



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 09:50 PM EDT

PDB ID : 4V8E / pdb_00004v8e
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

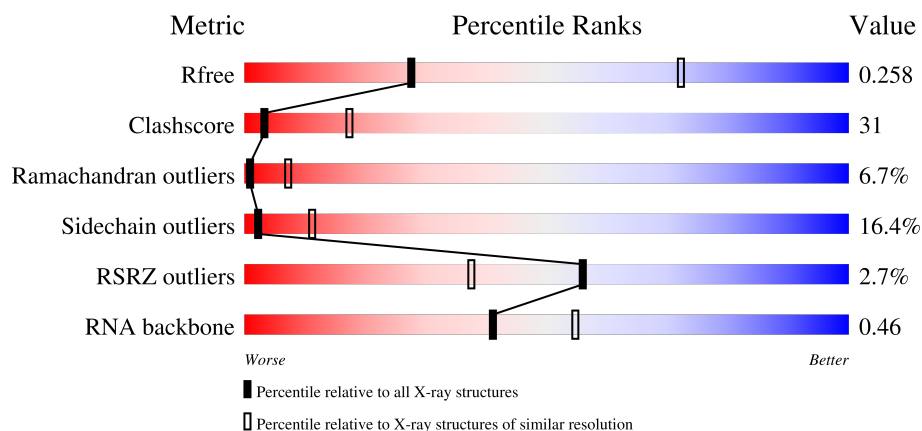
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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

Mol	Chain	Length	Quality of chain
1	AA	2912	36% 47% 17%
1	CA	2912	32% 50% 17%
2	AB	122	43% 48% 10%
2	CB	122	31% 48% 20%

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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	CA	3045	-	-	-	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 (CCD ID: MG) (formula: Mg).

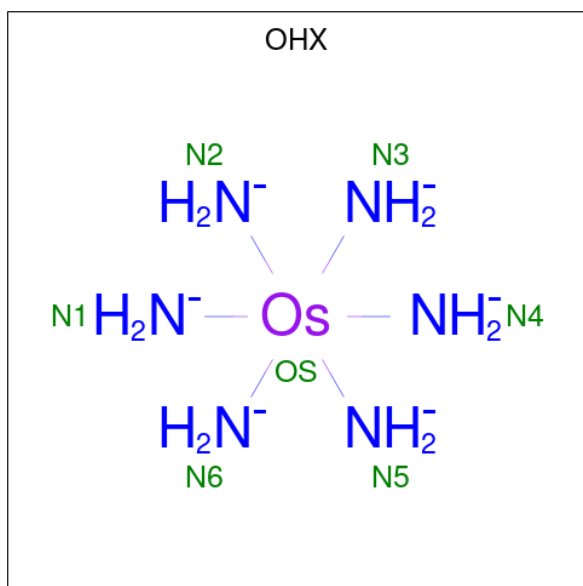
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	AA	331	Total Mg 331 331	0	0
55	AB	6	Total Mg 6 6	0	0
55	AE	3	Total Mg 3 3	0	0
55	AF	2	Total Mg 2 2	0	0
55	AO	3	Total Mg 3 3	0	0
55	A0	1	Total Mg 1 1	0	0
55	A1	1	Total Mg 1 1	0	0
55	A3	1	Total Mg 1 1	0	0
55	A5	1	Total Mg 1 1	0	0
55	BA	115	Total Mg 115 115	0	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 (CCD ID: 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		

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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		
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	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
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56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
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56	BA	1	Total	N	Os	0	0
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56	BA	1	Total	N	Os	0	0
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56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
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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
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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		
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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		
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			7	6	1		
56	BA	1	Total	N	Os	0	0
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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
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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
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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
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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		
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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		
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
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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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			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
			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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			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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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
56	CA	1	Total	N	Os	0	0
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			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
			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
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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		
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			7	6	1		
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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		
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
			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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			7	6	1		
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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		
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
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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		
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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
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			7	6	1		
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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
			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		
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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		

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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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			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		
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		
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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		
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	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		
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			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
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56	C6	1	Total	N	Os	0	0
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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		

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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		
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			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
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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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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		
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		

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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		
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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		
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		

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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		

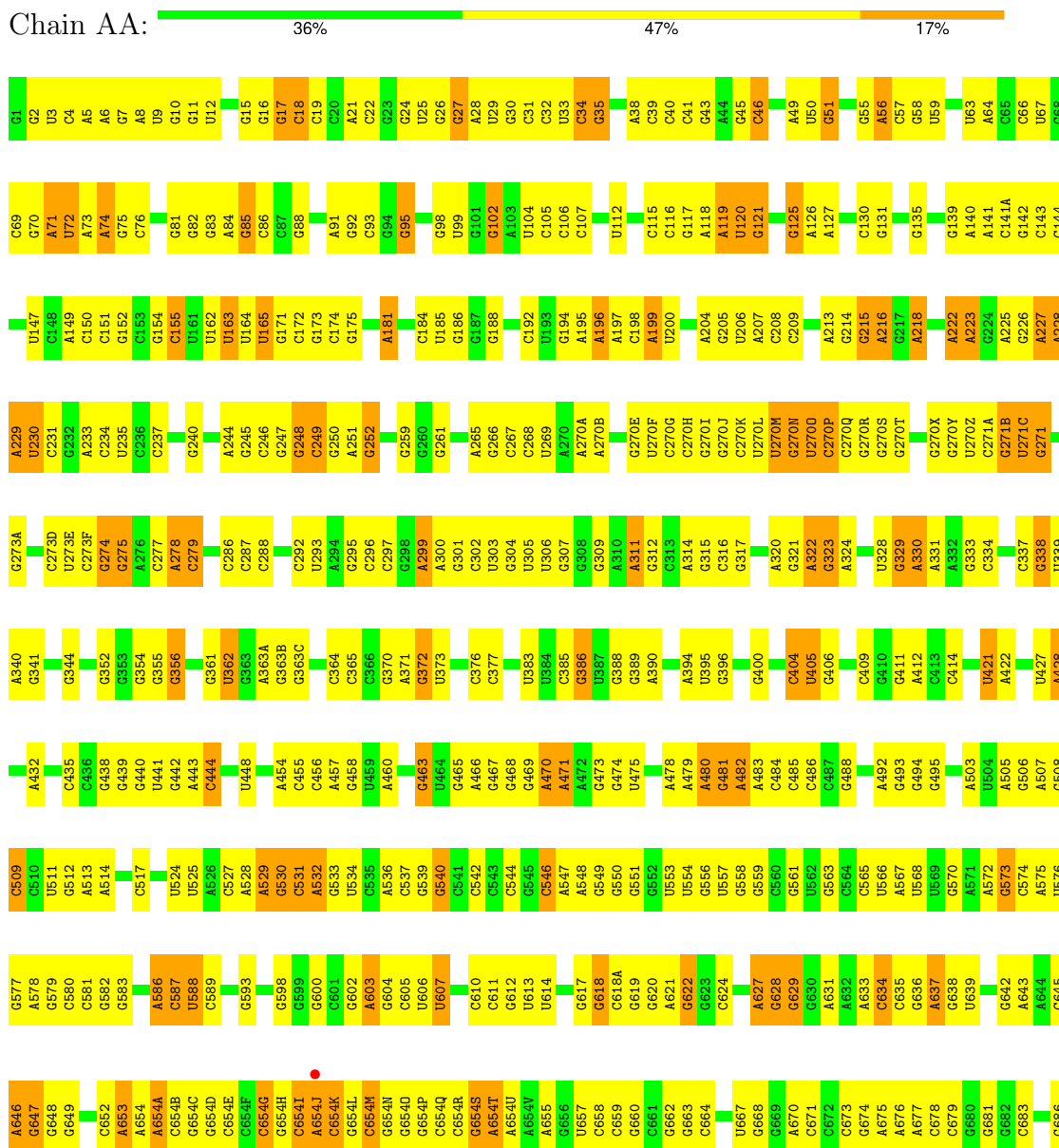
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

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)



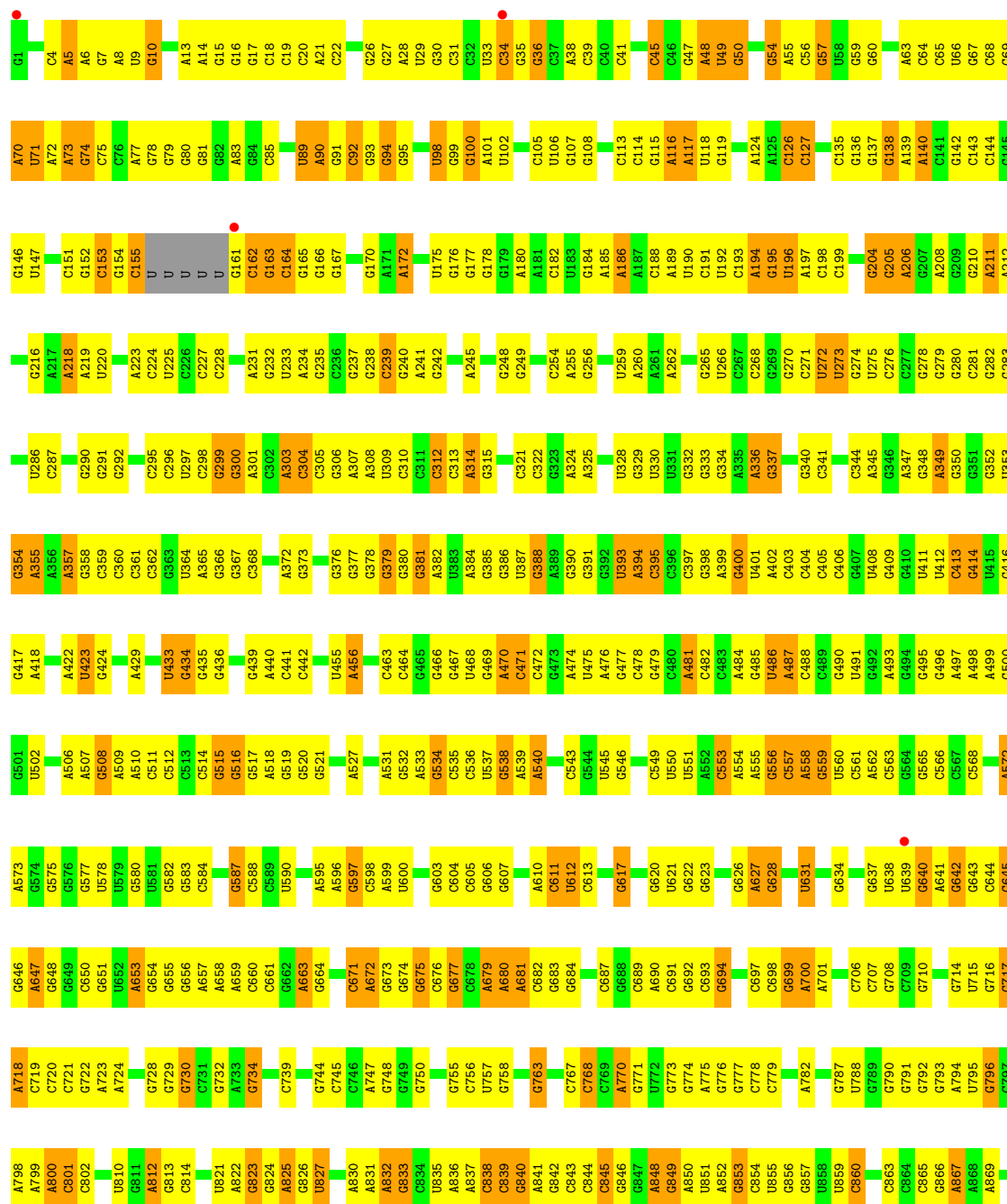
A1554	C1577	A1511	G1364	G1365	C1291	A1210	G1144	C1076	G1013	A945	A866	A769	G680
C1578	U1578	U1514	A1365	A1368	U1292	U1211	C1145	A1077	U1014	G946	C867	C790	C691
A1550	C1579	C1515	G1368	G1369	C1293	G1212	G1149	U1078	G1015	G948	U1014	G792	G696
G1581	U1516	U1516	G1369	G1370	U1294	A1214	G1152	A1080	G1017	G951	A870	A793	G695
C1582	G1517	C1518	U1372	U1373	G1295	G1215	C1153	U1081	C1018	G952	A871	G794	A705
A1583	C1450	C1451	A1373	A1374	G1296	G1216	C1154	U1082	U1019	A953	A872	C795	G717
C1585	C1451	C1452	G1374	G1375	C1297	G1219	C1155	U1083	A1020	G954	G873	C796	
A1586	A1453	U1520	A1378	A1379	C1298	G1221	A1156	U1084	G1022	C955	U877	C797	
A1587	U1455	G1522	A1378	A1379	U1300	C1221	U1159	A1086	U1023	G956	G798	G798	
G1591	C1458	G1525	G1379	G1380	A1301	C1222	U1160	G1087	G1024	G957	A802	G723	
C1592	G1459	G1526	G1380	G1381	A1302		C1161	A1088	G1025	U958	A802	U724	
G1593	A1460	A1527	G1382	G1383	G1303	G1230	G1162	G1089	U1026	A959	G805	G725	
A1594	G1461	A1528	C1383	C1384	G1309	G1231	G1163	U1090	A1027	A960	C806	G726	
A1596	C1464	G1530	G1384	G1385	G1310	G1235	U1165	C1091	A1028	G961	G809	A727	
G1600	G1465	G1531	G1386	G1387	G1311	G1236	C1166	C1092	G1029	G962	U810	G728	
G1601	G1466	C1532	C1387	C1388	U1312	G1244	U1167	U1094	A1030	C967	U811	C731	
C1605	C1467	C1533	G1388	G1389	U1313	G1247	G1168	A1095	U1033	G968	C812	G732	
G1606	C1468	U1535	G1389	G1390	C1314	U1248	G1169	U1096	G1036	U969	C813	G733	
C1607	A1469	A1536	G1390	G1391	U1316	G1249	G1170	U1097	G1037	C970	C814	G741	
A1608	G1470	C1537	U1394	U1395	G1317	G1250	C1171	A1098	C1038	G972	C817	G742	
A1609	A1471	G1538	A1396	A1397	C1318	A1247	G1172	C1100	G1039	A973	C818	G745	
U1610	A1472	G1539	U1396	U1397	G1319	U1248	A1174	U1101	G1042	G974	A819	G746	
G1615	G1473	G1540	C1399	C1400	C1320	G1249	U1175	A1102	C1043	C974A	A820	U747	
U1616	G1474	U1541	G1400	G1401	U1323	U1249	G1176	A1103	G1044	G975	A821	G748	
C1617	C1475	G1542	G1401	G1402	G1324	G1250	A1177	C1104	G1045	G978	U827	C749	
A1618	A1477	A1543	C1402	C1403	G1325	A1253	C1178	U1105	A1046	G979	U828	A750	
C1619	G1478	C1544	C1403	C1404	U1326	U1254	C1179	G1106	G1047	A980	A829	A751	
G1625	G1479	A1545	U1405	U1406	C1327	U1255	C1180	U1107	A1048	A981	A830	A752	
A1626	U1480	A1546	U1406	U1407	G1328	G1256	C1181	U1108	C1049	C982	G831	C753	
G1627	C1407	C1547	C1407	C1408	U1329	C1257	A1182	C1109	G1050	A983	U832	C754	
G1628	G1486	G1548	G1416	G1417	C1330	U1261	C1185	A1111	G1051	A984	C904	C755	
U1629	G1487	C1549	C1417	C1418	A1331	A1262	G1187	G1112	C1052	C985	A835	C756	
C1630A	U1488	C1550	G1418	G1419	G1332	U1263	U1188	U1113	C1053	G986	G836	G760	
A1631	U1489	G1551	A1418	A1419	A1336	A1264	A1189	G1114	A1054	G989	C837	A761	
G1632	A1490	G1552	A1419	A1420	G1337	A1265	G1190	G1222	G1055	A990	C838	U762	
G1633	G1491	A1554	U1420	U1421	G1338	U1266	G1191	A1057	G1056	C991	U839	A773	
A1637	G1492	C1555	G1421	G1422	U1340	A1267	G1192	G1225	G1058	C992	G845	G775	
C1638	C1493	C1556	G1422	G1423	U1341	A1269	A1194	A1126	G1059	G993	C846	G776	
U1639	A1494	C1557	G1423	G1424	G1344	C1270	G1195	U1127	U1060	C994	U847	C766	
C1640	A1495	A1558	G1424	G1425	G1345	G1271	C1196	U1130	U1061	C995	G848	U773	
A1641	A1496	G1559	G1425	G1426	G1346	A1272	G1197	G1131	G1062	A996	G849	A774	
G1642	U1497	G1560	G1426	G1427	G1347	U1273	U1198	A1132	C1063	C997	C850	G775	
G1643	C1498	G1561	A1427	A1428	G1347	A1274	U1199	U1133	U1065	U999	G928	G776	
C1644	G1499	A1566	C1428	G1429	G1348	A1275	C1200	C1135	U1066	A1000	G929	U851	
G1647	U1500	C1567	G1429	G1430	A1349	A1276	C1201	G1136	A1067	C998	C857	G780	
C1648	C1504	G1568	U1431	U1432	U1352	G1277	C1202	G1137	G1068	A933	U858	A781	
G1649	C1505	A1569	C1432	C1433	U1352	A1278	G1203	G1138	A1069	G1003	G859	A782	
G1650	C1506	A1570	U1433	U1434	G1356	G1279	A1204	G1139	A1070	G938	U860	A783	
G1651	A1507	A1571	A1434	A1435	G1356	G1280	U1205	C1140	G1071	C1005	A861	A784	
C1652	C1508	C1575	G1441	G1442	A1359	G1281	G1206	U1141	G1072	C1006	C862	G785	
A1749	A1509	U1576	G1442	G1443	A1360	A1287	C1207	U1142	A1073	G1011	A863	G786	
G1653	A1510		G1443	G1444	A1360	U1288	C1208	A142A	G1074	G1012	G864	U787	
							G1209	A143	C1075		G944	A788	





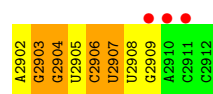
• Molecule 1: RNA (2912-MER)

Chain CA: 32% 50% 17%



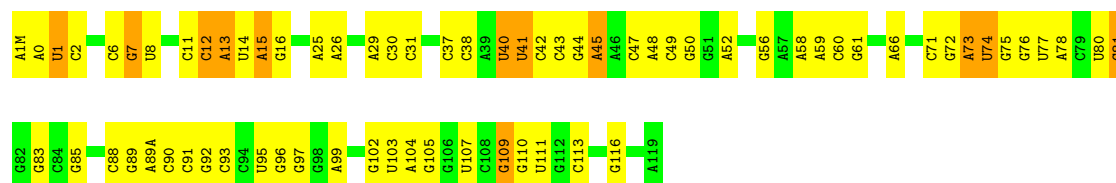
A1847	G1774	G1709	U1626	C1556	G1488	A1412	A1334	G1265	A1189	C1122	G1058	G996	A935	C873
G1848	C1775	A1712	A1627	A1557	G1489	G1415	U1335	A1266	A1190	C1123	U1059	C997	C936	U874
G1849		A1713		G1558	G1490	G1416	C1336	C1267		A1124	U1061	G998	C937	U875
U1850		G1714	A1631	G1559	G1491	G1417	C1337	C1268	C1193		U1062	A999	A938	U876
A1851	G1785	G1715	C1632	U1560	A1492	G1418	U1338	C1269	C1194	U1127	G1063	C1000	G939	A877
A1852	G1786	G1716	A1633	U1561	C1493	U1419	C1339	C1270	C1195	U1128	G1064	C1001	C940	G878
A1853	C1786	A1717	A1634	C1562	C1494	U1419	C1340	C1271	G1196		G1065	C1002	C941	G879
G1854		G1718	C1635	U1563	G1495			A1272	C1197		U1066	A1003	U942	G880
G1855	G1787	C1718	C1636		G1496	C1422	C1345	A1273	G1198	A1132	U1067	U1004	U943	U881
G1856	U1789	C1719	U1637	U1567	A1497	G1423	G1346	G1276	C1199	G1134	A1068	A1005	C944	C882
A1857	C1790	C1720	G1638	G1568	A1498	G1424	U1347	G1277	C1200	A1135	A1069	C945	C945	A883
G1858	G1791	U1721	C1639	G1569	C1499	A1425	A1348	C1278	G1201	G1136	G1069	C1007	A946	G884
A1859	A1792	G1722	G1640	U1501	C1500	A1426		G1279	A1202	U1137	U1070	G1008	A947	C885
G1860	C1793	C1723	G1641	G1502	A1501	G1427	C1351	C1279	A1203	G1138	G1071	U1009	A948	C886
A1861			G1642	U1503		G1428		A1280		C1139	G1072	C950	U949	U887
G1865	G1796	G1726		G1504	A1355	G1429	A1355	U1281	U1206	G1012	U1073	C951	C950	C888
U1866	G1797	U1727	C1645	G1505	C1356	A1430	G1357	G1282	G1207	C1013	A1074	C951	C951	C892
G1867	G1798	G1729	C1647	A1576	G1506	A1431	G1358	G1283	C1208	A1014	A1075	U952	U952	C893
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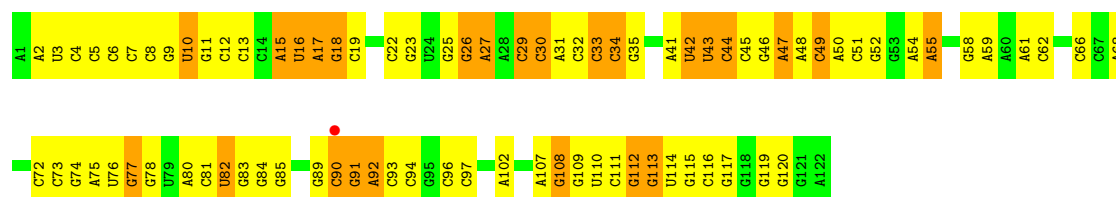
• Molecule 2: 5S RIBOSOMAL RNA

Chain AB: 43% 48% 10%



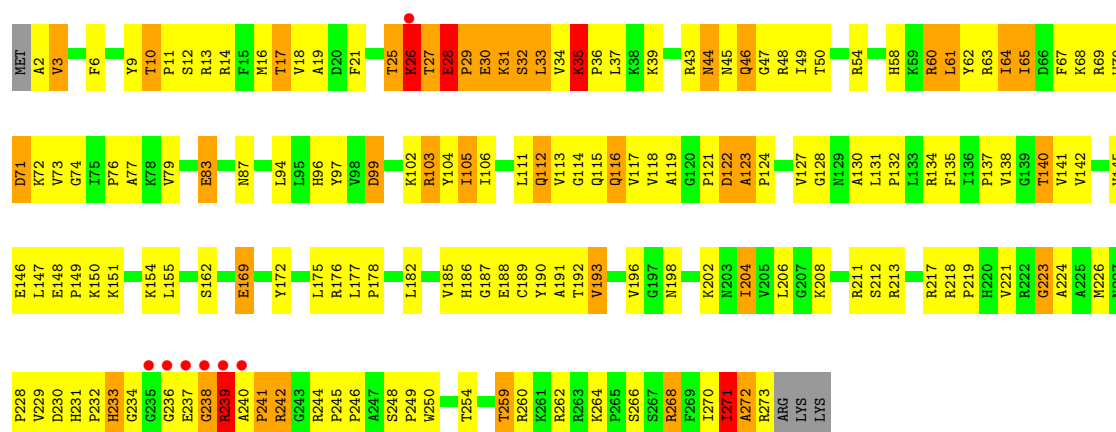
• Molecule 2: 5S RIBOSOMAL RNA

Chain CB: 31% 48% 20%



• Molecule 3: 50S ribosomal protein L2

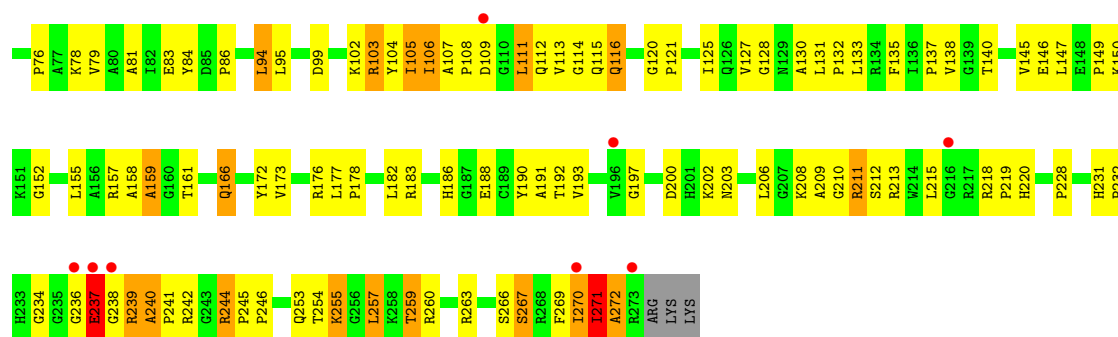
Chain AD: 3% 39% 44% 13% ..



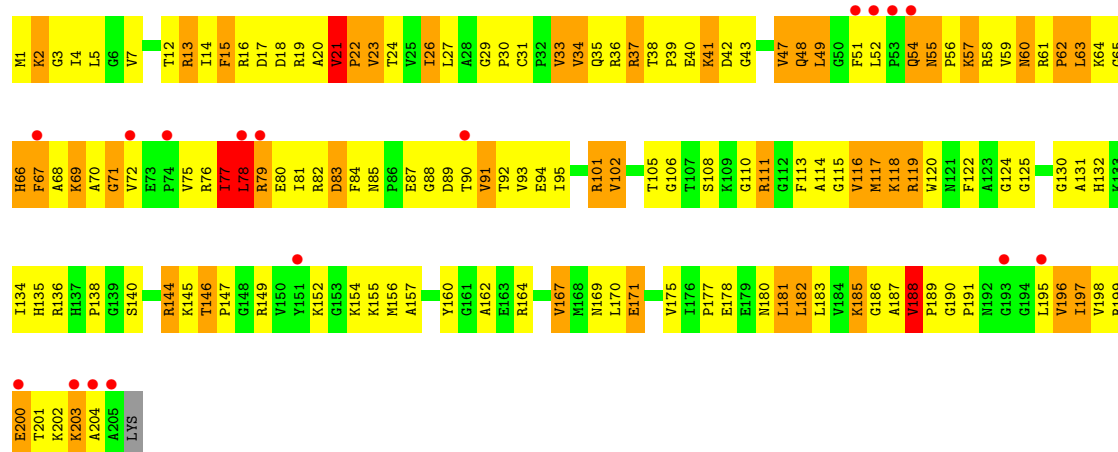
• Molecule 3: 50S ribosomal protein L2

Chain CD: 5% 44% 43% 10% ..

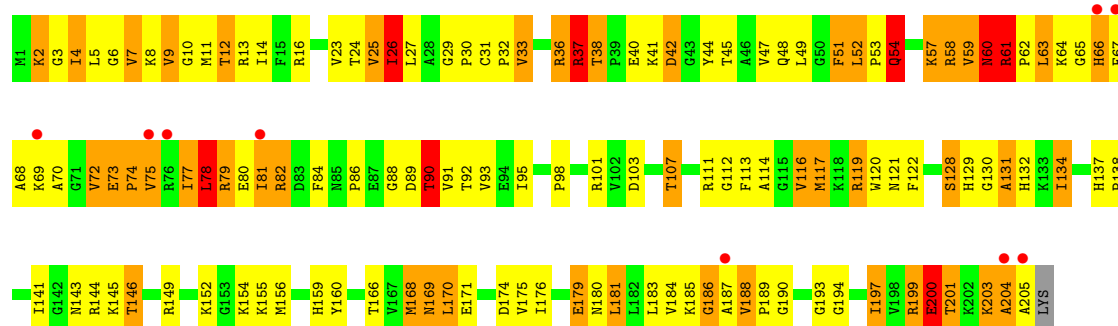




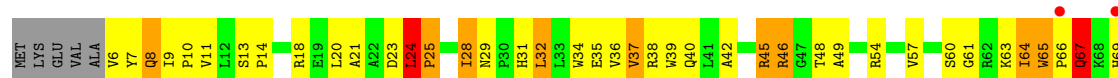
• Molecule 4: 50S ribosomal protein L3

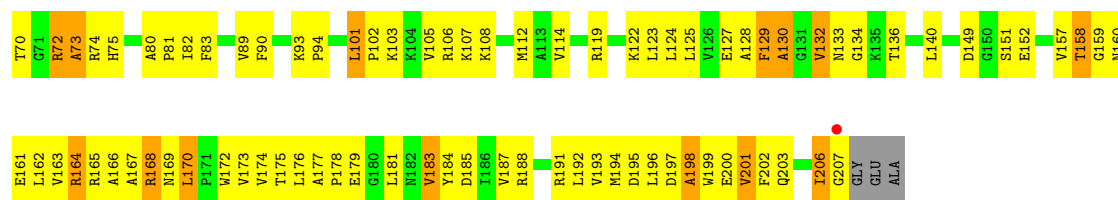


• Molecule 4: 50S ribosomal protein L3

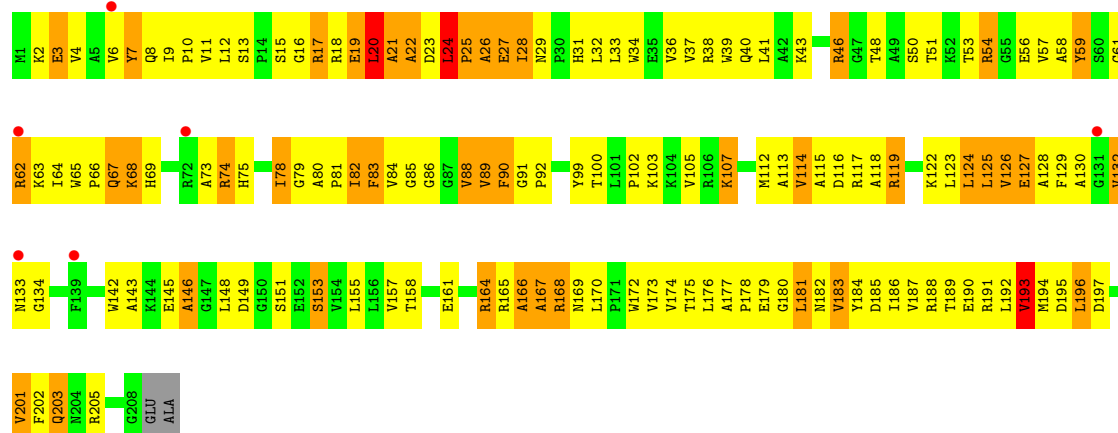


• Molecule 5: 50S ribosomal protein L4

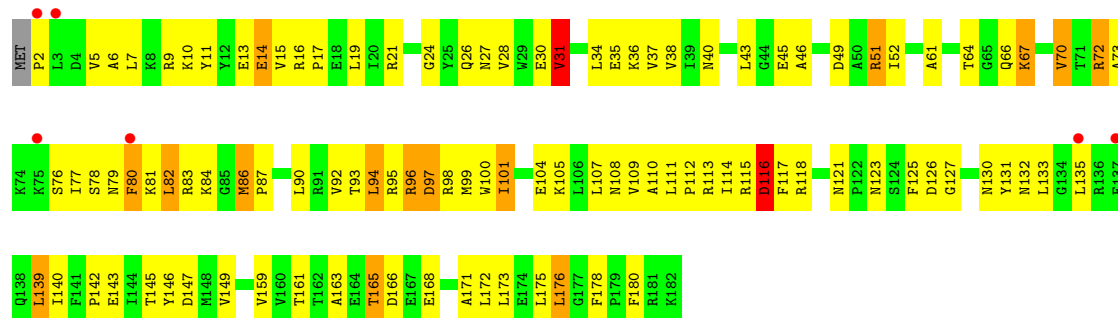
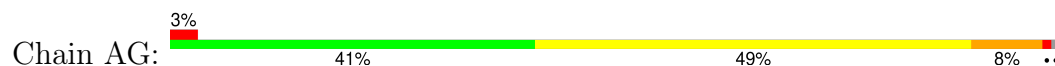




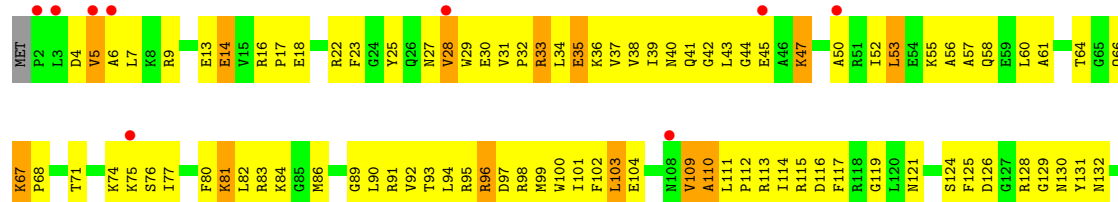
• Molecule 5: 50S ribosomal protein L4

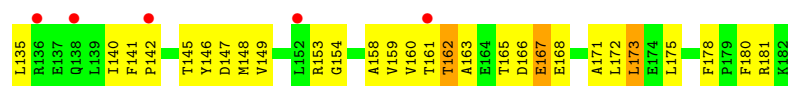


• Molecule 6: 50S ribosomal protein L5

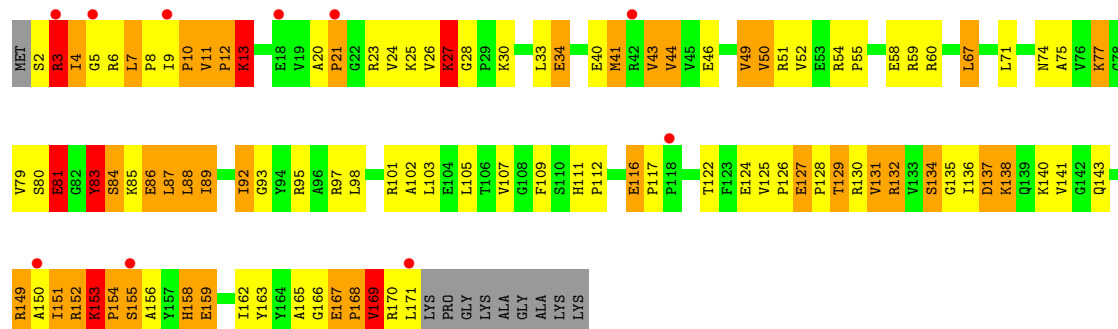


• Molecule 6: 50S ribosomal protein L5

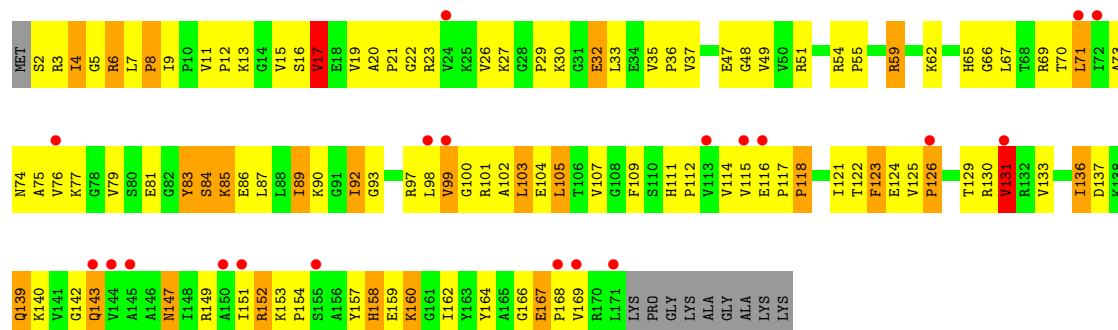




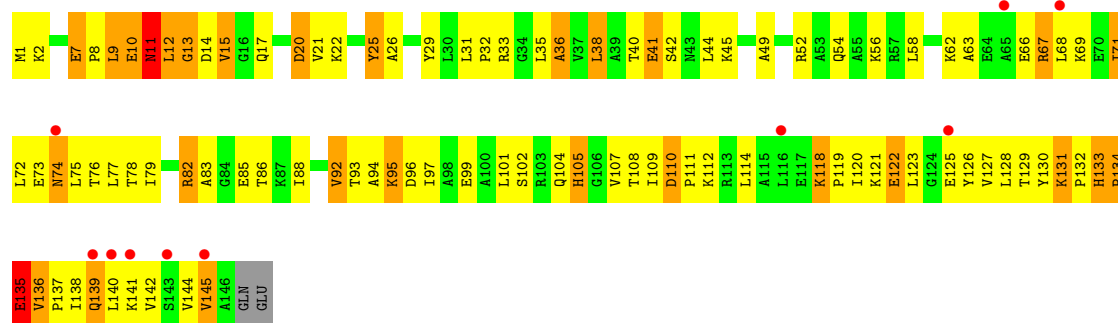
• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6

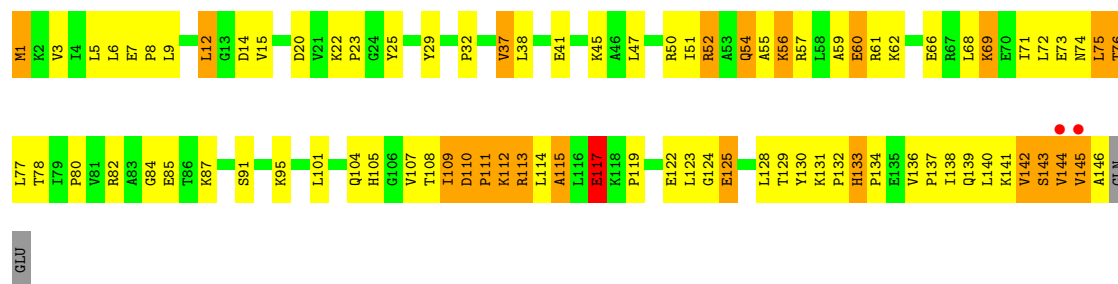


• Molecule 8: 50S ribosomal protein L9

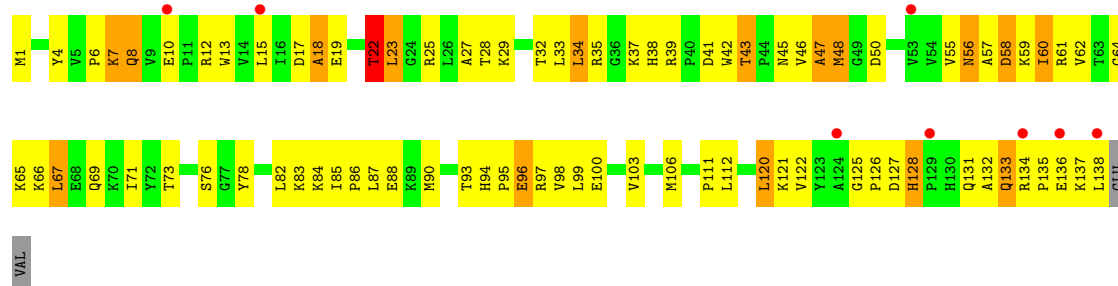


• Molecule 8: 50S ribosomal protein L9

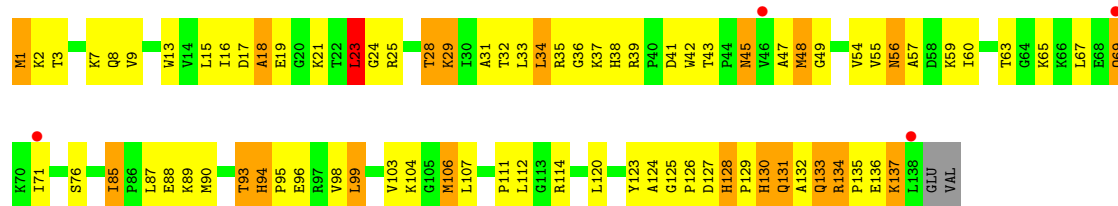




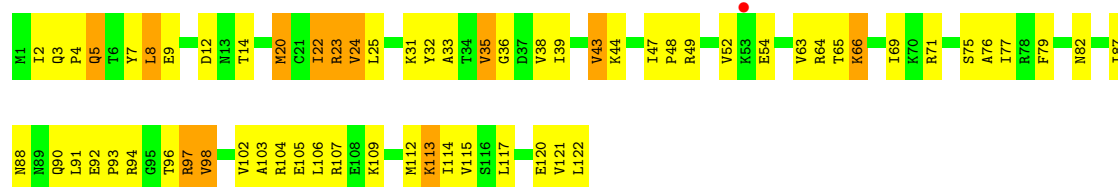
• Molecule 9: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L13

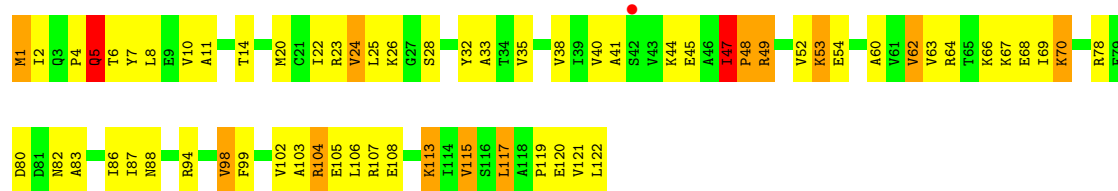


• Molecule 10: 50S ribosomal protein L14

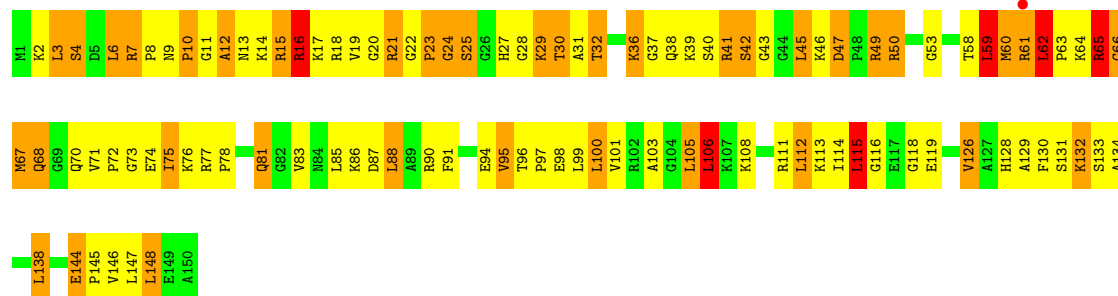


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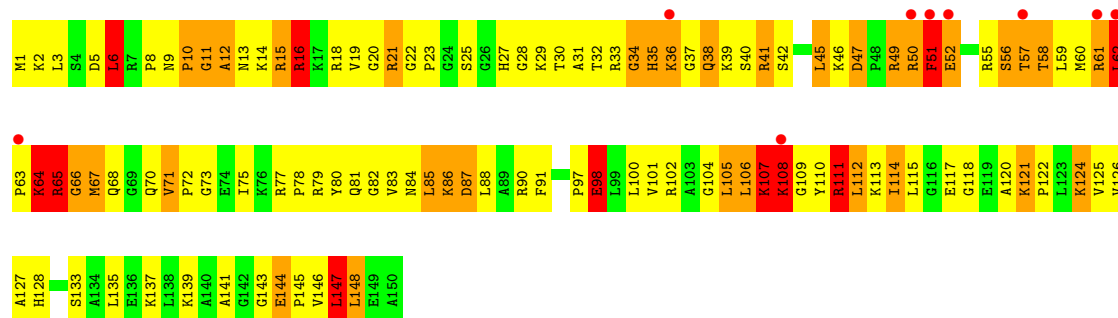




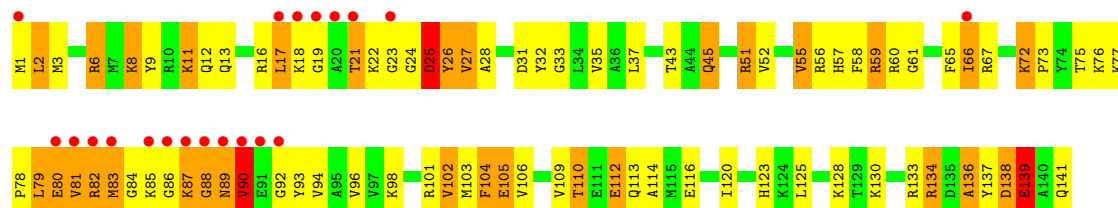
• Molecule 11: 50S ribosomal protein L15



• Molecule 11: 50S ribosomal protein L15

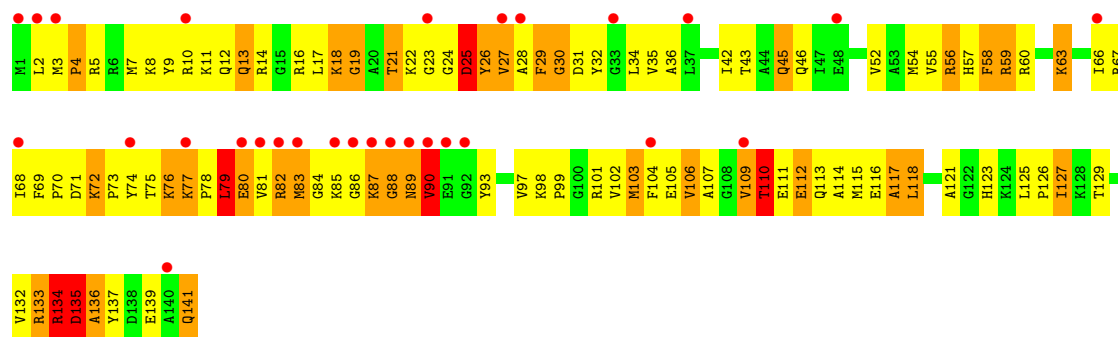


• Molecule 12: 50S ribosomal protein L16

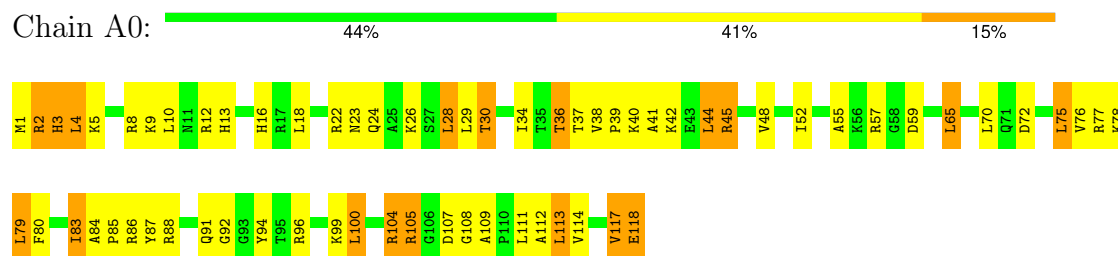


• Molecule 12: 50S ribosomal protein L16

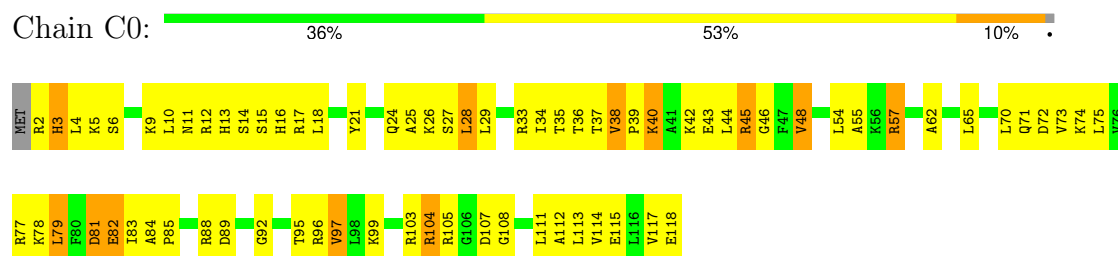




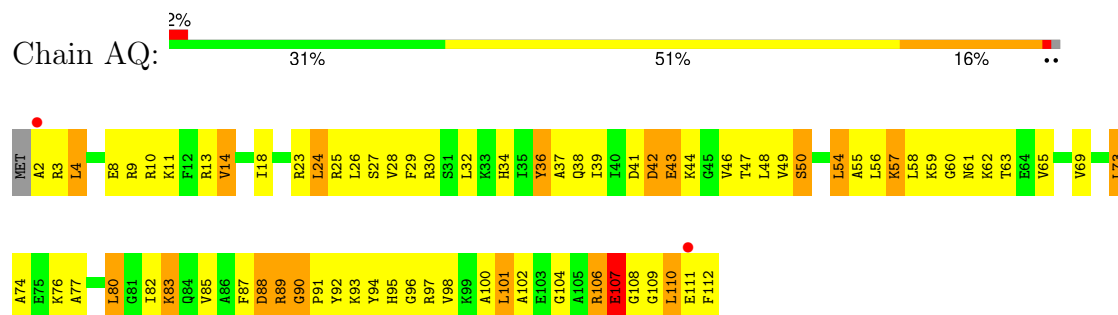
• Molecule 13: 50S ribosomal protein L17



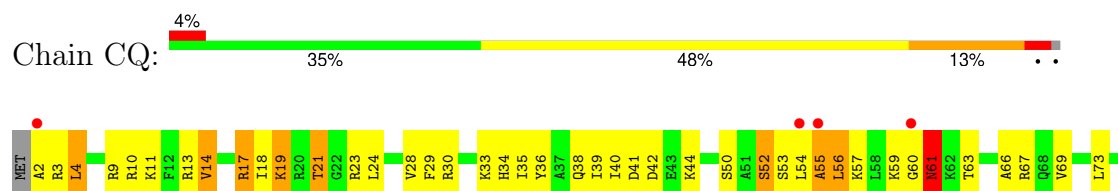
• Molecule 13: 50S ribosomal protein L17



• Molecule 14: 50S ribosomal protein L18

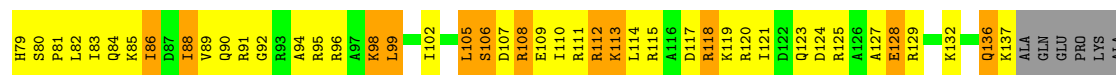
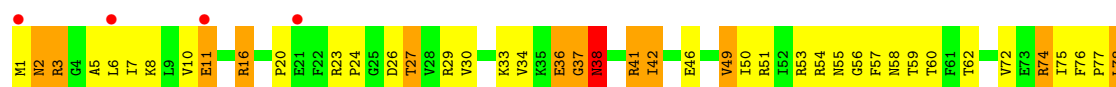


• Molecule 14: 50S ribosomal protein L18

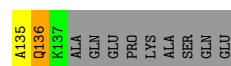
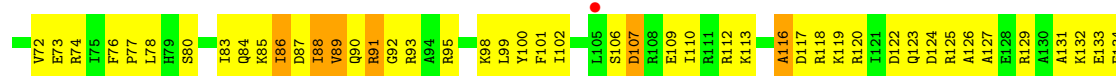
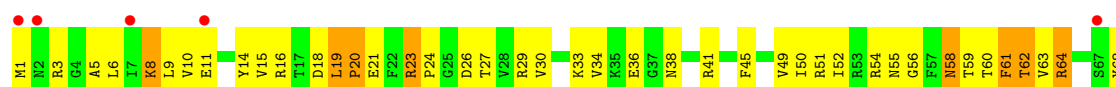




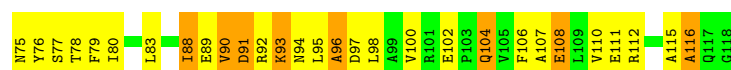
• Molecule 15: 50S ribosomal protein L19



• Molecule 15: 50S ribosomal protein L19



• Molecule 16: 50S ribosomal protein L20

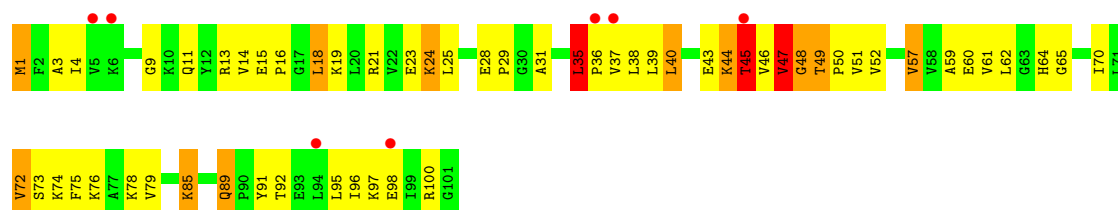


• Molecule 16: 50S ribosomal protein L20



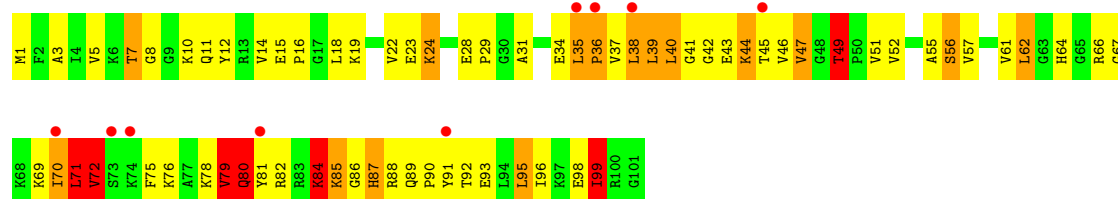
• Molecule 17: 50S ribosomal protein L21

Chain A2: 

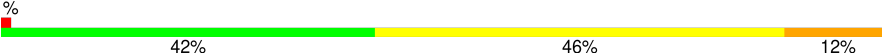


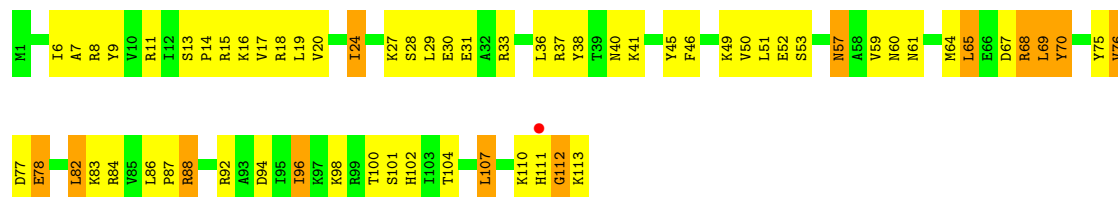
• Molecule 17: 50S ribosomal protein L21

Chain C2: 



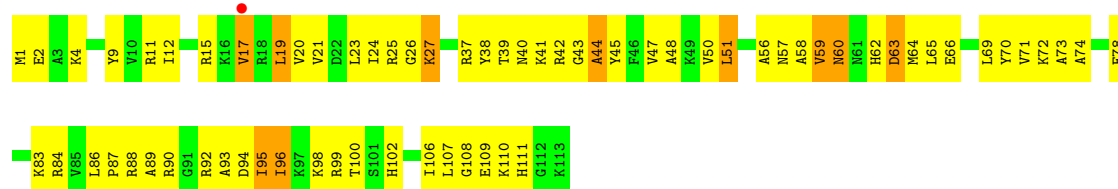
• Molecule 18: 50S ribosomal protein L22

Chain AS: 



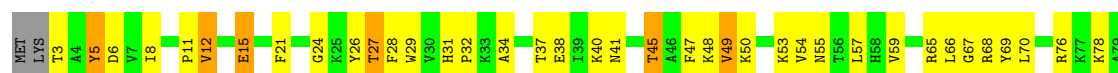
• Molecule 18: 50S ribosomal protein L22

Chain CS: 



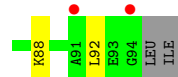
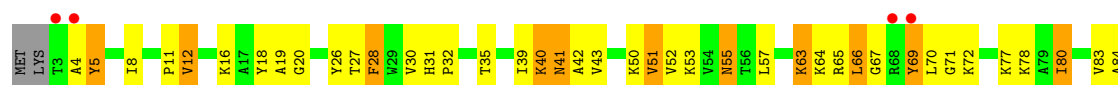
• Molecule 19: 50S ribosomal protein L23

Chain AT: 





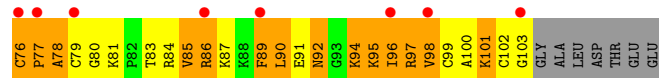
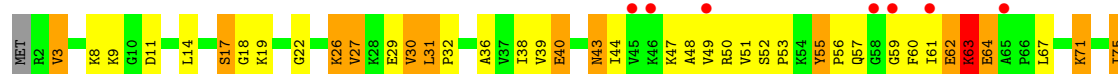
- Molecule 19: 50S ribosomal protein L23



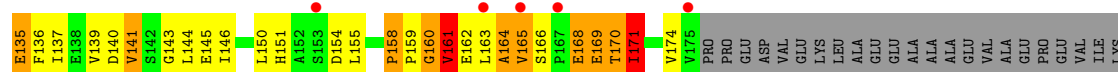
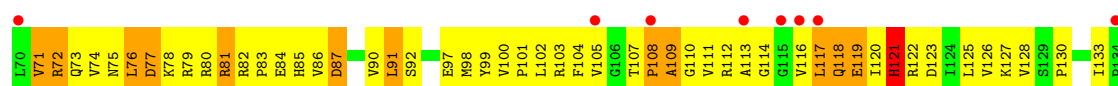
- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24

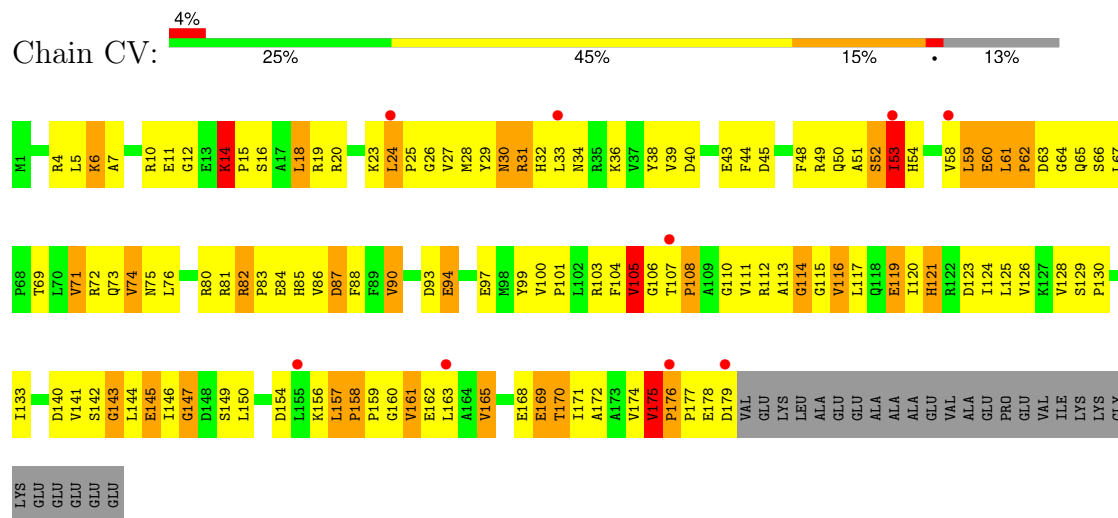


- Molecule 21: 50S ribosomal protein L25

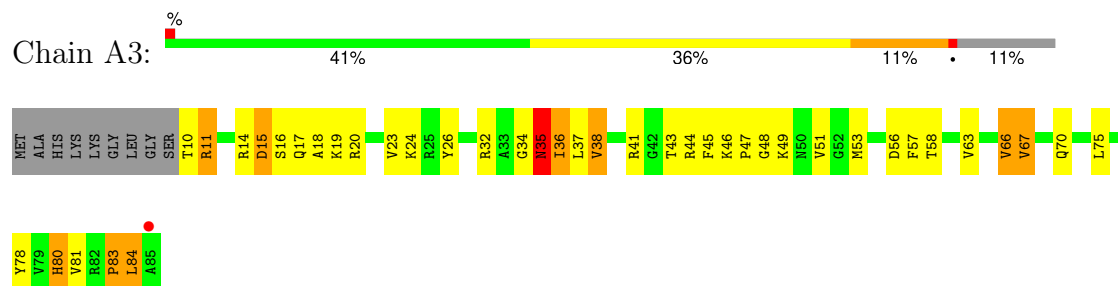


LYS
GLY
LYS
GLU
GLU
GLU
GLU

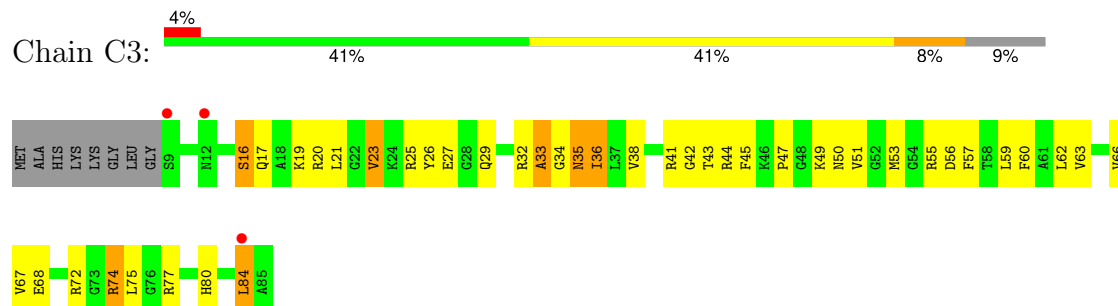
• Molecule 21: 50S ribosomal protein L25



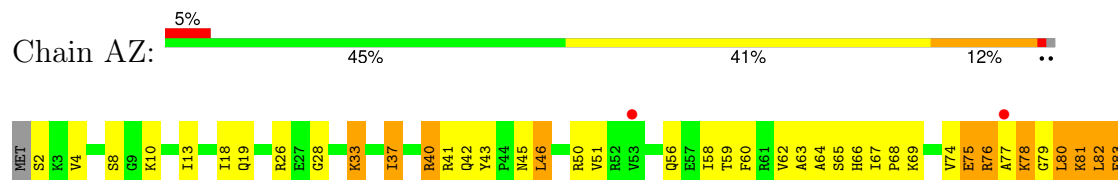
• Molecule 22: 50S ribosomal protein L27



• Molecule 22: 50S ribosomal protein L27



• Molecule 23: 50S ribosomal protein L28

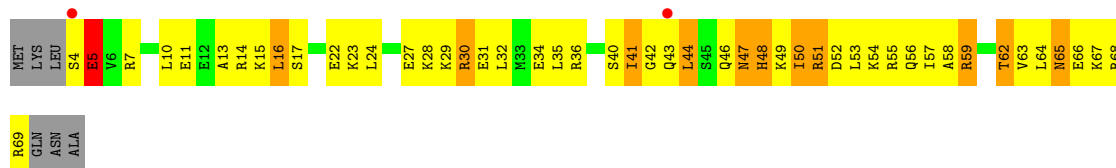




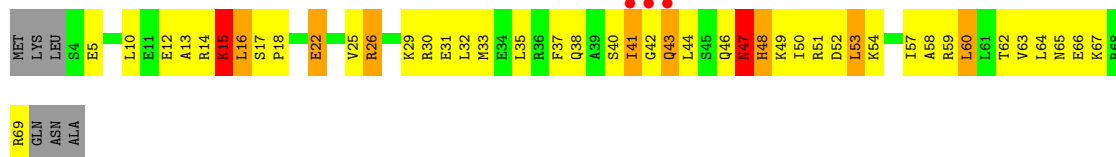
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



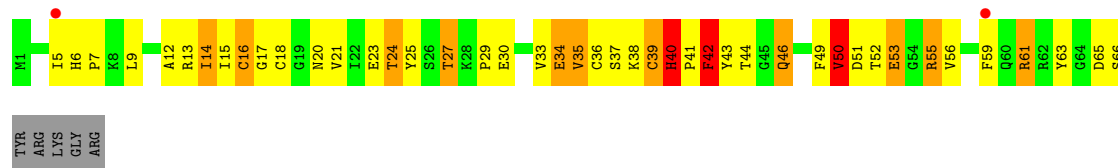
- Molecule 25: 50S ribosomal protein L30



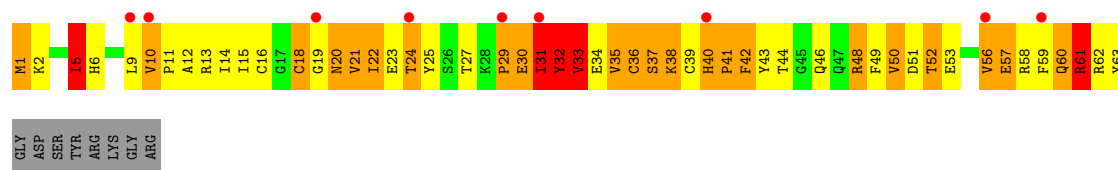
- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31



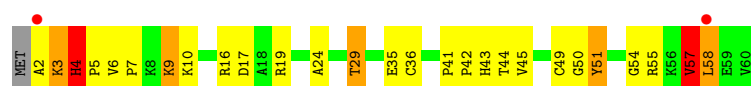
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



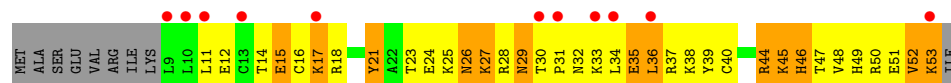
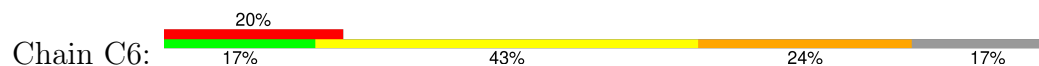
- Molecule 27: 50S ribosomal protein L32



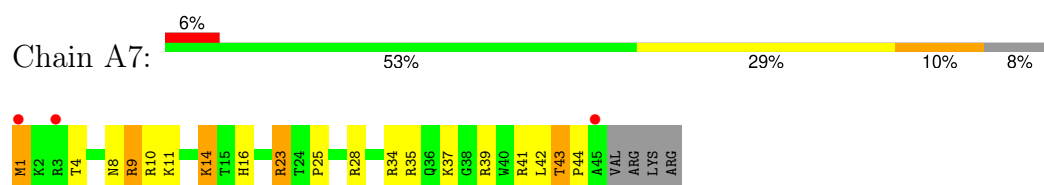
- Molecule 28: 50S ribosomal protein L33



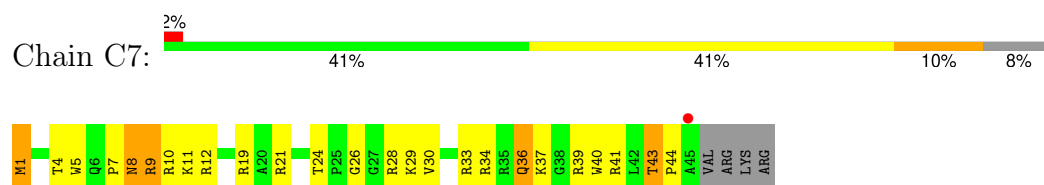
- Molecule 28: 50S ribosomal protein L33



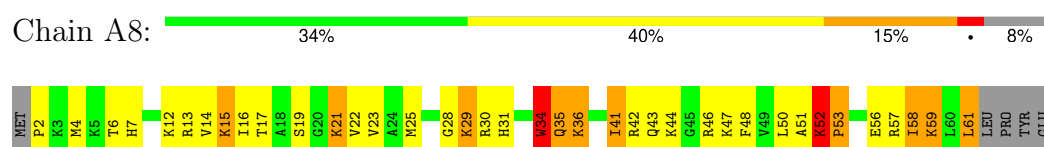
- Molecule 29: 50S ribosomal protein L34



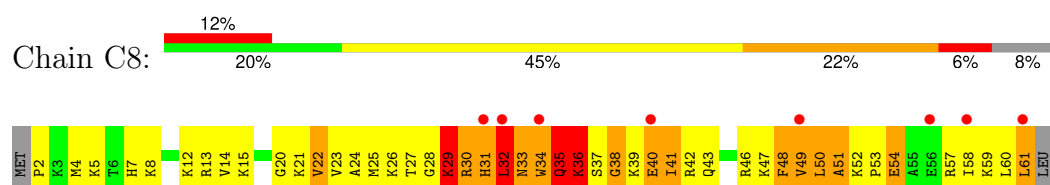
- Molecule 29: 50S ribosomal protein L34



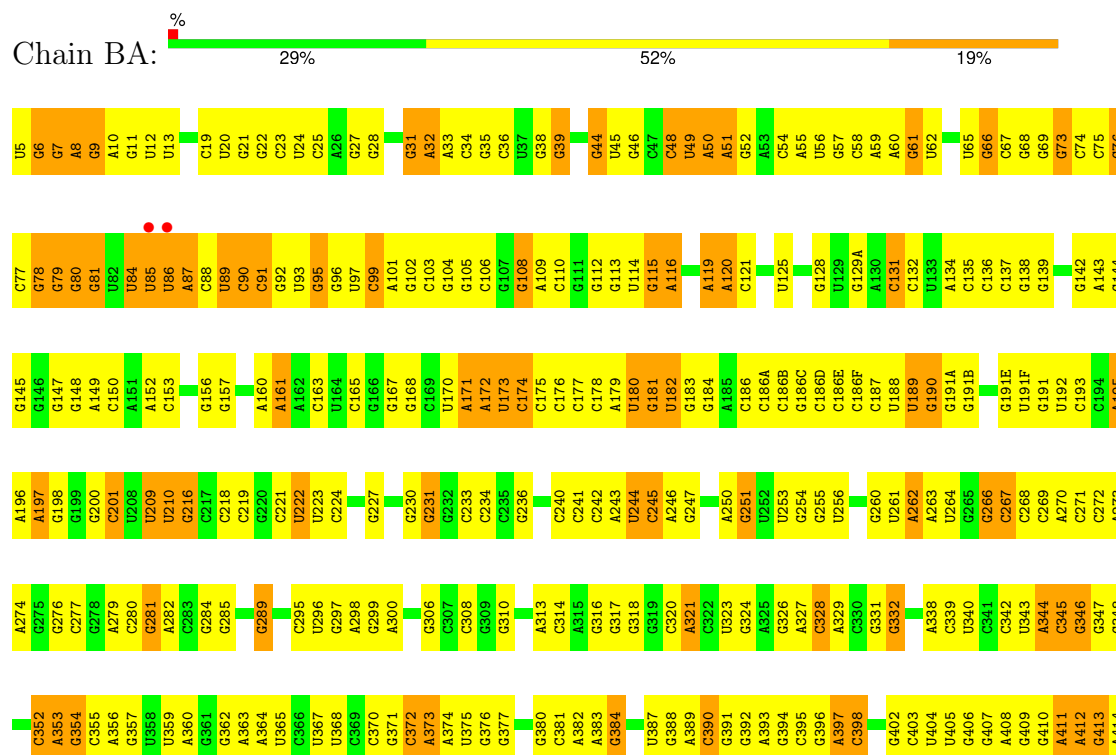
- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 16S ribosomal RNA

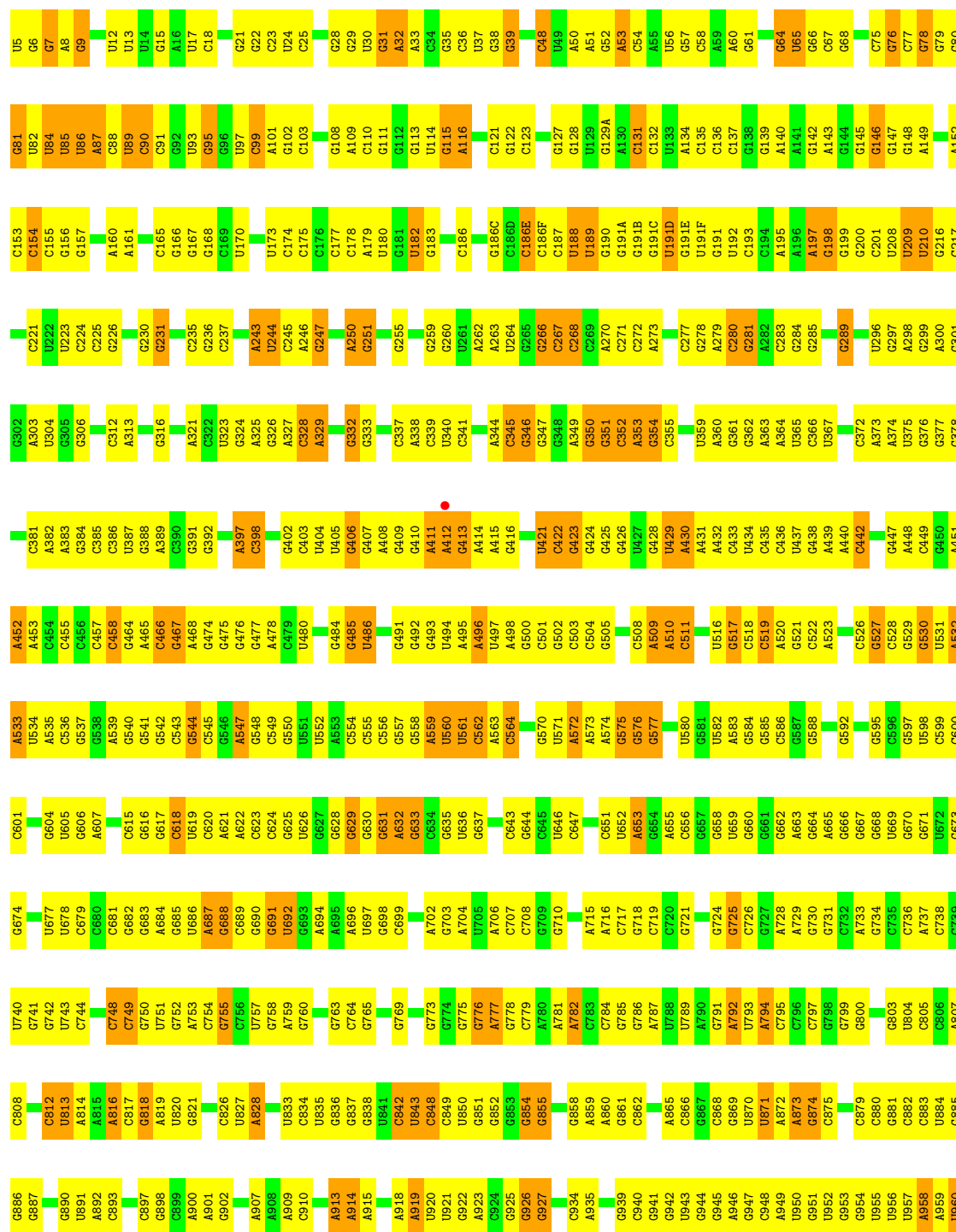


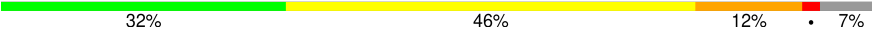
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C1395	C1328	C1262	U1195	G1130	G1061	G998	G933	G855	G775	A704	G630	G562	G492	C417
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C1397	U1330	C1264	U1196	G1132	U1065	U999	C935	G857	A777	C708	A632	C564	U494	C419
A1398	G1331	G1265	G1197	G1133	C1066	A1000	C936	G858	G778	G709	G633	U565	A495	C422
C1399	A1332	G1266	G1198	G1134	A1067	G1001	A937	A859	A782	G710	G637	G566	A496	G423
G1400	A1333	C1267	U1199	U1135	C1068	G1002	A938	G860	C783	G713	G638	G567	U497	G424
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C1402	C1335	A1269	A1201	G1137	U1070	G1004	C940	U862	G785	A572	C502	C503	C504	G426
C1403	C1336	G1270	G1202	G1138	U1071	A1005	G941	U863	C786	C719	A642	G505	U427	G427
G1404	G1337	G1271	G1206	G1139	G1074	C1006	G942	C868	U788	C720	C643	A574	G506	G428
G1405	G1338	G1272	G1207	C1141	C1075	C1007	U943	G869	U789	G721	C644	G575	G507	U429
U1406	G1273	G1273	G1207	C1142	C1076	G1008	G944	U870	A790	A722	G645	G576	G508	U430
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G1415	U1278	U1278	U1211	G1144	C1078	G1010	A946	A872	A792	G724	G650	C578	C507	A432
A1419	A1346	U1279	U1212	C1145	A1080	A1014	G947	A873	U793	G725	G651	G579	C508	C433
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G1422	C1282	G1282	G1215	U1148	U1083	A1017	U950	G876	G799	A728	A653	U582	C511	C436
G1423	A1350	G1283	G1216	C1149	G1084	G1017	G951	C877	G799	A729	G654	A583	U512	U437
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U1425	C1352	A1285	C1218	A1151	U1086	C1019	G953	C879	U804	G731	U659	G585	C514	A439
C1353	G1353	A1286	U1219	C1152	G1087	U1020	G954	C880	C905	C732	C660	G586	G515	A440
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U1358	A1288	A1288	C1223	G1154	C1089	G1022	U956	G886	C906	C736	A663	G588	G517	C443
C1359	A1289	G1289	C1224	G1155	U1090	G1023	U957	A807	C908	C737	A664	C589	C518	C444
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C1362A	G1294	G1294	C1228	G1160	U1095	C1028	U961	U891	U813	G741	U672	C594	C526	C449
A1363	C1295	G1295	C1161	C1161	C1096	C1028A	A964	A892	A814	C745	G673	G595	G527	G450
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G1365	C1297	C1297	G1163	A1101	A1101	C1030	C966	C896	C817	A747	C674	C600	A453	A454
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C1448	C1371	C1303	G1241	A1170	C1107	G1034	G973	A974	C826	C754	C681	U605	G538	A468
G1449	U1372	G1304	C1243	G1171	C1108	A1035	A974	A909	U827	G755	G682	G606	G539	G474
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C1462	A1318	G1253	G1253	A1182	C1119	G1048	A987	U921	G837	C765	A694	C621	C555	C483
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C1465	C1321	C1321	G1255	G1185	C1122	U1052	C990	G924	U843	G771	C701	G626	G558	C488
G1389	C1322	C1322	A1256	G1186	G1124	U1052	C989	A923	C842	A767	A696	G627	G559	C489
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A1468	U1391	A1324	C1258	G1187	U1126	C1054	U991	G925	C848	U772	C701	G627	G559	C489
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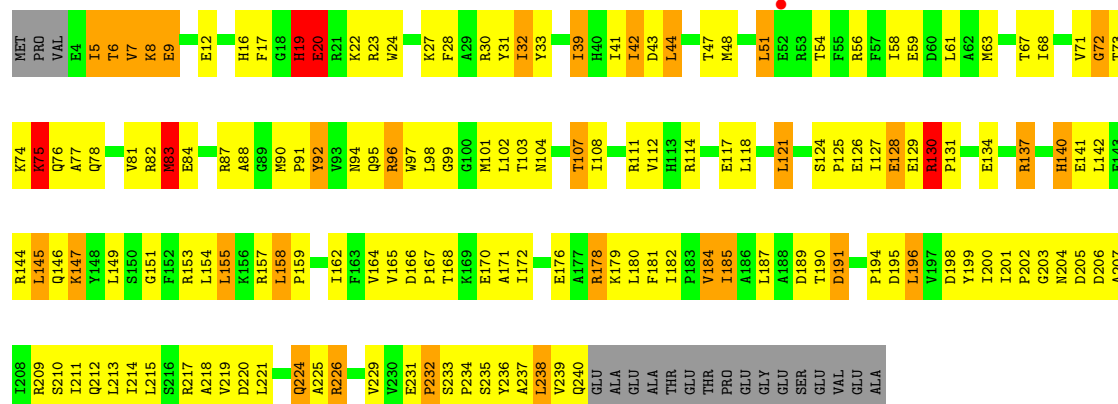


• Molecule 31: 16S ribosomal RNA

Chain DA: 28% 53% 19%

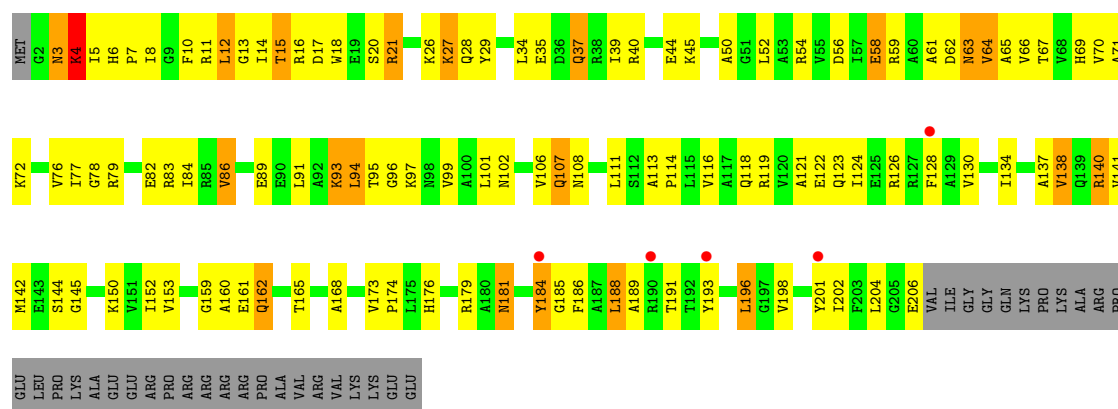


Chain DE: 



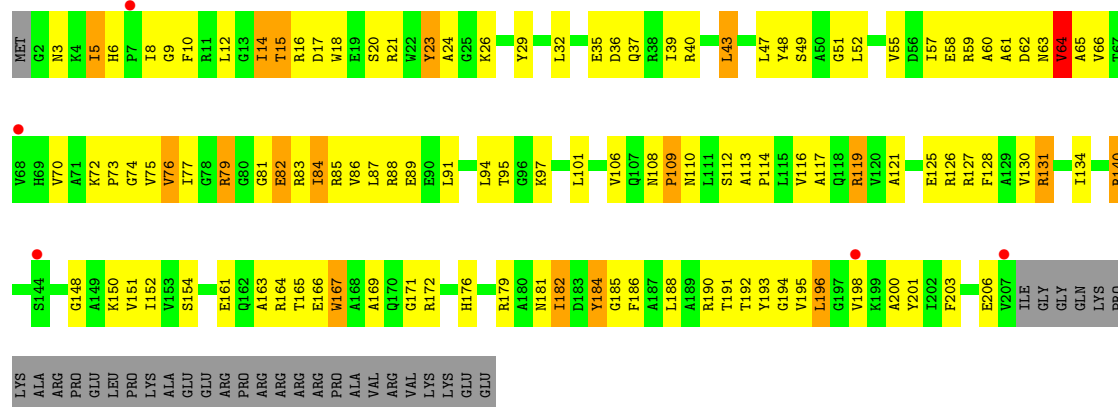
• Molecule 33: 30S RIBOSOMAL PROTEIN S3

Chain BF: 

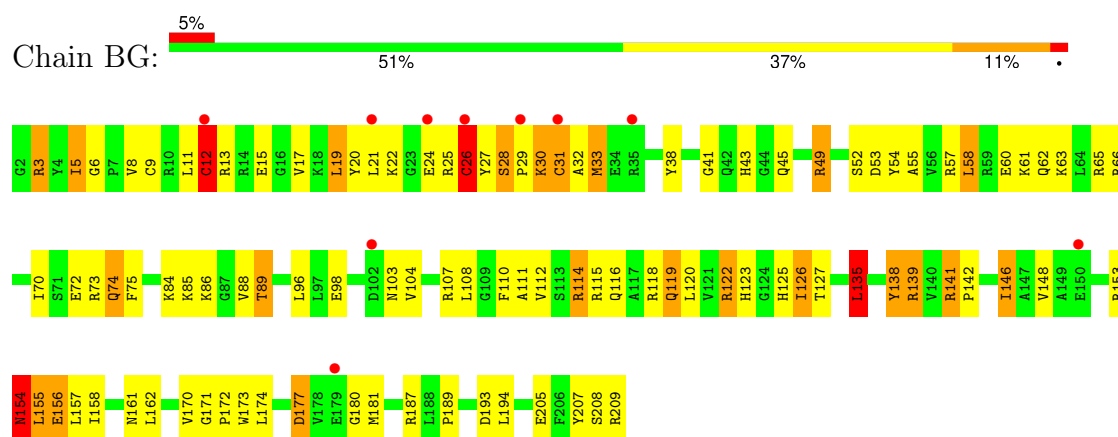


• Molecule 33: 30S RIBOSOMAL PROTEIN S3

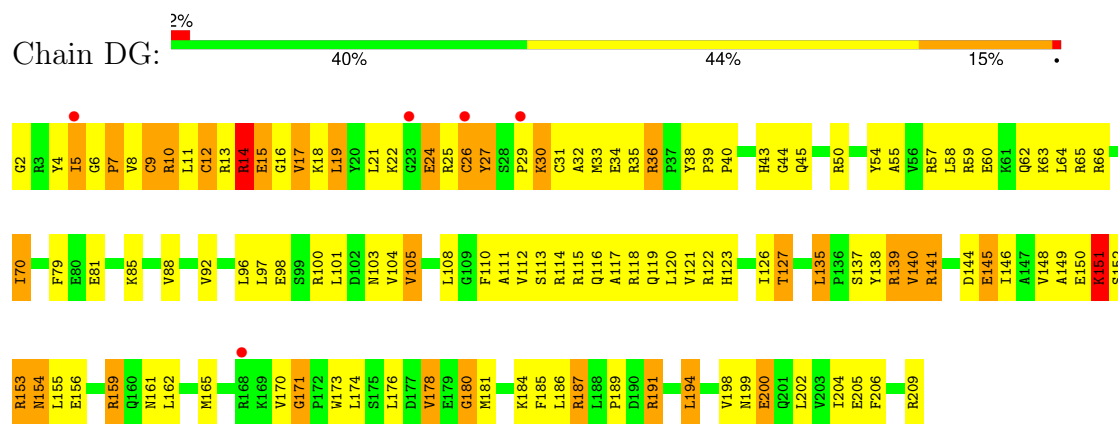
Chain DF: 



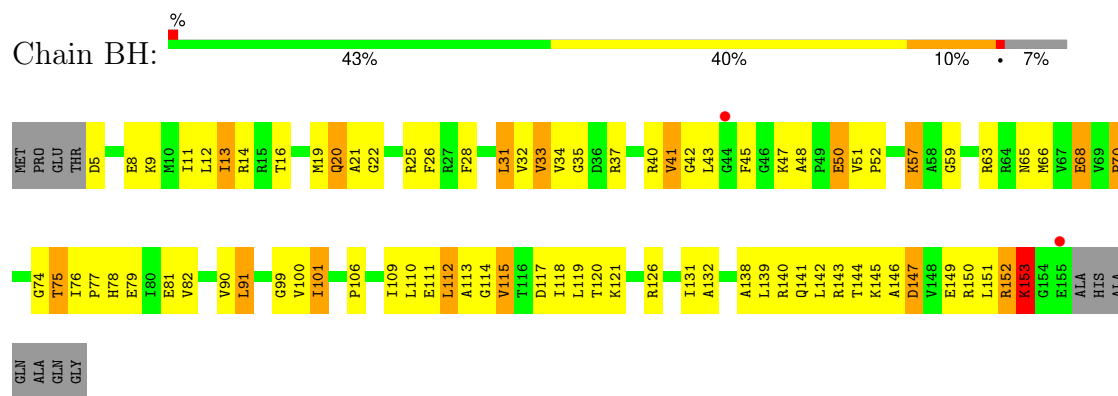
• Molecule 34: 30S RIBOSOMAL PROTEIN S4



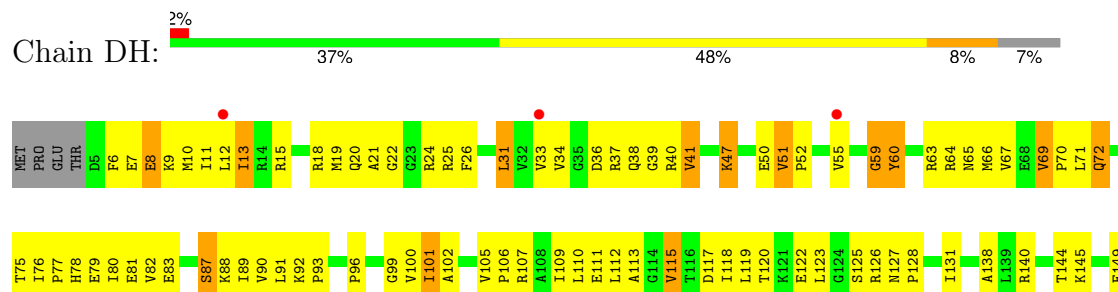
• Molecule 34: 30S RIBOSOMAL PROTEIN S4



• Molecule 35: 30S RIBOSOMAL PROTEIN S5



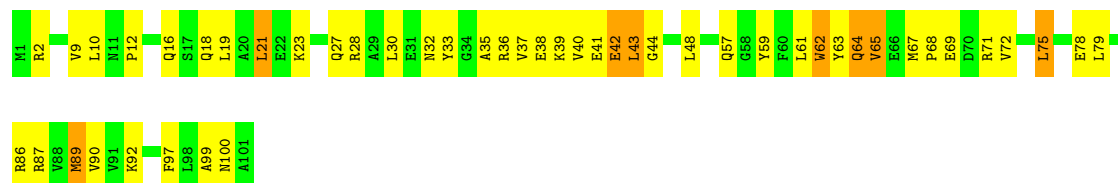
• Molecule 35: 30S RIBOSOMAL PROTEIN S5





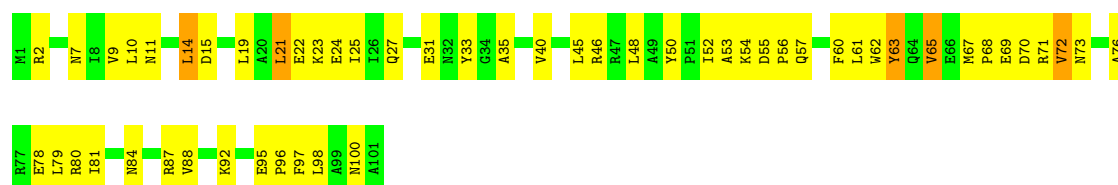
• Molecule 36: 30S RIBOSOMAL PROTEIN S6

Chain BI: 52% 40% 8%



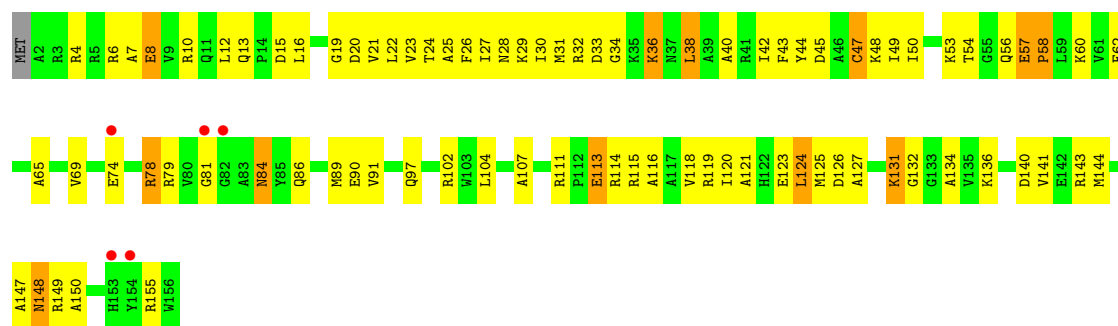
• Molecule 36: 30S RIBOSOMAL PROTEIN S6

Chain DI: 47% 49% 5%



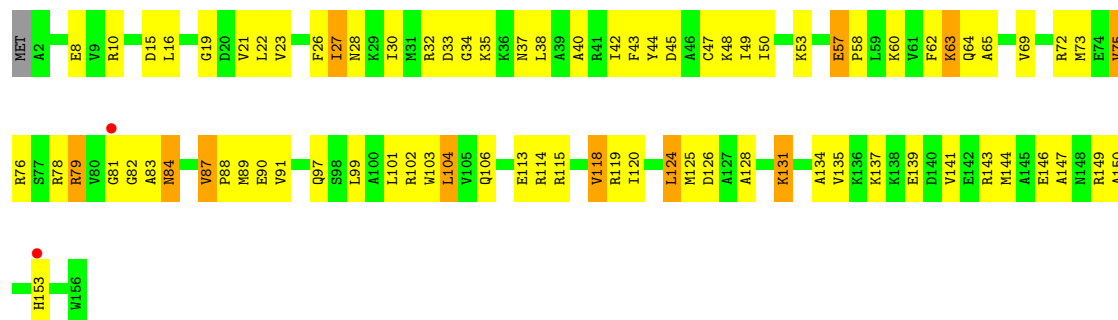
• Molecule 37: 30S RIBOSOMAL PROTEIN S7

Chain BJ: 3% 45% 47% 8%

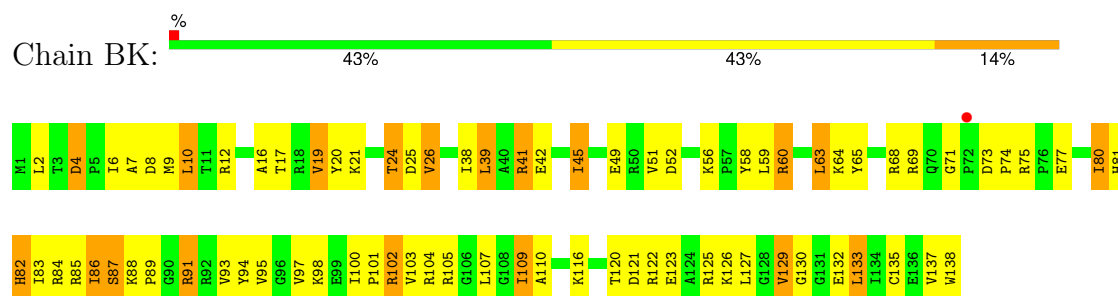


• Molecule 37: 30S RIBOSOMAL PROTEIN S7

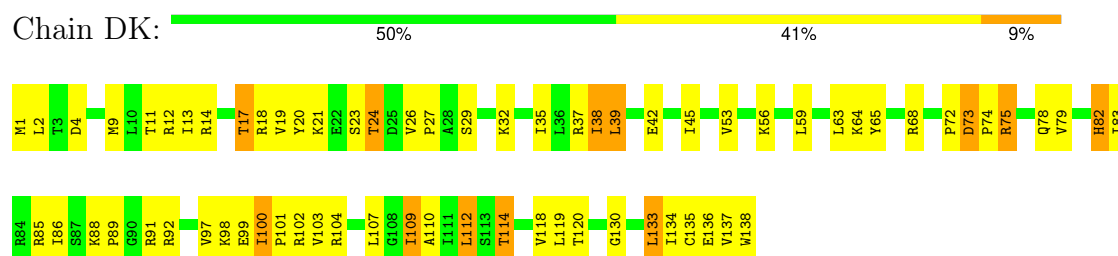
Chain DJ: % 47% 45% 7%



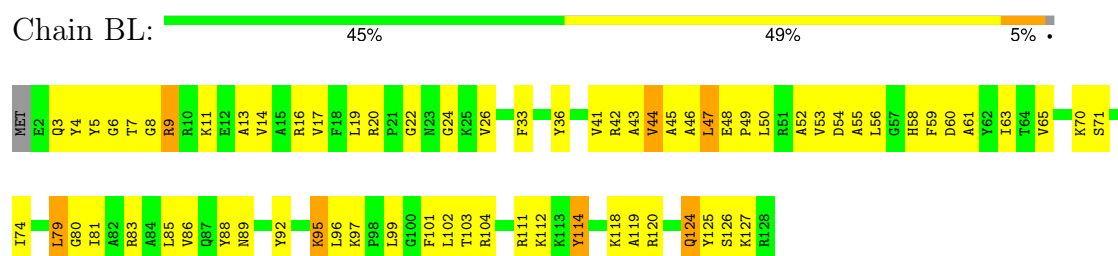
- Molecule 38: 30S RIBOSOMAL PROTEIN S8



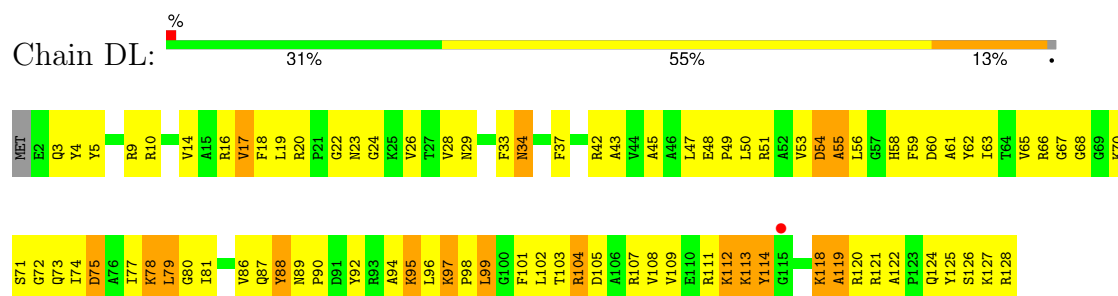
- Molecule 38: 30S RIBOSOMAL PROTEIN S8



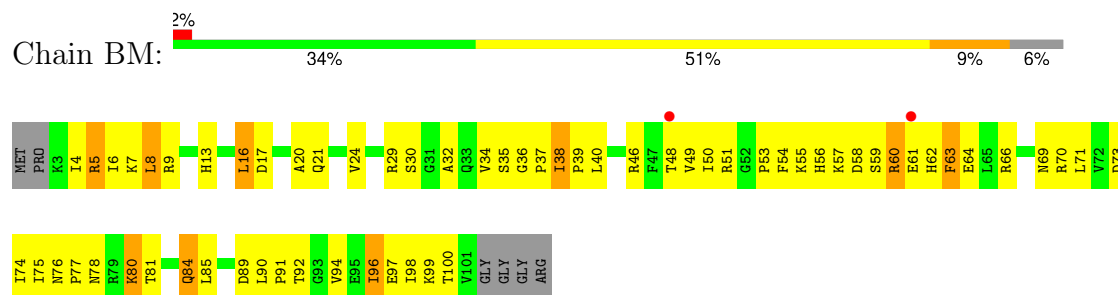
- Molecule 39: 30S RIBOSOMAL PROTEIN S9



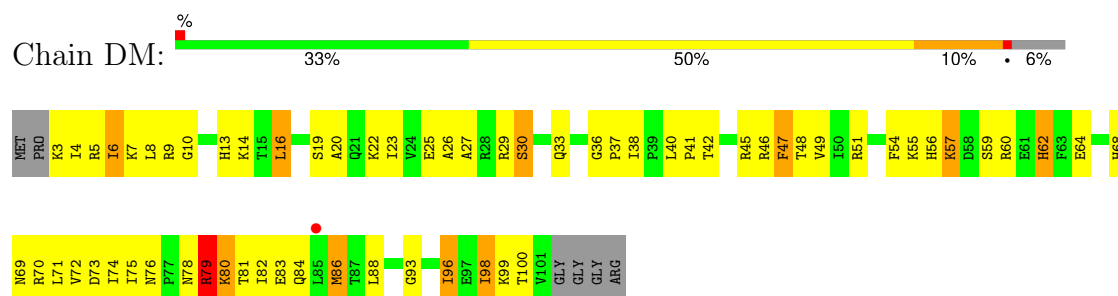
- Molecule 39: 30S RIBOSOMAL PROTEIN S9



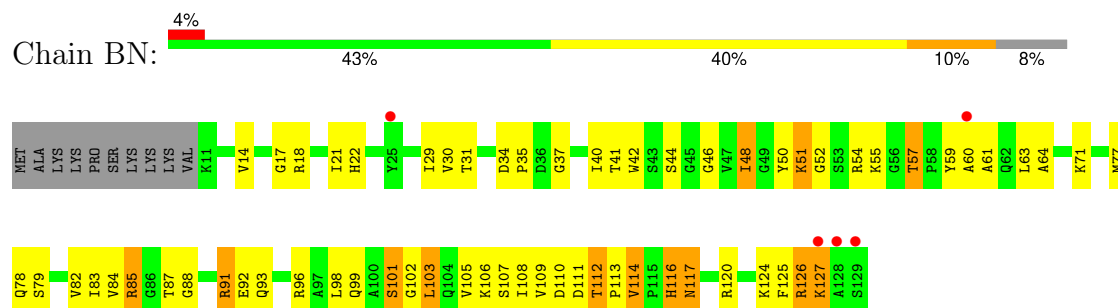
- Molecule 40: 30S RIBOSOMAL PROTEIN S10



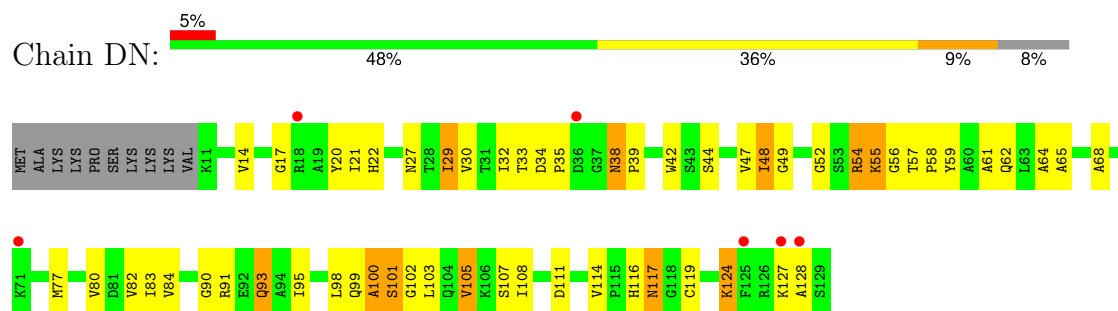
- Molecule 40: 30S RIBOSOMAL PROTEIN S10



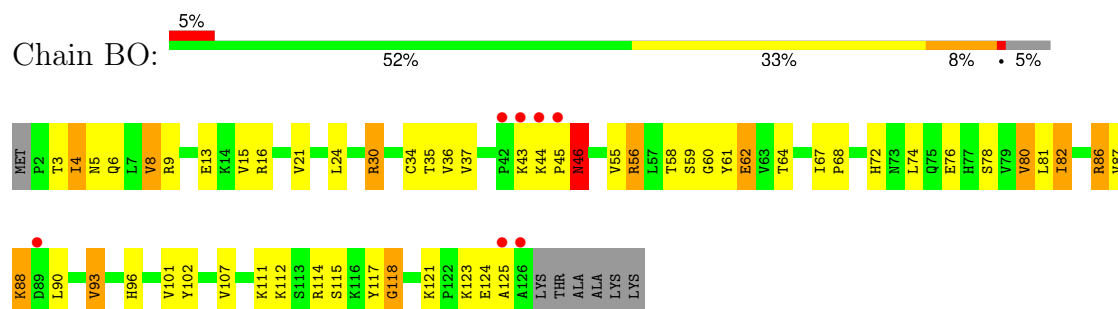
- Molecule 41: 30S RIBOSOMAL PROTEIN S11



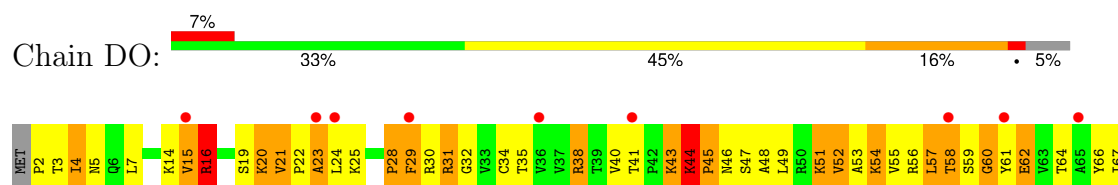
- Molecule 41: 30S RIBOSOMAL PROTEIN S11



- Molecule 42: 30S RIBOSOMAL PROTEIN S12

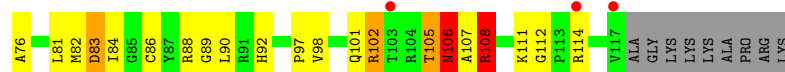
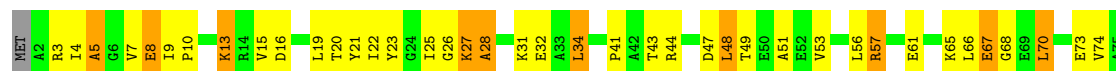
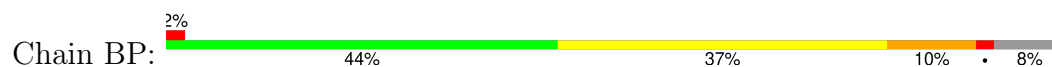


- Molecule 42: 30S RIBOSOMAL PROTEIN S12

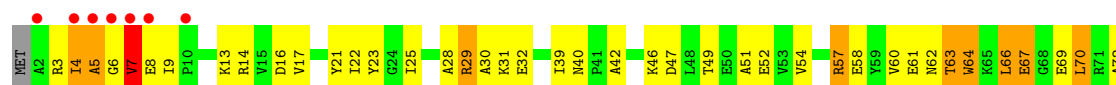




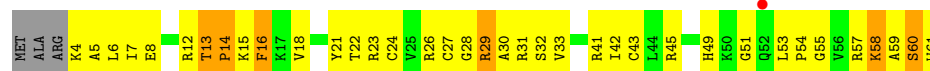
• Molecule 43: 30S RIBOSOMAL PROTEIN S13



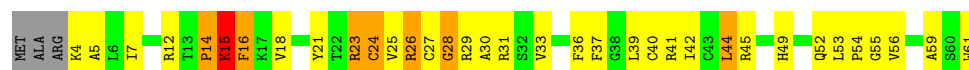
• Molecule 43: 30S RIBOSOMAL PROTEIN S13



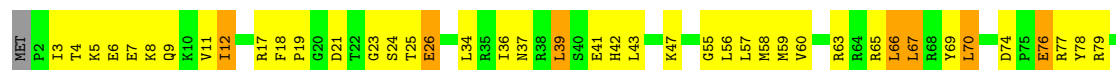
• Molecule 44: 30S RIBOSOMAL PROTEIN S14



• Molecule 44: 30S RIBOSOMAL PROTEIN S14

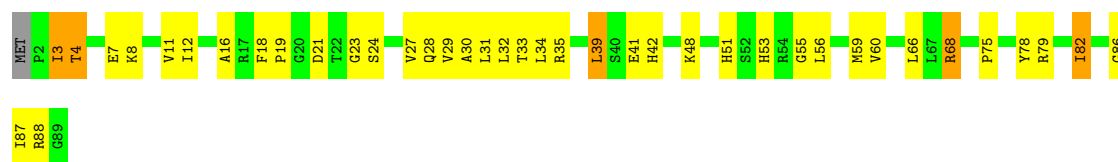


• Molecule 45: 30S RIBOSOMAL PROTEIN S15

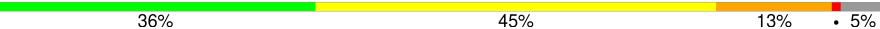


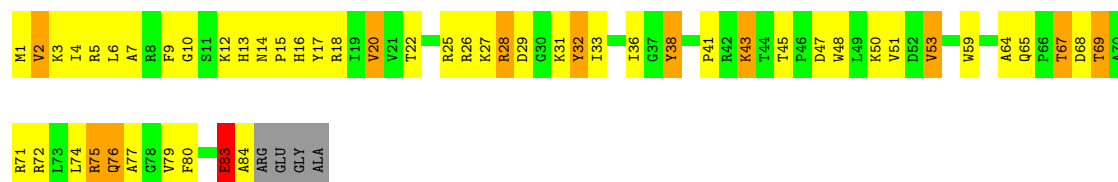
• Molecule 45: 30S RIBOSOMAL PROTEIN S15

Chain DR: 



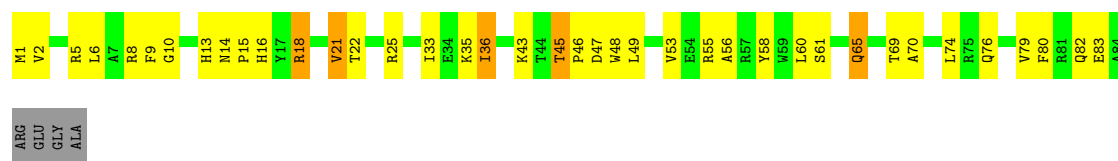
• Molecule 46: 30S RIBOSOMAL PROTEIN S16

Chain BS: 



• Molecule 46: 30S RIBOSOMAL PROTEIN S16

Chain DS: 



• Molecule 47: 30S RIBOSOMAL PROTEIN S17

Chain BT: 

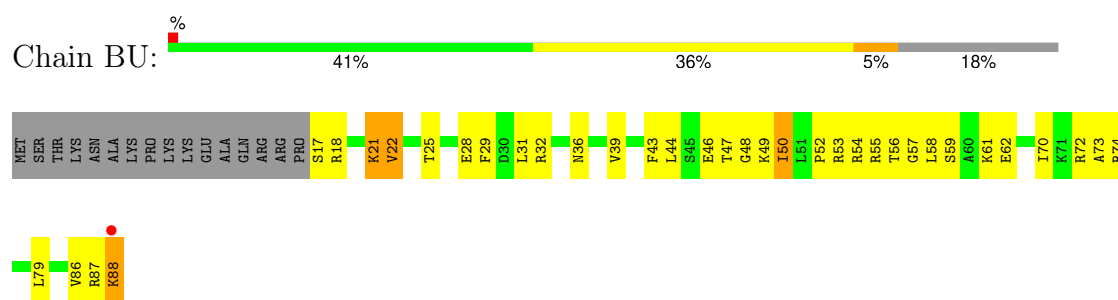


• Molecule 47: 30S RIBOSOMAL PROTEIN S17

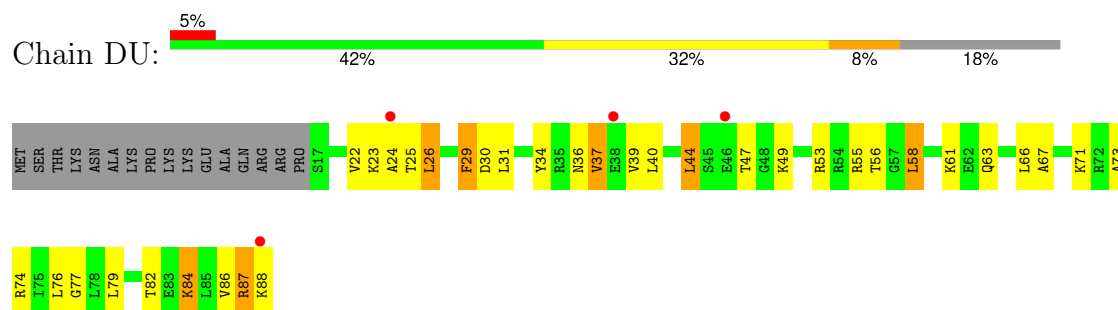
Chain DT: 



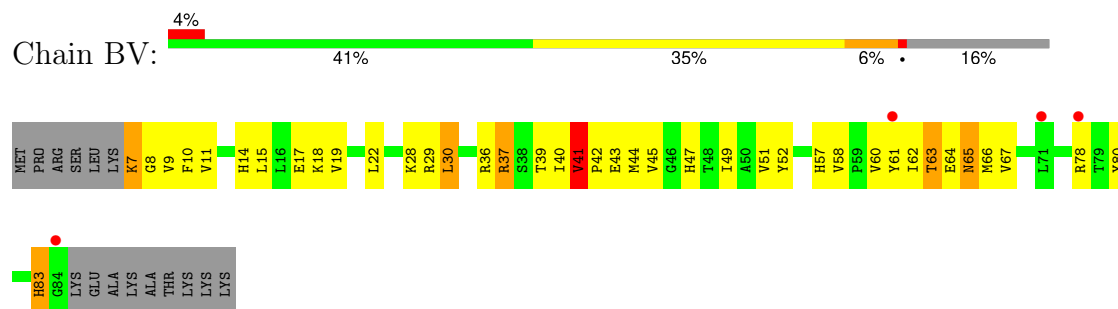
• Molecule 48: 30S RIBOSOMAL PROTEIN S18



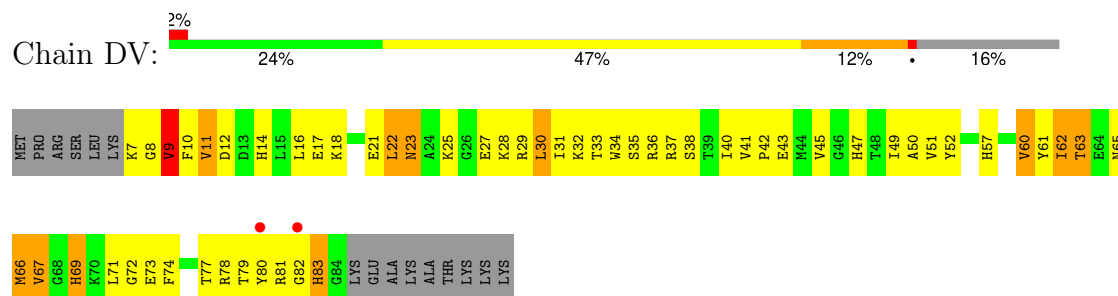
• Molecule 48: 30S RIBOSOMAL PROTEIN S18



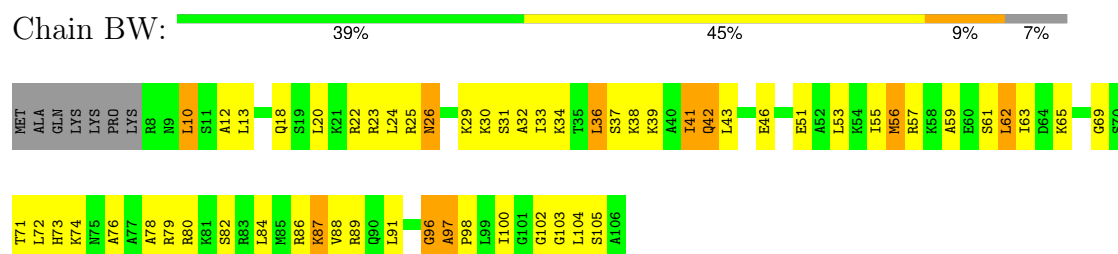
• Molecule 49: 30S RIBOSOMAL PROTEIN S19



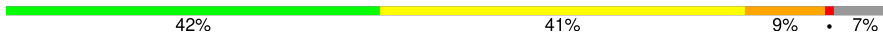
• Molecule 49: 30S RIBOSOMAL PROTEIN S19

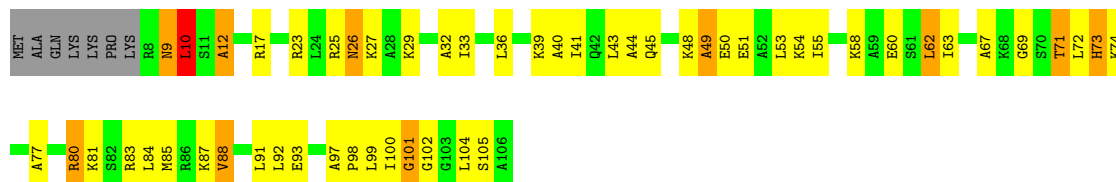


• Molecule 50: 30S RIBOSOMAL PROTEIN S20

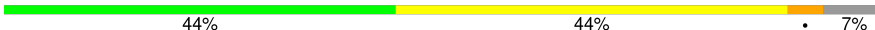


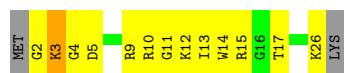
- Molecule 50: 30S RIBOSOMAL PROTEIN S20

Chain DW: 



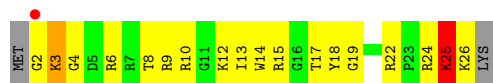
- Molecule 51: 30S RIBOSOMAL PROTEIN THX

Chain BX: 



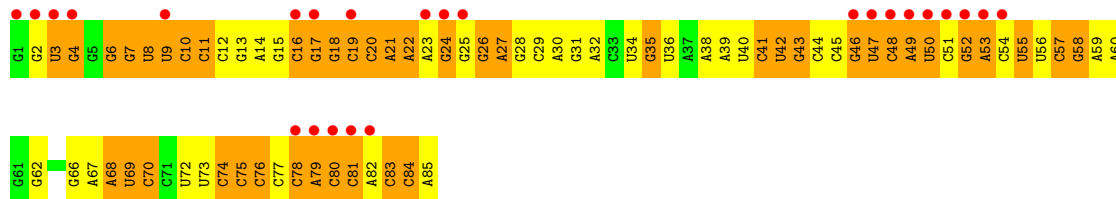
- Molecule 51: 30S RIBOSOMAL PROTEIN THX

Chain DX: 



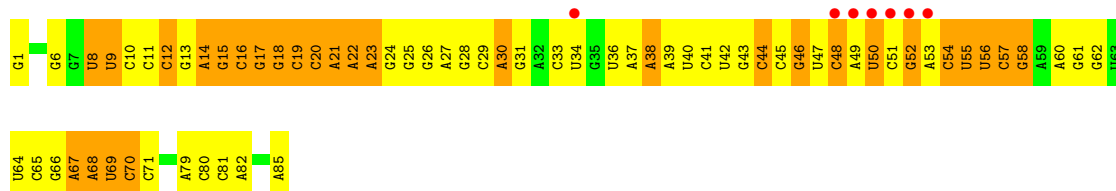
- Molecule 52: TRNA-TYR

Chain BB: 



- Molecule 52: TRNA-TYR

Chain BD: 

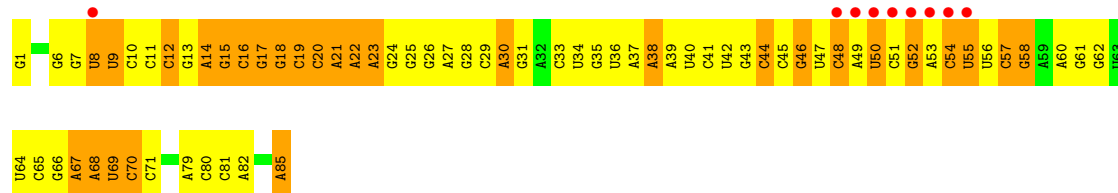
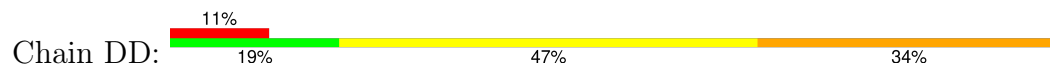


- Molecule 52: TRNA-TYR

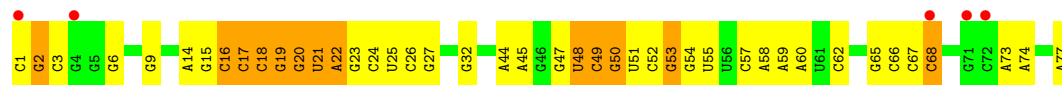
Chain DB: 



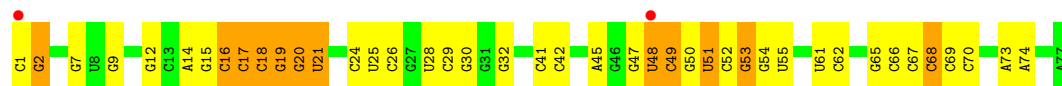
• Molecule 52: TRNA-TYR



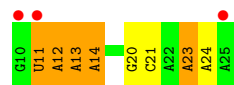
• Molecule 53: TRNA-FMET



• 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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	2000 reflections (0.21%)	wwPDB-VP
Wilson B-factor (Å ²)	90.6	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 72.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, OHX, 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	0.19	0/70233	0.35	0/109643
1	CA	0.17	0/70122	0.34	1/109469 (0.0%)
2	AB	0.17	0/2928	0.35	0/4568
2	CB	0.15	0/2928	0.34	0/4568
3	AD	0.39	0/2165	0.90	2/2919 (0.1%)
3	CD	0.35	0/2165	0.81	0/2919
4	AE	0.35	0/1601	0.92	10/2160 (0.5%)
4	CE	0.35	0/1601	0.88	5/2160 (0.2%)
5	AF	0.36	0/1620	0.82	6/2194 (0.3%)
5	CF	0.32	0/1662	0.89	8/2249 (0.4%)
6	AG	0.29	0/1499	0.81	3/2016 (0.1%)
6	CG	0.28	0/1499	0.80	1/2016 (0.0%)
7	AH	0.35	0/1332	0.82	0/1802
7	CH	0.31	0/1332	0.81	0/1802
8	AK	0.33	0/1151	0.82	3/1558 (0.2%)
8	CK	0.30	0/1151	0.84	5/1558 (0.3%)
9	AM	0.34	0/1131	0.79	0/1525
9	CM	0.30	0/1131	0.79	2/1525 (0.1%)
10	AN	0.32	0/943	0.80	0/1269
10	CN	0.31	0/943	0.79	2/1269 (0.2%)
11	AO	0.35	0/1162	0.93	4/1544 (0.3%)
11	CO	0.31	0/1162	0.78	0/1544
12	AP	0.33	0/1143	0.76	1/1527 (0.1%)
12	CP	0.28	0/1143	0.72	1/1527 (0.1%)
13	A0	0.33	0/982	0.76	1/1312 (0.1%)
13	C0	0.31	0/974	0.72	0/1302
14	AQ	0.32	0/892	0.78	0/1187
14	CQ	0.30	0/892	0.71	1/1187 (0.1%)
15	AR	0.34	0/1155	0.83	1/1542 (0.1%)
15	CR	0.30	0/1155	0.77	2/1542 (0.1%)
16	A1	0.33	0/982	0.86	2/1306 (0.2%)
16	C1	0.30	0/982	0.71	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	A2	0.32	0/790	0.82	2/1057 (0.2%)
17	C2	0.34	0/790	0.89	2/1057 (0.2%)
18	AS	0.35	0/911	0.76	0/1220
18	CS	0.33	0/911	0.77	0/1220
19	AT	0.35	0/739	0.79	1/993 (0.1%)
19	CT	0.34	0/739	0.82	2/993 (0.2%)
20	AU	0.34	0/798	0.82	0/1064
20	CU	0.33	0/798	0.77	0/1064
21	AV	0.31	0/1427	0.79	1/1935 (0.1%)
21	CV	0.30	0/1460	0.81	3/1982 (0.2%)
22	A3	0.30	0/615	0.75	0/819
22	C3	0.29	0/621	0.82	0/827
23	AZ	0.33	0/770	0.77	0/1022
23	CZ	0.32	0/770	0.81	0/1022
24	AW	0.35	0/560	0.85	1/741 (0.1%)
24	CW	0.29	0/560	0.73	0/741
25	AX	0.32	0/474	0.77	0/635
25	CX	0.26	0/474	0.83	2/635 (0.3%)
26	A4	0.31	0/545	0.88	3/733 (0.4%)
26	C4	0.37	0/527	0.84	2/709 (0.3%)
27	A5	0.34	0/473	0.90	2/639 (0.3%)
27	C5	0.34	0/473	0.83	0/639
28	A6	0.35	0/396	0.81	0/529
28	C6	0.37	0/396	0.87	1/529 (0.2%)
29	A7	0.40	0/399	0.76	0/526
29	C7	0.34	0/399	0.83	0/526
30	A8	0.44	0/486	0.98	3/638 (0.5%)
30	C8	0.34	0/486	0.83	1/638 (0.2%)
31	BA	0.15	0/36139	0.33	0/56406
31	DA	0.14	0/36142	0.32	0/56410
32	BE	0.27	0/1959	0.76	2/2642 (0.1%)
32	DE	0.29	0/1959	0.79	3/2642 (0.1%)
33	BF	0.29	0/1629	0.70	0/2195
33	DF	0.29	0/1636	0.73	0/2205
34	BG	0.32	0/1733	0.82	5/2318 (0.2%)
34	DG	0.29	0/1733	0.83	6/2318 (0.3%)
35	BH	0.30	0/1171	0.78	0/1576
35	DH	0.30	0/1171	0.79	0/1576
36	BI	0.28	0/856	0.72	0/1154
36	DI	0.29	0/856	0.76	0/1154
37	BJ	0.28	0/1276	0.72	0/1709
37	DJ	0.28	0/1276	0.71	0/1709
38	BK	0.30	0/1136	0.87	5/1527 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DK	0.27	0/1136	0.78	2/1527 (0.1%)
39	BL	0.29	0/1029	0.73	0/1379
39	DL	0.29	0/1029	0.81	3/1379 (0.2%)
40	BM	0.29	0/814	0.77	0/1095
40	DM	0.28	0/814	0.82	0/1095
41	BN	0.31	0/900	0.83	4/1213 (0.3%)
41	DN	0.29	0/900	0.80	2/1213 (0.2%)
42	BO	0.33	0/991	0.79	1/1327 (0.1%)
42	DO	0.29	0/991	0.74	0/1327
43	BP	0.28	0/938	0.76	1/1258 (0.1%)
43	DP	0.28	0/943	0.76	1/1265 (0.1%)
44	BQ	0.32	0/485	0.75	0/643
44	DQ	0.29	0/485	0.75	0/643
45	BR	0.30	0/745	0.70	0/992
45	DR	0.28	0/745	0.67	0/992
46	BS	0.28	0/721	0.76	2/970 (0.2%)
46	DS	0.28	0/721	0.73	0/970
47	BT	0.28	0/847	0.76	0/1131
47	DT	0.27	0/847	0.72	0/1131
48	BU	0.29	0/596	0.73	0/790
48	DU	0.29	0/596	0.72	0/790
49	BV	0.30	0/638	0.83	0/860
49	DV	0.31	0/638	0.82	0/860
50	BW	0.29	0/765	0.76	0/1007
50	DW	0.29	0/765	0.84	1/1007 (0.1%)
51	BX	0.29	0/221	0.67	0/288
51	DX	0.28	0/221	0.79	2/288 (0.7%)
52	BB	0.20	0/1992	0.37	0/3099
52	BD	0.17	0/1992	0.33	0/3099
52	DB	0.20	0/1992	0.36	0/3099
52	DD	0.18	0/1992	0.34	0/3099
53	BC	0.16	0/1835	0.31	0/2859
53	DC	0.14	0/1835	0.29	0/2859
54	B1	0.18	0/390	0.39	0/606
54	D1	0.17	0/390	0.40	0/606
All	All	0.22	0/324159	0.50	127/485455 (0.0%)

There are no bond length outliers.

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AE	65	GLY	N-CA-C	-9.11	104.64	114.67

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	DW	12	ALA	N-CA-C	-8.96	102.35	113.28
17	C2	49	THR	CA-C-N	-8.14	109.67	119.84
17	C2	49	THR	C-N-CA	-8.14	109.67	119.84
27	A5	46	CYS	CA-C-N	7.53	129.25	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	62707	0	31613	2358	0
1	CA	62607	0	31564	2409	0
2	AB	2617	0	1328	88	0
2	CB	2617	0	1328	129	0
3	AD	2115	0	2195	239	0
3	CD	2115	0	2195	202	0
4	AE	1568	0	1634	163	0
4	CE	1568	0	1634	171	0
5	AF	1585	0	1632	131	0
5	CF	1627	0	1680	195	0
6	AG	1474	0	1535	116	0
6	CG	1474	0	1535	125	0
7	AH	1307	0	1382	133	0
7	CH	1307	0	1382	113	1
8	AK	1136	0	1223	97	0
8	CK	1136	0	1223	82	0
9	AM	1104	0	1180	89	0
9	CM	1104	0	1180	75	0
10	AN	933	0	996	66	0
10	CN	933	0	996	56	0
11	AO	1145	0	1228	183	0
11	CO	1145	0	1228	273	0
12	AP	1122	0	1179	176	0
12	CP	1122	0	1179	199	0
13	A0	968	0	1033	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	C0	960	0	1021	73	0
14	AQ	882	0	943	87	0
14	CQ	882	0	943	92	0
15	AR	1141	0	1202	111	0
15	CR	1141	0	1202	94	0
16	A1	964	0	1022	90	0
16	C1	964	0	1022	85	0
17	A2	779	0	852	67	0
17	C2	779	0	852	103	0
18	AS	900	0	964	58	0
18	CS	900	0	964	60	0
19	AT	725	0	778	45	0
19	CT	725	0	778	43	0
20	AU	785	0	878	78	0
20	CU	785	0	878	82	0
21	AV	1397	0	1430	149	0
21	CV	1428	0	1454	157	0
22	A3	607	0	628	44	0
22	C3	613	0	633	47	0
23	AZ	763	0	848	53	0
23	CZ	763	0	848	46	0
24	AW	558	0	610	46	0
24	CW	558	0	610	52	0
25	AX	469	0	518	28	0
25	CX	469	0	518	29	0
26	A4	533	0	522	74	0
26	C4	515	0	510	102	0
27	A5	459	0	480	90	0
27	C5	459	0	478	36	0
28	A6	389	0	404	61	0
28	C6	389	0	404	52	0
29	A7	391	0	432	21	0
29	C7	391	0	432	32	0
30	A8	480	0	549	65	0
30	C8	480	0	549	123	0
31	BA	32284	0	16296	1470	1
31	DA	32287	0	16295	1439	0
32	BE	1924	0	1975	148	0
32	DE	1924	0	1975	166	0
33	BF	1605	0	1668	101	0
33	DF	1612	0	1677	118	0
34	BG	1703	0	1763	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	DG	1703	0	1763	135	0
35	BH	1155	0	1213	74	0
35	DH	1155	0	1213	82	0
36	BI	843	0	857	38	0
36	DI	843	0	857	48	0
37	BJ	1257	0	1296	76	0
37	DJ	1257	0	1296	93	0
38	BK	1116	0	1177	83	0
38	DK	1116	0	1177	58	0
39	BL	1010	0	1037	73	0
39	DL	1010	0	1037	117	0
40	BM	801	0	849	79	0
40	DM	801	0	849	92	0
41	BN	885	0	904	57	0
41	DN	885	0	904	60	0
42	BO	975	0	1062	54	0
42	DO	975	0	1062	92	0
43	BP	928	0	987	76	0
43	DP	933	0	992	83	0
44	BQ	476	0	511	47	0
44	DQ	476	0	511	54	0
45	BR	734	0	771	38	0
45	DR	734	0	771	40	0
46	BS	705	0	725	57	0
46	DS	705	0	725	36	0
47	BT	834	0	904	55	0
47	DT	834	0	904	41	0
48	BU	591	0	662	41	0
48	DU	591	0	662	40	0
49	BV	624	0	636	50	0
49	DV	624	0	636	84	0
50	BW	763	0	861	60	0
50	DW	763	0	861	50	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	153	0
52	DB	1814	0	932	174	0
52	DD	1814	0	932	173	0
53	BC	1643	0	837	47	0
53	DC	1643	0	837	52	0
54	B1	347	0	174	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
56	BB	14	0	0	1	0
56	BC	14	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	15360	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 31.

The worst 5 of 15360 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	13
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	9
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	30
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	13
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	43
18	CS	111/113 (98%)	99 (89%)	9 (8%)	3 (3%)	4	22
19	AT	90/96 (94%)	84 (93%)	5 (6%)	1 (1%)	11	39
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	15
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	12
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	18
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	20
33	DF	204/239 (85%)	163 (80%)	35 (17%)	6 (3%)	3	21
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	15
35	DH	149/162 (92%)	132 (89%)	15 (10%)	2 (1%)	9	35
36	BI	99/101 (98%)	89 (90%)	7 (7%)	3 (3%)	3	20
36	DI	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	6	27
37	BJ	153/156 (98%)	128 (84%)	21 (14%)	4 (3%)	4	23
37	DJ	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	9	35
38	BK	136/138 (99%)	116 (85%)	16 (12%)	4 (3%)	3	21
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	15
39	DL	125/128 (98%)	97 (78%)	21 (17%)	7 (6%)	1	9
40	BM	97/105 (92%)	83 (86%)	13 (13%)	1 (1%)	12	40
40	DM	97/105 (92%)	82 (84%)	14 (14%)	1 (1%)	12	40
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%)	1	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	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	DR	86/89 (97%)	77 (90%)	8 (9%)	1 (1%)	10	37
46	BS	82/88 (93%)	60 (73%)	20 (24%)	2 (2%)	4	24
46	DS	82/88 (93%)	70 (85%)	11 (13%)	1 (1%)	10	37
47	BT	98/105 (93%)	82 (84%)	13 (13%)	3 (3%)	3	20
47	DT	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	6	27
48	BU	70/88 (80%)	59 (84%)	10 (14%)	1 (1%)	9	33
48	DU	70/88 (80%)	57 (81%)	12 (17%)	1 (1%)	9	33
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	20
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%)	169 (79%)	45 (21%)	1	5
3	CD	214/218 (98%)	182 (85%)	32 (15%)	3	13
4	AE	165/166 (99%)	129 (78%)	36 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CE	165/166 (99%)	127 (77%)	38 (23%)	1	4
5	AF	161/166 (97%)	135 (84%)	26 (16%)	2	12
5	CF	165/166 (99%)	139 (84%)	26 (16%)	2	12
6	AG	155/156 (99%)	132 (85%)	23 (15%)	3	13
6	CG	155/156 (99%)	140 (90%)	15 (10%)	8	28
7	AH	142/148 (96%)	111 (78%)	31 (22%)	1	5
7	CH	142/148 (96%)	122 (86%)	20 (14%)	3	14
8	AK	122/124 (98%)	101 (83%)	21 (17%)	2	10
8	CK	122/124 (98%)	103 (84%)	19 (16%)	2	12
9	AM	117/119 (98%)	97 (83%)	20 (17%)	2	10
9	CM	117/119 (98%)	95 (81%)	22 (19%)	1	7
10	AN	100/100 (100%)	88 (88%)	12 (12%)	5	20
10	CN	100/100 (100%)	86 (86%)	14 (14%)	3	15
11	AO	116/116 (100%)	84 (72%)	32 (28%)	0	2
11	CO	116/116 (100%)	79 (68%)	37 (32%)	0	1
12	AP	111/111 (100%)	88 (79%)	23 (21%)	1	6
12	CP	111/111 (100%)	84 (76%)	27 (24%)	1	3
13	A0	101/101 (100%)	82 (81%)	19 (19%)	1	7
13	C0	100/101 (99%)	84 (84%)	16 (16%)	2	11
14	AQ	87/88 (99%)	71 (82%)	16 (18%)	1	7
14	CQ	87/88 (99%)	73 (84%)	14 (16%)	2	12
15	AR	120/127 (94%)	99 (82%)	21 (18%)	2	9
15	CR	120/127 (94%)	104 (87%)	16 (13%)	4	17
16	A1	93/94 (99%)	78 (84%)	15 (16%)	2	12
16	C1	93/94 (99%)	81 (87%)	12 (13%)	4	17
17	A2	82/82 (100%)	64 (78%)	18 (22%)	1	5
17	C2	82/82 (100%)	62 (76%)	20 (24%)	1	3
18	AS	92/92 (100%)	72 (78%)	20 (22%)	1	5
18	CS	92/92 (100%)	79 (86%)	13 (14%)	3	14
19	AT	74/78 (95%)	65 (88%)	9 (12%)	5	19
19	CT	74/78 (95%)	63 (85%)	11 (15%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AU	85/91 (93%)	68 (80%)	17 (20%)	1	6
20	CU	85/91 (93%)	60 (71%)	25 (29%)	0	2
21	AV	154/179 (86%)	126 (82%)	28 (18%)	2	8
21	CV	158/179 (88%)	138 (87%)	20 (13%)	4	18
22	A3	61/67 (91%)	52 (85%)	9 (15%)	3	13
22	C3	62/67 (92%)	56 (90%)	6 (10%)	8	28
23	AZ	82/83 (99%)	70 (85%)	12 (15%)	3	14
23	CZ	82/83 (99%)	65 (79%)	17 (21%)	1	6
24	AW	62/67 (92%)	47 (76%)	15 (24%)	1	3
24	CW	62/67 (92%)	52 (84%)	10 (16%)	2	12
25	AX	51/52 (98%)	43 (84%)	8 (16%)	2	12
25	CX	51/52 (98%)	43 (84%)	8 (16%)	2	12
26	A4	59/63 (94%)	51 (86%)	8 (14%)	3	16
26	C4	57/63 (90%)	43 (75%)	14 (25%)	1	3
27	A5	51/52 (98%)	41 (80%)	10 (20%)	1	6
27	C5	51/52 (98%)	42 (82%)	9 (18%)	2	9
28	A6	44/52 (85%)	31 (70%)	13 (30%)	0	2
28	C6	44/52 (85%)	38 (86%)	6 (14%)	3	16
29	A7	38/42 (90%)	32 (84%)	6 (16%)	2	12
29	C7	38/42 (90%)	31 (82%)	7 (18%)	1	7
30	A8	50/55 (91%)	39 (78%)	11 (22%)	1	5
30	C8	50/55 (91%)	37 (74%)	13 (26%)	0	2
32	BE	205/220 (93%)	171 (83%)	34 (17%)	2	11
32	DE	205/220 (93%)	174 (85%)	31 (15%)	3	13
33	BF	159/188 (85%)	130 (82%)	29 (18%)	2	8
33	DF	160/188 (85%)	141 (88%)	19 (12%)	5	20
34	BG	180/180 (100%)	155 (86%)	25 (14%)	3	15
34	DG	180/180 (100%)	153 (85%)	27 (15%)	3	13
35	BH	116/123 (94%)	96 (83%)	20 (17%)	2	10
35	DH	116/123 (94%)	96 (83%)	20 (17%)	2	10
36	BI	90/90 (100%)	81 (90%)	9 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	DI	90/90 (100%)	81 (90%)	9 (10%)	7	27
37	BJ	126/127 (99%)	106 (84%)	20 (16%)	2	12
37	DJ	126/127 (99%)	107 (85%)	19 (15%)	3	13
38	BK	119/119 (100%)	98 (82%)	21 (18%)	2	9
38	DK	119/119 (100%)	105 (88%)	14 (12%)	5	20
39	BL	98/99 (99%)	86 (88%)	12 (12%)	5	19
39	DL	98/99 (99%)	84 (86%)	14 (14%)	3	14
40	BM	89/92 (97%)	74 (83%)	15 (17%)	2	10
40	DM	89/92 (97%)	78 (88%)	11 (12%)	4	19
41	BN	90/99 (91%)	78 (87%)	12 (13%)	4	17
41	DN	90/99 (91%)	80 (89%)	10 (11%)	6	22
42	BO	104/109 (95%)	89 (86%)	15 (14%)	3	14
42	DO	104/109 (95%)	85 (82%)	19 (18%)	2	7
43	BP	94/101 (93%)	81 (86%)	13 (14%)	3	15
43	DP	94/101 (93%)	82 (87%)	12 (13%)	4	18
44	BQ	48/50 (96%)	44 (92%)	4 (8%)	10	34
44	DQ	48/50 (96%)	44 (92%)	4 (8%)	10	34
45	BR	79/80 (99%)	70 (89%)	9 (11%)	5	21
45	DR	79/80 (99%)	70 (89%)	9 (11%)	5	21
46	BS	72/74 (97%)	61 (85%)	11 (15%)	3	13
46	DS	72/74 (97%)	65 (90%)	7 (10%)	8	28
47	BT	95/97 (98%)	80 (84%)	15 (16%)	2	12
47	DT	95/97 (98%)	90 (95%)	5 (5%)	20	49
48	BU	63/77 (82%)	57 (90%)	6 (10%)	8	29
48	DU	63/77 (82%)	54 (86%)	9 (14%)	3	14
49	BV	67/80 (84%)	53 (79%)	14 (21%)	1	5
49	DV	67/80 (84%)	55 (82%)	12 (18%)	2	8
50	BW	76/82 (93%)	66 (87%)	10 (13%)	4	17
50	DW	76/82 (93%)	65 (86%)	11 (14%)	3	14
51	BX	20/22 (91%)	19 (95%)	1 (5%)	22	50
51	DX	20/22 (91%)	19 (95%)	1 (5%)	22	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9565/9996 (96%)	7996 (84%)	1569 (16%)	2 11

5 of 1569 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	CG	147	ASP
17	C2	99	ILE
8	CK	12	LEU
6	CG	109	VAL
11	CO	147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 306 such sidechains are listed below:

Mol	Chain	Res	Type
25	CX	46	ASN
42	DO	72	HIS
27	C5	4	HIS
36	DI	57	GLN
46	DS	76	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%)	326 (21%)	46 (3%)
52	BB	84/85 (98%)	47 (55%)	10 (11%)
52	BD	84/85 (98%)	32 (38%)	5 (5%)
52	DB	84/85 (98%)	49 (58%)	9 (10%)
52	DD	84/85 (98%)	31 (36%)	5 (5%)
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	9578/9606 (99%)	2137 (22%)	234 (2%)

5 of 2137 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	BB	38	52	28,31,32	1.95	3 (10%)	38,44,47	2.53	13 (34%)
52	MIA	DB	38	52	28,31,32	2.02	2 (7%)	38,44,47	2.70	13 (34%)
52	MIA	BD	38	52	28,31,32	1.90	3 (10%)	38,44,47	2.80	12 (31%)
52	MIA	DD	38	52	28,31,32	1.94	3 (10%)	38,44,47	2.58	12 (31%)

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	BB	38	52	-	3/15/33/34	0/3/3/3
52	MIA	DB	38	52	-	4/15/33/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	MIA	BD	38	52	-	8/15/33/34	0/3/3/3
52	MIA	DD	38	52	-	8/15/33/34	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	DB	38	MIA	C6-N6	7.70	1.46	1.34
52	BB	38	MIA	C6-N6	7.41	1.46	1.34
52	DD	38	MIA	C6-N6	7.37	1.45	1.34
52	BD	38	MIA	C6-N6	7.22	1.45	1.34
52	DB	38	MIA	C13-C14	6.06	1.50	1.32

The worst 5 of 50 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	BB	38	MIA	C5-C4-N3	-7.68	119.09	127.18
52	BD	38	MIA	C5-C4-N3	-7.57	119.20	127.18
52	DB	38	MIA	C5-C4-N3	-7.45	119.33	127.18

There are no chirality outliers.

5 of 23 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 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	DB	38	MIA	2	0
52	BD	38	MIA	3	0
52	DD	38	MIA	5	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	3523	-	0,6,6	-	-	-		
56	OHX	AA	3138	-	0,6,6	-	-	-		
56	OHX	CA	3291	-	0,6,6	-	-	-		
56	OHX	BA	1668	-	0,6,6	-	-	-		
56	OHX	BA	1682	-	0,6,6	-	-	-		
56	OHX	CB	215	-	0,6,6	-	-	-		
56	OHX	AA	3437	-	0,6,6	-	-	-		
56	OHX	BA	1662	-	0,6,6	-	-	-		
56	OHX	BA	1790	-	0,6,6	-	-	-		
56	OHX	AA	3506	-	0,6,6	-	-	-		
56	OHX	DA	1766	-	0,6,6	-	-	-		
56	OHX	CA	3342	-	0,6,6	-	-	-		
56	OHX	AA	3468	-	0,6,6	-	-	-		
56	OHX	CA	3335	-	0,6,6	-	-	-		
56	OHX	AB	212	-	0,6,6	-	-	-		
56	OHX	CA	3244	-	0,6,6	-	-	-		
56	OHX	DA	1776	-	0,6,6	-	-	-		
56	OHX	AB	216	-	0,6,6	-	-	-		
56	OHX	BA	1775	-	0,6,6	-	-	-		
56	OHX	BA	1771	-	0,6,6	-	-	-		
56	OHX	AA	3561	-	0,6,6	-	-	-		
56	OHX	CA	3273	-	0,6,6	-	-	-		
56	OHX	DA	1731	-	0,6,6	-	-	-		
56	OHX	AA	3490	-	0,6,6	-	-	-		
56	OHX	DA	1719	-	0,6,6	-	-	-		
56	OHX	CA	3302	-	0,6,6	-	-	-		
56	OHX	AB	218	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	CA	3280	-	0,6,6	-	-	-		
56	OHX	DA	1768	-	0,6,6	-	-	-		
56	OHX	AA	3434	-	0,6,6	-	-	-		
56	OHX	CA	3348	-	0,6,6	-	-	-		
56	OHX	AA	3312	-	0,6,6	-	-	-		
56	OHX	AA	3494	-	0,6,6	-	-	-		
56	OHX	AA	3497	-	0,6,6	-	-	-		
56	OHX	AA	3517	-	0,6,6	-	-	-		
56	OHX	CA	3467	55	0,6,6	-	-	-		
56	OHX	AW	101	-	0,6,6	-	-	-		
56	OHX	AF	303	-	0,6,6	-	-	-		
56	OHX	DA	1777	-	0,6,6	-	-	-		
56	OHX	BA	1688	-	0,6,6	-	-	-		
56	OHX	CA	3421	-	0,6,6	-	-	-		
56	OHX	CA	3390	-	0,6,6	-	-	-		
56	OHX	BA	1761	-	0,6,6	-	-	-		
56	OHX	DA	1757	-	0,6,6	-	-	-		
56	OHX	AA	3518	-	0,6,6	-	-	-		
56	OHX	CA	3491	-	0,6,6	-	-	-		
56	OHX	BA	1776	-	0,6,6	-	-	-		
56	OHX	AA	3535	-	0,6,6	-	-	-		
56	OHX	CA	3429	-	0,6,6	-	-	-		
56	OHX	DA	1791	-	0,6,6	-	-	-		
56	OHX	CA	3316	-	0,6,6	-	-	-		
56	OHX	AA	3560	-	0,6,6	-	-	-		
56	OHX	BA	1669	-	0,6,6	-	-	-		
56	OHX	CA	3321	-	0,6,6	-	-	-		
56	OHX	BA	1816	-	0,6,6	-	-	-		
56	OHX	BA	1767	-	0,6,6	-	-	-		
56	OHX	CB	208	-	0,6,6	-	-	-		
56	OHX	AA	3324	-	0,6,6	-	-	-		
56	OHX	CA	3345	-	0,6,6	-	-	-		
56	OHX	DA	1744	-	0,6,6	-	-	-		
56	OHX	CA	3481	-	0,6,6	-	-	-		
56	OHX	CA	3418	-	0,6,6	-	-	-		
56	OHX	AA	3310	-	0,6,6	-	-	-		
56	OHX	CA	3424	-	0,6,6	-	-	-		
56	OHX	DA	1793	-	0,6,6	-	-	-		
56	OHX	CA	3279	-	0,6,6	-	-	-		
56	OHX	DA	1780	-	0,6,6	-	-	-		
56	OHX	DA	1812	-	0,6,6	-	-	-		
56	OHX	AA	3428	-	0,6,6	-	-	-		
56	OHX	AA	3424	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	AA	3367	-	0,6,6	-	-	-		
56	OHX	CA	3306	-	0,6,6	-	-	-		
56	OHX	CA	3436	-	0,6,6	-	-	-		
56	OHX	AA	3370	-	0,6,6	-	-	-		
56	OHX	AA	3307	-	0,6,6	-	-	-		
56	OHX	CB	214	-	0,6,6	-	-	-		
56	OHX	AA	3432	-	0,6,6	-	-	-		
56	OHX	CA	3336	-	0,6,6	-	-	-		
56	OHX	CB	216	-	0,6,6	-	-	-		
56	OHX	DA	1781	-	0,6,6	-	-	-		
56	OHX	AA	3557	-	0,6,6	-	-	-		
56	OHX	CA	3238	-	0,6,6	-	-	-		
56	OHX	DA	1795	-	0,6,6	-	-	-		
56	OHX	BA	1674	55	0,6,6	-	-	-		
56	OHX	CA	3344	-	0,6,6	-	-	-		
56	OHX	CA	3403	-	0,6,6	-	-	-		
56	OHX	AA	3361	-	0,6,6	-	-	-		
56	OHX	AA	3474	-	0,6,6	-	-	-		
56	OHX	CA	3368	-	0,6,6	-	-	-		
56	OHX	AA	3365	-	0,6,6	-	-	-		
56	OHX	AA	3499	-	0,6,6	-	-	-		
56	OHX	AA	3462	-	0,6,6	-	-	-		
56	OHX	CA	3256	-	0,6,6	-	-	-		
56	OHX	CA	3242	-	0,6,6	-	-	-		
56	OHX	AB	210	55	0,6,6	-	-	-		
56	OHX	DA	1735	-	0,6,6	-	-	-		
56	OHX	DA	1759	-	0,6,6	-	-	-		
56	OHX	AA	3470	-	0,6,6	-	-	-		
56	OHX	BA	1789	-	0,6,6	-	-	-		
56	OHX	CA	3247	-	0,6,6	-	-	-		
56	OHX	CF	301	-	0,6,6	-	-	-		
56	OHX	CA	3369	-	0,6,6	-	-	-		
56	OHX	DA	1770	-	0,6,6	-	-	-		
56	OHX	DA	1782	-	0,6,6	-	-	-		
56	OHX	BA	1667	-	0,6,6	-	-	-		
56	OHX	BA	1755	-	0,6,6	-	-	-		
56	OHX	BR	101	-	0,6,6	-	-	-		
56	OHX	BA	1695	-	0,6,6	-	-	-		
56	OHX	CA	3393	-	0,6,6	-	-	-		
56	OHX	AA	3315	-	0,6,6	-	-	-		
56	OHX	CA	3326	-	0,6,6	-	-	-		
56	OHX	CA	3438	-	0,6,6	-	-	-		
56	OHX	AA	3473	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	BA	1797	-	0,6,6	-	-	-		
56	OHX	CA	3416	-	0,6,6	-	-	-		
56	OHX	AA	3504	-	0,6,6	-	-	-		
56	OHX	BA	1768	-	0,6,6	-	-	-		
56	OHX	CA	3489	-	0,6,6	-	-	-		
56	OHX	AA	3322	-	0,6,6	-	-	-		
56	OHX	CA	3236	-	0,6,6	-	-	-		
56	OHX	DA	1761	-	0,6,6	-	-	-		
56	OHX	BA	1678	-	0,6,6	-	-	-		
56	OHX	AA	3516	-	0,6,6	-	-	-		
56	OHX	AA	3496	-	0,6,6	-	-	-		
56	OHX	AA	3292	-	0,6,6	-	-	-		
56	OHX	AA	3426	-	0,6,6	-	-	-		
56	OHX	CA	3322	-	0,6,6	-	-	-		
56	OHX	DA	1756	-	0,6,6	-	-	-		
56	OHX	CA	3355	-	0,6,6	-	-	-		
56	OHX	BA	1759	-	0,6,6	-	-	-		
56	OHX	BA	1783	-	0,6,6	-	-	-		
56	OHX	BA	1659	-	0,6,6	-	-	-		
56	OHX	AA	3550	-	0,6,6	-	-	-		
56	OHX	AA	3419	-	0,6,6	-	-	-		
56	OHX	AA	3449	-	0,6,6	-	-	-		
56	OHX	BA	1758	-	0,6,6	-	-	-		
56	OHX	CA	3299	-	0,6,6	-	-	-		
56	OHX	BC	106	-	0,6,6	-	-	-		
56	OHX	AA	3534	-	0,6,6	-	-	-		
56	OHX	CA	3240	-	0,6,6	-	-	-		
56	OHX	CA	3337	-	0,6,6	-	-	-		
56	OHX	DB	103	-	0,6,6	-	-	-		
56	OHX	AA	3459	-	0,6,6	-	-	-		
56	OHX	CA	3372	-	0,6,6	-	-	-		
56	OHX	AA	3501	-	0,6,6	-	-	-		
56	OHX	AA	3301	-	0,6,6	-	-	-		
56	OHX	AA	3359	-	0,6,6	-	-	-		
56	OHX	C1	201	-	0,6,6	-	-	-		
56	OHX	AA	3425	-	0,6,6	-	-	-		
56	OHX	CA	3391	-	0,6,6	-	-	-		
56	OHX	AA	3469	-	0,6,6	-	-	-		
56	OHX	CA	3371	-	0,6,6	-	-	-		
56	OHX	BA	1766	-	0,6,6	-	-	-		
56	OHX	DA	1809	-	0,6,6	-	-	-		
56	OHX	AA	3407	-	0,6,6	-	-	-		
56	OHX	CA	3329	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	CA	3237	-	0,6,6	-	-	-		
56	OHX	CA	3303	-	0,6,6	-	-	-		
56	OHX	BA	1756	-	0,6,6	-	-	-		
56	OHX	BA	1815	-	0,6,6	-	-	-		
56	OHX	AA	3334	-	0,6,6	-	-	-		
56	OHX	CA	3485	-	0,6,6	-	-	-		
56	OHX	DA	1811	-	0,6,6	-	-	-		
56	OHX	AA	3545	-	0,6,6	-	-	-		
56	OHX	BA	1675	-	0,6,6	-	-	-		
56	OHX	CA	3435	-	0,6,6	-	-	-		
56	OHX	CA	3341	-	0,6,6	-	-	-		
56	OHX	CA	3354	-	0,6,6	-	-	-		
56	OHX	AA	3460	-	0,6,6	-	-	-		
56	OHX	BC	107	-	0,6,6	-	-	-		
56	OHX	DA	1802	-	0,6,6	-	-	-		
56	OHX	CA	3332	-	0,6,6	-	-	-		
56	OHX	DA	1810	-	0,6,6	-	-	-		
56	OHX	CA	3362	-	0,6,6	-	-	-		
56	OHX	CA	3283	-	0,6,6	-	-	-		
56	OHX	CA	3269	-	0,6,6	-	-	-		
56	OHX	AA	3363	-	0,6,6	-	-	-		
56	OHX	DC	110	-	0,6,6	-	-	-		
56	OHX	CA	3382	-	0,6,6	-	-	-		
56	OHX	CA	3308	-	0,6,6	-	-	-		
56	OHX	CA	3300	-	0,6,6	-	-	-		
56	OHX	DA	1758	-	0,6,6	-	-	-		
56	OHX	DA	1788	-	0,6,6	-	-	-		
56	OHX	CB	212	-	0,6,6	-	-	-		
56	OHX	AA	3309	-	0,6,6	-	-	-		
56	OHX	BA	1802	-	0,6,6	-	-	-		
56	OHX	CA	3398	-	0,6,6	-	-	-		
56	OHX	CA	3425	-	0,6,6	-	-	-		
56	OHX	AA	3368	-	0,6,6	-	-	-		
56	OHX	BA	1798	-	0,6,6	-	-	-		
56	OHX	CA	3340	-	0,6,6	-	-	-		
56	OHX	DA	1765	-	0,6,6	-	-	-		
56	OHX	BA	1696	-	0,6,6	-	-	-		
56	OHX	AA	3491	-	0,6,6	-	-	-		
56	OHX	BA	1760	-	0,6,6	-	-	-		
56	OHX	CA	3293	-	0,6,6	-	-	-		
56	OHX	CA	3378	-	0,6,6	-	-	-		
56	OHX	BA	1801	-	0,6,6	-	-	-		
56	OHX	BA	1811	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	AA	3540	-	0,6,6	-	-	-		
56	OHX	CB	218	-	0,6,6	-	-	-		
56	OHX	DA	1808	-	0,6,6	-	-	-		
56	OHX	CA	3252	-	0,6,6	-	-	-		
56	OHX	BA	1814	-	0,6,6	-	-	-		
56	OHX	AA	3327	-	0,6,6	-	-	-		
56	OHX	AA	3330	-	0,6,6	-	-	-		
56	OHX	BA	1685	-	0,6,6	-	-	-		
56	OHX	DA	1728	-	0,6,6	-	-	-		
56	OHX	DB	105	-	0,6,6	-	-	-		
56	OHX	AA	3302	-	0,6,6	-	-	-		
56	OHX	DA	1784	-	0,6,6	-	-	-		
56	OHX	AA	3531	-	0,6,6	-	-	-		
56	OHX	BA	1806	-	0,6,6	-	-	-		
56	OHX	BA	1774	-	0,6,6	-	-	-		
56	OHX	CA	3248	-	0,6,6	-	-	-		
56	OHX	AA	3364	-	0,6,6	-	-	-		
56	OHX	AA	3436	55	0,6,6	-	-	-		
56	OHX	BA	1677	-	0,6,6	-	-	-		
56	OHX	CA	3254	-	0,6,6	-	-	-		
56	OHX	AA	3448	-	0,6,6	-	-	-		
56	OHX	CA	3408	-	0,6,6	-	-	-		
56	OHX	AA	3332	-	0,6,6	-	-	-		
56	OHX	CA	3349	-	0,6,6	-	-	-		
56	OHX	AA	3304	-	0,6,6	-	-	-		
56	OHX	A3	102	-	0,6,6	-	-	-		
56	OHX	DA	1794	-	0,6,6	-	-	-		
56	OHX	AA	3482	-	0,6,6	-	-	-		
56	OHX	BA	1809	-	0,6,6	-	-	-		
56	OHX	AA	3372	-	0,6,6	-	-	-		
56	OHX	BA	1681	-	0,6,6	-	-	-		
56	OHX	CA	3434	-	0,6,6	-	-	-		
56	OHX	CA	3488	-	0,6,6	-	-	-		
56	OHX	AA	3299	-	0,6,6	-	-	-		
56	OHX	BA	1808	-	0,6,6	-	-	-		
56	OHX	CA	3310	-	0,6,6	-	-	-		
56	OHX	CA	3411	-	0,6,6	-	-	-		
56	OHX	CA	3466	-	0,6,6	-	-	-		
56	OHX	CA	3392	-	0,6,6	-	-	-		
56	OHX	CA	3292	-	0,6,6	-	-	-		
56	OHX	BA	1683	-	0,6,6	-	-	-		
56	OHX	AA	3486	-	0,6,6	-	-	-		
56	OHX	BA	1803	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	CA	3274	-	0,6,6	-	-	-		
56	OHX	CA	3307	-	0,6,6	-	-	-		
56	OHX	AA	3405	-	0,6,6	-	-	-		
56	OHX	AA	3433	-	0,6,6	-	-	-		
56	OHX	CA	3325	-	0,6,6	-	-	-		
56	OHX	DG	302	-	0,6,6	-	-	-		
56	OHX	CA	3358	-	0,6,6	-	-	-		
56	OHX	CA	3395	-	0,6,6	-	-	-		
56	OHX	CA	3353	-	0,6,6	-	-	-		
56	OHX	DR	101	-	0,6,6	-	-	-		
56	OHX	C3	101	-	0,6,6	-	-	-		
56	OHX	DA	1718	-	0,6,6	-	-	-		
56	OHX	BA	1813	-	0,6,6	-	-	-		
56	OHX	BA	1800	-	0,6,6	-	-	-		
56	OHX	AA	3287	-	0,6,6	-	-	-		
56	OHX	AA	3530	-	0,6,6	-	-	-		
56	OHX	CA	3484	-	0,6,6	-	-	-		
56	OHX	AA	3342	-	0,6,6	-	-	-		
56	OHX	CA	3461	-	0,6,6	-	-	-		
56	OHX	AA	3542	-	0,6,6	-	-	-		
56	OHX	CA	3311	-	0,6,6	-	-	-		
56	OHX	DA	1721	-	0,6,6	-	-	-		
56	OHX	AA	3263	-	0,6,6	-	-	-		
56	OHX	AA	3366	-	0,6,6	-	-	-		
56	OHX	AA	3519	-	0,6,6	-	-	-		
56	OHX	CA	3251	-	0,6,6	-	-	-		
56	OHX	BA	1661	-	0,6,6	-	-	-		
56	OHX	DA	1801	-	0,6,6	-	-	-		
56	OHX	CA	3249	55	0,6,6	-	-	-		
56	OHX	DA	1751	-	0,6,6	-	-	-		
56	OHX	CA	3414	-	0,6,6	-	-	-		
56	OHX	CA	3284	-	0,6,6	-	-	-		
56	OHX	AA	3360	-	0,6,6	-	-	-		
56	OHX	AA	3538	-	0,6,6	-	-	-		
56	OHX	BB	106	-	0,6,6	-	-	-		
56	OHX	AA	3521	-	0,6,6	-	-	-		
56	OHX	CA	3360	-	0,6,6	-	-	-		
56	OHX	CA	3423	-	0,6,6	-	-	-		
56	OHX	CA	3323	-	0,6,6	-	-	-		
56	OHX	CA	3359	-	0,6,6	-	-	-		
56	OHX	BA	1656	-	0,6,6	-	-	-		
56	OHX	CA	3365	-	0,6,6	-	-	-		
56	OHX	DA	1729	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	AA	3562	-	0,6,6	-	-	-		
56	OHX	CA	3298	-	0,6,6	-	-	-		
56	OHX	AA	3524	-	0,6,6	-	-	-		
56	OHX	CA	3318	-	0,6,6	-	-	-		
56	OHX	AA	3547	-	0,6,6	-	-	-		
56	OHX	AA	3323	-	0,6,6	-	-	-		
56	OHX	DA	1755	-	0,6,6	-	-	-		
56	OHX	AB	215	-	0,6,6	-	-	-		
56	OHX	DA	1743	-	0,6,6	-	-	-		
56	OHX	AA	3404	-	0,6,6	-	-	-		
56	OHX	AA	3328	-	0,6,6	-	-	-		
56	OHX	CA	3379	-	0,6,6	-	-	-		
56	OHX	CA	3410	-	0,6,6	-	-	-		
56	OHX	AA	3295	-	0,6,6	-	-	-		
56	OHX	BA	1691	-	0,6,6	-	-	-		
56	OHX	CA	3343	-	0,6,6	-	-	-		
56	OHX	BA	1794	-	0,6,6	-	-	-		
56	OHX	CA	3394	-	0,6,6	-	-	-		
56	OHX	DA	1797	-	0,6,6	-	-	-		
56	OHX	AA	3321	-	0,6,6	-	-	-		
56	OHX	AA	3447	-	0,6,6	-	-	-		
56	OHX	BA	1778	-	0,6,6	-	-	-		
56	OHX	AA	3485	-	0,6,6	-	-	-		
56	OHX	DA	1796	-	0,6,6	-	-	-		
56	OHX	AA	3406	-	0,6,6	-	-	-		
56	OHX	AA	3559	-	0,6,6	-	-	-		
56	OHX	CA	3386	-	0,6,6	-	-	-		
56	OHX	BB	107	-	0,6,6	-	-	-		
56	OHX	AA	3288	-	0,6,6	-	-	-		
56	OHX	AA	3466	-	0,6,6	-	-	-		
56	OHX	AA	3548	-	0,6,6	-	-	-		
56	OHX	DA	1779	-	0,6,6	-	-	-		
56	OHX	AA	3297	-	0,6,6	-	-	-		
56	OHX	AA	3509	-	0,6,6	-	-	-		
56	OHX	CA	3364	-	0,6,6	-	-	-		
56	OHX	CA	3287	-	0,6,6	-	-	-		
56	OHX	DA	1764	-	0,6,6	-	-	-		
56	OHX	BA	1763	-	0,6,6	-	-	-		
56	OHX	DA	1785	-	0,6,6	-	-	-		
56	OHX	AA	3450	-	0,6,6	-	-	-		
56	OHX	CA	3333	-	0,6,6	-	-	-		
56	OHX	AA	3160	-	0,6,6	-	-	-		
56	OHX	AA	3431	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	AO	204	-	0,6,6	-	-	-		
56	OHX	CA	3492	-	0,6,6	-	-	-		
56	OHX	AA	3300	-	0,6,6	-	-	-		
56	OHX	AA	3508	55	0,6,6	-	-	-		
56	OHX	AB	207	-	0,6,6	-	-	-		
56	OHX	CA	3427	-	0,6,6	-	-	-		
56	OHX	BA	1692	-	0,6,6	-	-	-		
56	OHX	CA	3350	-	0,6,6	-	-	-		
56	OHX	CA	3470	-	0,6,6	-	-	-		
56	OHX	AA	3427	-	0,6,6	-	-	-		
56	OHX	CB	219	-	0,6,6	-	-	-		
56	OHX	DA	1724	-	0,6,6	-	-	-		
56	OHX	CA	3377	-	0,6,6	-	-	-		
56	OHX	AA	3296	-	0,6,6	-	-	-		
56	OHX	AA	3453	-	0,6,6	-	-	-		
56	OHX	AA	3498	-	0,6,6	-	-	-		
56	OHX	CA	3363	-	0,6,6	-	-	-		
56	OHX	CA	3415	-	0,6,6	-	-	-		
56	OHX	AB	211	-	0,6,6	-	-	-		
56	OHX	DA	1763	-	0,6,6	-	-	-		
56	OHX	BA	1793	-	0,6,6	-	-	-		
56	OHX	CA	3276	-	0,6,6	-	-	-		
56	OHX	BA	1780	-	0,6,6	-	-	-		
56	OHX	CB	220	-	0,6,6	-	-	-		
56	OHX	AA	3336	-	0,6,6	-	-	-		
56	OHX	CA	3331	-	0,6,6	-	-	-		
56	OHX	AA	3539	-	0,6,6	-	-	-		
56	OHX	CA	3419	-	0,6,6	-	-	-		
56	OHX	BA	1785	-	0,6,6	-	-	-		
56	OHX	AA	3339	-	0,6,6	-	-	-		
56	OHX	CA	3367	-	0,6,6	-	-	-		
56	OHX	DA	1726	-	0,6,6	-	-	-		
56	OHX	CA	3426	-	0,6,6	-	-	-		
56	OHX	AA	3511	-	0,6,6	-	-	-		
56	OHX	AA	3326	-	0,6,6	-	-	-		
56	OHX	AA	3438	-	0,6,6	-	-	-		
56	OHX	AA	3565	-	0,6,6	-	-	-		
56	OHX	AA	3489	-	0,6,6	-	-	-		
56	OHX	DC	108	-	0,6,6	-	-	-		
56	OHX	DV	101	-	0,6,6	-	-	-		
56	OHX	BA	1676	-	0,6,6	-	-	-		
56	OHX	CA	3243	-	0,6,6	-	-	-		
56	OHX	AA	3507	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	CA	3420	-	0,6,6	-	-	-		
56	OHX	AA	3476	-	0,6,6	-	-	-		
56	OHX	AA	3429	-	0,6,6	-	-	-		
56	OHX	CA	3304	-	0,6,6	-	-	-		
56	OHX	DA	1749	-	0,6,6	-	-	-		
56	OHX	AA	3316	-	0,6,6	-	-	-		
56	OHX	AA	3446	-	0,6,6	-	-	-		
56	OHX	CA	3375	-	0,6,6	-	-	-		
56	OHX	BA	1791	-	0,6,6	-	-	-		
56	OHX	CA	3431	-	0,6,6	-	-	-		
56	OHX	DA	1727	-	0,6,6	-	-	-		
56	OHX	CA	3255	-	0,6,6	-	-	-		
56	OHX	AA	3541	-	0,6,6	-	-	-		
56	OHX	DA	1787	-	0,6,6	-	-	-		
56	OHX	CA	3234	-	0,6,6	-	-	-		
56	OHX	CA	3278	-	0,6,6	-	-	-		
56	OHX	CA	3245	-	0,6,6	-	-	-		
56	OHX	AA	3454	-	0,6,6	-	-	-		
56	OHX	AA	3527	-	0,6,6	-	-	-		
56	OHX	CA	3433	-	0,6,6	-	-	-		
56	OHX	AA	3484	-	0,6,6	-	-	-		
56	OHX	AA	3401	-	0,6,6	-	-	-		
56	OHX	CA	3246	-	0,6,6	-	-	-		
56	OHX	AA	3313	-	0,6,6	-	-	-		
56	OHX	DA	1739	-	0,6,6	-	-	-		
56	OHX	BA	1665	-	0,6,6	-	-	-		
56	OHX	BA	1670	-	0,6,6	-	-	-		
56	OHX	CA	3397	-	0,6,6	-	-	-		
56	OHX	BA	1795	-	0,6,6	-	-	-		
56	OHX	CA	3486	-	0,6,6	-	-	-		
56	OHX	AA	3329	-	0,6,6	-	-	-		
56	OHX	DA	1807	-	0,6,6	-	-	-		
56	OHX	CA	3400	-	0,6,6	-	-	-		
56	OHX	AA	3502	-	0,6,6	-	-	-		
56	OHX	CA	3357	-	0,6,6	-	-	-		
56	OHX	AA	3311	-	0,6,6	-	-	-		
56	OHX	BA	1777	-	0,6,6	-	-	-		
56	OHX	CA	3272	-	0,6,6	-	-	-		
56	OHX	AA	3566	-	0,6,6	-	-	-		
56	OHX	AA	3317	-	0,6,6	-	-	-		
56	OHX	AA	3417	-	0,6,6	-	-	-		
56	OHX	AA	3505	-	0,6,6	-	-	-		
56	OHX	BA	1757	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	CA	3428	-	0,6,6	-	-	-		
56	OHX	DA	1790	-	0,6,6	-	-	-		
56	OHX	BA	1787	-	0,6,6	-	-	-		
56	OHX	CA	3235	-	0,6,6	-	-	-		
56	OHX	CA	3490	-	0,6,6	-	-	-		
56	OHX	DA	1771	-	0,6,6	-	-	-		
56	OHX	BA	1684	-	0,6,6	-	-	-		
56	OHX	AA	3555	-	0,6,6	-	-	-		
56	OHX	CA	3463	-	0,6,6	-	-	-		
56	OHX	AA	3455	-	0,6,6	-	-	-		
56	OHX	AA	3503	-	0,6,6	-	-	-		
56	OHX	AA	3333	55	0,6,6	-	-	-		
56	OHX	AA	3495	-	0,6,6	-	-	-		
56	OHX	AA	3546	-	0,6,6	-	-	-		
56	OHX	AA	3522	-	0,6,6	-	-	-		
56	OHX	CA	3380	-	0,6,6	-	-	-		
56	OHX	DC	107	-	0,6,6	-	-	-		
56	OHX	CA	3399	-	0,6,6	-	-	-		
56	OHX	AA	3493	-	0,6,6	-	-	-		
56	OHX	AA	3471	-	0,6,6	-	-	-		
56	OHX	DA	1745	-	0,6,6	-	-	-		
56	OHX	CA	3389	-	0,6,6	-	-	-		
56	OHX	BA	1657	-	0,6,6	-	-	-		
56	OHX	CA	3384	-	0,6,6	-	-	-		
56	OHX	DA	1762	-	0,6,6	-	-	-		
56	OHX	AA	3481	-	0,6,6	-	-	-		
56	OHX	AA	3418	-	0,6,6	-	-	-		
56	OHX	BA	1807	-	0,6,6	-	-	-		
56	OHX	BD	103	-	0,6,6	-	-	-		
56	OHX	CA	3327	-	0,6,6	-	-	-		
56	OHX	CA	3385	-	0,6,6	-	-	-		
56	OHX	AA	3154	-	0,6,6	-	-	-		
56	OHX	CA	3338	-	0,6,6	-	-	-		
56	OHX	AA	3563	-	0,6,6	-	-	-		
56	OHX	AA	3294	-	0,6,6	-	-	-		
56	OHX	AA	3293	-	0,6,6	-	-	-		
56	OHX	DA	1767	-	0,6,6	-	-	-		
56	OHX	AA	3305	-	0,6,6	-	-	-		
56	OHX	BA	1773	-	0,6,6	-	-	-		
56	OHX	AA	3472	-	0,6,6	-	-	-		
56	OHX	CA	3430	-	0,6,6	-	-	-		
56	OHX	CA	3324	-	0,6,6	-	-	-		
56	OHX	CA	3374	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	BG	302	-	0,6,6	-	-	-		
56	OHX	AA	3564	-	0,6,6	-	-	-		
56	OHX	DA	1734	-	0,6,6	-	-	-		
56	OHX	DA	1760	-	0,6,6	-	-	-		
56	OHX	AE	304	-	0,6,6	-	-	-		
56	OHX	CA	3297	-	0,6,6	-	-	-		
56	OHX	CA	3253	-	0,6,6	-	-	-		
56	OHX	AA	3337	-	0,6,6	-	-	-		
56	OHX	DA	1774	-	0,6,6	-	-	-		
56	OHX	BA	1762	-	0,6,6	-	-	-		
56	OHX	AA	3445	-	0,6,6	-	-	-		
56	OHX	CA	3290	55	0,6,6	-	-	-		
56	OHX	CA	3432	-	0,6,6	-	-	-		
56	OHX	AA	3458	-	0,6,6	-	-	-		
56	OHX	AO	205	-	0,6,6	-	-	-		
56	OHX	AA	3452	-	0,6,6	-	-	-		
56	OHX	AA	3526	55	0,6,6	-	-	-		
56	OHX	CA	3413	-	0,6,6	-	-	-		
56	OHX	AA	3556	-	0,6,6	-	-	-		
56	OHX	BD	102	-	0,6,6	-	-	-		
56	OHX	DA	1792	-	0,6,6	-	-	-		
56	OHX	DA	1732	-	0,6,6	-	-	-		
56	OHX	DA	1737	-	0,6,6	-	-	-		
56	OHX	AA	3399	-	0,6,6	-	-	-		
56	OHX	CA	3361	-	0,6,6	-	-	-		
56	OHX	BA	1772	-	0,6,6	-	-	-		
56	OHX	AA	3303	-	0,6,6	-	-	-		
56	OHX	BD	104	-	0,6,6	-	-	-		
56	OHX	DA	1804	-	0,6,6	-	-	-		
56	OHX	CA	3402	-	0,6,6	-	-	-		
56	OHX	AA	3500	-	0,6,6	-	-	-		
56	OHX	AA	3537	-	0,6,6	-	-	-		
56	OHX	AA	3536	-	0,6,6	-	-	-		
56	OHX	AA	3544	-	0,6,6	-	-	-		
56	OHX	CA	3412	-	0,6,6	-	-	-		
56	OHX	DA	1741	-	0,6,6	-	-	-		
56	OHX	CA	3296	-	0,6,6	-	-	-		
56	OHX	AA	3552	-	0,6,6	-	-	-		
56	OHX	CA	3401	-	0,6,6	-	-	-		
56	OHX	CA	3315	-	0,6,6	-	-	-		
56	OHX	CA	3404	-	0,6,6	-	-	-		
56	OHX	AA	3478	-	0,6,6	-	-	-		
56	OHX	AB	219	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	A1	202	-	0,6,6	-	-	-		
56	OHX	AA	3463	-	0,6,6	-	-	-		
56	OHX	BA	1810	-	0,6,6	-	-	-		
56	OHX	CA	3352	-	0,6,6	-	-	-		
56	OHX	CA	3450	-	0,6,6	-	-	-		
56	OHX	CA	3285	-	0,6,6	-	-	-		
56	OHX	DA	1769	-	0,6,6	-	-	-		
56	OHX	DA	1789	-	0,6,6	-	-	-		
56	OHX	AA	3440	-	0,6,6	-	-	-		
56	OHX	CA	3396	-	0,6,6	-	-	-		
56	OHX	AA	3549	-	0,6,6	-	-	-		
56	OHX	CA	3465	-	0,6,6	-	-	-		
56	OHX	AA	3457	-	0,6,6	-	-	-		
56	OHX	AA	3439	-	0,6,6	-	-	-		
56	OHX	CA	3232	-	0,6,6	-	-	-		
56	OHX	DA	1805	-	0,6,6	-	-	-		
56	OHX	AA	3520	-	0,6,6	-	-	-		
56	OHX	AA	3475	-	0,6,6	-	-	-		
56	OHX	AA	3558	-	0,6,6	-	-	-		
56	OHX	BA	1666	-	0,6,6	-	-	-		
56	OHX	DA	1806	-	0,6,6	-	-	-		
56	OHX	BA	1779	-	0,6,6	-	-	-		
56	OHX	AA	3403	-	0,6,6	-	-	-		
56	OHX	BA	1765	-	0,6,6	-	-	-		
56	OHX	DA	1750	-	0,6,6	-	-	-		
56	OHX	CA	3351	-	0,6,6	-	-	-		
56	OHX	DA	1773	-	0,6,6	-	-	-		
56	OHX	CA	3356	-	0,6,6	-	-	-		
56	OHX	AA	3314	-	0,6,6	-	-	-		
56	OHX	AA	3529	-	0,6,6	-	-	-		
56	OHX	CB	211	-	0,6,6	-	-	-		
56	OHX	DK	201	-	0,6,6	-	-	-		
56	OHX	DA	1733	-	0,6,6	-	-	-		
56	OHX	BA	1686	-	0,6,6	-	-	-		
56	OHX	AA	3554	-	0,6,6	-	-	-		
56	OHX	AA	3318	-	0,6,6	-	-	-		
56	OHX	BA	1689	-	0,6,6	-	-	-		
56	OHX	BA	1769	-	0,6,6	-	-	-		
56	OHX	BA	1799	-	0,6,6	-	-	-		
56	OHX	AA	3430	-	0,6,6	-	-	-		
56	OHX	C6	101	-	0,6,6	-	-	-		
56	OHX	DA	1783	-	0,6,6	-	-	-		
56	OHX	AA	3442	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	BA	1784	-	0,6,6	-	-	-		
56	OHX	CA	3277	-	0,6,6	-	-	-		
56	OHX	DA	1748	-	0,6,6	-	-	-		
56	OHX	CA	3319	-	0,6,6	-	-	-		
56	OHX	CA	3328	-	0,6,6	-	-	-		
56	OHX	A1	203	-	0,6,6	-	-	-		
56	OHX	BA	1694	-	0,6,6	-	-	-		
56	OHX	CA	3281	-	0,6,6	-	-	-		
56	OHX	DA	1753	-	0,6,6	-	-	-		
56	OHX	CA	3469	-	0,6,6	-	-	-		
56	OHX	CB	217	-	0,6,6	-	-	-		
56	OHX	AA	3362	-	0,6,6	-	-	-		
56	OHX	CA	3294	-	0,6,6	-	-	-		
56	OHX	CA	3388	-	0,6,6	-	-	-		
56	OHX	AA	3289	-	0,6,6	-	-	-		
56	OHX	BA	1680	55	0,6,6	-	-	-		
56	OHX	CA	3464	-	0,6,6	-	-	-		
56	OHX	DA	1772	-	0,6,6	-	-	-		
56	OHX	AA	3567	-	0,6,6	-	-	-		
56	OHX	AA	3477	-	0,6,6	-	-	-		
56	OHX	CA	3366	-	0,6,6	-	-	-		
56	OHX	BA	1671	-	0,6,6	-	-	-		
56	OHX	CA	3334	-	0,6,6	-	-	-		
56	OHX	AA	3444	-	0,6,6	-	-	-		
56	OHX	CA	3233	-	0,6,6	-	-	-		
56	OHX	BA	1792	-	0,6,6	-	-	-		
56	OHX	CA	3487	-	0,6,6	-	-	-		
56	OHX	AA	3290	-	0,6,6	-	-	-		
56	OHX	AA	3488	-	0,6,6	-	-	-		
56	OHX	CO	201	-	0,6,6	-	-	-		
56	OHX	AA	3568	-	0,6,6	-	-	-		
56	OHX	AA	3402	-	0,6,6	-	-	-		
56	OHX	BA	1804	-	0,6,6	-	-	-		
56	OHX	CA	3381	-	0,6,6	-	-	-		
56	OHX	A6	101	-	0,6,6	-	-	-		
56	OHX	CA	3320	55	0,6,6	-	-	-		
56	OHX	CA	3286	-	0,6,6	-	-	-		
56	OHX	DA	1722	-	0,6,6	-	-	-		
56	OHX	CA	3387	-	0,6,6	-	-	-		
56	OHX	AA	3291	-	0,6,6	-	-	-		
56	OHX	CA	3309	-	0,6,6	-	-	-		
56	OHX	CA	3317	-	0,6,6	-	-	-		
56	OHX	AA	3569	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	AA	3543	55	0,6,6	-	-	-		
56	OHX	AA	3480	-	0,6,6	-	-	-		
56	OHX	BA	1664	-	0,6,6	-	-	-		
56	OHX	AA	3320	-	0,6,6	-	-	-		
56	OHX	AA	3461	-	0,6,6	-	-	-		
56	OHX	AA	3335	-	0,6,6	-	-	-		
56	OHX	AA	3479	-	0,6,6	-	-	-		
56	OHX	DA	1803	-	0,6,6	-	-	-		
56	OHX	AA	3319	-	0,6,6	-	-	-		
56	OHX	BA	1672	-	0,6,6	-	-	-		
56	OHX	AA	3525	55	0,6,6	-	-	-		
56	OHX	CA	3295	-	0,6,6	-	-	-		
56	OHX	AA	3513	-	0,6,6	-	-	-		
56	OHX	CA	3339	-	0,6,6	-	-	-		
56	OHX	DA	1746	-	0,6,6	-	-	-		
56	OHX	AA	3435	-	0,6,6	-	-	-		
56	OHX	AA	3341	-	0,6,6	-	-	-		
56	OHX	BA	1690	-	0,6,6	-	-	-		
56	OHX	CA	3383	-	0,6,6	-	-	-		
56	OHX	BA	1764	-	0,6,6	-	-	-		
56	OHX	CA	3288	-	0,6,6	-	-	-		
56	OHX	AA	3528	55	0,6,6	-	-	-		
56	OHX	CA	3239	-	0,6,6	-	-	-		
56	OHX	CA	3312	-	0,6,6	-	-	-		
56	OHX	DA	1800	-	0,6,6	-	-	-		
56	OHX	AB	208	-	0,6,6	-	-	-		
56	OHX	AA	3422	55	0,6,6	-	-	-		
56	OHX	AA	3456	-	0,6,6	-	-	-		
56	OHX	AA	3423	-	0,6,6	-	-	-		
56	OHX	AA	3551	-	0,6,6	-	-	-		
56	OHX	BA	1679	-	0,6,6	-	-	-		
56	OHX	BA	1693	-	0,6,6	-	-	-		
56	OHX	CA	3409	-	0,6,6	-	-	-		
56	OHX	DA	1730	-	0,6,6	-	-	-		
56	OHX	DA	1742	-	0,6,6	-	-	-		
56	OHX	AA	3421	-	0,6,6	-	-	-		
56	OHX	CA	3482	-	0,6,6	-	-	-		
56	OHX	AB	214	-	0,6,6	-	-	-		
56	OHX	BA	1663	-	0,6,6	-	-	-		
56	OHX	CA	3407	-	0,6,6	-	-	-		
56	OHX	AA	3306	-	0,6,6	-	-	-		
56	OHX	DA	1752	-	0,6,6	-	-	-		
56	OHX	DA	1786	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	AA	3483	-	0,6,6	-	-	-		
56	OHX	CA	3483	-	0,6,6	-	-	-		
56	OHX	DA	1740	-	0,6,6	-	-	-		
56	OHX	AB	209	-	0,6,6	-	-	-		
56	OHX	BA	1805	-	0,6,6	-	-	-		
56	OHX	CA	3282	-	0,6,6	-	-	-		
56	OHX	BA	1812	-	0,6,6	-	-	-		
56	OHX	CA	3250	-	0,6,6	-	-	-		
56	OHX	CA	3271	-	0,6,6	-	-	-		
56	OHX	BA	1687	-	0,6,6	-	-	-		
56	OHX	CA	3346	-	0,6,6	-	-	-		
56	OHX	CA	3313	-	0,6,6	-	-	-		
56	OHX	AA	3371	-	0,6,6	-	-	-		
56	OHX	AA	3514	-	0,6,6	-	-	-		
56	OHX	AB	213	-	0,6,6	-	-	-		
56	OHX	DA	1736	-	0,6,6	-	-	-		
56	OHX	AA	3451	-	0,6,6	-	-	-		
56	OHX	CA	3468	-	0,6,6	-	-	-		
56	OHX	AA	3441	-	0,6,6	-	-	-		
56	OHX	AA	3443	-	0,6,6	-	-	-		
56	OHX	CA	3437	-	0,6,6	-	-	-		
56	OHX	DA	1723	-	0,6,6	-	-	-		
56	OHX	CA	3370	-	0,6,6	-	-	-		
56	OHX	CB	210	-	0,6,6	-	-	-		
56	OHX	CA	3241	-	0,6,6	-	-	-		
56	OHX	AA	3147	-	0,6,6	-	-	-		
56	OHX	AA	3308	-	0,6,6	-	-	-		
56	OHX	BA	1781	-	0,6,6	-	-	-		
56	OHX	AA	3369	-	0,6,6	-	-	-		
56	OHX	CA	3275	-	0,6,6	-	-	-		
56	OHX	CA	3373	-	0,6,6	-	-	-		
56	OHX	BA	1788	55	0,6,6	-	-	-		
56	OHX	AA	3465	-	0,6,6	-	-	-		
56	OHX	AA	3492	-	0,6,6	-	-	-		
56	OHX	AA	3467	-	0,6,6	-	-	-		
56	OHX	AB	217	-	0,6,6	-	-	-		
56	OHX	AA	3400	-	0,6,6	-	-	-		
56	OHX	AA	3510	-	0,6,6	-	-	-		
56	OHX	AA	3373	-	0,6,6	-	-	-		
56	OHX	DA	1754	-	0,6,6	-	-	-		
56	OHX	AA	3298	-	0,6,6	-	-	-		
56	OHX	C5	102	-	0,6,6	-	-	-		
56	OHX	CA	3405	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	AA	3325	-	0,6,6	-	-	-		
56	OHX	AA	3340	-	0,6,6	-	-	-		
56	OHX	CA	3376	-	0,6,6	-	-	-		
56	OHX	AA	3512	-	0,6,6	-	-	-		
56	OHX	BA	1770	-	0,6,6	-	-	-		
56	OHX	AA	3532	-	0,6,6	-	-	-		
56	OHX	BA	1782	-	0,6,6	-	-	-		
56	OHX	AA	3331	-	0,6,6	-	-	-		
56	OHX	BA	1796	-	0,6,6	-	-	-		
56	OHX	DA	1799	-	0,6,6	-	-	-		
56	OHX	AA	3553	-	0,6,6	-	-	-		
56	OHX	CA	3330	-	0,6,6	-	-	-		
56	OHX	CA	3305	-	0,6,6	-	-	-		
56	OHX	CB	209	-	0,6,6	-	-	-		
56	OHX	CA	3314	-	0,6,6	-	-	-		
56	OHX	DA	1738	-	0,6,6	-	-	-		
56	OHX	AA	3338	-	0,6,6	-	-	-		
56	OHX	BA	1786	-	0,6,6	-	-	-		
56	OHX	AA	3420	-	0,6,6	-	-	-		
56	OHX	CA	3270	-	0,6,6	-	-	-		
56	OHX	AA	3464	55	0,6,6	-	-	-		
56	OHX	DC	109	-	0,6,6	-	-	-		
56	OHX	DD	101	-	0,6,6	-	-	-		
56	OHX	DA	1747	-	0,6,6	-	-	-		
56	OHX	DB	104	-	0,6,6	-	-	-		
56	OHX	CA	3289	-	0,6,6	-	-	-		
56	OHX	CA	3417	-	0,6,6	-	-	-		
56	OHX	CA	3406	-	0,6,6	-	-	-		
56	OHX	DA	1775	55	0,6,6	-	-	-		
56	OHX	CA	3347	-	0,6,6	-	-	-		
56	OHX	BA	1673	-	0,6,6	-	-	-		
56	OHX	AA	3487	-	0,6,6	-	-	-		
56	OHX	CB	213	-	0,6,6	-	-	-		
56	OHX	CA	3462	-	0,6,6	-	-	-		
56	OHX	CA	3422	-	0,6,6	-	-	-		
56	OHX	AA	3515	-	0,6,6	-	-	-		
56	OHX	DA	1798	-	0,6,6	-	-	-		
56	OHX	AA	3533	-	0,6,6	-	-	-		
56	OHX	DA	1778	-	0,6,6	-	-	-		
56	OHX	CA	3301	-	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	AB	212	OHX	1	0
56	CA	3244	OHX	1	0
56	BA	1775	OHX	2	0
56	DA	1731	OHX	4	0
56	DA	1719	OHX	1	0
56	DA	1768	OHX	1	0
56	AA	3434	OHX	1	0
56	AA	3312	OHX	1	0
56	AF	303	OHX	1	0
56	BA	1688	OHX	1	0
56	AA	3518	OHX	1	0
56	CA	3316	OHX	1	0
56	AA	3560	OHX	2	0
56	CA	3321	OHX	1	0
56	CA	3481	OHX	1	0
56	CA	3418	OHX	1	0
56	CA	3279	OHX	2	0
56	DA	1812	OHX	1	0
56	AA	3424	OHX	2	0
56	AA	3370	OHX	1	0
56	AA	3557	OHX	1	0
56	DA	1795	OHX	1	0
56	CA	3403	OHX	1	0
56	AA	3499	OHX	1	0
56	DA	1759	OHX	1	0
56	CA	3247	OHX	1	0
56	DA	1770	OHX	2	0
56	BA	1755	OHX	1	0
56	BA	1695	OHX	1	0
56	CA	3326	OHX	1	0
56	AA	3473	OHX	2	0
56	BA	1797	OHX	2	0
56	CA	3416	OHX	1	0
56	BA	1768	OHX	1	0
56	AA	3322	OHX	1	0
56	CA	3236	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	BA	1678	OHX	1	0
56	AA	3292	OHX	1	0
56	AA	3426	OHX	2	0
56	DA	1756	OHX	1	0
56	BA	1783	OHX	1	0
56	AA	3419	OHX	1	0
56	AA	3449	OHX	1	0
56	BC	106	OHX	2	0
56	AA	3534	OHX	1	0
56	CA	3240	OHX	1	0
56	DB	103	OHX	1	0
56	AA	3425	OHX	1	0
56	AA	3407	OHX	1	0
56	BA	1756	OHX	1	0
56	BA	1675	OHX	1	0
56	CA	3435	OHX	1	0
56	CA	3354	OHX	1	0
56	AA	3460	OHX	1	0
56	CA	3332	OHX	3	0
56	CA	3362	OHX	1	0
56	CA	3283	OHX	1	0
56	CA	3269	OHX	1	0
56	DC	110	OHX	2	0
56	CA	3300	OHX	2	0
56	CB	212	OHX	1	0
56	CA	3425	OHX	1	0
56	AA	3368	OHX	1	0
56	BA	1798	OHX	1	0
56	AA	3491	OHX	1	0
56	BA	1760	OHX	2	0
56	CA	3293	OHX	1	0
56	DA	1808	OHX	1	0
56	AA	3330	OHX	1	0
56	AA	3531	OHX	2	0
56	BA	1774	OHX	1	0
56	AA	3299	OHX	1	0
56	CA	3310	OHX	1	0
56	CA	3411	OHX	1	0
56	BA	1683	OHX	1	0
56	CA	3274	OHX	1	0
56	AA	3433	OHX	1	0
56	DG	302	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	DA	1718	OHX	1	0
56	BA	1813	OHX	1	0
56	BA	1800	OHX	1	0
56	CA	3484	OHX	1	0
56	DA	1721	OHX	2	0
56	BA	1661	OHX	1	0
56	DA	1751	OHX	1	0
56	AA	3538	OHX	1	0
56	BB	106	OHX	1	0
56	CA	3365	OHX	1	0
56	AA	3562	OHX	1	0
56	DA	1755	OHX	1	0
56	AA	3447	OHX	1	0
56	BA	1778	OHX	1	0
56	AA	3485	OHX	1	0
56	AA	3559	OHX	1	0
56	DA	1779	OHX	1	0
56	DA	1764	OHX	2	0
56	AA	3450	OHX	3	0
56	CA	3333	OHX	1	0
56	AA	3431	OHX	1	0
56	CA	3492	OHX	1	0
56	AA	3300	OHX	1	0
56	AA	3508	OHX	1	0
56	CA	3350	OHX	1	0
56	DA	1724	OHX	1	0
56	CA	3377	OHX	2	0
56	CA	3363	OHX	1	0
56	CA	3415	OHX	1	0
56	CA	3276	OHX	1	0
56	CA	3331	OHX	1	0
56	AA	3438	OHX	2	0
56	AA	3489	OHX	1	0
56	DC	108	OHX	1	0
56	DV	101	OHX	1	0
56	AA	3429	OHX	1	0
56	CA	3304	OHX	1	0
56	DA	1749	OHX	1	0
56	AA	3446	OHX	1	0
56	CA	3375	OHX	1	0
56	DA	1727	OHX	1	0
56	DA	1787	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	CA	3234	OHX	3	0
56	CA	3278	OHX	2	0
56	AA	3313	OHX	1	0
56	BA	1670	OHX	1	0
56	BA	1795	OHX	2	0
56	CA	3486	OHX	2	0
56	AA	3329	OHX	1	0
56	AA	3311	OHX	1	0
56	CA	3272	OHX	1	0
56	AA	3566	OHX	1	0
56	CA	3428	OHX	1	0
56	CA	3490	OHX	1	0
56	BA	1684	OHX	7	0
56	AA	3455	OHX	1	0
56	AA	3333	OHX	1	0
56	DC	107	OHX	6	0
56	CA	3399	OHX	1	0
56	DA	1745	OHX	1	0
56	CA	3384	OHX	1	0
56	DA	1762	OHX	1	0
56	AA	3418	OHX	1	0
56	CA	3327	OHX	1	0
56	AA	3154	OHX	2	0
56	AA	3294	OHX	2	0
56	DA	1767	OHX	4	0
56	AA	3305	OHX	1	0
56	CA	3324	OHX	1	0
56	BG	302	OHX	2	0
56	DA	1734	OHX	3	0
56	DA	1760	OHX	7	0
56	BA	1762	OHX	1	0
56	CA	3432	OHX	1	0
56	AA	3458	OHX	3	0
56	AO	205	OHX	1	0
56	AA	3452	OHX	2	0
56	AA	3526	OHX	1	0
56	AA	3556	OHX	1	0
56	BD	102	OHX	1	0
56	DA	1792	OHX	1	0
56	DA	1737	OHX	1	0
56	AA	3399	OHX	2	0
56	BA	1772	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	AA	3536	OHX	2	0
56	CA	3296	OHX	1	0
56	AA	3478	OHX	1	0
56	AB	219	OHX	1	0
56	CA	3396	OHX	1	0
56	CA	3232	OHX	1	0
56	AA	3475	OHX	1	0
56	BA	1666	OHX	3	0
56	CA	3351	OHX	1	0
56	CB	211	OHX	1	0
56	DK	201	OHX	1	0
56	DA	1733	OHX	1	0
56	AA	3318	OHX	1	0
56	AA	3430	OHX	1	0
56	C6	101	OHX	4	0
56	DA	1783	OHX	2	0
56	DA	1748	OHX	1	0
56	CA	3281	OHX	1	0
56	CB	217	OHX	1	0
56	AA	3362	OHX	1	0
56	AA	3567	OHX	1	0
56	BA	1671	OHX	1	0
56	CA	3233	OHX	1	0
56	CA	3487	OHX	1	0
56	AA	3568	OHX	5	0
56	AA	3402	OHX	1	0
56	BA	1804	OHX	2	0
56	A6	101	OHX	3	0
56	CA	3320	OHX	1	0
56	AA	3291	OHX	2	0
56	AA	3480	OHX	1	0
56	AA	3320	OHX	1	0
56	AA	3461	OHX	1	0
56	BA	1672	OHX	1	0
56	AA	3513	OHX	1	0
56	CA	3383	OHX	1	0
56	DA	1800	OHX	1	0
56	AA	3456	OHX	1	0
56	BA	1693	OHX	1	0
56	DA	1730	OHX	1	0
56	DA	1742	OHX	1	0
56	AA	3421	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	DA	1752	OHX	1	0
56	DA	1740	OHX	1	0
56	BA	1805	OHX	1	0
56	BA	1812	OHX	2	0
56	AA	3514	OHX	1	0
56	CA	3468	OHX	1	0
56	CA	3275	OHX	1	0
56	AB	217	OHX	2	0
56	AA	3510	OHX	1	0
56	AA	3373	OHX	1	0
56	DA	1754	OHX	1	0
56	C5	102	OHX	1	0
56	AA	3325	OHX	1	0
56	CA	3376	OHX	1	0
56	AA	3512	OHX	1	0
56	BA	1782	OHX	1	0
56	CA	3305	OHX	1	0
56	CB	209	OHX	1	0
56	AA	3338	OHX	1	0
56	BA	1786	OHX	1	0
56	AA	3420	OHX	1	0
56	CA	3270	OHX	2	0
56	DC	109	OHX	1	0
56	DD	101	OHX	1	0
56	DA	1775	OHX	1	0
56	BA	1673	OHX	5	0
56	AA	3487	OHX	1	0
56	CA	3462	OHX	1	0
56	AA	3533	OHX	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	2912/2912 (100%)	-0.73	7 (0%) 91 86	45, 76, 209, 243	0
1	CA	2907/2912 (99%)	-0.49	10 (0%) 90 82	58, 92, 230, 245	0
2	AB	122/122 (100%)	-0.68	0 100 100	73, 95, 116, 177	0
2	CB	122/122 (100%)	-0.42	1 (0%) 82 68	92, 126, 146, 198	0
3	AD	272/276 (98%)	0.10	7 (2%) 57 38	39, 66, 84, 105	0
3	CD	272/276 (98%)	0.39	15 (5%) 30 21	55, 78, 96, 128	0
4	AE	205/206 (99%)	0.40	17 (8%) 17 13	51, 86, 130, 142	0
4	CE	205/206 (99%)	0.30	9 (4%) 39 25	64, 100, 148, 165	0
5	AF	202/210 (96%)	-0.22	3 (1%) 72 53	47, 81, 118, 130	0
5	CF	208/210 (99%)	0.26	6 (2%) 53 35	62, 106, 160, 184	0
6	AG	181/182 (99%)	0.15	6 (3%) 49 33	84, 107, 138, 149	0
6	CG	181/182 (99%)	0.70	14 (7%) 19 14	120, 141, 164, 171	0
7	AH	170/180 (94%)	0.43	10 (5%) 28 19	86, 112, 130, 157	0
7	CH	170/180 (94%)	0.76	20 (11%) 9 8	155, 198, 220, 229	0
8	AK	146/148 (98%)	0.30	10 (6%) 23 16	79, 131, 147, 150	0
8	CK	146/148 (98%)	0.25	2 (1%) 73 55	84, 130, 152, 158	0
9	AM	138/140 (98%)	0.40	8 (5%) 29 19	66, 87, 124, 136	0
9	CM	138/140 (98%)	0.53	4 (2%) 53 35	83, 114, 140, 156	0
10	AN	122/122 (100%)	0.06	1 (0%) 82 68	57, 78, 93, 101	0
10	CN	122/122 (100%)	0.31	1 (0%) 82 68	75, 95, 111, 124	0
11	AO	150/150 (100%)	-0.07	1 (0%) 84 70	48, 88, 117, 160	0
11	CO	150/150 (100%)	0.36	9 (6%) 27 19	45, 108, 146, 178	0
12	AP	141/141 (100%)	0.88	20 (14%) 6 5	58, 83, 105, 127	0
12	CP	141/141 (100%)	1.21	29 (20%) 2 2	58, 109, 140, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	A0	118/118 (100%)	-0.22	0 100 100	61, 81, 103, 113	0
13	C0	117/118 (99%)	-0.32	0 100 100	69, 87, 106, 121	0
14	AQ	111/112 (99%)	-0.06	2 (1%) 67 49	70, 92, 117, 131	0
14	CQ	111/112 (99%)	0.13	5 (4%) 38 25	86, 123, 147, 162	0
15	AR	137/146 (93%)	0.10	4 (2%) 53 35	73, 93, 143, 170	0
15	CR	137/146 (93%)	0.12	6 (4%) 39 25	84, 104, 163, 183	0
16	A1	117/118 (99%)	-0.07	0 100 100	52, 75, 108, 139	0
16	C1	117/118 (99%)	0.22	1 (0%) 81 65	67, 106, 143, 162	0
17	A2	101/101 (100%)	0.51	7 (6%) 23 16	53, 98, 122, 141	0
17	C2	101/101 (100%)	0.97	9 (8%) 15 12	67, 129, 142, 151	0
18	AS	113/113 (100%)	-0.08	1 (0%) 81 65	54, 73, 104, 156	0
18	CS	113/113 (100%)	0.03	1 (0%) 81 65	64, 80, 114, 158	0
19	AT	92/96 (95%)	-0.02	2 (2%) 62 43	57, 71, 95, 107	0
19	CT	92/96 (95%)	0.46	6 (6%) 25 17	74, 88, 113, 127	0
20	AU	102/110 (92%)	0.38	6 (5%) 28 19	74, 101, 152, 162	0
20	CU	102/110 (92%)	0.85	15 (14%) 6 5	95, 118, 166, 181	0
21	AV	175/206 (84%)	0.75	15 (8%) 16 12	87, 126, 188, 191	0
21	CV	179/206 (86%)	0.73	9 (5%) 34 23	122, 160, 208, 216	0
22	A3	76/85 (89%)	-0.16	1 (1%) 75 56	59, 77, 91, 132	0
22	C3	77/85 (90%)	0.12	3 (3%) 43 29	83, 95, 117, 147	0
23	AZ	97/98 (98%)	0.01	5 (5%) 33 22	58, 78, 126, 156	0
23	CZ	97/98 (98%)	0.51	5 (5%) 33 22	68, 86, 132, 155	0
24	AW	66/72 (91%)	0.05	2 (3%) 52 35	63, 84, 98, 125	0
24	CW	66/72 (91%)	0.28	3 (4%) 38 25	84, 107, 130, 139	0
25	AX	59/60 (98%)	-0.02	1 (1%) 69 50	63, 83, 112, 130	0
25	CX	59/60 (98%)	0.34	2 (3%) 48 32	80, 110, 141, 162	0
26	A4	66/71 (92%)	0.48	2 (3%) 52 35	120, 156, 173, 179	0
26	C4	63/71 (88%)	1.11	9 (14%) 6 5	146, 185, 194, 199	0
27	A5	59/60 (98%)	0.67	9 (15%) 5 5	49, 88, 168, 171	0
27	C5	59/60 (98%)	0.33	2 (3%) 48 32	65, 92, 173, 187	0
28	A6	45/54 (83%)	1.00	8 (17%) 4 3	124, 151, 168, 177	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	C6	45/54 (83%)	1.36	11 (24%) 2 1	141, 169, 183, 186	0
29	A7	45/49 (91%)	-0.22	3 (6%) 24 16	47, 55, 69, 78	0
29	C7	45/49 (91%)	0.02	1 (2%) 62 43	56, 66, 77, 100	0
30	A8	60/65 (92%)	-0.04	0 100 100	55, 73, 90, 114	0
30	C8	60/65 (92%)	0.61	8 (13%) 7 6	78, 90, 112, 137	0
31	BA	1502/1506 (99%)	-0.57	10 (0%) 84 70	58, 107, 187, 244	0
31	DA	1502/1506 (99%)	-0.65	2 (0%) 92 90	71, 119, 189, 244	0
32	BE	237/256 (92%)	0.46	8 (3%) 48 32	111, 144, 182, 193	0
32	DE	237/256 (92%)	0.20	1 (0%) 88 79	126, 161, 196, 211	0
33	BF	205/239 (85%)	0.36	5 (2%) 59 40	96, 119, 152, 160	0
33	DF	206/239 (86%)	0.29	5 (2%) 59 40	127, 147, 175, 180	0
34	BG	208/208 (100%)	0.55	10 (4%) 35 24	92, 116, 136, 147	0
34	DG	208/208 (100%)	0.25	5 (2%) 59 40	93, 111, 132, 145	0
35	BH	151/162 (93%)	0.31	2 (1%) 75 56	81, 105, 127, 161	0
35	DH	151/162 (93%)	0.18	3 (1%) 65 46	104, 121, 142, 165	0
36	BI	101/101 (100%)	0.12	0 100 100	81, 108, 122, 145	0
36	DI	101/101 (100%)	0.39	0 100 100	81, 106, 124, 149	0
37	BJ	155/156 (99%)	0.20	5 (3%) 50 34	106, 121, 149, 158	0
37	DJ	155/156 (99%)	0.10	2 (1%) 75 56	113, 131, 153, 164	0
38	BK	138/138 (100%)	-0.05	1 (0%) 84 70	89, 110, 123, 129	0
38	DK	138/138 (100%)	-0.24	0 100 100	104, 125, 136, 146	0
39	BL	127/128 (99%)	-0.12	0 100 100	87, 142, 160, 169	0
39	DL	127/128 (99%)	-0.16	1 (0%) 82 68	117, 155, 168, 174	0
40	BM	99/105 (94%)	0.10	2 (2%) 65 46	91, 142, 170, 174	0
40	DM	99/105 (94%)	0.17	1 (1%) 79 63	124, 159, 175, 179	0
41	BN	119/129 (92%)	0.27	5 (4%) 40 26	72, 104, 133, 161	0
41	DN	119/129 (92%)	0.46	6 (5%) 34 23	91, 112, 139, 167	0
42	BO	125/132 (94%)	0.45	7 (5%) 30 20	69, 83, 112, 158	0
42	DO	125/132 (94%)	0.57	9 (7%) 21 15	93, 110, 134, 166	0
43	BP	116/126 (92%)	0.13	3 (2%) 57 38	92, 128, 145, 153	0
43	DP	117/126 (92%)	0.38	7 (5%) 27 19	106, 156, 169, 171	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	58/61 (95%)	0.06	1 (1%) 69 50	91, 108, 122, 129	0
44	DQ	58/61 (95%)	-0.14	0 100 100	126, 140, 157, 160	0
45	BR	88/89 (98%)	-0.18	0 100 100	80, 100, 121, 125	0
45	DR	88/89 (98%)	0.01	0 100 100	85, 112, 133, 140	0
46	BS	84/88 (95%)	0.09	0 100 100	100, 118, 139, 175	0
46	DS	84/88 (95%)	-0.04	0 100 100	96, 107, 127, 158	0
47	BT	100/105 (95%)	0.01	4 (4%) 42 28	93, 112, 125, 133	0
47	DT	100/105 (95%)	0.05	3 (3%) 52 35	94, 114, 135, 143	0
48	BU	72/88 (81%)	0.29	1 (1%) 73 55	88, 106, 139, 164	0
48	DU	72/88 (81%)	0.43	4 (5%) 30 20	97, 114, 155, 169	0
49	BV	78/93 (83%)	0.38	4 (5%) 33 22	109, 130, 147, 152	0
49	DV	78/93 (83%)	0.36	2 (2%) 57 38	145, 163, 182, 185	0
50	BW	99/106 (93%)	-0.07	0 100 100	105, 124, 155, 160	0
50	DW	99/106 (93%)	-0.25	0 100 100	95, 117, 153, 163	0
51	BX	25/27 (92%)	-0.34	0 100 100	102, 117, 137, 154	0
51	DX	25/27 (92%)	-0.05	1 (4%) 42 28	122, 143, 158, 168	0
52	BB	84/85 (98%)	1.23	25 (29%) 1 1	82, 123, 154, 169	0
52	BD	84/85 (98%)	0.20	7 (8%) 17 13	75, 137, 217, 227	0
52	DB	84/85 (98%)	1.23	17 (20%) 3 2	93, 128, 156, 171	0
52	DD	84/85 (98%)	0.53	9 (10%) 11 9	84, 137, 217, 225	0
53	BC	77/77 (100%)	0.23	5 (6%) 25 17	77, 114, 139, 153	0
53	DC	77/77 (100%)	0.17	2 (2%) 57 38	88, 122, 150, 157	0
54	B1	16/16 (100%)	0.82	3 (18%) 3 3	76, 104, 156, 163	0
54	D1	16/16 (100%)	0.36	2 (12%) 8 6	85, 109, 157, 165	0
All	All	21100/21658 (97%)	-0.10	564 (2%) 56 37	39, 105, 182, 245	0

The worst 5 of 564 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	CW	41	ILE	7.6
27	A5	2	ALA	7.3
11	CO	61	ARG	7.2
12	AP	86	GLY	7.1
27	C5	2	ALA	6.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	CA	3213	1/1	0.26	0.15	121,121,121,121	0
55	MG	AA	3095	1/1	0.40	0.24	89,89,89,89	0
55	MG	AA	3086	1/1	0.43	0.31	95,95,95,95	0
55	MG	DA	1631	1/1	0.43	0.28	111,111,111,111	0
55	MG	DA	1619	1/1	0.48	0.31	98,98,98,98	0
55	MG	CA	3455	1/1	0.52	0.61	97,97,97,97	0
55	MG	BA	1699	1/1	0.54	0.37	79,79,79,79	0
55	MG	DA	1681	1/1	0.54	0.18	100,100,100,100	0
55	MG	DA	1622	1/1	0.57	0.21	122,122,122,122	0
55	MG	BA	1648	1/1	0.58	0.25	99,99,99,99	0
55	MG	AA	3100	1/1	0.58	0.23	108,108,108,108	0
55	MG	BB	104	1/1	0.58	0.44	87,87,87,87	0
55	MG	BA	1632	1/1	0.59	0.21	108,108,108,108	0
55	MG	AA	3247	1/1	0.60	0.26	81,81,81,81	0
55	MG	DA	1714	1/1	0.60	0.20	97,97,97,97	0
55	MG	DA	1618	1/1	0.61	0.25	105,105,105,105	0
55	MG	AA	3137	1/1	0.62	0.38	51,51,51,51	0
55	MG	AA	3067	1/1	0.62	0.19	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	DA	1673	1/1	0.62	0.20	80,80,80,80	0
55	MG	CA	3034	1/1	0.62	0.25	91,91,91,91	0
55	MG	CA	3209	1/1	0.62	0.33	85,85,85,85	0
56	OHX	AA	3526	7/7	0.62	0.12	120,129,136,176	1
55	MG	BA	1629	1/1	0.63	0.18	112,112,112,112	0
55	MG	BC	102	1/1	0.63	0.18	68,68,68,68	0
55	MG	CA	3220	1/1	0.63	0.35	85,85,85,85	0
55	MG	AA	3245	1/1	0.63	0.26	68,68,68,68	0
56	OHX	DB	104	7/7	0.63	0.09	129,133,143,205	2
55	MG	BA	1634	1/1	0.64	0.34	74,74,74,74	0
55	MG	AA	3087	1/1	0.64	0.29	83,83,83,83	0
55	MG	DA	1642	1/1	0.64	0.21	112,112,112,112	0
56	OHX	DA	1794	7/7	0.64	0.09	124,130,139,205	1
55	MG	CA	3198	1/1	0.64	0.23	118,118,118,118	0
55	MG	DA	1659	1/1	0.65	0.22	89,89,89,89	0
55	MG	DA	1641	1/1	0.65	0.27	130,130,130,130	0
55	MG	DA	1643	1/1	0.65	0.24	136,136,136,136	0
55	MG	DA	1682	1/1	0.65	0.35	87,87,87,87	0
55	MG	AA	3248	1/1	0.66	0.25	86,86,86,86	0
55	MG	CA	3085	1/1	0.66	0.28	102,102,102,102	0
55	MG	CA	3107	1/1	0.66	0.25	82,82,82,82	0
55	MG	DB	102	1/1	0.66	0.21	102,102,102,102	0
55	MG	CA	3197	1/1	0.66	0.32	79,79,79,79	0
55	MG	BA	1749	1/1	0.66	0.27	88,88,88,88	0
55	MG	BC	105	1/1	0.66	0.40	87,87,87,87	0
55	MG	CA	3264	1/1	0.67	0.40	49,49,49,49	0
56	OHX	CB	218	7/7	0.67	0.10	141,159,166,235	1
55	MG	DA	1720	1/1	0.67	0.25	105,105,105,105	0
55	MG	DA	1688	1/1	0.67	0.30	101,101,101,101	0
55	MG	AA	3009	1/1	0.68	0.16	89,89,89,89	0
55	MG	DA	1717	1/1	0.68	0.20	100,100,100,100	0
55	MG	BA	1746	1/1	0.68	0.28	82,82,82,82	0
55	MG	AA	3108	1/1	0.68	0.19	82,82,82,82	0
55	MG	AA	3347	1/1	0.68	0.32	70,70,70,70	0
55	MG	CA	3141	1/1	0.68	0.32	77,77,77,77	0
55	MG	BA	1622	1/1	0.68	0.16	123,123,123,123	0
55	MG	DA	1705	1/1	0.68	0.24	108,108,108,108	0
55	MG	DA	1649	1/1	0.69	0.27	87,87,87,87	0
55	MG	CA	3458	1/1	0.69	0.20	82,82,82,82	0
55	MG	DA	1668	1/1	0.69	0.22	86,86,86,86	0
55	MG	BA	1607	1/1	0.69	0.24	93,93,93,93	0
55	MG	DA	1623	1/1	0.70	0.24	124,124,124,124	0

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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	CE	301	1/1	0.70	0.39	56,56,56,56	0
55	MG	DA	1617	1/1	0.70	0.20	115,115,115,115	0
56	OHX	BD	104	7/7	0.70	0.12	82,85,90,147	2
55	MG	CA	3146	1/1	0.70	0.29	77,77,77,77	0
55	MG	CA	3062	1/1	0.70	0.14	78,78,78,78	0
55	MG	CA	3457	1/1	0.70	0.20	66,66,66,66	0
56	OHX	DB	105	7/7	0.70	0.14	88,91,103,175	5
55	MG	BA	1611	1/1	0.71	0.34	84,84,84,84	0
55	MG	DC	103	1/1	0.71	0.34	96,96,96,96	0
55	MG	AA	3131	1/1	0.71	0.20	94,94,94,94	0
55	MG	CA	3448	1/1	0.71	0.25	63,63,63,63	0
55	MG	AA	3144	1/1	0.72	0.45	71,71,71,71	0
55	MG	CA	3079	1/1	0.72	0.28	73,73,73,73	0
55	MG	BA	1602	1/1	0.72	0.29	75,75,75,75	0
55	MG	AA	3232	1/1	0.72	0.23	75,75,75,75	0
55	MG	CA	3215	1/1	0.72	0.15	137,137,137,137	0
55	MG	CA	3023	1/1	0.72	0.30	85,85,85,85	0
55	MG	AA	3065	1/1	0.72	0.40	49,49,49,49	0
55	MG	CA	3172	1/1	0.72	0.22	86,86,86,86	0
55	MG	BA	1615	1/1	0.73	0.21	113,113,113,113	0
56	OHX	AA	3536	7/7	0.73	0.10	116,124,157,192	1
55	MG	CA	3196	1/1	0.73	0.36	92,92,92,92	0
56	OHX	CA	3429	7/7	0.73	0.10	127,129,142,209	1
55	MG	DA	1678	1/1	0.73	0.13	118,118,118,118	0
55	MG	AA	3141	1/1	0.73	0.32	44,44,44,44	0
55	MG	AA	3098	1/1	0.73	0.23	77,77,77,77	0
55	MG	AA	3218	1/1	0.73	0.27	82,82,82,82	0
55	MG	BA	1712	1/1	0.74	0.29	95,95,95,95	0
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	1745	1/1	0.74	0.44	83,83,83,83	0
55	MG	AA	3282	1/1	0.74	0.18	69,69,69,69	0
55	MG	AA	3037	1/1	0.74	0.30	63,63,63,63	0
55	MG	DA	1630	1/1	0.74	0.20	95,95,95,95	0
55	MG	AA	3045	1/1	0.74	0.28	65,65,65,65	0
56	OHX	AA	3534	7/7	0.74	0.10	136,141,145,222	1
55	MG	CA	3086	1/1	0.75	0.29	68,68,68,68	0
55	MG	BA	1722	1/1	0.75	0.34	91,91,91,91	0
55	MG	CA	3136	1/1	0.75	0.19	91,91,91,91	0
55	MG	BA	1704	1/1	0.75	0.13	88,88,88,88	0
55	MG	AA	3268	1/1	0.75	0.30	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	BA	1720	1/1	0.75	0.30	58,58,58,58	0
55	MG	DA	1634	1/1	0.75	0.09	118,118,118,118	0
55	MG	DA	1637	1/1	0.75	0.23	106,106,106,106	0
55	MG	CA	3193	1/1	0.75	0.25	80,80,80,80	0
55	MG	AA	3273	1/1	0.76	0.31	66,66,66,66	0
55	MG	BA	1601	1/1	0.76	0.11	81,81,81,81	0
55	MG	CA	3183	1/1	0.76	0.29	93,93,93,93	0
55	MG	CA	3187	1/1	0.76	0.36	86,86,86,86	0
56	OHX	AA	3562	7/7	0.76	0.10	98,105,127,189	1
55	MG	BA	1747	1/1	0.76	0.28	74,74,74,74	0
55	MG	AA	3125	1/1	0.76	0.20	92,92,92,92	0
56	OHX	CA	3421	7/7	0.76	0.10	113,126,135,198	1
55	MG	BA	1605	1/1	0.76	0.16	104,104,104,104	0
55	MG	AA	3209	1/1	0.76	0.26	57,57,57,57	0
55	MG	CA	3117	1/1	0.76	0.17	69,69,69,69	0
55	MG	BA	1609	1/1	0.76	0.22	73,73,73,73	0
55	MG	BA	1744	1/1	0.76	0.16	90,90,90,90	0
55	MG	AA	3058	1/1	0.77	0.20	73,73,73,73	0
55	MG	AA	3150	1/1	0.77	0.27	68,68,68,68	0
55	MG	AA	3397	1/1	0.77	0.14	80,80,80,80	0
55	MG	DC	104	1/1	0.77	0.28	77,77,77,77	0
56	OHX	AA	3523	7/7	0.77	0.12	109,114,123,180	1
55	MG	CA	3460	1/1	0.77	0.36	72,72,72,72	0
55	MG	BA	1718	1/1	0.77	0.20	78,78,78,78	0
55	MG	BA	1633	1/1	0.77	0.18	59,59,59,59	0
55	MG	CA	3201	1/1	0.77	0.29	79,79,79,79	0
55	MG	CA	3129	1/1	0.77	0.39	81,81,81,81	0
55	MG	AA	3190	1/1	0.77	0.32	69,69,69,69	0
55	MG	BA	1729	1/1	0.77	0.33	73,73,73,73	0
55	MG	BA	1640	1/1	0.77	0.26	73,73,73,73	0
55	MG	DA	1694	1/1	0.77	0.20	104,104,104,104	0
55	MG	CA	3045	1/1	0.77	0.41	91,91,91,91	0
55	MG	CA	3266	1/1	0.77	0.30	64,64,64,64	0
55	MG	DA	1715	1/1	0.77	0.22	89,89,89,89	0
55	MG	AA	3076	1/1	0.77	0.37	72,72,72,72	0
55	MG	CA	3046	1/1	0.78	0.18	76,76,76,76	0
55	MG	DA	1675	1/1	0.78	0.19	92,92,92,92	0
55	MG	DA	1676	1/1	0.78	0.29	83,83,83,83	0
55	MG	BA	1706	1/1	0.78	0.32	79,79,79,79	0
56	OHX	AA	3535	7/7	0.78	0.10	104,112,123,191	1
55	MG	DA	1627	1/1	0.78	0.32	77,77,77,77	0
56	OHX	AA	3545	7/7	0.78	0.14	90,96,105,167	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	1631	1/1	0.78	0.15	78,78,78,78	0
55	MG	CA	3200	1/1	0.78	0.24	56,56,56,56	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	3159	1/1	0.78	0.19	65,65,65,65	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	CA	3202	1/1	0.78	0.33	79,79,79,79	0
56	OHX	CA	3396	7/7	0.78	0.08	135,136,150,198	1
55	MG	AA	3164	1/1	0.78	0.17	70,70,70,70	0
55	MG	CA	3095	1/1	0.78	0.16	54,54,54,54	0
55	MG	DA	1609	1/1	0.78	0.25	91,91,91,91	0
55	MG	AA	3074	1/1	0.78	0.24	73,73,73,73	0
55	MG	CA	3216	1/1	0.78	0.28	91,91,91,91	0
55	MG	BA	1728	1/1	0.78	0.28	90,90,90,90	0
55	MG	AA	3391	1/1	0.79	0.27	59,59,59,59	0
55	MG	CA	3170	1/1	0.79	0.12	65,65,65,65	0
55	MG	CA	3217	1/1	0.79	0.28	58,58,58,58	0
55	MG	BA	1612	1/1	0.79	0.28	81,81,81,81	0
55	MG	CA	3053	1/1	0.79	0.12	99,99,99,99	0
55	MG	AA	3187	1/1	0.79	0.32	86,86,86,86	0
55	MG	AO	201	1/1	0.79	0.23	80,80,80,80	0
55	MG	DA	1635	1/1	0.79	0.36	96,96,96,96	0
56	OHX	BA	1677	7/7	0.79	0.10	141,145,154,220	1
55	MG	AA	3035	1/1	0.79	0.31	64,64,64,64	0
55	MG	BA	1751	1/1	0.79	0.35	95,95,95,95	0
55	MG	AA	3258	1/1	0.79	0.25	65,65,65,65	0
55	MG	AA	3176	1/1	0.79	0.17	60,60,60,60	0
56	OHX	CA	3420	7/7	0.79	0.09	131,141,152,216	1
55	MG	DA	1647	1/1	0.79	0.30	90,90,90,90	0
55	MG	BA	1606	1/1	0.79	0.24	92,92,92,92	0
56	OHX	CA	3470	7/7	0.79	0.10	113,126,137,181	1
55	MG	AA	3350	1/1	0.79	0.32	80,80,80,80	0
55	MG	DA	1660	1/1	0.79	0.33	88,88,88,88	0
55	MG	AA	3378	1/1	0.79	0.25	47,47,47,47	0
55	MG	CA	3035	1/1	0.79	0.18	92,92,92,92	0
55	MG	DA	1662	1/1	0.80	0.29	73,73,73,73	0
55	MG	BA	1610	1/1	0.80	0.19	92,92,92,92	0
55	MG	CA	3207	1/1	0.80	0.23	68,68,68,68	0
55	MG	CA	3042	1/1	0.80	0.24	67,67,67,67	0
56	OHX	AA	3552	7/7	0.80	0.13	105,122,135,199	1
55	MG	CA	3044	1/1	0.80	0.20	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3231	1/1	0.80	0.30	66,66,66,66	0
55	MG	AA	3169	1/1	0.80	0.30	76,76,76,76	0
55	MG	DA	1629	1/1	0.80	0.15	93,93,93,93	0
55	MG	CA	3164	1/1	0.80	0.26	97,97,97,97	0
55	MG	AA	3062	1/1	0.80	0.34	73,73,73,73	0
55	MG	DA	1696	1/1	0.80	0.16	112,112,112,112	0
55	MG	CA	3223	1/1	0.80	0.29	88,88,88,88	0
55	MG	DA	1708	1/1	0.80	0.27	87,87,87,87	0
55	MG	BA	1724	1/1	0.80	0.24	59,59,59,59	0
55	MG	CA	3072	1/1	0.80	0.36	43,43,43,43	0
55	MG	CA	3076	1/1	0.80	0.37	64,64,64,64	0
55	MG	AA	3217	1/1	0.80	0.23	60,60,60,60	0
55	MG	BA	1625	1/1	0.80	0.32	65,65,65,65	0
55	MG	AA	3132	1/1	0.80	0.34	81,81,81,81	0
56	OHX	DA	1753	7/7	0.80	0.13	120,124,134,196	1
55	MG	CA	3088	1/1	0.80	0.30	86,86,86,86	0
55	MG	CA	3028	1/1	0.80	0.19	73,73,73,73	0
55	MG	AA	3285	1/1	0.80	0.32	80,80,80,80	0
55	MG	DA	1657	1/1	0.81	0.33	70,70,70,70	0
55	MG	AA	3235	1/1	0.81	0.21	50,50,50,50	0
55	MG	CA	3225	1/1	0.81	0.18	48,48,48,48	0
55	MG	BA	1725	1/1	0.81	0.35	69,69,69,69	0
55	MG	AB	201	1/1	0.81	0.27	73,73,73,73	0
55	MG	CA	3267	1/1	0.81	0.22	65,65,65,65	0
55	MG	CA	3440	1/1	0.81	0.31	54,54,54,54	0
55	MG	CA	3060	1/1	0.81	0.16	75,75,75,75	0
55	MG	CA	3206	1/1	0.81	0.30	90,90,90,90	0
55	MG	AB	206	1/1	0.81	0.37	83,83,83,83	0
55	MG	BQ	101	1/1	0.81	0.41	96,96,96,96	0
55	MG	CA	3191	1/1	0.81	0.28	72,72,72,72	0
55	MG	CA	3192	1/1	0.81	0.23	87,87,87,87	0
55	MG	BA	1703	1/1	0.81	0.27	108,108,108,108	0
55	MG	BA	1635	1/1	0.81	0.23	96,96,96,96	0
55	MG	CA	3081	1/1	0.81	0.34	63,63,63,63	0
56	OHX	AA	3565	7/7	0.81	0.09	117,122,134,195	1
56	OHX	DC	108	7/7	0.81	0.10	120,132,142,180	1
55	MG	CA	3221	1/1	0.82	0.29	69,69,69,69	0
55	MG	CA	3171	1/1	0.82	0.20	82,82,82,82	0
55	MG	AA	3019	1/1	0.82	0.31	72,72,72,72	0
56	OHX	AA	3522	7/7	0.82	0.10	118,131,145,201	1
55	MG	CA	3262	1/1	0.82	0.41	74,74,74,74	0
55	MG	CA	3178	1/1	0.82	0.19	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	3064	1/1	0.82	0.12	89,89,89,89	0
55	MG	AA	3130	1/1	0.82	0.17	75,75,75,75	0
55	MG	AA	3354	1/1	0.82	0.33	57,57,57,57	0
55	MG	CA	3441	1/1	0.82	0.33	99,99,99,99	0
55	MG	AA	3165	1/1	0.82	0.24	84,84,84,84	0
55	MG	CA	3449	1/1	0.82	0.32	54,54,54,54	0
55	MG	AA	3066	1/1	0.82	0.26	83,83,83,83	0
55	MG	BA	1709	1/1	0.82	0.24	100,100,100,100	0
55	MG	DA	1672	1/1	0.82	0.26	83,83,83,83	0
55	MG	AA	3096	1/1	0.82	0.27	71,71,71,71	0
55	MG	DA	1674	1/1	0.82	0.22	99,99,99,99	0
55	MG	AA	3080	1/1	0.82	0.31	55,55,55,55	0
55	MG	AB	203	1/1	0.82	0.29	71,71,71,71	0
55	MG	AA	3083	1/1	0.82	0.15	88,88,88,88	0
55	MG	AA	3014	1/1	0.82	0.34	44,44,44,44	0
55	MG	AA	3276	1/1	0.82	0.21	69,69,69,69	0
56	OHX	CA	3419	7/7	0.82	0.08	153,156,164,238	1
55	MG	AA	3145	1/1	0.82	0.32	56,56,56,56	0
55	MG	BA	1604	1/1	0.82	0.22	72,72,72,72	0
56	OHX	CA	3427	7/7	0.82	0.08	114,126,136,203	1
55	MG	CA	3144	1/1	0.82	0.30	54,54,54,54	0
55	MG	DA	1626	1/1	0.82	0.33	84,84,84,84	0
55	MG	CA	3145	1/1	0.82	0.42	74,74,74,74	0
55	MG	DA	1710	1/1	0.82	0.15	103,103,103,103	0
56	OHX	DA	1765	7/7	0.82	0.15	117,133,141,227	1
55	MG	AA	3119	1/1	0.82	0.28	64,64,64,64	0
55	MG	AA	3156	1/1	0.82	0.27	45,45,45,45	0
55	MG	BA	1646	1/1	0.82	0.24	95,95,95,95	0
55	MG	DA	1633	1/1	0.82	0.32	74,74,74,74	0
55	MG	CA	3477	1/1	0.83	0.27	60,60,60,60	0
55	MG	CB	206	1/1	0.83	0.23	83,83,83,83	0
55	MG	AA	3021	1/1	0.83	0.30	80,80,80,80	0
55	MG	AA	3129	1/1	0.83	0.20	83,83,83,83	0
55	MG	CA	3163	1/1	0.83	0.28	80,80,80,80	0
55	MG	BA	1710	1/1	0.83	0.25	97,97,97,97	0
55	MG	CA	3065	1/1	0.83	0.29	55,55,55,55	0
55	MG	AA	3091	1/1	0.83	0.20	77,77,77,77	0
55	MG	AA	3072	1/1	0.83	0.22	65,65,65,65	0
55	MG	AA	3166	1/1	0.83	0.25	66,66,66,66	0
55	MG	AA	3351	1/1	0.83	0.30	53,53,53,53	0
55	MG	CA	3227	1/1	0.83	0.32	79,79,79,79	0
55	MG	CA	3230	1/1	0.83	0.27	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	BB	107	7/7	0.83	0.12	71,92,103,147	3
55	MG	DA	1703	1/1	0.83	0.30	73,73,73,73	0
55	MG	AA	3052	1/1	0.83	0.24	85,85,85,85	0
55	MG	AA	3024	1/1	0.83	0.27	63,63,63,63	0
55	MG	BA	1644	1/1	0.83	0.49	94,94,94,94	0
55	MG	CA	3091	1/1	0.83	0.29	74,74,74,74	0
55	MG	CA	3268	1/1	0.83	0.16	52,52,52,52	0
55	MG	CA	3040	1/1	0.83	0.31	70,70,70,70	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	3252	1/1	0.83	0.32	47,47,47,47	0
55	MG	AA	3034	1/1	0.83	0.27	56,56,56,56	0
56	OHX	C3	101	7/7	0.83	0.10	119,129,151,179	2
55	MG	DA	1644	1/1	0.83	0.10	149,149,149,149	0
55	MG	AA	3017	1/1	0.83	0.23	100,100,100,100	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	AA	3110	1/1	0.83	0.38	48,48,48,48	0
55	MG	AA	3005	1/1	0.83	0.29	43,43,43,43	0
55	MG	CA	3142	1/1	0.83	0.27	71,71,71,71	0
55	MG	CA	3054	1/1	0.83	0.19	54,54,54,54	0
55	MG	BA	1723	1/1	0.84	0.20	82,82,82,82	0
55	MG	DA	1624	1/1	0.84	0.07	73,73,73,73	0
56	OHX	AA	3564	7/7	0.84	0.07	102,105,128,167	1
55	MG	AB	205	1/1	0.84	0.17	50,50,50,50	0
55	MG	AA	3026	1/1	0.84	0.26	92,92,92,92	0
55	MG	CA	3039	1/1	0.84	0.28	65,65,65,65	0
55	MG	BA	1647	1/1	0.84	0.18	112,112,112,112	0
55	MG	AE	301	1/1	0.84	0.32	52,52,52,52	0
55	MG	DA	1698	1/1	0.84	0.31	95,95,95,95	0
55	MG	DA	1701	1/1	0.84	0.36	90,90,90,90	0
55	MG	AA	3220	1/1	0.84	0.26	64,64,64,64	0
55	MG	AA	3139	1/1	0.84	0.30	48,48,48,48	0
56	OHX	CA	3250	7/7	0.84	0.13	106,109,126,164	1
55	MG	DA	1706	1/1	0.84	0.09	100,100,100,100	0
56	OHX	CA	3399	7/7	0.84	0.13	97,104,115,165	2
55	MG	CA	3134	1/1	0.84	0.25	65,65,65,65	0
55	MG	AA	3015	1/1	0.84	0.26	76,76,76,76	0
55	MG	AA	3038	1/1	0.84	0.15	46,46,46,46	0
55	MG	AA	3208	1/1	0.84	0.23	65,65,65,65	0
55	MG	AA	3281	1/1	0.84	0.38	70,70,70,70	0
55	MG	BA	1753	1/1	0.84	0.24	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3059	1/1	0.84	0.26	85,85,85,85	0
55	MG	DC	101	1/1	0.84	0.34	85,85,85,85	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	CA	3214	1/1	0.84	0.22	65,65,65,65	0
55	MG	CB	204	1/1	0.84	0.24	73,73,73,73	0
55	MG	BA	1715	1/1	0.84	0.26	74,74,74,74	0
55	MG	AB	202	1/1	0.84	0.13	72,72,72,72	0
55	MG	BA	1639	1/1	0.84	0.10	102,102,102,102	0
55	MG	DA	1613	1/1	0.84	0.20	87,87,87,87	0
55	MG	CA	3078	1/1	0.84	0.37	76,76,76,76	0
55	MG	AA	3148	1/1	0.84	0.23	65,65,65,65	0
55	MG	CA	3175	1/1	0.84	0.43	64,64,64,64	0
55	MG	CA	3027	1/1	0.84	0.26	81,81,81,81	0
55	MG	DA	1712	1/1	0.85	0.33	98,98,98,98	0
55	MG	DA	1670	1/1	0.85	0.24	64,64,64,64	0
55	MG	CA	3037	1/1	0.85	0.23	89,89,89,89	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	DA	1632	1/1	0.85	0.20	83,83,83,83	0
55	MG	CA	3057	1/1	0.85	0.26	95,95,95,95	0
55	MG	DA	1601	1/1	0.85	0.25	87,87,87,87	0
55	MG	DA	1603	1/1	0.85	0.39	71,71,71,71	0
55	MG	CA	3189	1/1	0.85	0.31	67,67,67,67	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	BA	1608	1/1	0.85	0.23	55,55,55,55	0
56	OHX	AA	3333	7/7	0.85	0.12	91,114,128,179	2
56	OHX	AA	3369	7/7	0.85	0.14	80,102,119,165	1
56	OHX	CA	3422	7/7	0.85	0.09	126,137,143,193	1
56	OHX	AA	3513	7/7	0.85	0.09	80,88,116,153	1
55	MG	AA	3216	1/1	0.85	0.28	71,71,71,71	0
55	MG	DA	1686	1/1	0.85	0.14	73,73,73,73	0
55	MG	BA	1660	1/1	0.85	0.20	97,97,97,97	0
56	OHX	AA	3530	7/7	0.85	0.12	101,121,143,206	1
55	MG	CA	3195	1/1	0.85	0.17	68,68,68,68	0
56	OHX	CA	3491	7/7	0.85	0.11	92,108,117,175	1
55	MG	AA	3107	1/1	0.85	0.11	79,79,79,79	0
55	MG	DA	1697	1/1	0.85	0.25	72,72,72,72	0
56	OHX	CB	219	7/7	0.85	0.08	145,151,161,232	1
55	MG	CA	3071	1/1	0.85	0.26	51,51,51,51	0
55	MG	DA	1656	1/1	0.85	0.28	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	1702	1/1	0.85	0.11	122,122,122,122	0
55	MG	CA	3114	1/1	0.85	0.32	57,57,57,57	0
55	MG	AA	3126	1/1	0.85	0.21	85,85,85,85	0
56	OHX	DA	1783	7/7	0.85	0.09	123,123,145,185	1
55	MG	AA	3105	1/1	0.85	0.23	124,124,124,124	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	DA	1707	1/1	0.85	0.26	85,85,85,85	0
55	MG	CA	3051	1/1	0.85	0.31	69,69,69,69	0
55	MG	AA	3379	1/1	0.85	0.35	55,55,55,55	0
55	MG	AA	3079	1/1	0.86	0.26	88,88,88,88	0
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	BA	1714	1/1	0.86	0.18	56,56,56,56	0
55	MG	CA	3109	1/1	0.86	0.23	56,56,56,56	0
55	MG	AA	3046	1/1	0.86	0.24	68,68,68,68	0
55	MG	BB	102	1/1	0.86	0.19	85,85,85,85	0
56	OHX	BA	1790	7/7	0.86	0.11	96,123,133,185	1
55	MG	DA	1640	1/1	0.86	0.20	83,83,83,83	0
55	MG	CA	3118	1/1	0.86	0.26	69,69,69,69	0
55	MG	DA	1709	1/1	0.86	0.36	80,80,80,80	0
55	MG	CA	3124	1/1	0.86	0.29	44,44,44,44	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	AO	203	1/1	0.86	0.19	56,56,56,56	0
55	MG	DA	1713	1/1	0.86	0.30	79,79,79,79	0
56	OHX	CA	3409	7/7	0.86	0.11	97,100,119,183	1
55	MG	BA	1641	1/1	0.86	0.16	85,85,85,85	0
55	MG	BA	1721	1/1	0.86	0.25	70,70,70,70	0
56	OHX	CA	3415	7/7	0.86	0.10	134,135,143,187	1
55	MG	DA	1716	1/1	0.86	0.26	85,85,85,85	0
55	MG	CA	3014	1/1	0.86	0.22	76,76,76,76	0
55	MG	CA	3479	1/1	0.86	0.33	64,64,64,64	0
55	MG	DA	1725	1/1	0.86	0.32	87,87,87,87	0
55	MG	AA	3382	1/1	0.86	0.27	36,36,36,36	0
55	MG	BA	1617	1/1	0.86	0.25	71,71,71,71	0
55	MG	BA	1618	1/1	0.86	0.27	63,63,63,63	0
55	MG	AA	3157	1/1	0.86	0.35	49,49,49,49	0
55	MG	CA	3151	1/1	0.86	0.22	76,76,76,76	0
55	MG	DA	1607	1/1	0.86	0.23	82,82,82,82	0
56	OHX	CA	3487	7/7	0.86	0.08	135,139,147,210	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	3156	1/1	0.86	0.38	84,84,84,84	0
55	MG	AA	3256	1/1	0.86	0.33	53,53,53,53	0
55	MG	DA	1614	1/1	0.86	0.17	91,91,91,91	0
55	MG	BA	1628	1/1	0.86	0.28	80,80,80,80	0
55	MG	CA	3218	1/1	0.86	0.26	83,83,83,83	0
55	MG	AA	3211	1/1	0.86	0.36	62,62,62,62	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	DA	1684	1/1	0.86	0.29	79,79,79,79	0
55	MG	AA	3048	1/1	0.86	0.34	94,94,94,94	0
55	MG	DA	1687	1/1	0.86	0.15	63,63,63,63	0
55	MG	CA	3177	1/1	0.86	0.21	57,57,57,57	0
55	MG	AA	3270	1/1	0.86	0.09	94,94,94,94	0
55	MG	AA	3084	1/1	0.86	0.23	58,58,58,58	0
55	MG	AA	3275	1/1	0.86	0.28	64,64,64,64	0
56	OHX	BA	1666	7/7	0.86	0.09	117,122,134,158	2
55	MG	CA	3188	1/1	0.86	0.33	60,60,60,60	0
55	MG	BA	1649	1/1	0.87	0.14	74,74,74,74	0
55	MG	AA	3392	1/1	0.87	0.35	64,64,64,64	0
55	MG	CA	3056	1/1	0.87	0.28	79,79,79,79	0
55	MG	BA	1698	1/1	0.87	0.30	62,62,62,62	0
55	MG	AA	3040	1/1	0.87	0.27	47,47,47,47	0
55	MG	CA	3125	1/1	0.87	0.16	52,52,52,52	0
55	MG	CA	3446	1/1	0.87	0.33	47,47,47,47	0
55	MG	A1	201	1/1	0.87	0.30	71,71,71,71	0
55	MG	A3	101	1/1	0.87	0.31	60,60,60,60	0
55	MG	AA	3171	1/1	0.87	0.20	48,48,48,48	0
55	MG	CA	3456	1/1	0.87	0.23	66,66,66,66	0
55	MG	CA	3066	1/1	0.87	0.38	56,56,56,56	0
55	MG	BA	1734	1/1	0.87	0.32	70,70,70,70	0
55	MG	CA	3029	1/1	0.87	0.19	76,76,76,76	0
56	OHX	CA	3348	7/7	0.87	0.15	104,111,132,178	1
55	MG	CA	3471	1/1	0.87	0.30	57,57,57,57	0
56	OHX	CA	3379	7/7	0.87	0.07	134,137,155,207	1
55	MG	DA	1655	1/1	0.87	0.24	78,78,78,78	0
56	OHX	CA	3397	7/7	0.87	0.07	128,138,154,219	1
55	MG	BA	1741	1/1	0.87	0.38	73,73,73,73	0
55	MG	CA	3478	1/1	0.87	0.29	82,82,82,82	0
55	MG	BA	1708	1/1	0.87	0.28	77,77,77,77	0
55	MG	CA	3036	1/1	0.87	0.22	87,87,87,87	0
55	MG	AA	3106	1/1	0.87	0.24	70,70,70,70	0
55	MG	DA	1665	1/1	0.87	0.27	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	AA	3331	7/7	0.87	0.14	72,87,130,163	3
55	MG	AA	3267	1/1	0.87	0.30	80,80,80,80	0
55	MG	AA	3068	1/1	0.87	0.20	61,61,61,61	0
56	OHX	AA	3403	7/7	0.87	0.10	109,110,128,178	1
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	CA	3434	7/7	0.87	0.10	96,110,126,177	1
56	OHX	AA	3512	7/7	0.87	0.11	99,114,126,166	2
56	OHX	CA	3436	7/7	0.87	0.08	115,121,137,192	1
55	MG	CA	3041	1/1	0.87	0.14	73,73,73,73	0
55	MG	AA	3053	1/1	0.87	0.26	60,60,60,60	0
55	MG	DA	1608	1/1	0.87	0.19	78,78,78,78	0
55	MG	BA	1626	1/1	0.87	0.14	81,81,81,81	0
55	MG	CA	3219	1/1	0.87	0.44	79,79,79,79	0
56	OHX	CB	217	7/7	0.87	0.08	128,135,146,182	1
56	OHX	AA	3532	7/7	0.87	0.08	89,105,116,172	1
55	MG	AA	3061	1/1	0.87	0.22	49,49,49,49	0
55	MG	CA	3176	1/1	0.87	0.40	67,67,67,67	0
55	MG	CA	3222	1/1	0.87	0.20	81,81,81,81	0
55	MG	DA	1683	1/1	0.87	0.37	71,71,71,71	0
55	MG	AF	302	1/1	0.87	0.23	81,81,81,81	0
55	MG	DA	1620	1/1	0.87	0.32	79,79,79,79	0
55	MG	CA	3101	1/1	0.87	0.31	59,59,59,59	0
55	MG	CA	3102	1/1	0.87	0.31	67,67,67,67	0
56	OHX	DA	1801	7/7	0.87	0.08	141,143,154,216	1
55	MG	CA	3184	1/1	0.87	0.35	60,60,60,60	0
56	OHX	DA	1808	7/7	0.87	0.10	119,124,131,178	1
56	OHX	AA	3566	7/7	0.87	0.09	92,97,126,175	2
56	OHX	DK	201	7/7	0.87	0.08	137,138,149,200	1
56	OHX	AB	216	7/7	0.87	0.12	88,124,141,184	1
55	MG	CA	3231	1/1	0.87	0.27	89,89,89,89	0
56	OHX	BA	1661	7/7	0.87	0.09	108,124,128,170	1
55	MG	BS	101	1/1	0.87	0.20	93,93,93,93	0
55	MG	AA	3381	1/1	0.88	0.27	59,59,59,59	0
55	MG	CA	3258	1/1	0.88	0.33	56,56,56,56	0
55	MG	CA	3050	1/1	0.88	0.24	65,65,65,65	0
55	MG	AA	3226	1/1	0.88	0.28	42,42,42,42	0
55	MG	CA	3052	1/1	0.88	0.28	66,66,66,66	0
55	MG	BA	1603	1/1	0.88	0.20	63,63,63,63	0
55	MG	BA	1711	1/1	0.88	0.29	94,94,94,94	0
56	OHX	AA	3524	7/7	0.88	0.07	111,120,128,172	1
55	MG	AA	3013	1/1	0.88	0.22	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3143	1/1	0.88	0.30	46,46,46,46	0
56	OHX	CA	3417	7/7	0.88	0.07	151,167,187,222	1
55	MG	AA	3396	1/1	0.88	0.40	71,71,71,71	0
55	MG	AA	3279	1/1	0.88	0.25	81,81,81,81	0
55	MG	CA	3140	1/1	0.88	0.27	59,59,59,59	0
55	MG	CA	3003	1/1	0.88	0.22	51,51,51,51	0
56	OHX	CA	3426	7/7	0.88	0.06	142,146,155,215	1
55	MG	CA	3008	1/1	0.88	0.23	52,52,52,52	0
55	MG	CA	3204	1/1	0.88	0.29	73,73,73,73	0
56	OHX	CA	3431	7/7	0.88	0.08	105,117,132,179	1
56	OHX	AA	3554	7/7	0.88	0.07	116,128,150,205	1
55	MG	AA	3193	1/1	0.88	0.08	58,58,58,58	0
55	MG	AA	3206	1/1	0.88	0.34	64,64,64,64	0
55	MG	CA	3208	1/1	0.88	0.29	70,70,70,70	0
55	MG	BA	1643	1/1	0.88	0.10	78,78,78,78	0
55	MG	AA	3163	1/1	0.88	0.20	61,61,61,61	0
56	OHX	AA	3567	7/7	0.88	0.08	103,106,118,172	1
55	MG	AA	3115	1/1	0.88	0.20	51,51,51,51	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	1650	1/1	0.88	0.23	67,67,67,67	0
55	MG	CB	201	1/1	0.88	0.12	77,77,77,77	0
55	MG	CA	3033	1/1	0.88	0.15	71,71,71,71	0
55	MG	AA	3057	1/1	0.88	0.29	72,72,72,72	0
55	MG	AA	3123	1/1	0.88	0.18	72,72,72,72	0
55	MG	AE	302	1/1	0.88	0.22	71,71,71,71	0
55	MG	BA	1652	1/1	0.88	0.20	63,63,63,63	0
55	MG	DA	1663	1/1	0.88	0.19	66,66,66,66	0
55	MG	AA	3049	1/1	0.88	0.25	64,64,64,64	0
55	MG	AA	3353	1/1	0.88	0.21	39,39,39,39	0
55	MG	AA	3151	1/1	0.88	0.21	62,62,62,62	0
55	MG	AA	3044	1/1	0.88	0.33	72,72,72,72	0
56	OHX	BA	1816	7/7	0.88	0.09	127,130,142,194	1
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
55	MG	D1	101	1/1	0.88	0.28	78,78,78,78	0
55	MG	CA	3179	1/1	0.88	0.09	73,73,73,73	0
55	MG	BA	1627	1/1	0.88	0.29	80,80,80,80	0
55	MG	AA	3224	1/1	0.88	0.22	68,68,68,68	0
56	OHX	CA	3284	7/7	0.88	0.09	136,147,155,216	1
55	MG	BA	1650	1/1	0.89	0.36	72,72,72,72	0
55	MG	CA	3018	1/1	0.89	0.34	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	1651	1/1	0.89	0.10	90,90,90,90	0
55	MG	CA	3211	1/1	0.89	0.12	116,116,116,116	0
55	MG	CA	3026	1/1	0.89	0.10	58,58,58,58	0
55	MG	CA	3157	1/1	0.89	0.31	76,76,76,76	0
55	MG	AA	3234	1/1	0.89	0.13	56,56,56,56	0
55	MG	BA	1727	1/1	0.89	0.28	70,70,70,70	0
55	MG	CB	202	1/1	0.89	0.14	99,99,99,99	0
56	OHX	CA	3269	7/7	0.89	0.14	98,100,123,153	2
55	MG	AA	3063	1/1	0.89	0.20	76,76,76,76	0
55	MG	DC	106	1/1	0.89	0.41	91,91,91,91	0
56	OHX	CA	3358	7/7	0.89	0.07	128,130,147,230	1
55	MG	CB	205	1/1	0.89	0.33	74,74,74,74	0
56	OHX	CA	3378	7/7	0.89	0.09	128,141,148,178	1
56	OHX	AA	3138	7/7	0.89	0.12	88,92,127,173	1
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
55	MG	CA	3030	1/1	0.89	0.22	89,89,89,89	0
56	OHX	CA	3407	7/7	0.89	0.08	142,149,155,227	1
55	MG	AA	3244	1/1	0.89	0.21	49,49,49,49	0
56	OHX	AA	3366	7/7	0.89	0.13	85,90,106,173	1
55	MG	BA	1730	1/1	0.89	0.30	73,73,73,73	0
56	OHX	AA	3370	7/7	0.89	0.10	115,126,140,200	1
55	MG	DA	1667	1/1	0.89	0.32	68,68,68,68	0
55	MG	AA	3102	1/1	0.89	0.25	79,79,79,79	0
56	OHX	AA	3490	7/7	0.89	0.07	94,113,129,158	1
55	MG	DA	1669	1/1	0.89	0.31	64,64,64,64	0
55	MG	BA	1702	1/1	0.89	0.17	62,62,62,62	0
55	MG	AA	3167	1/1	0.89	0.32	53,53,53,53	0
55	MG	AA	3155	1/1	0.89	0.10	85,85,85,85	0
55	MG	AA	3212	1/1	0.89	0.24	35,35,35,35	0
55	MG	AA	3128	1/1	0.89	0.23	54,54,54,54	0
55	MG	DA	1615	1/1	0.89	0.15	98,98,98,98	0
55	MG	DA	1677	1/1	0.89	0.23	76,76,76,76	0
55	MG	DA	1616	1/1	0.89	0.24	88,88,88,88	0
55	MG	AA	3175	1/1	0.89	0.25	39,39,39,39	0
55	MG	CA	3257	1/1	0.89	0.21	60,60,60,60	0
55	MG	AA	3023	1/1	0.89	0.24	52,52,52,52	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
56	OHX	CB	214	7/7	0.89	0.09	129,139,146,186	1
55	MG	CA	3260	1/1	0.89	0.22	71,71,71,71	0
55	MG	AA	3117	1/1	0.89	0.19	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	1613	1/1	0.89	0.17	65,65,65,65	0
55	MG	BA	1713	1/1	0.89	0.15	59,59,59,59	0
55	MG	DA	1625	1/1	0.89	0.12	97,97,97,97	0
55	MG	DA	1695	1/1	0.89	0.30	76,76,76,76	0
55	MG	BB	101	1/1	0.89	0.34	70,70,70,70	0
55	MG	BA	1614	1/1	0.89	0.25	73,73,73,73	0
56	OHX	DA	1775	7/7	0.89	0.08	133,145,148,215	1
55	MG	DA	1628	1/1	0.89	0.31	78,78,78,78	0
55	MG	CA	3439	1/1	0.89	0.32	63,63,63,63	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
56	OHX	AB	218	7/7	0.89	0.07	128,132,146,199	1
56	OHX	DA	1796	7/7	0.89	0.07	134,139,149,195	1
55	MG	AA	3070	1/1	0.89	0.13	52,52,52,52	0
56	OHX	DA	1803	7/7	0.89	0.07	135,141,144,207	1
55	MG	AA	3041	1/1	0.89	0.15	49,49,49,49	0
55	MG	CA	3443	1/1	0.89	0.36	49,49,49,49	0
55	MG	AA	3199	1/1	0.89	0.33	76,76,76,76	0
55	MG	BD	101	1/1	0.89	0.24	93,93,93,93	0
56	OHX	DA	1812	7/7	0.89	0.08	149,158,168,252	1
55	MG	CA	3059	1/1	0.89	0.32	63,63,63,63	0
55	MG	DA	1636	1/1	0.89	0.21	75,75,75,75	0
55	MG	AA	3390	1/1	0.89	0.28	46,46,46,46	0
55	MG	CA	3005	1/1	0.89	0.15	48,48,48,48	0
55	MG	AA	3201	1/1	0.89	0.22	45,45,45,45	0
56	OHX	BA	1690	7/7	0.89	0.08	118,127,134,188	1
55	MG	CA	3476	1/1	0.90	0.26	52,52,52,52	0
55	MG	BA	1623	1/1	0.90	0.20	67,67,67,67	0
55	MG	AA	3221	1/1	0.90	0.13	68,68,68,68	0
55	MG	DA	1658	1/1	0.90	0.31	64,64,64,64	0
55	MG	AA	3127	1/1	0.90	0.27	57,57,57,57	0
55	MG	CA	3119	1/1	0.90	0.19	61,61,61,61	0
56	OHX	CA	3306	7/7	0.90	0.09	98,106,119,148	1
55	MG	AA	3261	1/1	0.90	0.36	64,64,64,64	0
56	OHX	AA	3365	7/7	0.90	0.14	90,106,114,161	2
55	MG	AA	3109	1/1	0.90	0.34	47,47,47,47	0
55	MG	CB	203	1/1	0.90	0.11	111,111,111,111	0
55	MG	AA	3229	1/1	0.90	0.28	59,59,59,59	0
56	OHX	CA	3380	7/7	0.90	0.07	106,119,130,170	1
55	MG	CA	3131	1/1	0.90	0.27	65,65,65,65	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3380	1/1	0.90	0.21	66,66,66,66	0
55	MG	CA	3212	1/1	0.90	0.29	75,75,75,75	0
56	OHX	CA	3411	7/7	0.90	0.07	117,123,138,184	1
56	OHX	AA	3505	7/7	0.90	0.12	86,108,110,156	1
55	MG	AA	3060	1/1	0.90	0.13	70,70,70,70	0
55	MG	AA	3114	1/1	0.90	0.22	47,47,47,47	0
55	MG	DA	1604	1/1	0.90	0.28	82,82,82,82	0
56	OHX	AA	3519	7/7	0.90	0.08	140,146,150,214	1
55	MG	BB	103	1/1	0.90	0.27	91,91,91,91	0
55	MG	CA	3055	1/1	0.90	0.17	66,66,66,66	0
55	MG	AA	3386	1/1	0.90	0.14	42,42,42,42	0
55	MG	DA	1611	1/1	0.90	0.18	92,92,92,92	0
55	MG	DA	1679	1/1	0.90	0.17	69,69,69,69	0
55	MG	BB	105	1/1	0.90	0.39	63,63,63,63	0
55	MG	AA	3274	1/1	0.90	0.28	89,89,89,89	0
55	MG	AA	3078	1/1	0.90	0.24	59,59,59,59	0
56	OHX	CA	3433	7/7	0.90	0.07	121,129,144,183	1
55	MG	CA	3153	1/1	0.90	0.23	56,56,56,56	0
56	OHX	AA	3537	7/7	0.90	0.07	171,189,202,242	1
55	MG	AA	3103	1/1	0.90	0.08	97,97,97,97	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	CA	3002	1/1	0.90	0.29	50,50,50,50	0
55	MG	BA	1716	1/1	0.90	0.21	55,55,55,55	0
55	MG	AA	3243	1/1	0.90	0.30	51,51,51,51	0
55	MG	CA	3229	1/1	0.90	0.27	80,80,80,80	0
56	OHX	CB	213	7/7	0.90	0.08	131,144,166,188	1
55	MG	CA	3165	1/1	0.90	0.25	57,57,57,57	0
56	OHX	CB	215	7/7	0.90	0.08	108,133,144,220	1
56	OHX	AA	3560	7/7	0.90	0.07	102,104,127,184	1
55	MG	CA	3166	1/1	0.90	0.35	58,58,58,58	0
55	MG	CA	3067	1/1	0.90	0.26	49,49,49,49	0
55	MG	BA	1642	1/1	0.90	0.10	102,102,102,102	0
55	MG	AA	3071	1/1	0.90	0.33	68,68,68,68	0
55	MG	AA	3409	1/1	0.90	0.30	56,56,56,56	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	CA	3021	1/1	0.90	0.12	60,60,60,60	0
55	MG	BA	1645	1/1	0.90	0.33	51,51,51,51	0
55	MG	AA	3020	1/1	0.90	0.39	44,44,44,44	0
56	OHX	DA	1785	7/7	0.90	0.09	110,114,129,164	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3158	1/1	0.90	0.26	50,50,50,50	0
55	MG	CA	3083	1/1	0.90	0.27	44,44,44,44	0
55	MG	AA	3284	1/1	0.90	0.11	66,66,66,66	0
55	MG	CA	3185	1/1	0.90	0.39	75,75,75,75	0
55	MG	AA	3073	1/1	0.90	0.18	69,69,69,69	0
55	MG	AA	3250	1/1	0.90	0.35	56,56,56,56	0
55	MG	AA	3348	1/1	0.90	0.36	46,46,46,46	0
56	OHX	DA	1807	7/7	0.90	0.07	117,126,135,195	1
55	MG	AA	3069	1/1	0.90	0.26	62,62,62,62	0
55	MG	BA	1735	1/1	0.90	0.15	48,48,48,48	0
55	MG	CA	3096	1/1	0.90	0.18	64,64,64,64	0
55	MG	BA	1739	1/1	0.90	0.32	70,70,70,70	0
55	MG	DA	1645	1/1	0.90	0.26	91,91,91,91	0
56	OHX	BA	1783	7/7	0.90	0.14	77,87,125,141	2
55	MG	BA	1658	1/1	0.90	0.25	71,71,71,71	0
56	OHX	BA	1805	7/7	0.90	0.11	90,105,122,143	3
55	MG	BA	1621	1/1	0.90	0.27	55,55,55,55	0
55	MG	AF	301	1/1	0.90	0.23	83,83,83,83	0
55	MG	AA	3077	1/1	0.91	0.22	73,73,73,73	0
56	OHX	AA	3487	7/7	0.91	0.07	95,110,116,167	1
55	MG	AA	3124	1/1	0.91	0.24	70,70,70,70	0
56	OHX	CA	3375	7/7	0.91	0.10	103,118,131,145	1
55	MG	CA	3143	1/1	0.91	0.24	60,60,60,60	0
55	MG	DA	1605	1/1	0.91	0.23	63,63,63,63	0
55	MG	AA	3101	1/1	0.91	0.22	63,63,63,63	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	CA	3025	1/1	0.91	0.12	83,83,83,83	0
55	MG	AA	3249	1/1	0.91	0.31	58,58,58,58	0
56	OHX	AA	3515	7/7	0.91	0.08	100,121,139,211	1
56	OHX	CA	3404	7/7	0.91	0.09	149,155,166,217	1
55	MG	CA	3148	1/1	0.91	0.21	57,57,57,57	0
55	MG	BA	1742	1/1	0.91	0.37	86,86,86,86	0
55	MG	AA	3036	1/1	0.91	0.26	36,36,36,36	0
55	MG	CA	3154	1/1	0.91	0.26	46,46,46,46	0
55	MG	CA	3155	1/1	0.91	0.20	58,58,58,58	0
55	MG	AA	3162	1/1	0.91	0.33	38,38,38,38	0
55	MG	AA	3398	1/1	0.91	0.23	51,51,51,51	0
55	MG	CA	3224	1/1	0.91	0.25	77,77,77,77	0
55	MG	CA	3159	1/1	0.91	0.28	75,75,75,75	0
55	MG	CA	3031	1/1	0.91	0.08	53,53,53,53	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	AA	3012	1/1	0.91	0.20	46,46,46,46	0
55	MG	AA	3414	1/1	0.91	0.24	57,57,57,57	0
56	OHX	AA	3542	7/7	0.91	0.08	118,127,135,189	1
55	MG	CA	3167	1/1	0.91	0.29	75,75,75,75	0
55	MG	BA	1750	1/1	0.91	0.24	72,72,72,72	0
55	MG	AA	3416	1/1	0.91	0.25	74,74,74,74	0
55	MG	AA	3227	1/1	0.91	0.26	63,63,63,63	0
55	MG	DA	1704	1/1	0.91	0.31	73,73,73,73	0
55	MG	CA	3087	1/1	0.91	0.06	70,70,70,70	0
55	MG	CA	3038	1/1	0.91	0.15	74,74,74,74	0
55	MG	AA	3349	1/1	0.91	0.32	61,61,61,61	0
55	MG	AA	3033	1/1	0.91	0.18	48,48,48,48	0
55	MG	AA	3266	1/1	0.91	0.12	78,78,78,78	0
55	MG	CA	3099	1/1	0.91	0.24	51,51,51,51	0
56	OHX	AA	3569	7/7	0.91	0.07	116,117,125,191	1
55	MG	CA	3100	1/1	0.91	0.36	63,63,63,63	0
55	MG	BA	1717	1/1	0.91	0.26	51,51,51,51	0
55	MG	CA	3186	1/1	0.91	0.17	75,75,75,75	0
55	MG	AA	3064	1/1	0.91	0.11	66,66,66,66	0
55	MG	CA	3103	1/1	0.91	0.23	70,70,70,70	0
55	MG	AA	3149	1/1	0.91	0.15	74,74,74,74	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	AA	3356	1/1	0.91	0.34	58,58,58,58	0
55	MG	AA	3118	1/1	0.91	0.20	53,53,53,53	0
55	MG	DB	101	1/1	0.91	0.33	78,78,78,78	0
56	OHX	BA	1673	7/7	0.91	0.08	117,123,127,191	1
55	MG	CA	3116	1/1	0.91	0.24	69,69,69,69	0
55	MG	AA	3056	1/1	0.91	0.16	36,36,36,36	0
55	MG	DC	102	1/1	0.91	0.41	69,69,69,69	0
56	OHX	DA	1784	7/7	0.91	0.07	150,153,166,225	1
56	OHX	BA	1680	7/7	0.91	0.07	120,125,145,238	1
55	MG	AA	3241	1/1	0.91	0.22	60,60,60,60	0
55	MG	DA	1654	1/1	0.91	0.26	61,61,61,61	0
55	MG	BA	1624	1/1	0.91	0.20	70,70,70,70	0
55	MG	CA	3121	1/1	0.91	0.28	55,55,55,55	0
56	OHX	DA	1798	7/7	0.91	0.07	128,133,140,212	1
55	MG	BA	1653	1/1	0.91	0.17	63,63,63,63	0
55	MG	AA	3122	1/1	0.91	0.22	62,62,62,62	0
55	MG	AA	3174	1/1	0.91	0.29	76,76,76,76	0
55	MG	CA	3203	1/1	0.91	0.21	47,47,47,47	0
55	MG	DA	1661	1/1	0.91	0.39	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	3009	1/1	0.91	0.24	39,39,39,39	0
55	MG	CA	3013	1/1	0.91	0.15	47,47,47,47	0
56	OHX	CA	3245	7/7	0.91	0.09	99,120,129,189	1
55	MG	AA	3383	1/1	0.91	0.22	46,46,46,46	0
55	MG	CA	3138	1/1	0.91	0.43	53,53,53,53	0
55	MG	CA	3061	1/1	0.91	0.30	64,64,64,64	0
56	OHX	AA	3406	7/7	0.91	0.13	84,92,109,162	1
56	OHX	CA	3304	7/7	0.91	0.09	113,122,141,181	2
55	MG	CA	3210	1/1	0.91	0.34	74,74,74,74	0
56	OHX	CA	3340	7/7	0.92	0.09	115,122,140,168	1
55	MG	CA	3068	1/1	0.92	0.29	44,44,44,44	0
55	MG	CA	3069	1/1	0.92	0.36	69,69,69,69	0
56	OHX	CA	3359	7/7	0.92	0.07	115,123,136,171	2
55	MG	AA	3152	1/1	0.92	0.23	56,56,56,56	0
56	OHX	CA	3373	7/7	0.92	0.09	113,122,129,160	1
56	OHX	AA	3525	7/7	0.92	0.09	100,109,122,187	1
55	MG	CA	3139	1/1	0.92	0.21	56,56,56,56	0
56	OHX	AA	3527	7/7	0.92	0.06	130,134,147,188	1
55	MG	AA	3255	1/1	0.92	0.16	64,64,64,64	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	CA	3452	1/1	0.92	0.13	51,51,51,51	0
56	OHX	CA	3392	7/7	0.92	0.08	126,132,142,192	1
56	OHX	AA	3533	7/7	0.92	0.10	98,103,114,150	2
56	OHX	CA	3395	7/7	0.92	0.09	106,111,125,156	1
55	MG	CA	3454	1/1	0.92	0.30	51,51,51,51	0
55	MG	CA	3074	1/1	0.92	0.35	64,64,64,64	0
55	MG	BA	1754	1/1	0.92	0.29	61,61,61,61	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	CA	3077	1/1	0.92	0.16	57,57,57,57	0
55	MG	AA	3153	1/1	0.92	0.36	64,64,64,64	0
56	OHX	CA	3408	7/7	0.92	0.05	136,139,143,209	1
55	MG	CA	3459	1/1	0.92	0.17	56,56,56,56	0
56	OHX	AA	3541	7/7	0.92	0.09	102,114,134,158	2
55	MG	AA	3135	1/1	0.92	0.20	67,67,67,67	0
55	MG	AA	3177	1/1	0.92	0.23	37,37,37,37	0
56	OHX	AA	3546	7/7	0.92	0.09	98,103,119,179	1
56	OHX	AA	3551	7/7	0.92	0.06	141,143,149,194	1
56	OHX	CA	3418	7/7	0.92	0.08	115,119,129,166	1
55	MG	CA	3473	1/1	0.92	0.22	50,50,50,50	0
55	MG	CA	3475	1/1	0.92	0.18	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3136	1/1	0.92	0.15	57,57,57,57	0
56	OHX	AA	3559	7/7	0.92	0.05	124,133,143,186	1
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	3055	1/1	0.92	0.26	65,65,65,65	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	3357	1/1	0.92	0.36	73,73,73,73	0
55	MG	BC	101	1/1	0.92	0.37	69,69,69,69	0
55	MG	AA	3097	1/1	0.92	0.11	59,59,59,59	0
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	CA	3093	1/1	0.92	0.32	81,81,81,81	0
55	MG	CA	3001	1/1	0.92	0.18	46,46,46,46	0
55	MG	AO	202	1/1	0.92	0.24	55,55,55,55	0
55	MG	AA	3161	1/1	0.92	0.19	50,50,50,50	0
56	OHX	AO	205	7/7	0.92	0.08	83,89,107,180	1
56	OHX	CA	3468	7/7	0.92	0.08	115,126,133,180	1
55	MG	C0	201	1/1	0.92	0.16	61,61,61,61	0
55	MG	DC	105	1/1	0.92	0.36	54,54,54,54	0
55	MG	AA	3142	1/1	0.92	0.40	45,45,45,45	0
55	MG	CA	3007	1/1	0.92	0.16	45,45,45,45	0
55	MG	AA	3028	1/1	0.92	0.24	66,66,66,66	0
55	MG	AA	3384	1/1	0.92	0.31	59,59,59,59	0
55	MG	CA	3106	1/1	0.92	0.24	61,61,61,61	0
55	MG	CA	3011	1/1	0.92	0.24	46,46,46,46	0
55	MG	BA	1630	1/1	0.92	0.11	90,90,90,90	0
55	MG	CA	3228	1/1	0.92	0.10	65,65,65,65	0
55	MG	CA	3110	1/1	0.92	0.37	85,85,85,85	0
56	OHX	BA	1676	7/7	0.92	0.07	143,151,156,210	1
56	OHX	C5	102	7/7	0.92	0.07	114,118,133,165	1
55	MG	AA	3006	1/1	0.92	0.36	45,45,45,45	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
56	OHX	BA	1678	7/7	0.92	0.07	115,118,134,165	1
55	MG	CA	3182	1/1	0.92	0.34	59,59,59,59	0
56	OHX	AA	3371	7/7	0.92	0.10	93,107,117,177	1
56	OHX	DA	1781	7/7	0.92	0.08	107,126,135,195	1
55	MG	CA	3115	1/1	0.92	0.23	63,63,63,63	0
56	OHX	AA	3404	7/7	0.92	0.10	74,98,116,164	1
55	MG	CA	3015	1/1	0.92	0.21	54,54,54,54	0
55	MG	AA	3051	1/1	0.92	0.17	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	BA	1784	7/7	0.92	0.09	122,129,148,203	0
56	OHX	BA	1787	7/7	0.92	0.09	107,117,138,149	2
55	MG	AA	3027	1/1	0.92	0.21	42,42,42,42	0
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
56	OHX	DA	1799	7/7	0.92	0.06	122,127,139,209	1
56	OHX	AA	3485	7/7	0.92	0.07	104,114,127,171	1
55	MG	CA	3022	1/1	0.92	0.20	55,55,55,55	0
55	MG	AA	3215	1/1	0.92	0.36	50,50,50,50	0
55	MG	AA	3090	1/1	0.92	0.14	85,85,85,85	0
56	OHX	AA	3493	7/7	0.92	0.07	109,111,123,166	1
55	MG	AA	3283	1/1	0.92	0.25	55,55,55,55	0
56	OHX	CA	3247	7/7	0.92	0.11	95,104,117,152	1
56	OHX	AA	3509	7/7	0.92	0.07	92,96,122,175	1
55	MG	AA	3047	1/1	0.92	0.26	54,54,54,54	0
55	MG	AA	3092	1/1	0.92	0.04	73,73,73,73	0
55	MG	DA	1689	1/1	0.92	0.17	87,87,87,87	0
56	OHX	DB	103	7/7	0.92	0.09	166,171,179,191	1
56	OHX	CA	3302	7/7	0.92	0.10	79,86,104,139	1
55	MG	DA	1690	1/1	0.92	0.27	63,63,63,63	0
55	MG	DA	1692	1/1	0.92	0.30	70,70,70,70	0
55	MG	DA	1711	1/1	0.93	0.15	107,107,107,107	0
55	MG	CA	3147	1/1	0.93	0.27	51,51,51,51	0
56	OHX	CA	3382	7/7	0.93	0.07	129,131,148,199	1
55	MG	AA	3387	1/1	0.93	0.22	42,42,42,42	0
56	OHX	CA	3384	7/7	0.93	0.07	118,124,135,184	1
55	MG	CA	3090	1/1	0.93	0.19	55,55,55,55	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
56	OHX	AA	3544	7/7	0.93	0.06	103,105,124,176	1
55	MG	DA	1648	1/1	0.93	0.07	91,91,91,91	0
55	MG	CA	3152	1/1	0.93	0.35	54,54,54,54	0
56	OHX	AA	3547	7/7	0.93	0.07	69,84,101,157	2
55	MG	CA	3048	1/1	0.93	0.29	44,44,44,44	0
55	MG	DA	1653	1/1	0.93	0.37	73,73,73,73	0
56	OHX	AA	3553	7/7	0.93	0.06	113,118,133,183	1
55	MG	AA	3259	1/1	0.93	0.20	35,35,35,35	0
55	MG	DL	201	1/1	0.93	0.28	92,92,92,92	0
55	MG	BA	1736	1/1	0.93	0.41	64,64,64,64	0
55	MG	CA	3010	1/1	0.93	0.13	47,47,47,47	0
56	OHX	AA	3561	7/7	0.93	0.07	152,158,173,226	1
55	MG	CA	3097	1/1	0.93	0.25	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	AA	3563	7/7	0.93	0.06	124,125,134,183	1
56	OHX	CA	3412	7/7	0.93	0.11	99,116,129,164	2
55	MG	AA	3260	1/1	0.93	0.37	58,58,58,58	0
55	MG	CA	3162	1/1	0.93	0.32	65,65,65,65	0
55	MG	BA	1740	1/1	0.93	0.34	61,61,61,61	0
56	OHX	CA	3416	7/7	0.93	0.07	114,117,128,182	1
55	MG	CB	207	1/1	0.93	0.33	76,76,76,76	0
55	MG	AA	3286	1/1	0.93	0.33	68,68,68,68	0
55	MG	AA	3395	1/1	0.93	0.13	40,40,40,40	0
55	MG	CA	3016	1/1	0.93	0.20	55,55,55,55	0
56	OHX	AB	215	7/7	0.93	0.10	105,114,120,153	1
55	MG	DA	1602	1/1	0.93	0.23	68,68,68,68	0
56	OHX	AB	217	7/7	0.93	0.09	85,105,116,146	1
55	MG	CA	3104	1/1	0.93	0.32	41,41,41,41	0
56	OHX	AB	219	7/7	0.93	0.08	104,111,125,162	1
55	MG	CA	3169	1/1	0.93	0.18	71,71,71,71	0
55	MG	BA	1707	1/1	0.93	0.21	70,70,70,70	0
55	MG	DA	1671	1/1	0.93	0.12	64,64,64,64	0
56	OHX	CA	3430	7/7	0.93	0.08	96,106,114,197	1
55	MG	AA	3344	1/1	0.93	0.24	48,48,48,48	0
55	MG	AA	3032	1/1	0.93	0.23	41,41,41,41	0
55	MG	AA	3264	1/1	0.93	0.27	76,76,76,76	0
55	MG	CA	3112	1/1	0.93	0.28	41,41,41,41	0
55	MG	AA	3408	1/1	0.93	0.30	47,47,47,47	0
55	MG	AA	3184	1/1	0.93	0.16	38,38,38,38	0
56	OHX	BA	1672	7/7	0.93	0.07	156,159,170,224	1
56	OHX	CA	3464	7/7	0.93	0.12	78,109,122,137	3
55	MG	AA	3413	1/1	0.93	0.20	57,57,57,57	0
55	MG	CA	3259	1/1	0.93	0.28	65,65,65,65	0
56	OHX	AA	3476	7/7	0.93	0.10	102,122,137,175	1
56	OHX	AA	3482	7/7	0.93	0.07	105,118,127,177	1
56	OHX	AA	3483	7/7	0.93	0.07	124,141,146,196	1
55	MG	AA	3113	1/1	0.93	0.20	32,32,32,32	0
55	MG	AA	3188	1/1	0.93	0.16	40,40,40,40	0
56	OHX	CB	211	7/7	0.93	0.07	122,128,152,168	1
55	MG	AA	3189	1/1	0.93	0.27	42,42,42,42	0
55	MG	AA	3134	1/1	0.93	0.15	82,82,82,82	0
55	MG	DA	1685	1/1	0.93	0.10	59,59,59,59	0
56	OHX	BA	1694	7/7	0.93	0.06	159,161,173,226	1
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	DA	1621	1/1	0.93	0.17	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	AA	3495	7/7	0.93	0.09	86,93,120,158	1
55	MG	CA	3123	1/1	0.93	0.14	36,36,36,36	0
56	OHX	BA	1797	7/7	0.93	0.13	71,104,132,136	3
56	OHX	AA	3506	7/7	0.93	0.06	97,110,123,157	1
56	OHX	DA	1756	7/7	0.93	0.06	145,145,160,212	1
56	OHX	AA	3507	7/7	0.93	0.07	101,111,128,158	1
55	MG	AA	3120	1/1	0.93	0.15	71,71,71,71	0
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	BA	1719	1/1	0.93	0.31	51,51,51,51	0
55	MG	CA	3075	1/1	0.93	0.21	45,45,45,45	0
56	OHX	DA	1777	7/7	0.93	0.06	150,152,155,232	1
56	OHX	BR	101	7/7	0.93	0.06	117,129,143,169	1
55	MG	AB	204	1/1	0.93	0.33	68,68,68,68	0
56	OHX	AA	3514	7/7	0.93	0.08	84,93,104,149	1
55	MG	CA	3133	1/1	0.93	0.23	48,48,48,48	0
55	MG	AA	3197	1/1	0.93	0.27	50,50,50,50	0
56	OHX	CA	3248	7/7	0.93	0.06	116,128,134,203	1
55	MG	AA	3198	1/1	0.93	0.22	54,54,54,54	0
55	MG	CA	3137	1/1	0.93	0.33	74,74,74,74	0
55	MG	CA	3451	1/1	0.93	0.22	46,46,46,46	0
55	MG	AA	3004	1/1	0.93	0.23	37,37,37,37	0
55	MG	CA	3080	1/1	0.93	0.10	57,57,57,57	0
55	MG	AA	3008	1/1	0.93	0.27	42,42,42,42	0
56	OHX	AA	3529	7/7	0.93	0.08	90,106,115,167	1
56	OHX	DA	1804	7/7	0.93	0.07	107,115,128,173	1
55	MG	AA	3203	1/1	0.93	0.18	50,50,50,50	0
56	OHX	DA	1806	7/7	0.93	0.05	142,150,160,228	1
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	3531	7/7	0.93	0.06	119,124,135,185	1
56	OHX	CA	3350	7/7	0.93	0.08	112,134,144,175	1
55	MG	AA	3204	1/1	0.93	0.12	61,61,61,61	0
55	MG	AA	3228	1/1	0.93	0.18	67,67,67,67	0
55	MG	AA	3089	1/1	0.93	0.47	84,84,84,84	0
55	MG	CA	3205	1/1	0.93	0.15	63,63,63,63	0
55	MG	AA	3230	1/1	0.93	0.19	66,66,66,66	0
56	OHX	CA	3376	7/7	0.93	0.07	113,130,136,172	1
56	OHX	DC	107	7/7	0.93	0.09	131,132,141,177	1
55	MG	BA	1731	1/1	0.93	0.33	57,57,57,57	0
57	ZN	DG	301	1/1	0.93	0.20	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3093	1/1	0.94	0.26	91,91,91,91	0
55	MG	AA	3003	1/1	0.94	0.17	39,39,39,39	0
56	OHX	AA	3452	7/7	0.94	0.11	61,75,91,137	2
55	MG	AA	3233	1/1	0.94	0.16	59,59,59,59	0
56	OHX	AA	3477	7/7	0.94	0.06	108,119,125,208	1
56	OHX	A1	202	7/7	0.94	0.08	85,95,114,146	1
56	OHX	CA	3403	7/7	0.94	0.08	88,108,114,167	1
55	MG	AA	3210	1/1	0.94	0.33	41,41,41,41	0
56	OHX	CA	3405	7/7	0.94	0.06	112,116,119,187	1
56	OHX	BA	1656	7/7	0.94	0.07	160,162,176,267	0
55	MG	AA	3082	1/1	0.94	0.12	50,50,50,50	0
55	MG	CA	3181	1/1	0.94	0.21	62,62,62,62	0
55	MG	CA	3017	1/1	0.94	0.15	92,92,92,92	0
56	OHX	AA	3486	7/7	0.94	0.07	127,135,138,199	1
55	MG	AA	3236	1/1	0.94	0.26	40,40,40,40	0
55	MG	CA	3122	1/1	0.94	0.19	40,40,40,40	0
55	MG	CA	3020	1/1	0.94	0.21	70,70,70,70	0
55	MG	AA	3237	1/1	0.94	0.23	45,45,45,45	0
55	MG	BA	1737	1/1	0.94	0.18	46,46,46,46	0
55	MG	CA	3126	1/1	0.94	0.20	54,54,54,54	0
56	OHX	AA	3494	7/7	0.94	0.08	59,86,128,185	1
55	MG	AA	3238	1/1	0.94	0.29	50,50,50,50	0
56	OHX	AA	3504	7/7	0.94	0.06	112,118,129,179	1
55	MG	CA	3445	1/1	0.94	0.19	38,38,38,38	0
55	MG	AA	3191	1/1	0.94	0.19	45,45,45,45	0
56	OHX	BA	1681	7/7	0.94	0.06	153,163,173,229	1
55	MG	AA	3278	1/1	0.94	0.24	35,35,35,35	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
56	OHX	AA	3508	7/7	0.94	0.07	122,129,136,204	1
56	OHX	BA	1691	7/7	0.94	0.06	148,150,156,215	1
55	MG	AA	3214	1/1	0.94	0.21	46,46,46,46	0
56	OHX	BA	1693	7/7	0.94	0.08	112,112,134,152	1
55	MG	DA	1699	1/1	0.94	0.21	78,78,78,78	0
55	MG	AA	3192	1/1	0.94	0.27	48,48,48,48	0
56	OHX	BA	1771	7/7	0.94	0.11	77,100,122,150	1
55	MG	AA	3104	1/1	0.94	0.31	68,68,68,68	0
55	MG	BA	1616	1/1	0.94	0.15	61,61,61,61	0
56	OHX	BA	1785	7/7	0.94	0.08	109,122,129,170	1
55	MG	AA	3246	1/1	0.94	0.21	36,36,36,36	0
55	MG	CA	3199	1/1	0.94	0.23	62,62,62,62	0
56	OHX	BA	1791	7/7	0.94	0.10	82,106,122,150	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	BA	1793	7/7	0.94	0.07	95,105,117,163	1
56	OHX	CA	3482	7/7	0.94	0.07	84,120,131,181	0
55	MG	AA	3195	1/1	0.94	0.25	43,43,43,43	0
55	MG	DA	1639	1/1	0.94	0.24	70,70,70,70	0
56	OHX	CA	3489	7/7	0.94	0.09	91,101,112,140	1
55	MG	AA	3030	1/1	0.94	0.18	44,44,44,44	0
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	BA	1705	1/1	0.94	0.18	63,63,63,63	0
55	MG	AA	3011	1/1	0.94	0.21	49,49,49,49	0
56	OHX	BA	1811	7/7	0.94	0.09	88,104,115,154	1
55	MG	AA	3180	1/1	0.94	0.19	65,65,65,65	0
55	MG	CA	3472	1/1	0.94	0.10	59,59,59,59	0
56	OHX	BB	106	7/7	0.94	0.12	164,167,173,198	1
55	MG	AA	3251	1/1	0.94	0.28	49,49,49,49	0
56	OHX	BD	102	7/7	0.94	0.07	153,174,197,228	0
55	MG	AA	3345	1/1	0.94	0.48	47,47,47,47	0
56	OHX	CA	3244	7/7	0.94	0.07	94,113,121,172	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	3222	1/1	0.94	0.28	64,64,64,64	0
55	MG	CA	3089	1/1	0.94	0.15	60,60,60,60	0
55	MG	AA	3254	1/1	0.94	0.20	42,42,42,42	0
55	MG	AA	3223	1/1	0.94	0.21	56,56,56,56	0
56	OHX	DA	1760	7/7	0.94	0.07	142,145,152,204	1
55	MG	CA	3092	1/1	0.94	0.35	52,52,52,52	0
55	MG	AA	3182	1/1	0.94	0.29	45,45,45,45	0
55	MG	AA	3257	1/1	0.94	0.22	57,57,57,57	0
56	OHX	DA	1773	7/7	0.94	0.06	122,126,137,197	1
55	MG	AA	3225	1/1	0.94	0.16	63,63,63,63	0
55	MG	AA	3183	1/1	0.94	0.24	88,88,88,88	0
56	OHX	DA	1776	7/7	0.94	0.07	114,116,125,160	1
55	MG	AA	3039	1/1	0.94	0.21	40,40,40,40	0
56	OHX	DA	1778	7/7	0.94	0.07	142,148,154,267	0
56	OHX	CA	3318	7/7	0.94	0.11	34,112,130,183	1
55	MG	CA	3161	1/1	0.94	0.20	71,71,71,71	0
55	MG	CA	3049	1/1	0.94	0.19	62,62,62,62	0
55	MG	AA	3205	1/1	0.94	0.18	40,40,40,40	0
55	MG	AA	3358	1/1	0.94	0.24	51,51,51,51	0
56	OHX	CA	3346	7/7	0.94	0.09	99,104,119,151	1
56	OHX	AA	3548	7/7	0.94	0.06	113,118,133,172	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	DA	1790	7/7	0.94	0.06	135,136,148,199	1
56	OHX	CA	3349	7/7	0.94	0.07	115,117,131,178	1
56	OHX	AA	3550	7/7	0.94	0.07	111,121,131,187	1
56	OHX	CA	3355	7/7	0.94	0.09	108,110,119,149	1
55	MG	BA	1636	1/1	0.94	0.14	61,61,61,61	0
55	MG	DA	1666	1/1	0.94	0.30	62,62,62,62	0
56	OHX	CA	3365	7/7	0.94	0.07	164,171,176,213	1
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	BA	1638	1/1	0.94	0.20	57,57,57,57	0
55	MG	AA	3374	1/1	0.94	0.22	29,29,29,29	0
56	OHX	CA	3377	7/7	0.94	0.10	90,95,111,135	2
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	3168	1/1	0.94	0.24	72,72,72,72	0
55	MG	AA	3377	1/1	0.94	0.23	51,51,51,51	0
55	MG	DA	1606	1/1	0.94	0.13	84,84,84,84	0
55	MG	CA	3226	1/1	0.94	0.41	65,65,65,65	0
56	OHX	DV	101	7/7	0.94	0.07	162,169,185,231	1
55	MG	AA	3168	1/1	0.94	0.26	89,89,89,89	0
55	MG	AA	3265	1/1	0.94	0.30	85,85,85,85	0
55	MG	AA	3207	1/1	0.94	0.31	57,57,57,57	0
56	OHX	AA	3402	7/7	0.94	0.14	87,110,129,141	3
55	MG	DA	1612	1/1	0.94	0.21	86,86,86,86	0
56	OHX	DD	101	7/7	0.94	0.08	155,165,187,227	0
57	ZN	BQ	102	1/1	0.94	0.12	130,130,130,130	0
55	MG	CA	3173	1/1	0.94	0.16	53,53,53,53	0
55	MG	AA	3240	1/1	0.95	0.17	43,43,43,43	0
55	MG	CA	3174	1/1	0.95	0.32	52,52,52,52	0
55	MG	BA	1619	1/1	0.95	0.18	50,50,50,50	0
55	MG	AA	3173	1/1	0.95	0.19	52,52,52,52	0
55	MG	AA	3242	1/1	0.95	0.21	37,37,37,37	0
55	MG	BA	1726	1/1	0.95	0.27	61,61,61,61	0
56	OHX	AA	3528	7/7	0.95	0.07	112,118,137,160	2
56	OHX	BA	1778	7/7	0.95	0.08	99,120,131,182	0
55	MG	AA	3262	1/1	0.95	0.28	52,52,52,52	0
55	MG	CA	3130	1/1	0.95	0.41	58,58,58,58	0
55	MG	BA	1654	1/1	0.95	0.24	47,47,47,47	0
55	MG	AA	3002	1/1	0.95	0.28	41,41,41,41	0
55	MG	AA	3010	1/1	0.95	0.17	40,40,40,40	0
55	MG	DA	1610	1/1	0.95	0.14	96,96,96,96	0
55	MG	CA	3135	1/1	0.95	0.29	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	BA	1794	7/7	0.95	0.06	118,138,149,184	1
55	MG	CA	3043	1/1	0.95	0.11	82,82,82,82	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	CA	3263	1/1	0.95	0.25	69,69,69,69	0
56	OHX	AA	3304	7/7	0.95	0.06	109,115,135,200	1
55	MG	CA	3004	1/1	0.95	0.13	49,49,49,49	0
55	MG	BA	1697	1/1	0.95	0.26	37,37,37,37	0
56	OHX	BA	1807	7/7	0.95	0.06	135,141,150,224	0
56	OHX	AA	3313	7/7	0.95	0.08	96,112,122,174	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
56	OHX	BA	1815	7/7	0.95	0.07	110,125,133,172	1
56	OHX	AA	3543	7/7	0.95	0.05	113,117,131,189	1
56	OHX	AA	3319	7/7	0.95	0.08	87,95,122,151	1
55	MG	CA	3006	1/1	0.95	0.19	47,47,47,47	0
56	OHX	AA	3330	7/7	0.95	0.07	102,112,122,166	1
55	MG	CA	3190	1/1	0.95	0.11	60,60,60,60	0
56	OHX	CA	3488	7/7	0.95	0.06	113,123,127,179	1
55	MG	AA	3343	1/1	0.95	0.28	34,34,34,34	0
55	MG	AA	3099	1/1	0.95	0.18	65,65,65,65	0
55	MG	AA	3389	1/1	0.95	0.29	44,44,44,44	0
55	MG	CA	3442	1/1	0.95	0.18	61,61,61,61	0
55	MG	CA	3194	1/1	0.95	0.26	63,63,63,63	0
56	OHX	CB	212	7/7	0.95	0.07	101,120,135,155	1
55	MG	AA	3029	1/1	0.95	0.24	38,38,38,38	0
56	OHX	AA	3373	7/7	0.95	0.08	75,103,110,155	1
56	OHX	AA	3557	7/7	0.95	0.09	75,87,101,114	1
55	MG	CA	3094	1/1	0.95	0.35	79,79,79,79	0
56	OHX	CA	3285	7/7	0.95	0.12	94,107,126,147	1
55	MG	A5	101	1/1	0.95	0.19	41,41,41,41	0
55	MG	AA	3178	1/1	0.95	0.31	39,39,39,39	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
55	MG	AA	3269	1/1	0.95	0.23	72,72,72,72	0
55	MG	AA	3179	1/1	0.95	0.32	60,60,60,60	0
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	3325	7/7	0.95	0.13	108,122,148,156	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	CA	3334	7/7	0.95	0.07	110,115,136,183	0
56	OHX	DA	1751	7/7	0.95	0.13	66,109,137,183	2
55	MG	CA	3149	1/1	0.95	0.27	55,55,55,55	0
56	OHX	AA	3474	7/7	0.95	0.09	51,85,127,151	2
56	OHX	DA	1754	7/7	0.95	0.07	98,102,118,156	1
56	OHX	AA	3475	7/7	0.95	0.07	67,93,111,167	1
55	MG	CA	3150	1/1	0.95	0.23	55,55,55,55	0
55	MG	DA	1691	1/1	0.95	0.22	54,54,54,54	0
56	OHX	AA	3479	7/7	0.95	0.07	106,122,142,174	1
56	OHX	DA	1762	7/7	0.95	0.08	107,112,122,180	1
56	OHX	AB	209	7/7	0.95	0.08	63,88,125,152	2
55	MG	BA	1743	1/1	0.95	0.26	69,69,69,69	0
56	OHX	DA	1771	7/7	0.95	0.10	97,105,129,152	1
55	MG	AA	3025	1/1	0.95	0.20	59,59,59,59	0
55	MG	AA	3146	1/1	0.95	0.20	41,41,41,41	0
55	MG	CA	3019	1/1	0.95	0.13	46,46,46,46	0
56	OHX	CA	3362	7/7	0.95	0.05	129,136,141,186	1
56	OHX	CA	3364	7/7	0.95	0.07	117,120,133,182	1
55	MG	AA	3352	1/1	0.95	0.13	41,41,41,41	0
56	OHX	CA	3368	7/7	0.95	0.07	108,126,135,177	1
56	OHX	DA	1780	7/7	0.95	0.07	127,131,138,167	1
56	OHX	CA	3370	7/7	0.95	0.07	116,120,142,180	1
55	MG	AA	3088	1/1	0.95	0.09	60,60,60,60	0
55	MG	AA	3202	1/1	0.95	0.27	45,45,45,45	0
56	OHX	CA	3374	7/7	0.95	0.08	106,124,128,169	1
55	MG	CA	3158	1/1	0.95	0.21	56,56,56,56	0
55	MG	CA	3474	1/1	0.95	0.16	70,70,70,70	0
56	OHX	AW	101	7/7	0.95	0.09	103,112,128,156	1
56	OHX	DA	1788	7/7	0.95	0.08	96,113,128,168	1
55	MG	CA	3108	1/1	0.95	0.22	52,52,52,52	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	AA	3412	1/1	0.95	0.23	39,39,39,39	0
56	OHX	DA	1795	7/7	0.95	0.06	112,118,132,167	1
56	OHX	BA	1659	7/7	0.95	0.07	114,130,135,179	1
56	OHX	DA	1797	7/7	0.95	0.05	149,152,159,218	1
56	OHX	CA	3381	7/7	0.95	0.07	102,112,121,159	1
55	MG	AA	3018	1/1	0.95	0.20	43,43,43,43	0
55	MG	BA	1752	1/1	0.95	0.31	53,53,53,53	0
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
55	MG	CA	3113	1/1	0.95	0.21	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	BA	1668	7/7	0.95	0.07	116,121,137,182	1
55	MG	DA	1646	1/1	0.95	0.16	64,64,64,64	0
56	OHX	CA	3391	7/7	0.95	0.06	140,144,157,182	1
56	OHX	BA	1670	7/7	0.95	0.06	135,143,147,201	1
55	MG	AA	3186	1/1	0.95	0.21	49,49,49,49	0
55	MG	AA	3277	1/1	0.95	0.27	46,46,46,46	0
55	MG	AA	3170	1/1	0.95	0.14	50,50,50,50	0
55	MG	AA	3375	1/1	0.95	0.25	31,31,31,31	0
56	OHX	CA	3398	7/7	0.95	0.06	129,132,142,192	1
55	MG	DA	1651	1/1	0.95	0.38	62,62,62,62	0
55	MG	DA	1652	1/1	0.95	0.33	52,52,52,52	0
55	MG	AA	3376	1/1	0.95	0.25	33,33,33,33	0
55	MG	AA	3121	1/1	0.95	0.30	53,53,53,53	0
55	MG	CA	3120	1/1	0.95	0.25	48,48,48,48	0
56	OHX	BA	1683	7/7	0.95	0.06	124,130,146,183	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
55	MG	AA	3239	1/1	0.95	0.15	44,44,44,44	0
55	MG	AA	3043	1/1	0.96	0.23	46,46,46,46	0
55	MG	AA	3050	1/1	0.96	0.20	60,60,60,60	0
56	OHX	AA	3558	7/7	0.96	0.06	95,121,125,156	1
55	MG	CA	3012	1/1	0.96	0.18	53,53,53,53	0
55	MG	CA	3047	1/1	0.96	0.33	41,41,41,41	0
56	OHX	CA	3423	7/7	0.96	0.04	123,126,136,189	1
56	OHX	BA	1810	7/7	0.96	0.07	106,108,121,152	1
55	MG	BA	1748	1/1	0.96	0.20	66,66,66,66	0
56	OHX	BA	1812	7/7	0.96	0.06	151,164,170,231	1
55	MG	AA	3415	1/1	0.96	0.12	52,52,52,52	0
55	MG	AA	3007	1/1	0.96	0.11	31,31,31,31	0
55	MG	BA	1655	1/1	0.96	0.19	60,60,60,60	0
55	MG	AA	3133	1/1	0.96	0.15	54,54,54,54	0
55	MG	AA	3385	1/1	0.96	0.29	34,34,34,34	0
55	MG	AA	3111	1/1	0.96	0.22	35,35,35,35	0
55	MG	BN	201	1/1	0.96	0.11	80,80,80,80	0
55	MG	AA	3112	1/1	0.96	0.13	47,47,47,47	0
56	OHX	BD	103	7/7	0.96	0.06	86,95,103,174	1
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	CA	3463	7/7	0.96	0.10	107,129,139,156	1
55	MG	CA	3180	1/1	0.96	0.17	75,75,75,75	0
56	OHX	CA	3465	7/7	0.96	0.07	131,136,147,181	1
55	MG	AA	3022	1/1	0.96	0.12	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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	3469	7/7	0.96	0.07	89,110,121,162	1
56	OHX	AB	214	7/7	0.96	0.07	110,118,132,162	1
56	OHX	CA	3253	7/7	0.96	0.08	107,120,133,155	1
55	MG	BA	1701	1/1	0.96	0.20	57,57,57,57	0
56	OHX	AA	3496	7/7	0.96	0.06	117,124,142,215	0
55	MG	CA	3024	1/1	0.96	0.11	48,48,48,48	0
55	MG	AA	3181	1/1	0.96	0.25	61,61,61,61	0
56	OHX	CA	3490	7/7	0.96	0.07	102,105,118,156	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
56	OHX	CA	3314	7/7	0.96	0.10	84,93,97,114	1
55	MG	DA	1680	1/1	0.96	0.18	72,72,72,72	0
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	A3	102	7/7	0.96	0.10	90,98,113,134	2
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
55	MG	CA	3063	1/1	0.96	0.15	70,70,70,70	0
56	OHX	A6	101	7/7	0.96	0.07	113,122,137,155	1
55	MG	AA	3016	1/1	0.96	0.20	39,39,39,39	0
55	MG	AA	3200	1/1	0.96	0.27	45,45,45,45	0
56	OHX	C6	101	7/7	0.96	0.07	132,145,157,184	1
55	MG	CA	3105	1/1	0.96	0.41	68,68,68,68	0
55	MG	BA	1732	1/1	0.96	0.27	52,52,52,52	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	AA	3305	7/7	0.96	0.10	83,97,103,135	1
55	MG	AE	303	1/1	0.96	0.15	32,32,32,32	0
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	DA	1750	7/7	0.96	0.07	127,137,146,202	1
56	OHX	CA	3353	7/7	0.96	0.07	81,96,110,140	1
56	OHX	BA	1665	7/7	0.96	0.08	82,92,111,128	1
56	OHX	CA	3356	7/7	0.96	0.06	96,109,118,157	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BC	103	1/1	0.96	0.31	62,62,62,62	0
55	MG	BC	104	1/1	0.96	0.34	57,57,57,57	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
56	OHX	AA	3317	7/7	0.96	0.07	79,88,118,156	1
56	OHX	CA	3363	7/7	0.96	0.08	94,99,114,167	1
56	OHX	DA	1763	7/7	0.96	0.05	154,159,173,250	0
55	MG	CA	3070	1/1	0.96	0.14	44,44,44,44	0
56	OHX	DA	1768	7/7	0.96	0.06	121,132,163,218	0
55	MG	CA	3261	1/1	0.96	0.36	48,48,48,48	0
56	OHX	DA	1770	7/7	0.96	0.05	136,142,156,217	1
56	OHX	CA	3366	7/7	0.96	0.07	140,148,168,207	0
56	OHX	CA	3367	7/7	0.96	0.05	129,137,147,194	1
56	OHX	AA	3327	7/7	0.96	0.06	107,115,135,188	1
56	OHX	CA	3369	7/7	0.96	0.08	97,113,121,158	1
56	OHX	AA	3328	7/7	0.96	0.09	89,97,114,142	1
55	MG	AA	3393	1/1	0.96	0.13	56,56,56,56	0
55	MG	DA	1693	1/1	0.96	0.32	54,54,54,54	0
55	MG	C5	101	1/1	0.96	0.24	50,50,50,50	0
56	OHX	AA	3334	7/7	0.96	0.09	66,79,94,105	1
56	OHX	AA	3336	7/7	0.96	0.07	146,153,168,218	0
56	OHX	BA	1679	7/7	0.96	0.05	116,125,129,189	1
55	MG	AA	3394	1/1	0.96	0.23	43,43,43,43	0
55	MG	CA	3073	1/1	0.96	0.18	54,54,54,54	0
56	OHX	BA	1682	7/7	0.96	0.06	119,124,130,186	1
56	OHX	AA	3368	7/7	0.96	0.10	76,83,98,126	1
55	MG	AA	3054	1/1	0.96	0.13	49,49,49,49	0
56	OHX	BA	1687	7/7	0.96	0.08	94,99,108,140	1
55	MG	BA	1738	1/1	0.96	0.09	41,41,41,41	0
56	OHX	CA	3385	7/7	0.96	0.06	115,124,135,193	1
55	MG	AA	3140	1/1	0.96	0.09	41,41,41,41	0
56	OHX	AA	3372	7/7	0.96	0.07	93,103,121,167	1
55	MG	CA	3160	1/1	0.96	0.28	49,49,49,49	0
55	MG	AA	3185	1/1	0.96	0.26	36,36,36,36	0
56	OHX	AA	3538	7/7	0.96	0.09	88,94,114,159	1
55	MG	AA	3116	1/1	0.96	0.17	45,45,45,45	0
55	MG	AA	3001	1/1	0.96	0.25	28,28,28,28	0
56	OHX	DA	1800	7/7	0.96	0.05	137,140,150,220	1
56	OHX	AA	3405	7/7	0.96	0.06	103,111,138,161	1
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
55	MG	AA	3346	1/1	0.96	0.16	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	3444	1/1	0.96	0.21	52,52,52,52	0
56	OHX	AA	3447	7/7	0.96	0.07	91,102,120,163	1
56	OHX	CA	3401	7/7	0.96	0.06	136,149,158,185	1
55	MG	AA	3410	1/1	0.96	0.23	61,61,61,61	0
56	OHX	AA	3458	7/7	0.96	0.10	34,48,113,148	3
56	OHX	BA	1788	7/7	0.96	0.07	118,118,132,157	1
56	OHX	BA	1789	7/7	0.96	0.07	108,112,133,182	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	3549	7/7	0.96	0.08	97,102,111,165	1
56	OHX	CA	3410	7/7	0.96	0.06	114,125,132,190	1
56	OHX	AA	3466	7/7	0.96	0.07	89,94,108,128	1
56	OHX	BA	1796	7/7	0.96	0.06	143,156,164,225	0
56	OHX	AA	3470	7/7	0.96	0.07	107,109,130,160	1
56	OHX	AA	3473	7/7	0.96	0.08	66,95,102,124	1
55	MG	AA	3042	1/1	0.96	0.17	43,43,43,43	0
55	MG	CA	3447	1/1	0.96	0.43	58,58,58,58	0
56	OHX	BA	1802	7/7	0.96	0.06	107,121,133,185	1
55	MG	CA	3127	1/1	0.97	0.18	53,53,53,53	0
56	OHX	AA	3480	7/7	0.97	0.07	90,100,124,135	1
56	OHX	AA	3481	7/7	0.97	0.06	95,108,126,156	2
56	OHX	CA	3372	7/7	0.97	0.07	112,137,145,182	0
56	OHX	AA	3332	7/7	0.97	0.08	77,106,123,134	1
55	MG	CA	3128	1/1	0.97	0.07	72,72,72,72	0
55	MG	AA	3075	1/1	0.97	0.34	44,44,44,44	0
56	OHX	BA	1663	7/7	0.97	0.05	132,137,143,190	1
56	OHX	BA	1808	7/7	0.97	0.11	84,90,96,110	2
56	OHX	BA	1809	7/7	0.97	0.05	141,153,160,232	0
56	OHX	AA	3335	7/7	0.97	0.06	94,101,113,136	1
56	OHX	CO	201	7/7	0.97	0.06	104,109,121,141	1
55	MG	AA	3085	1/1	0.97	0.12	58,58,58,58	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	AA	3489	7/7	0.97	0.07	72,78,92,128	1
56	OHX	DA	1728	7/7	0.97	0.07	78,116,123,162	0
56	OHX	AA	3363	7/7	0.97	0.09	90,99,133,145	1
55	MG	AA	3196	1/1	0.97	0.20	36,36,36,36	0
56	OHX	BG	302	7/7	0.97	0.06	128,137,145,186	1
56	OHX	BA	1671	7/7	0.97	0.04	127,131,133,210	1
55	MG	C7	101	1/1	0.97	0.28	54,54,54,54	0
56	OHX	CA	3389	7/7	0.97	0.06	101,110,123,155	1
56	OHX	AA	3367	7/7	0.97	0.06	121,129,147,173	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	3132	1/1	0.97	0.14	80,80,80,80	0
55	MG	AA	3253	1/1	0.97	0.20	53,53,53,53	0
56	OHX	AA	3263	7/7	0.97	0.06	76,102,114,143	1
56	OHX	DA	1748	7/7	0.97	0.06	95,111,122,149	1
56	OHX	CA	3394	7/7	0.97	0.07	97,100,116,155	1
56	OHX	AA	3288	7/7	0.97	0.08	76,85,101,127	1
56	OHX	AA	3498	7/7	0.97	0.07	92,94,127,136	1
56	OHX	CA	3246	7/7	0.97	0.10	113,116,120,151	1
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	AA	3556	7/7	0.97	0.05	212,217,223,266	1
56	OHX	AA	3502	7/7	0.97	0.07	97,102,112,146	1
56	OHX	AA	3401	7/7	0.97	0.05	93,112,116,173	1
56	OHX	CA	3254	7/7	0.97	0.06	167,174,181,211	0
56	OHX	DA	1761	7/7	0.97	0.05	130,132,145,205	0
56	OHX	BA	1685	7/7	0.97	0.05	198,199,207,267	1
55	MG	AA	3094	1/1	0.97	0.31	39,39,39,39	0
56	OHX	CA	3406	7/7	0.97	0.06	151,161,169,211	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	3303	7/7	0.97	0.07	93,102,117,145	1
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
55	MG	DA	1638	1/1	0.97	0.11	89,89,89,89	0
55	MG	AA	3411	1/1	0.97	0.17	63,63,63,63	0
55	MG	CA	3453	1/1	0.97	0.24	58,58,58,58	0
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
56	OHX	AA	3307	7/7	0.97	0.07	85,90,103,127	1
56	OHX	CA	3317	7/7	0.97	0.07	116,126,142,180	1
55	MG	CA	3098	1/1	0.97	0.13	63,63,63,63	0
56	OHX	AA	3448	7/7	0.97	0.08	87,90,112,131	1
56	OHX	AA	3450	7/7	0.97	0.07	65,94,112,113	3
55	MG	CA	3058	1/1	0.97	0.29	50,50,50,50	0
56	OHX	BA	1764	7/7	0.97	0.08	88,94,120,157	0
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	3336	7/7	0.97	0.06	114,127,138,191	0
55	MG	CA	3111	1/1	0.97	0.28	30,30,30,30	0
56	OHX	CA	3338	7/7	0.97	0.08	95,103,117,121	1
56	OHX	DA	1789	7/7	0.97	0.04	176,179,184,242	1
56	OHX	AA	3318	7/7	0.97	0.08	92,102,113,133	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	BA	1773	7/7	0.97	0.08	101,102,110,142	1
56	OHX	CA	3341	7/7	0.97	0.08	74,100,107,145	2
56	OHX	DA	1793	7/7	0.97	0.06	146,150,161,207	1
55	MG	DA	1700	1/1	0.97	0.35	70,70,70,70	0
56	OHX	AA	3322	7/7	0.97	0.06	89,98,107,146	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	BA	1782	7/7	0.97	0.07	133,144,159,198	0
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	AA	3467	7/7	0.97	0.06	100,105,117,133	1
56	OHX	DA	1802	7/7	0.97	0.07	120,122,140,196	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	1786	7/7	0.97	0.07	93,97,101,149	1
56	OHX	AA	3468	7/7	0.97	0.06	99,111,119,167	1
56	OHX	AA	3469	7/7	0.97	0.08	79,91,98,161	1
55	MG	AA	3388	1/1	0.97	0.25	41,41,41,41	0
56	OHX	CA	3357	7/7	0.97	0.07	86,98,106,151	1
56	OHX	DA	1811	7/7	0.97	0.04	137,141,149,222	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
56	OHX	BA	1792	7/7	0.97	0.06	150,163,168,209	1
56	OHX	CA	3481	7/7	0.97	0.08	35,87,114,138	2
56	OHX	AA	3325	7/7	0.97	0.07	91,103,115,154	1
56	OHX	CA	3484	7/7	0.97	0.06	104,113,129,146	1
56	OHX	AA	3326	7/7	0.97	0.09	83,94,100,118	1
56	OHX	BA	1795	7/7	0.97	0.06	109,127,134,173	1
55	MG	BA	1700	1/1	0.97	0.34	61,61,61,61	0
55	MG	DA	1664	1/1	0.97	0.32	31,31,31,31	0
55	MG	AA	3219	1/1	0.97	0.15	48,48,48,48	0
56	OHX	BA	1799	7/7	0.97	0.06	158,163,176,213	1
56	OHX	AA	3478	7/7	0.97	0.06	77,90,100,131	1
55	MG	AA	3172	1/1	0.98	0.32	38,38,38,38	0
56	OHX	AA	3323	7/7	0.98	0.07	72,87,96,117	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	3307	7/7	0.98	0.06	92,104,131,164	0
56	OHX	DA	1729	7/7	0.98	0.06	104,108,118,152	1
55	MG	BA	1620	1/1	0.98	0.37	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	AA	3518	7/7	0.98	0.06	67,73,103,130	1
56	OHX	CA	3310	7/7	0.98	0.06	74,88,107,129	1
56	OHX	CA	3311	7/7	0.98	0.07	79,95,105,127	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
56	OHX	AA	3300	7/7	0.98	0.06	67,91,120,167	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	3315	7/7	0.98	0.07	90,101,110,160	1
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
55	MG	AA	3031	1/1	0.98	0.20	35,35,35,35	0
56	OHX	DA	1746	7/7	0.98	0.05	126,134,146,189	1
56	OHX	AA	3400	7/7	0.98	0.08	69,80,83,116	1
56	OHX	CA	3319	7/7	0.98	0.06	87,97,106,138	1
56	OHX	CA	3320	7/7	0.98	0.06	140,142,153,174	0
56	OHX	CA	3321	7/7	0.98	0.06	111,119,144,156	0
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
55	MG	DN	201	1/1	0.98	0.10	80,80,80,80	0
56	OHX	CA	3326	7/7	0.98	0.06	97,110,130,136	2
55	MG	BA	1733	1/1	0.98	0.35	60,60,60,60	0
56	OHX	CA	3329	7/7	0.98	0.06	102,103,123,146	1
56	OHX	AA	3329	7/7	0.98	0.06	85,90,103,133	1
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	CA	3332	7/7	0.98	0.07	70,82,93,103	1
55	MG	AA	3213	1/1	0.98	0.10	49,49,49,49	0
56	OHX	AA	3154	7/7	0.98	0.08	76,89,110,133	1
55	MG	CA	3265	1/1	0.98	0.14	55,55,55,55	0
56	OHX	DA	1764	7/7	0.98	0.05	115,121,127,171	1
56	OHX	AA	3308	7/7	0.98	0.06	66,73,104,120	2
56	OHX	AA	3440	7/7	0.98	0.07	59,88,102,124	0
56	OHX	BA	1684	7/7	0.98	0.05	109,118,126,149	1
56	OHX	AA	3441	7/7	0.98	0.07	84,93,115,140	0
56	OHX	AA	3443	7/7	0.98	0.06	69,76,84,127	1
56	OHX	AB	211	7/7	0.98	0.07	74,85,113,121	0
56	OHX	AA	3309	7/7	0.98	0.07	64,84,90,112	1
55	MG	A0	201	1/1	0.98	0.14	48,48,48,48	0
56	OHX	AA	3287	7/7	0.98	0.06	75,88,103,129	2
56	OHX	CA	3345	7/7	0.98	0.05	91,108,114,146	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	AA	3451	7/7	0.98	0.07	75,85,92,125	1
56	OHX	CA	3347	7/7	0.98	0.06	86,102,110,148	1
56	OHX	AA	3314	7/7	0.98	0.07	81,93,123,149	1
56	OHX	AA	3454	7/7	0.98	0.07	68,93,112,112	1
56	OHX	DA	1779	7/7	0.98	0.04	144,146,155,215	1
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	BA	1761	7/7	0.98	0.06	102,104,115,161	0
56	OHX	AA	3338	7/7	0.98	0.07	82,93,108,126	1
56	OHX	CA	3354	7/7	0.98	0.08	78,88,98,105	1
56	OHX	BA	1765	7/7	0.98	0.07	111,119,130,164	0
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	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	3499	7/7	0.98	0.05	101,113,131,183	1
56	OHX	BA	1769	7/7	0.98	0.07	102,107,127,145	0
56	OHX	AA	3459	7/7	0.98	0.07	71,92,105,129	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	3460	7/7	0.98	0.06	87,98,107,140	0
56	OHX	CA	3483	7/7	0.98	0.07	84,93,103,136	1
56	OHX	AA	3461	7/7	0.98	0.06	60,78,98,143	1
56	OHX	CA	3485	7/7	0.98	0.07	88,102,109,144	1
56	OHX	AA	3463	7/7	0.98	0.07	77,89,96,134	1
56	OHX	BA	1774	7/7	0.98	0.06	80,98,111,147	1
56	OHX	AA	3315	7/7	0.98	0.09	89,99,111,137	1
56	OHX	CA	3249	7/7	0.98	0.08	86,90,104,128	1
56	OHX	AA	3340	7/7	0.98	0.05	159,167,171,209	0
56	OHX	CA	3251	7/7	0.98	0.06	88,107,125,141	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	3341	7/7	0.98	0.06	75,103,114,126	1
56	OHX	AA	3342	7/7	0.98	0.06	78,85,104,123	1
55	MG	AA	3355	1/1	0.98	0.29	36,36,36,36	0
56	OHX	AA	3364	7/7	0.98	0.07	92,103,108,119	1
56	OHX	AA	3295	7/7	0.98	0.07	84,98,116,152	0
56	OHX	AA	3511	7/7	0.98	0.05	133,145,154,207	0
56	OHX	CA	3288	7/7	0.98	0.07	87,95,104,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	AA	3297	7/7	0.98	0.10	87,98,102,106	1
56	OHX	CA	3294	7/7	0.98	0.08	91,93,107,125	1
56	OHX	AA	3320	7/7	0.98	0.09	69,81,96,121	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	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	CA	3299	7/7	0.98	0.06	99,105,124,141	1
57	ZN	BG	301	1/1	0.98	0.18	79,79,79,79	0
56	OHX	CA	3301	7/7	0.98	0.07	55,85,123,136	3
56	OHX	AA	3321	7/7	0.98	0.04	97,109,121,173	1
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	CA	3303	7/7	0.99	0.04	92,96,123,138	0
56	OHX	AA	3435	7/7	0.99	0.07	61,70,93,100	3
56	OHX	CA	3305	7/7	0.99	0.06	70,83,99,129	1
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	AA	3310	7/7	0.99	0.04	94,104,125,156	0
56	OHX	DA	1740	7/7	0.99	0.05	139,153,162,184	0
56	OHX	AA	3311	7/7	0.99	0.06	97,106,117,155	1
56	OHX	AA	3442	7/7	0.99	0.05	70,87,119,140	0
56	OHX	AA	3301	7/7	0.99	0.06	88,89,93,110	1
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	CA	3316	7/7	0.99	0.05	119,122,129,158	0
56	OHX	AA	3446	7/7	0.99	0.07	68,90,101,115	2
56	OHX	AA	3293	7/7	0.99	0.07	54,82,88,102	2
56	OHX	AA	3294	7/7	0.99	0.05	94,100,117,120	0
56	OHX	AA	3449	7/7	0.99	0.04	64,74,89,112	2
55	MG	B1	101	1/1	0.99	0.33	26,26,26,26	0
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	3324	7/7	0.99	0.07	65,83,94,110	2
56	OHX	BA	1756	7/7	0.99	0.08	59,79,107,108	0
56	OHX	BA	1757	7/7	0.99	0.07	57,66,87,98	2
56	OHX	CA	3327	7/7	0.99	0.05	76,83,103,129	1
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	CA	3330	7/7	0.99	0.04	102,106,115,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	BA	1760	7/7	0.99	0.06	71,106,126,148	0
56	OHX	AE	304	7/7	0.99	0.06	74,87,107,110	1
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	AO	204	7/7	0.99	0.05	83,94,106,121	1
56	OHX	AA	3316	7/7	0.99	0.05	80,95,97,136	0
56	OHX	AA	3296	7/7	0.99	0.05	115,120,123,158	0
56	OHX	AA	3453	7/7	0.99	0.06	95,106,114,148	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	3399	7/7	0.99	0.10	42,51,73,98	0
56	OHX	CA	3236	7/7	0.99	0.06	81,104,120,146	0
56	OHX	AA	3289	7/7	0.99	0.07	53,58,81,93	0
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	AA	3359	7/7	0.99	0.05	61,75,93,113	0
56	OHX	AA	3457	7/7	0.99	0.04	73,83,101,131	1
56	OHX	CA	3461	7/7	0.99	0.08	38,55,94,109	0
56	OHX	AA	3360	7/7	0.99	0.07	58,67,70,97	1
56	OHX	CA	3243	7/7	0.99	0.05	121,128,140,172	0
56	OHX	AA	3361	7/7	0.99	0.06	51,71,83,107	0
56	OHX	AA	3362	7/7	0.99	0.08	40,81,119,136	1
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	3290	7/7	0.99	0.06	10,72,91,128	0
56	OHX	AA	3462	7/7	0.99	0.06	75,85,103,106	1
56	OHX	BA	1779	7/7	0.99	0.05	102,112,125,152	1
56	OHX	AA	3291	7/7	0.99	0.07	68,75,102,108	3
56	OHX	AA	3292	7/7	0.99	0.06	50,75,88,112	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	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	3422	7/7	0.99	0.07	74,81,107,116	0
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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	3423	7/7	0.99	0.08	44,66,84,86	1
56	OHX	AA	3424	7/7	0.99	0.06	92,97,108,112	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
56	OHX	AA	3426	7/7	0.99	0.08	70,84,89,118	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	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	AA	3429	7/7	0.99	0.06	69,73,84,102	1
56	OHX	CA	3296	7/7	0.99	0.06	65,90,108,135	2
56	OHX	DA	1718	7/7	0.99	0.08	73,98,100,135	0
56	OHX	AA	3430	7/7	0.99	0.06	63,78,92,111	1
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	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	1727	7/7	0.99	0.05	114,126,131,160	0
56	OHX	CA	3300	7/7	0.99	0.07	66,75,91,101	1
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.