,6	-	-	-		
56	OHX	AA	3526	-	0,6,6	-	-	-		
56	OHX	AA	3306	-	0,6,6	-	-	-		
56	OHX	AB	213	-	0,6,6	-	-	-		
56	OHX	BA	1810	-	0,6,6	-	-	-		
56	OHX	BA	1657	-	0,6,6	-	-	-		
56	OHX	CA	3469	-	0,6,6	-	-	-		
56	OHX	AE	304	-	0,6,6	-	-	-		
56	OHX	DA	1734	-	0,6,6	-	-	-		
56	OHX	CA	3286	-	0,6,6	-	-	-		
56	OHX	CA	3287	-	0,6,6	-	-	-		
56	OHX	AA	3317	-	0,6,6	-	-	-		
56	OHX	AA	3320	-	0,6,6	-	-	-		
56	OHX	AA	3455	-	0,6,6	-	-	-		
56	OHX	AA	3365	-	0,6,6	-	-	-		
56	OHX	BA	1782	-	0,6,6	-	-	-		
56	OHX	CA	3462	-	0,6,6	-	-	-		
56	OHX	AA	3466	-	0,6,6	-	-	-		
56	OHX	AA	3300	-	0,6,6	-	-	-		
56	OHX	AA	3305	-	0,6,6	-	-	-		
56	OHX	AA	3510	-	0,6,6	-	-	-		
56	OHX	DA	1791	-	0,6,6	-	-	-		
56	OHX	AB	207	-	0,6,6	-	-	-		
56	OHX	CA	3345	-	0,6,6	-	-	-		
56	OHX	AA	3536	-	0,6,6	-	-	-		
56	OHX	CA	3401	-	0,6,6	-	-	-		
56	OHX	AA	3370	-	0,6,6	-	-	-		
56	OHX	AA	3545	-	0,6,6	-	-	-		
56	OHX	AA	3427	-	0,6,6	-	-	-		
56	OHX	AB	216	-	0,6,6	-	-	-		
56	OHX	CA	3464	-	0,6,6	-	-	-		
56	OHX	AA	3336	-	0,6,6	-	-	-		
56	OHX	CA	3357	-	0,6,6	-	-	-		
56	OHX	AA	3339	-	0,6,6	-	-	-		
56	OHX	AA	3334	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	CA	3388	-	0,6,6	-	-	-		
56	OHX	DA	1810	-	0,6,6	-	-	-		
56	OHX	AA	3405	-	0,6,6	-	-	-		
56	OHX	AA	3479	-	0,6,6	-	-	-		
56	OHX	CA	3276	-	0,6,6	-	-	-		
56	OHX	AA	3330	-	0,6,6	-	-	-		
56	OHX	AA	3431	-	0,6,6	-	-	-		
56	OHX	BA	1659	-	0,6,6	-	-	-		
56	OHX	CA	3332	-	0,6,6	-	-	-		
56	OHX	CA	3405	-	0,6,6	-	-	-		
56	OHX	CA	3298	-	0,6,6	-	-	-		
56	OHX	DA	1803	-	0,6,6	-	-	-		
56	OHX	BA	1673	-	0,6,6	-	-	-		
56	OHX	CA	3354	-	0,6,6	-	-	-		
56	OHX	CA	3337	-	0,6,6	-	-	-		
56	OHX	DA	1754	-	0,6,6	-	-	-		
56	OHX	CB	212	-	0,6,6	-	-	-		
56	OHX	CA	3274	-	0,6,6	-	-	-		
56	OHX	CA	3385	-	0,6,6	-	-	-		
56	OHX	DA	1785	-	0,6,6	-	-	-		
56	OHX	AA	3401	-	0,6,6	-	-	-		
56	OHX	DA	1744	-	0,6,6	-	-	-		
56	OHX	CA	3242	-	0,6,6	-	-	-		
56	OHX	BA	1793	-	0,6,6	-	-	-		
56	OHX	AA	3519	-	0,6,6	-	-	-		
56	OHX	AA	3552	-	0,6,6	-	-	-		
56	OHX	AA	3485	-	0,6,6	-	-	-		
56	OHX	AA	3528	-	0,6,6	-	-	-		
56	OHX	CA	3252	-	0,6,6	-	-	-		
56	OHX	CA	3331	-	0,6,6	-	-	-		
56	OHX	DA	1726	-	0,6,6	-	-	-		
56	OHX	CB	214	-	0,6,6	-	-	-		
56	OHX	CA	3489	-	0,6,6	-	-	-		
56	OHX	DA	1782	-	0,6,6	-	-	-		
56	OHX	AA	3468	-	0,6,6	-	-	-		
56	OHX	CA	3314	-	0,6,6	-	-	-		
56	OHX	DA	1747	-	0,6,6	-	-	-		
56	OHX	AA	3546	-	0,6,6	-	-	-		
56	OHX	DK	201	-	0,6,6	-	-	-		
56	OHX	AA	3325	-	0,6,6	-	-	-		

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.

233 monomers are involved in 316 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	AA	3438	OHX	2	0
56	AA	3568	OHX	5	0
56	BA	1671	OHX	1	0
56	AA	3424	OHX	2	0
56	DA	1733	OHX	1	0
56	DA	1751	OHX	1	0
56	CA	3272	OHX	1	0
56	DB	103	OHX	1	0
56	AA	3426	OHX	2	0
56	BA	1672	OHX	1	0
56	BA	1760	OHX	2	0
56	CA	3300	OHX	2	0
56	BA	1762	OHX	1	0
56	DA	1727	OHX	1	0
56	CA	3293	OHX	1	0
56	DA	1755	OHX	1	0
56	AA	3430	OHX	1	0
56	AA	3407	OHX	1	0
56	AA	3456	OHX	1	0
56	CA	3362	OHX	1	0
56	CA	3376	OHX	1	0
56	CA	3279	OHX	2	0
56	AB	219	OHX	1	0
56	AA	3447	OHX	1	0
56	DA	1787	OHX	2	0
56	DA	1745	OHX	1	0
56	DA	1721	OHX	2	0
56	AA	3421	OHX	3	0
56	CA	3481	OHX	1	0
56	CA	3486	OHX	2	0
56	BA	1755	OHX	1	0
56	AA	3567	OHX	1	0
56	AA	3402	OHX	1	0
56	CA	3350	OHX	1	0
56	CA	3236	OHX	1	0
56	AA	3566	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	DA	1760	OHX	7	0
56	AA	3491	OHX	1	0
56	BA	1775	OHX	2	0
56	AA	3154	OHX	2	0
56	DA	1764	OHX	2	0
56	BA	1813	OHX	1	0
56	BA	1804	OHX	2	0
56	CA	3233	OHX	1	0
56	DA	1779	OHX	1	0
56	DA	1775	OHX	1	0
56	CA	3377	OHX	2	0
56	AA	3556	OHX	1	0
56	AA	3338	OHX	1	0
56	BA	1797	OHX	2	0
56	CA	3383	OHX	1	0
56	CA	3283	OHX	1	0
56	DA	1742	OHX	1	0
56	CA	3351	OHX	1	0
56	AA	3291	OHX	2	0
56	AA	3433	OHX	1	0
56	CA	3321	OHX	1	0
56	DA	1740	OHX	1	0
56	BA	1661	OHX	1	0
56	CB	209	OHX	1	0
56	DA	1770	OHX	2	0
56	CA	3365	OHX	1	0
56	AA	3513	OHX	1	0
56	CA	3234	OHX	3	0
56	AA	3333	OHX	1	0
56	AA	3499	OHX	1	0
56	BA	1678	OHX	1	0
56	BA	1812	OHX	2	0
56	BA	1683	OHX	1	0
56	CA	3428	OHX	1	0
56	CA	3232	OHX	1	0
56	BB	106	OHX	1	0
56	CA	3244	OHX	1	0
56	CA	3415	OHX	1	0
56	AA	3487	OHX	1	0
56	AA	3311	OHX	1	0
56	BA	1778	OHX	1	0
56	CA	3468	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	AB	212	OHX	1	0
56	BA	1800	OHX	1	0
56	BA	1695	OHX	1	0
56	DA	1731	OHX	4	0
56	AA	3368	OHX	1	0
56	BA	1786	OHX	1	0
56	DD	101	OHX	1	0
56	DA	1795	OHX	1	0
56	DA	1767	OHX	4	0
56	CA	3326	OHX	1	0
56	CA	3490	OHX	1	0
56	AA	3489	OHX	1	0
56	BA	1798	OHX	1	0
56	CA	3416	OHX	1	0
56	DA	1800	OHX	1	0
56	CA	3324	OHX	1	0
56	AA	3373	OHX	1	0
56	AA	3322	OHX	1	0
56	AA	3559	OHX	1	0
56	AA	3418	OHX	1	0
56	AA	3533	OHX	2	0
56	BA	1693	OHX	1	0
56	CA	3333	OHX	1	0
56	AA	3562	OHX	1	0
56	AA	3329	OHX	1	0
56	CA	3484	OHX	1	0
56	AA	3446	OHX	1	0
56	DA	1756	OHX	1	0
56	AA	3299	OHX	1	0
56	DA	1808	OHX	1	0
56	AA	3429	OHX	1	0
56	AA	3425	OHX	1	0
56	CB	217	OHX	1	0
56	CA	3247	OHX	1	0
56	AA	3420	OHX	1	0
56	DA	1759	OHX	1	0
56	AA	3313	OHX	1	0
56	CA	3316	OHX	1	0
56	AA	3534	OHX	1	0
56	DA	1752	OHX	1	0
56	DC	110	OHX	2	0
56	DA	1762	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	AA	3419	OHX	1	0
56	AA	3478	OHX	1	0
56	DV	101	OHX	1	0
56	CA	3411	OHX	1	0
56	BA	1783	OHX	1	0
56	AA	3461	OHX	1	0
56	DG	302	OHX	2	0
56	C6	101	OHX	4	0
56	CA	3418	OHX	1	0
56	AA	3362	OHX	1	0
56	AF	303	OHX	1	0
56	CA	3281	OHX	1	0
56	DA	1724	OHX	1	0
56	CA	3487	OHX	1	0
56	AA	3475	OHX	1	0
56	C5	102	OHX	1	0
56	CA	3425	OHX	1	0
56	CA	3240	OHX	1	0
56	BA	1772	OHX	1	0
56	BA	1688	OHX	1	0
56	DA	1718	OHX	1	0
56	DC	108	OHX	1	0
56	BA	1795	OHX	2	0
56	CA	3363	OHX	1	0
56	AA	3452	OHX	2	0
56	CA	3275	OHX	1	0
56	CA	3435	OHX	1	0
56	AA	3512	OHX	1	0
56	DA	1792	OHX	1	0
56	BD	102	OHX	1	0
56	DA	1812	OHX	1	0
56	CA	3375	OHX	1	0
56	DA	1719	OHX	1	0
56	BA	1666	OHX	3	0
56	AA	3318	OHX	1	0
56	AA	3531	OHX	2	0
56	AA	3434	OHX	1	0
56	AA	3557	OHX	1	0
56	CA	3304	OHX	1	0
56	CA	3403	OHX	1	0
56	CA	3310	OHX	1	0
56	AA	3449	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	DA	1748	OHX	1	0
56	DA	1749	OHX	1	0
56	BA	1774	OHX	1	0
56	AA	3460	OHX	1	0
56	BA	1684	OHX	7	0
56	AA	3480	OHX	1	0
56	CA	3432	OHX	1	0
56	CA	3396	OHX	1	0
56	CA	3399	OHX	1	0
56	BA	1768	OHX	1	0
56	AA	3458	OHX	3	0
56	AA	3518	OHX	1	0
56	AA	3538	OHX	1	0
56	AA	3560	OHX	2	0
56	AA	3514	OHX	1	0
56	CA	3492	OHX	1	0
56	AA	3312	OHX	1	0
56	AB	217	OHX	2	0
56	AA	3294	OHX	2	0
56	AA	3399	OHX	2	0
56	AA	3473	OHX	2	0
56	AA	3292	OHX	1	0
56	CA	3305	OHX	1	0
56	DA	1730	OHX	1	0
56	DA	1783	OHX	2	0
56	DC	107	OHX	6	0
56	A6	101	OHX	3	0
56	AA	3450	OHX	3	0
56	BA	1670	OHX	1	0
56	DA	1768	OHX	1	0
56	CA	3270	OHX	2	0
56	BC	106	OHX	2	0
56	CA	3278	OHX	2	0
56	CA	3296	OHX	1	0
56	CA	3384	OHX	1	0
56	CB	211	OHX	1	0
56	BG	302	OHX	2	0
56	BA	1805	OHX	1	0
56	AO	205	OHX	1	0
56	BA	1675	OHX	1	0
56	CA	3269	OHX	1	0
56	BA	1756	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	CA	3327	OHX	1	0
56	AA	3508	OHX	1	0
56	DA	1737	OHX	1	0
56	CA	3320	OHX	1	0
56	DC	109	OHX	1	0
56	AA	3526	OHX	1	0
56	DA	1734	OHX	3	0
56	AA	3320	OHX	1	0
56	AA	3455	OHX	1	0
56	BA	1782	OHX	1	0
56	CA	3462	OHX	1	0
56	AA	3300	OHX	1	0
56	AA	3305	OHX	1	0
56	AA	3510	OHX	1	0
56	AA	3536	OHX	2	0
56	AA	3370	OHX	1	0
56	CA	3276	OHX	1	0
56	AA	3330	OHX	1	0
56	AA	3431	OHX	1	0
56	CA	3332	OHX	3	0
56	BA	1673	OHX	5	0
56	CA	3354	OHX	1	0
56	DA	1754	OHX	1	0
56	CB	212	OHX	1	0
56	CA	3274	OHX	1	0
56	AA	3485	OHX	1	0
56	CA	3331	OHX	1	0
56	DK	201	OHX	1	0
56	AA	3325	OHX	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	AA	2912/2912 (100%)	-0.77	5 (0%) 92 88	45, 76, 209, 243	0
1	CA	2907/2912 (99%)	-0.54	8 (0%) 90 85	58, 92, 230, 245	0
2	AB	122/122 (100%)	-0.72	0 100 100	73, 95, 116, 177	0
2	CB	122/122 (100%)	-0.46	1 (0%) 82 72	92, 126, 146, 198	0
3	AD	272/276 (98%)	-0.04	7 (2%) 57 42	39, 66, 84, 105	0
3	CD	272/276 (98%)	0.25	15 (5%) 32 25	55, 78, 96, 128	0
4	AE	205/206 (99%)	0.26	14 (6%) 25 20	51, 86, 130, 142	0
4	CE	205/206 (99%)	0.16	7 (3%) 48 35	64, 100, 148, 165	0
5	AF	202/210 (96%)	-0.36	3 (1%) 71 58	47, 81, 118, 130	0
5	CF	208/210 (99%)	0.12	6 (2%) 54 40	62, 106, 160, 184	0
6	AG	181/182 (99%)	0.00	5 (2%) 55 40	84, 107, 138, 149	0
6	CG	181/182 (99%)	0.55	11 (6%) 28 23	120, 141, 164, 171	0
7	AH	170/180 (94%)	0.29	8 (4%) 37 28	86, 112, 130, 157	0
7	CH	170/180 (94%)	0.61	15 (8%) 17 16	155, 198, 220, 229	0
8	AK	146/148 (98%)	0.16	9 (6%) 28 22	79, 131, 147, 150	0
8	CK	146/148 (98%)	0.11	2 (1%) 73 60	84, 130, 152, 158	0
9	AM	138/140 (98%)	0.26	7 (5%) 34 27	66, 87, 124, 136	0
9	CM	138/140 (98%)	0.38	4 (2%) 54 40	83, 114, 140, 156	0
10	AN	122/122 (100%)	-0.08	1 (0%) 82 72	57, 78, 93, 101	0
10	CN	122/122 (100%)	0.17	1 (0%) 82 72	75, 95, 111, 124	0
11	AO	150/150 (100%)	-0.21	1 (0%) 84 75	48, 88, 117, 160	0
11	CO	150/150 (100%)	0.22	8 (5%) 33 26	45, 108, 146, 178	0
12	AP	141/141 (100%)	0.74	19 (13%) 8 8	58, 83, 105, 127	0
12	CP	141/141 (100%)	1.07	25 (17%) 4 4	58, 109, 140, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	A0	118/118 (100%)	-0.36	0 100 100	61, 81, 103, 113	0
13	C0	117/118 (99%)	-0.46	0 100 100	69, 87, 106, 121	0
14	AQ	111/112 (99%)	-0.20	2 (1%) 67 53	70, 92, 117, 131	0
14	CQ	111/112 (99%)	-0.01	4 (3%) 46 34	86, 123, 147, 162	0
15	AR	137/146 (93%)	-0.04	3 (2%) 62 47	73, 93, 143, 170	0
15	CR	137/146 (93%)	-0.03	5 (3%) 46 34	84, 104, 163, 183	0
16	A1	117/118 (99%)	-0.21	0 100 100	52, 75, 108, 139	0
16	C1	117/118 (99%)	0.08	1 (0%) 81 70	67, 106, 143, 162	0
17	A2	101/101 (100%)	0.37	5 (4%) 35 28	53, 98, 122, 141	0
17	C2	101/101 (100%)	0.83	8 (7%) 20 18	67, 129, 142, 151	0
18	AS	113/113 (100%)	-0.22	1 (0%) 81 70	54, 73, 104, 156	0
18	CS	113/113 (100%)	-0.11	1 (0%) 81 70	64, 80, 114, 158	0
19	AT	92/96 (95%)	-0.16	2 (2%) 62 47	57, 71, 95, 107	0
19	CT	92/96 (95%)	0.31	6 (6%) 26 21	74, 88, 113, 127	0
20	AU	102/110 (92%)	0.24	5 (4%) 36 28	74, 101, 152, 162	0
20	CU	102/110 (92%)	0.71	10 (9%) 14 14	95, 118, 166, 181	0
21	AV	175/206 (84%)	0.60	11 (6%) 27 22	87, 126, 188, 191	0
21	CV	179/206 (86%)	0.58	6 (3%) 48 35	122, 160, 208, 216	0
22	A3	76/85 (89%)	-0.30	1 (1%) 74 61	59, 77, 91, 132	0
22	C3	77/85 (90%)	-0.02	3 (3%) 44 33	83, 95, 117, 147	0
23	AZ	97/98 (98%)	-0.14	5 (5%) 34 27	58, 78, 126, 156	0
23	CZ	97/98 (98%)	0.37	5 (5%) 34 27	68, 86, 132, 155	0
24	AW	66/72 (91%)	-0.10	1 (1%) 71 58	63, 84, 98, 125	0
24	CW	66/72 (91%)	0.13	3 (4%) 39 29	84, 107, 130, 139	0
25	AX	59/60 (98%)	-0.16	1 (1%) 69 55	63, 83, 112, 130	0
25	CX	59/60 (98%)	0.20	0 100 100	80, 110, 141, 162	0
26	A4	66/71 (92%)	0.33	2 (3%) 52 39	120, 156, 173, 179	0
26	C4	63/71 (88%)	0.96	8 (12%) 9 9	146, 185, 194, 199	0
27	A5	59/60 (98%)	0.52	7 (11%) 10 10	49, 88, 168, 171	0
27	C5	59/60 (98%)	0.18	2 (3%) 48 35	65, 92, 173, 187	0
28	A6	45/54 (83%)	0.86	7 (15%) 6 6	124, 151, 168, 177	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	C6	45/54 (83%)	1.22	9 (20%) 3 3	141, 169, 183, 186	0
29	A7	45/49 (91%)	-0.36	3 (6%) 25 20	47, 55, 69, 78	0
29	C7	45/49 (91%)	-0.12	1 (2%) 62 47	56, 66, 77, 100	0
30	A8	60/65 (92%)	-0.18	0 100 100	55, 73, 90, 114	0
30	C8	60/65 (92%)	0.47	8 (13%) 8 8	78, 90, 112, 137	0
31	BA	1502/1506 (99%)	-0.61	9 (0%) 85 78	58, 107, 187, 244	0
31	DA	1502/1506 (99%)	-0.69	1 (0%) 92 91	71, 119, 189, 244	0
32	BE	237/256 (92%)	0.31	7 (2%) 52 39	111, 144, 182, 193	0
32	DE	237/256 (92%)	0.06	0 100 100	126, 161, 196, 211	0
33	BF	205/239 (85%)	0.22	2 (0%) 79 68	96, 119, 152, 160	0
33	DF	206/239 (86%)	0.15	4 (1%) 66 51	127, 147, 175, 180	0
34	BG	208/208 (100%)	0.40	7 (3%) 48 35	92, 116, 136, 147	0
34	DG	208/208 (100%)	0.10	4 (1%) 66 51	93, 111, 132, 145	0
35	BH	151/162 (93%)	0.17	2 (1%) 74 61	81, 105, 127, 161	0
35	DH	151/162 (93%)	0.04	0 100 100	104, 121, 142, 165	0
36	BI	101/101 (100%)	-0.02	0 100 100	81, 108, 122, 145	0
36	DI	101/101 (100%)	0.24	0 100 100	81, 106, 124, 149	0
37	BJ	155/156 (99%)	0.06	5 (3%) 50 37	106, 121, 149, 158	0
37	DJ	155/156 (99%)	-0.05	2 (1%) 74 61	113, 131, 153, 164	0
38	BK	138/138 (100%)	-0.19	0 100 100	89, 110, 123, 129	0
38	DK	138/138 (100%)	-0.39	0 100 100	104, 125, 136, 146	0
39	BL	127/128 (99%)	-0.26	0 100 100	87, 142, 160, 169	0
39	DL	127/128 (99%)	-0.31	1 (0%) 82 72	117, 155, 168, 174	0
40	BM	99/105 (94%)	-0.04	1 (1%) 79 68	91, 142, 170, 174	0
40	DM	99/105 (94%)	0.02	1 (1%) 79 68	124, 159, 175, 179	0
41	BN	119/129 (92%)	0.12	4 (3%) 48 35	72, 104, 133, 161	0
41	DN	119/129 (92%)	0.32	6 (5%) 35 28	91, 112, 139, 167	0
42	BO	125/132 (94%)	0.30	7 (5%) 31 25	69, 83, 112, 158	0
42	DO	125/132 (94%)	0.43	9 (7%) 23 19	93, 110, 134, 166	0
43	BP	116/126 (92%)	-0.01	2 (1%) 69 55	92, 128, 145, 153	0
43	DP	117/126 (92%)	0.23	7 (5%) 29 23	106, 156, 169, 171	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
44	BQ	58/61 (95%)	-0.08	0	100	100	91, 108, 122, 129	0
44	DQ	58/61 (95%)	-0.28	0	100	100	126, 140, 157, 160	0
45	BR	88/89 (98%)	-0.32	0	100	100	80, 100, 121, 125	0
45	DR	88/89 (98%)	-0.14	0	100	100	85, 112, 133, 140	0
46	BS	84/88 (95%)	-0.06	0	100	100	100, 118, 139, 175	0
46	DS	84/88 (95%)	-0.18	0	100	100	96, 107, 127, 158	0
47	BT	100/105 (95%)	-0.14	3 (3%)	52	39	93, 112, 125, 133	0
47	DT	100/105 (95%)	-0.10	3 (3%)	52	39	94, 114, 135, 143	0
48	BU	72/88 (81%)	0.15	1 (1%)	73	60	88, 106, 139, 164	0
48	DU	72/88 (81%)	0.29	4 (5%)	31	25	97, 114, 155, 169	0
49	BV	78/93 (83%)	0.23	3 (3%)	44	33	109, 130, 147, 152	0
49	DV	78/93 (83%)	0.21	2 (2%)	57	42	145, 163, 182, 185	0
50	BW	99/106 (93%)	-0.21	0	100	100	105, 124, 155, 160	0
50	DW	99/106 (93%)	-0.39	0	100	100	95, 117, 153, 163	0
51	BX	25/27 (92%)	-0.48	0	100	100	102, 117, 137, 154	0
51	DX	25/27 (92%)	-0.19	1 (4%)	43	32	122, 143, 158, 168	0
52	BB	84/85 (98%)	1.14	24 (28%)	1	1	82, 123, 154, 169	0
52	BD	84/85 (98%)	0.14	5 (5%)	29	23	75, 137, 217, 227	0
52	DB	84/85 (98%)	1.13	17 (20%)	3	3	93, 128, 156, 171	0
52	DD	84/85 (98%)	0.45	7 (8%)	19	17	84, 137, 217, 225	0
53	BC	77/77 (100%)	0.16	5 (6%)	26	21	77, 114, 139, 153	0
53	DC	77/77 (100%)	0.11	2 (2%)	57	42	88, 122, 150, 157	0
54	B1	16/16 (100%)	0.73	3 (18%)	4	3	76, 104, 156, 163	0
54	D1	16/16 (100%)	0.28	2 (12%)	9	9	85, 109, 157, 165	0
All	All	21100/21658 (97%)	-0.20	481 (2%)	61	46	39, 105, 182, 245	0

The worst 5 of 481 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	CW	41	ILE	7.5
27	A5	2	ALA	7.2
11	CO	61	ARG	7.2
12	AP	86	GLY	6.9
27	C5	2	ALA	6.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å <sup>2</sup> )	Q<0.9
52	MIA	DB	38	29/30	0.79	0.12	84,93,111,126	0
52	MIA	BD	38	29/30	0.87	0.15	116,135,182,198	0
52	MIA	DD	38	29/30	0.88	0.12	120,140,186,205	0
52	MIA	BB	38	29/30	0.93	0.12	68,83,97,106	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å <sup>2</sup> )	Q<0.9
55	MG	CA	3213	1/1	0.28	0.15	121,121,121,121	0
55	MG	DA	1631	1/1	0.43	0.29	111,111,111,111	0
55	MG	AA	3086	1/1	0.45	0.31	95,95,95,95	0
55	MG	AA	3095	1/1	0.45	0.24	89,89,89,89	0
55	MG	CA	3455	1/1	0.48	0.63	97,97,97,97	0
55	MG	BA	1699	1/1	0.50	0.38	79,79,79,79	0
55	MG	BA	1648	1/1	0.52	0.25	99,99,99,99	0
55	MG	DA	1619	1/1	0.53	0.31	98,98,98,98	0
55	MG	AA	3100	1/1	0.54	0.24	108,108,108,108	0
55	MG	DA	1622	1/1	0.57	0.20	122,122,122,122	0
55	MG	BB	104	1/1	0.58	0.44	87,87,87,87	0
55	MG	BA	1632	1/1	0.58	0.22	108,108,108,108	0
55	MG	DA	1714	1/1	0.58	0.20	97,97,97,97	0
55	MG	AA	3137	1/1	0.60	0.38	51,51,51,51	0
55	MG	DA	1643	1/1	0.61	0.24	136,136,136,136	0
55	MG	BA	1629	1/1	0.61	0.18	112,112,112,112	0
55	MG	AA	3067	1/1	0.62	0.19	97,97,97,97	0
55	MG	CA	3198	1/1	0.63	0.23	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	1641	1/1	0.63	0.27	130,130,130,130	0
55	MG	CA	3034	1/1	0.63	0.25	91,91,91,91	0
55	MG	DA	1673	1/1	0.63	0.20	80,80,80,80	0
55	MG	DA	1681	1/1	0.63	0.18	100,100,100,100	0
55	MG	CA	3220	1/1	0.63	0.35	85,85,85,85	0
56	OHX	AA	3526	7/7	0.63	0.12	120,129,136,176	1
56	OHX	DB	104	7/7	0.63	0.09	129,133,143,205	2
56	OHX	DA	1794	7/7	0.64	0.09	124,130,139,205	1
55	MG	AA	3247	1/1	0.65	0.25	81,81,81,81	0
55	MG	DA	1642	1/1	0.65	0.21	112,112,112,112	0
55	MG	BA	1634	1/1	0.65	0.37	74,74,74,74	0
55	MG	DA	1659	1/1	0.65	0.22	89,89,89,89	0
55	MG	DA	1618	1/1	0.65	0.24	105,105,105,105	0
55	MG	DA	1705	1/1	0.66	0.24	108,108,108,108	0
55	MG	CA	3209	1/1	0.66	0.34	85,85,85,85	0
55	MG	AA	3245	1/1	0.66	0.26	68,68,68,68	0
55	MG	DA	1682	1/1	0.66	0.36	87,87,87,87	0
55	MG	DA	1688	1/1	0.66	0.29	101,101,101,101	0
55	MG	BA	1607	1/1	0.67	0.24	93,93,93,93	0
56	OHX	CB	218	7/7	0.67	0.10	141,159,166,235	1
55	MG	AA	3108	1/1	0.67	0.20	82,82,82,82	0
55	MG	AA	3087	1/1	0.67	0.29	83,83,83,83	0
55	MG	CA	3197	1/1	0.68	0.32	79,79,79,79	0
55	MG	CE	301	1/1	0.68	0.39	56,56,56,56	0
55	MG	AA	3248	1/1	0.68	0.25	86,86,86,86	0
55	MG	DA	1720	1/1	0.68	0.25	105,105,105,105	0
55	MG	DB	102	1/1	0.68	0.22	102,102,102,102	0
55	MG	BA	1615	1/1	0.68	0.21	113,113,113,113	0
55	MG	AA	3347	1/1	0.68	0.34	70,70,70,70	0
55	MG	DA	1623	1/1	0.68	0.23	124,124,124,124	0
55	MG	CA	3085	1/1	0.68	0.29	102,102,102,102	0
55	MG	CA	3107	1/1	0.69	0.25	82,82,82,82	0
55	MG	CA	3458	1/1	0.69	0.20	82,82,82,82	0
55	MG	BA	1746	1/1	0.69	0.28	82,82,82,82	0
55	MG	AA	3144	1/1	0.69	0.44	71,71,71,71	0
55	MG	AA	3098	1/1	0.70	0.24	77,77,77,77	0
55	MG	BA	1622	1/1	0.70	0.16	123,123,123,123	0
55	MG	BA	1749	1/1	0.70	0.27	88,88,88,88	0
55	MG	CA	3146	1/1	0.70	0.28	77,77,77,77	0
55	MG	CA	3172	1/1	0.70	0.22	86,86,86,86	0
55	MG	DA	1617	1/1	0.70	0.19	115,115,115,115	0
56	OHX	BD	104	7/7	0.70	0.12	82,85,90,147	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3280	1/1	0.70	0.24	77,77,77,77	0
55	MG	BC	102	1/1	0.70	0.19	68,68,68,68	0
55	MG	BC	105	1/1	0.70	0.42	87,87,87,87	0
56	OHX	DB	105	7/7	0.70	0.14	88,91,103,175	5
55	MG	BA	1602	1/1	0.71	0.31	75,75,75,75	0
55	MG	DA	1717	1/1	0.71	0.19	100,100,100,100	0
55	MG	CA	3457	1/1	0.71	0.20	66,66,66,66	0
55	MG	DA	1668	1/1	0.71	0.22	86,86,86,86	0
55	MG	AA	3009	1/1	0.71	0.16	89,89,89,89	0
55	MG	AA	3037	1/1	0.72	0.31	63,63,63,63	0
55	MG	CA	3193	1/1	0.72	0.25	80,80,80,80	0
55	MG	DA	1649	1/1	0.72	0.28	87,87,87,87	0
55	MG	BA	1611	1/1	0.72	0.34	84,84,84,84	0
55	MG	CA	3079	1/1	0.73	0.29	73,73,73,73	0
55	MG	CA	3023	1/1	0.73	0.30	85,85,85,85	0
56	OHX	CA	3429	7/7	0.73	0.10	127,129,142,209	1
55	MG	CA	3187	1/1	0.73	0.35	86,86,86,86	0
55	MG	AA	3131	1/1	0.73	0.20	94,94,94,94	0
55	MG	CA	3448	1/1	0.73	0.26	63,63,63,63	0
55	MG	CA	3117	1/1	0.73	0.17	69,69,69,69	0
56	OHX	AA	3536	7/7	0.74	0.10	116,124,157,192	1
56	OHX	AA	3555	7/7	0.74	0.10	112,114,124,192	1
56	OHX	BA	1669	7/7	0.74	0.14	124,127,142,200	1
55	MG	BA	1712	1/1	0.74	0.30	95,95,95,95	0
55	MG	CA	3201	1/1	0.74	0.30	79,79,79,79	0
55	MG	BA	1728	1/1	0.74	0.28	90,90,90,90	0
55	MG	DA	1634	1/1	0.74	0.09	118,118,118,118	0
55	MG	CA	3460	1/1	0.74	0.37	72,72,72,72	0
56	OHX	AA	3534	7/7	0.74	0.10	136,141,145,222	1
55	MG	DA	1630	1/1	0.75	0.20	95,95,95,95	0
55	MG	DA	1715	1/1	0.75	0.23	89,89,89,89	0
55	MG	CA	3215	1/1	0.75	0.15	137,137,137,137	0
55	MG	CA	3141	1/1	0.75	0.33	77,77,77,77	0
55	MG	CA	3145	1/1	0.75	0.42	74,74,74,74	0
55	MG	BA	1704	1/1	0.75	0.12	88,88,88,88	0
55	MG	BA	1605	1/1	0.75	0.15	104,104,104,104	0
55	MG	BA	1720	1/1	0.75	0.30	58,58,58,58	0
55	MG	AA	3045	1/1	0.75	0.28	65,65,65,65	0
55	MG	CA	3196	1/1	0.75	0.36	92,92,92,92	0
55	MG	CA	3045	1/1	0.75	0.42	91,91,91,91	0
55	MG	DA	1678	1/1	0.75	0.12	118,118,118,118	0
55	MG	BA	1729	1/1	0.75	0.34	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3065	1/1	0.75	0.40	49,49,49,49	0
55	MG	BA	1601	1/1	0.75	0.12	81,81,81,81	0
55	MG	AA	3232	1/1	0.75	0.23	75,75,75,75	0
55	MG	CA	3129	1/1	0.76	0.39	81,81,81,81	0
55	MG	AA	3397	1/1	0.76	0.14	80,80,80,80	0
55	MG	DC	104	1/1	0.76	0.28	77,77,77,77	0
55	MG	AA	3141	1/1	0.76	0.32	44,44,44,44	0
55	MG	BA	1633	1/1	0.76	0.18	59,59,59,59	0
55	MG	CA	3062	1/1	0.76	0.15	78,78,78,78	0
55	MG	CA	3266	1/1	0.76	0.29	64,64,64,64	0
56	OHX	AA	3562	7/7	0.76	0.10	98,105,127,189	1
55	MG	DA	1627	1/1	0.76	0.33	77,77,77,77	0
55	MG	BA	1751	1/1	0.76	0.35	95,95,95,95	0
56	OHX	CA	3421	7/7	0.76	0.10	113,126,135,198	1
55	MG	AA	3058	1/1	0.76	0.20	73,73,73,73	0
55	MG	CA	3088	1/1	0.76	0.30	86,86,86,86	0
55	MG	DA	1635	1/1	0.76	0.36	96,96,96,96	0
55	MG	BA	1722	1/1	0.76	0.34	91,91,91,91	0
55	MG	AA	3150	1/1	0.76	0.27	68,68,68,68	0
55	MG	DA	1696	1/1	0.77	0.17	112,112,112,112	0
55	MG	BA	1609	1/1	0.77	0.21	73,73,73,73	0
55	MG	CA	3136	1/1	0.77	0.19	91,91,91,91	0
55	MG	CA	3216	1/1	0.77	0.28	91,91,91,91	0
55	MG	BA	1610	1/1	0.77	0.20	92,92,92,92	0
55	MG	CA	3264	1/1	0.77	0.44	49,49,49,49	0
55	MG	BA	1640	1/1	0.77	0.26	73,73,73,73	0
55	MG	DA	1637	1/1	0.77	0.23	106,106,106,106	0
56	OHX	AA	3523	7/7	0.77	0.12	109,114,123,180	1
55	MG	BA	1744	1/1	0.77	0.18	90,90,90,90	0
55	MG	CA	3046	1/1	0.77	0.18	76,76,76,76	0
55	MG	BA	1745	1/1	0.77	0.45	83,83,83,83	0
55	MG	AA	3273	1/1	0.77	0.31	66,66,66,66	0
55	MG	AA	3275	1/1	0.77	0.29	64,64,64,64	0
55	MG	CB	204	1/1	0.77	0.24	73,73,73,73	0
55	MG	CA	3086	1/1	0.77	0.29	68,68,68,68	0
55	MG	DA	1675	1/1	0.77	0.19	92,92,92,92	0
55	MG	AA	3074	1/1	0.77	0.24	73,73,73,73	0
55	MG	CA	3200	1/1	0.77	0.25	56,56,56,56	0
55	MG	AA	3187	1/1	0.77	0.32	86,86,86,86	0
55	MG	AA	3350	1/1	0.77	0.33	80,80,80,80	0
55	MG	DA	1694	1/1	0.77	0.20	104,104,104,104	0
55	MG	CA	3164	1/1	0.78	0.26	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3095	1/1	0.78	0.17	54,54,54,54	0
56	OHX	AA	3535	7/7	0.78	0.10	104,112,123,191	1
55	MG	CA	3183	1/1	0.78	0.28	93,93,93,93	0
56	OHX	AA	3545	7/7	0.78	0.14	90,96,105,167	2
55	MG	DA	1609	1/1	0.78	0.24	91,91,91,91	0
55	MG	AA	3218	1/1	0.78	0.27	82,82,82,82	0
56	OHX	BA	1657	7/7	0.78	0.15	116,125,141,215	1
56	OHX	BA	1667	7/7	0.78	0.12	118,130,146,200	1
55	MG	AA	3062	1/1	0.78	0.35	73,73,73,73	0
56	OHX	BA	1686	7/7	0.78	0.09	141,143,153,230	1
56	OHX	BA	1692	7/7	0.78	0.10	126,131,140,209	1
55	MG	BA	1703	1/1	0.78	0.27	108,108,108,108	0
56	OHX	CA	3396	7/7	0.78	0.08	135,136,150,198	1
55	MG	AA	3159	1/1	0.78	0.19	65,65,65,65	0
55	MG	AA	3035	1/1	0.78	0.32	64,64,64,64	0
55	MG	AA	3209	1/1	0.78	0.26	57,57,57,57	0
55	MG	BA	1747	1/1	0.78	0.29	74,74,74,74	0
55	MG	DA	1676	1/1	0.78	0.29	83,83,83,83	0
55	MG	CA	3202	1/1	0.78	0.32	79,79,79,79	0
55	MG	CA	3076	1/1	0.79	0.39	64,64,64,64	0
55	MG	CA	3028	1/1	0.79	0.19	73,73,73,73	0
55	MG	CA	3192	1/1	0.79	0.23	87,87,87,87	0
55	MG	CA	3081	1/1	0.79	0.34	63,63,63,63	0
55	MG	AA	3076	1/1	0.79	0.38	72,72,72,72	0
55	MG	CA	3040	1/1	0.79	0.33	70,70,70,70	0
55	MG	DA	1706	1/1	0.79	0.09	100,100,100,100	0
56	OHX	BA	1677	7/7	0.79	0.10	141,145,154,220	1
55	MG	DA	1647	1/1	0.79	0.29	90,90,90,90	0
55	MG	BA	1606	1/1	0.79	0.24	92,92,92,92	0
55	MG	CA	3441	1/1	0.79	0.33	99,99,99,99	0
55	MG	DA	1660	1/1	0.79	0.34	88,88,88,88	0
56	OHX	CA	3420	7/7	0.79	0.09	131,141,152,216	1
55	MG	DA	1662	1/1	0.79	0.29	73,73,73,73	0
55	MG	AO	201	1/1	0.79	0.23	80,80,80,80	0
56	OHX	CA	3470	7/7	0.79	0.10	113,126,137,181	1
55	MG	CA	3170	1/1	0.79	0.12	65,65,65,65	0
55	MG	DA	1629	1/1	0.79	0.15	93,93,93,93	0
55	MG	BA	1604	1/1	0.79	0.22	72,72,72,72	0
55	MG	CA	3206	1/1	0.79	0.31	90,90,90,90	0
55	MG	BQ	101	1/1	0.80	0.41	96,96,96,96	0
55	MG	AA	3208	1/1	0.80	0.25	65,65,65,65	0
55	MG	CA	3267	1/1	0.80	0.22	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	AA	3552	7/7	0.80	0.13	105,122,135,199	1
55	MG	BA	1706	1/1	0.80	0.32	79,79,79,79	0
55	MG	AA	3145	1/1	0.80	0.33	56,56,56,56	0
55	MG	AA	3282	1/1	0.80	0.20	69,69,69,69	0
55	MG	BA	1631	1/1	0.80	0.15	78,78,78,78	0
55	MG	AA	3165	1/1	0.80	0.25	84,84,84,84	0
55	MG	AA	3258	1/1	0.80	0.25	65,65,65,65	0
55	MG	DA	1708	1/1	0.80	0.27	87,87,87,87	0
55	MG	AA	3351	1/1	0.80	0.29	53,53,53,53	0
55	MG	BA	1635	1/1	0.80	0.23	96,96,96,96	0
55	MG	AA	3391	1/1	0.80	0.27	59,59,59,59	0
55	MG	CA	3065	1/1	0.80	0.30	55,55,55,55	0
55	MG	DA	1725	1/1	0.80	0.33	87,87,87,87	0
55	MG	AA	3268	1/1	0.80	0.31	73,73,73,73	0
55	MG	DC	103	1/1	0.80	0.34	96,96,96,96	0
55	MG	AA	3024	1/1	0.80	0.28	63,63,63,63	0
56	OHX	DA	1753	7/7	0.80	0.13	120,124,134,196	1
55	MG	CA	3217	1/1	0.80	0.28	58,58,58,58	0
55	MG	BA	1612	1/1	0.80	0.28	81,81,81,81	0
55	MG	DA	1624	1/1	0.80	0.08	73,73,73,73	0
55	MG	CA	3191	1/1	0.81	0.27	72,72,72,72	0
55	MG	CA	3035	1/1	0.81	0.18	92,92,92,92	0
55	MG	CA	3037	1/1	0.81	0.24	89,89,89,89	0
55	MG	BA	1718	1/1	0.81	0.20	78,78,78,78	0
55	MG	CA	3042	1/1	0.81	0.25	67,67,67,67	0
56	OHX	AA	3565	7/7	0.81	0.09	117,122,134,195	1
55	MG	AB	203	1/1	0.81	0.30	71,71,71,71	0
55	MG	DA	1698	1/1	0.81	0.31	95,95,95,95	0
55	MG	AB	206	1/1	0.81	0.38	83,83,83,83	0
55	MG	CA	3060	1/1	0.81	0.16	75,75,75,75	0
55	MG	AA	3132	1/1	0.81	0.34	81,81,81,81	0
55	MG	CA	3478	1/1	0.81	0.30	82,82,82,82	0
55	MG	AA	3354	1/1	0.81	0.33	57,57,57,57	0
55	MG	CA	3207	1/1	0.81	0.23	68,68,68,68	0
55	MG	DA	1657	1/1	0.81	0.33	70,70,70,70	0
55	MG	CA	3156	1/1	0.81	0.38	84,84,84,84	0
55	MG	AA	3169	1/1	0.81	0.30	76,76,76,76	0
55	MG	AA	3231	1/1	0.81	0.30	66,66,66,66	0
55	MG	CA	3027	1/1	0.81	0.26	81,81,81,81	0
55	MG	BA	1709	1/1	0.81	0.24	100,100,100,100	0
55	MG	DA	1674	1/1	0.81	0.22	99,99,99,99	0
55	MG	AB	201	1/1	0.81	0.27	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3223	1/1	0.81	0.29	88,88,88,88	0
56	OHX	DC	108	7/7	0.81	0.10	120,132,142,180	1
55	MG	CA	3134	1/1	0.82	0.26	65,65,65,65	0
55	MG	CB	206	1/1	0.82	0.23	83,83,83,83	0
55	MG	CA	3044	1/1	0.82	0.19	74,74,74,74	0
55	MG	AA	3079	1/1	0.82	0.26	88,88,88,88	0
55	MG	CA	3142	1/1	0.82	0.27	71,71,71,71	0
55	MG	CA	3144	1/1	0.82	0.30	54,54,54,54	0
55	MG	AA	3235	1/1	0.82	0.22	50,50,50,50	0
55	MG	AA	3285	1/1	0.82	0.33	80,80,80,80	0
55	MG	BA	1626	1/1	0.82	0.15	81,81,81,81	0
55	MG	AA	3176	1/1	0.82	0.17	60,60,60,60	0
55	MG	AA	3096	1/1	0.82	0.27	71,71,71,71	0
55	MG	AA	3190	1/1	0.82	0.34	69,69,69,69	0
55	MG	CA	3227	1/1	0.82	0.34	79,79,79,79	0
55	MG	AA	3148	1/1	0.82	0.23	65,65,65,65	0
55	MG	CA	3184	1/1	0.82	0.36	60,60,60,60	0
55	MG	AA	3066	1/1	0.82	0.26	83,83,83,83	0
55	MG	CA	3440	1/1	0.82	0.31	54,54,54,54	0
55	MG	DA	1710	1/1	0.82	0.15	103,103,103,103	0
56	OHX	CA	3419	7/7	0.82	0.08	153,156,164,238	1
55	MG	BA	1724	1/1	0.82	0.25	59,59,59,59	0
55	MG	AA	3017	1/1	0.82	0.24	100,100,100,100	0
56	OHX	CA	3427	7/7	0.82	0.08	114,126,136,203	1
55	MG	CA	3091	1/1	0.82	0.30	74,74,74,74	0
55	MG	DA	1644	1/1	0.82	0.10	149,149,149,149	0
55	MG	AA	3105	1/1	0.82	0.23	124,124,124,124	0
55	MG	BA	1644	1/1	0.82	0.49	94,94,94,94	0
56	OHX	DA	1765	7/7	0.82	0.15	117,133,141,227	1
55	MG	DC	101	1/1	0.82	0.33	85,85,85,85	0
55	MG	BA	1646	1/1	0.82	0.24	95,95,95,95	0
55	MG	AA	3276	1/1	0.82	0.21	69,69,69,69	0
56	OHX	AA	3522	7/7	0.82	0.10	118,131,145,201	1
55	MG	AA	3125	1/1	0.83	0.21	92,92,92,92	0
55	MG	CA	3114	1/1	0.83	0.33	57,57,57,57	0
55	MG	DA	1661	1/1	0.83	0.39	76,76,76,76	0
55	MG	AA	3129	1/1	0.83	0.21	83,83,83,83	0
55	MG	AA	3156	1/1	0.83	0.27	45,45,45,45	0
55	MG	DA	1672	1/1	0.83	0.26	83,83,83,83	0
55	MG	CA	3039	1/1	0.83	0.28	65,65,65,65	0
55	MG	BA	1725	1/1	0.83	0.38	69,69,69,69	0
55	MG	DA	1613	1/1	0.83	0.20	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3234	1/1	0.83	0.15	56,56,56,56	0
55	MG	AA	3130	1/1	0.83	0.17	75,75,75,75	0
55	MG	AA	3026	1/1	0.83	0.26	92,92,92,92	0
55	MG	BA	1641	1/1	0.83	0.16	85,85,85,85	0
55	MG	CA	3057	1/1	0.83	0.27	95,95,95,95	0
55	MG	AA	3019	1/1	0.83	0.31	72,72,72,72	0
55	MG	DA	1626	1/1	0.83	0.33	84,84,84,84	0
55	MG	CA	3163	1/1	0.83	0.28	80,80,80,80	0
56	OHX	BB	107	7/7	0.83	0.12	71,92,103,147	3
55	MG	DA	1702	1/1	0.83	0.11	122,122,122,122	0
55	MG	AA	3059	1/1	0.83	0.26	85,85,85,85	0
55	MG	CA	3225	1/1	0.83	0.19	48,48,48,48	0
55	MG	AA	3252	1/1	0.83	0.32	47,47,47,47	0
55	MG	AA	3396	1/1	0.83	0.41	71,71,71,71	0
55	MG	DA	1712	1/1	0.83	0.33	98,98,98,98	0
55	MG	CA	3175	1/1	0.83	0.43	64,64,64,64	0
56	OHX	CA	3432	7/7	0.83	0.08	119,135,143,173	1
56	OHX	CA	3435	7/7	0.83	0.13	105,108,131,192	1
55	MG	AA	3139	1/1	0.83	0.30	48,48,48,48	0
55	MG	CA	3268	1/1	0.83	0.16	52,52,52,52	0
56	OHX	C3	101	7/7	0.83	0.10	119,129,151,179	2
55	MG	AA	3072	1/1	0.83	0.21	65,65,65,65	0
55	MG	AA	3015	1/1	0.83	0.26	76,76,76,76	0
56	OHX	DA	1774	7/7	0.83	0.12	131,135,155,208	1
56	OHX	DA	1782	7/7	0.83	0.08	117,128,138,207	1
55	MG	BA	1625	1/1	0.83	0.32	65,65,65,65	0
55	MG	BA	1710	1/1	0.83	0.24	97,97,97,97	0
55	MG	AA	3110	1/1	0.83	0.39	48,48,48,48	0
55	MG	AE	301	1/1	0.83	0.32	52,52,52,52	0
55	MG	CA	3214	1/1	0.84	0.22	65,65,65,65	0
55	MG	AA	3217	1/1	0.84	0.23	60,60,60,60	0
55	MG	CA	3053	1/1	0.84	0.13	99,99,99,99	0
56	OHX	CA	3250	7/7	0.84	0.13	106,109,126,164	1
55	MG	CA	3477	1/1	0.84	0.28	60,60,60,60	0
56	OHX	CA	3399	7/7	0.84	0.13	97,104,115,165	2
55	MG	BA	1639	1/1	0.84	0.10	102,102,102,102	0
55	MG	AA	3021	1/1	0.84	0.31	80,80,80,80	0
55	MG	CA	3222	1/1	0.84	0.20	81,81,81,81	0
55	MG	CA	3195	1/1	0.84	0.18	68,68,68,68	0
55	MG	CA	3101	1/1	0.84	0.30	59,59,59,59	0
55	MG	AA	3379	1/1	0.84	0.36	55,55,55,55	0
55	MG	DA	1701	1/1	0.84	0.36	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3262	1/1	0.84	0.43	74,74,74,74	0
56	OHX	CA	3486	7/7	0.84	0.13	87,109,129,181	2
56	OHX	CB	216	7/7	0.84	0.10	117,132,146,206	1
55	MG	DA	1656	1/1	0.84	0.28	68,68,68,68	0
55	MG	CA	3064	1/1	0.84	0.12	89,89,89,89	0
55	MG	AA	3083	1/1	0.84	0.15	88,88,88,88	0
56	OHX	AA	3564	7/7	0.84	0.07	102,105,128,167	1
55	MG	CA	3171	1/1	0.84	0.21	82,82,82,82	0
55	MG	AA	3014	1/1	0.84	0.34	44,44,44,44	0
55	MG	BA	1647	1/1	0.84	0.18	112,112,112,112	0
55	MG	CA	3178	1/1	0.84	0.19	52,52,52,52	0
55	MG	BA	1715	1/1	0.84	0.26	74,74,74,74	0
55	MG	AA	3052	1/1	0.84	0.24	85,85,85,85	0
55	MG	AA	3107	1/1	0.85	0.11	79,79,79,79	0
55	MG	DA	1607	1/1	0.85	0.23	82,82,82,82	0
55	MG	CA	3072	1/1	0.85	0.38	43,43,43,43	0
55	MG	AA	3091	1/1	0.85	0.20	77,77,77,77	0
55	MG	CA	3078	1/1	0.85	0.39	76,76,76,76	0
55	MG	CA	3218	1/1	0.85	0.27	83,83,83,83	0
55	MG	AA	3270	1/1	0.85	0.09	94,94,94,94	0
55	MG	CA	3221	1/1	0.85	0.31	69,69,69,69	0
55	MG	AA	3163	1/1	0.85	0.21	61,61,61,61	0
55	MG	CA	3177	1/1	0.85	0.21	57,57,57,57	0
55	MG	DA	1686	1/1	0.85	0.14	73,73,73,73	0
55	MG	DA	1687	1/1	0.85	0.16	63,63,63,63	0
55	MG	BA	1723	1/1	0.85	0.20	82,82,82,82	0
55	MG	AA	3102	1/1	0.85	0.26	79,79,79,79	0
55	MG	BA	1628	1/1	0.85	0.28	80,80,80,80	0
56	OHX	BA	1695	7/7	0.85	0.07	129,147,158,217	1
56	OHX	BA	1806	7/7	0.85	0.14	97,127,142,180	2
55	MG	BA	1660	1/1	0.85	0.20	97,97,97,97	0
55	MG	AA	3382	1/1	0.85	0.27	36,36,36,36	0
55	MG	DA	1632	1/1	0.85	0.20	83,83,83,83	0
55	MG	DA	1703	1/1	0.85	0.29	73,73,73,73	0
55	MG	DA	1633	1/1	0.85	0.32	74,74,74,74	0
56	OHX	CA	3413	7/7	0.85	0.10	121,130,144,215	1
56	OHX	CA	3414	7/7	0.85	0.09	155,156,163,215	1
55	MG	AA	3211	1/1	0.85	0.37	62,62,62,62	0
55	MG	CA	3041	1/1	0.85	0.15	73,73,73,73	0
55	MG	AA	3005	1/1	0.85	0.30	43,43,43,43	0
56	OHX	CA	3422	7/7	0.85	0.09	126,137,143,193	1
55	MG	DA	1640	1/1	0.85	0.20	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	1713	1/1	0.85	0.29	79,79,79,79	0
55	MG	AA	3281	1/1	0.85	0.38	70,70,70,70	0
55	MG	BA	1708	1/1	0.85	0.28	77,77,77,77	0
55	MG	CA	3449	1/1	0.85	0.32	54,54,54,54	0
55	MG	AA	3106	1/1	0.85	0.24	70,70,70,70	0
56	OHX	CA	3491	7/7	0.85	0.11	92,108,117,175	1
55	MG	AB	202	1/1	0.85	0.13	72,72,72,72	0
55	MG	CA	3054	1/1	0.85	0.19	54,54,54,54	0
56	OHX	CB	219	7/7	0.85	0.08	145,151,161,232	1
55	MG	DA	1650	1/1	0.85	0.24	67,67,67,67	0
55	MG	CA	3056	1/1	0.85	0.28	79,79,79,79	0
55	MG	BA	1711	1/1	0.85	0.29	94,94,94,94	0
56	OHX	AA	3369	7/7	0.85	0.14	80,102,119,165	1
56	OHX	AA	3513	7/7	0.85	0.09	80,88,116,153	1
56	OHX	DA	1783	7/7	0.85	0.09	123,123,145,185	1
55	MG	BS	101	1/1	0.85	0.20	93,93,93,93	0
56	OHX	DA	1805	7/7	0.85	0.07	155,158,165,245	1
56	OHX	DA	1809	7/7	0.85	0.07	124,126,139,221	1
56	OHX	DR	101	7/7	0.85	0.07	135,141,146,189	1
55	MG	AA	3221	1/1	0.85	0.14	68,68,68,68	0
55	MG	BB	105	1/1	0.85	0.40	63,63,63,63	0
56	OHX	AA	3530	7/7	0.85	0.12	101,121,143,206	1
56	OHX	BA	1674	7/7	0.86	0.09	117,122,137,199	1
56	OHX	BA	1675	7/7	0.86	0.09	120,128,140,197	1
55	MG	AA	3166	1/1	0.86	0.25	66,66,66,66	0
55	MG	AA	3034	1/1	0.86	0.28	56,56,56,56	0
55	MG	BA	1741	1/1	0.86	0.38	73,73,73,73	0
55	MG	DA	1707	1/1	0.86	0.26	85,85,85,85	0
56	OHX	BA	1790	7/7	0.86	0.11	96,123,133,185	1
55	MG	CA	3071	1/1	0.86	0.26	51,51,51,51	0
55	MG	AA	3080	1/1	0.86	0.33	55,55,55,55	0
55	MG	AA	3216	1/1	0.86	0.28	71,71,71,71	0
55	MG	CA	3479	1/1	0.86	0.33	64,64,64,64	0
56	OHX	CA	3252	7/7	0.86	0.13	108,118,136,203	1
56	OHX	CA	3371	7/7	0.86	0.14	67,90,123,162	1
55	MG	AA	3053	1/1	0.86	0.25	60,60,60,60	0
55	MG	AA	3378	1/1	0.86	0.26	47,47,47,47	0
56	OHX	CA	3409	7/7	0.86	0.11	97,100,119,183	1
55	MG	DA	1716	1/1	0.86	0.26	85,85,85,85	0
55	MG	BA	1649	1/1	0.86	0.14	74,74,74,74	0
56	OHX	CA	3415	7/7	0.86	0.10	134,135,143,187	1
55	MG	DA	1658	1/1	0.86	0.30	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	DA	1601	1/1	0.86	0.25	87,87,87,87	0
55	MG	DB	101	1/1	0.86	0.32	78,78,78,78	0
55	MG	CA	3082	1/1	0.86	0.34	62,62,62,62	0
55	MG	CA	3084	1/1	0.86	0.39	60,60,60,60	0
55	MG	AA	3068	1/1	0.86	0.21	61,61,61,61	0
55	MG	DA	1614	1/1	0.86	0.17	91,91,91,91	0
56	OHX	AA	3333	7/7	0.86	0.12	91,114,128,179	2
55	MG	BA	1753	1/1	0.86	0.24	67,67,67,67	0
55	MG	CA	3176	1/1	0.86	0.44	67,67,67,67	0
56	OHX	CA	3487	7/7	0.86	0.08	135,139,147,210	1
55	MG	BA	1721	1/1	0.86	0.25	70,70,70,70	0
55	MG	AE	302	1/1	0.86	0.23	71,71,71,71	0
55	MG	BB	102	1/1	0.86	0.19	85,85,85,85	0
55	MG	AA	3199	1/1	0.86	0.34	76,76,76,76	0
55	MG	CA	3230	1/1	0.86	0.28	79,79,79,79	0
55	MG	AA	3206	1/1	0.86	0.33	64,64,64,64	0
55	MG	DA	1684	1/1	0.86	0.29	79,79,79,79	0
55	MG	CA	3188	1/1	0.86	0.33	60,60,60,60	0
55	MG	CA	3109	1/1	0.86	0.22	56,56,56,56	0
55	MG	BA	1618	1/1	0.86	0.27	63,63,63,63	0
55	MG	BA	1727	1/1	0.86	0.30	70,70,70,70	0
55	MG	CA	3118	1/1	0.86	0.26	69,69,69,69	0
55	MG	DA	1697	1/1	0.86	0.25	72,72,72,72	0
55	MG	CA	3124	1/1	0.86	0.29	44,44,44,44	0
56	OHX	BA	1666	7/7	0.86	0.09	117,122,134,158	2
55	MG	CA	3059	1/1	0.86	0.32	63,63,63,63	0
55	MG	CA	3014	1/1	0.86	0.23	76,76,76,76	0
55	MG	CA	3439	1/1	0.87	0.32	63,63,63,63	0
55	MG	DA	1670	1/1	0.87	0.24	64,64,64,64	0
55	MG	BA	1617	1/1	0.87	0.25	71,71,71,71	0
55	MG	BA	1698	1/1	0.87	0.31	62,62,62,62	0
55	MG	AA	3164	1/1	0.87	0.17	70,70,70,70	0
55	MG	CA	3125	1/1	0.87	0.16	52,52,52,52	0
55	MG	DA	1628	1/1	0.87	0.32	78,78,78,78	0
56	OHX	CA	3348	7/7	0.87	0.15	104,111,132,178	1
55	MG	DA	1677	1/1	0.87	0.24	76,76,76,76	0
56	OHX	CA	3379	7/7	0.87	0.07	134,137,155,207	1
56	OHX	AA	3331	7/7	0.87	0.14	72,87,130,163	3
56	OHX	CA	3397	7/7	0.87	0.07	128,138,154,219	1
55	MG	AB	205	1/1	0.87	0.17	50,50,50,50	0
55	MG	CA	3456	1/1	0.87	0.23	66,66,66,66	0
56	OHX	AA	3403	7/7	0.87	0.10	109,110,128,178	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	AA	3488	7/7	0.87	0.10	86,101,105,150	1
56	OHX	AA	3510	7/7	0.87	0.12	92,103,113,152	2
56	OHX	AA	3512	7/7	0.87	0.11	99,114,126,166	2
55	MG	CA	3179	1/1	0.87	0.10	73,73,73,73	0
55	MG	AA	3126	1/1	0.87	0.21	85,85,85,85	0
55	MG	CA	3050	1/1	0.87	0.24	65,65,65,65	0
55	MG	CA	3471	1/1	0.87	0.30	57,57,57,57	0
55	MG	CA	3140	1/1	0.87	0.27	59,59,59,59	0
56	OHX	AA	3532	7/7	0.87	0.08	89,105,116,172	1
56	OHX	CA	3434	7/7	0.87	0.10	96,110,126,177	1
55	MG	AA	3084	1/1	0.87	0.23	58,58,58,58	0
56	OHX	CA	3436	7/7	0.87	0.08	115,121,137,192	1
55	MG	CA	3189	1/1	0.87	0.33	67,67,67,67	0
55	MG	AA	3220	1/1	0.87	0.25	64,64,64,64	0
55	MG	CA	3029	1/1	0.87	0.20	76,76,76,76	0
55	MG	CA	3033	1/1	0.87	0.15	71,71,71,71	0
55	MG	AA	3049	1/1	0.87	0.27	64,64,64,64	0
56	OHX	CB	217	7/7	0.87	0.08	128,135,146,182	1
55	MG	DA	1603	1/1	0.87	0.39	71,71,71,71	0
55	MG	CA	3151	1/1	0.87	0.22	76,76,76,76	0
55	MG	DA	1608	1/1	0.87	0.19	78,78,78,78	0
56	OHX	AA	3566	7/7	0.87	0.09	92,97,126,175	2
56	OHX	AB	216	7/7	0.87	0.12	88,124,141,184	1
55	MG	DA	1655	1/1	0.87	0.24	78,78,78,78	0
56	OHX	BA	1661	7/7	0.87	0.09	108,124,128,170	1
55	MG	CA	3231	1/1	0.87	0.27	89,89,89,89	0
55	MG	DA	1709	1/1	0.87	0.36	80,80,80,80	0
56	OHX	DA	1801	7/7	0.87	0.08	141,143,154,216	1
55	MG	DA	1611	1/1	0.87	0.19	92,92,92,92	0
56	OHX	DA	1808	7/7	0.87	0.10	119,124,131,178	1
55	MG	A3	101	1/1	0.87	0.31	60,60,60,60	0
56	OHX	DK	201	7/7	0.87	0.08	137,138,149,200	1
55	MG	CA	3036	1/1	0.87	0.22	87,87,87,87	0
55	MG	AA	3115	1/1	0.87	0.20	51,51,51,51	0
55	MG	AA	3048	1/1	0.87	0.34	94,94,94,94	0
55	MG	BA	1734	1/1	0.87	0.32	70,70,70,70	0
55	MG	DC	102	1/1	0.88	0.42	69,69,69,69	0
55	MG	AA	3013	1/1	0.88	0.22	41,41,41,41	0
55	MG	BA	1608	1/1	0.88	0.23	55,55,55,55	0
56	OHX	CA	3284	7/7	0.88	0.09	136,147,155,216	1
55	MG	D1	101	1/1	0.88	0.29	78,78,78,78	0
55	MG	AA	3392	1/1	0.88	0.35	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	CA	3038	1/1	0.88	0.16	74,74,74,74	0
55	MG	DA	1620	1/1	0.88	0.31	79,79,79,79	0
55	MG	CA	3185	1/1	0.88	0.40	75,75,75,75	0
55	MG	AA	3038	1/1	0.88	0.16	46,46,46,46	0
55	MG	BA	1650	1/1	0.88	0.35	72,72,72,72	0
55	MG	AA	3224	1/1	0.88	0.22	68,68,68,68	0
55	MG	AA	3226	1/1	0.88	0.28	42,42,42,42	0
55	MG	DA	1683	1/1	0.88	0.37	71,71,71,71	0
56	OHX	CA	3417	7/7	0.88	0.07	151,167,187,222	1
55	MG	AA	3151	1/1	0.88	0.21	62,62,62,62	0
56	OHX	AA	3524	7/7	0.88	0.07	111,120,128,172	1
55	MG	AA	3193	1/1	0.88	0.08	58,58,58,58	0
55	MG	AA	3040	1/1	0.88	0.27	47,47,47,47	0
56	OHX	CA	3426	7/7	0.88	0.06	142,146,155,215	1
55	MG	AA	3044	1/1	0.88	0.33	72,72,72,72	0
55	MG	AA	3057	1/1	0.88	0.29	72,72,72,72	0
56	OHX	CA	3431	7/7	0.88	0.08	105,117,132,179	1
55	MG	DA	1695	1/1	0.88	0.31	76,76,76,76	0
55	MG	AA	3119	1/1	0.88	0.28	64,64,64,64	0
55	MG	AF	302	1/1	0.88	0.24	81,81,81,81	0
55	MG	AA	3036	1/1	0.88	0.27	36,36,36,36	0
56	OHX	AA	3554	7/7	0.88	0.07	116,128,150,205	1
55	MG	AO	203	1/1	0.88	0.19	56,56,56,56	0
55	MG	A1	201	1/1	0.88	0.31	71,71,71,71	0
55	MG	CA	3476	1/1	0.88	0.27	52,52,52,52	0
55	MG	AA	3353	1/1	0.88	0.21	39,39,39,39	0
55	MG	BD	101	1/1	0.88	0.24	93,93,93,93	0
56	OHX	AA	3567	7/7	0.88	0.08	103,106,118,172	1
55	MG	CA	3002	1/1	0.88	0.31	50,50,50,50	0
56	OHX	A1	203	7/7	0.88	0.11	100,107,140,182	3
55	MG	CA	3480	1/1	0.88	0.17	72,72,72,72	0
55	MG	DA	1648	1/1	0.88	0.08	91,91,91,91	0
55	MG	CA	3066	1/1	0.88	0.38	56,56,56,56	0
55	MG	CB	205	1/1	0.88	0.33	74,74,74,74	0
55	MG	CA	3008	1/1	0.88	0.24	52,52,52,52	0
55	MG	AA	3046	1/1	0.88	0.25	68,68,68,68	0
55	MG	AA	3256	1/1	0.88	0.33	53,53,53,53	0
55	MG	BA	1603	1/1	0.88	0.20	63,63,63,63	0
55	MG	AA	3128	1/1	0.88	0.23	54,54,54,54	0
55	MG	AA	3381	1/1	0.88	0.27	59,59,59,59	0
56	OHX	DA	1810	7/7	0.88	0.05	134,135,143,197	1
56	OHX	DG	302	7/7	0.88	0.07	133,142,147,197	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3030	1/1	0.88	0.22	89,89,89,89	0
55	MG	BA	1643	1/1	0.88	0.11	78,78,78,78	0
55	MG	DA	1665	1/1	0.88	0.28	70,70,70,70	0
56	OHX	BA	1816	7/7	0.88	0.09	127,130,142,194	1
55	MG	AA	3171	1/1	0.88	0.20	48,48,48,48	0
55	MG	AA	3201	1/1	0.89	0.22	45,45,45,45	0
55	MG	CA	3153	1/1	0.89	0.23	56,56,56,56	0
55	MG	CA	3155	1/1	0.89	0.20	58,58,58,58	0
55	MG	BA	1742	1/1	0.89	0.37	86,86,86,86	0
56	OHX	AA	3138	7/7	0.89	0.12	88,92,127,173	1
56	OHX	CA	3269	7/7	0.89	0.14	98,100,123,153	2
56	OHX	AA	3302	7/7	0.89	0.10	88,114,124,193	1
56	OHX	AA	3306	7/7	0.89	0.08	134,139,151,214	1
56	OHX	CA	3358	7/7	0.89	0.07	128,130,147,230	1
55	MG	DA	1669	1/1	0.89	0.34	64,64,64,64	0
56	OHX	CA	3378	7/7	0.89	0.09	128,141,148,178	1
55	MG	AA	3070	1/1	0.89	0.13	52,52,52,52	0
56	OHX	AA	3366	7/7	0.89	0.13	85,90,106,173	1
55	MG	AA	3279	1/1	0.89	0.26	81,81,81,81	0
56	OHX	AA	3370	7/7	0.89	0.10	115,126,140,200	1
56	OHX	CA	3407	7/7	0.89	0.08	142,149,155,227	1
55	MG	AA	3175	1/1	0.89	0.28	39,39,39,39	0
55	MG	AA	3250	1/1	0.89	0.35	56,56,56,56	0
56	OHX	AA	3490	7/7	0.89	0.07	94,113,129,158	1
55	MG	BA	1645	1/1	0.89	0.34	51,51,51,51	0
55	MG	AA	3117	1/1	0.89	0.18	48,48,48,48	0
55	MG	DA	1616	1/1	0.89	0.24	88,88,88,88	0
55	MG	BA	1713	1/1	0.89	0.15	59,59,59,59	0
55	MG	CA	3087	1/1	0.89	0.06	70,70,70,70	0
55	MG	BA	1714	1/1	0.89	0.19	56,56,56,56	0
55	MG	BA	1627	1/1	0.89	0.30	80,80,80,80	0
55	MG	CA	3258	1/1	0.89	0.33	56,56,56,56	0
55	MG	BB	101	1/1	0.89	0.34	70,70,70,70	0
55	MG	AA	3020	1/1	0.89	0.39	44,44,44,44	0
55	MG	BB	103	1/1	0.89	0.28	91,91,91,91	0
55	MG	AA	3157	1/1	0.89	0.36	49,49,49,49	0
56	OHX	AA	3539	7/7	0.89	0.07	116,125,136,193	1
56	OHX	AA	3540	7/7	0.89	0.08	109,134,164,188	2
55	MG	AA	3167	1/1	0.89	0.32	53,53,53,53	0
55	MG	CA	3051	1/1	0.89	0.33	69,69,69,69	0
55	MG	CA	3052	1/1	0.89	0.28	66,66,66,66	0
55	MG	BA	1651	1/1	0.89	0.10	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	CB	214	7/7	0.89	0.09	129,139,146,186	1
55	MG	CA	3443	1/1	0.89	0.38	49,49,49,49	0
55	MG	CA	3446	1/1	0.89	0.35	47,47,47,47	0
55	MG	BA	1652	1/1	0.89	0.21	63,63,63,63	0
55	MG	BA	1658	1/1	0.89	0.26	71,71,71,71	0
55	MG	CA	3454	1/1	0.89	0.31	51,51,51,51	0
55	MG	CA	3131	1/1	0.89	0.28	65,65,65,65	0
56	OHX	AB	218	7/7	0.89	0.07	128,132,146,199	1
55	MG	AA	3064	1/1	0.89	0.12	66,66,66,66	0
56	OHX	DA	1775	7/7	0.89	0.08	133,145,148,215	1
55	MG	CA	3003	1/1	0.89	0.22	51,51,51,51	0
55	MG	CA	3005	1/1	0.89	0.16	48,48,48,48	0
56	OHX	DA	1786	7/7	0.89	0.08	143,151,161,223	1
56	OHX	DA	1787	7/7	0.89	0.09	95,113,121,162	2
55	MG	AA	3244	1/1	0.89	0.22	49,49,49,49	0
56	OHX	DA	1796	7/7	0.89	0.07	134,139,149,195	1
55	MG	BA	1613	1/1	0.89	0.17	65,65,65,65	0
56	OHX	DA	1803	7/7	0.89	0.07	135,141,144,207	1
55	MG	CA	3204	1/1	0.89	0.29	73,73,73,73	0
55	MG	CA	3205	1/1	0.89	0.17	63,63,63,63	0
55	MG	BA	1702	1/1	0.89	0.17	62,62,62,62	0
55	MG	BA	1614	1/1	0.89	0.25	73,73,73,73	0
56	OHX	DA	1812	7/7	0.89	0.08	149,158,168,252	1
55	MG	BA	1739	1/1	0.89	0.32	70,70,70,70	0
56	OHX	BA	1690	7/7	0.89	0.08	118,127,134,188	1
55	MG	CB	201	1/1	0.89	0.13	77,77,77,77	0
55	MG	CB	202	1/1	0.89	0.15	99,99,99,99	0
55	MG	CA	3211	1/1	0.89	0.12	116,116,116,116	0
55	MG	CA	3212	1/1	0.89	0.30	75,75,75,75	0
55	MG	DA	1711	1/1	0.90	0.15	107,107,107,107	0
55	MG	AA	3071	1/1	0.90	0.34	68,68,68,68	0
55	MG	CA	3260	1/1	0.90	0.22	71,71,71,71	0
56	OHX	BA	1783	7/7	0.90	0.14	77,87,125,141	2
55	MG	AA	3383	1/1	0.90	0.23	46,46,46,46	0
56	OHX	BA	1805	7/7	0.90	0.11	90,105,122,143	3
55	MG	AA	3386	1/1	0.90	0.14	42,42,42,42	0
55	MG	AA	3122	1/1	0.90	0.23	62,62,62,62	0
55	MG	CA	3165	1/1	0.90	0.26	57,57,57,57	0
55	MG	DA	1636	1/1	0.90	0.20	75,75,75,75	0
55	MG	AA	3261	1/1	0.90	0.37	64,64,64,64	0
55	MG	AA	3267	1/1	0.90	0.32	80,80,80,80	0
55	MG	AA	3123	1/1	0.90	0.18	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3409	1/1	0.90	0.30	56,56,56,56	0
56	OHX	CA	3306	7/7	0.90	0.09	98,106,119,148	1
55	MG	AA	3103	1/1	0.90	0.08	97,97,97,97	0
55	MG	AA	3060	1/1	0.90	0.13	70,70,70,70	0
55	MG	DA	1645	1/1	0.90	0.26	91,91,91,91	0
55	MG	DC	105	1/1	0.90	0.37	54,54,54,54	0
55	MG	AA	3274	1/1	0.90	0.28	89,89,89,89	0
56	OHX	CA	3380	7/7	0.90	0.07	106,119,130,170	1
55	MG	AA	3149	1/1	0.90	0.15	74,74,74,74	0
55	MG	AA	3073	1/1	0.90	0.19	69,69,69,69	0
55	MG	AA	3229	1/1	0.90	0.28	59,59,59,59	0
55	MG	AA	3061	1/1	0.90	0.22	49,49,49,49	0
55	MG	BA	1716	1/1	0.90	0.21	55,55,55,55	0
56	OHX	CA	3411	7/7	0.90	0.07	117,123,138,184	1
56	OHX	AA	3365	7/7	0.90	0.14	90,106,114,161	2
55	MG	CA	3083	1/1	0.90	0.27	44,44,44,44	0
55	MG	CA	3459	1/1	0.90	0.17	56,56,56,56	0
55	MG	AF	301	1/1	0.90	0.23	83,83,83,83	0
55	MG	CA	3018	1/1	0.90	0.35	55,55,55,55	0
56	OHX	AA	3407	7/7	0.90	0.10	108,117,126,165	1
56	OHX	AA	3484	7/7	0.90	0.11	76,100,111,147	2
55	MG	CA	3021	1/1	0.90	0.12	60,60,60,60	0
55	MG	AA	3155	1/1	0.90	0.11	85,85,85,85	0
55	MG	DA	1663	1/1	0.90	0.20	66,66,66,66	0
55	MG	CA	3026	1/1	0.90	0.10	58,58,58,58	0
55	MG	AA	3023	1/1	0.90	0.24	52,52,52,52	0
56	OHX	AA	3519	7/7	0.90	0.08	140,146,150,214	1
56	OHX	CA	3433	7/7	0.90	0.07	121,129,144,183	1
55	MG	AO	202	1/1	0.90	0.25	55,55,55,55	0
55	MG	CA	3096	1/1	0.90	0.19	64,64,64,64	0
55	MG	CA	3097	1/1	0.90	0.26	67,67,67,67	0
56	OHX	CA	3437	7/7	0.90	0.10	98,105,117,166	2
56	OHX	CA	3466	7/7	0.90	0.12	96,98,116,157	1
56	OHX	CA	3467	7/7	0.90	0.11	131,146,152,199	1
55	MG	CB	203	1/1	0.90	0.10	111,111,111,111	0
55	MG	CA	3100	1/1	0.90	0.36	63,63,63,63	0
55	MG	AA	3284	1/1	0.90	0.11	66,66,66,66	0
55	MG	AA	3063	1/1	0.90	0.20	76,76,76,76	0
56	OHX	CB	213	7/7	0.90	0.08	131,144,166,188	1
55	MG	CA	3031	1/1	0.90	0.08	53,53,53,53	0
56	OHX	CB	215	7/7	0.90	0.08	108,133,144,220	1
55	MG	BA	1642	1/1	0.90	0.10	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	AA	3537	7/7	0.90	0.07	171,189,202,242	1
55	MG	DA	1679	1/1	0.90	0.17	69,69,69,69	0
55	MG	AA	3345	1/1	0.90	0.49	47,47,47,47	0
55	MG	CA	3208	1/1	0.90	0.30	70,70,70,70	0
55	MG	AA	3158	1/1	0.90	0.27	50,50,50,50	0
55	MG	CA	3119	1/1	0.90	0.19	61,61,61,61	0
55	MG	AA	3348	1/1	0.90	0.36	46,46,46,46	0
56	OHX	AA	3560	7/7	0.90	0.07	102,104,127,184	1
55	MG	BA	1730	1/1	0.90	0.30	73,73,73,73	0
55	MG	AA	3069	1/1	0.90	0.26	62,62,62,62	0
56	OHX	DA	1785	7/7	0.90	0.09	110,114,129,164	1
55	MG	DA	1692	1/1	0.90	0.30	70,70,70,70	0
55	MG	DA	1615	1/1	0.90	0.15	98,98,98,98	0
55	MG	BA	1735	1/1	0.90	0.15	48,48,48,48	0
56	OHX	AA	3568	7/7	0.90	0.09	78,93,100,118	1
56	OHX	AB	210	7/7	0.90	0.10	83,107,129,146	3
55	MG	BA	1737	1/1	0.90	0.19	46,46,46,46	0
55	MG	AA	3246	1/1	0.90	0.22	36,36,36,36	0
56	OHX	DA	1807	7/7	0.90	0.07	117,126,135,195	1
55	MG	AA	3162	1/1	0.90	0.34	38,38,38,38	0
55	MG	AA	3136	1/1	0.90	0.16	57,57,57,57	0
55	MG	AA	3041	1/1	0.90	0.16	49,49,49,49	0
55	MG	CA	3143	1/1	0.90	0.24	60,60,60,60	0
55	MG	AA	3212	1/1	0.90	0.24	35,35,35,35	0
55	MG	DA	1625	1/1	0.90	0.13	97,97,97,97	0
55	MG	AA	3380	1/1	0.90	0.22	66,66,66,66	0
55	MG	BA	1653	1/1	0.90	0.18	63,63,63,63	0
55	MG	AA	3255	1/1	0.90	0.16	64,64,64,64	0
55	MG	BA	1750	1/1	0.90	0.25	72,72,72,72	0
55	MG	CA	3167	1/1	0.91	0.30	75,75,75,75	0
56	OHX	CA	3375	7/7	0.91	0.10	103,118,131,145	1
56	OHX	AA	3505	7/7	0.91	0.12	86,108,110,156	1
55	MG	CA	3224	1/1	0.91	0.25	77,77,77,77	0
55	MG	AA	3077	1/1	0.91	0.23	73,73,73,73	0
56	OHX	CA	3390	7/7	0.91	0.07	117,128,152,209	1
56	OHX	CA	3393	7/7	0.91	0.12	93,114,121,181	1
55	MG	AA	3114	1/1	0.91	0.22	47,47,47,47	0
56	OHX	AA	3515	7/7	0.91	0.08	100,121,139,211	1
55	MG	CA	3228	1/1	0.91	0.10	65,65,65,65	0
56	OHX	CA	3404	7/7	0.91	0.09	149,155,166,217	1
55	MG	AA	3127	1/1	0.91	0.27	57,57,57,57	0
55	MG	AA	3413	1/1	0.91	0.22	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3257	1/1	0.91	0.22	60,60,60,60	0
55	MG	CA	3001	1/1	0.91	0.18	46,46,46,46	0
55	MG	AA	3414	1/1	0.91	0.24	57,57,57,57	0
55	MG	AA	3416	1/1	0.91	0.26	74,74,74,74	0
55	MG	AA	3264	1/1	0.91	0.26	76,76,76,76	0
55	MG	CA	3182	1/1	0.91	0.34	59,59,59,59	0
55	MG	AA	3349	1/1	0.91	0.34	61,61,61,61	0
55	MG	CA	3102	1/1	0.91	0.31	67,67,67,67	0
55	MG	CA	3009	1/1	0.91	0.24	39,39,39,39	0
55	MG	CA	3186	1/1	0.91	0.17	75,75,75,75	0
56	OHX	AA	3542	7/7	0.91	0.08	118,127,135,189	1
55	MG	CA	3013	1/1	0.91	0.16	47,47,47,47	0
55	MG	DA	1704	1/1	0.91	0.32	73,73,73,73	0
55	MG	CA	3110	1/1	0.91	0.40	85,85,85,85	0
55	MG	AA	3266	1/1	0.91	0.12	78,78,78,78	0
55	MG	CA	3055	1/1	0.91	0.18	66,66,66,66	0
55	MG	CA	3015	1/1	0.91	0.21	54,54,54,54	0
55	MG	AA	3174	1/1	0.91	0.31	76,76,76,76	0
55	MG	CA	3121	1/1	0.91	0.29	55,55,55,55	0
55	MG	AA	3143	1/1	0.91	0.30	46,46,46,46	0
55	MG	AA	3241	1/1	0.91	0.23	60,60,60,60	0
55	MG	CA	3061	1/1	0.91	0.31	64,64,64,64	0
56	OHX	AA	3569	7/7	0.91	0.07	116,117,125,191	1
55	MG	CA	3025	1/1	0.91	0.12	83,83,83,83	0
55	MG	AA	3051	1/1	0.91	0.17	49,49,49,49	0
55	MG	AA	3056	1/1	0.91	0.17	36,36,36,36	0
55	MG	CA	3203	1/1	0.91	0.22	47,47,47,47	0
55	MG	CA	3137	1/1	0.91	0.34	74,74,74,74	0
55	MG	AA	3027	1/1	0.91	0.21	42,42,42,42	0
56	OHX	BA	1662	7/7	0.91	0.08	105,117,141,193	1
56	OHX	BA	1664	7/7	0.91	0.07	108,126,142,197	1
55	MG	DA	1654	1/1	0.91	0.26	61,61,61,61	0
55	MG	CA	3067	1/1	0.91	0.27	49,49,49,49	0
55	MG	CA	3069	1/1	0.91	0.38	69,69,69,69	0
56	OHX	BA	1673	7/7	0.91	0.08	117,123,127,191	1
55	MG	AA	3120	1/1	0.91	0.15	71,71,71,71	0
55	MG	AA	3092	1/1	0.91	0.04	73,73,73,73	0
55	MG	CA	3074	1/1	0.91	0.36	64,64,64,64	0
55	MG	BA	1754	1/1	0.91	0.31	61,61,61,61	0
56	OHX	DA	1784	7/7	0.91	0.07	150,153,166,225	1
55	MG	DC	106	1/1	0.91	0.42	91,91,91,91	0
55	MG	CA	3032	1/1	0.91	0.33	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	1623	1/1	0.91	0.20	67,67,67,67	0
55	MG	BA	1624	1/1	0.91	0.20	70,70,70,70	0
55	MG	C0	201	1/1	0.91	0.16	61,61,61,61	0
56	OHX	DA	1798	7/7	0.91	0.07	128,133,140,212	1
55	MG	DA	1667	1/1	0.91	0.33	68,68,68,68	0
55	MG	AA	3249	1/1	0.91	0.31	58,58,58,58	0
55	MG	DA	1602	1/1	0.91	0.24	68,68,68,68	0
55	MG	CA	3159	1/1	0.91	0.28	75,75,75,75	0
55	MG	DA	1604	1/1	0.91	0.28	82,82,82,82	0
56	OHX	CA	3245	7/7	0.91	0.09	99,120,129,189	1
55	MG	AA	3109	1/1	0.91	0.35	47,47,47,47	0
55	MG	CA	3219	1/1	0.91	0.46	79,79,79,79	0
56	OHX	AA	3406	7/7	0.91	0.13	84,92,109,162	1
55	MG	AA	3203	1/1	0.91	0.19	50,50,50,50	0
56	OHX	CA	3304	7/7	0.91	0.09	113,122,141,181	2
55	MG	AA	3227	1/1	0.91	0.27	63,63,63,63	0
56	OHX	AA	3487	7/7	0.91	0.07	95,110,116,167	1
55	MG	CA	3166	1/1	0.91	0.35	58,58,58,58	0
56	OHX	CA	3373	7/7	0.92	0.09	113,122,129,160	1
56	OHX	AA	3533	7/7	0.92	0.10	98,103,114,150	2
55	MG	AA	3161	1/1	0.92	0.20	50,50,50,50	0
55	MG	AA	3357	1/1	0.92	0.38	73,73,73,73	0
55	MG	CA	3099	1/1	0.92	0.25	51,51,51,51	0
56	OHX	CA	3383	7/7	0.92	0.07	111,116,132,194	1
56	OHX	CA	3386	7/7	0.92	0.08	110,116,134,181	1
55	MG	BA	1736	1/1	0.92	0.42	64,64,64,64	0
56	OHX	CA	3392	7/7	0.92	0.08	126,132,142,192	1
55	MG	CA	3010	1/1	0.92	0.14	47,47,47,47	0
56	OHX	CA	3395	7/7	0.92	0.09	106,111,125,156	1
55	MG	CA	3011	1/1	0.92	0.23	46,46,46,46	0
56	OHX	AA	3541	7/7	0.92	0.09	102,114,134,158	2
55	MG	CA	3103	1/1	0.92	0.23	70,70,70,70	0
56	OHX	CA	3400	7/7	0.92	0.08	116,133,145,220	1
56	OHX	CA	3402	7/7	0.92	0.07	159,162,170,218	1
55	MG	AA	3118	1/1	0.92	0.20	53,53,53,53	0
56	OHX	AA	3546	7/7	0.92	0.09	98,103,119,179	1
56	OHX	CA	3408	7/7	0.92	0.05	136,139,143,209	1
56	OHX	AA	3551	7/7	0.92	0.06	141,143,149,194	1
55	MG	AA	3271	1/1	0.92	0.12	39,39,39,39	0
55	MG	AA	3272	1/1	0.92	0.27	50,50,50,50	0
55	MG	DA	1605	1/1	0.92	0.23	63,63,63,63	0
56	OHX	AA	3559	7/7	0.92	0.05	124,133,143,186	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3229	1/1	0.92	0.28	80,80,80,80	0
56	OHX	CA	3418	7/7	0.92	0.08	115,119,129,166	1
55	MG	AA	3097	1/1	0.92	0.10	59,59,59,59	0
55	MG	CA	3115	1/1	0.92	0.24	63,63,63,63	0
55	MG	AA	3090	1/1	0.92	0.14	85,85,85,85	0
55	MG	CA	3022	1/1	0.92	0.20	55,55,55,55	0
56	OHX	CA	3424	7/7	0.92	0.06	141,145,151,214	1
56	OHX	CA	3425	7/7	0.92	0.06	101,110,125,187	1
55	MG	AA	3078	1/1	0.92	0.25	59,59,59,59	0
55	MG	AA	3081	1/1	0.92	0.39	56,56,56,56	0
56	OHX	CA	3428	7/7	0.92	0.07	123,134,138,182	1
55	MG	AA	3390	1/1	0.92	0.28	46,46,46,46	0
55	MG	AA	3134	1/1	0.92	0.15	82,82,82,82	0
55	MG	AA	3168	1/1	0.92	0.26	89,89,89,89	0
55	MG	CA	3068	1/1	0.92	0.29	44,44,44,44	0
56	OHX	AO	205	7/7	0.92	0.08	83,89,107,180	1
55	MG	AA	3215	1/1	0.92	0.36	50,50,50,50	0
55	MG	AA	3135	1/1	0.92	0.20	67,67,67,67	0
55	MG	AA	3398	1/1	0.92	0.24	51,51,51,51	0
55	MG	AA	3283	1/1	0.92	0.25	55,55,55,55	0
55	MG	BA	1717	1/1	0.92	0.28	51,51,51,51	0
56	OHX	CA	3468	7/7	0.92	0.08	115,126,133,180	1
55	MG	CA	3077	1/1	0.92	0.16	57,57,57,57	0
55	MG	AA	3152	1/1	0.92	0.23	56,56,56,56	0
56	OHX	AA	3371	7/7	0.92	0.10	93,107,117,177	1
55	MG	CA	3452	1/1	0.92	0.13	51,51,51,51	0
56	OHX	AA	3404	7/7	0.92	0.10	74,98,116,164	1
55	MG	AA	3153	1/1	0.92	0.36	64,64,64,64	0
56	OHX	BA	1676	7/7	0.92	0.07	143,151,156,210	1
55	MG	CA	3080	1/1	0.92	0.10	57,57,57,57	0
56	OHX	BA	1678	7/7	0.92	0.07	115,118,134,165	1
56	OHX	BA	1680	7/7	0.92	0.07	120,125,145,238	1
55	MG	AA	3344	1/1	0.92	0.24	48,48,48,48	0
56	OHX	AA	3485	7/7	0.92	0.07	104,114,127,171	1
56	OHX	C5	102	7/7	0.92	0.07	114,118,133,165	1
55	MG	DA	1690	1/1	0.92	0.27	63,63,63,63	0
56	OHX	DA	1755	7/7	0.92	0.10	103,120,143,191	1
56	OHX	DA	1757	7/7	0.92	0.10	123,127,134,157	1
55	MG	AA	3124	1/1	0.92	0.25	70,70,70,70	0
55	MG	AA	3093	1/1	0.92	0.25	91,91,91,91	0
56	OHX	BA	1784	7/7	0.92	0.09	122,129,148,203	0
56	OHX	DA	1781	7/7	0.92	0.08	107,126,135,195	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	BA	1787	7/7	0.92	0.09	107,117,138,149	2
56	OHX	AA	3493	7/7	0.92	0.07	109,111,123,166	1
56	OHX	BA	1803	7/7	0.92	0.09	101,126,136,190	1
56	OHX	BA	1804	7/7	0.92	0.09	134,142,150,227	1
55	MG	BC	101	1/1	0.92	0.37	69,69,69,69	0
56	OHX	AA	3509	7/7	0.92	0.07	92,96,122,175	1
55	MG	AA	3177	1/1	0.92	0.23	37,37,37,37	0
55	MG	CA	3210	1/1	0.92	0.34	74,74,74,74	0
55	MG	CA	3475	1/1	0.92	0.17	55,55,55,55	0
56	OHX	DA	1799	7/7	0.92	0.06	122,127,139,209	1
55	MG	DA	1639	1/1	0.92	0.24	70,70,70,70	0
56	OHX	CA	3247	7/7	0.92	0.11	95,104,117,152	1
55	MG	CA	3157	1/1	0.92	0.32	76,76,76,76	0
55	MG	AA	3012	1/1	0.92	0.22	46,46,46,46	0
55	MG	CA	3162	1/1	0.92	0.33	65,65,65,65	0
55	MG	AA	3089	1/1	0.92	0.47	84,84,84,84	0
56	OHX	CA	3302	7/7	0.92	0.10	79,86,104,139	1
56	OHX	AA	3525	7/7	0.92	0.09	100,109,122,187	1
55	MG	BA	1621	1/1	0.92	0.27	55,55,55,55	0
56	OHX	CA	3340	7/7	0.92	0.09	115,122,140,168	1
56	OHX	AA	3527	7/7	0.92	0.06	130,134,147,188	1
56	OHX	DB	103	7/7	0.92	0.09	166,171,179,191	1
55	MG	AA	3142	1/1	0.92	0.41	45,45,45,45	0
56	OHX	CA	3359	7/7	0.92	0.07	115,123,136,171	2
55	MG	AA	3195	1/1	0.92	0.25	43,43,43,43	0
56	OHX	CA	3376	7/7	0.93	0.07	113,130,136,172	1
55	MG	CA	3017	1/1	0.93	0.16	92,92,92,92	0
55	MG	AA	3260	1/1	0.93	0.38	58,58,58,58	0
55	MG	BA	1740	1/1	0.93	0.35	61,61,61,61	0
56	OHX	CA	3382	7/7	0.93	0.07	129,131,148,199	1
55	MG	AA	3228	1/1	0.93	0.19	67,67,67,67	0
56	OHX	CA	3384	7/7	0.93	0.07	118,124,135,184	1
55	MG	CA	3123	1/1	0.93	0.15	36,36,36,36	0
56	OHX	CA	3387	7/7	0.93	0.07	111,127,150,170	2
56	OHX	CA	3388	7/7	0.93	0.11	112,116,127,180	1
55	MG	AA	3029	1/1	0.93	0.23	38,38,38,38	0
55	MG	AA	3230	1/1	0.93	0.19	66,66,66,66	0
56	OHX	AA	3544	7/7	0.93	0.06	103,105,124,176	1
55	MG	CA	3126	1/1	0.93	0.20	54,54,54,54	0
55	MG	AA	3032	1/1	0.93	0.23	41,41,41,41	0
56	OHX	AA	3547	7/7	0.93	0.07	69,84,101,157	2
55	MG	CA	3130	1/1	0.93	0.42	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3356	1/1	0.93	0.35	58,58,58,58	0
56	OHX	AA	3553	7/7	0.93	0.06	113,118,133,183	1
55	MG	CA	3473	1/1	0.93	0.22	50,50,50,50	0
55	MG	AA	3204	1/1	0.93	0.12	61,61,61,61	0
55	MG	BA	1707	1/1	0.93	0.21	70,70,70,70	0
55	MG	DL	201	1/1	0.93	0.28	92,92,92,92	0
56	OHX	AA	3561	7/7	0.93	0.07	152,158,173,226	1
56	OHX	CA	3412	7/7	0.93	0.11	99,116,129,164	2
55	MG	CA	3075	1/1	0.93	0.21	45,45,45,45	0
56	OHX	AA	3563	7/7	0.93	0.06	124,125,134,183	1
55	MG	DA	1651	1/1	0.93	0.39	62,62,62,62	0
56	OHX	CA	3416	7/7	0.93	0.07	114,117,128,182	1
55	MG	DA	1653	1/1	0.93	0.38	73,73,73,73	0
55	MG	CA	3138	1/1	0.93	0.46	53,53,53,53	0
55	MG	CA	3139	1/1	0.93	0.21	56,56,56,56	0
55	MG	AA	3374	1/1	0.93	0.22	29,29,29,29	0
55	MG	AA	3033	1/1	0.93	0.18	48,48,48,48	0
55	MG	BA	1630	1/1	0.93	0.11	90,90,90,90	0
56	OHX	AB	215	7/7	0.93	0.10	105,114,120,153	1
55	MG	AA	3121	1/1	0.93	0.31	53,53,53,53	0
56	OHX	AB	217	7/7	0.93	0.09	85,105,116,146	1
55	MG	AA	3238	1/1	0.93	0.30	50,50,50,50	0
56	OHX	AB	219	7/7	0.93	0.08	104,111,125,162	1
55	MG	AA	3001	1/1	0.93	0.26	28,28,28,28	0
56	OHX	CA	3430	7/7	0.93	0.08	96,106,114,197	1
55	MG	AA	3243	1/1	0.93	0.31	51,51,51,51	0
55	MG	CB	207	1/1	0.93	0.33	76,76,76,76	0
55	MG	CA	3147	1/1	0.93	0.27	51,51,51,51	0
55	MG	CA	3148	1/1	0.93	0.23	57,57,57,57	0
55	MG	AA	3055	1/1	0.93	0.26	65,65,65,65	0
55	MG	CA	3152	1/1	0.93	0.37	54,54,54,54	0
55	MG	BA	1636	1/1	0.93	0.15	61,61,61,61	0
56	OHX	CA	3464	7/7	0.93	0.12	78,109,122,137	3
55	MG	AA	3384	1/1	0.93	0.32	59,59,59,59	0
56	OHX	BA	1672	7/7	0.93	0.07	156,159,170,224	1
55	MG	AA	3179	1/1	0.93	0.34	60,60,60,60	0
55	MG	BA	1719	1/1	0.93	0.31	51,51,51,51	0
55	MG	AA	3183	1/1	0.93	0.24	88,88,88,88	0
55	MG	CA	3090	1/1	0.93	0.20	55,55,55,55	0
56	OHX	AA	3476	7/7	0.93	0.10	102,122,137,175	1
56	OHX	CB	211	7/7	0.93	0.07	122,128,152,168	1
56	OHX	AA	3482	7/7	0.93	0.07	105,118,127,177	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	AA	3483	7/7	0.93	0.07	124,141,146,196	1
55	MG	AA	3184	1/1	0.93	0.17	38,38,38,38	0
55	MG	CA	3093	1/1	0.93	0.32	81,81,81,81	0
55	MG	AA	3006	1/1	0.93	0.37	45,45,45,45	0
56	OHX	BA	1694	7/7	0.93	0.06	159,161,173,226	1
55	MG	AA	3188	1/1	0.93	0.16	40,40,40,40	0
55	MG	AA	3002	1/1	0.93	0.28	41,41,41,41	0
56	OHX	AA	3491	7/7	0.93	0.08	162,182,190,220	1
56	OHX	AA	3492	7/7	0.93	0.09	79,89,95,107	3
55	MG	CA	3168	1/1	0.93	0.24	72,72,72,72	0
56	OHX	DA	1756	7/7	0.93	0.06	145,145,160,212	1
56	OHX	BA	1797	7/7	0.93	0.13	71,104,132,136	3
56	OHX	AA	3495	7/7	0.93	0.09	86,93,120,158	1
56	OHX	DA	1769	7/7	0.93	0.07	133,140,147,188	1
56	OHX	DA	1772	7/7	0.93	0.07	131,135,143,214	1
55	MG	CA	3169	1/1	0.93	0.18	71,71,71,71	0
56	OHX	AA	3506	7/7	0.93	0.06	97,110,123,157	1
56	OHX	DA	1777	7/7	0.93	0.06	150,152,155,232	1
56	OHX	AA	3507	7/7	0.93	0.07	101,111,128,158	1
55	MG	AA	3251	1/1	0.93	0.29	49,49,49,49	0
56	OHX	BR	101	7/7	0.93	0.06	117,129,143,169	1
55	MG	AA	3408	1/1	0.93	0.31	47,47,47,47	0
55	MG	DA	1621	1/1	0.93	0.17	98,98,98,98	0
55	MG	DA	1689	1/1	0.93	0.17	87,87,87,87	0
56	OHX	AA	3514	7/7	0.93	0.08	84,93,104,149	1
56	OHX	CA	3248	7/7	0.93	0.06	116,128,134,203	1
55	MG	AA	3047	1/1	0.93	0.26	54,54,54,54	0
55	MG	AA	3286	1/1	0.93	0.33	68,68,68,68	0
55	MG	AA	3101	1/1	0.93	0.23	63,63,63,63	0
55	MG	CA	3104	1/1	0.93	0.33	41,41,41,41	0
55	MG	CA	3106	1/1	0.93	0.25	61,61,61,61	0
56	OHX	DA	1804	7/7	0.93	0.07	107,115,128,173	1
55	MG	AA	3198	1/1	0.93	0.23	54,54,54,54	0
56	OHX	DA	1806	7/7	0.93	0.05	142,150,160,228	1
55	MG	CA	3181	1/1	0.93	0.21	62,62,62,62	0
55	MG	BA	1616	1/1	0.93	0.15	61,61,61,61	0
56	OHX	CA	3342	7/7	0.93	0.07	116,123,130,201	1
56	OHX	CA	3343	7/7	0.93	0.09	109,118,132,184	1
56	OHX	CA	3344	7/7	0.93	0.10	96,110,117,162	1
56	OHX	AA	3529	7/7	0.93	0.08	90,106,115,167	1
56	OHX	CA	3350	7/7	0.93	0.08	112,134,144,175	1
55	MG	AA	3028	1/1	0.93	0.23	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	AA	3531	7/7	0.93	0.06	119,124,135,185	1
55	MG	AA	3259	1/1	0.93	0.21	35,35,35,35	0
55	MG	CA	3016	1/1	0.93	0.20	55,55,55,55	0
56	OHX	DC	107	7/7	0.93	0.09	131,132,141,177	1
55	MG	CA	3116	1/1	0.93	0.24	69,69,69,69	0
55	MG	AA	3269	1/1	0.94	0.23	72,72,72,72	0
55	MG	AA	3236	1/1	0.94	0.26	40,40,40,40	0
55	MG	AA	3237	1/1	0.94	0.23	45,45,45,45	0
55	MG	AA	3030	1/1	0.94	0.18	44,44,44,44	0
55	MG	AA	3214	1/1	0.94	0.21	46,46,46,46	0
55	MG	AA	3008	1/1	0.94	0.28	42,42,42,42	0
56	OHX	AA	3147	7/7	0.94	0.09	89,98,103,163	1
56	OHX	AA	3160	7/7	0.94	0.06	116,121,130,182	1
55	MG	AA	3189	1/1	0.94	0.27	42,42,42,42	0
55	MG	CA	3150	1/1	0.94	0.22	55,55,55,55	0
56	OHX	AA	3312	7/7	0.94	0.08	64,87,123,173	1
56	OHX	AA	3324	7/7	0.94	0.09	92,110,118,165	1
55	MG	CA	3089	1/1	0.94	0.15	60,60,60,60	0
55	MG	AA	3082	1/1	0.94	0.12	50,50,50,50	0
56	OHX	CA	3403	7/7	0.94	0.08	88,108,114,167	1
55	MG	AA	3387	1/1	0.94	0.23	42,42,42,42	0
56	OHX	CA	3405	7/7	0.94	0.06	112,116,119,187	1
55	MG	CA	3154	1/1	0.94	0.27	46,46,46,46	0
55	MG	DA	1666	1/1	0.94	0.31	62,62,62,62	0
55	MG	AA	3192	1/1	0.94	0.27	48,48,48,48	0
55	MG	AA	3003	1/1	0.94	0.17	39,39,39,39	0
56	OHX	AA	3402	7/7	0.94	0.14	87,110,129,141	3
56	OHX	A1	202	7/7	0.94	0.08	85,95,114,146	1
55	MG	AA	3173	1/1	0.94	0.20	52,52,52,52	0
56	OHX	BA	1656	7/7	0.94	0.07	160,162,176,267	0
55	MG	CA	3158	1/1	0.94	0.22	56,56,56,56	0
55	MG	DA	1671	1/1	0.94	0.12	64,64,64,64	0
55	MG	AA	3395	1/1	0.94	0.13	40,40,40,40	0
56	OHX	AA	3452	7/7	0.94	0.11	61,75,91,137	2
55	MG	CA	3161	1/1	0.94	0.21	71,71,71,71	0
56	OHX	AA	3477	7/7	0.94	0.06	108,119,125,208	1
55	MG	DA	1606	1/1	0.94	0.14	84,84,84,84	0
55	MG	CA	3048	1/1	0.94	0.29	44,44,44,44	0
55	MG	CA	3049	1/1	0.94	0.19	62,62,62,62	0
55	MG	AA	3222	1/1	0.94	0.29	64,64,64,64	0
56	OHX	AA	3486	7/7	0.94	0.07	127,135,138,199	1
55	MG	DA	1610	1/1	0.94	0.14	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	AA	3223	1/1	0.94	0.21	56,56,56,56	0
55	MG	BA	1726	1/1	0.94	0.27	61,61,61,61	0
55	MG	CA	3226	1/1	0.94	0.41	65,65,65,65	0
56	OHX	BA	1681	7/7	0.94	0.06	153,163,173,229	1
55	MG	AA	3197	1/1	0.94	0.28	50,50,50,50	0
56	OHX	BA	1688	7/7	0.94	0.09	107,112,123,154	1
56	OHX	BA	1689	7/7	0.94	0.07	113,130,139,190	1
55	MG	CA	3007	1/1	0.94	0.17	45,45,45,45	0
56	OHX	BA	1691	7/7	0.94	0.06	148,150,156,215	1
56	OHX	AA	3494	7/7	0.94	0.08	59,86,128,185	1
56	OHX	BA	1693	7/7	0.94	0.08	112,112,134,152	1
55	MG	DA	1685	1/1	0.94	0.10	59,59,59,59	0
56	OHX	AA	3504	7/7	0.94	0.06	112,118,129,179	1
56	OHX	BA	1771	7/7	0.94	0.11	77,100,122,150	1
56	OHX	CA	3482	7/7	0.94	0.07	84,120,131,181	0
55	MG	AA	3225	1/1	0.94	0.16	63,63,63,63	0
55	MG	AA	3254	1/1	0.94	0.21	42,42,42,42	0
56	OHX	CA	3489	7/7	0.94	0.09	91,101,112,140	1
56	OHX	BA	1785	7/7	0.94	0.08	109,122,129,170	1
56	OHX	CB	209	7/7	0.94	0.09	117,133,147,190	1
56	OHX	CB	210	7/7	0.94	0.08	104,124,140,171	1
55	MG	AA	3054	1/1	0.94	0.14	49,49,49,49	0
56	OHX	AA	3508	7/7	0.94	0.07	122,129,136,204	1
56	OHX	BA	1791	7/7	0.94	0.10	82,106,122,150	2
56	OHX	BA	1793	7/7	0.94	0.07	95,105,117,163	1
55	MG	CA	3112	1/1	0.94	0.29	41,41,41,41	0
55	MG	CA	3174	1/1	0.94	0.33	52,52,52,52	0
55	MG	CA	3113	1/1	0.94	0.21	61,61,61,61	0
55	MG	BA	1731	1/1	0.94	0.35	57,57,57,57	0
55	MG	CA	3263	1/1	0.94	0.25	69,69,69,69	0
56	OHX	BA	1811	7/7	0.94	0.09	88,104,115,154	1
56	OHX	DA	1747	7/7	0.94	0.09	109,122,155,200	1
56	OHX	DA	1749	7/7	0.94	0.10	91,120,126,173	1
56	OHX	DA	1752	7/7	0.94	0.06	107,121,128,186	1
55	MG	AA	3039	1/1	0.94	0.21	40,40,40,40	0
55	MG	AA	3257	1/1	0.94	0.22	57,57,57,57	0
56	OHX	BB	106	7/7	0.94	0.12	164,167,173,198	1
55	MG	AA	3004	1/1	0.94	0.23	37,37,37,37	0
56	OHX	DA	1760	7/7	0.94	0.07	142,145,152,204	1
56	OHX	BD	102	7/7	0.94	0.07	153,174,197,228	0
55	MG	DA	1699	1/1	0.94	0.22	78,78,78,78	0
56	OHX	CA	3244	7/7	0.94	0.07	94,113,121,172	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	DA	1773	7/7	0.94	0.06	122,126,137,197	1
55	MG	CA	3063	1/1	0.94	0.16	70,70,70,70	0
55	MG	BA	1619	1/1	0.94	0.19	50,50,50,50	0
56	OHX	DA	1776	7/7	0.94	0.07	114,116,125,160	1
55	MG	CA	3120	1/1	0.94	0.26	48,48,48,48	0
56	OHX	DA	1778	7/7	0.94	0.07	142,148,154,267	0
55	MG	BA	1697	1/1	0.94	0.26	37,37,37,37	0
55	MG	CA	3122	1/1	0.94	0.19	40,40,40,40	0
55	MG	AA	3088	1/1	0.94	0.09	60,60,60,60	0
55	MG	CA	3019	1/1	0.94	0.14	46,46,46,46	0
55	MG	CA	3020	1/1	0.94	0.21	70,70,70,70	0
55	MG	CA	3451	1/1	0.94	0.23	46,46,46,46	0
55	MG	AA	3099	1/1	0.94	0.19	65,65,65,65	0
56	OHX	DA	1790	7/7	0.94	0.06	135,136,148,199	1
56	OHX	CA	3318	7/7	0.94	0.11	34,112,130,183	1
55	MG	AB	204	1/1	0.94	0.34	68,68,68,68	0
55	MG	BA	1743	1/1	0.94	0.26	69,69,69,69	0
55	MG	AA	3181	1/1	0.94	0.26	61,61,61,61	0
55	MG	AA	3352	1/1	0.94	0.13	41,41,41,41	0
56	OHX	CA	3346	7/7	0.94	0.09	99,104,119,151	1
55	MG	AA	3182	1/1	0.94	0.29	45,45,45,45	0
56	OHX	CA	3349	7/7	0.94	0.07	115,117,131,178	1
55	MG	AA	3265	1/1	0.94	0.29	85,85,85,85	0
56	OHX	CA	3355	7/7	0.94	0.09	108,110,119,149	1
55	MG	AA	3233	1/1	0.94	0.16	59,59,59,59	0
55	MG	DA	1646	1/1	0.94	0.16	64,64,64,64	0
56	OHX	CA	3365	7/7	0.94	0.07	164,171,176,213	1
55	MG	CA	3199	1/1	0.94	0.23	62,62,62,62	0
55	MG	CA	3472	1/1	0.94	0.10	59,59,59,59	0
55	MG	AA	3113	1/1	0.94	0.21	32,32,32,32	0
56	OHX	AA	3548	7/7	0.94	0.06	113,118,133,172	1
56	OHX	DV	101	7/7	0.94	0.07	162,169,185,231	1
56	OHX	CA	3377	7/7	0.94	0.10	90,95,111,135	2
56	OHX	AA	3550	7/7	0.94	0.07	111,121,131,187	1
55	MG	AA	3025	1/1	0.94	0.21	59,59,59,59	0
55	MG	BA	1752	1/1	0.94	0.31	53,53,53,53	0
55	MG	DA	1652	1/1	0.94	0.34	52,52,52,52	0
56	OHX	DD	101	7/7	0.94	0.08	155,165,187,227	0
57	ZN	BQ	102	1/1	0.94	0.11	130,130,130,130	0
57	ZN	DG	301	1/1	0.94	0.20	122,122,122,122	0
56	OHX	BA	1813	7/7	0.95	0.07	128,130,137,174	1
56	OHX	BA	1814	7/7	0.95	0.06	101,109,125,174	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	BA	1815	7/7	0.95	0.07	110,125,133,172	1
55	MG	CA	3445	1/1	0.95	0.19	38,38,38,38	0
55	MG	BA	1654	1/1	0.95	0.24	47,47,47,47	0
55	MG	BA	1655	1/1	0.95	0.19	60,60,60,60	0
55	MG	AA	3210	1/1	0.95	0.33	41,41,41,41	0
55	MG	AA	3240	1/1	0.95	0.17	43,43,43,43	0
55	MG	AA	3104	1/1	0.95	0.32	68,68,68,68	0
55	MG	AA	3010	1/1	0.95	0.17	40,40,40,40	0
55	MG	AA	3018	1/1	0.95	0.20	43,43,43,43	0
55	MG	CA	3092	1/1	0.95	0.36	52,52,52,52	0
55	MG	CA	3133	1/1	0.95	0.24	48,48,48,48	0
55	MG	CA	3173	1/1	0.95	0.16	53,53,53,53	0
56	OHX	AB	209	7/7	0.95	0.08	63,88,125,152	2
56	OHX	AA	3497	7/7	0.95	0.08	94,106,111,138	2
56	OHX	AA	3500	7/7	0.95	0.07	94,114,122,159	1
56	OHX	CA	3285	7/7	0.95	0.12	94,107,126,147	1
55	MG	AA	3085	1/1	0.95	0.13	58,58,58,58	0
55	MG	CA	3135	1/1	0.95	0.30	45,45,45,45	0
55	MG	CA	3094	1/1	0.95	0.35	79,79,79,79	0
56	OHX	CA	3488	7/7	0.95	0.06	113,123,127,179	1
55	MG	AA	3389	1/1	0.95	0.30	44,44,44,44	0
56	OHX	CA	3325	7/7	0.95	0.13	108,122,148,156	1
56	OHX	CA	3334	7/7	0.95	0.07	110,115,136,183	0
55	MG	BA	1638	1/1	0.95	0.21	57,57,57,57	0
55	MG	CA	3474	1/1	0.95	0.16	70,70,70,70	0
56	OHX	CB	212	7/7	0.95	0.07	101,120,135,155	1
55	MG	BA	1705	1/1	0.95	0.18	63,63,63,63	0
56	OHX	AW	101	7/7	0.95	0.09	103,112,128,156	1
55	MG	BA	1732	1/1	0.95	0.27	52,52,52,52	0
55	MG	AE	303	1/1	0.95	0.16	32,32,32,32	0
56	OHX	BA	1659	7/7	0.95	0.07	114,130,135,179	1
55	MG	AA	3277	1/1	0.95	0.28	46,46,46,46	0
55	MG	AA	3278	1/1	0.95	0.25	35,35,35,35	0
56	OHX	CB	220	7/7	0.95	0.07	133,142,154,201	0
56	OHX	C1	201	7/7	0.95	0.08	102,111,123,165	1
56	OHX	AA	3516	7/7	0.95	0.06	101,109,121,183	1
56	OHX	AA	3517	7/7	0.95	0.10	88,111,115,145	1
56	OHX	DA	1730	7/7	0.95	0.09	102,111,123,157	0
56	OHX	DA	1731	7/7	0.95	0.07	129,139,145,172	1
56	OHX	DA	1741	7/7	0.95	0.08	97,116,128,170	1
56	OHX	DA	1745	7/7	0.95	0.07	115,123,143,223	0
56	OHX	CA	3362	7/7	0.95	0.05	129,136,141,186	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	CA	3364	7/7	0.95	0.07	117,120,133,182	1
56	OHX	DA	1751	7/7	0.95	0.13	66,109,137,183	2
55	MG	AA	3186	1/1	0.95	0.21	49,49,49,49	0
56	OHX	CA	3368	7/7	0.95	0.07	108,126,135,177	1
56	OHX	DA	1754	7/7	0.95	0.07	98,102,118,156	1
56	OHX	CA	3370	7/7	0.95	0.07	116,120,142,180	1
56	OHX	BA	1668	7/7	0.95	0.07	116,121,137,182	1
55	MG	AA	3133	1/1	0.95	0.15	54,54,54,54	0
56	OHX	CA	3374	7/7	0.95	0.08	106,124,128,169	1
56	OHX	DA	1762	7/7	0.95	0.08	107,112,122,180	1
56	OHX	BA	1670	7/7	0.95	0.06	135,143,147,201	1
55	MG	CA	3105	1/1	0.95	0.42	68,68,68,68	0
56	OHX	DA	1771	7/7	0.95	0.10	97,105,129,152	1
56	OHX	AA	3304	7/7	0.95	0.06	109,115,135,200	1
55	MG	AA	3011	1/1	0.95	0.21	49,49,49,49	0
55	MG	CA	3004	1/1	0.95	0.14	49,49,49,49	0
56	OHX	AA	3313	7/7	0.95	0.08	96,112,122,174	0
56	OHX	CA	3381	7/7	0.95	0.07	102,112,121,159	1
56	OHX	AA	3528	7/7	0.95	0.07	112,118,137,160	2
56	OHX	AA	3319	7/7	0.95	0.08	87,95,122,151	1
56	OHX	DA	1780	7/7	0.95	0.07	127,131,138,167	1
55	MG	CA	3190	1/1	0.95	0.11	60,60,60,60	0
56	OHX	AA	3330	7/7	0.95	0.07	102,112,122,166	1
56	OHX	BA	1683	7/7	0.95	0.06	124,130,146,183	1
55	MG	CA	3108	1/1	0.95	0.23	52,52,52,52	0
55	MG	AA	3178	1/1	0.95	0.31	39,39,39,39	0
56	OHX	CA	3391	7/7	0.95	0.06	140,144,157,182	1
55	MG	CA	3006	1/1	0.95	0.19	47,47,47,47	0
56	OHX	DA	1788	7/7	0.95	0.08	96,113,128,168	1
55	MG	CA	3259	1/1	0.95	0.28	65,65,65,65	0
56	OHX	DA	1791	7/7	0.95	0.09	103,104,121,153	1
56	OHX	DA	1792	7/7	0.95	0.07	110,118,129,172	1
55	MG	C5	101	1/1	0.95	0.24	50,50,50,50	0
56	OHX	DA	1795	7/7	0.95	0.06	112,118,132,167	1
55	MG	CA	3194	1/1	0.95	0.26	63,63,63,63	0
56	OHX	DA	1797	7/7	0.95	0.05	149,152,159,218	1
55	MG	AA	3205	1/1	0.95	0.18	40,40,40,40	0
56	OHX	CA	3398	7/7	0.95	0.06	129,132,142,192	1
56	OHX	AA	3373	7/7	0.95	0.08	75,103,110,155	1
55	MG	A5	101	1/1	0.95	0.19	41,41,41,41	0
55	MG	AA	3375	1/1	0.95	0.25	31,31,31,31	0
56	OHX	BA	1778	7/7	0.95	0.08	99,120,131,182	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	OHX	AA	3543	7/7	0.95	0.05	113,117,131,189	1
55	MG	AA	3376	1/1	0.95	0.25	33,33,33,33	0
55	MG	AA	3377	1/1	0.95	0.23	51,51,51,51	0
55	MG	CA	3012	1/1	0.95	0.19	53,53,53,53	0
55	MG	AA	3116	1/1	0.95	0.17	45,45,45,45	0
56	OHX	AA	3474	7/7	0.95	0.09	51,85,127,151	2
56	OHX	AA	3475	7/7	0.95	0.07	67,93,111,167	1
56	OHX	BA	1794	7/7	0.95	0.06	118,138,149,184	1
55	MG	BA	1748	1/1	0.95	0.21	66,66,66,66	0
56	OHX	BA	1798	7/7	0.95	0.06	140,143,151,221	1
56	OHX	BA	1800	7/7	0.95	0.08	106,107,118,143	1
56	OHX	BA	1801	7/7	0.95	0.06	118,138,142,207	1
55	MG	AA	3191	1/1	0.95	0.20	45,45,45,45	0
56	OHX	AA	3479	7/7	0.95	0.07	106,122,142,174	1
55	MG	AA	3180	1/1	0.95	0.20	65,65,65,65	0
55	MG	DA	1612	1/1	0.95	0.21	86,86,86,86	0
56	OHX	BA	1807	7/7	0.95	0.06	135,141,150,224	0
56	OHX	AA	3557	7/7	0.95	0.09	75,87,101,114	1
55	MG	AA	3111	1/1	0.96	0.22	35,35,35,35	0
56	OHX	BA	1810	7/7	0.96	0.07	106,108,121,152	1
55	MG	CA	3149	1/1	0.96	0.29	55,55,55,55	0
56	OHX	CA	3423	7/7	0.96	0.04	123,126,136,189	1
56	OHX	BA	1812	7/7	0.96	0.06	151,164,170,231	1
55	MG	AA	3146	1/1	0.96	0.20	41,41,41,41	0
55	MG	AA	3415	1/1	0.96	0.13	52,52,52,52	0
55	MG	CA	3043	1/1	0.96	0.11	82,82,82,82	0
55	MG	AA	3343	1/1	0.96	0.29	34,34,34,34	0
55	MG	AA	3112	1/1	0.96	0.14	47,47,47,47	0
55	MG	AA	3043	1/1	0.96	0.23	46,46,46,46	0
56	OHX	AB	207	7/7	0.96	0.07	89,99,126,152	1
56	OHX	AB	208	7/7	0.96	0.07	113,119,131,170	1
56	OHX	BD	103	7/7	0.96	0.06	86,95,103,174	1
55	MG	CA	3047	1/1	0.96	0.33	41,41,41,41	0
56	OHX	AA	3496	7/7	0.96	0.06	117,124,142,215	0
56	OHX	AB	212	7/7	0.96	0.08	81,99,131,153	1
56	OHX	AB	213	7/7	0.96	0.10	85,93,130,132	3
56	OHX	CA	3463	7/7	0.96	0.10	107,129,139,156	1
56	OHX	AB	214	7/7	0.96	0.07	110,118,132,162	1
56	OHX	CA	3465	7/7	0.96	0.07	131,136,147,181	1
55	MG	AA	3346	1/1	0.96	0.16	42,42,42,42	0
55	MG	BN	201	1/1	0.96	0.11	80,80,80,80	0
56	OHX	CA	3253	7/7	0.96	0.08	107,120,133,155	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	CA	3469	7/7	0.96	0.07	89,110,121,162	1
56	OHX	AA	3501	7/7	0.96	0.08	101,109,129,149	1
56	OHX	AA	3503	7/7	0.96	0.06	99,121,138,179	1
55	MG	BA	1701	1/1	0.96	0.20	57,57,57,57	0
55	MG	CA	3261	1/1	0.96	0.37	48,48,48,48	0
55	MG	CA	3160	1/1	0.96	0.28	49,49,49,49	0
55	MG	AA	3207	1/1	0.96	0.32	57,57,57,57	0
56	OHX	CA	3490	7/7	0.96	0.07	102,105,118,156	1
56	OHX	CA	3314	7/7	0.96	0.10	84,93,97,114	1
56	OHX	A3	102	7/7	0.96	0.10	90,98,113,134	2
55	MG	BA	1637	1/1	0.96	0.06	83,83,83,83	0
56	OHX	CA	3328	7/7	0.96	0.07	50,117,131,206	0
56	OHX	CA	3331	7/7	0.96	0.09	101,112,120,147	1
56	OHX	CA	3333	7/7	0.96	0.07	104,127,133,184	1
56	OHX	A6	101	7/7	0.96	0.07	113,122,137,155	1
56	OHX	CA	3335	7/7	0.96	0.07	96,110,125,200	0
56	OHX	CA	3337	7/7	0.96	0.08	109,124,136,185	0
56	OHX	CA	3339	7/7	0.96	0.08	100,105,127,171	1
56	OHX	AA	3305	7/7	0.96	0.10	83,97,103,135	1
55	MG	AA	3170	1/1	0.96	0.14	50,50,50,50	0
55	MG	AA	3239	1/1	0.96	0.16	44,44,44,44	0
55	MG	DA	1691	1/1	0.96	0.22	54,54,54,54	0
56	OHX	AA	3317	7/7	0.96	0.07	79,88,118,156	1
55	MG	AA	3094	1/1	0.96	0.31	39,39,39,39	0
56	OHX	C6	101	7/7	0.96	0.07	132,145,157,184	1
56	OHX	BA	1665	7/7	0.96	0.08	82,92,111,128	1
55	MG	DA	1693	1/1	0.96	0.32	54,54,54,54	0
56	OHX	DA	1732	7/7	0.96	0.07	134,143,157,195	0
56	OHX	DA	1733	7/7	0.96	0.07	146,151,163,202	0
56	OHX	DA	1735	7/7	0.96	0.07	110,115,118,170	1
56	OHX	DA	1736	7/7	0.96	0.07	130,135,157,193	0
56	OHX	DA	1737	7/7	0.96	0.08	87,110,131,158	1
56	OHX	CA	3351	7/7	0.96	0.07	102,107,134,173	1
56	OHX	CA	3352	7/7	0.96	0.05	133,145,147,191	1
56	OHX	CA	3353	7/7	0.96	0.07	81,96,110,140	1
56	OHX	AA	3327	7/7	0.96	0.06	107,115,135,188	1
56	OHX	DA	1750	7/7	0.96	0.07	127,137,146,202	1
56	OHX	CA	3356	7/7	0.96	0.06	96,109,118,157	1
56	OHX	AA	3328	7/7	0.96	0.09	89,97,114,142	1
55	MG	CA	3127	1/1	0.96	0.17	53,53,53,53	0
56	OHX	CA	3360	7/7	0.96	0.06	116,124,135,193	1
56	OHX	CA	3361	7/7	0.96	0.06	113,119,132,166	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3024	1/1	0.96	0.12	48,48,48,48	0
56	OHX	CA	3363	7/7	0.96	0.08	94,99,114,167	1
55	MG	AA	3050	1/1	0.96	0.20	60,60,60,60	0
56	OHX	AA	3334	7/7	0.96	0.09	66,79,94,105	1
56	OHX	DA	1763	7/7	0.96	0.05	154,159,173,250	0
56	OHX	CA	3366	7/7	0.96	0.07	140,148,168,207	0
56	OHX	DA	1768	7/7	0.96	0.06	121,132,163,218	0
56	OHX	CA	3367	7/7	0.96	0.05	129,137,147,194	1
56	OHX	DA	1770	7/7	0.96	0.05	136,142,156,217	1
56	OHX	AA	3336	7/7	0.96	0.07	146,153,168,218	0
56	OHX	CA	3369	7/7	0.96	0.08	97,113,121,158	1
55	MG	CA	3442	1/1	0.96	0.19	61,61,61,61	0
55	MG	AA	3242	1/1	0.96	0.23	37,37,37,37	0
56	OHX	AA	3368	7/7	0.96	0.10	76,83,98,126	1
55	MG	CA	3444	1/1	0.96	0.22	52,52,52,52	0
56	OHX	BA	1679	7/7	0.96	0.05	116,125,129,189	1
55	MG	AA	3075	1/1	0.96	0.34	44,44,44,44	0
55	MG	BC	103	1/1	0.96	0.32	62,62,62,62	0
56	OHX	BA	1682	7/7	0.96	0.06	119,124,130,186	1
56	OHX	AA	3372	7/7	0.96	0.07	93,103,121,167	1
55	MG	CA	3447	1/1	0.96	0.46	58,58,58,58	0
56	OHX	BA	1687	7/7	0.96	0.08	94,99,108,140	1
55	MG	AA	3185	1/1	0.96	0.27	36,36,36,36	0
55	MG	BA	1738	1/1	0.96	0.09	41,41,41,41	0
55	MG	AA	3393	1/1	0.96	0.13	56,56,56,56	0
56	OHX	CA	3385	7/7	0.96	0.06	115,124,135,193	1
56	OHX	AA	3538	7/7	0.96	0.09	88,94,114,159	1
56	OHX	AA	3405	7/7	0.96	0.06	103,111,138,161	1
55	MG	AA	3262	1/1	0.96	0.28	52,52,52,52	0
55	MG	CA	3453	1/1	0.96	0.25	58,58,58,58	0
56	OHX	AA	3447	7/7	0.96	0.07	91,102,120,163	1
55	MG	AA	3007	1/1	0.96	0.12	31,31,31,31	0
56	OHX	BA	1772	7/7	0.96	0.07	106,118,144,175	0
56	OHX	BA	1777	7/7	0.96	0.07	114,118,140,171	1
56	OHX	AA	3458	7/7	0.96	0.10	34,48,113,148	3
56	OHX	DA	1800	7/7	0.96	0.05	137,140,150,220	1
56	OHX	AA	3464	7/7	0.96	0.07	117,125,139,188	0
56	OHX	AA	3465	7/7	0.96	0.08	85,99,124,159	1
56	OHX	AA	3466	7/7	0.96	0.07	89,94,108,128	1
56	OHX	AA	3470	7/7	0.96	0.07	107,109,130,160	1
56	OHX	CA	3401	7/7	0.96	0.06	136,149,158,185	1
56	OHX	BA	1788	7/7	0.96	0.07	118,118,132,157	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	BA	1789	7/7	0.96	0.07	108,112,133,182	1
56	OHX	AA	3549	7/7	0.96	0.08	97,102,111,165	1
56	OHX	AA	3473	7/7	0.96	0.08	66,95,102,124	1
55	MG	AA	3358	1/1	0.96	0.25	51,51,51,51	0
55	MG	AA	3200	1/1	0.96	0.28	45,45,45,45	0
56	OHX	BA	1796	7/7	0.96	0.06	143,156,164,225	0
56	OHX	CA	3410	7/7	0.96	0.06	114,125,132,190	1
55	MG	AA	3042	1/1	0.96	0.17	43,43,43,43	0
55	MG	CA	3180	1/1	0.96	0.17	75,75,75,75	0
55	MG	CA	3070	1/1	0.96	0.14	44,44,44,44	0
55	MG	AA	3202	1/1	0.96	0.27	45,45,45,45	0
56	OHX	BA	1802	7/7	0.96	0.06	107,121,133,185	1
56	OHX	AA	3558	7/7	0.96	0.06	95,121,125,156	1
55	MG	AA	3411	1/1	0.96	0.17	63,63,63,63	0
55	MG	CA	3073	1/1	0.96	0.18	54,54,54,54	0
55	MG	AA	3412	1/1	0.96	0.23	39,39,39,39	0
56	OHX	BA	1792	7/7	0.97	0.06	150,163,168,209	1
55	MG	CA	3128	1/1	0.97	0.07	72,72,72,72	0
55	MG	CA	3098	1/1	0.97	0.14	63,63,63,63	0
56	OHX	BA	1795	7/7	0.97	0.06	109,127,134,173	1
55	MG	BC	104	1/1	0.97	0.35	57,57,57,57	0
56	OHX	AA	3467	7/7	0.97	0.06	100,105,117,133	1
56	OHX	AA	3468	7/7	0.97	0.06	99,111,119,167	1
56	OHX	BA	1799	7/7	0.97	0.06	158,163,176,213	1
56	OHX	AA	3469	7/7	0.97	0.08	79,91,98,161	1
56	OHX	CA	3372	7/7	0.97	0.07	112,137,145,182	0
56	OHX	AA	3318	7/7	0.97	0.08	92,102,113,133	1
56	OHX	AA	3471	7/7	0.97	0.05	98,107,114,163	1
56	OHX	AA	3472	7/7	0.97	0.07	120,126,137,153	1
55	MG	C7	101	1/1	0.97	0.29	54,54,54,54	0
56	OHX	CO	201	7/7	0.97	0.06	104,109,121,141	1
56	OHX	AA	3322	7/7	0.97	0.06	89,98,107,146	1
55	MG	AA	3385	1/1	0.97	0.29	34,34,34,34	0
56	OHX	AA	3325	7/7	0.97	0.07	91,103,115,154	1
56	OHX	BA	1808	7/7	0.97	0.11	84,90,96,110	2
56	OHX	DA	1728	7/7	0.97	0.07	78,116,123,162	0
56	OHX	BA	1809	7/7	0.97	0.05	141,153,160,232	0
56	OHX	AA	3326	7/7	0.97	0.09	83,94,100,118	1
56	OHX	AA	3478	7/7	0.97	0.06	77,90,100,131	1
56	OHX	BA	1663	7/7	0.97	0.05	132,137,143,190	1
55	MG	DA	1638	1/1	0.97	0.11	89,89,89,89	0
56	OHX	AA	3480	7/7	0.97	0.07	90,100,124,135	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	AA	3481	7/7	0.97	0.06	95,108,126,156	2
55	MG	DN	201	1/1	0.97	0.10	80,80,80,80	0
56	OHX	CA	3389	7/7	0.97	0.06	101,110,123,155	1
56	OHX	BG	302	7/7	0.97	0.06	128,137,145,186	1
56	OHX	DA	1748	7/7	0.97	0.06	95,111,122,149	1
55	MG	CA	3132	1/1	0.97	0.14	80,80,80,80	0
55	MG	DA	1700	1/1	0.97	0.36	70,70,70,70	0
56	OHX	AA	3332	7/7	0.97	0.08	77,106,123,134	1
56	OHX	CA	3394	7/7	0.97	0.07	97,100,116,155	1
56	OHX	BA	1671	7/7	0.97	0.04	127,131,133,210	1
55	MG	BA	1700	1/1	0.97	0.35	61,61,61,61	0
55	MG	DA	1680	1/1	0.97	0.18	72,72,72,72	0
56	OHX	AA	3335	7/7	0.97	0.06	94,101,113,136	1
56	OHX	AA	3489	7/7	0.97	0.07	72,78,92,128	1
56	OHX	CA	3246	7/7	0.97	0.10	113,116,120,151	1
56	OHX	DA	1761	7/7	0.97	0.05	130,132,145,205	0
55	MG	AA	3394	1/1	0.97	0.24	43,43,43,43	0
56	OHX	AA	3337	7/7	0.97	0.06	97,106,127,177	1
56	OHX	AA	3339	7/7	0.97	0.06	151,155,164,211	1
56	OHX	DA	1766	7/7	0.97	0.06	118,124,133,175	1
56	OHX	DA	1767	7/7	0.97	0.05	120,124,135,184	1
56	OHX	AA	3363	7/7	0.97	0.09	90,99,133,145	1
55	MG	AA	3016	1/1	0.97	0.21	39,39,39,39	0
56	OHX	CA	3406	7/7	0.97	0.06	151,161,169,211	1
56	OHX	CA	3254	7/7	0.97	0.06	167,174,181,211	0
55	MG	AA	3253	1/1	0.97	0.21	53,53,53,53	0
56	OHX	AA	3367	7/7	0.97	0.06	121,129,147,173	1
55	MG	AA	3388	1/1	0.97	0.26	41,41,41,41	0
56	OHX	CA	3293	7/7	0.97	0.09	100,117,128,163	0
56	OHX	CA	3295	7/7	0.97	0.08	102,105,117,137	1
56	OHX	BA	1685	7/7	0.97	0.05	198,199,207,267	1
56	OHX	AA	3556	7/7	0.97	0.05	212,217,223,266	1
56	OHX	AA	3498	7/7	0.97	0.07	92,94,127,136	1
56	OHX	CA	3308	7/7	0.97	0.07	88,90,121,161	0
56	OHX	CA	3309	7/7	0.97	0.07	92,108,125,150	1
55	MG	DA	1664	1/1	0.97	0.33	31,31,31,31	0
56	OHX	CA	3317	7/7	0.97	0.07	116,126,142,180	1
55	MG	AA	3022	1/1	0.97	0.12	15,15,15,15	0
56	OHX	AA	3502	7/7	0.97	0.07	97,102,112,146	1
55	MG	AA	3219	1/1	0.97	0.15	48,48,48,48	0
55	MG	AA	3140	1/1	0.97	0.09	41,41,41,41	0
56	OHX	DA	1789	7/7	0.97	0.04	176,179,184,242	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	OHX	AA	3263	7/7	0.97	0.06	76,102,114,143	1
56	OHX	AA	3401	7/7	0.97	0.05	93,112,116,173	1
56	OHX	AA	3288	7/7	0.97	0.08	76,85,101,127	1
56	OHX	DA	1793	7/7	0.97	0.06	146,150,161,207	1
56	OHX	CA	3336	7/7	0.97	0.06	114,127,138,191	0
56	OHX	BA	1764	7/7	0.97	0.08	88,94,120,157	0
56	OHX	CA	3338	7/7	0.97	0.08	95,103,117,121	1
56	OHX	BA	1768	7/7	0.97	0.07	128,139,147,175	0
56	OHX	BA	1770	7/7	0.97	0.07	102,113,126,149	1
56	OHX	CA	3341	7/7	0.97	0.08	74,100,107,145	2
56	OHX	AA	3298	7/7	0.97	0.11	71,88,99,110	1
56	OHX	AA	3299	7/7	0.97	0.07	54,81,94,118	1
56	OHX	DA	1802	7/7	0.97	0.07	120,122,140,196	1
56	OHX	BA	1773	7/7	0.97	0.08	101,102,110,142	1
55	MG	AA	3410	1/1	0.97	0.24	61,61,61,61	0
56	OHX	AA	3303	7/7	0.97	0.07	93,102,117,145	1
56	OHX	CA	3438	7/7	0.97	0.05	97,104,116,167	1
56	OHX	CA	3450	7/7	0.97	0.06	112,125,137,206	0
56	OHX	CA	3462	7/7	0.97	0.09	71,82,94,110	1
56	OHX	BA	1780	7/7	0.97	0.09	94,102,115,117	1
56	OHX	BA	1781	7/7	0.97	0.06	91,111,121,156	1
56	OHX	DA	1811	7/7	0.97	0.04	137,141,149,222	1
56	OHX	BA	1782	7/7	0.97	0.07	133,144,159,198	0
55	MG	AA	3031	1/1	0.97	0.21	35,35,35,35	0
55	MG	CA	3111	1/1	0.97	0.29	30,30,30,30	0
56	OHX	AA	3448	7/7	0.97	0.08	87,90,112,131	1
56	OHX	BA	1786	7/7	0.97	0.07	93,97,101,149	1
56	OHX	CA	3357	7/7	0.97	0.07	86,98,106,151	1
56	OHX	CA	3481	7/7	0.97	0.08	35,87,114,138	2
56	OHX	AA	3450	7/7	0.97	0.07	65,94,112,113	3
56	OHX	CA	3484	7/7	0.97	0.06	104,113,129,146	1
55	MG	CA	3058	1/1	0.97	0.29	50,50,50,50	0
56	OHX	AA	3307	7/7	0.97	0.07	85,90,103,127	1
56	OHX	AA	3520	7/7	0.97	0.05	127,132,145,185	1
56	OHX	AA	3521	7/7	0.97	0.06	87,94,107,160	1
56	OHX	DA	1719	7/7	0.98	0.07	79,99,112,124	0
56	OHX	DA	1724	7/7	0.98	0.07	84,106,133,148	1
56	OHX	DA	1726	7/7	0.98	0.08	87,101,123,159	0
56	OHX	CA	3311	7/7	0.98	0.07	79,95,105,127	1
56	OHX	DA	1729	7/7	0.98	0.06	104,108,118,152	1
56	OHX	CA	3312	7/7	0.98	0.07	85,101,114,134	1
56	OHX	CA	3313	7/7	0.98	0.05	103,112,124,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	AA	3443	7/7	0.98	0.06	69,76,84,127	1
56	OHX	CA	3315	7/7	0.98	0.07	90,101,110,160	1
56	OHX	AA	3315	7/7	0.98	0.09	89,99,111,137	1
56	OHX	AA	3297	7/7	0.98	0.10	87,98,102,106	1
56	OHX	CA	3319	7/7	0.98	0.06	87,97,106,138	1
56	OHX	DA	1738	7/7	0.98	0.05	115,122,137,171	1
56	OHX	DA	1739	7/7	0.98	0.04	98,110,124,155	1
56	OHX	CA	3320	7/7	0.98	0.06	140,142,153,174	0
56	OHX	DA	1742	7/7	0.98	0.05	117,127,141,176	1
56	OHX	DA	1743	7/7	0.98	0.06	109,113,118,148	1
56	OHX	DA	1744	7/7	0.98	0.06	103,108,120,148	1
56	OHX	CA	3321	7/7	0.98	0.06	111,119,144,156	0
56	OHX	DA	1746	7/7	0.98	0.05	126,134,146,189	1
56	OHX	CA	3322	7/7	0.98	0.06	104,117,127,154	1
56	OHX	CA	3323	7/7	0.98	0.05	107,111,118,169	0
56	OHX	AA	3338	7/7	0.98	0.07	82,93,108,126	1
56	OHX	CA	3326	7/7	0.98	0.06	97,110,130,136	2
56	OHX	AA	3451	7/7	0.98	0.07	75,85,92,125	1
56	OHX	CA	3329	7/7	0.98	0.06	102,103,123,146	1
55	MG	A0	201	1/1	0.98	0.14	48,48,48,48	0
56	OHX	CA	3332	7/7	0.98	0.07	70,82,93,103	1
56	OHX	AA	3454	7/7	0.98	0.07	68,93,112,112	1
56	OHX	BA	1684	7/7	0.98	0.05	109,118,126,149	1
56	OHX	AB	211	7/7	0.98	0.07	74,85,113,121	0
56	OHX	DA	1758	7/7	0.98	0.04	132,137,143,204	0
56	OHX	DA	1759	7/7	0.98	0.05	120,137,147,190	0
56	OHX	AA	3455	7/7	0.98	0.06	56,75,100,119	2
56	OHX	AA	3456	7/7	0.98	0.07	59,75,90,132	2
56	OHX	AA	3340	7/7	0.98	0.05	159,167,171,209	0
56	OHX	AA	3459	7/7	0.98	0.07	71,92,105,129	1
56	OHX	DA	1764	7/7	0.98	0.05	115,121,127,171	1
56	OHX	AA	3460	7/7	0.98	0.06	87,98,107,140	0
56	OHX	AA	3499	7/7	0.98	0.05	101,113,131,183	1
56	OHX	AA	3461	7/7	0.98	0.06	60,78,98,143	1
56	OHX	AA	3463	7/7	0.98	0.07	77,89,96,134	1
56	OHX	AA	3341	7/7	0.98	0.06	75,103,114,126	1
56	OHX	CA	3345	7/7	0.98	0.05	91,108,114,146	1
56	OHX	AA	3342	7/7	0.98	0.06	78,85,104,123	1
56	OHX	CA	3347	7/7	0.98	0.06	86,102,110,148	1
56	OHX	BA	1761	7/7	0.98	0.06	102,104,115,161	0
55	MG	CA	3265	1/1	0.98	0.14	55,55,55,55	0
56	OHX	BA	1765	7/7	0.98	0.07	111,119,130,164	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	BA	1766	7/7	0.98	0.08	89,96,106,129	1
56	OHX	BA	1767	7/7	0.98	0.06	92,119,140,142	0
56	OHX	AA	3364	7/7	0.98	0.07	92,103,108,119	1
56	OHX	DA	1779	7/7	0.98	0.04	144,146,155,215	1
56	OHX	CA	3354	7/7	0.98	0.08	78,88,98,105	1
56	OHX	BA	1769	7/7	0.98	0.07	102,107,127,145	0
56	OHX	BC	106	7/7	0.98	0.07	110,133,144,147	1
56	OHX	BC	107	7/7	0.98	0.06	105,124,134,145	1
56	OHX	AA	3320	7/7	0.98	0.09	69,81,96,121	1
56	OHX	AA	3321	7/7	0.98	0.04	97,109,121,173	1
56	OHX	AA	3300	7/7	0.98	0.06	67,91,120,167	1
56	OHX	CA	3235	7/7	0.98	0.06	43,79,99,118	0
56	OHX	CA	3237	7/7	0.98	0.06	109,109,122,166	0
56	OHX	CA	3240	7/7	0.98	0.07	96,99,103,148	1
56	OHX	CA	3241	7/7	0.98	0.08	90,96,101,122	1
56	OHX	CA	3242	7/7	0.98	0.07	95,107,117,129	1
56	OHX	AA	3323	7/7	0.98	0.07	72,87,96,117	1
56	OHX	BA	1774	7/7	0.98	0.06	80,98,111,147	1
55	MG	AA	3196	1/1	0.98	0.20	36,36,36,36	0
56	OHX	AA	3511	7/7	0.98	0.05	133,145,154,207	0
55	MG	BA	1733	1/1	0.98	0.35	60,60,60,60	0
56	OHX	CA	3483	7/7	0.98	0.07	84,93,103,136	1
56	OHX	CA	3249	7/7	0.98	0.08	86,90,104,128	1
56	OHX	CA	3485	7/7	0.98	0.07	88,102,109,144	1
56	OHX	AA	3154	7/7	0.98	0.08	76,89,110,133	1
56	OHX	CA	3251	7/7	0.98	0.06	88,107,125,141	1
55	MG	AA	3213	1/1	0.98	0.10	49,49,49,49	0
55	MG	BA	1620	1/1	0.98	0.37	70,70,70,70	0
56	OHX	AA	3400	7/7	0.98	0.08	69,80,83,116	1
56	OHX	AA	3329	7/7	0.98	0.06	85,90,103,133	1
56	OHX	CA	3492	7/7	0.98	0.06	97,102,115,126	1
56	OHX	CB	208	7/7	0.98	0.06	105,109,142,147	0
56	OHX	AA	3518	7/7	0.98	0.06	67,73,103,130	1
56	OHX	AA	3287	7/7	0.98	0.06	75,88,103,129	2
56	OHX	CA	3288	7/7	0.98	0.07	87,95,104,133	0
56	OHX	AA	3308	7/7	0.98	0.06	66,73,104,120	2
56	OHX	CA	3294	7/7	0.98	0.08	91,93,107,125	1
56	OHX	AA	3309	7/7	0.98	0.07	64,84,90,112	1
56	OHX	CA	3297	7/7	0.98	0.05	84,94,129,142	1
56	OHX	CA	3298	7/7	0.98	0.05	90,98,134,148	0
56	OHX	CA	3299	7/7	0.98	0.06	99,105,124,141	1
56	OHX	CA	3301	7/7	0.98	0.07	55,85,123,136	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3355	1/1	0.98	0.31	36,36,36,36	0
56	OHX	AA	3295	7/7	0.98	0.07	84,98,116,152	0
56	OHX	AA	3314	7/7	0.98	0.07	81,93,123,149	1
56	OHX	CA	3307	7/7	0.98	0.06	92,104,131,164	0
56	OHX	DC	109	7/7	0.98	0.05	88,92,104,159	3
56	OHX	DC	110	7/7	0.98	0.07	78,91,106,144	4
56	OHX	AA	3440	7/7	0.98	0.07	59,88,102,124	0
57	ZN	BG	301	1/1	0.98	0.18	79,79,79,79	0
56	OHX	AA	3441	7/7	0.98	0.07	84,93,115,140	0
56	OHX	CA	3310	7/7	0.98	0.06	74,88,107,129	1
56	OHX	AA	3424	7/7	0.99	0.06	92,97,108,112	0
56	OHX	AA	3426	7/7	0.99	0.08	70,84,89,118	0
56	OHX	CA	3300	7/7	0.99	0.07	66,75,91,101	1
56	OHX	AA	3427	7/7	0.99	0.05	29,70,88,108	0
56	OHX	AA	3428	7/7	0.99	0.07	67,79,86,113	0
56	OHX	CA	3303	7/7	0.99	0.04	92,96,123,138	0
56	OHX	AA	3429	7/7	0.99	0.06	69,73,84,102	1
56	OHX	CA	3305	7/7	0.99	0.06	70,83,99,129	1
56	OHX	AA	3430	7/7	0.99	0.06	63,78,92,111	1
56	OHX	AA	3431	7/7	0.99	0.05	74,81,100,115	0
56	OHX	AA	3432	7/7	0.99	0.05	72,98,103,107	0
56	OHX	DA	1740	7/7	0.99	0.05	139,153,162,184	0
56	OHX	AA	3433	7/7	0.99	0.04	63,65,104,122	1
56	OHX	AA	3434	7/7	0.99	0.06	62,71,94,101	1
56	OHX	AA	3435	7/7	0.99	0.07	61,70,93,100	3
56	OHX	AA	3436	7/7	0.99	0.05	78,91,117,117	0
56	OHX	AA	3437	7/7	0.99	0.05	81,95,107,131	0
56	OHX	AA	3438	7/7	0.99	0.06	51,64,72,96	2
56	OHX	AA	3439	7/7	0.99	0.04	69,82,92,115	1
56	OHX	CA	3316	7/7	0.99	0.05	119,122,129,158	0
56	OHX	AA	3296	7/7	0.99	0.05	115,120,123,158	0
55	MG	B1	101	1/1	0.99	0.36	26,26,26,26	0
56	OHX	AA	3442	7/7	0.99	0.05	70,87,119,140	0
56	OHX	AA	3289	7/7	0.99	0.07	53,58,81,93	0
56	OHX	AA	3444	7/7	0.99	0.05	80,103,116,131	1
56	OHX	AA	3445	7/7	0.99	0.05	75,87,109,120	1
56	OHX	AA	3446	7/7	0.99	0.07	68,90,101,115	2
56	OHX	CA	3324	7/7	0.99	0.07	65,83,94,110	2
56	OHX	BA	1696	7/7	0.99	0.04	47,75,99,113	0
56	OHX	BA	1755	7/7	0.99	0.06	72,74,97,109	0
56	OHX	CA	3327	7/7	0.99	0.05	76,83,103,129	1
56	OHX	BA	1756	7/7	0.99	0.08	59,79,107,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	BA	1757	7/7	0.99	0.07	57,66,87,98	2
56	OHX	CA	3330	7/7	0.99	0.04	102,106,115,169	0
56	OHX	BA	1758	7/7	0.99	0.07	69,88,100,119	0
56	OHX	BA	1759	7/7	0.99	0.07	78,93,120,156	0
56	OHX	BA	1760	7/7	0.99	0.06	71,106,126,148	0
56	OHX	AA	3290	7/7	0.99	0.06	10,72,91,128	0
56	OHX	BA	1762	7/7	0.99	0.07	72,94,107,136	0
56	OHX	BA	1763	7/7	0.99	0.05	94,115,123,136	0
56	OHX	AE	304	7/7	0.99	0.06	74,87,107,110	1
56	OHX	AO	204	7/7	0.99	0.05	83,94,106,121	1
56	OHX	AA	3310	7/7	0.99	0.04	94,104,125,156	0
56	OHX	CA	3232	7/7	0.99	0.10	72,77,83,137	0
56	OHX	CA	3233	7/7	0.99	0.08	74,85,95,121	0
56	OHX	CA	3234	7/7	0.99	0.06	77,91,119,122	2
56	OHX	AA	3449	7/7	0.99	0.04	64,74,89,112	2
56	OHX	CA	3236	7/7	0.99	0.06	81,104,120,146	0
56	OHX	AA	3311	7/7	0.99	0.06	97,106,117,155	1
56	OHX	CA	3238	7/7	0.99	0.08	80,102,103,125	1
56	OHX	CA	3239	7/7	0.99	0.06	66,92,107,113	1
56	OHX	CA	3461	7/7	0.99	0.08	38,55,94,109	0
56	OHX	AA	3291	7/7	0.99	0.07	68,75,102,108	3
56	OHX	AA	3301	7/7	0.99	0.06	88,89,93,110	1
56	OHX	AA	3453	7/7	0.99	0.06	95,106,114,148	0
56	OHX	CA	3243	7/7	0.99	0.05	121,128,140,172	0
56	OHX	AA	3292	7/7	0.99	0.06	50,75,88,112	0
56	OHX	AA	3399	7/7	0.99	0.10	42,51,73,98	0
56	OHX	AA	3293	7/7	0.99	0.07	54,82,88,102	2
56	OHX	BA	1775	7/7	0.99	0.04	111,114,129,169	1
56	OHX	BA	1776	7/7	0.99	0.05	102,114,119,153	1
56	OHX	AA	3457	7/7	0.99	0.04	73,83,101,131	1
56	OHX	AA	3316	7/7	0.99	0.05	80,95,97,136	0
56	OHX	BA	1779	7/7	0.99	0.05	102,112,125,152	1
56	OHX	AA	3359	7/7	0.99	0.05	61,75,93,113	0
56	OHX	AA	3360	7/7	0.99	0.07	58,67,70,97	1
56	OHX	AA	3361	7/7	0.99	0.06	51,71,83,107	0
56	OHX	CA	3255	7/7	0.99	0.05	103,107,122,145	1
56	OHX	CA	3256	7/7	0.99	0.06	88,101,112,126	1
56	OHX	AA	3462	7/7	0.99	0.06	75,85,103,106	1
56	OHX	CA	3270	7/7	0.99	0.05	73,87,105,117	0
56	OHX	CA	3272	7/7	0.99	0.08	54,70,84,85	1
56	OHX	CA	3273	7/7	0.99	0.06	58,69,86,110	0
56	OHX	CA	3274	7/7	0.99	0.07	67,83,114,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	OHX	CA	3276	7/7	0.99	0.06	81,100,117,133	0
56	OHX	CA	3277	7/7	0.99	0.06	73,81,99,107	1
56	OHX	CA	3278	7/7	0.99	0.05	81,96,114,120	0
56	OHX	CA	3279	7/7	0.99	0.07	80,89,109,118	0
56	OHX	CA	3280	7/7	0.99	0.07	82,87,100,129	0
56	OHX	CA	3283	7/7	0.99	0.07	81,83,86,120	1
56	OHX	AA	3362	7/7	0.99	0.08	40,81,119,136	1
56	OHX	AA	3294	7/7	0.99	0.05	94,100,117,120	0
56	OHX	CA	3286	7/7	0.99	0.04	87,94,108,115	0
56	OHX	CA	3287	7/7	0.99	0.08	69,74,104,109	3
55	MG	AA	3172	1/1	0.99	0.34	38,38,38,38	0
56	OHX	CA	3289	7/7	0.99	0.04	69,83,106,125	0
56	OHX	CA	3290	7/7	0.99	0.05	94,101,123,130	0
56	OHX	CA	3291	7/7	0.99	0.07	86,105,118,139	0
56	OHX	CA	3292	7/7	0.99	0.08	69,105,113,146	0
56	OHX	AA	3420	7/7	0.99	0.08	63,69,102,115	0
56	OHX	AA	3421	7/7	0.99	0.07	50,71,87,114	0
56	OHX	DA	1718	7/7	0.99	0.08	73,98,100,135	0
56	OHX	AA	3422	7/7	0.99	0.07	74,81,107,116	0
56	OHX	DA	1721	7/7	0.99	0.04	94,108,116,135	0
56	OHX	DA	1722	7/7	0.99	0.06	84,90,106,116	0
56	OHX	DA	1723	7/7	0.99	0.06	107,111,116,151	0
56	OHX	CA	3296	7/7	0.99	0.06	65,90,108,135	2
56	OHX	AA	3423	7/7	0.99	0.08	44,66,84,86	1
56	OHX	DA	1727	7/7	0.99	0.05	114,126,131,160	0
57	ZN	DQ	101	1/1	0.99	0.04	123,123,123,123	0
56	OHX	CA	3282	7/7	1.00	0.03	79,83,97,109	0
56	OHX	DA	1734	7/7	1.00	0.03	102,105,122,149	1
56	OHX	AA	3425	7/7	1.00	0.04	45,61,75,79	0
56	OHX	AA	3417	7/7	1.00	0.06	68,72,82,103	0
56	OHX	CF	301	7/7	1.00	0.07	54,58,79,92	0
56	OHX	CA	3275	7/7	1.00	0.04	56,80,112,114	1
56	OHX	AA	3418	7/7	1.00	0.06	39,61,82,95	0
56	OHX	AA	3419	7/7	1.00	0.05	67,75,91,95	0
56	OHX	AF	303	7/7	1.00	0.07	45,52,58,77	0
56	OHX	CA	3271	7/7	1.00	0.09	67,82,101,115	0
55	MG	AA	3194	1/1	1.00	0.04	26,26,26,26	0
56	OHX	CA	3281	7/7	1.00	0.06	101,105,126,132	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.