



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 04:10 PM UTC

PDB ID : 4V8F / pdb_00004v8f
Title : Crystal structure analysis of ribosomal decoding (near-cognate tRNA-ttyr complex with paromomycin).
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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

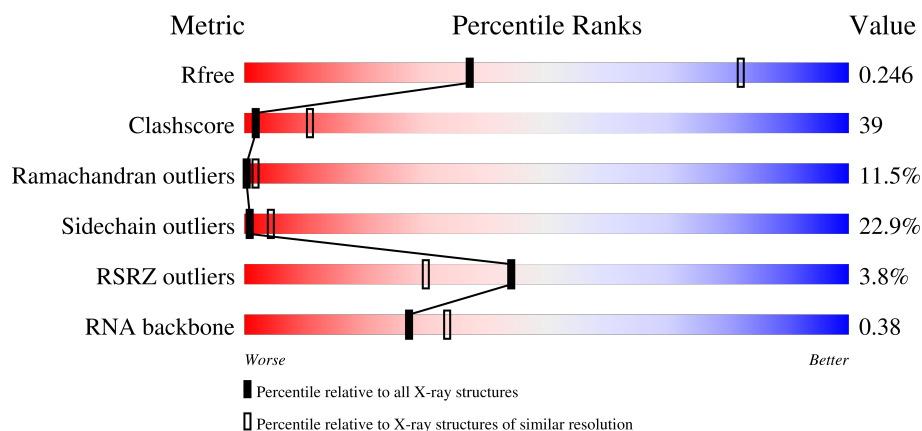
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	29%52%19%
1	DA	2912	% 28%52%20%
2	AB	122	24%60%16%
2	DB	122	% 24%56%20%

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Mol	Chain	Length	Quality of chain
3	AD	276	
3	DD	276	
4	AE	206	
4	DE	206	
5	AF	210	
5	DF	210	
6	AG	182	
6	DG	182	
7	AH	180	
7	DH	180	
8	AK	148	
8	DK	148	
9	AM	140	
9	DM	140	
10	AN	122	
10	DN	122	
11	AO	150	
11	DO	150	
12	AP	141	
12	DP	141	
13	A0	118	
13	D0	118	
14	AQ	112	
14	DQ	112	
15	AR	146	

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Mol	Chain	Length	Quality of chain
15	DR	146	
16	A1	118	
16	D1	118	
17	A2	101	
17	D2	101	
18	AS	113	
18	DS	113	
19	AT	96	
19	DT	96	
20	AU	110	
20	DU	110	
21	AV	206	
21	DV	206	
22	A3	85	
22	D3	85	
23	AZ	98	
23	DZ	98	
24	AW	72	
24	DW	72	
25	AX	60	
25	DX	60	
26	A4	71	
26	D4	71	
27	A5	60	
27	D5	60	

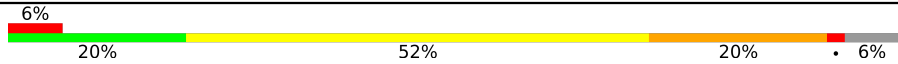
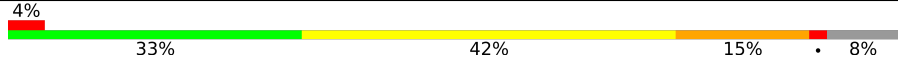
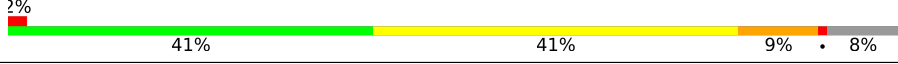
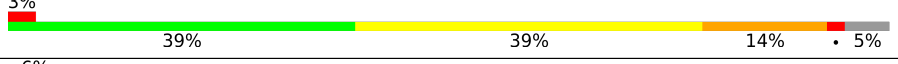
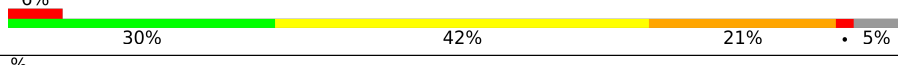
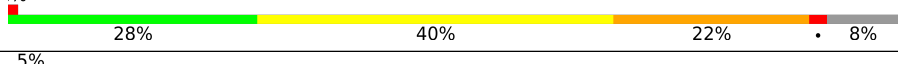
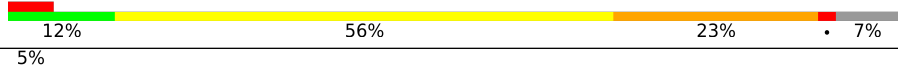
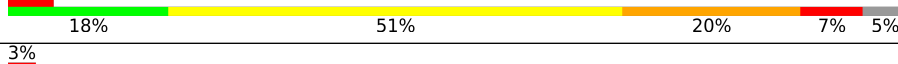
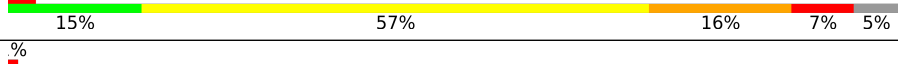
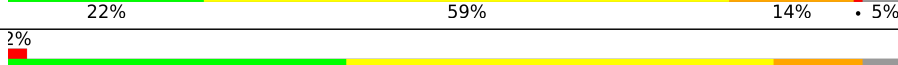
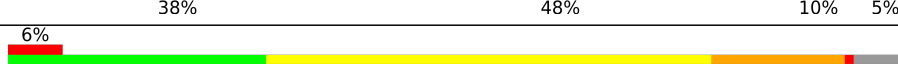
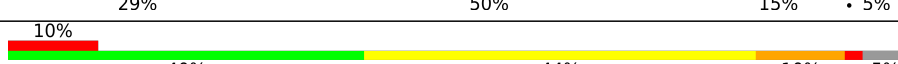
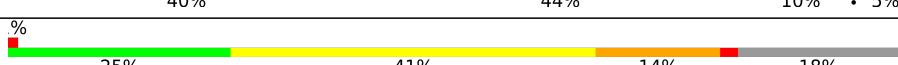
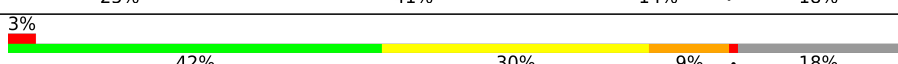
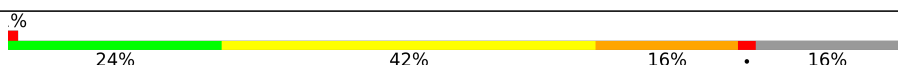
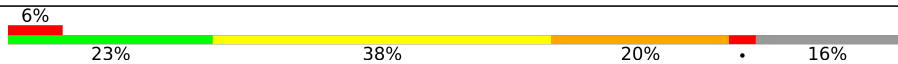
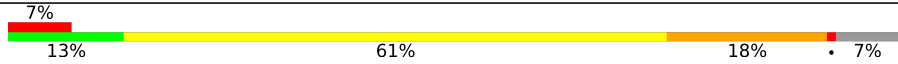
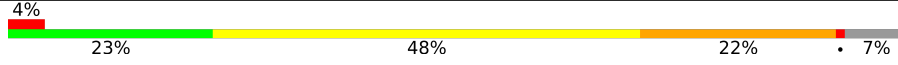
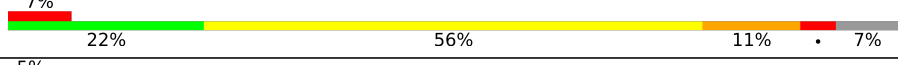
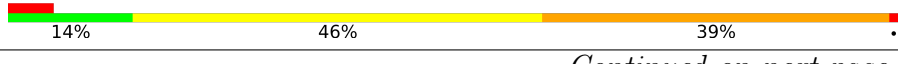
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Mol	Chain	Length	Quality of chain
28	A6	54	
28	D6	54	
29	A7	49	
29	D7	49	
30	A8	65	
30	D8	65	
31	BA	1506	
31	CA	1506	
32	BE	256	
32	CE	256	
33	BF	239	
33	CF	239	
34	BG	208	
34	CG	208	
35	BH	162	
35	CH	162	
36	BI	101	
36	CI	101	
37	BJ	156	
37	CJ	156	
38	BK	138	
38	CK	138	
39	BL	128	
39	CL	128	
40	BM	105	

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Mol	Chain	Length	Quality of chain
40	CM	105	
41	BN	129	
41	CN	129	
42	BO	132	
42	CO	132	
43	BP	126	
43	CP	126	
44	BQ	61	
44	CQ	61	
45	BR	89	
45	CR	89	
46	BS	88	
46	CS	88	
47	BT	105	
47	CT	105	
48	BU	88	
48	CU	88	
49	BV	93	
49	CV	93	
50	BW	106	
50	CW	106	
51	BX	27	
51	CX	27	
52	BB	85	
52	BD	85	

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Mol	Chain	Length	Quality of chain
52	CB	85	
52	CD	85	
53	BC	77	
53	CC	77	
54	B1	16	
54	C1	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	CA	1641	-	-	-	X
55	MG	CA	1674	-	-	-	X
55	MG	DA	3076	-	-	-	X
55	MG	DA	3158	-	-	-	X
55	MG	DA	3199	-	-	-	X
55	MG	DA	3200	-	-	-	X
56	OHX	AA	3330	-	-	X	-
56	OHX	AA	3365	-	-	X	-
56	OHX	AA	3504	-	-	X	-
56	OHX	AA	3547	-	-	X	-
56	OHX	BA	1785	-	-	X	-
56	OHX	BA	1802	-	-	X	-
56	OHX	CA	1762	-	-	X	-
56	OHX	CA	1798	-	-	X	-
56	OHX	CC	108	-	-	X	-
56	OHX	D8	101	-	-	X	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 304031 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	DA	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
DA	168	U	-	insertion	GB AP008226.1
DA	654A	A	G	conflict	GB AP008226.1
DA	654E	C	G	conflict	GB AP008226.1
DA	654P	G	C	conflict	GB AP008226.1
DA	654T	A	C	conflict	GB AP008226.1
DA	1058	U	G	conflict	GB AP008226.1
DA	1080	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	DB	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	DD	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	DE	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	DF	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	DG	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	DH	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	DK	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	DM	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	DN	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	DO	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	DP	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	D0	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	DQ	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	DR	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	D1	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	D2	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	DS	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	DT	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	DU	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	DV	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	D3	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	DZ	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	DW	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	DX	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	D4	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	D5	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	D6	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	D7	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	D8	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	CA	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	CE	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	CF	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	CG	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	CH	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	CI	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	CJ	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	CK	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	CL	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	CM	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	CN	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	CO	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	CP	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	CQ	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	CR	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	CS	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	CT	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	CU	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	CV	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	CW	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	CX	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	CB	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			
52	CD	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	CC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			

- 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	C1	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	332	Total	Mg	0	0
			332	332		
55	AB	6	Total	Mg	0	0
			6	6		
55	AE	3	Total	Mg	0	0
			3	3		

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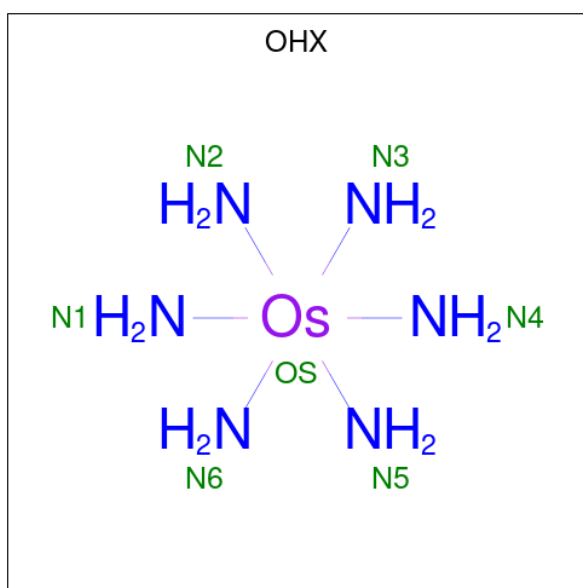
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AF	2	Total 2	Mg 2	0	0
55	AO	1	Total 1	Mg 1	0	0
55	A0	1	Total 1	Mg 1	0	0
55	A1	2	Total 2	Mg 2	0	0
55	A3	1	Total 1	Mg 1	0	0
55	A5	1	Total 1	Mg 1	0	0
55	A7	1	Total 1	Mg 1	0	0
55	BA	114	Total 114	Mg 114	0	0
55	BF	1	Total 1	Mg 1	0	0
55	BS	1	Total 1	Mg 1	0	0
55	BW	1	Total 1	Mg 1	0	0
55	BB	13	Total 13	Mg 13	0	0
55	BC	4	Total 4	Mg 4	0	0
55	BD	1	Total 1	Mg 1	0	0
55	B1	1	Total 1	Mg 1	0	0
55	CA	121	Total 121	Mg 121	0	0
55	CN	1	Total 1	Mg 1	0	0
55	CB	3	Total 3	Mg 3	0	0
55	CC	7	Total 7	Mg 7	0	0
55	C1	2	Total 2	Mg 2	0	0
55	DA	272	Total 272	Mg 272	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	DB	7	Total	Mg	0	0
			7	7		
55	DE	1	Total	Mg	0	0
			1	1		
55	D0	1	Total	Mg	0	0
			1	1		
55	D5	1	Total	Mg	0	0
			1	1		
55	D7	1	Total	Mg	0	0
			1	1		

- 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	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	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	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	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	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		
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		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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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
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56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		

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

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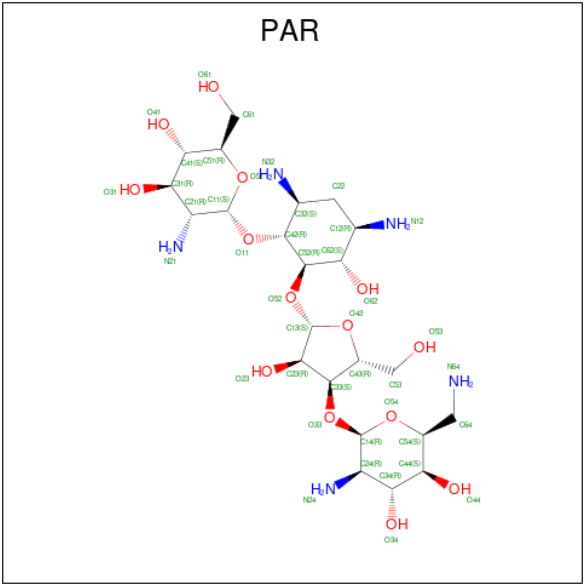
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	DB	1	Total	N	Os	0	0
			7	6	1		
56	DB	1	Total	N	Os	0	0
			7	6	1		
56	DF	1	Total	N	Os	0	0
			7	6	1		
56	DO	1	Total	N	Os	0	0
			7	6	1		
56	D1	1	Total	N	Os	0	0
			7	6	1		
56	D3	1	Total	N	Os	0	0
			7	6	1		
56	D5	1	Total	N	Os	0	0
			7	6	1		
56	D8	1	Total	N	Os	0	0
			7	6	1		

- Molecule 57 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	BA	1	Total	C	N	O	0	0
			42	23	5	14		
57	CA	1	Total	C	N	O	0	0
			42	23	5	14		

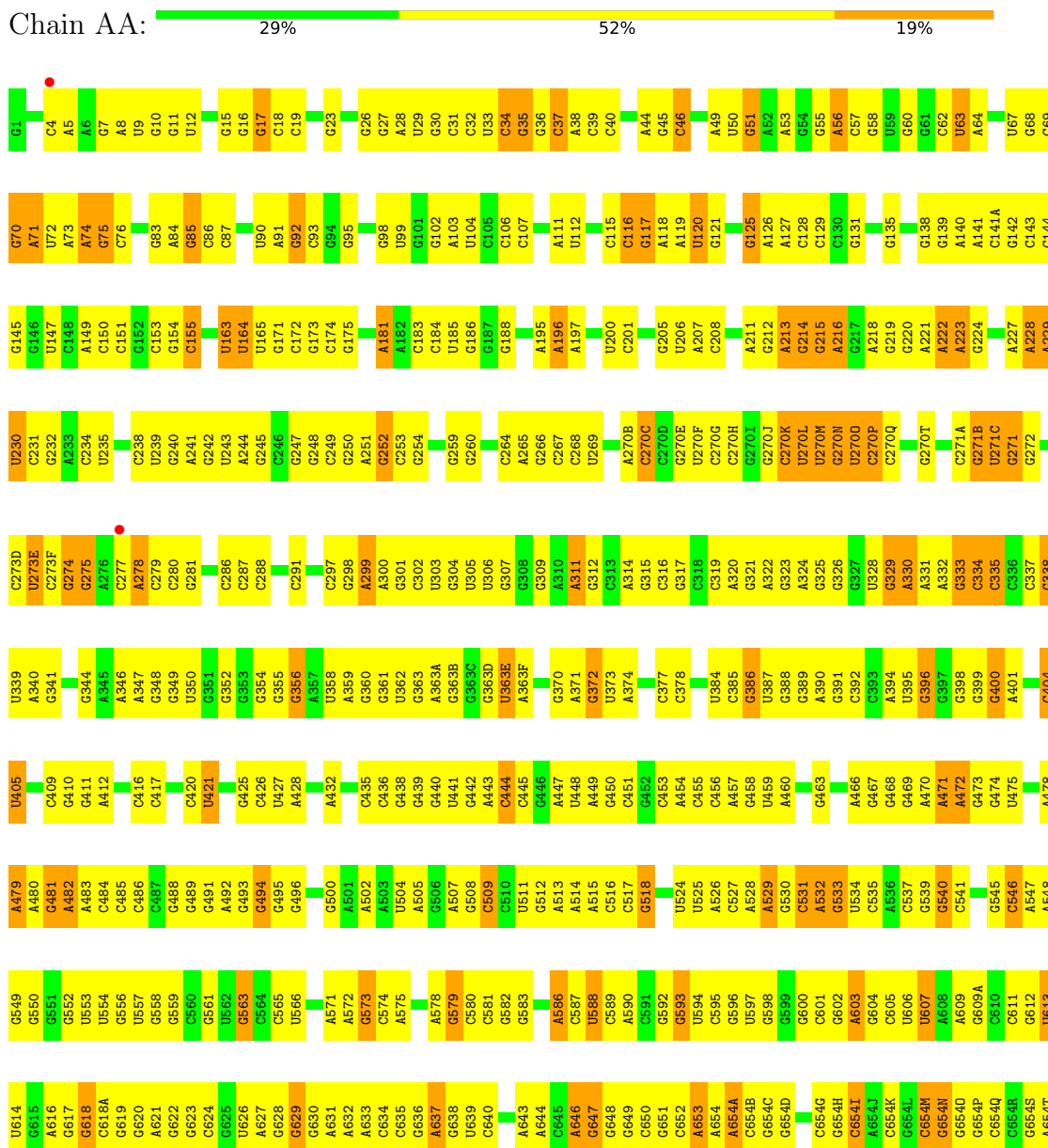
- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	BG	1	Total	Zn	0	0
			1	1		
58	BQ	1	Total	Zn	0	0
			1	1		
58	CG	1	Total	Zn	0	0
			1	1		
58	CQ	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

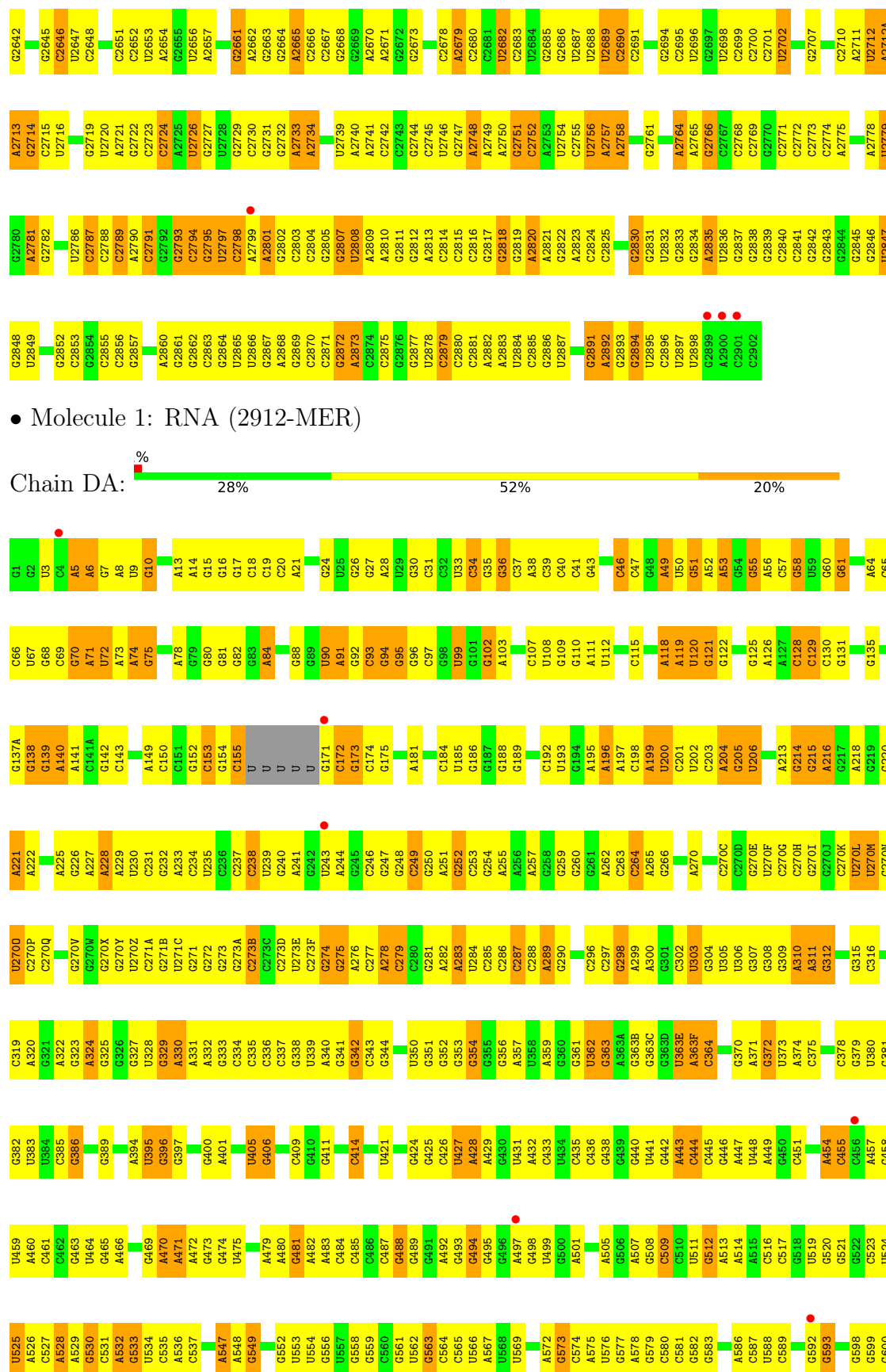
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



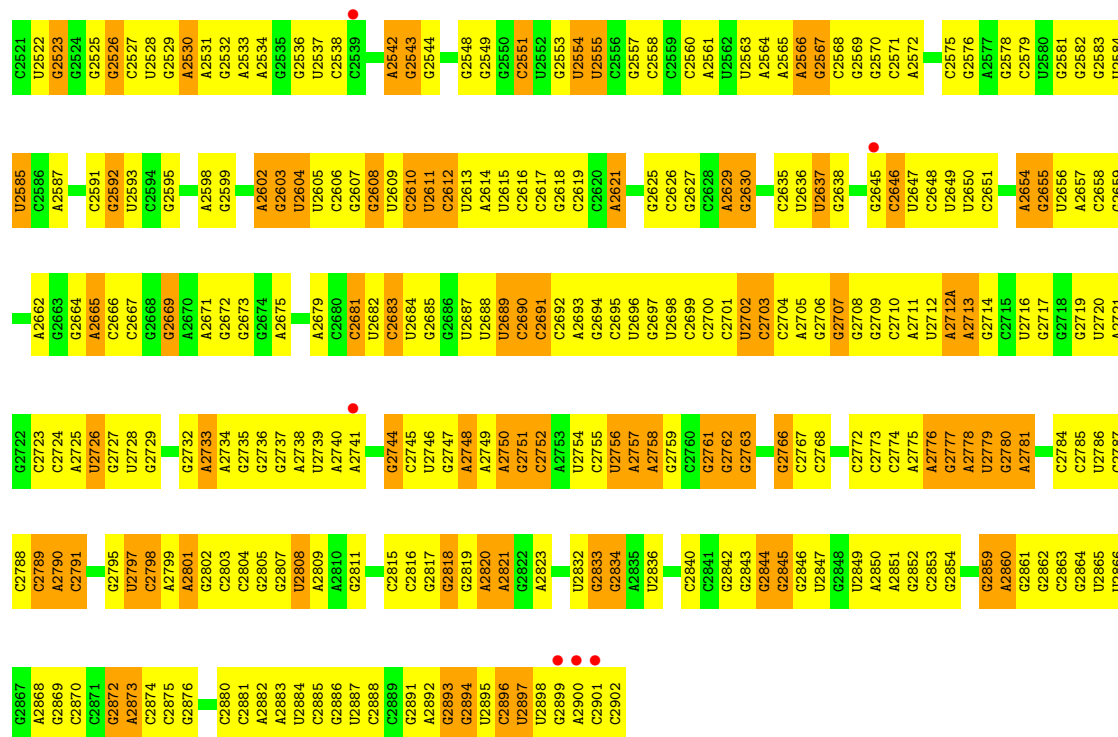
C1537	G1538	C1539	G1540	U1541	G1542	A1543	G1544	A1545	A1545A	G1546	C1547	C1548	C1549	C1550	G1551	G1552	A1553	A1554	G1555	C1556	A1557	G1558	A1559	G1560	G1561	A1566	A1567	G1568	A1569	C1575	U1576	C1577	U1578	A1579	A1580	G1581	C1582	A1583	C1585	A1586	A1587	C1588	G1591	C1592	G1593	G1594	G1595	C1598	C1599	C1600	C1601	U1602	A1603	C1604	C1605		
A1471	A1472	C1473	C1474	G1475	G1478	G1479	G1480	U1482	G1483	G1484	G1485	A1486	G1487	G1488	C1489	G1490	G1491	G1492	C1493	A1494	A1495	A1496	U1497	C1498	C1499	G1500	C1504	C1505	C1506	A1507	A1508	C1509	A1510	A1511	C1515	U1516	G1517	C1518	G1519	U1520	G1521	G1522	U1523	G1524	G1525	G1526	G1527	A1528	A1529	G1530	C1531	C1532	C1533	G1534	U1535	A1536	U1537
C1408	C1411	A1412	G1413	G1414	U1415	G1416	C1417	G1418	A1419	U1420	G1421	G1422	G1423	G1424	G1425	G1426	A1427	C1428	G1429	C1430	U1431	C1432	U1433	A1434	G1435	C1436	C1437	U1438	A1439	G1440	G1441	G1442	G1443	G1444	C1445	C1446	G1447	G1448	A1449	G1449A	C1450	U1454	G1455	C1458	G1459	A1460	G1461	C1464	G1465	C1466	C1467	C1468	U1469	G1470			
U1340	U1341	A1342	G1343	G1344	C1345	A1349	U1352	U1357	G1358	A1359	A1360	G1361	C1362	C1363	C1364	A1365	G1368	G1369	C1370	U1372	A1373	G1374	C1375	C1376	C1377	A1378	A1379	G1380	G1381	G1382	C1383	A1384	G1385	C1386	C1387	G1388	G1389	U1390	U1391	A1392	A1393	U1394	A1395	U1396	U1397	G1400	G1401	C1402	C1403	C1404	U1405	U1406	C1407				
U1276	G1277	A1278	G1279	G1280	G1281	U1282	G1283	A1284	G1285	A1286	U1287	U1288	C1289	C1290	C1291	C1292	C1293	U1294	C1295	G1296	C1297	C1298	G1299	U1300	A1301	A1302	C1306	U1307	U1312	U1313	C1314	C1315	U1316	U1317	U1255	G1256	C1261	U1262	U1263	G1264	A1265	G1266	U1267	A1268	A1269	G1270	G1271	A1272	A1273	A1274	A1275						
C1140	U1141	U1142	A1142A	A1143	G1144	C1145	C1146	A1147	A1148	G1149	G1150	G1151	C1152	C1153	G1154	A1155	A1156	G1157	C1158	U1159	G1160	C1161	G1162	G1163	G1164	U1165	U1166	U1167	G1168	G1169	G1170	G1171	A1173	A1174	U1175	G1176	A1177	C1178	C1179	C1180	C1181	A1182	G1183	G1184	C1185	G1186	G1187	U1188	A1189	A1194	G1195	C1196	G1197	U1198	C1201	G1203	
C1072	A1073	C1075	A1076	C1077	A1077	U1078	C1079	U1080	A1081	U1082	U1083	A1084	A1085	A1086	G1087	A1088	G1089	U1090	G1091	C1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	G1115	C1116	G1117	G1122	A1126	A1127	U1130	G1131	U1065	U1066	U1067	G1068	A1069	G1070	
C1006	A1010	G1011	U1012	C1013	U1014	U1015	G1016	G1017	C1018	U1019	A1020	A1021	A1022	U1023	G1024	G1025	U1026	A1027	A1028	G1029	G1030	U1033	G1036	G1037	C1041	C1042	C1043	G1044	A1045	A1046	G1047	A1048	C1049	A1050	G1051	C1052	C1053	A1054	G1055	G1056	A1057	U1058	G1059	U1060	U1061	G1062	G1063	C1064	U1065	U1066	A1000	A1001	G1002	G1003	C1004	C1005	
G938	A941	G942	U943	G944	A945	G946	G947	G948	G956	A957	U958	A959	A960	C961	G962	U963	G966	C967	G968	U969	C970	C971	G972	G974	G975	G978	G979	A981	C982	A983	A984	C985	C986	G987	A988	G989	A990	C991	G992	G993	C994	C995	A996	G997	C998	U999	A1000	A1001	G1002	G1003	C1004	C1005					
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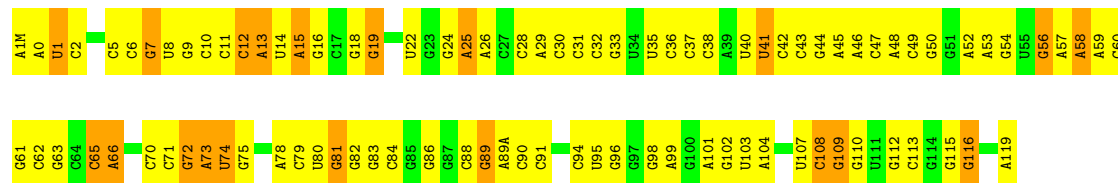
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G1380	G1381	G1382	G1383	G1384	G1385	C1386	C1387	G1388	G1389	A1392	A1393	U1394	C1395	U1396	U1397	C1398	C1399	C1400	C1404	U1405	C1406	C1407	C1408	C1409	C1415	U1416	C1417	C1418	A1419	U1420	C1421	C1422	C1423	C1424	C1425	G1426	A1427	C1428	C1429	C1430	U1431	C1432	U1433	A1434	C1435	C1436	C1437	C1438	A1439	C1506	A1507	C1508	C1509	A1510	A1511	C1445			

WORLDWIDE
PDB
PROTEIN DATA BANK



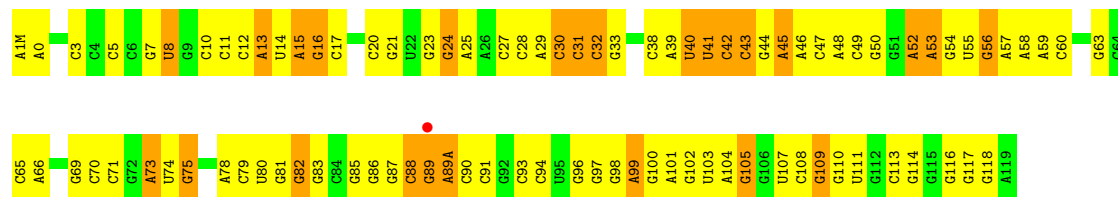
• Molecule 2: 5S RIBOSOMAL RNA

Chain AB: 24% 60% 16%



• Molecule 2: 5S RIBOSOMAL RNA

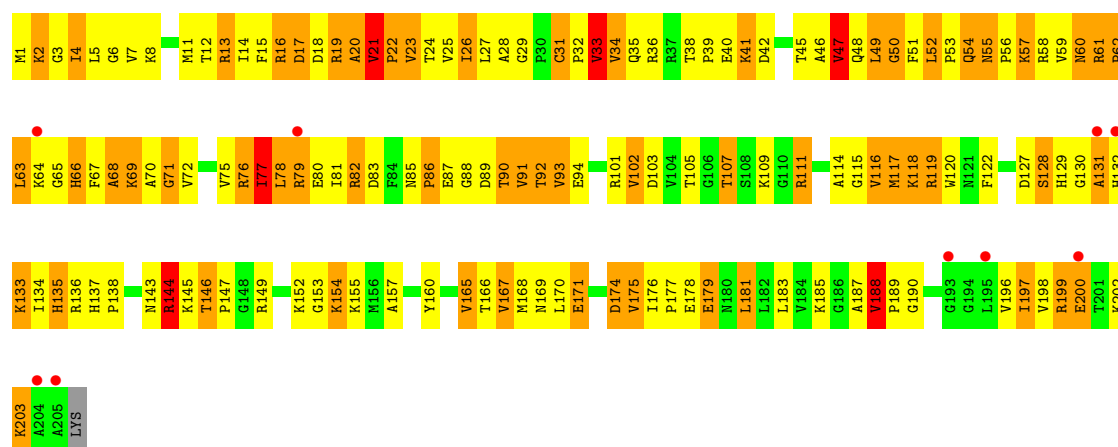
Chain DB: 24% 56% 20%



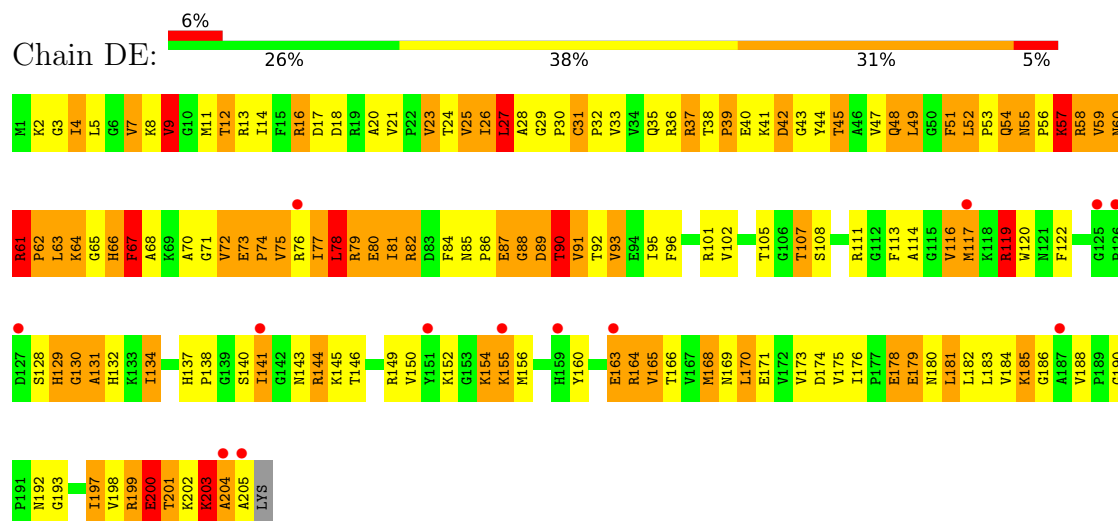
• Molecule 3: 50S ribosomal protein L2

Chain AD: 4% 33% 44% 16% 6%

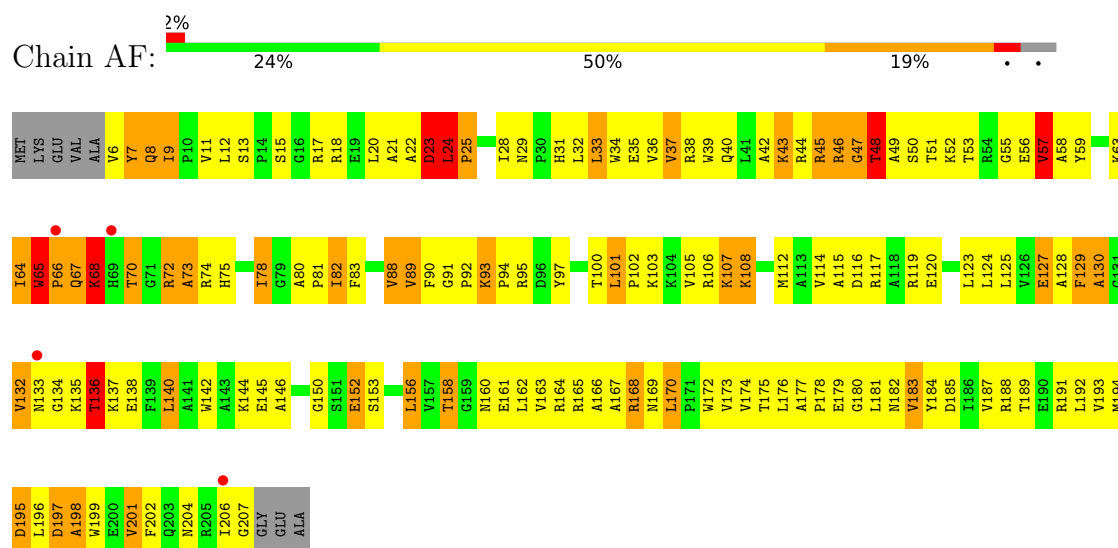




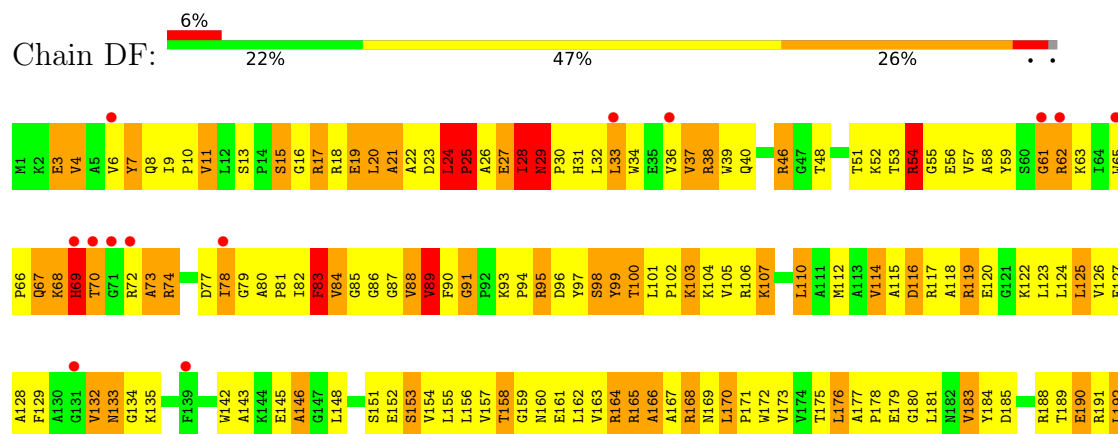
• Molecule 4: 50S ribosomal protein L3



• Molecule 5: 50S ribosomal protein L4

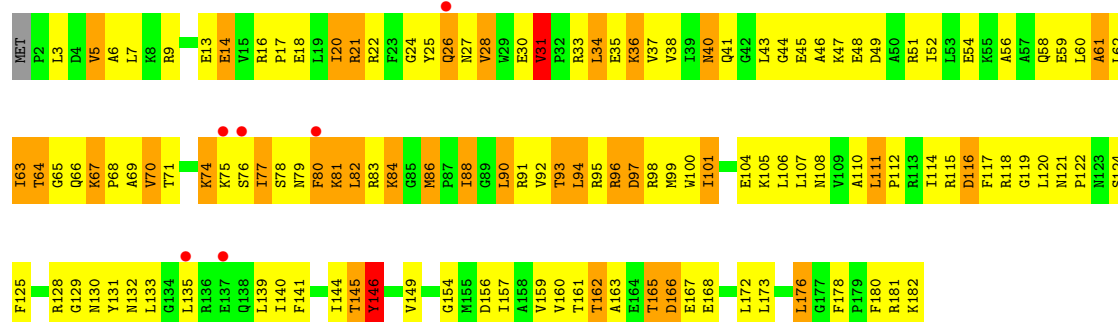


• Molecule 5: 50S ribosomal protein L4

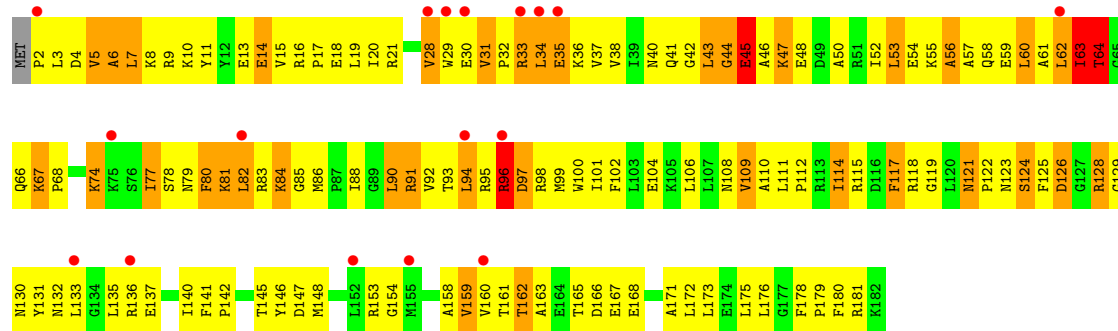




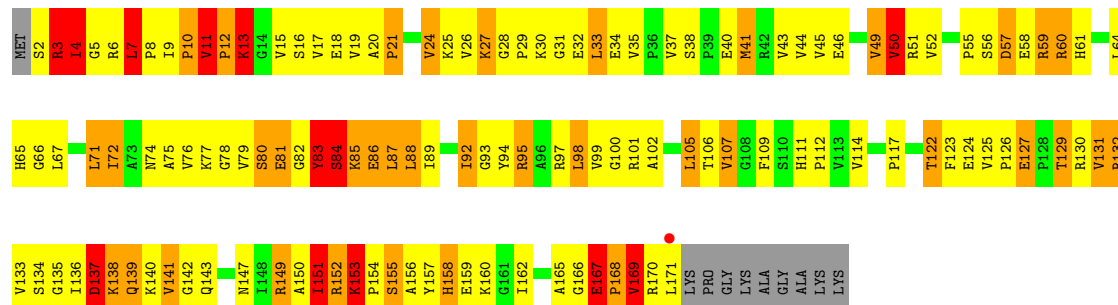
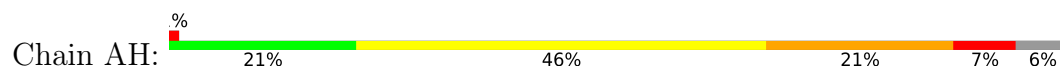
• Molecule 6: 50S ribosomal protein L5



• Molecule 6: 50S ribosomal protein L5

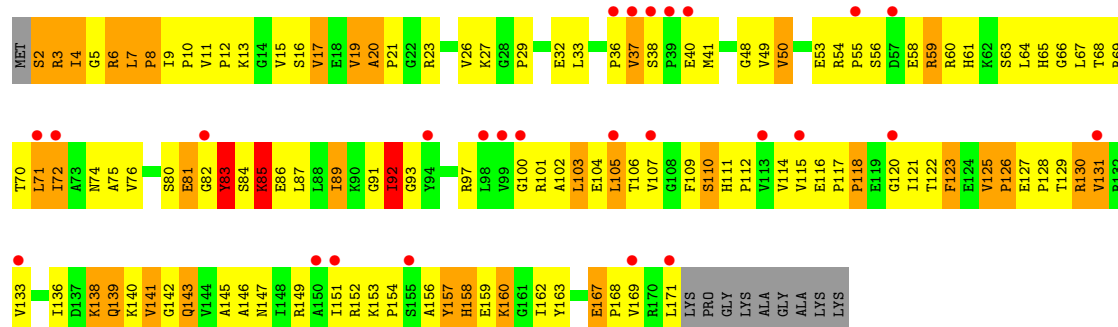


• Molecule 7: 50S ribosomal protein L6

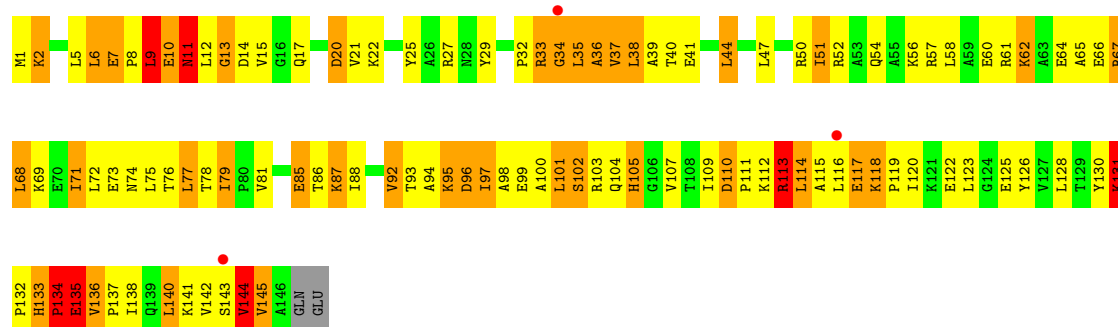


• Molecule 7: 50S ribosomal protein L6

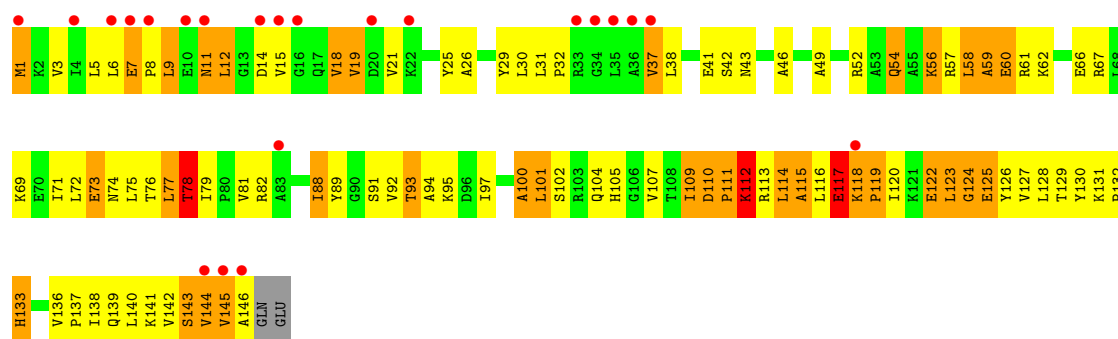




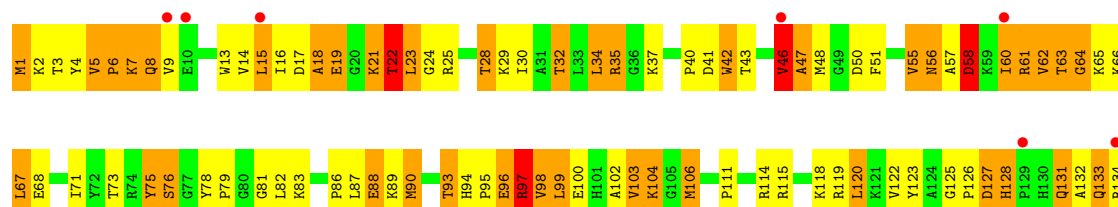
• Molecule 8: 50S ribosomal protein L9

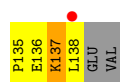


• Molecule 8: 50S ribosomal protein L9

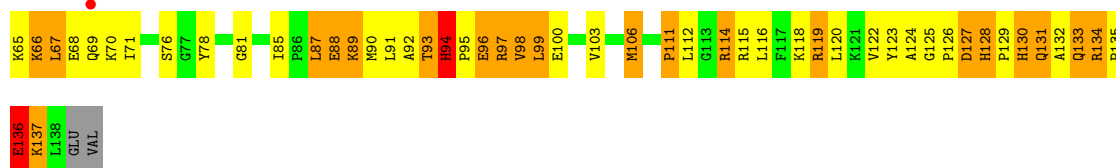
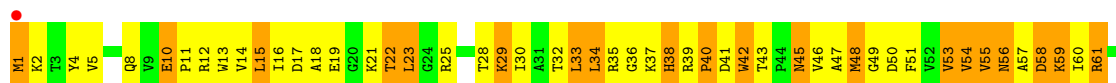


• Molecule 9: 50S ribosomal protein L13

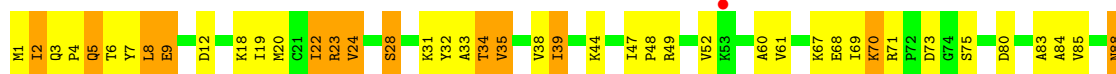




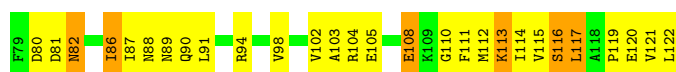
• Molecule 9: 50S ribosomal protein L13



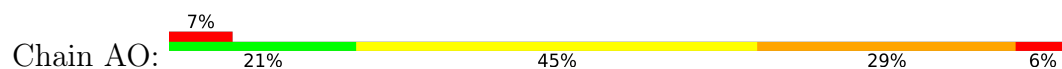
• Molecule 10: 50S ribosomal protein L14

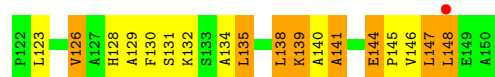


• Molecule 10: 50S ribosomal protein L14

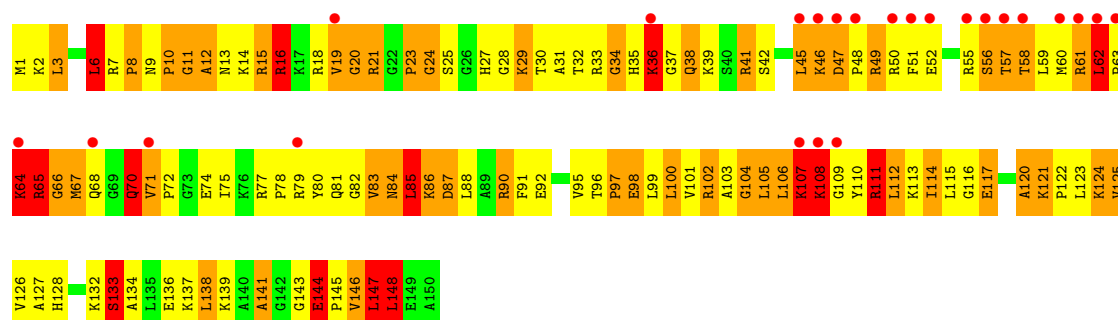
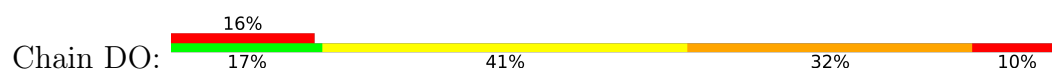


• Molecule 11: 50S ribosomal protein L15

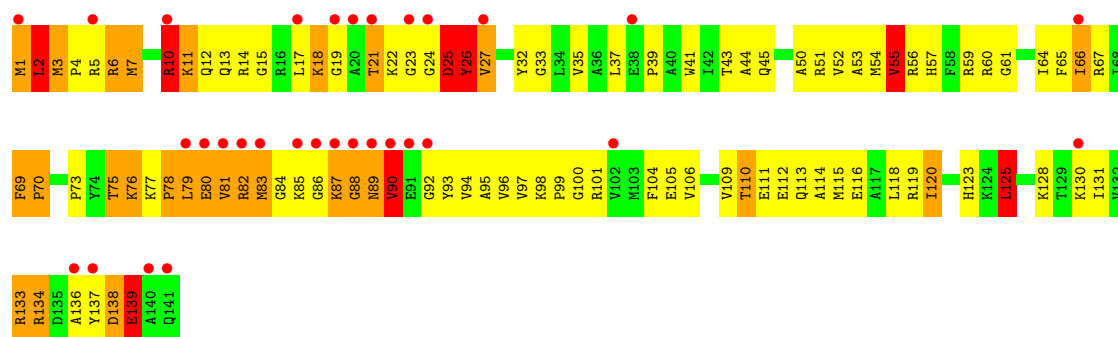




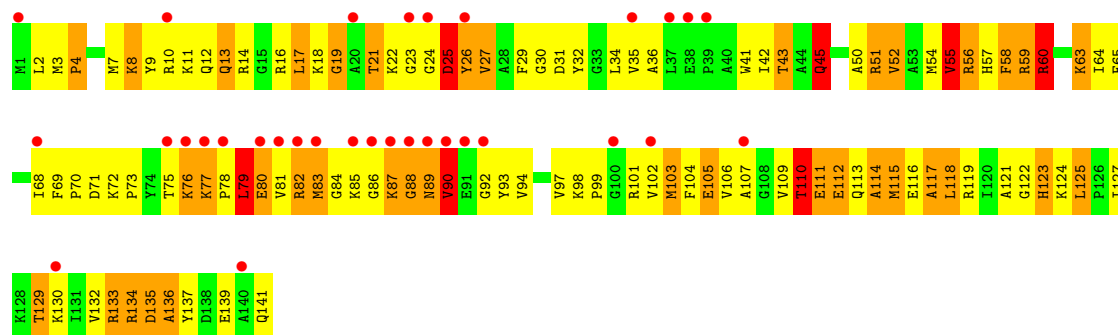
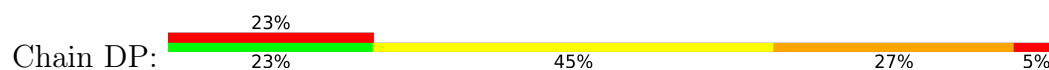
• Molecule 11: 50S ribosomal protein L15



• Molecule 12: 50S ribosomal protein L16

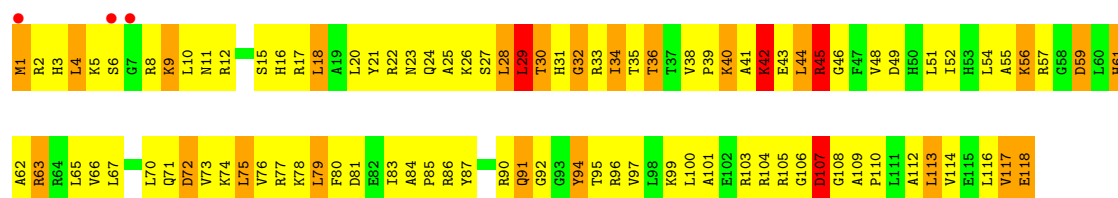


• Molecule 12: 50S ribosomal protein L16

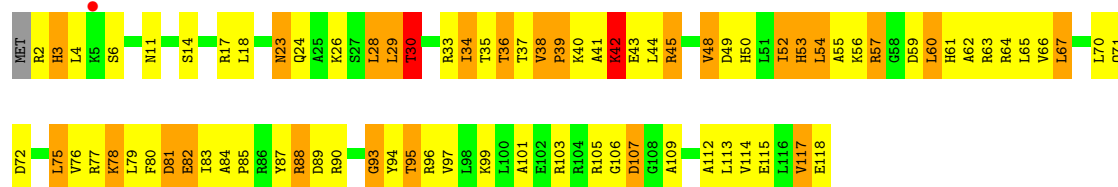


• Molecule 13: 50S ribosomal protein L17

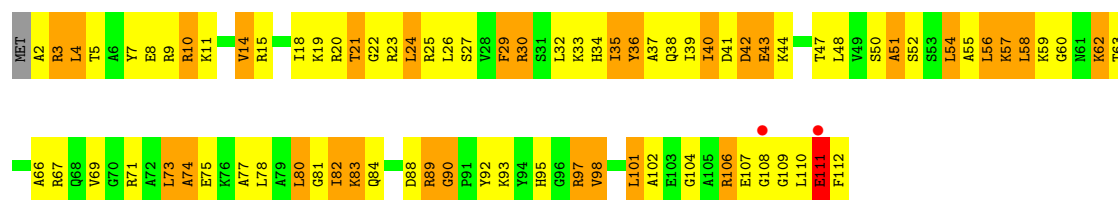




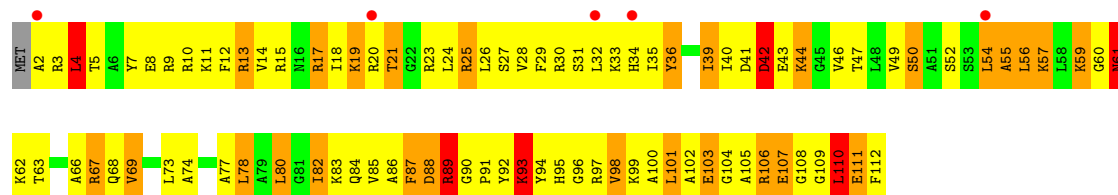
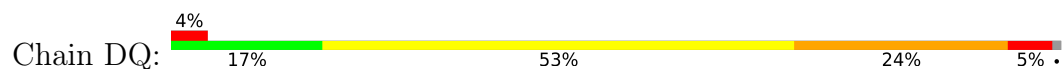
• Molecule 13: 50S ribosomal protein L17



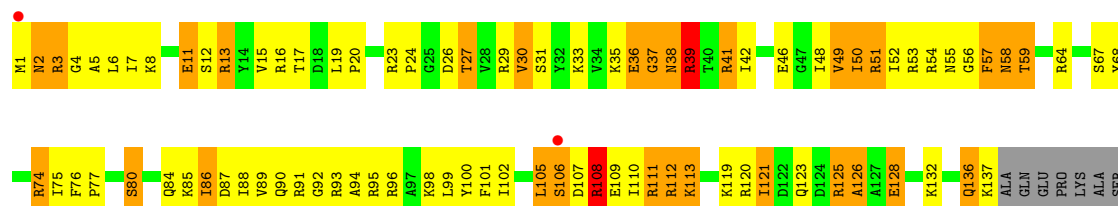
• Molecule 14: 50S ribosomal protein L18



• Molecule 14: 50S ribosomal protein L18

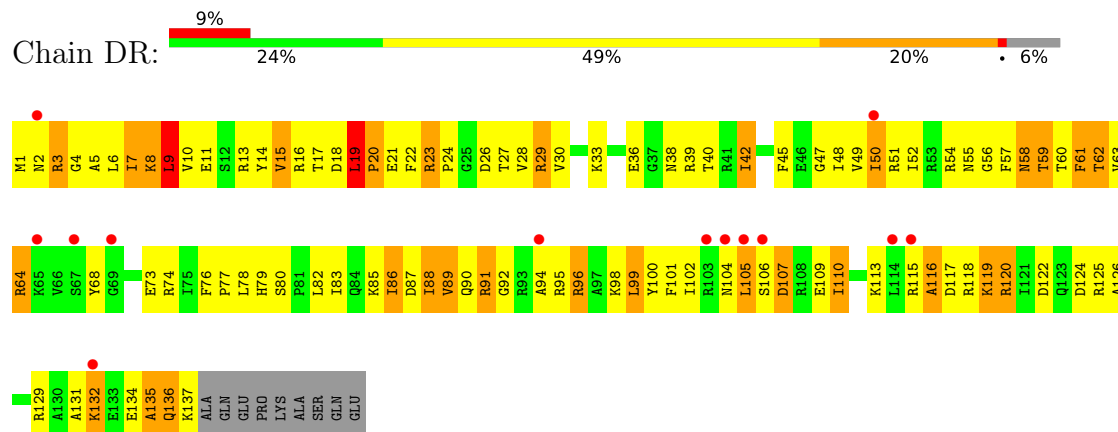


• Molecule 15: 50S ribosomal protein L19

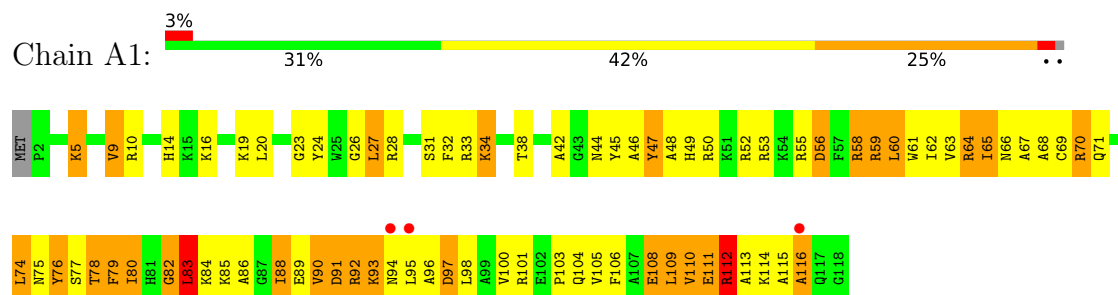


GLN
GLU

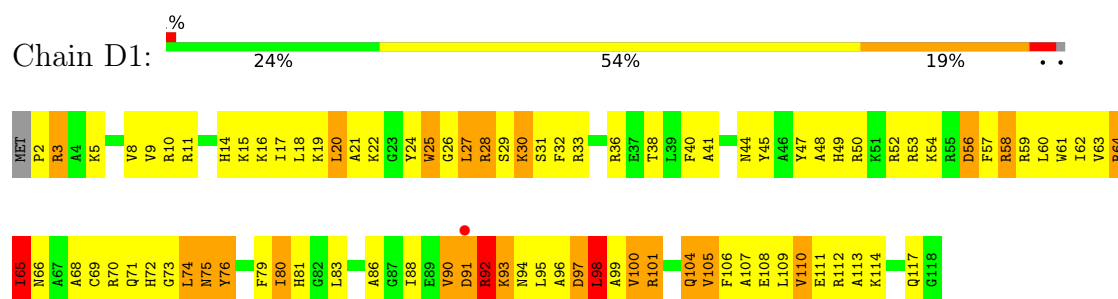
- Molecule 15: 50S ribosomal protein L19



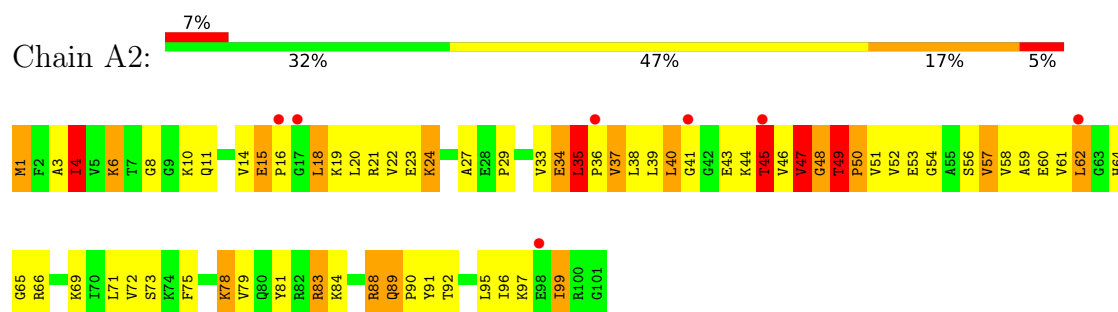
- Molecule 16: 50S ribosomal protein L20



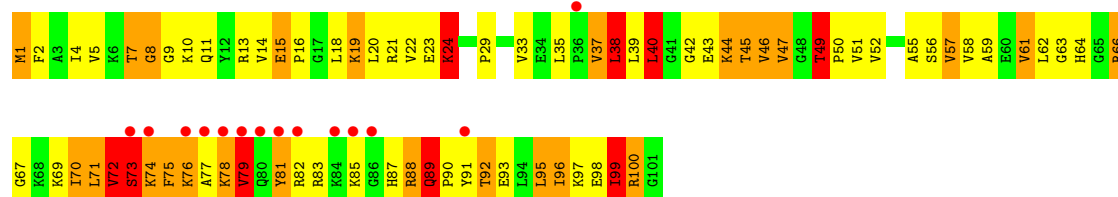
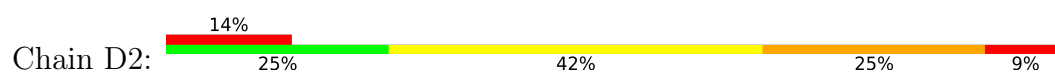
- Molecule 16: 50S ribosomal protein L20



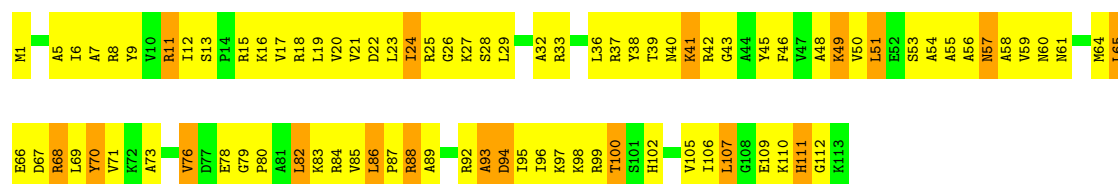
- Molecule 17: 50S ribosomal protein L21



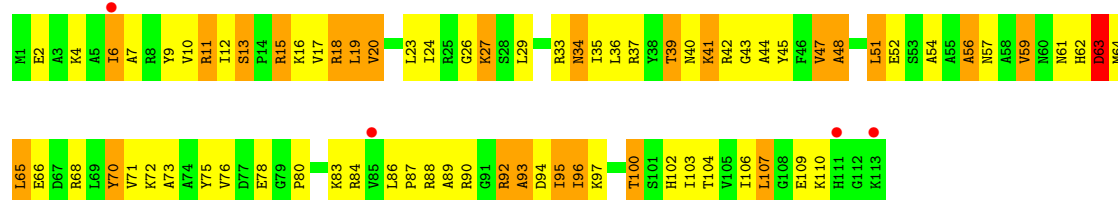
- Molecule 17: 50S ribosomal protein L21



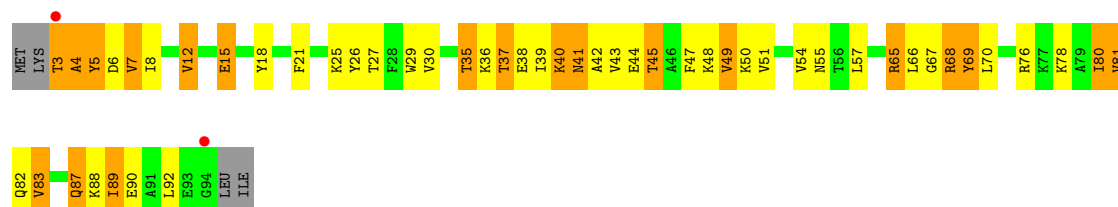
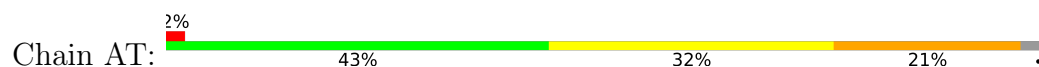
• Molecule 18: 50S ribosomal protein L22



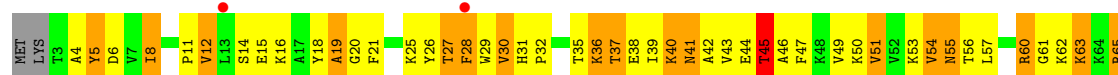
• Molecule 18: 50S ribosomal protein L22



• Molecule 19: 50S ribosomal protein L23

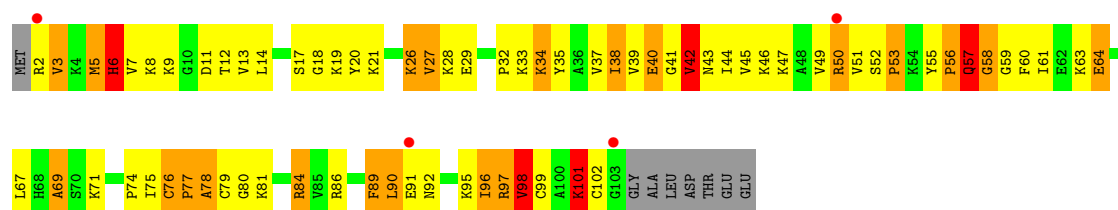


• Molecule 19: 50S ribosomal protein L23

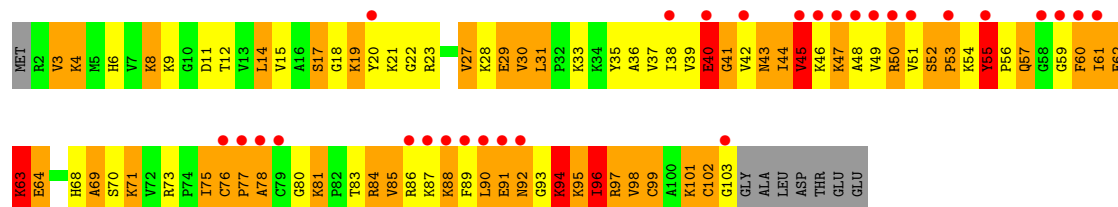




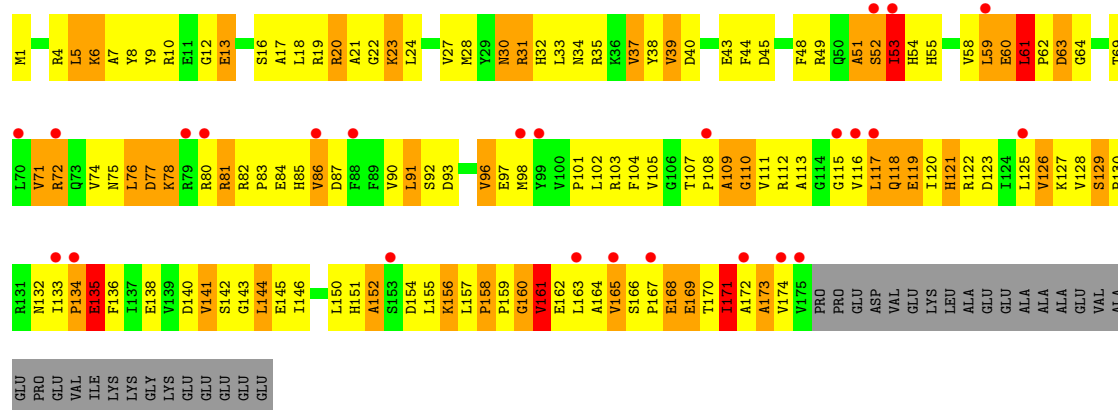
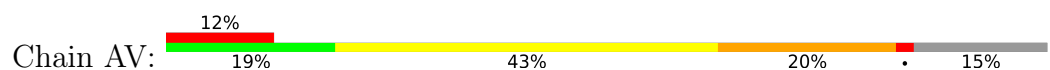
• Molecule 20: 50S ribosomal protein L24



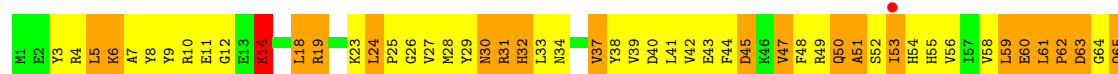
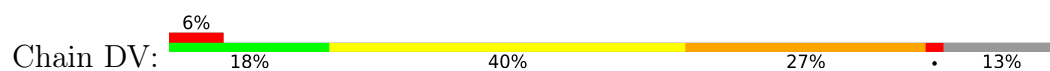
• Molecule 20: 50S ribosomal protein L24

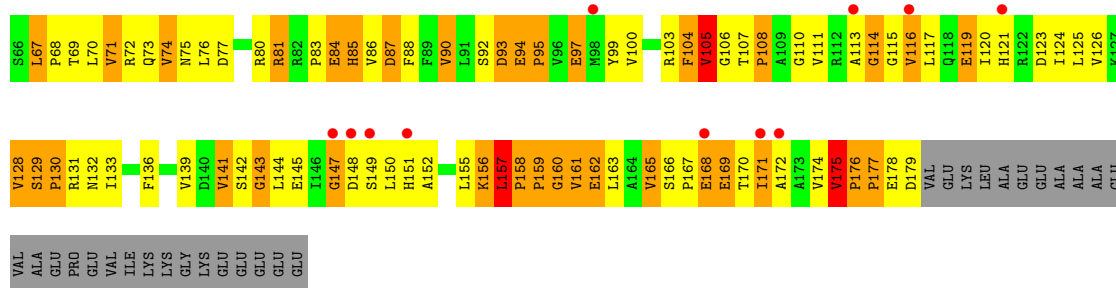


• Molecule 21: 50S ribosomal protein L25



• Molecule 21: 50S ribosomal protein L25

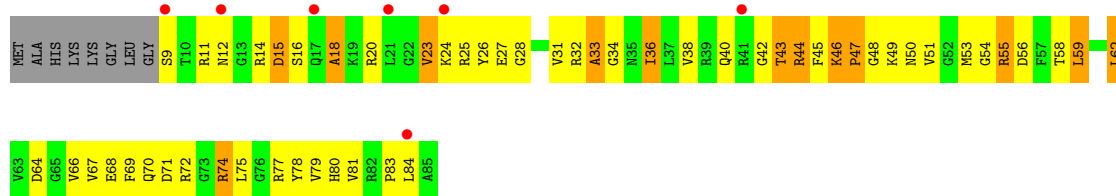




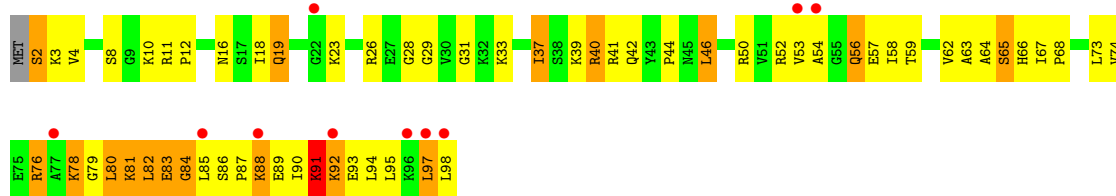
- Molecule 22: 50S ribosomal protein L27



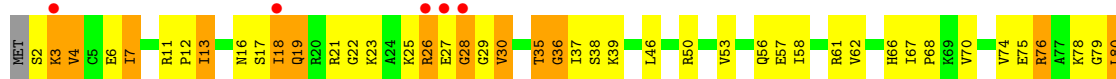
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28

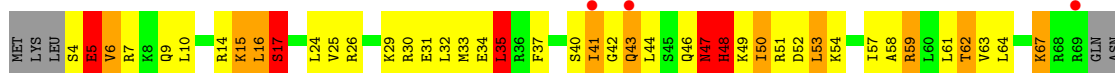


- Molecule 23: 50S ribosomal protein L28

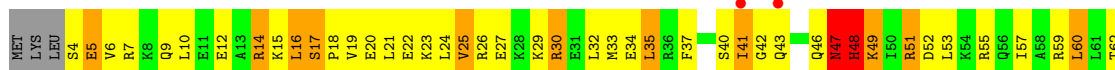




- Molecule 24: 50S ribosomal protein L29



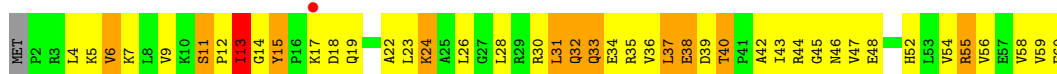
- Molecule 24: 50S ribosomal protein L29



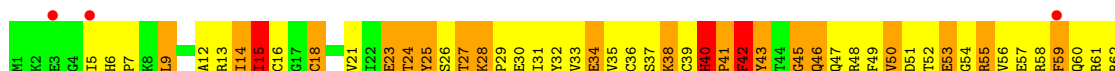
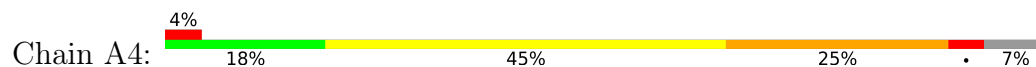
- Molecule 25: 50S ribosomal protein L30



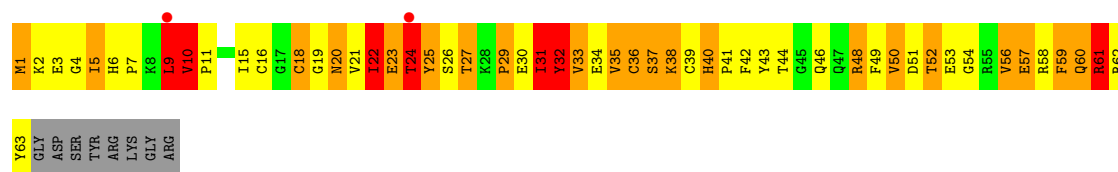
- Molecule 25: 50S ribosomal protein L30



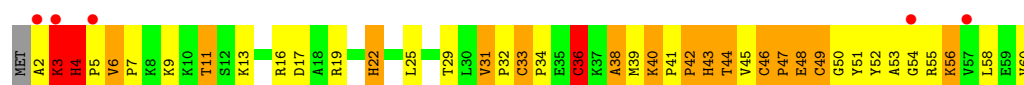
- Molecule 26: 50S ribosomal protein L31



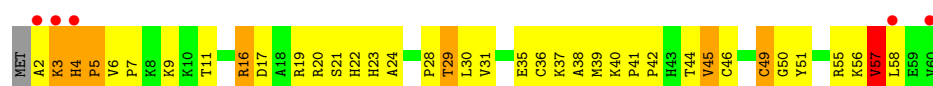
- Molecule 26: 50S ribosomal protein L31



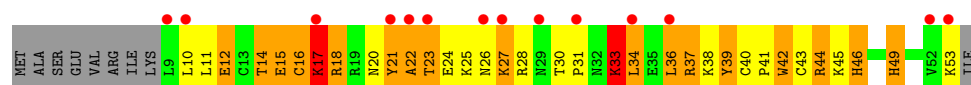
- Molecule 27: 50S ribosomal protein L32



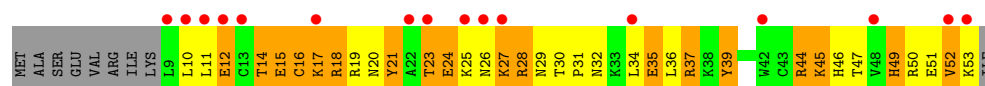
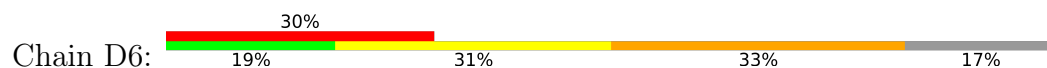
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34

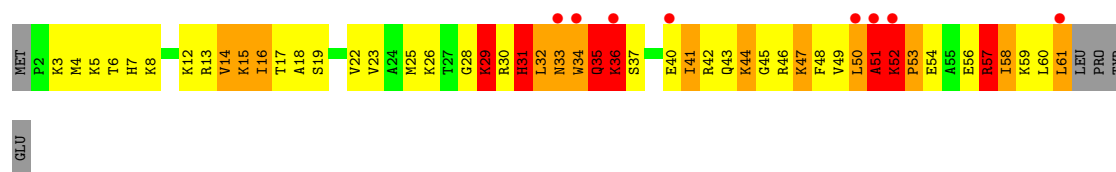
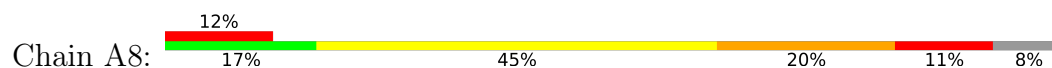


- Molecule 29: 50S ribosomal protein L34

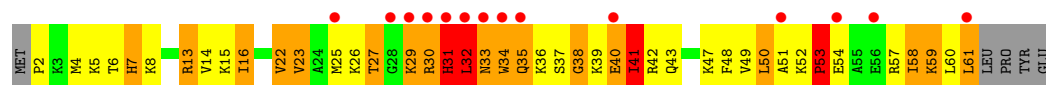
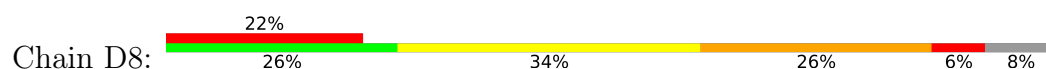




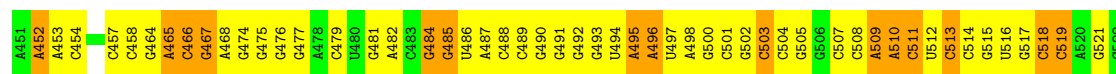
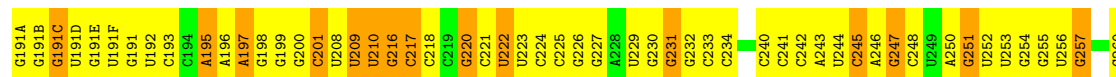
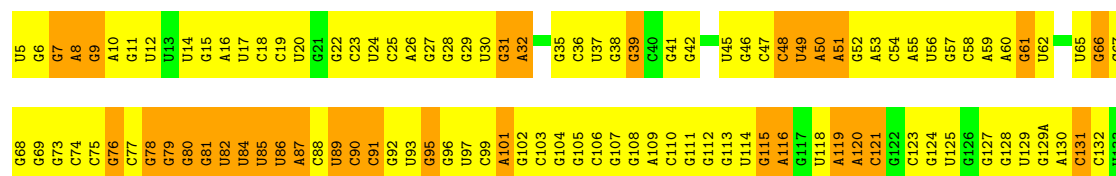
- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35

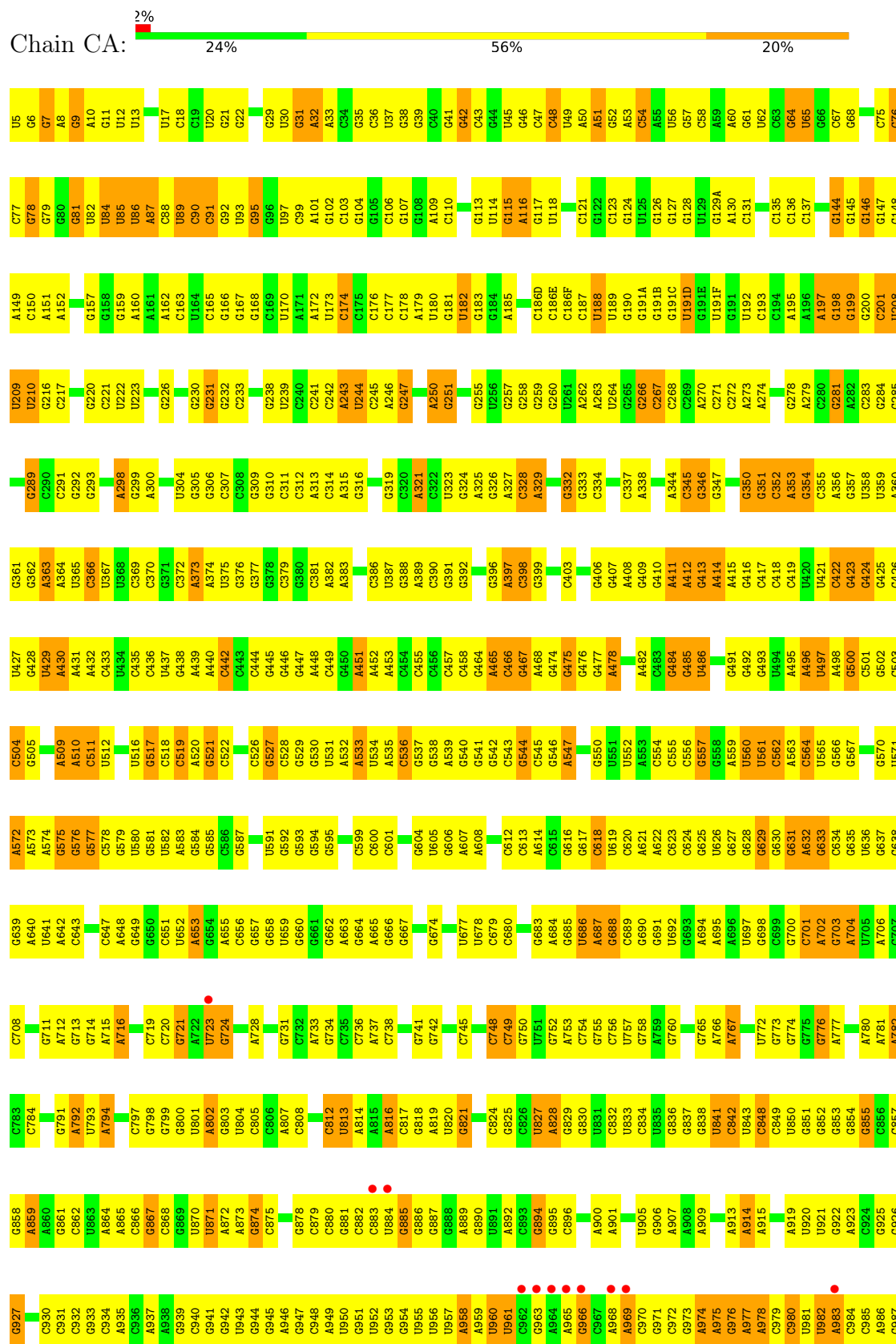


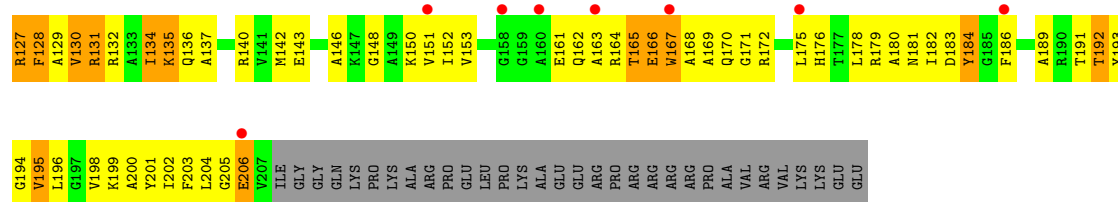
- Molecule 31: 16S ribosomal RNA



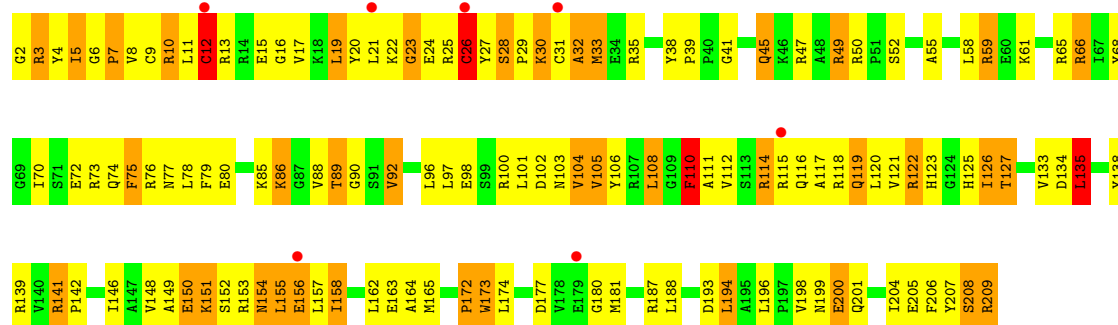
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G1379	C1320	G1379	C1259	G1197	U1135	C1076	A1016	U952	C877	U952	G730	G659	C525
U1380	C1321	U1380	A1261	G1198	C1136	G1077	G1017	G953	C880	G809	G731	G660	G594
C1322	G1323	C1322	G1262	C1200	G1138	U1078	C1018	U955	G881	C810	C735	A663	G595
G1386	G1387	G1323	C1263	A1201	G1139	U1079	C1019	U956	C882	C811	C736	A664	C596
G1388	A1324	C1324	C1264	G1202	C1140	A1080	U1020	U957	C883	C812	A737	A665	G597
G1389	C1325	G1388	G1265	C1203	C1141	G1081	G1021	A958	U884	U813	C738	A532	U580
U1390	C1326	C1326	G1266	A1204	G1142	G1082	G1022	A959	G885	A814	C739	A533	G589
G1438	C1327	G1438	C1267	U1205	G1143	U1083	G1023	U960	A889	A815	U740	C600	C600
U1391	C1328	C1328	A1268	G1206	G1144	G1084	G1024	U961	U889	A816	G741	G670	A601
C1392	A1329	A1329	A1269	G1207	C1145	U1085	U1025	C962	G890	C817	G742	G671	C602
U1393	C1330	U1330	C1270	U1211	A1146	U1086	G1026	A964	U891	A818	C745	U672	U603
A1394	G1331	G1331	C1271	U1212	C1147	G1087	C1027	G963	A892	A819	A746	G673	G603
C1395	A1332	A1332	G1272	U1213	U1148	G1088	G1028	A965	C893	U820	G747	A674	U605
A1396	C1333	C1333	G1273	C1213	C1149	G1089	C1028A	G966	G894	G821	C748	A675	G606
C1397	G1334	G1334	G1274	G1214	U1150	U1090	C1028B	C967	A900	G825	C749	A676	G610
A1398	C1335	C1335	A1275	G1215	A1151	U1091	G1030	A968	A901	C826	G750	U677	A611
C1399	C1336	C1336	G1276	C1216	A1152	A1092	C1031	A969	G902	U827	G751	G682	C615
A1400	G1401	G1337	C1277	C1217	C1153	A1093	G1031	G971	G903	G830	G752	G685	G616
U1500	G1401	G1338	U1278	G1218	G1154	G1094	A1032	A977	C904	G829	A753	U686	U619
C1501	C1402	A1339	A1279	U1219	G1155	U1095	G1032A	A978	U905	G830	C754	A687	C620
A1502	C1403	A1340	A1280	G1220	G1156	C1096	G1032B	A979	G906	G831	G755	C688	A621
A1503	U1341	U1341	A1281	G1221	A1157	C1097	G1033	A974	A909	U833	C756	G689	C622
G1504	C1342	G1342	C1282	G1222	C1158	C1098	G1034	A975	C910	U833	G757	G690	A622
G1505	G1343	G1343	G1283	C1223	U1159	G1099	A1035	G976	A914	G837	G758	G691	C623
U1506	C1344	U1344	A1284	G1224	C1160	C1100	C1036	A978	U911	U835	A759	U692	C624
A1507	U1415	U1345	A1285	A1225	G1161	A1101	C1037	A978	C912	G836	C762	G693	C625
G1508	G1416	A1346	A1286	C1226	C1162	A1102	C1038	C979	A918	G837	A766	G694	C626
U1509	G1417	U1347	A1287	A1227	G1163	A1103	C1039	C980	U919	U841	A767	C695	U626
U1510	A1418	U1348	A1288	C1228	C1164	G1104	U1040	U981	C926	G854	C765	G637	G557
G1511	G1419	A1349	A1289	A1229	C1165	A1105	A1041	U982	U921	U843	A768	C699	G629
U1512	A1350	A1350	G1290	C1230	G1166	G1106	G1042	A983	U920	U843	C769	G700	U619
C1513	U1351	U1351	G1291	G1231	A1167	C1107	G1047	C984	U920	C849	A768	C701	C630
A1514	G1422	C1352	U1292	U1232	A1169	G1108	U1047	G988	U921	C849	C769	G709	U619
C1515	C1423	G1353	G1293	C1233	A1170	C1109	G1048	C989	G922	C849	A768	G710	C631
G1517	U1425	C1354	C1294	U1234	G1171	A1110	U1049	C989	G922	C849	C769	G711	C632
A1518	C1355	G1355	G1295	C1235	C1172	A1111	U1052	C990	A923	G851	G771	A712	A563
U1519	A1428	G1356	C1296	A1236	G1173	C1112	U1052	U991	C924	G852	G772	G713	C633
G1520	C1429	A1357	C1297	G1237	G1174	C1113	G1053	U992	C924	G853	G773	A704	C634
G1521	C1430	U1358	C1298	A1238	C1175	C1114	C1054	G993	G926	G854	G774	U705	G635
U1522	G1431	C1359	A1299	A1239	A1176	C1115	A1055	G993	G927	G855	G775	A706	U636
G1523	A1360	C1360	G1300	U1240	G1177	C1116	U1056	A996	U921	C856	G776	G637	G637
C1524	C1361	C1361	U1301	G1241	G1178	G1117	G1057	U997	C934	C857	G777	G709	G638
G1525	A1434	G1362	U1302	C1242	A1179	C1118	G1058	A935	A935	C857	G778	G710	C639
U1526	G1435	C1362A	C1303	C1243	A1180	C1119	C1059	C998A	C936	A859	A781	A712	G643
G1527	A1363	A1363	G1304	C1244	G1181	G1120	C1060	U999	A937	A860	A782	G713	C644
U1528	C1364	U1364	G1305	A1245	G1182	U1121	G1061	A1000	A938	G861	G714	G713	C645
G1529	C1365	C1365	A1306	C1246	A1183	U1122	U1062	G1001	G939	C862	U789	A715	U646
G	G1442	C1366	U1307	U1247	C1247	A1123	C1063	G1002	C940	U863	A790	C647	C647
A	G1443	C1367	U1308	A1248	G1186	G1124	G1064	A1003	G941	C864	G791	C719	A648
U	A1446	G1368	G1309	C1249	G1187	U1125	U1065	A1004	G942	A864	A792	C720	U580
C	C1449	C1369	G1310	A1250	A1188	U1126	C1066	A1005	U943	U943	U793	G721	G581
U1450	U1450	G1370	G1311	A1251	C1189	U1127	A1067	C1006	G944	G869	A794	U722	C651
A1451	C1371	G1312	C1312	A1252	G1190	C1128	G1068	C1007	G945	U870	C795	U723	U582
C1452	U1372	G1313	U1313	G1253	A1191	C1129	C1069	C1008	A946	U871	G796	U724	A583
G1453	G1373	C1314	C1314	C1254	C1192	A1130	U1070	G1009	G947	A872	C797	G725	G584
U1454	A1374	U1374	U1315	G1255	G1193	G1131	C1071	G1011	C948	A873	G798	C726	G585
G1455	G1454	A1375	C1316	A1256	U1194	C1132	C1072	G1011	A940	C874	G799	C727	C656

● Molecule 31: 16S ribosomal RNA

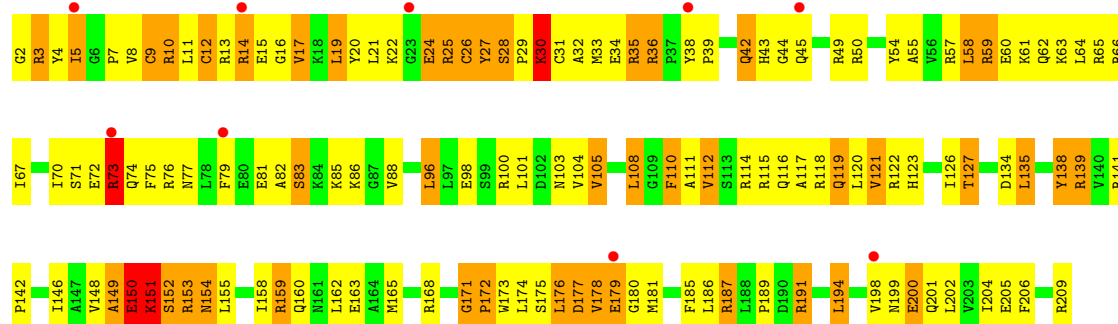




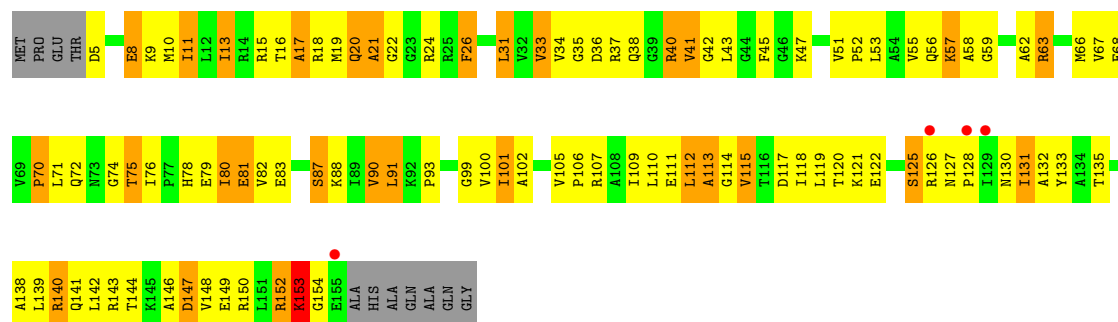
• Molecule 34: 30S RIBOSOMAL PROTEIN S4



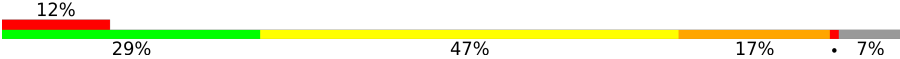
• Molecule 34: 30S RIBOSOMAL PROTEIN S4

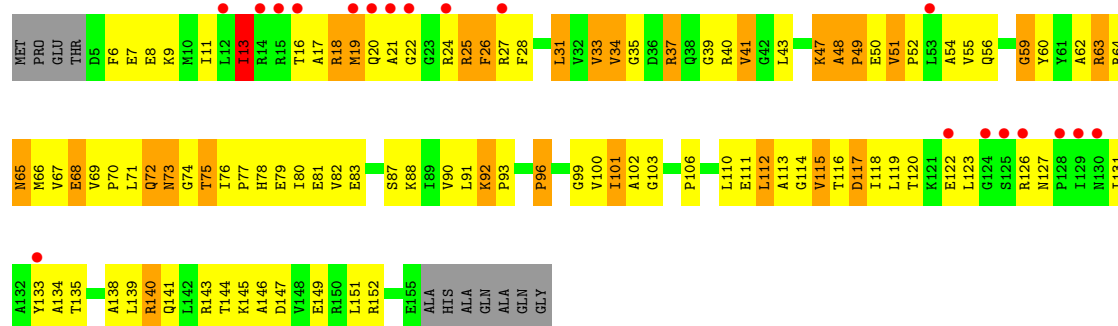


• Molecule 35: 30S RIBOSOMAL PROTEIN S5



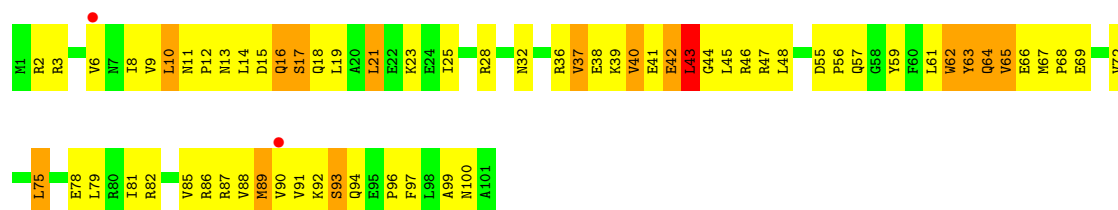
• Molecule 35: 30S RIBOSOMAL PROTEIN S5

Chain CH: 



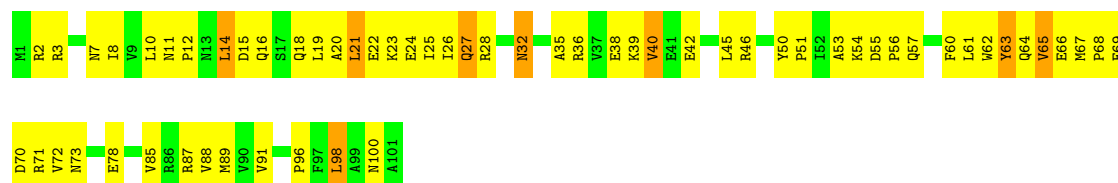
• Molecule 36: 30S RIBOSOMAL PROTEIN S6

Chain BI: 



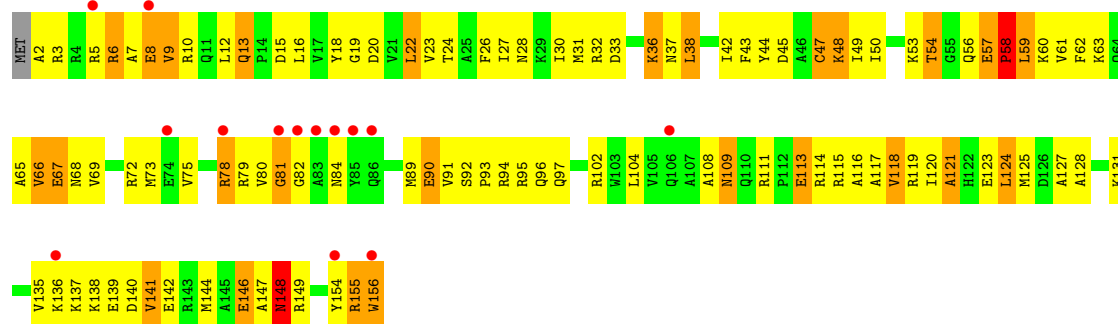
• Molecule 36: 30S RIBOSOMAL PROTEIN S6

Chain CI: 

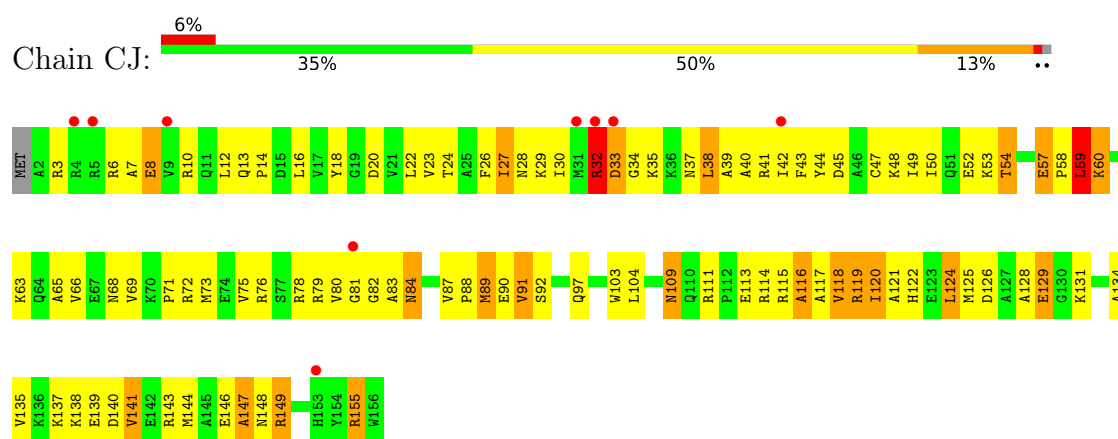


• Molecule 37: 30S RIBOSOMAL PROTEIN S7

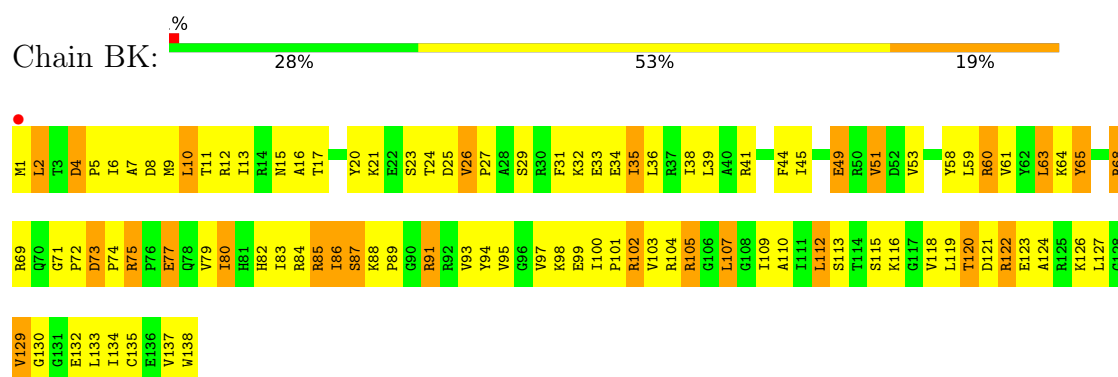
Chain BJ: 



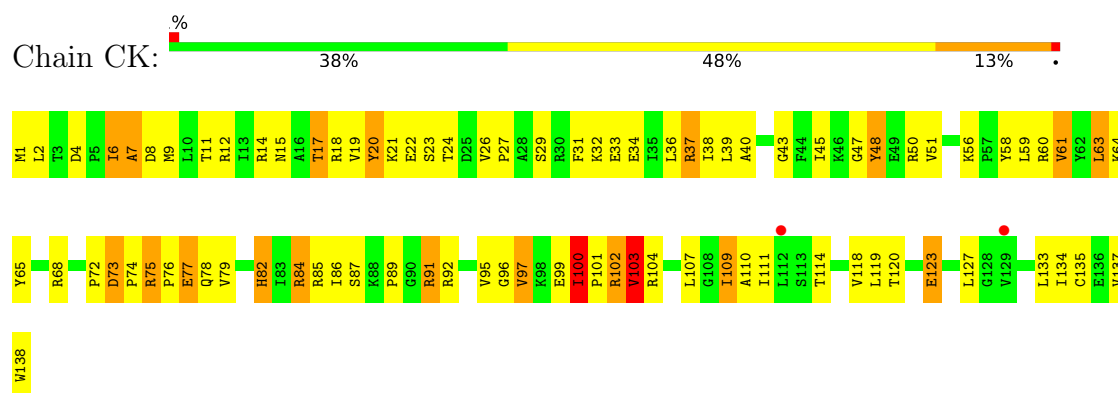
• Molecule 37: 30S RIBOSOMAL PROTEIN S7



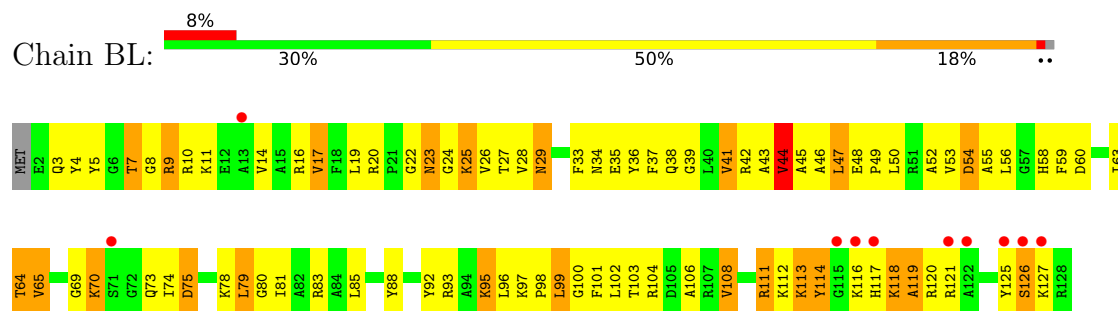
- Molecule 38: 30S RIBOSOMAL PROTEIN S8



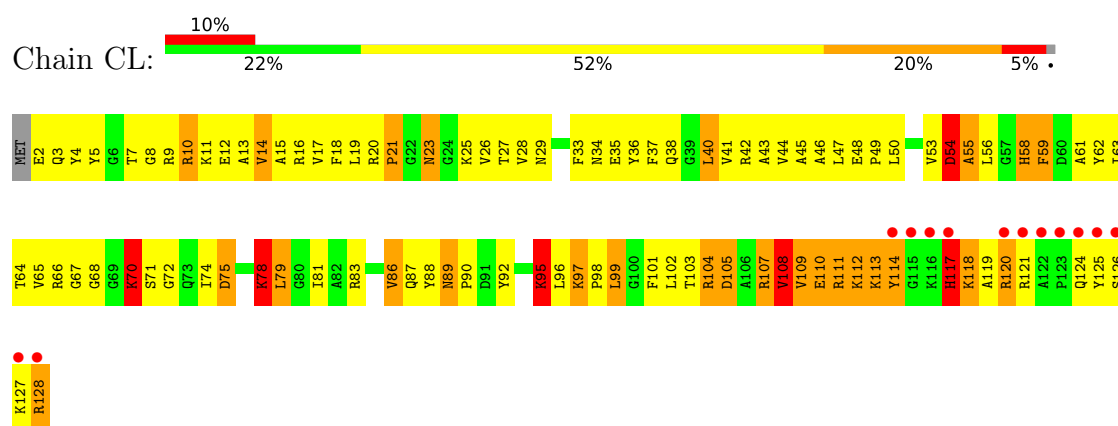
- Molecule 38: 30S RIBOSOMAL PROTEIN S8



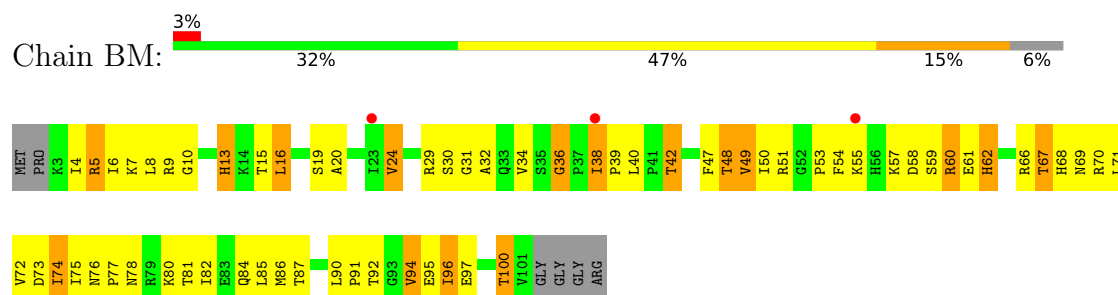
- Molecule 39: 30S RIBOSOMAL PROTEIN S9



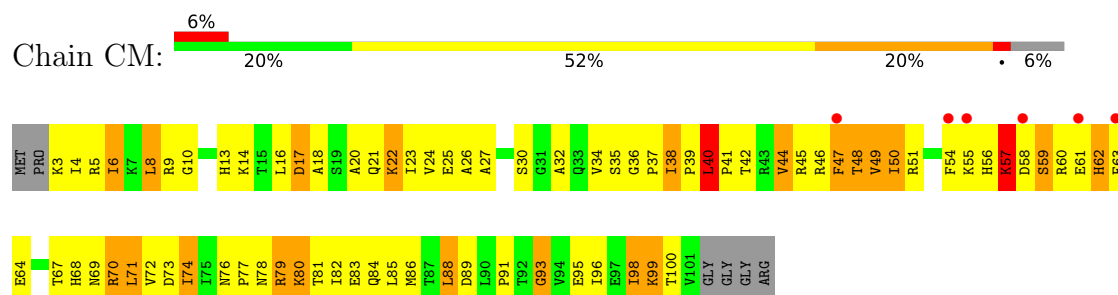
- Molecule 39: 30S RIBOSOMAL PROTEIN S9



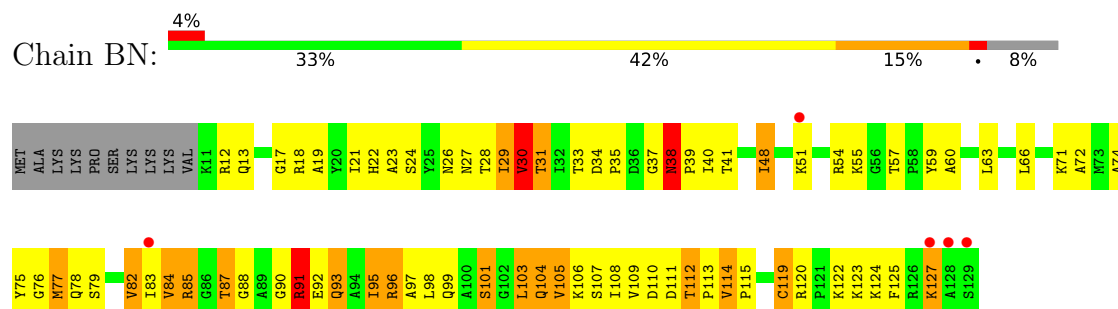
• Molecule 40: 30S RIBOSOMAL PROTEIN S10



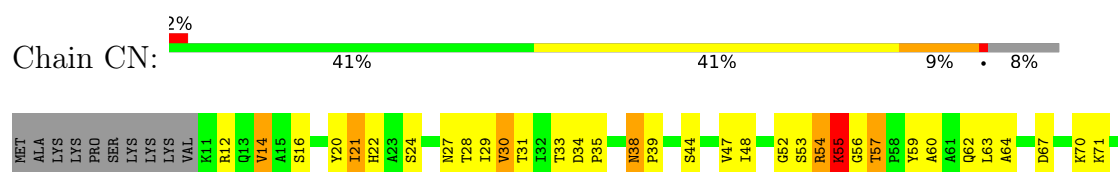
• Molecule 40: 30S RIBOSOMAL PROTEIN S10



• Molecule 41: 30S RIBOSOMAL PROTEIN S11

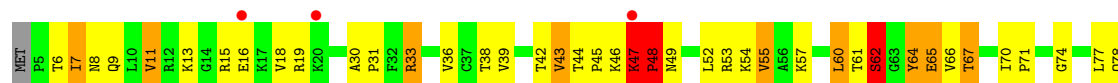


• Molecule 41: 30S RIBOSOMAL PROTEIN S11

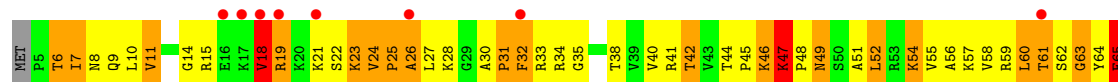




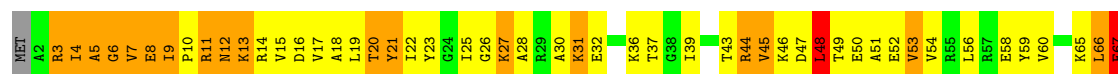
• Molecule 42: 30S RIBOSOMAL PROTEIN S12



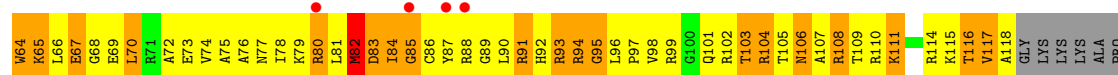
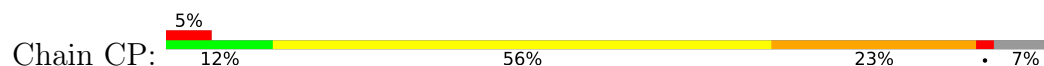
• Molecule 42: 30S RIBOSOMAL PROTEIN S12



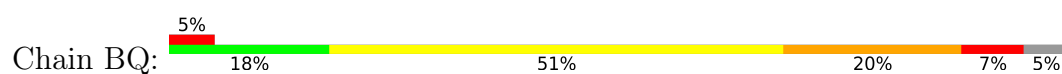
• Molecule 43: 30S RIBOSOMAL PROTEIN S13



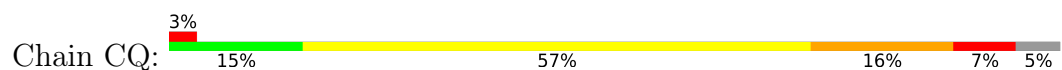
• Molecule 43: 30S RIBOSOMAL PROTEIN S13



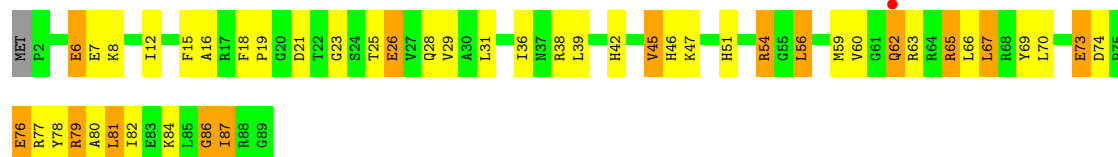
• Molecule 44: 30S RIBOSOMAL PROTEIN S14



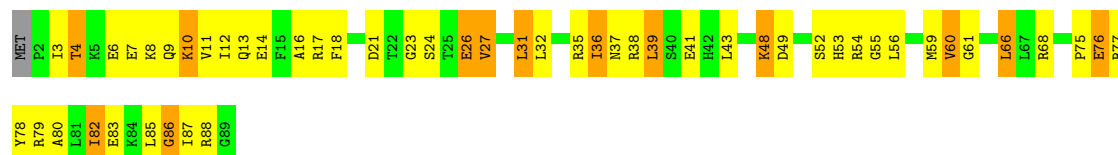
• Molecule 44: 30S RIBOSOMAL PROTEIN S14



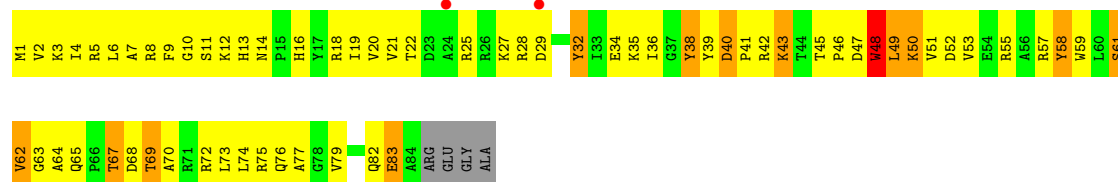
• Molecule 45: 30S RIBOSOMAL PROTEIN S15



• Molecule 45: 30S RIBOSOMAL PROTEIN S15

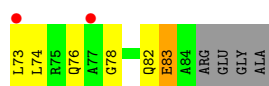


• Molecule 46: 30S RIBOSOMAL PROTEIN S16

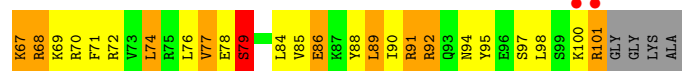
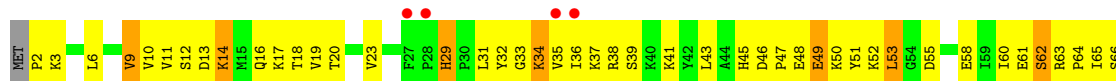


• Molecule 46: 30S RIBOSOMAL PROTEIN S16

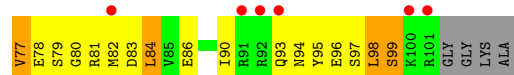
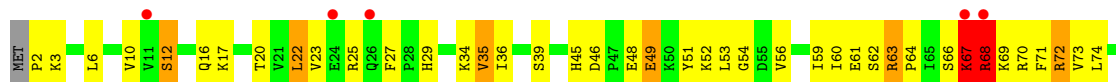




• Molecule 47: 30S RIBOSOMAL PROTEIN S17



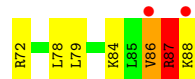
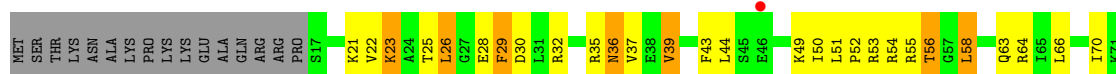
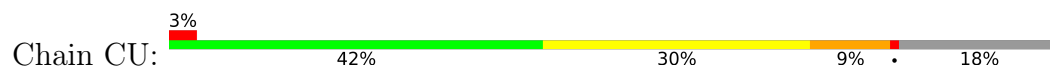
• Molecule 47: 30S RIBOSOMAL PROTEIN S17



• Molecule 48: 30S RIBOSOMAL PROTEIN S18

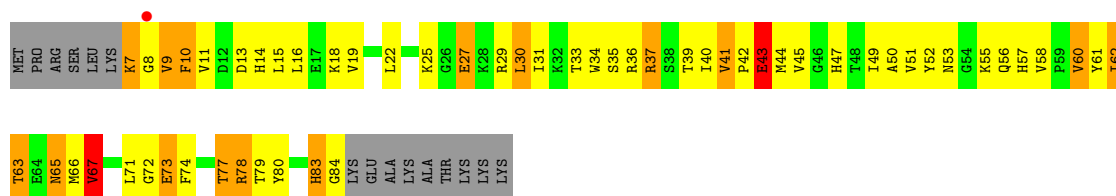


• Molecule 48: 30S RIBOSOMAL PROTEIN S18

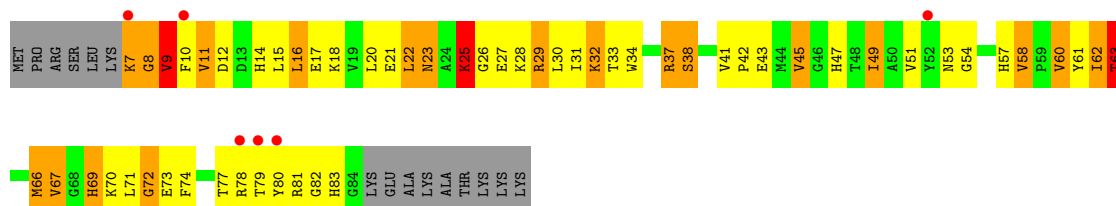
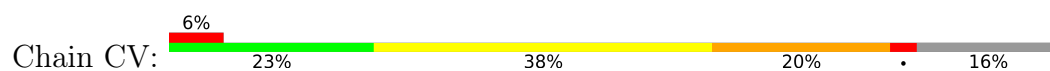


• Molecule 49: 30S RIBOSOMAL PROTEIN S19

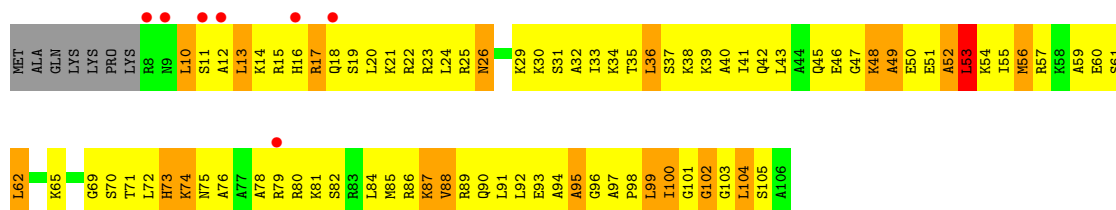
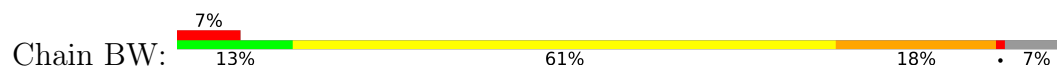




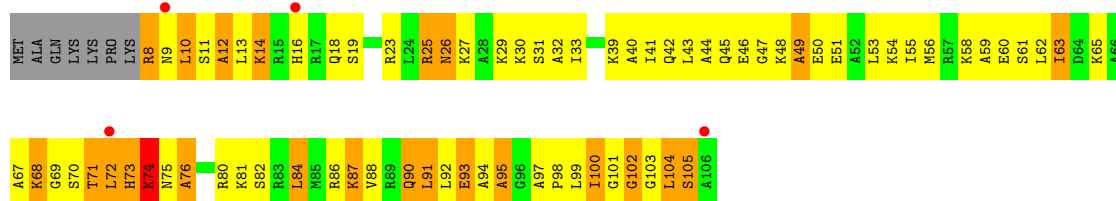
• Molecule 49: 30S RIBOSOMAL PROTEIN S19



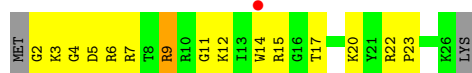
• Molecule 50: 30S RIBOSOMAL PROTEIN S20



• Molecule 50: 30S RIBOSOMAL PROTEIN S20

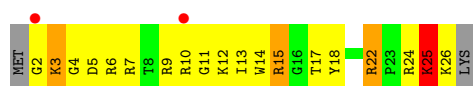


• Molecule 51: 30S RIBOSOMAL PROTEIN THX



• Molecule 51: 30S RIBOSOMAL PROTEIN THX

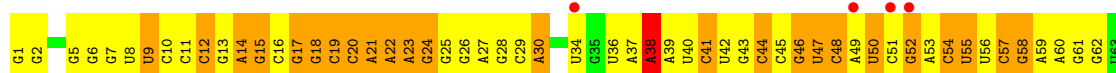
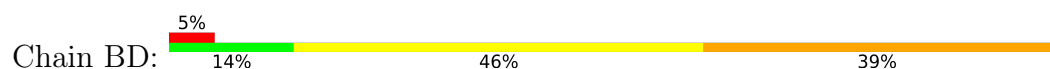




• Molecule 52: TRNA-TYR



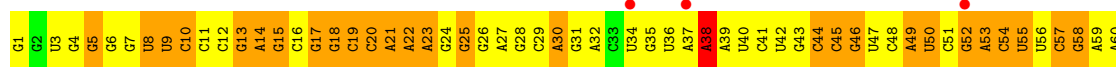
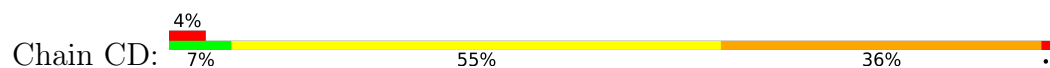
• Molecule 52: TRNA-TYR



• Molecule 52: TRNA-TYR

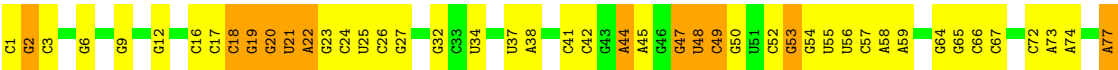


• Molecule 52: TRNA-TYR

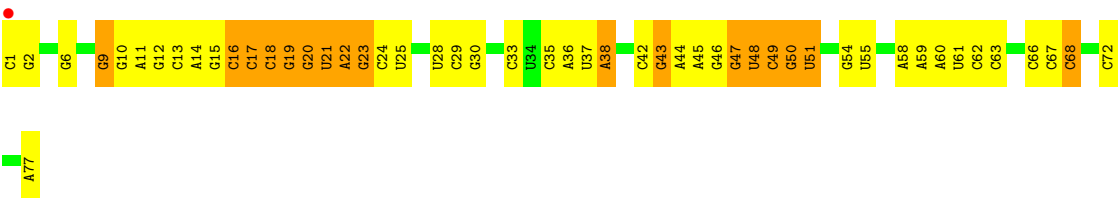


• Molecule 53: TRNA-FMET

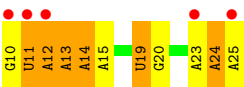
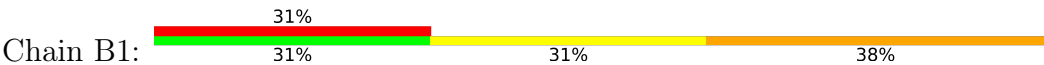




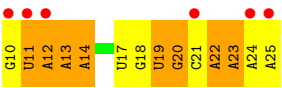
● Molecule 53: TRNA-FMET



● Molecule 54: MRNA



● Molecule 54: MRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.00Å 450.33Å 622.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.64 – 3.30 152.64 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (152.64-3.30) 94.3 (152.64-3.30)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.57 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.196 , 0.247 0.200 , 0.246	Depositor DCC
R_{free} test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å ²)	76.1	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 78.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	304031	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.35% 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: OHX, MIA, PAR, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.40	0/70233	0.48	1/109643 (0.0%)
1	DA	0.35	0/70122	0.45	4/109469 (0.0%)
2	AB	0.34	0/2928	0.47	1/4568 (0.0%)
2	DB	0.29	0/2928	0.45	0/4568
3	AD	0.72	0/2165	1.14	14/2919 (0.5%)
3	DD	0.64	0/2165	1.13	16/2919 (0.5%)
4	AE	0.58	0/1601	1.10	12/2160 (0.6%)
4	DE	0.57	0/1601	1.07	11/2160 (0.5%)
5	AF	0.63	0/1620	1.07	12/2194 (0.5%)
5	DF	0.49	0/1662	1.06	16/2249 (0.7%)
6	AG	0.46	0/1499	0.94	7/2016 (0.3%)
6	DG	0.38	0/1499	0.90	7/2016 (0.3%)
7	AH	0.56	0/1332	0.99	4/1802 (0.2%)
7	DH	0.42	0/1332	0.94	6/1802 (0.3%)
8	AK	0.50	0/1151	0.99	7/1558 (0.4%)
8	DK	0.48	0/1151	0.99	6/1558 (0.4%)
9	AM	0.53	0/1131	0.96	4/1525 (0.3%)
9	DM	0.44	0/1131	0.95	3/1525 (0.2%)
10	AN	0.59	0/943	1.00	1/1269 (0.1%)
10	DN	0.53	0/943	0.95	0/1269
11	AO	0.59	0/1162	1.12	10/1544 (0.6%)
11	DO	0.41	0/1162	0.86	2/1544 (0.1%)
12	AP	0.56	0/1143	1.01	7/1527 (0.5%)
12	DP	0.42	0/1143	0.87	6/1527 (0.4%)
13	A0	0.58	0/982	0.98	1/1312 (0.1%)
13	D0	0.54	0/974	0.93	0/1302
14	AQ	0.56	0/892	1.02	2/1187 (0.2%)
14	DQ	0.42	0/892	0.83	2/1187 (0.2%)
15	AR	0.57	0/1155	0.99	5/1542 (0.3%)
15	DR	0.52	0/1155	0.96	5/1542 (0.3%)
16	A1	0.56	0/982	1.02	6/1306 (0.5%)
16	D1	0.47	0/982	0.89	2/1306 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	A2	0.54	0/790	1.01	3/1057 (0.3%)
17	D2	0.42	0/790	1.02	4/1057 (0.4%)
18	AS	0.58	0/911	0.99	0/1220
18	DS	0.60	0/911	0.92	2/1220 (0.2%)
19	AT	0.67	1/739 (0.1%)	0.98	1/993 (0.1%)
19	DT	0.57	0/739	0.97	1/993 (0.1%)
20	AU	0.67	1/798 (0.1%)	1.09	5/1064 (0.5%)
20	DU	0.57	0/798	0.98	1/1064 (0.1%)
21	AV	0.46	0/1427	0.96	2/1935 (0.1%)
21	DV	0.40	0/1460	0.90	9/1982 (0.5%)
22	A3	0.58	0/615	0.99	0/819
22	D3	0.53	0/621	1.03	3/827 (0.4%)
23	AZ	0.58	0/770	1.01	1/1022 (0.1%)
23	DZ	0.54	0/770	1.04	2/1022 (0.2%)
24	AW	0.57	0/560	1.12	2/741 (0.3%)
24	DW	0.46	0/560	0.83	0/741
25	AX	0.53	0/474	1.03	5/635 (0.8%)
25	DX	0.41	0/474	0.93	2/635 (0.3%)
26	A4	0.49	0/545	0.91	3/733 (0.4%)
26	D4	0.49	0/527	0.98	3/709 (0.4%)
27	A5	0.54	0/473	1.16	5/639 (0.8%)
27	D5	0.52	0/473	0.95	1/639 (0.2%)
28	A6	0.69	0/396	1.02	2/529 (0.4%)
28	D6	0.68	0/396	1.02	3/529 (0.6%)
29	A7	0.73	0/399	1.07	1/526 (0.2%)
29	D7	0.69	0/399	1.08	2/526 (0.4%)
30	A8	0.71	0/486	1.21	6/638 (0.9%)
30	D8	0.52	0/486	0.95	2/638 (0.3%)
31	BA	0.31	0/36139	0.44	1/56406 (0.0%)
31	CA	0.29	0/36142	0.42	0/56410
32	BE	0.38	0/1959	0.86	9/2642 (0.3%)
32	CE	0.37	0/1959	0.90	8/2642 (0.3%)
33	BF	0.44	0/1629	0.81	1/2195 (0.0%)
33	CF	0.39	0/1636	0.82	1/2205 (0.0%)
34	BG	0.50	0/1733	0.93	3/2318 (0.1%)
34	CG	0.44	0/1733	0.94	3/2318 (0.1%)
35	BH	0.49	0/1171	0.88	0/1576
35	CH	0.46	0/1171	0.96	7/1576 (0.4%)
36	BI	0.47	0/856	0.84	0/1154
36	CI	0.43	0/856	0.84	0/1154
37	BJ	0.42	0/1276	0.82	3/1709 (0.2%)
37	CJ	0.40	0/1276	0.85	1/1709 (0.1%)
38	BK	0.45	0/1136	1.01	7/1527 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	CK	0.39	0/1136	0.87	4/1527 (0.3%)
39	BL	0.38	0/1029	0.82	1/1379 (0.1%)
39	CL	0.39	0/1029	0.97	6/1379 (0.4%)
40	BM	0.44	0/814	0.88	0/1095
40	CM	0.40	0/814	0.94	4/1095 (0.4%)
41	BN	0.47	0/900	0.94	5/1213 (0.4%)
41	CN	0.48	0/900	0.90	3/1213 (0.2%)
42	BO	0.58	0/991	1.04	4/1327 (0.3%)
42	CO	0.50	0/991	0.96	4/1327 (0.3%)
43	BP	0.43	0/938	0.90	3/1258 (0.2%)
43	CP	0.36	0/943	0.85	1/1265 (0.1%)
44	BQ	0.50	0/485	0.94	0/643
44	CQ	0.39	0/485	0.82	0/643
45	BR	0.49	0/745	0.88	1/992 (0.1%)
45	CR	0.46	0/745	0.81	0/992
46	BS	0.40	0/721	0.87	1/970 (0.1%)
46	CS	0.46	0/721	0.87	0/970
47	BT	0.46	0/847	0.85	2/1131 (0.2%)
47	CT	0.41	0/847	0.88	2/1131 (0.2%)
48	BU	0.48	0/596	0.93	1/790 (0.1%)
48	CU	0.46	0/596	0.81	0/790
49	BV	0.44	0/638	0.91	1/860 (0.1%)
49	CV	0.44	0/638	0.98	5/860 (0.6%)
50	BW	0.40	0/765	0.83	2/1007 (0.2%)
50	CW	0.43	0/765	0.94	4/1007 (0.4%)
51	BX	0.45	0/221	0.74	0/288
51	CX	0.41	0/221	0.86	2/288 (0.7%)
52	BB	0.40	0/1992	0.43	0/3099
52	BD	0.37	0/1992	0.39	0/3099
52	CB	0.47	0/1992	0.40	0/3099
52	CD	0.38	0/1992	0.42	0/3099
53	BC	0.29	0/1835	0.39	0/2859
53	CC	0.27	0/1835	0.39	0/2859
54	B1	0.39	0/390	0.42	0/606
54	C1	0.38	0/390	0.53	0/606
All	All	0.40	2/324159 (0.0%)	0.62	351/485455 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	AD	0	3
3	DD	0	1
4	AE	0	1
5	AF	0	1
5	DF	0	1
7	AH	0	1
8	AK	0	1
8	DK	0	1
11	AO	0	1
11	DO	0	1
24	AW	0	1
30	A8	0	1
30	D8	0	1
42	BO	0	1
All	All	0	16

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	AU	99	CYS	CA-C	6.75	1.55	1.52
19	AT	3	THR	CA-CB	5.76	1.70	1.54

The worst 5 of 351 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D2	49	THR	CA-C-N	-11.68	106.83	118.97
17	D2	49	THR	C-N-CA	-11.68	106.83	118.97
11	AO	64	LYS	N-CA-C	-10.40	102.76	114.62
4	AE	58	ARG	N-CA-C	-9.74	99.40	112.26
5	AF	65	TRP	CA-C-N	9.64	131.89	119.84

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AD	197	GLY	Peptide
3	AD	27	THR	Peptide
3	AD	47	GLY	Peptide
4	AE	20	ALA	Peptide
5	AF	47	GLY	Peptide

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	31614	2890	0
1	DA	62607	0	31564	2915	0
2	AB	2617	0	1328	137	0
2	DB	2617	0	1328	161	0
3	AD	2115	0	2195	282	0
3	DD	2115	0	2195	247	0
4	AE	1568	0	1634	217	0
4	DE	1568	0	1634	226	0
5	AF	1585	0	1632	187	0
5	DF	1627	0	1680	249	0
6	AG	1474	0	1535	165	0
6	DG	1474	0	1535	175	0
7	AH	1307	0	1382	182	0
7	DH	1307	0	1382	144	1
8	AK	1136	0	1223	130	0
8	DK	1136	0	1223	113	0
9	AM	1104	0	1180	138	0
9	DM	1104	0	1180	150	0
10	AN	933	0	996	70	0
10	DN	933	0	996	77	0
11	AO	1145	0	1228	250	0
11	DO	1145	0	1227	320	0
12	AP	1122	0	1179	194	0
12	DP	1122	0	1179	194	0
13	A0	968	0	1033	133	0
13	D0	960	0	1021	95	0
14	AQ	882	0	943	124	0
14	DQ	882	0	943	148	0
15	AR	1141	0	1202	123	0
15	DR	1141	0	1202	138	0
16	A1	964	0	1022	126	0
16	D1	964	0	1019	166	0
17	A2	779	0	852	104	0
17	D2	779	0	852	138	0
18	AS	900	0	964	99	0
18	DS	900	0	964	78	0
19	AT	725	0	778	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	DT	725	0	778	103	0
20	AU	785	0	878	105	0
20	DU	785	0	878	133	0
21	AV	1397	0	1430	183	0
21	DV	1428	0	1454	190	0
22	A3	607	0	628	65	0
22	D3	613	0	633	70	0
23	AZ	763	0	848	76	0
23	DZ	763	0	848	57	0
24	AW	558	0	610	42	0
24	DW	558	0	610	60	0
25	AX	469	0	518	39	0
25	DX	469	0	518	40	0
26	A4	533	0	522	92	0
26	D4	515	0	510	94	0
27	A5	459	0	480	88	0
27	D5	459	0	478	52	0
28	A6	389	0	404	58	0
28	D6	389	0	404	65	0
29	A7	391	0	432	41	0
29	D7	391	0	432	39	0
30	A8	480	0	549	130	0
30	D8	480	0	549	137	0
31	BA	32284	0	16296	1831	1
31	CA	32287	0	16295	1776	0
32	BE	1924	0	1975	212	0
32	CE	1924	0	1975	239	0
33	BF	1605	0	1668	140	0
33	CF	1612	0	1677	191	0
34	BG	1703	0	1763	182	0
34	CG	1703	0	1763	193	0
35	BH	1155	0	1213	123	0
35	CH	1155	0	1213	119	0
36	BI	843	0	857	71	0
36	CI	843	0	857	56	0
37	BJ	1257	0	1296	117	0
37	CJ	1257	0	1296	113	0
38	BK	1116	0	1177	117	0
38	CK	1116	0	1177	84	0
39	BL	1010	0	1037	110	0
39	CL	1010	0	1037	159	0
40	BM	801	0	849	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	CM	801	0	849	134	0
41	BN	885	0	904	68	0
41	CN	885	0	904	79	0
42	BO	975	0	1062	68	0
42	CO	975	0	1062	128	0
43	BP	928	0	987	110	0
43	CP	933	0	992	141	0
44	BQ	476	0	511	62	0
44	CQ	476	0	512	84	0
45	BR	734	0	771	51	0
45	CR	734	0	771	56	0
46	BS	705	0	725	79	0
46	CS	705	0	725	58	0
47	BT	834	0	904	87	0
47	CT	834	0	904	60	0
48	BU	591	0	662	63	0
48	CU	591	0	662	40	0
49	BV	624	0	636	75	0
49	CV	624	0	636	87	0
50	BW	763	0	861	108	0
50	CW	763	0	861	84	0
51	BX	217	0	234	16	0
51	CX	217	0	234	22	0
52	BB	1814	0	931	140	0
52	BD	1814	0	932	151	0
52	CB	1814	0	931	149	0
52	CD	1814	0	932	157	0
53	BC	1643	0	837	55	0
53	CC	1643	0	837	79	0
54	B1	347	0	174	20	0
54	C1	347	0	174	48	0
55	A0	1	0	0	0	0
55	A1	2	0	0	0	0
55	A3	1	0	0	0	0
55	A5	1	0	0	0	0
55	A7	1	0	0	0	0
55	AA	332	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	1	0	0	0	0
55	B1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	BA	114	0	0	0	0
55	BB	13	0	0	0	0
55	BC	4	0	0	0	0
55	BD	1	0	0	0	0
55	BF	1	0	0	0	0
55	BS	1	0	0	0	0
55	BW	1	0	0	0	0
55	C1	2	0	0	0	0
55	CA	121	0	0	0	0
55	CB	3	0	0	0	0
55	CC	7	0	0	0	0
55	CN	1	0	0	0	0
55	D0	1	0	0	0	0
55	D5	1	0	0	0	0
55	D7	1	0	0	0	0
55	DA	272	0	0	0	0
55	DB	7	0	0	0	0
55	DE	1	0	0	0	0
56	A1	14	0	0	0	0
56	A3	7	0	0	1	0
56	A6	7	0	0	1	0
56	AA	1659	0	0	140	0
56	AB	91	0	0	6	0
56	AE	7	0	0	0	0
56	AF	7	0	0	3	0
56	AO	14	0	0	2	0
56	AW	7	0	0	0	0
56	BA	693	0	0	66	0
56	BB	14	0	0	0	0
56	BC	21	0	0	2	0
56	BD	21	0	0	1	0
56	BG	7	0	0	2	0
56	BL	7	0	0	0	0
56	BR	7	0	0	0	0
56	CA	651	0	0	83	0
56	CB	21	0	0	2	0
56	CC	21	0	0	7	0
56	CD	7	0	0	1	0
56	CK	7	0	0	1	0
56	CR	7	0	0	0	0
56	CV	7	0	0	1	0
56	D1	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	D3	7	0	0	1	0
56	D5	7	0	0	1	0
56	D8	7	0	0	5	0
56	DA	1533	0	0	128	0
56	DB	91	0	0	6	0
56	DF	7	0	0	1	0
56	DO	7	0	0	0	0
57	BA	42	0	45	3	0
57	CA	42	0	45	1	0
58	BG	1	0	0	0	0
58	BQ	1	0	0	0	0
58	CG	1	0	0	0	0
58	CQ	1	0	0	0	0
All	All	304031	0	201063	19813	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 39.

The worst 5 of 19813 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)
11:DO:71:VAL:CG1	11:DO:72:PRO:HD3	1.34	1.57
30:A8:34:TRP:CB	30:A8:35:GLN:HB2	1.34	1.53
20:DU:89:PHE:CE1	20:DU:90:LEU:HG	1.40	1.50
9:DM:17:ASP:HA	9:DM:55:VAL:CG2	1.36	1.49
27:D5:4:HIS:HB3	27:D5:5:PRO:CD	1.40	1.48

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:DH:100:GLY:O[3_555]	1.86	0.34

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%)	208 (77%)	45 (17%)	17 (6%)	1	8
3	DD	270/276 (98%)	226 (84%)	31 (12%)	13 (5%)	2	12
4	AE	203/206 (98%)	138 (68%)	33 (16%)	32 (16%)	0	1
4	DE	203/206 (98%)	128 (63%)	34 (17%)	41 (20%)	0	0
5	AF	200/210 (95%)	153 (76%)	28 (14%)	19 (10%)	0	3
5	DF	206/210 (98%)	133 (65%)	46 (22%)	27 (13%)	0	1
6	AG	179/182 (98%)	127 (71%)	36 (20%)	16 (9%)	0	4
6	DG	179/182 (98%)	128 (72%)	30 (17%)	21 (12%)	0	1
7	AH	168/180 (93%)	111 (66%)	25 (15%)	32 (19%)	0	0
7	DH	168/180 (93%)	92 (55%)	52 (31%)	24 (14%)	0	1
8	AK	144/148 (97%)	75 (52%)	44 (31%)	25 (17%)	0	0
8	DK	144/148 (97%)	98 (68%)	27 (19%)	19 (13%)	0	1
9	AM	136/140 (97%)	96 (71%)	21 (15%)	19 (14%)	0	1
9	DM	136/140 (97%)	98 (72%)	21 (15%)	17 (12%)	0	1
10	AN	120/122 (98%)	101 (84%)	15 (12%)	4 (3%)	3	19
10	DN	120/122 (98%)	97 (81%)	15 (12%)	8 (7%)	1	7
11	AO	148/150 (99%)	91 (62%)	29 (20%)	28 (19%)	0	0
11	DO	148/150 (99%)	83 (56%)	21 (14%)	44 (30%)	0	0
12	AP	139/141 (99%)	93 (67%)	27 (19%)	19 (14%)	0	1
12	DP	139/141 (99%)	88 (63%)	29 (21%)	22 (16%)	0	1
13	A0	116/118 (98%)	86 (74%)	21 (18%)	9 (8%)	1	5
13	D0	115/118 (98%)	83 (72%)	18 (16%)	14 (12%)	0	1
14	AQ	109/112 (97%)	74 (68%)	26 (24%)	9 (8%)	0	5
14	DQ	109/112 (97%)	60 (55%)	32 (29%)	17 (16%)	0	1
15	AR	135/146 (92%)	101 (75%)	19 (14%)	15 (11%)	0	2
15	DR	135/146 (92%)	101 (75%)	23 (17%)	11 (8%)	1	5
16	A1	115/118 (98%)	82 (71%)	19 (16%)	14 (12%)	0	1
16	D1	115/118 (98%)	73 (64%)	29 (25%)	13 (11%)	0	2
17	A2	99/101 (98%)	81 (82%)	10 (10%)	8 (8%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	D2	99/101 (98%)	64 (65%)	19 (19%)	16 (16%)	0	1
18	AS	111/113 (98%)	94 (85%)	13 (12%)	4 (4%)	2	17
18	DS	111/113 (98%)	89 (80%)	13 (12%)	9 (8%)	1	5
19	AT	90/96 (94%)	78 (87%)	8 (9%)	4 (4%)	2	13
19	DT	90/96 (94%)	67 (74%)	15 (17%)	8 (9%)	0	4
20	AU	100/110 (91%)	65 (65%)	18 (18%)	17 (17%)	0	1
20	DU	100/110 (91%)	56 (56%)	18 (18%)	26 (26%)	0	0
21	AV	173/206 (84%)	105 (61%)	42 (24%)	26 (15%)	0	1
21	DV	177/206 (86%)	100 (56%)	35 (20%)	42 (24%)	0	0
22	A3	74/85 (87%)	58 (78%)	11 (15%)	5 (7%)	1	7
22	D3	75/85 (88%)	54 (72%)	15 (20%)	6 (8%)	1	5
23	AZ	95/98 (97%)	75 (79%)	14 (15%)	6 (6%)	1	8
23	DZ	95/98 (97%)	72 (76%)	12 (13%)	11 (12%)	0	2
24	AW	64/72 (89%)	55 (86%)	3 (5%)	6 (9%)	0	3
24	DW	64/72 (89%)	46 (72%)	11 (17%)	7 (11%)	0	2
25	AX	57/60 (95%)	47 (82%)	8 (14%)	2 (4%)	3	18
25	DX	57/60 (95%)	44 (77%)	9 (16%)	4 (7%)	1	7
26	A4	64/71 (90%)	33 (52%)	14 (22%)	17 (27%)	0	0
26	D4	61/71 (86%)	23 (38%)	12 (20%)	26 (43%)	0	0
27	A5	57/60 (95%)	39 (68%)	10 (18%)	8 (14%)	0	1
27	D5	57/60 (95%)	44 (77%)	7 (12%)	6 (10%)	0	2
28	A6	43/54 (80%)	21 (49%)	13 (30%)	9 (21%)	0	0
28	D6	43/54 (80%)	23 (54%)	9 (21%)	11 (26%)	0	0
29	A7	43/49 (88%)	41 (95%)	0	2 (5%)	2	12
29	D7	43/49 (88%)	38 (88%)	3 (7%)	2 (5%)	2	12
30	A8	58/65 (89%)	39 (67%)	11 (19%)	8 (14%)	0	1
30	D8	58/65 (89%)	40 (69%)	8 (14%)	10 (17%)	0	1
32	BE	235/256 (92%)	155 (66%)	44 (19%)	36 (15%)	0	1
32	CE	235/256 (92%)	152 (65%)	49 (21%)	34 (14%)	0	1
33	BF	203/239 (85%)	137 (68%)	47 (23%)	19 (9%)	0	3
33	CF	204/239 (85%)	124 (61%)	55 (27%)	25 (12%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	BG	206/208 (99%)	152 (74%)	34 (16%)	20 (10%)	0	3
34	CG	206/208 (99%)	152 (74%)	31 (15%)	23 (11%)	0	2
35	BH	149/162 (92%)	115 (77%)	26 (17%)	8 (5%)	1	10
35	CH	149/162 (92%)	115 (77%)	25 (17%)	9 (6%)	1	9
36	BI	99/101 (98%)	71 (72%)	23 (23%)	5 (5%)	1	11
36	CI	99/101 (98%)	85 (86%)	12 (12%)	2 (2%)	6	27
37	BJ	153/156 (98%)	111 (72%)	32 (21%)	10 (6%)	1	8
37	CJ	153/156 (98%)	118 (77%)	22 (14%)	13 (8%)	0	4
38	BK	136/138 (99%)	105 (77%)	24 (18%)	7 (5%)	1	11
38	CK	136/138 (99%)	100 (74%)	24 (18%)	12 (9%)	0	4
39	BL	125/128 (98%)	89 (71%)	25 (20%)	11 (9%)	0	4
39	CL	125/128 (98%)	80 (64%)	29 (23%)	16 (13%)	0	1
40	BM	97/105 (92%)	76 (78%)	20 (21%)	1 (1%)	12	40
40	CM	97/105 (92%)	73 (75%)	19 (20%)	5 (5%)	1	11
41	BN	117/129 (91%)	85 (73%)	24 (20%)	8 (7%)	1	7
41	CN	117/129 (91%)	93 (80%)	19 (16%)	5 (4%)	2	14
42	BO	123/132 (93%)	93 (76%)	18 (15%)	12 (10%)	0	3
42	CO	123/132 (93%)	79 (64%)	27 (22%)	17 (14%)	0	1
43	BP	114/126 (90%)	69 (60%)	27 (24%)	18 (16%)	0	1
43	CP	115/126 (91%)	71 (62%)	24 (21%)	20 (17%)	0	0
44	BQ	56/61 (92%)	38 (68%)	5 (9%)	13 (23%)	0	0
44	CQ	56/61 (92%)	32 (57%)	13 (23%)	11 (20%)	0	0
45	BR	86/89 (97%)	62 (72%)	19 (22%)	5 (6%)	1	9
45	CR	86/89 (97%)	72 (84%)	11 (13%)	3 (4%)	3	18
46	BS	82/88 (93%)	57 (70%)	15 (18%)	10 (12%)	0	1
46	CS	82/88 (93%)	55 (67%)	21 (26%)	6 (7%)	1	6
47	BT	98/105 (93%)	74 (76%)	17 (17%)	7 (7%)	1	6
47	CT	98/105 (93%)	83 (85%)	9 (9%)	6 (6%)	1	9
48	BU	70/88 (80%)	53 (76%)	11 (16%)	6 (9%)	0	4
48	CU	70/88 (80%)	58 (83%)	10 (14%)	2 (3%)	3	21
49	BV	76/93 (82%)	56 (74%)	13 (17%)	7 (9%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	CV	76/93 (82%)	49 (64%)	18 (24%)	9 (12%)	0	1
50	BW	97/106 (92%)	65 (67%)	21 (22%)	11 (11%)	0	2
50	CW	97/106 (92%)	70 (72%)	13 (13%)	14 (14%)	0	1
51	BX	23/27 (85%)	15 (65%)	5 (22%)	3 (13%)	0	1
51	CX	23/27 (85%)	15 (65%)	6 (26%)	2 (9%)	0	4
All	All	11319/12052 (94%)	7969 (70%)	2044 (18%)	1306 (12%)	0	2

5 of 1306 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AD	3	VAL
3	AD	28	GLU
3	AD	29	PRO
3	AD	33	LEU
3	AD	37	LEU

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%)	149 (70%)	65 (30%)	0	1
3	DD	214/218 (98%)	156 (73%)	58 (27%)	0	2
4	AE	165/166 (99%)	120 (73%)	45 (27%)	0	2
4	DE	165/166 (99%)	120 (73%)	45 (27%)	0	2
5	AF	161/166 (97%)	117 (73%)	44 (27%)	0	2
5	DF	165/166 (99%)	124 (75%)	41 (25%)	1	3
6	AG	155/156 (99%)	121 (78%)	34 (22%)	1	5
6	DG	155/156 (99%)	127 (82%)	28 (18%)	2	8
7	AH	142/148 (96%)	105 (74%)	37 (26%)	0	2
7	DH	142/148 (96%)	118 (83%)	24 (17%)	2	10
8	AK	122/124 (98%)	94 (77%)	28 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	DK	122/124 (98%)	97 (80%)	25 (20%)	1	6
9	AM	117/119 (98%)	84 (72%)	33 (28%)	0	2
9	DM	117/119 (98%)	80 (68%)	37 (32%)	0	1
10	AN	100/100 (100%)	78 (78%)	22 (22%)	1	5
10	DN	100/100 (100%)	80 (80%)	20 (20%)	1	6
11	AO	116/116 (100%)	82 (71%)	34 (29%)	0	2
11	DO	116/116 (100%)	74 (64%)	42 (36%)	0	1
12	AP	111/111 (100%)	85 (77%)	26 (23%)	1	4
12	DP	111/111 (100%)	75 (68%)	36 (32%)	0	1
13	A0	101/101 (100%)	72 (71%)	29 (29%)	0	2
13	D0	100/101 (99%)	79 (79%)	21 (21%)	1	5
14	AQ	87/88 (99%)	62 (71%)	25 (29%)	0	2
14	DQ	87/88 (99%)	64 (74%)	23 (26%)	0	2
15	AR	120/127 (94%)	98 (82%)	22 (18%)	2	7
15	DR	120/127 (94%)	90 (75%)	30 (25%)	0	3
16	A1	93/94 (99%)	72 (77%)	21 (23%)	1	5
16	D1	93/94 (99%)	72 (77%)	21 (23%)	1	5
17	A2	82/82 (100%)	57 (70%)	25 (30%)	0	1
17	D2	82/82 (100%)	54 (66%)	28 (34%)	0	1
18	AS	92/92 (100%)	66 (72%)	26 (28%)	0	2
18	DS	92/92 (100%)	69 (75%)	23 (25%)	0	3
19	AT	74/78 (95%)	56 (76%)	18 (24%)	1	3
19	DT	74/78 (95%)	54 (73%)	20 (27%)	0	2
20	AU	85/91 (93%)	62 (73%)	23 (27%)	0	2
20	DU	85/91 (93%)	52 (61%)	33 (39%)	0	0
21	AV	154/179 (86%)	122 (79%)	32 (21%)	1	6
21	DV	158/179 (88%)	134 (85%)	24 (15%)	3	13
22	A3	61/67 (91%)	47 (77%)	14 (23%)	1	4
22	D3	62/67 (92%)	54 (87%)	8 (13%)	4	17
23	AZ	82/83 (99%)	61 (74%)	21 (26%)	0	2
23	DZ	82/83 (99%)	55 (67%)	27 (33%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	AW	62/67 (92%)	43 (69%)	19 (31%)	0	1
24	DW	62/67 (92%)	44 (71%)	18 (29%)	0	2
25	AX	51/52 (98%)	39 (76%)	12 (24%)	1	4
25	DX	51/52 (98%)	37 (72%)	14 (28%)	0	2
26	A4	59/63 (94%)	50 (85%)	9 (15%)	3	13
26	D4	57/63 (90%)	43 (75%)	14 (25%)	1	3
27	A5	51/52 (98%)	39 (76%)	12 (24%)	1	4
27	D5	51/52 (98%)	42 (82%)	9 (18%)	2	9
28	A6	44/52 (85%)	32 (73%)	12 (27%)	0	2
28	D6	44/52 (85%)	38 (86%)	6 (14%)	3	16
29	A7	38/42 (90%)	29 (76%)	9 (24%)	1	4
29	D7	38/42 (90%)	29 (76%)	9 (24%)	1	4
30	A8	50/55 (91%)	34 (68%)	16 (32%)	0	1
30	D8	50/55 (91%)	35 (70%)	15 (30%)	0	1
32	BE	205/220 (93%)	163 (80%)	42 (20%)	1	6
32	CE	205/220 (93%)	167 (82%)	38 (18%)	1	7
33	BF	159/188 (85%)	124 (78%)	35 (22%)	1	5
33	CF	160/188 (85%)	130 (81%)	30 (19%)	1	7
34	BG	180/180 (100%)	149 (83%)	31 (17%)	2	10
34	CG	180/180 (100%)	142 (79%)	38 (21%)	1	5
35	BH	116/123 (94%)	88 (76%)	28 (24%)	1	3
35	CH	116/123 (94%)	92 (79%)	24 (21%)	1	6
36	BI	90/90 (100%)	77 (86%)	13 (14%)	3	14
36	CI	90/90 (100%)	78 (87%)	12 (13%)	4	17
37	BJ	126/127 (99%)	93 (74%)	33 (26%)	0	2
37	CJ	126/127 (99%)	103 (82%)	23 (18%)	2	7
38	BK	119/119 (100%)	97 (82%)	22 (18%)	1	7
38	CK	119/119 (100%)	101 (85%)	18 (15%)	3	13
39	BL	98/99 (99%)	78 (80%)	20 (20%)	1	6
39	CL	98/99 (99%)	74 (76%)	24 (24%)	1	3
40	BM	89/92 (97%)	71 (80%)	18 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	CM	89/92 (97%)	68 (76%)	21 (24%)	1	4
41	BN	90/99 (91%)	72 (80%)	18 (20%)	1	6
41	CN	90/99 (91%)	77 (86%)	13 (14%)	3	14
42	BO	104/109 (95%)	81 (78%)	23 (22%)	1	5
42	CO	104/109 (95%)	80 (77%)	24 (23%)	1	4
43	BP	94/101 (93%)	74 (79%)	20 (21%)	1	5
43	CP	94/101 (93%)	73 (78%)	21 (22%)	1	5
44	BQ	48/50 (96%)	34 (71%)	14 (29%)	0	2
44	CQ	48/50 (96%)	39 (81%)	9 (19%)	1	7
45	BR	79/80 (99%)	69 (87%)	10 (13%)	4	18
45	CR	79/80 (99%)	65 (82%)	14 (18%)	2	8
46	BS	72/74 (97%)	60 (83%)	12 (17%)	2	11
46	CS	72/74 (97%)	61 (85%)	11 (15%)	3	13
47	BT	95/97 (98%)	78 (82%)	17 (18%)	2	8
47	CT	95/97 (98%)	83 (87%)	12 (13%)	4	18
48	BU	63/77 (82%)	51 (81%)	12 (19%)	1	7
48	CU	63/77 (82%)	51 (81%)	12 (19%)	1	7
49	BV	67/80 (84%)	49 (73%)	18 (27%)	0	2
49	CV	67/80 (84%)	49 (73%)	18 (27%)	0	2
50	BW	76/82 (93%)	62 (82%)	14 (18%)	1	7
50	CW	76/82 (93%)	60 (79%)	16 (21%)	1	5
51	BX	20/22 (91%)	20 (100%)	0	100	100
51	CX	20/22 (91%)	18 (90%)	2 (10%)	7	27
All	All	9565/9996 (96%)	7373 (77%)	2192 (23%)	1	4

5 of 2192 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	D0	29	LEU
15	DR	48	ILE
13	D0	23	ASN
23	DZ	3	LYS
33	BF	161	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 331 such sidechains are listed below:

Mol	Chain	Res	Type
3	DD	112	GLN
16	D1	75	ASN
3	DD	198	ASN
8	DK	54	GLN
19	DT	87	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2911/2912 (99%)	697 (23%)	62 (2%)
1	DA	2905/2912 (99%)	733 (25%)	60 (2%)
2	AB	121/122 (99%)	23 (19%)	0
2	DB	121/122 (99%)	28 (23%)	1 (0%)
31	BA	1501/1506 (99%)	351 (23%)	39 (2%)
31	CA	1501/1506 (99%)	352 (23%)	49 (3%)
52	BB	84/85 (98%)	45 (53%)	5 (5%)
52	BD	84/85 (98%)	39 (46%)	5 (5%)
52	CB	84/85 (98%)	49 (58%)	8 (9%)
52	CD	84/85 (98%)	36 (42%)	6 (7%)
53	BC	76/77 (98%)	17 (22%)	3 (3%)
53	CC	76/77 (98%)	20 (26%)	3 (3%)
54	B1	15/16 (93%)	7 (46%)	2 (13%)
54	C1	15/16 (93%)	8 (53%)	3 (20%)
All	All	9578/9606 (99%)	2405 (25%)	246 (2%)

5 of 2405 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	U
1	AA	17	G
1	AA	23	G
1	AA	34	C
1	AA	35	G

5 of 246 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	B1	13	A
1	DA	1980	G
31	CA	913	A

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Mol	Chain	Res	Type
1	DA	1899	G
1	DA	2610	C

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	CD	38	52	28,31,32	1.95	2 (7%)	38,44,47	2.84	12 (31%)
52	MIA	BD	38	52	28,31,32	1.95	3 (10%)	38,44,47	3.06	13 (34%)
52	MIA	BB	38	52	28,31,32	2.02	3 (10%)	38,44,47	2.42	12 (31%)
52	MIA	CB	38	52	28,31,32	2.19	4 (14%)	38,44,47	2.85	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	CD	38	52	-	7/15/33/34	0/3/3/3
52	MIA	BD	38	52	-	6/15/33/34	0/3/3/3
52	MIA	BB	38	52	-	2/15/33/34	0/3/3/3
52	MIA	CB	38	52	-	2/15/33/34	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	CB	38	MIA	C6-N6	8.33	1.47	1.34
52	BB	38	MIA	C6-N6	7.54	1.46	1.34
52	BD	38	MIA	C6-N6	7.49	1.46	1.34
52	CD	38	MIA	C6-N6	7.41	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	CB	38	MIA	C13-C14	6.31	1.51	1.32

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	BD	38	MIA	C11-S10-C2	11.87	111.16	102.25
52	CD	38	MIA	C11-S10-C2	10.68	110.27	102.25
52	CB	38	MIA	C11-S10-C2	9.99	109.75	102.25
52	CB	38	MIA	C5-C4-N3	-8.51	118.22	127.18
52	BD	38	MIA	C5-C4-N3	-8.04	118.71	127.18

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	BB	38	MIA	C12-C13-C14-C15
52	BB	38	MIA	C12-C13-C14-C16
52	BD	38	MIA	O4'-C4'-C5'-O5'
52	BD	38	MIA	N1-C2-S10-C11
52	BD	38	MIA	N3-C2-S10-C11

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	CD	38	MIA	3	0
52	BD	38	MIA	8	0
52	BB	38	MIA	2	0
52	CB	38	MIA	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1619 ligands modelled in this entry, 907 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	CB	106	-	0,6,6	-	-	-		
56	OHX	DA	3094	-	0,6,6	-	-	-		
56	OHX	BD	104	-	0,6,6	-	-	-		
56	OHX	AB	211	-	0,6,6	-	-	-		
56	OHX	BA	1724	-	0,6,6	-	-	-		
56	OHX	AA	3380	-	0,6,6	-	-	-		
56	OHX	AA	3428	-	0,6,6	-	-	-		
56	OHX	DA	3422	-	0,6,6	-	-	-		
56	OHX	AA	3443	-	0,6,6	-	-	-		
56	OHX	BA	1745	-	0,6,6	-	-	-		
56	OHX	DA	3398	-	0,6,6	-	-	-		
56	OHX	CA	1773	-	0,6,6	-	-	-		
56	OHX	CV	101	-	0,6,6	-	-	-		
56	OHX	CA	1778	-	0,6,6	-	-	-		
56	OHX	DA	3394	-	0,6,6	-	-	-		
56	OHX	DA	3407	-	0,6,6	-	-	-		
56	OHX	BA	1760	-	0,6,6	-	-	-		
56	OHX	AB	218	-	0,6,6	-	-	-		
56	OHX	AA	3564	-	0,6,6	-	-	-		
56	OHX	AA	3342	-	0,6,6	-	-	-		
56	OHX	AA	3451	-	0,6,6	-	-	-		
56	OHX	AA	3500	-	0,6,6	-	-	-		
56	OHX	AA	3554	-	0,6,6	-	-	-		
56	OHX	DA	3399	-	0,6,6	-	-	-		
56	OHX	DA	3345	-	0,6,6	-	-	-		
56	OHX	AA	3465	-	0,6,6	-	-	-		
56	OHX	AA	3529	-	0,6,6	-	-	-		
56	OHX	AA	3548	-	0,6,6	-	-	-		
56	OHX	BA	1730	-	0,6,6	-	-	-		
56	OHX	AA	3348	-	0,6,6	-	-	-		
56	OHX	DA	3364	-	0,6,6	-	-	-		
56	OHX	AA	3553	-	0,6,6	-	-	-		
56	OHX	DA	3127	-	0,6,6	-	-	-		
56	OHX	AA	3526	-	0,6,6	-	-	-		
56	OHX	BA	1798	-	0,6,6	-	-	-		
56	OHX	DA	3382	-	0,6,6	-	-	-		
56	OHX	CA	1766	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	DA	3363	-	0,6,6	-	-	-		
56	OHX	AA	3496	-	0,6,6	-	-	-		
56	OHX	DA	3360	-	0,6,6	-	-	-		
56	OHX	AA	3327	-	0,6,6	-	-	-		
56	OHX	DA	3157	-	0,6,6	-	-	-		
56	OHX	DA	3412	-	0,6,6	-	-	-		
56	OHX	BA	1788	-	0,6,6	-	-	-		
56	OHX	DA	3444	-	0,6,6	-	-	-		
56	OHX	AA	3519	-	0,6,6	-	-	-		
56	OHX	AA	3445	-	0,6,6	-	-	-		
56	OHX	AA	3535	-	0,6,6	-	-	-		
56	OHX	DB	216	-	0,6,6	-	-	-		
56	OHX	AA	3497	-	0,6,6	-	-	-		
56	OHX	DA	3136	-	0,6,6	-	-	-		
56	OHX	DA	3482	-	0,6,6	-	-	-		
56	OHX	BR	101	-	0,6,6	-	-	-		
56	OHX	AA	3448	-	0,6,6	-	-	-		
56	OHX	DA	3480	-	0,6,6	-	-	-		
56	OHX	BA	1754	-	0,6,6	-	-	-		
56	OHX	CA	1767	-	0,6,6	-	-	-		
56	OHX	DA	3414	-	0,6,6	-	-	-		
56	OHX	DA	3450	-	0,6,6	-	-	-		
56	OHX	DA	3427	-	0,6,6	-	-	-		
56	OHX	BA	1756	-	0,6,6	-	-	-		
56	OHX	AA	3424	-	0,6,6	-	-	-		
56	OHX	AA	3544	-	0,6,6	-	-	-		
56	OHX	DA	3469	-	0,6,6	-	-	-		
56	OHX	BA	1785	-	0,6,6	-	-	-		
56	OHX	BA	1732	-	0,6,6	-	-	-		
56	OHX	AA	3501	-	0,6,6	-	-	-		
56	OHX	AA	3559	-	0,6,6	-	-	-		
56	OHX	AA	3461	-	0,6,6	-	-	-		
56	OHX	AA	3498	-	0,6,6	-	-	-		
56	OHX	CA	1779	-	0,6,6	-	-	-		
56	OHX	CA	1775	-	0,6,6	-	-	-		
56	OHX	CA	1751	-	0,6,6	-	-	-		
56	OHX	AA	3476	-	0,6,6	-	-	-		
56	OHX	DA	3431	-	0,6,6	-	-	-		
56	OHX	DA	3411	-	0,6,6	-	-	-		
56	OHX	CA	1770	-	0,6,6	-	-	-		
56	OHX	BA	1803	-	0,6,6	-	-	-		
56	OHX	AA	3507	-	0,6,6	-	-	-		
56	OHX	AA	3362	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	DA	3224	-	0,6,6	-	-	-		
56	OHX	DA	3470	-	0,6,6	-	-	-		
56	OHX	AA	3439	-	0,6,6	-	-	-		
56	OHX	DA	3468	-	0,6,6	-	-	-		
56	OHX	AB	215	-	0,6,6	-	-	-		
56	OHX	BB	114	-	0,6,6	-	-	-		
56	OHX	CA	1750	-	0,6,6	-	-	-		
56	OHX	DA	3434	-	0,6,6	-	-	-		
56	OHX	AA	3336	-	0,6,6	-	-	-		
56	OHX	DA	3471	-	0,6,6	-	-	-		
57	PAR	CA	1722	-	44,45,45	0.69	0	63,67,67	1.84	14 (22%)
56	OHX	DA	3348	-	0,6,6	-	-	-		
56	OHX	BA	1740	-	0,6,6	-	-	-		
56	OHX	AA	3422	-	0,6,6	-	-	-		
56	OHX	AA	3474	-	0,6,6	-	-	-		
56	OHX	AA	3396	-	0,6,6	-	-	-		
56	OHX	AA	3514	-	0,6,6	-	-	-		
56	OHX	AF	303	-	0,6,6	-	-	-		
56	OHX	BA	1739	-	0,6,6	-	-	-		
56	OHX	CA	1790	-	0,6,6	-	-	-		
56	OHX	AA	3495	-	0,6,6	-	-	-		
56	OHX	AA	3414	-	0,6,6	-	-	-		
56	OHX	DA	3426	-	0,6,6	-	-	-		
56	OHX	CA	1789	-	0,6,6	-	-	-		
56	OHX	AA	3450	-	0,6,6	-	-	-		
56	OHX	BA	1806	-	0,6,6	-	-	-		
56	OHX	DA	3478	-	0,6,6	-	-	-		
56	OHX	DA	3068	-	0,6,6	-	-	-		
56	OHX	DA	3371	-	0,6,6	-	-	-		
56	OHX	AE	304	-	0,6,6	-	-	-		
56	OHX	DA	3467	-	0,6,6	-	-	-		
56	OHX	DB	215	-	0,6,6	-	-	-		
56	OHX	DA	3489	-	0,6,6	-	-	-		
56	OHX	BA	1734	-	0,6,6	-	-	-		
56	OHX	AA	3386	-	0,6,6	-	-	-		
56	OHX	AA	3430	-	0,6,6	-	-	-		
56	OHX	AA	3463	-	0,6,6	-	-	-		
56	OHX	AA	3528	-	0,6,6	-	-	-		
56	OHX	DA	3459	-	0,6,6	-	-	-		
56	OHX	DA	3253	-	0,6,6	-	-	-		
56	OHX	AA	3389	-	0,6,6	-	-	-		
56	OHX	CA	1764	-	0,6,6	-	-	-		
56	OHX	AA	3558	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	AA	3425	-	0,6,6	-	-	-		
56	OHX	AA	3375	-	0,6,6	-	-	-		
56	OHX	AA	3516	-	0,6,6	-	-	-		
56	OHX	BD	102	-	0,6,6	-	-	-		
56	OHX	DA	3457	-	0,6,6	-	-	-		
56	OHX	CA	1804	-	0,6,6	-	-	-		
56	OHX	AA	3552	-	0,6,6	-	-	-		
56	OHX	BA	1787	-	0,6,6	-	-	-		
56	OHX	AA	3468	-	0,6,6	-	-	-		
56	OHX	BA	1805	-	0,6,6	-	-	-		
56	OHX	CA	1811	-	0,6,6	-	-	-		
56	OHX	CC	110	-	0,6,6	-	-	-		
56	OHX	BB	115	-	0,6,6	-	-	-		
56	OHX	CA	1733	-	0,6,6	-	-	-		
56	OHX	DA	3423	-	0,6,6	-	-	-		
56	OHX	DA	3462	-	0,6,6	-	-	-		
56	OHX	AA	3490	-	0,6,6	-	-	-		
56	OHX	AB	214	-	0,6,6	-	-	-		
56	OHX	AA	3525	-	0,6,6	-	-	-		
56	OHX	AA	3331	-	0,6,6	-	-	-		
56	OHX	AO	203	-	0,6,6	-	-	-		
56	OHX	AA	3376	-	0,6,6	-	-	-		
56	OHX	DA	3217	-	0,6,6	-	-	-		
56	OHX	AA	3408	-	0,6,6	-	-	-		
56	OHX	DA	3460	-	0,6,6	-	-	-		
56	OHX	AA	3426	-	0,6,6	-	-	-		
56	OHX	DA	3124	-	0,6,6	-	-	-		
56	OHX	DA	3404	-	0,6,6	-	-	-		
56	OHX	DA	3370	-	0,6,6	-	-	-		
56	OHX	BA	1757	-	0,6,6	-	-	-		
56	OHX	BA	1728	-	0,6,6	-	-	-		
56	OHX	AA	3538	-	0,6,6	-	-	-		
56	OHX	AA	3543	-	0,6,6	-	-	-		
56	OHX	AA	3407	-	0,6,6	-	-	-		
56	OHX	BA	1716	-	0,6,6	-	-	-		
56	OHX	DA	3168	-	0,6,6	-	-	-		
56	OHX	DA	3439	-	0,6,6	-	-	-		
56	OHX	AB	213	-	0,6,6	-	-	-		
56	OHX	CC	109	-	0,6,6	-	-	-		
56	OHX	DA	3061	-	0,6,6	-	-	-		
56	OHX	CA	1787	-	0,6,6	-	-	-		
56	OHX	AA	3441	-	0,6,6	-	-	-		
56	OHX	AA	3489	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	OHX	DA	3111	-	0,6,6	-	-	-		
56	OHX	DA	3429	-	0,6,6	-	-	-		
56	OHX	BA	1731	-	0,6,6	-	-	-		
56	OHX	AA	3459	-	0,6,6	-	-	-		
56	OHX	CA	1752	-	0,6,6	-	-	-		
56	OHX	DA	3424	-	0,6,6	-	-	-		
56	OHX	DB	214	-	0,6,6	-	-	-		
56	OHX	CA	1748	-	0,6,6	-	-	-		
56	OHX	BA	1751	-	0,6,6	-	-	-		
56	OHX	AA	3520	-	0,6,6	-	-	-		
56	OHX	DA	3353	-	0,6,6	-	-	-		
56	OHX	AA	3382	-	0,6,6	-	-	-		
56	OHX	CA	1754	-	0,6,6	-	-	-		
56	OHX	CA	1784	-	0,6,6	-	-	-		
56	OHX	DA	3159	-	0,6,6	-	-	-		
56	OHX	DA	3248	-	0,6,6	-	-	-		
56	OHX	DA	3390	-	0,6,6	-	-	-		
56	OHX	AA	3488	-	0,6,6	-	-	-		
56	OHX	BA	1807	-	0,6,6	-	-	-		
56	OHX	A1	203	-	0,6,6	-	-	-		
56	OHX	BA	1737	-	0,6,6	-	-	-		
56	OHX	CA	1723	-	0,6,6	-	-	-		
56	OHX	BA	1808	-	0,6,6	-	-	-		
56	OHX	DA	3162	-	0,6,6	-	-	-		
56	OHX	CA	1756	-	0,6,6	-	-	-		
56	OHX	DA	3376	-	0,6,6	-	-	-		
56	OHX	DA	3341	-	0,6,6	-	-	-		
56	OHX	CB	104	-	0,6,6	-	-	-		
56	OHX	AA	3480	-	0,6,6	-	-	-		
56	OHX	BA	1772	-	0,6,6	-	-	-		
56	OHX	BC	107	-	0,6,6	-	-	-		
56	OHX	CA	1753	-	0,6,6	-	-	-		
56	OHX	AA	3381	-	0,6,6	-	-	-		
56	OHX	BC	106	-	0,6,6	-	-	-		
56	OHX	AA	3346	-	0,6,6	-	-	-		
56	OHX	DA	3428	-	0,6,6	-	-	-		
56	OHX	AA	3377	-	0,6,6	-	-	-		
56	OHX	AA	3469	-	0,6,6	-	-	-		
56	OHX	DA	3073	-	0,6,6	-	-	-		
56	OHX	DA	3446	-	0,6,6	-	-	-		
56	OHX	AA	3419	-	0,6,6	-	-	-		
56	OHX	BA	1779	-	0,6,6	-	-	-		
56	OHX	DA	3214	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	AA	3551	-	0,6,6	-	-	-		
56	OHX	DA	3396	-	0,6,6	-	-	-		
56	OHX	DA	3491	-	0,6,6	-	-	-		
56	OHX	AA	3477	-	0,6,6	-	-	-		
56	OHX	CA	1763	-	0,6,6	-	-	-		
56	OHX	BA	1776	-	0,6,6	-	-	-		
56	OHX	AA	3326	-	0,6,6	-	-	-		
56	OHX	CA	1785	-	0,6,6	-	-	-		
56	OHX	DB	213	-	0,6,6	-	-	-		
56	OHX	BA	1717	-	0,6,6	-	-	-		
56	OHX	AA	3517	-	0,6,6	-	-	-		
56	OHX	DA	3425	-	0,6,6	-	-	-		
56	OHX	BA	1761	-	0,6,6	-	-	-		
56	OHX	DA	3105	-	0,6,6	-	-	-		
56	OHX	DA	3386	-	0,6,6	-	-	-		
56	OHX	CA	1806	-	0,6,6	-	-	-		
56	OHX	A6	101	-	0,6,6	-	-	-		
56	OHX	AA	3361	-	0,6,6	-	-	-		
56	OHX	DA	3452	-	0,6,6	-	-	-		
56	OHX	AA	3444	-	0,6,6	-	-	-		
56	OHX	BA	1770	-	0,6,6	-	-	-		
56	OHX	AA	3383	-	0,6,6	-	-	-		
56	OHX	CA	1795	-	0,6,6	-	-	-		
56	OHX	CR	101	-	0,6,6	-	-	-		
56	OHX	DA	3165	-	0,6,6	-	-	-		
56	OHX	DF	301	-	0,6,6	-	-	-		
56	OHX	BA	1763	-	0,6,6	-	-	-		
56	OHX	DA	3171	-	0,6,6	-	-	-		
56	OHX	BA	1768	-	0,6,6	-	-	-		
56	OHX	DA	3369	-	0,6,6	-	-	-		
56	OHX	DA	3413	-	0,6,6	-	-	-		
56	OHX	BA	1771	-	0,6,6	-	-	-		
56	OHX	AA	3403	-	0,6,6	-	-	-		
56	OHX	BC	105	-	0,6,6	-	-	-		
56	OHX	AA	3393	-	0,6,6	-	-	-		
56	OHX	AB	217	-	0,6,6	-	-	-		
56	OHX	BA	1814	-	0,6,6	-	-	-		
56	OHX	AA	3511	-	0,6,6	-	-	-		
56	OHX	BA	1769	-	0,6,6	-	-	-		
56	OHX	BA	1812	-	0,6,6	-	-	-		
56	OHX	AA	3330	-	0,6,6	-	-	-		
56	OHX	AA	3434	-	0,6,6	-	-	-		
56	OHX	AA	3545	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	AB	216	-	0,6,6	-	-	-		
56	OHX	CA	1759	-	0,6,6	-	-	-		
56	OHX	DA	3368	-	0,6,6	-	-	-		
56	OHX	DA	3437	-	0,6,6	-	-	-		
56	OHX	DA	3346	-	0,6,6	-	-	-		
56	OHX	AA	3562	-	0,6,6	-	-	-		
56	OHX	AA	3378	-	0,6,6	-	-	-		
56	OHX	AA	3467	-	0,6,6	-	-	-		
56	OHX	DA	3448	-	0,6,6	-	-	-		
56	OHX	AA	3416	-	0,6,6	-	-	-		
56	OHX	BA	1720	-	0,6,6	-	-	-		
56	OHX	CA	1803	-	0,6,6	-	-	-		
56	OHX	CA	1807	-	0,6,6	-	-	-		
56	OHX	AA	3400	-	0,6,6	-	-	-		
56	OHX	AA	3354	-	0,6,6	-	-	-		
56	OHX	AA	3539	-	0,6,6	-	-	-		
56	OHX	AA	3555	-	0,6,6	-	-	-		
56	OHX	CK	201	-	0,6,6	-	-	-		
56	OHX	AA	3335	-	0,6,6	-	-	-		
56	OHX	AA	3473	-	0,6,6	-	-	-		
56	OHX	AA	3492	-	0,6,6	-	-	-		
56	OHX	BA	1789	-	0,6,6	-	-	-		
56	OHX	CA	1765	-	0,6,6	-	-	-		
56	OHX	DB	220	-	0,6,6	-	-	-		
56	OHX	CA	1737	-	0,6,6	-	-	-		
56	OHX	AA	3510	-	0,6,6	-	-	-		
56	OHX	AA	3542	-	0,6,6	-	-	-		
56	OHX	DA	3257	-	0,6,6	-	-	-		
56	OHX	AA	3328	-	0,6,6	-	-	-		
56	OHX	DA	3215	-	0,6,6	-	-	-		
56	OHX	CA	1776	-	0,6,6	-	-	-		
56	OHX	DB	212	-	0,6,6	-	-	-		
56	OHX	DA	3391	-	0,6,6	-	-	-		
56	OHX	AA	3413	-	0,6,6	-	-	-		
56	OHX	AA	3513	-	0,6,6	-	-	-		
56	OHX	DA	3455	-	0,6,6	-	-	-		
56	OHX	AA	3521	-	0,6,6	-	-	-		
56	OHX	AA	3432	-	0,6,6	-	-	-		
56	OHX	AA	3421	-	0,6,6	-	-	-		
56	OHX	DA	3134	-	0,6,6	-	-	-		
56	OHX	AA	3352	-	0,6,6	-	-	-		
56	OHX	DA	3082	-	0,6,6	-	-	-		
56	OHX	DA	3409	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	BA	1786	-	0,6,6	-	-	-		
56	OHX	AA	3481	-	0,6,6	-	-	-		
56	OHX	AA	3366	-	0,6,6	-	-	-		
56	OHX	AA	3399	-	0,6,6	-	-	-		
56	OHX	AA	3442	-	0,6,6	-	-	-		
56	OHX	AA	3370	-	0,6,6	-	-	-		
56	OHX	DA	3418	-	0,6,6	-	-	-		
56	OHX	CA	1732	-	0,6,6	-	-	-		
56	OHX	DA	3367	-	0,6,6	-	-	-		
56	OHX	BA	1797	-	0,6,6	-	-	-		
56	OHX	CA	1725	-	0,6,6	-	-	-		
56	OHX	AA	3353	-	0,6,6	-	-	-		
57	PAR	BA	1715	-	44,45,45	0.71	2 (4%)	63,67,67	1.74	12 (19%)
56	OHX	AA	3379	-	0,6,6	-	-	-		
56	OHX	AA	3478	-	0,6,6	-	-	-		
56	OHX	DB	211	-	0,6,6	-	-	-		
56	OHX	DA	3392	-	0,6,6	-	-	-		
56	OHX	BA	1743	-	0,6,6	-	-	-		
56	OHX	DB	217	-	0,6,6	-	-	-		
56	OHX	DA	3465	-	0,6,6	-	-	-		
56	OHX	AB	207	-	0,6,6	-	-	-		
56	OHX	BA	1796	-	0,6,6	-	-	-		
56	OHX	CA	1730	-	0,6,6	-	-	-		
56	OHX	CA	1810	-	0,6,6	-	-	-		
56	OHX	BA	1793	-	0,6,6	-	-	-		
56	OHX	BA	1725	-	0,6,6	-	-	-		
56	OHX	DA	3430	-	0,6,6	-	-	-		
56	OHX	AA	3452	-	0,6,6	-	-	-		
56	OHX	BA	1747	-	0,6,6	-	-	-		
56	OHX	CA	1812	-	0,6,6	-	-	-		
56	OHX	CA	1805	-	0,6,6	-	-	-		
56	OHX	BA	1752	-	0,6,6	-	-	-		
56	OHX	CA	1726	-	0,6,6	-	-	-		
56	OHX	DA	3435	-	0,6,6	-	-	-		
56	OHX	AA	3404	-	0,6,6	-	-	-		
56	OHX	BA	1800	-	0,6,6	-	-	-		
56	OHX	AA	3531	-	0,6,6	-	-	-		
56	OHX	AA	3537	-	0,6,6	-	-	-		
56	OHX	DA	3375	-	0,6,6	-	-	-		
56	OHX	AA	3561	-	0,6,6	-	-	-		
56	OHX	BA	1729	-	0,6,6	-	-	-		
56	OHX	CA	1780	-	0,6,6	-	-	-		
56	OHX	DA	3403	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	DA	3440	-	0,6,6	-	-	-		
56	OHX	DA	3453	-	0,6,6	-	-	-		
56	OHX	BG	302	-	0,6,6	-	-	-		
56	OHX	AA	3365	-	0,6,6	-	-	-		
56	OHX	AB	212	-	0,6,6	-	-	-		
56	OHX	DA	3490	-	0,6,6	-	-	-		
56	OHX	AA	3367	-	0,6,6	-	-	-		
56	OHX	BA	1794	-	0,6,6	-	-	-		
56	OHX	DA	3103	-	0,6,6	-	-	-		
56	OHX	AA	3333	-	0,6,6	-	-	-		
56	OHX	BA	1804	-	0,6,6	-	-	-		
56	OHX	CA	1762	-	0,6,6	-	-	-		
56	OHX	BA	1726	-	0,6,6	-	-	-		
56	OHX	DA	3254	-	0,6,6	-	-	-		
56	OHX	DA	3166	-	0,6,6	-	-	-		
56	OHX	DA	3461	-	0,6,6	-	-	-		
56	OHX	DA	3246	-	0,6,6	-	-	-		
56	OHX	DA	3226	-	0,6,6	-	-	-		
56	OHX	DA	3485	-	0,6,6	-	-	-		
56	OHX	BA	1774	-	0,6,6	-	-	-		
56	OHX	CA	1768	-	0,6,6	-	-	-		
56	OHX	DA	3372	-	0,6,6	-	-	-		
56	OHX	AA	3530	-	0,6,6	-	-	-		
56	OHX	BA	1809	-	0,6,6	-	-	-		
56	OHX	CA	1799	-	0,6,6	-	-	-		
56	OHX	CA	1788	-	0,6,6	-	-	-		
56	OHX	AA	3479	-	0,6,6	-	-	-		
56	OHX	CA	1792	-	0,6,6	-	-	-		
56	OHX	CA	1739	-	0,6,6	-	-	-		
56	OHX	DA	3160	-	0,6,6	-	-	-		
56	OHX	DA	3221	-	0,6,6	-	-	-		
56	OHX	CA	1746	-	0,6,6	-	-	-		
56	OHX	DA	3483	-	0,6,6	-	-	-		
56	OHX	DA	3350	-	0,6,6	-	-	-		
56	OHX	AA	3499	-	0,6,6	-	-	-		
56	OHX	AA	3438	-	0,6,6	-	-	-		
56	OHX	AA	3401	-	0,6,6	-	-	-		
56	OHX	AA	3557	-	0,6,6	-	-	-		
56	OHX	AA	3524	-	0,6,6	-	-	-		
56	OHX	AA	3446	-	0,6,6	-	-	-		
56	OHX	AA	3394	-	0,6,6	-	-	-		
56	OHX	AA	3540	-	0,6,6	-	-	-		
56	OHX	BA	1778	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	DA	3378	-	0,6,6	-	-	-		
56	OHX	AA	3437	-	0,6,6	-	-	-		
56	OHX	AA	3405	-	0,6,6	-	-	-		
56	OHX	BA	1733	-	0,6,6	-	-	-		
56	OHX	AA	3340	-	0,6,6	-	-	-		
56	OHX	AA	3409	-	0,6,6	-	-	-		
56	OHX	DA	3339	-	0,6,6	-	-	-		
56	OHX	DA	3486	-	0,6,6	-	-	-		
56	OHX	DA	3062	-	0,6,6	-	-	-		
56	OHX	CA	1802	-	0,6,6	-	-	-		
56	OHX	DA	3255	-	0,6,6	-	-	-		
56	OHX	CA	1798	-	0,6,6	-	-	-		
56	OHX	BA	1719	-	0,6,6	-	-	-		
56	OHX	DA	3380	-	0,6,6	-	-	-		
56	OHX	DA	3099	-	0,6,6	-	-	-		
56	OHX	DA	3433	-	0,6,6	-	-	-		
56	OHX	DA	3352	-	0,6,6	-	-	-		
56	OHX	DA	3388	-	0,6,6	-	-	-		
56	OHX	BA	1765	-	0,6,6	-	-	-		
56	OHX	AA	3369	-	0,6,6	-	-	-		
56	OHX	DA	3340	-	0,6,6	-	-	-		
56	OHX	DA	3402	-	0,6,6	-	-	-		
56	OHX	CA	1747	-	0,6,6	-	-	-		
56	OHX	CC	108	-	0,6,6	-	-	-		
56	OHX	CA	1740	-	0,6,6	-	-	-		
56	OHX	DA	3212	-	0,6,6	-	-	-		
56	OHX	CA	1741	-	0,6,6	-	-	-		
56	OHX	D1	201	-	0,6,6	-	-	-		
56	OHX	AA	3391	-	0,6,6	-	-	-		
56	OHX	AA	3332	-	0,6,6	-	-	-		
56	OHX	BA	1736	-	0,6,6	-	-	-		
56	OHX	BA	1746	-	0,6,6	-	-	-		
56	OHX	AA	3350	-	0,6,6	-	-	-		
56	OHX	BA	1738	-	0,6,6	-	-	-		
56	OHX	AA	3351	-	0,6,6	-	-	-		
56	OHX	DA	3379	-	0,6,6	-	-	-		
56	OHX	DA	3447	-	0,6,6	-	-	-		
56	OHX	AA	3523	-	0,6,6	-	-	-		
56	OHX	CA	1758	-	0,6,6	-	-	-		
56	OHX	DA	3075	-	0,6,6	-	-	-		
56	OHX	BA	1791	-	0,6,6	-	-	-		
56	OHX	AA	3502	-	0,6,6	-	-	-		
56	OHX	BA	1784	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	AA	3536	-	0,6,6	-	-	-		
56	OHX	BA	1766	-	0,6,6	-	-	-		
56	OHX	BA	1718	-	0,6,6	-	-	-		
56	OHX	AA	3482	-	0,6,6	-	-	-		
56	OHX	AA	3515	-	0,6,6	-	-	-		
56	OHX	AA	3402	-	0,6,6	-	-	-		
56	OHX	BA	1777	-	0,6,6	-	-	-		
56	OHX	AA	3453	-	0,6,6	-	-	-		
56	OHX	BA	1782	-	0,6,6	-	-	-		
56	OHX	DA	3118	-	0,6,6	-	-	-		
56	OHX	DA	3344	-	0,6,6	-	-	-		
56	OHX	AA	3338	-	0,6,6	-	-	-		
56	OHX	DA	3383	-	0,6,6	-	-	-		
56	OHX	AA	3512	-	0,6,6	-	-	-		
56	OHX	CA	1744	-	0,6,6	-	-	-		
56	OHX	CA	1794	-	0,6,6	-	-	-		
56	OHX	AA	3464	-	0,6,6	-	-	-		
56	OHX	BA	1810	-	0,6,6	-	-	-		
56	OHX	DA	3109	-	0,6,6	-	-	-		
56	OHX	CA	1736	-	0,6,6	-	-	-		
56	OHX	CA	1783	-	0,6,6	-	-	-		
56	OHX	BA	1735	-	0,6,6	-	-	-		
56	OHX	DA	3393	-	0,6,6	-	-	-		
56	OHX	DA	3170	-	0,6,6	-	-	-		
56	OHX	AA	3418	-	0,6,6	-	-	-		
56	OHX	AA	3435	-	0,6,6	-	-	-		
56	OHX	AA	3411	-	0,6,6	-	-	-		
56	OHX	BL	201	-	0,6,6	-	-	-		
56	OHX	AA	3364	-	0,6,6	-	-	-		
56	OHX	AA	3506	-	0,6,6	-	-	-		
56	OHX	DA	3464	-	0,6,6	-	-	-		
56	OHX	DA	3484	-	0,6,6	-	-	-		
56	OHX	CA	1786	-	0,6,6	-	-	-		
56	OHX	AA	3371	-	0,6,6	-	-	-		
56	OHX	AA	3344	-	0,6,6	-	-	-		
56	OHX	AA	3494	-	0,6,6	-	-	-		
56	OHX	DA	3488	-	0,6,6	-	-	-		
56	OHX	DA	3397	-	0,6,6	-	-	-		
56	OHX	D5	102	-	0,6,6	-	-	-		
56	OHX	DA	3335	-	0,6,6	-	-	-		
56	OHX	AA	3567	-	0,6,6	-	-	-		
56	OHX	AA	3363	-	0,6,6	-	-	-		
56	OHX	BA	1750	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	BA	1749	-	0,6,6	-	-	-		
56	OHX	AA	3347	-	0,6,6	-	-	-		
56	OHX	AA	3440	-	0,6,6	-	-	-		
56	OHX	DA	3223	-	0,6,6	-	-	-		
56	OHX	DA	3438	-	0,6,6	-	-	-		
56	OHX	AA	3541	-	0,6,6	-	-	-		
56	OHX	DA	3401	-	0,6,6	-	-	-		
56	OHX	AA	3534	-	0,6,6	-	-	-		
56	OHX	BA	1741	-	0,6,6	-	-	-		
56	OHX	CA	1813	-	0,6,6	-	-	-		
56	OHX	CA	1743	-	0,6,6	-	-	-		
56	OHX	AA	3415	-	0,6,6	-	-	-		
56	OHX	AA	3518	-	0,6,6	-	-	-		
56	OHX	BA	1742	-	0,6,6	-	-	-		
56	OHX	DA	3474	-	0,6,6	-	-	-		
56	OHX	AA	3449	-	0,6,6	-	-	-		
56	OHX	DA	3220	-	0,6,6	-	-	-		
56	OHX	DA	3362	-	0,6,6	-	-	-		
56	OHX	DA	3163	-	0,6,6	-	-	-		
56	OHX	CA	1760	-	0,6,6	-	-	-		
56	OHX	DA	3172	-	0,6,6	-	-	-		
56	OHX	CA	1781	-	0,6,6	-	-	-		
56	OHX	AA	3427	-	0,6,6	-	-	-		
56	OHX	AA	3388	-	0,6,6	-	-	-		
56	OHX	CA	1749	-	0,6,6	-	-	-		
56	OHX	CA	1796	-	0,6,6	-	-	-		
56	OHX	AA	3475	-	0,6,6	-	-	-		
56	OHX	BA	1759	-	0,6,6	-	-	-		
56	OHX	CA	1731	-	0,6,6	-	-	-		
56	OHX	AA	3509	-	0,6,6	-	-	-		
56	OHX	CA	1793	-	0,6,6	-	-	-		
56	OHX	DA	3421	-	0,6,6	-	-	-		
56	OHX	DB	210	-	0,6,6	-	-	-		
56	OHX	DA	3083	-	0,6,6	-	-	-		
56	OHX	BA	1758	-	0,6,6	-	-	-		
56	OHX	AA	3532	-	0,6,6	-	-	-		
56	OHX	DA	3366	-	0,6,6	-	-	-		
56	OHX	AB	208	-	0,6,6	-	-	-		
56	OHX	AA	3485	-	0,6,6	-	-	-		
56	OHX	BA	1790	-	0,6,6	-	-	-		
56	OHX	AA	3533	-	0,6,6	-	-	-		
56	OHX	AA	3483	-	0,6,6	-	-	-		
56	OHX	DA	3361	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	OHX	DA	3356	-	0,6,6	-	-	-		
56	OHX	DA	3385	-	0,6,6	-	-	-		
56	OHX	CA	1727	-	0,6,6	-	-	-		
56	OHX	DB	218	-	0,6,6	-	-	-		
56	OHX	BA	1748	-	0,6,6	-	-	-		
56	OHX	DA	3387	-	0,6,6	-	-	-		
56	OHX	AA	3460	-	0,6,6	-	-	-		
56	OHX	BA	1723	-	0,6,6	-	-	-		
56	OHX	DA	3258	-	0,6,6	-	-	-		
56	OHX	AA	3329	-	0,6,6	-	-	-		
56	OHX	AA	3420	-	0,6,6	-	-	-		
56	OHX	CA	1772	-	0,6,6	-	-	-		
56	OHX	AA	3462	-	0,6,6	-	-	-		
56	OHX	AA	3472	-	0,6,6	-	-	-		
56	OHX	DA	3384	-	0,6,6	-	-	-		
56	OHX	BA	1753	-	0,6,6	-	-	-		
56	OHX	DA	3338	-	0,6,6	-	-	-		
56	OHX	DA	3343	-	0,6,6	-	-	-		
56	OHX	DA	3377	-	0,6,6	-	-	-		
56	OHX	AA	3358	-	0,6,6	-	-	-		
56	OHX	AA	3550	-	0,6,6	-	-	-		
56	OHX	AA	3565	-	0,6,6	-	-	-		
56	OHX	DA	3355	-	0,6,6	-	-	-		
56	OHX	AA	3429	-	0,6,6	-	-	-		
56	OHX	DA	3419	-	0,6,6	-	-	-		
56	OHX	AA	3563	-	0,6,6	-	-	-		
56	OHX	CA	1738	-	0,6,6	-	-	-		
56	OHX	BA	1802	-	0,6,6	-	-	-		
56	OHX	BA	1813	-	0,6,6	-	-	-		
56	OHX	BA	1727	-	0,6,6	-	-	-		
56	OHX	DA	3436	-	0,6,6	-	-	-		
56	OHX	DA	3169	-	0,6,6	-	-	-		
56	OHX	AA	3359	-	0,6,6	-	-	-		
56	OHX	DA	3354	-	0,6,6	-	-	-		
56	OHX	DA	3466	-	0,6,6	-	-	-		
56	OHX	DA	3395	-	0,6,6	-	-	-		
56	OHX	AA	3360	-	0,6,6	-	-	-		
56	OHX	AA	3447	-	0,6,6	-	-	-		
56	OHX	DA	3071	-	0,6,6	-	-	-		
56	OHX	AA	3458	-	0,6,6	-	-	-		
56	OHX	DA	3174	-	0,6,6	-	-	-		
56	OHX	CA	1801	-	0,6,6	-	-	-		
56	OHX	AA	3556	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	OHX	DA	3406	-	0,6,6	-	-	-		
56	OHX	CD	101	-	0,6,6	-	-	-		
56	OHX	CA	1815	-	0,6,6	-	-	-		
56	OHX	AA	3423	-	0,6,6	-	-	-		
56	OHX	AB	209	-	0,6,6	-	-	-		
56	OHX	DA	3347	-	0,6,6	-	-	-		
56	OHX	AA	3546	-	0,6,6	-	-	-		
56	OHX	DB	208	-	0,6,6	-	-	-		
56	OHX	BA	1744	-	0,6,6	-	-	-		
56	OHX	DA	3381	-	0,6,6	-	-	-		
56	OHX	AA	3568	-	0,6,6	-	-	-		
56	OHX	CA	1782	-	0,6,6	-	-	-		
56	OHX	AA	3547	-	0,6,6	-	-	-		
56	OHX	AA	3486	-	0,6,6	-	-	-		
56	OHX	AA	3569	-	0,6,6	-	-	-		
56	OHX	DA	3342	-	0,6,6	-	-	-		
56	OHX	DA	3454	-	0,6,6	-	-	-		
56	OHX	AA	3373	-	0,6,6	-	-	-		
56	OHX	CA	1774	-	0,6,6	-	-	-		
56	OHX	BA	1764	-	0,6,6	-	-	-		
56	OHX	DA	3481	-	0,6,6	-	-	-		
56	OHX	DA	3442	-	0,6,6	-	-	-		
56	OHX	DA	3064	-	0,6,6	-	-	-		
56	OHX	DA	3349	-	0,6,6	-	-	-		
56	OHX	BA	1795	-	0,6,6	-	-	-		
56	OHX	AA	3431	-	0,6,6	-	-	-		
56	OHX	DB	209	-	0,6,6	-	-	-		
56	OHX	DA	3475	-	0,6,6	-	-	-		
56	OHX	DA	3472	-	0,6,6	-	-	-		
56	OHX	CA	1797	-	0,6,6	-	-	-		
56	OHX	DA	3415	-	0,6,6	-	-	-		
56	OHX	AA	3466	-	0,6,6	-	-	-		
56	OHX	DA	3417	-	0,6,6	-	-	-		
56	OHX	CA	1735	-	0,6,6	-	-	-		
56	OHX	DA	3449	-	0,6,6	-	-	-		
56	OHX	DA	3358	-	0,6,6	-	-	-		
56	OHX	CA	1761	-	0,6,6	-	-	-		
56	OHX	DA	3400	-	0,6,6	-	-	-		
56	OHX	BA	1781	-	0,6,6	-	-	-		
56	OHX	DA	3477	-	0,6,6	-	-	-		
56	OHX	AB	219	-	0,6,6	-	-	-		
56	OHX	BA	1801	-	0,6,6	-	-	-		
56	OHX	AA	3390	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	DA	3473	-	0,6,6	-	-	-		
56	OHX	AA	3398	-	0,6,6	-	-	-		
56	OHX	CA	1769	-	0,6,6	-	-	-		
56	OHX	AA	3522	-	0,6,6	-	-	-		
56	OHX	CA	1728	-	0,6,6	-	-	-		
56	OHX	AA	3484	-	0,6,6	-	-	-		
56	OHX	DA	3456	-	0,6,6	-	-	-		
56	OHX	AA	3341	-	0,6,6	-	-	-		
56	OHX	CA	1742	-	0,6,6	-	-	-		
56	OHX	AA	3454	-	0,6,6	-	-	-		
56	OHX	CA	1814	-	0,6,6	-	-	-		
56	OHX	AA	3433	-	0,6,6	-	-	-		
56	OHX	DA	3410	-	0,6,6	-	-	-		
56	OHX	BA	1811	-	0,6,6	-	-	-		
56	OHX	BA	1799	-	0,6,6	-	-	-		
56	OHX	AA	3384	-	0,6,6	-	-	-		
56	OHX	AA	3503	-	0,6,6	-	-	-		
56	OHX	BA	1755	-	0,6,6	-	-	-		
56	OHX	DA	3336	-	0,6,6	-	-	-		
56	OHX	AA	3566	-	0,6,6	-	-	-		
56	OHX	DA	3351	-	0,6,6	-	-	-		
56	OHX	DA	3365	-	0,6,6	-	-	-		
56	OHX	CA	1757	-	0,6,6	-	-	-		
56	OHX	BA	1792	-	0,6,6	-	-	-		
56	OHX	AA	3349	-	0,6,6	-	-	-		
56	OHX	AA	3397	-	0,6,6	-	-	-		
56	OHX	AA	3455	-	0,6,6	-	-	-		
56	OHX	AA	3345	-	0,6,6	-	-	-		
56	OHX	DA	3420	-	0,6,6	-	-	-		
56	OHX	AA	3491	-	0,6,6	-	-	-		
56	OHX	AA	3406	-	0,6,6	-	-	-		
56	OHX	DA	3084	-	0,6,6	-	-	-		
56	OHX	AA	3487	-	0,6,6	-	-	-		
56	OHX	AA	3417	-	0,6,6	-	-	-		
56	OHX	AA	3457	-	0,6,6	-	-	-		
56	OHX	DA	3176	-	0,6,6	-	-	-		
56	OHX	AA	3470	-	0,6,6	-	-	-		
56	OHX	CA	1808	-	0,6,6	-	-	-		
56	OHX	DB	219	-	0,6,6	-	-	-		
56	OHX	DA	3359	-	0,6,6	-	-	-		
56	OHX	BA	1721	-	0,6,6	-	-	-		
56	OHX	AA	3471	-	0,6,6	-	-	-		
56	OHX	DA	3243	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	AA	3387	-	0,6,6	-	-	-		
56	OHX	DA	3487	-	0,6,6	-	-	-		
56	OHX	BA	1773	-	0,6,6	-	-	-		
56	OHX	DA	3476	-	0,6,6	-	-	-		
56	OHX	CA	1755	-	0,6,6	-	-	-		
56	OHX	AA	3505	-	0,6,6	-	-	-		
56	OHX	BA	1783	-	0,6,6	-	-	-		
56	OHX	DA	3357	-	0,6,6	-	-	-		
56	OHX	CA	1771	-	0,6,6	-	-	-		
56	OHX	D3	101	-	0,6,6	-	-	-		
56	OHX	AA	3412	-	0,6,6	-	-	-		
56	OHX	DA	3173	-	0,6,6	-	-	-		
56	OHX	CA	1791	-	0,6,6	-	-	-		
56	OHX	DA	3479	-	0,6,6	-	-	-		
56	OHX	CA	1729	-	0,6,6	-	-	-		
56	OHX	AA	3410	-	0,6,6	-	-	-		
56	OHX	DA	3087	-	0,6,6	-	-	-		
56	OHX	AA	3436	-	0,6,6	-	-	-		
56	OHX	DA	3416	-	0,6,6	-	-	-		
56	OHX	DA	3458	-	0,6,6	-	-	-		
56	OHX	AW	101	-	0,6,6	-	-	-		
56	OHX	AB	210	-	0,6,6	-	-	-		
56	OHX	AA	3508	-	0,6,6	-	-	-		
56	OHX	DA	3065	-	0,6,6	-	-	-		
56	OHX	AA	3385	-	0,6,6	-	-	-		
56	OHX	BA	1775	-	0,6,6	-	-	-		
56	OHX	DA	3373	-	0,6,6	-	-	-		
56	OHX	CB	105	-	0,6,6	-	-	-		
56	OHX	DA	3405	-	0,6,6	-	-	-		
56	OHX	AA	3527	-	0,6,6	-	-	-		
56	OHX	DA	3132	-	0,6,6	-	-	-		
56	OHX	DA	3445	-	0,6,6	-	-	-		
56	OHX	DA	3389	-	0,6,6	-	-	-		
56	OHX	DA	3408	-	0,6,6	-	-	-		
56	OHX	DA	3443	-	0,6,6	-	-	-		
56	OHX	AA	3504	-	0,6,6	-	-	-		
56	OHX	DA	3091	-	0,6,6	-	-	-		
56	OHX	DA	3251	-	0,6,6	-	-	-		
56	OHX	AO	202	-	0,6,6	-	-	-		
56	OHX	AA	3493	-	0,6,6	-	-	-		
56	OHX	A1	204	-	0,6,6	-	-	-		
56	OHX	AA	3395	-	0,6,6	-	-	-		
56	OHX	D8	101	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	DA	3451	-	0,6,6	-	-	-		
56	OHX	DA	3081	-	0,6,6	-	-	-		
56	OHX	DA	3432	-	0,6,6	-	-	-		
56	OHX	CA	1800	-	0,6,6	-	-	-		
56	OHX	AA	3549	-	0,6,6	-	-	-		
56	OHX	AA	3392	-	0,6,6	-	-	-		
56	OHX	AA	3560	-	0,6,6	-	-	-		
56	OHX	AA	3355	-	0,6,6	-	-	-		
56	OHX	BA	1780	-	0,6,6	-	-	-		
56	OHX	CA	1724	-	0,6,6	-	-	-		
56	OHX	DA	3441	-	0,6,6	-	-	-		
56	OHX	DA	3218	-	0,6,6	-	-	-		
56	OHX	DA	3337	-	0,6,6	-	-	-		
56	OHX	BA	1722	-	0,6,6	-	-	-		
56	OHX	DO	201	-	0,6,6	-	-	-		
56	OHX	AA	3374	-	0,6,6	-	-	-		
56	OHX	BA	1762	-	0,6,6	-	-	-		
56	OHX	CA	1745	-	0,6,6	-	-	-		
56	OHX	DA	3374	-	0,6,6	-	-	-		
56	OHX	CA	1734	-	0,6,6	-	-	-		
56	OHX	AA	3368	-	0,6,6	-	-	-		
56	OHX	DA	3463	-	0,6,6	-	-	-		
56	OHX	BD	103	-	0,6,6	-	-	-		
56	OHX	BA	1767	-	0,6,6	-	-	-		
56	OHX	DA	3249	-	0,6,6	-	-	-		
56	OHX	CA	1809	-	0,6,6	-	-	-		
56	OHX	A3	102	-	0,6,6	-	-	-		
56	OHX	CA	1777	-	0,6,6	-	-	-		
56	OHX	AA	3456	-	0,6,6	-	-	-		
56	OHX	DA	3245	-	0,6,6	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PAR	BA	1715	-	-	5/18/94/94	0/4/4/4
57	PAR	CA	1722	-	-	4/18/94/94	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	BA	1715	PAR	C21-N21	-2.30	1.43	1.47
57	BA	1715	PAR	C31-C21	-2.16	1.50	1.53

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	CA	1722	PAR	C11-O51-C51	5.05	123.58	113.72
57	CA	1722	PAR	C13-O52-C52	-4.64	106.98	117.98
57	BA	1715	PAR	C44-C34-C24	4.52	118.49	110.99
57	BA	1715	PAR	C11-O51-C51	4.28	122.08	113.72
57	CA	1722	PAR	C62-C12-N12	-4.23	102.59	110.94

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	CA	1722	PAR	O43-C43-C53-O53
57	CA	1722	PAR	C33-C43-C53-O53
57	CA	1722	PAR	C41-C51-C61-O61
57	BA	1715	PAR	C41-C51-C61-O61
57	BA	1715	PAR	O43-C43-C53-O53

There are no ring outliers.

332 monomers are involved in 465 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	BA	1724	OHX	1	0
56	DA	3422	OHX	1	0
56	BA	1745	OHX	2	0
56	DA	3398	OHX	1	0
56	CA	1773	OHX	1	0
56	CV	101	OHX	1	0
56	CA	1778	OHX	1	0
56	DA	3407	OHX	1	0
56	BA	1760	OHX	1	0
56	AB	218	OHX	1	0
56	AA	3342	OHX	2	0
56	AA	3554	OHX	1	0
56	DA	3399	OHX	1	0
56	AA	3529	OHX	1	0
56	DA	3364	OHX	1	0
56	AA	3553	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	DA	3127	OHX	1	0
56	DA	3382	OHX	1	0
56	CA	1766	OHX	1	0
56	AA	3496	OHX	1	0
56	DA	3412	OHX	1	0
56	BA	1788	OHX	1	0
56	DA	3444	OHX	2	0
56	AA	3445	OHX	1	0
56	AA	3535	OHX	1	0
56	AA	3497	OHX	2	0
56	DA	3427	OHX	3	0
56	BA	1756	OHX	1	0
56	BA	1785	OHX	5	0
56	BA	1732	OHX	1	0
56	CA	1779	OHX	3	0
56	CA	1775	OHX	1	0
56	CA	1751	OHX	1	0
56	DA	3411	OHX	1	0
56	CA	1770	OHX	1	0
56	AA	3507	OHX	2	0
56	AA	3362	OHX	2	0
56	DA	3470	OHX	2	0
56	DA	3468	OHX	1	0
56	AB	215	OHX	1	0
56	CA	1750	OHX	1	0
56	DA	3471	OHX	2	0
57	CA	1722	PAR	1	0
56	DA	3348	OHX	1	0
56	AA	3422	OHX	1	0
56	AA	3514	OHX	1	0
56	AF	303	OHX	3	0
56	CA	1790	OHX	2	0
56	AA	3414	OHX	1	0
56	DA	3426	OHX	1	0
56	BA	1806	OHX	2	0
56	DA	3478	OHX	2	0
56	DA	3068	OHX	1	0
56	DA	3489	OHX	2	0
56	BA	1734	OHX	1	0
56	AA	3463	OHX	1	0
56	DA	3459	OHX	1	0
56	DA	3253	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	CA	1764	OHX	1	0
56	AA	3558	OHX	2	0
56	AA	3375	OHX	1	0
56	AA	3516	OHX	1	0
56	BD	102	OHX	1	0
56	DA	3457	OHX	1	0
56	AA	3468	OHX	1	0
56	BA	1805	OHX	1	0
56	CA	1811	OHX	1	0
56	CC	110	OHX	1	0
56	CA	1733	OHX	1	0
56	AA	3525	OHX	1	0
56	AA	3331	OHX	1	0
56	AO	203	OHX	1	0
56	AA	3376	OHX	1	0
56	BA	1757	OHX	1	0
56	BA	1728	OHX	1	0
56	AA	3538	OHX	2	0
56	AA	3407	OHX	1	0
56	BA	1716	OHX	1	0
56	DA	3439	OHX	1	0
56	AB	213	OHX	1	0
56	DA	3061	OHX	1	0
56	AA	3441	OHX	1	0
56	DA	3111	OHX	2	0
56	CA	1784	OHX	1	0
56	DA	3159	OHX	1	0
56	DA	3248	OHX	1	0
56	DA	3390	OHX	1	0
56	BA	1807	OHX	1	0
56	CA	1723	OHX	2	0
56	DA	3162	OHX	1	0
56	CA	1756	OHX	2	0
56	DA	3376	OHX	1	0
56	DA	3341	OHX	1	0
56	CB	104	OHX	1	0
56	BA	1772	OHX	2	0
56	CA	1753	OHX	1	0
56	BC	106	OHX	1	0
56	AA	3346	OHX	1	0
56	DA	3428	OHX	2	0
56	AA	3377	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	AA	3419	OHX	1	0
56	DA	3214	OHX	2	0
56	AA	3551	OHX	2	0
56	CA	1785	OHX	3	0
56	DB	213	OHX	1	0
56	BA	1717	OHX	1	0
56	BA	1761	OHX	1	0
56	A6	101	OHX	1	0
56	AA	3361	OHX	1	0
56	BA	1770	OHX	1	0
56	AA	3383	OHX	1	0
56	DF	301	OHX	1	0
56	BA	1763	OHX	1	0
56	BC	105	OHX	1	0
56	BA	1812	OHX	1	0
56	AA	3330	OHX	5	0
56	AA	3545	OHX	1	0
56	CA	1759	OHX	1	0
56	DA	3368	OHX	1	0
56	DA	3437	OHX	1	0
56	DA	3346	OHX	1	0
56	AA	3467	OHX	1	0
56	AA	3416	OHX	3	0
56	BA	1720	OHX	1	0
56	CA	1803	OHX	1	0
56	AA	3555	OHX	1	0
56	CK	201	OHX	1	0
56	AA	3335	OHX	1	0
56	AA	3473	OHX	2	0
56	BA	1789	OHX	1	0
56	DB	220	OHX	1	0
56	CA	1737	OHX	2	0
56	DA	3257	OHX	1	0
56	DA	3215	OHX	1	0
56	CA	1776	OHX	1	0
56	DB	212	OHX	1	0
56	DA	3391	OHX	1	0
56	AA	3432	OHX	1	0
56	AA	3481	OHX	1	0
56	AA	3399	OHX	2	0
56	AA	3370	OHX	1	0
56	DA	3418	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	CA	1725	OHX	2	0
57	BA	1715	PAR	3	0
56	DA	3465	OHX	1	0
56	BA	1796	OHX	1	0
56	CA	1730	OHX	1	0
56	CA	1810	OHX	2	0
56	BA	1793	OHX	2	0
56	DA	3430	OHX	1	0
56	BA	1747	OHX	1	0
56	CA	1805	OHX	1	0
56	CA	1726	OHX	1	0
56	AA	3531	OHX	1	0
56	AA	3561	OHX	2	0
56	DA	3403	OHX	2	0
56	BG	302	OHX	2	0
56	AA	3365	OHX	4	0
56	AA	3367	OHX	3	0
56	BA	1794	OHX	1	0
56	DA	3103	OHX	3	0
56	AA	3333	OHX	1	0
56	CA	1762	OHX	7	0
56	DA	3461	OHX	1	0
56	DA	3246	OHX	1	0
56	CA	1768	OHX	1	0
56	AA	3530	OHX	1	0
56	CA	1788	OHX	2	0
56	AA	3479	OHX	1	0
56	CA	1792	OHX	2	0
56	CA	1739	OHX	1	0
56	DA	3221	OHX	2	0
56	CA	1746	OHX	1	0
56	DA	3483	OHX	1	0
56	AA	3438	OHX	1	0
56	AA	3557	OHX	2	0
56	AA	3524	OHX	1	0
56	AA	3540	OHX	1	0
56	AA	3405	OHX	1	0
56	BA	1733	OHX	3	0
56	AA	3409	OHX	2	0
56	DA	3486	OHX	1	0
56	DA	3062	OHX	1	0
56	DA	3255	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	CA	1798	OHX	4	0
56	DA	3099	OHX	1	0
56	DA	3388	OHX	2	0
56	DA	3340	OHX	1	0
56	CC	108	OHX	6	0
56	CA	1740	OHX	1	0
56	DA	3212	OHX	1	0
56	CA	1741	OHX	2	0
56	AA	3391	OHX	2	0
56	BA	1746	OHX	1	0
56	AA	3350	OHX	1	0
56	AA	3351	OHX	1	0
56	DA	3379	OHX	2	0
56	AA	3523	OHX	1	0
56	CA	1758	OHX	1	0
56	BA	1791	OHX	3	0
56	AA	3502	OHX	2	0
56	BA	1784	OHX	2	0
56	AA	3536	OHX	2	0
56	BA	1766	OHX	1	0
56	AA	3453	OHX	2	0
56	DA	3118	OHX	1	0
56	DA	3344	OHX	3	0
56	AA	3512	OHX	1	0
56	AA	3464	OHX	1	0
56	BA	1735	OHX	1	0
56	AA	3418	OHX	1	0
56	AA	3364	OHX	1	0
56	AA	3506	OHX	1	0
56	DA	3484	OHX	1	0
56	CA	1786	OHX	1	0
56	AA	3371	OHX	1	0
56	AA	3494	OHX	1	0
56	DA	3488	OHX	3	0
56	D5	102	OHX	1	0
56	AA	3567	OHX	1	0
56	AA	3347	OHX	1	0
56	DA	3223	OHX	1	0
56	DA	3438	OHX	1	0
56	DA	3401	OHX	1	0
56	AA	3415	OHX	3	0
56	DA	3362	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	CA	1760	OHX	1	0
56	DA	3172	OHX	2	0
56	AA	3388	OHX	2	0
56	CA	1749	OHX	1	0
56	AA	3475	OHX	1	0
56	CA	1731	OHX	1	0
56	AA	3509	OHX	1	0
56	CA	1793	OHX	1	0
56	DB	210	OHX	1	0
56	DA	3083	OHX	1	0
56	BA	1790	OHX	1	0
56	DA	3385	OHX	2	0
56	CA	1727	OHX	1	0
56	DA	3258	OHX	1	0
56	AA	3329	OHX	1	0
56	AA	3462	OHX	1	0
56	DA	3384	OHX	1	0
56	DA	3343	OHX	3	0
56	DA	3377	OHX	2	0
56	AA	3550	OHX	1	0
56	AA	3565	OHX	1	0
56	DA	3419	OHX	2	0
56	CA	1738	OHX	2	0
56	BA	1802	OHX	4	0
56	BA	1813	OHX	2	0
56	DA	3169	OHX	1	0
56	DA	3395	OHX	1	0
56	AA	3447	OHX	1	0
56	AA	3458	OHX	1	0
56	AA	3556	OHX	1	0
56	DA	3406	OHX	1	0
56	CD	101	OHX	1	0
56	CA	1815	OHX	1	0
56	AA	3423	OHX	1	0
56	AB	209	OHX	1	0
56	AA	3546	OHX	1	0
56	AA	3568	OHX	1	0
56	CA	1782	OHX	1	0
56	AA	3547	OHX	6	0
56	AA	3569	OHX	3	0
56	DA	3454	OHX	1	0
56	AA	3373	OHX	1	0

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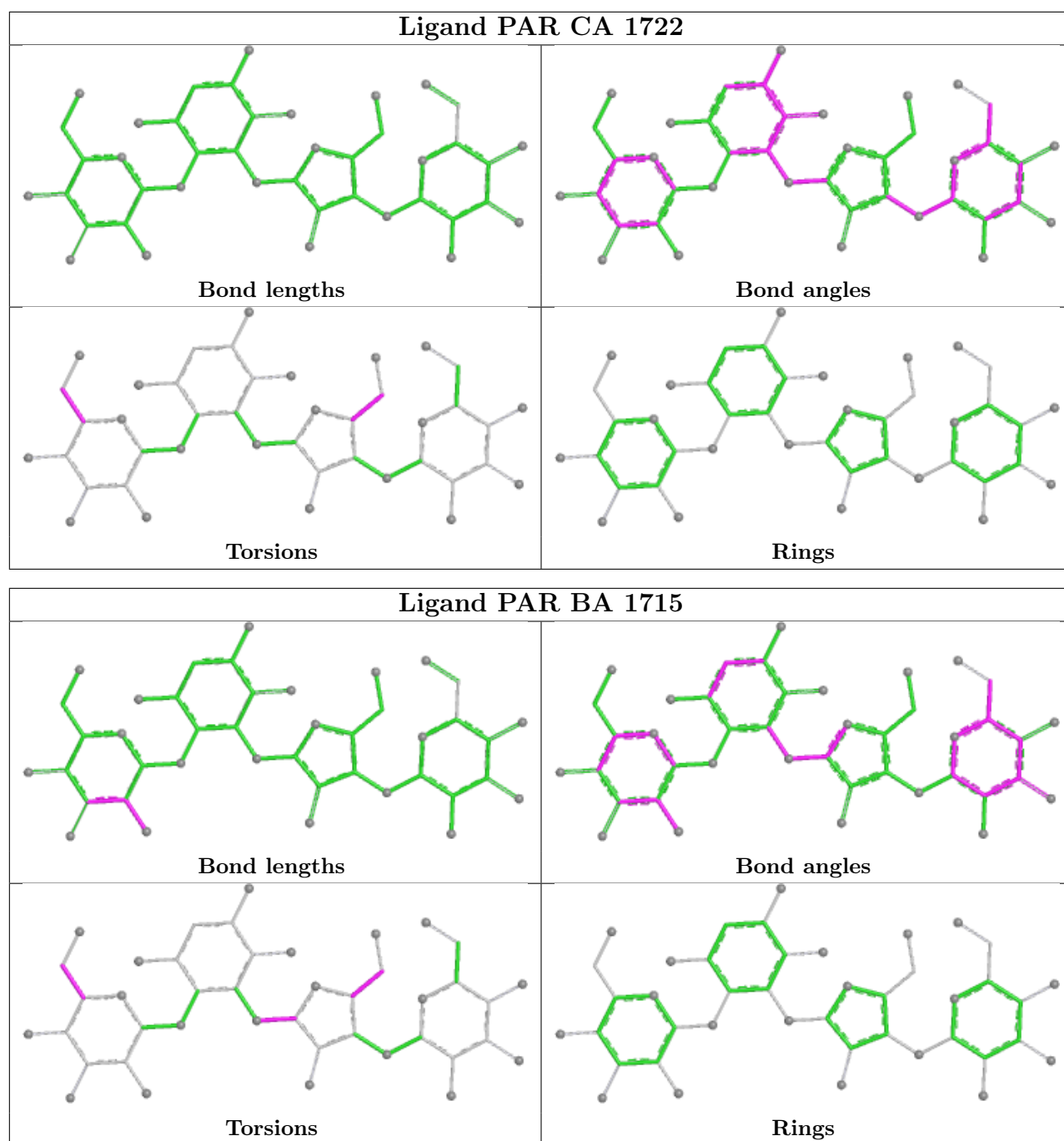
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	CA	1774	OHX	1	0
56	DA	3064	OHX	3	0
56	DB	209	OHX	1	0
56	CA	1797	OHX	2	0
56	DA	3415	OHX	1	0
56	AA	3466	OHX	1	0
56	CA	1735	OHX	1	0
56	DA	3400	OHX	2	0
56	AB	219	OHX	2	0
56	BA	1801	OHX	1	0
56	DA	3473	OHX	1	0
56	CA	1769	OHX	1	0
56	CA	1728	OHX	1	0
56	CA	1742	OHX	1	0
56	AA	3433	OHX	3	0
56	DA	3410	OHX	2	0
56	BA	1811	OHX	2	0
56	BA	1799	OHX	1	0
56	AA	3384	OHX	1	0
56	BA	1755	OHX	1	0
56	DA	3336	OHX	1	0
56	AA	3566	OHX	1	0
56	CA	1757	OHX	1	0
56	BA	1792	OHX	1	0
56	AA	3487	OHX	1	0
56	AA	3417	OHX	1	0
56	DA	3176	OHX	1	0
56	DB	219	OHX	1	0
56	BA	1721	OHX	3	0
56	DA	3487	OHX	1	0
56	BA	1773	OHX	2	0
56	CA	1755	OHX	1	0
56	AA	3505	OHX	1	0
56	CA	1771	OHX	1	0
56	D3	101	OHX	1	0
56	AA	3412	OHX	2	0
56	DA	3173	OHX	2	0
56	DA	3087	OHX	1	0
56	DA	3416	OHX	1	0
56	BA	1775	OHX	1	0
56	CB	105	OHX	1	0
56	AA	3527	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	DA	3132	OHX	1	0
56	DA	3445	OHX	1	0
56	DA	3389	OHX	3	0
56	DA	3443	OHX	1	0
56	AA	3504	OHX	4	0
56	DA	3251	OHX	1	0
56	AO	202	OHX	1	0
56	D8	101	OHX	5	0
56	DA	3081	OHX	1	0
56	AA	3392	OHX	1	0
56	AA	3560	OHX	1	0
56	BA	1780	OHX	1	0
56	CA	1724	OHX	1	0
56	DA	3441	OHX	1	0
56	DA	3337	OHX	1	0
56	AA	3374	OHX	2	0
56	BA	1762	OHX	1	0
56	DA	3374	OHX	3	0
56	CA	1734	OHX	2	0
56	CA	1809	OHX	1	0
56	A3	102	OHX	1	0
56	CA	1777	OHX	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	2912/2912 (100%)	-0.57	13 (0%) 88 79	44, 79, 216, 250	0
1	DA	2907/2912 (99%)	-0.35	26 (0%) 81 65	56, 94, 236, 252	0
2	AB	122/122 (100%)	-0.59	0 100 100	77, 99, 118, 184	0
2	DB	122/122 (100%)	-0.29	1 (0%) 82 68	98, 129, 153, 204	0
3	AD	272/276 (98%)	0.08	10 (3%) 45 31	42, 67, 88, 106	0
3	DD	272/276 (98%)	0.04	8 (2%) 53 35	52, 78, 98, 130	0
4	AE	205/206 (99%)	0.22	9 (4%) 39 25	54, 90, 135, 147	0
4	DE	205/206 (99%)	0.37	13 (6%) 26 17	61, 102, 153, 167	0
5	AF	202/210 (96%)	-0.14	4 (1%) 65 46	49, 84, 121, 136	0
5	DF	208/210 (99%)	0.20	13 (6%) 26 17	63, 108, 164, 189	0
6	AG	181/182 (99%)	-0.06	6 (3%) 49 33	90, 112, 143, 155	0
6	DG	181/182 (99%)	0.66	17 (9%) 14 11	122, 146, 169, 175	0
7	AH	170/180 (94%)	0.08	1 (0%) 85 73	89, 116, 133, 162	0
7	DH	170/180 (94%)	0.96	26 (15%) 5 5	162, 204, 226, 236	0
8	AK	146/148 (98%)	0.13	3 (2%) 63 44	78, 134, 153, 155	0
8	DK	146/148 (98%)	0.65	22 (15%) 5 5	88, 135, 157, 163	0
9	AM	138/140 (98%)	0.27	8 (5%) 29 19	68, 92, 129, 141	0
9	DM	138/140 (98%)	0.26	2 (1%) 73 55	83, 117, 146, 159	0
10	AN	122/122 (100%)	0.02	1 (0%) 82 68	61, 79, 96, 107	0
10	DN	122/122 (100%)	0.24	1 (0%) 82 68	75, 97, 114, 124	0
11	AO	150/150 (100%)	0.28	11 (7%) 21 15	46, 93, 120, 166	0
11	DO	150/150 (100%)	0.70	24 (16%) 5 4	45, 106, 147, 183	0
12	AP	141/141 (100%)	0.92	31 (21%) 2 2	58, 86, 108, 136	0
12	DP	141/141 (100%)	1.30	32 (22%) 2 2	58, 111, 143, 164	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	A0	118/118 (100%)	-0.02	3 (2%) 58 39	57, 86, 110, 118	0
13	D0	117/118 (99%)	-0.15	1 (0%) 81 65	68, 89, 109, 124	0
14	AQ	111/112 (99%)	-0.18	2 (1%) 67 49	67, 97, 120, 133	0
14	DQ	111/112 (99%)	0.15	5 (4%) 38 25	85, 126, 150, 162	0
15	AR	137/146 (93%)	0.17	2 (1%) 72 53	75, 96, 149, 175	0
15	DR	137/146 (93%)	0.69	13 (9%) 14 11	81, 106, 168, 189	0
16	A1	117/118 (99%)	0.09	3 (2%) 57 38	58, 81, 110, 142	0
16	D1	117/118 (99%)	-0.01	1 (0%) 81 65	71, 109, 145, 167	0
17	A2	101/101 (100%)	0.47	7 (6%) 23 16	51, 104, 126, 143	0
17	D2	101/101 (100%)	0.49	14 (13%) 6 5	65, 134, 147, 155	0
18	AS	113/113 (100%)	-0.02	0 100 100	61, 77, 108, 161	0
18	DS	113/113 (100%)	0.21	4 (3%) 47 31	66, 82, 116, 162	0
19	AT	92/96 (95%)	-0.06	2 (2%) 62 43	59, 73, 99, 111	0
19	DT	92/96 (95%)	0.38	6 (6%) 25 17	74, 92, 117, 133	0
20	AU	102/110 (92%)	0.41	4 (3%) 43 29	79, 105, 156, 168	0
20	DU	102/110 (92%)	1.44	29 (28%) 1 1	97, 122, 169, 185	0
21	AV	175/206 (84%)	0.92	25 (14%) 6 5	90, 131, 195, 198	0
21	DV	179/206 (86%)	0.62	12 (6%) 24 16	127, 165, 214, 226	0
22	A3	76/85 (89%)	-0.09	1 (1%) 75 56	65, 78, 95, 130	0
22	D3	77/85 (90%)	0.53	7 (9%) 15 11	78, 97, 119, 152	0
23	AZ	97/98 (98%)	0.40	10 (10%) 12 10	59, 79, 131, 161	0
23	DZ	97/98 (98%)	0.62	8 (8%) 17 13	69, 89, 136, 157	0
24	AW	66/72 (91%)	-0.01	3 (4%) 38 25	63, 87, 103, 128	0
24	DW	66/72 (91%)	0.16	2 (3%) 52 35	88, 112, 132, 142	0
25	AX	59/60 (98%)	-0.09	0 100 100	66, 86, 119, 134	0
25	DX	59/60 (98%)	0.10	1 (1%) 69 50	87, 113, 146, 167	0
26	A4	66/71 (92%)	0.23	3 (4%) 38 25	130, 162, 180, 188	0
26	D4	63/71 (88%)	0.44	2 (3%) 50 34	149, 192, 200, 204	0
27	A5	59/60 (98%)	0.81	5 (8%) 16 13	54, 95, 172, 174	0
27	D5	59/60 (98%)	0.52	5 (8%) 16 13	61, 96, 179, 195	0
28	A6	45/54 (83%)	1.47	14 (31%) 1 1	129, 159, 174, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	D6	45/54 (83%)	1.72	16 (35%) 1 1	146, 174, 190, 192	0
29	A7	45/49 (91%)	-0.10	2 (4%) 39 25	46, 55, 72, 78	0
29	D7	45/49 (91%)	-0.03	1 (2%) 62 43	56, 66, 79, 96	0
30	A8	60/65 (92%)	0.53	8 (13%) 7 6	56, 74, 97, 120	0
30	D8	60/65 (92%)	1.37	14 (23%) 2 2	75, 91, 113, 138	0
31	BA	1502/1506 (99%)	-0.29	11 (0%) 84 70	58, 111, 193, 251	0
31	CA	1502/1506 (99%)	-0.20	29 (1%) 66 48	69, 122, 195, 251	0
32	BE	237/256 (92%)	0.23	10 (4%) 40 26	117, 150, 188, 200	0
32	CE	237/256 (92%)	0.25	8 (3%) 48 32	128, 166, 201, 216	0
33	BF	205/239 (85%)	0.30	11 (5%) 31 21	95, 124, 157, 167	0
33	CF	206/239 (86%)	0.58	16 (7%) 19 14	130, 151, 179, 185	0
34	BG	208/208 (100%)	0.31	7 (3%) 48 32	95, 119, 141, 152	0
34	CG	208/208 (100%)	0.36	9 (4%) 40 25	94, 114, 136, 151	0
35	BH	151/162 (93%)	0.07	4 (2%) 57 38	81, 109, 130, 166	0
35	CH	151/162 (93%)	0.62	19 (12%) 8 6	106, 124, 148, 171	0
36	BI	101/101 (100%)	-0.16	2 (1%) 65 46	86, 111, 127, 152	0
36	CI	101/101 (100%)	-0.26	0 100 100	83, 108, 131, 149	0
37	BJ	155/156 (99%)	0.32	14 (9%) 15 11	109, 127, 154, 167	0
37	CJ	155/156 (99%)	0.37	9 (5%) 29 19	120, 136, 159, 167	0
38	BK	138/138 (100%)	0.01	1 (0%) 84 70	90, 115, 128, 133	0
38	CK	138/138 (100%)	0.21	2 (1%) 73 55	105, 129, 141, 151	0
39	BL	127/128 (99%)	0.41	10 (7%) 18 14	98, 148, 166, 173	0
39	CL	127/128 (99%)	0.66	13 (10%) 12 10	118, 160, 175, 179	0
40	BM	99/105 (94%)	0.42	3 (3%) 52 35	93, 149, 177, 178	0
40	CM	99/105 (94%)	0.30	6 (6%) 27 18	128, 165, 180, 184	0
41	BN	119/129 (92%)	0.34	5 (4%) 40 26	81, 109, 138, 167	0
41	CN	119/129 (92%)	0.36	3 (2%) 58 39	89, 116, 144, 172	0
42	BO	125/132 (94%)	0.13	4 (3%) 50 34	73, 86, 118, 162	0
42	CO	125/132 (94%)	0.29	8 (6%) 25 17	91, 113, 138, 172	0
43	BP	116/126 (92%)	-0.01	1 (0%) 81 65	97, 135, 151, 157	0
43	CP	117/126 (92%)	0.40	6 (5%) 33 22	108, 162, 175, 177	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	58/61 (95%)	0.49	3 (5%) 33 22	96, 113, 128, 134	0
44	CQ	58/61 (95%)	0.50	2 (3%) 48 32	132, 145, 162, 167	0
45	BR	88/89 (98%)	-0.01	1 (1%) 78 60	81, 103, 125, 130	0
45	CR	88/89 (98%)	0.27	0 100 100	88, 116, 138, 145	0
46	BS	84/88 (95%)	0.65	2 (2%) 59 40	105, 122, 147, 180	0
46	CS	84/88 (95%)	0.35	2 (2%) 59 40	96, 108, 131, 164	0
47	BT	100/105 (95%)	0.21	6 (6%) 27 19	95, 114, 128, 135	0
47	CT	100/105 (95%)	0.56	11 (11%) 10 9	96, 117, 138, 149	0
48	BU	72/88 (81%)	-0.12	1 (1%) 73 55	94, 111, 147, 169	0
48	CU	72/88 (81%)	-0.26	3 (4%) 40 26	98, 120, 160, 178	0
49	BV	78/93 (83%)	0.14	1 (1%) 75 56	113, 135, 155, 159	0
49	CV	78/93 (83%)	0.56	6 (7%) 19 14	146, 170, 187, 192	0
50	BW	99/106 (93%)	0.44	7 (7%) 22 15	113, 129, 159, 167	0
50	CW	99/106 (93%)	0.41	4 (4%) 42 28	100, 122, 157, 170	0
51	BX	25/27 (92%)	0.40	1 (4%) 42 28	110, 123, 139, 157	0
51	CX	25/27 (92%)	1.02	2 (8%) 18 14	126, 148, 165, 175	0
52	BB	84/85 (98%)	0.44	4 (4%) 35 24	98, 138, 163, 176	0
52	BD	84/85 (98%)	0.57	4 (4%) 35 24	78, 144, 223, 233	0
52	CB	84/85 (98%)	0.79	8 (9%) 14 11	113, 143, 166, 176	0
52	CD	84/85 (98%)	0.34	3 (3%) 46 31	86, 144, 222, 230	0
53	BC	77/77 (100%)	-0.06	0 100 100	82, 117, 146, 159	0
53	CC	77/77 (100%)	-0.15	1 (1%) 75 56	92, 127, 156, 164	0
54	B1	16/16 (100%)	1.22	5 (31%) 1 1	81, 117, 161, 169	0
54	C1	16/16 (100%)	1.82	6 (37%) 1 1	90, 122, 168, 176	0
All	All	21100/21658 (97%)	0.02	811 (3%) 44 30	42, 108, 188, 252	0

The worst 5 of 811 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
39	CL	115	GLY	12.2
27	A5	2	ALA	11.2
39	CL	127	LYS	8.8
39	CL	125	TYR	8.4
8	DK	11	ASN	8.3

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	CB	38	29/30	0.79	0.15	99,111,127,136	0
52	MIA	CD	38	29/30	0.88	0.13	127,140,183,200	0
52	MIA	BB	38	29/30	0.92	0.12	92,99,110,128	0
52	MIA	BD	38	29/30	0.92	0.14	126,140,181,195	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	1628	1/1	0.20	0.29	137,137,137,137	0
55	MG	CA	1672	1/1	0.23	0.16	125,125,125,125	0
55	MG	BB	105	1/1	0.30	0.12	94,94,94,94	0
55	MG	BA	1706	1/1	0.36	0.31	111,111,111,111	0
55	MG	BA	1704	1/1	0.36	0.18	127,127,127,127	0
55	MG	BA	1630	1/1	0.41	0.34	109,109,109,109	0
55	MG	DA	3320	1/1	0.42	0.18	132,132,132,132	0
55	MG	BB	108	1/1	0.43	0.15	80,80,80,80	0
55	MG	BB	104	1/1	0.44	0.17	100,100,100,100	0
55	MG	DA	3323	1/1	0.45	0.28	100,100,100,100	0
56	OHX	CB	105	7/7	0.45	0.14	139,142,156,183	2
55	MG	CA	1616	1/1	0.46	0.39	100,100,100,100	0
55	MG	AA	3071	1/1	0.47	0.32	84,84,84,84	0
55	MG	CA	1665	1/1	0.47	0.29	114,114,114,114	0
55	MG	AA	3055	1/1	0.47	0.30	88,88,88,88	0
55	MG	DA	3053	1/1	0.48	0.32	116,116,116,116	0
55	MG	BA	1695	1/1	0.48	0.20	132,132,132,132	0
55	MG	DA	3200	1/1	0.49	0.57	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3291	1/1	0.51	0.22	99,99,99,99	0
55	MG	BB	113	1/1	0.52	0.14	80,80,80,80	0
55	MG	DA	3259	1/1	0.53	0.29	114,114,114,114	0
55	MG	CA	1687	1/1	0.54	0.35	104,104,104,104	0
55	MG	BA	1700	1/1	0.55	0.15	119,119,119,119	0
55	MG	CA	1626	1/1	0.55	0.28	124,124,124,124	0
55	MG	DA	3303	1/1	0.56	0.15	97,97,97,97	0
55	MG	AA	3083	1/1	0.56	0.32	94,94,94,94	0
56	OHX	DB	220	7/7	0.56	0.09	159,162,171,208	1
56	OHX	BA	1804	7/7	0.57	0.12	147,154,164,208	1
56	OHX	CB	106	7/7	0.58	0.12	97,107,117,126	6
55	MG	DA	3307	1/1	0.58	0.26	119,119,119,119	0
55	MG	AA	3200	1/1	0.59	0.26	82,82,82,82	0
55	MG	BC	104	1/1	0.59	0.32	88,88,88,88	0
56	OHX	CR	101	7/7	0.59	0.09	143,150,160,179	1
55	MG	CA	1686	1/1	0.60	0.27	110,110,110,110	0
55	MG	CA	1681	1/1	0.60	0.25	111,111,111,111	0
55	MG	BA	1613	1/1	0.62	0.22	116,116,116,116	0
56	OHX	AA	3505	7/7	0.63	0.09	143,150,161,212	1
55	MG	BA	1709	1/1	0.63	0.12	68,68,68,68	0
55	MG	BA	1670	1/1	0.63	0.19	100,100,100,100	0
55	MG	CA	1719	1/1	0.63	0.32	94,94,94,94	0
55	MG	BA	1685	1/1	0.63	0.34	93,93,93,93	0
55	MG	AA	3078	1/1	0.63	0.27	97,97,97,97	0
55	MG	DA	3044	1/1	0.64	0.22	100,100,100,100	0
55	MG	DA	3298	1/1	0.64	0.23	102,102,102,102	0
55	MG	BA	1612	1/1	0.65	0.31	100,100,100,100	0
55	MG	DB	201	1/1	0.65	0.17	95,95,95,95	0
55	MG	DA	3284	1/1	0.65	0.30	89,89,89,89	0
55	MG	BA	1649	1/1	0.65	0.36	92,92,92,92	0
55	MG	DA	3205	1/1	0.66	0.22	106,106,106,106	0
55	MG	AA	3306	1/1	0.66	0.24	100,100,100,100	0
55	MG	AA	3321	1/1	0.66	0.30	41,41,41,41	0
55	MG	AA	3301	1/1	0.66	0.12	97,97,97,97	0
55	MG	CA	1615	1/1	0.66	0.27	109,109,109,109	0
55	MG	DA	3158	1/1	0.67	0.42	88,88,88,88	0
56	OHX	AA	3507	7/7	0.67	0.14	120,135,161,172	2
55	MG	BB	111	1/1	0.67	0.08	80,80,80,80	0
55	MG	BA	1686	1/1	0.67	0.22	100,100,100,100	0
55	MG	DA	3048	1/1	0.67	0.39	93,93,93,93	0
55	MG	CA	1708	1/1	0.67	0.12	95,95,95,95	0
55	MG	DA	3296	1/1	0.67	0.21	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3343	1/1	0.68	0.16	92,92,92,92	0
55	MG	AA	3372	1/1	0.68	0.18	80,80,80,80	0
55	MG	CC	104	1/1	0.68	0.25	89,89,89,89	0
55	MG	BB	102	1/1	0.68	0.11	92,92,92,92	0
56	OHX	DB	219	7/7	0.68	0.09	147,161,178,209	1
55	MG	CA	1691	1/1	0.68	0.19	128,128,128,128	0
55	MG	CA	1720	1/1	0.69	0.34	110,110,110,110	0
55	MG	DA	3153	1/1	0.69	0.38	69,69,69,69	0
56	OHX	CA	1797	7/7	0.69	0.17	129,132,139,171	1
55	MG	AA	3209	1/1	0.69	0.25	86,86,86,86	0
55	MG	AA	3090	1/1	0.70	0.34	78,78,78,78	0
55	MG	CA	1674	1/1	0.70	0.42	97,97,97,97	0
55	MG	BA	1708	1/1	0.70	0.13	80,80,80,80	0
55	MG	CA	1629	1/1	0.70	0.08	166,166,166,166	0
55	MG	CA	1623	1/1	0.70	0.33	96,96,96,96	0
55	MG	C1	101	1/1	0.70	0.26	102,102,102,102	0
56	OHX	AA	3538	7/7	0.70	0.13	95,101,128,162	1
55	MG	BA	1625	1/1	0.71	0.20	66,66,66,66	0
56	OHX	CB	104	7/7	0.71	0.09	175,181,183,194	1
55	MG	CA	1630	1/1	0.71	0.27	86,86,86,86	0
55	MG	AA	3048	1/1	0.71	0.20	91,91,91,91	0
55	MG	CA	1627	1/1	0.71	0.19	126,126,126,126	0
55	MG	AA	3079	1/1	0.71	0.36	67,67,67,67	0
55	MG	AA	3054	1/1	0.72	0.28	83,83,83,83	0
56	OHX	BA	1813	7/7	0.72	0.09	151,161,170,205	1
55	MG	DA	3242	1/1	0.72	0.19	99,99,99,99	0
55	MG	DA	3049	1/1	0.72	0.23	104,104,104,104	0
55	MG	DA	3325	1/1	0.72	0.24	91,91,91,91	0
55	MG	BA	1655	1/1	0.72	0.29	84,84,84,84	0
55	MG	BB	107	1/1	0.72	0.10	80,80,80,80	0
55	MG	C1	102	1/1	0.72	0.24	104,104,104,104	0
55	MG	AA	3106	1/1	0.72	0.26	72,72,72,72	0
55	MG	AA	3322	1/1	0.73	0.19	81,81,81,81	0
56	OHX	AA	3492	7/7	0.73	0.11	139,142,151,196	1
55	MG	BA	1636	1/1	0.73	0.28	111,111,111,111	0
55	MG	BA	1639	1/1	0.73	0.32	101,101,101,101	0
55	MG	CA	1660	1/1	0.73	0.29	97,97,97,97	0
55	MG	AA	3096	1/1	0.73	0.37	76,76,76,76	0
55	MG	AA	3178	1/1	0.73	0.36	76,76,76,76	0
56	OHX	CA	1784	7/7	0.73	0.12	127,135,151,190	1
55	MG	AA	3230	1/1	0.73	0.36	72,72,72,72	0
55	MG	BA	1677	1/1	0.73	0.32	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	1685	1/1	0.73	0.33	104,104,104,104	0
55	MG	BB	103	1/1	0.73	0.11	105,105,105,105	0
55	MG	DA	3322	1/1	0.73	0.17	152,152,152,152	0
55	MG	AA	3311	1/1	0.73	0.26	90,90,90,90	0
55	MG	AA	3282	1/1	0.73	0.17	103,103,103,103	0
55	MG	AA	3313	1/1	0.74	0.35	82,82,82,82	0
55	MG	BA	1602	1/1	0.74	0.14	66,66,66,66	0
55	MG	AA	3310	1/1	0.74	0.28	71,71,71,71	0
55	MG	BA	1680	1/1	0.74	0.22	64,64,64,64	0
55	MG	DA	3039	1/1	0.74	0.23	102,102,102,102	0
55	MG	DA	3201	1/1	0.74	0.38	86,86,86,86	0
56	OHX	AA	3512	7/7	0.74	0.13	110,115,138,180	2
56	OHX	DA	3223	7/7	0.74	0.12	126,133,144,169	1
56	OHX	DA	3453	7/7	0.74	0.08	145,153,160,191	1
55	MG	CA	1609	1/1	0.74	0.30	112,112,112,112	0
55	MG	BA	1711	1/1	0.74	0.34	90,90,90,90	0
55	MG	AA	3112	1/1	0.75	0.21	87,87,87,87	0
55	MG	DA	3030	1/1	0.75	0.37	94,94,94,94	0
55	MG	AA	3215	1/1	0.75	0.26	69,69,69,69	0
56	OHX	AA	3530	7/7	0.75	0.13	117,123,125,163	1
55	MG	AA	3295	1/1	0.75	0.30	89,89,89,89	0
55	MG	AA	3118	1/1	0.75	0.16	69,69,69,69	0
55	MG	AB	202	1/1	0.75	0.21	80,80,80,80	0
55	MG	CA	1631	1/1	0.75	0.26	74,74,74,74	0
55	MG	DA	3310	1/1	0.75	0.19	73,73,73,73	0
55	MG	DA	3060	1/1	0.75	0.34	77,77,77,77	0
55	MG	CA	1654	1/1	0.75	0.21	89,89,89,89	0
55	MG	CA	1617	1/1	0.75	0.16	126,126,126,126	0
55	MG	CA	1662	1/1	0.75	0.37	92,92,92,92	0
55	MG	DA	3327	1/1	0.75	0.19	73,73,73,73	0
55	MG	BA	1673	1/1	0.75	0.36	75,75,75,75	0
56	OHX	AA	3456	7/7	0.75	0.11	111,115,132,161	3
55	MG	CA	1624	1/1	0.75	0.20	114,114,114,114	0
55	MG	DA	3294	1/1	0.76	0.16	74,74,74,74	0
55	MG	AA	3236	1/1	0.76	0.40	66,66,66,66	0
55	MG	CA	1682	1/1	0.76	0.25	107,107,107,107	0
55	MG	DA	3072	1/1	0.76	0.09	93,93,93,93	0
56	OHX	AB	218	7/7	0.76	0.09	138,141,157,181	1
56	OHX	BA	1795	7/7	0.76	0.10	152,159,163,204	1
55	MG	CA	1683	1/1	0.76	0.36	79,79,79,79	0
55	MG	AA	3162	1/1	0.76	0.21	48,48,48,48	0
55	MG	BA	1696	1/1	0.76	0.28	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3334	1/1	0.76	0.14	90,90,90,90	0
55	MG	AA	3043	1/1	0.76	0.33	75,75,75,75	0
55	MG	CA	1704	1/1	0.76	0.10	135,135,135,135	0
55	MG	DA	3326	1/1	0.76	0.38	90,90,90,90	0
55	MG	DA	3256	1/1	0.76	0.23	89,89,89,89	0
55	MG	CA	1649	1/1	0.76	0.21	92,92,92,92	0
55	MG	DA	3266	1/1	0.76	0.20	88,88,88,88	0
56	OHX	DB	213	7/7	0.76	0.10	125,144,157,169	2
55	MG	CA	1712	1/1	0.76	0.14	83,83,83,83	0
55	MG	DA	3293	1/1	0.76	0.28	88,88,88,88	0
55	MG	AA	3092	1/1	0.77	0.15	92,92,92,92	0
55	MG	DA	3288	1/1	0.77	0.21	82,82,82,82	0
55	MG	DA	3035	1/1	0.77	0.27	95,95,95,95	0
55	MG	CA	1640	1/1	0.77	0.29	77,77,77,77	0
56	OHX	CA	1788	7/7	0.77	0.12	138,144,149,176	1
55	MG	CA	1713	1/1	0.77	0.23	114,114,114,114	0
55	MG	CA	1641	1/1	0.77	0.45	85,85,85,85	0
55	MG	DA	3210	1/1	0.77	0.38	73,73,73,73	0
55	MG	DA	3304	1/1	0.77	0.11	89,89,89,89	0
55	MG	BA	1683	1/1	0.77	0.33	85,85,85,85	0
55	MG	CA	1689	1/1	0.77	0.23	80,80,80,80	0
55	MG	DA	3313	1/1	0.77	0.26	88,88,88,88	0
55	MG	AA	3148	1/1	0.77	0.23	69,69,69,69	0
55	MG	BA	1657	1/1	0.77	0.28	87,87,87,87	0
56	OHX	BA	1794	7/7	0.77	0.10	156,163,165,204	1
55	MG	AA	3127	1/1	0.78	0.31	45,45,45,45	0
56	OHX	BA	1792	7/7	0.78	0.10	118,131,146,181	1
55	MG	DA	3033	1/1	0.78	0.24	82,82,82,82	0
55	MG	DA	3076	1/1	0.78	0.42	54,54,54,54	0
55	MG	DA	3096	1/1	0.78	0.12	85,85,85,85	0
55	MG	DA	3279	1/1	0.78	0.24	68,68,68,68	0
55	MG	DA	3117	1/1	0.78	0.22	82,82,82,82	0
55	MG	DA	3287	1/1	0.78	0.22	102,102,102,102	0
55	MG	DA	3145	1/1	0.78	0.38	82,82,82,82	0
56	OHX	CA	1804	7/7	0.78	0.13	145,149,162,192	1
55	MG	BA	1703	1/1	0.78	0.24	90,90,90,90	0
56	OHX	AA	3451	7/7	0.78	0.14	79,96,106,142	1
55	MG	BA	1688	1/1	0.78	0.15	79,79,79,79	0
55	MG	AA	3039	1/1	0.78	0.30	50,50,50,50	0
55	MG	AA	3062	1/1	0.78	0.21	97,97,97,97	0
56	OHX	DA	3441	7/7	0.78	0.15	114,122,135,176	1
55	MG	DA	3302	1/1	0.78	0.32	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BB	106	1/1	0.78	0.36	102,102,102,102	0
56	OHX	DB	217	7/7	0.78	0.12	135,139,157,196	1
55	MG	DA	3209	1/1	0.78	0.24	64,64,64,64	0
55	MG	BA	1699	1/1	0.78	0.29	84,84,84,84	0
55	MG	CA	1601	1/1	0.79	0.30	75,75,75,75	0
55	MG	DA	3244	1/1	0.79	0.32	82,82,82,82	0
55	MG	CA	1675	1/1	0.79	0.36	94,94,94,94	0
55	MG	AA	3249	1/1	0.79	0.17	81,81,81,81	0
55	MG	DA	3199	1/1	0.79	0.42	77,77,77,77	0
56	OHX	BA	1778	7/7	0.79	0.16	125,131,152,191	1
56	OHX	BA	1786	7/7	0.79	0.09	133,136,154,188	1
56	OHX	DA	3124	7/7	0.79	0.10	144,164,170,220	1
56	OHX	DA	3127	7/7	0.79	0.11	118,132,150,170	2
55	MG	AA	3269	1/1	0.79	0.22	59,59,59,59	0
55	MG	AA	3270	1/1	0.79	0.23	90,90,90,90	0
55	MG	BA	1638	1/1	0.79	0.30	104,104,104,104	0
56	OHX	DA	3473	7/7	0.79	0.09	138,151,163,196	1
55	MG	AA	3135	1/1	0.79	0.30	66,66,66,66	0
55	MG	AA	3226	1/1	0.79	0.37	68,68,68,68	0
56	OHX	DB	218	7/7	0.79	0.11	134,141,153,171	1
56	OHX	CA	1755	7/7	0.79	0.11	119,128,149,178	1
56	OHX	AA	3506	7/7	0.79	0.13	104,115,126,178	1
55	MG	BA	1681	1/1	0.80	0.35	64,64,64,64	0
55	MG	DA	3267	1/1	0.80	0.20	82,82,82,82	0
56	OHX	CA	1785	7/7	0.80	0.15	125,126,143,155	1
55	MG	DA	3276	1/1	0.80	0.32	78,78,78,78	0
55	MG	AA	3051	1/1	0.80	0.37	69,69,69,69	0
56	OHX	CA	1799	7/7	0.80	0.11	142,145,160,170	1
56	OHX	AA	3529	7/7	0.80	0.11	114,130,134,179	1
56	OHX	CA	1812	7/7	0.80	0.11	134,141,149,203	1
55	MG	CA	1664	1/1	0.80	0.18	57,57,57,57	0
55	MG	AA	3296	1/1	0.80	0.27	69,69,69,69	0
56	OHX	AA	3539	7/7	0.80	0.09	130,133,143,179	1
56	OHX	AA	3541	7/7	0.80	0.08	131,134,141,173	1
56	OHX	AA	3546	7/7	0.80	0.12	101,114,120,164	2
56	OHX	AA	3567	7/7	0.80	0.08	125,135,148,181	2
55	MG	CC	107	1/1	0.80	0.23	80,80,80,80	0
56	OHX	DA	3413	7/7	0.80	0.19	103,122,138,176	1
56	OHX	BA	1750	7/7	0.80	0.12	112,129,139,168	1
55	MG	DA	3291	1/1	0.80	0.18	66,66,66,66	0
55	MG	CA	1621	1/1	0.80	0.12	110,110,110,110	0
56	OHX	DA	3482	7/7	0.80	0.09	128,142,154,190	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	1628	1/1	0.80	0.46	95,95,95,95	0
55	MG	CA	1699	1/1	0.80	0.30	86,86,86,86	0
55	MG	AA	3137	1/1	0.80	0.24	74,74,74,74	0
55	MG	BA	1691	1/1	0.80	0.32	87,87,87,87	0
55	MG	BA	1633	1/1	0.80	0.28	77,77,77,77	0
55	MG	DA	3311	1/1	0.81	0.25	63,63,63,63	0
55	MG	CA	1619	1/1	0.81	0.29	92,92,92,92	0
55	MG	AA	3302	1/1	0.81	0.31	72,72,72,72	0
55	MG	BA	1692	1/1	0.81	0.25	73,73,73,73	0
55	MG	AA	3277	1/1	0.81	0.49	94,94,94,94	0
56	OHX	BB	115	7/7	0.81	0.07	90,109,116,116	3
55	MG	CA	1678	1/1	0.81	0.13	97,97,97,97	0
56	OHX	CA	1774	7/7	0.81	0.14	137,150,161,190	1
55	MG	AA	3279	1/1	0.81	0.53	90,90,90,90	0
55	MG	AA	3120	1/1	0.81	0.35	74,74,74,74	0
56	OHX	CA	1786	7/7	0.81	0.09	163,163,175,198	1
55	MG	AA	3285	1/1	0.81	0.26	77,77,77,77	0
55	MG	AA	3222	1/1	0.81	0.23	85,85,85,85	0
55	MG	AA	3256	1/1	0.81	0.39	52,52,52,52	0
56	OHX	AA	3480	7/7	0.81	0.10	111,119,135,158	2
56	OHX	CA	1811	7/7	0.81	0.10	126,129,137,159	1
55	MG	AA	3157	1/1	0.81	0.35	86,86,86,86	0
56	OHX	CA	1813	7/7	0.81	0.07	138,144,151,179	1
55	MG	AA	3300	1/1	0.81	0.21	81,81,81,81	0
55	MG	CA	1605	1/1	0.81	0.29	75,75,75,75	0
55	MG	CA	1643	1/1	0.81	0.28	68,68,68,68	0
55	MG	CA	1700	1/1	0.81	0.21	97,97,97,97	0
56	OHX	AA	3520	7/7	0.81	0.15	88,95,98,151	2
55	MG	CA	1608	1/1	0.81	0.23	76,76,76,76	0
55	MG	DA	3112	1/1	0.81	0.42	85,85,85,85	0
56	OHX	DA	3251	7/7	0.81	0.14	102,112,141,176	3
55	MG	BA	1637	1/1	0.81	0.28	99,99,99,99	0
56	OHX	DA	3423	7/7	0.81	0.08	127,140,151,201	1
55	MG	AA	3089	1/1	0.81	0.23	130,130,130,130	0
55	MG	DA	3148	1/1	0.81	0.50	50,50,50,50	0
55	MG	DA	3151	1/1	0.81	0.20	62,62,62,62	0
56	OHX	DA	3479	7/7	0.81	0.06	150,159,164,201	1
56	OHX	DA	3480	7/7	0.81	0.11	125,130,144,190	1
56	OHX	AA	3551	7/7	0.81	0.14	97,115,123,153	1
56	OHX	DA	3489	7/7	0.81	0.10	117,121,134,153	1
55	MG	CA	1661	1/1	0.81	0.51	83,83,83,83	0
55	MG	BB	101	1/1	0.81	0.11	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3181	1/1	0.81	0.29	98,98,98,98	0
55	MG	DA	3191	1/1	0.81	0.28	66,66,66,66	0
55	MG	AB	201	1/1	0.81	0.22	85,85,85,85	0
56	OHX	AA	3484	7/7	0.82	0.10	123,137,150,203	1
55	MG	BA	1647	1/1	0.82	0.29	66,66,66,66	0
56	OHX	AA	3497	7/7	0.82	0.12	105,127,139,145	1
55	MG	DA	3295	1/1	0.82	0.32	77,77,77,77	0
55	MG	BA	1635	1/1	0.82	0.17	86,86,86,86	0
55	MG	CA	1614	1/1	0.82	0.21	118,118,118,118	0
55	MG	DA	3237	1/1	0.82	0.26	85,85,85,85	0
55	MG	DA	3239	1/1	0.82	0.14	79,79,79,79	0
56	OHX	AA	3523	7/7	0.82	0.08	112,123,137,155	1
55	MG	DA	3010	1/1	0.82	0.32	47,47,47,47	0
55	MG	AA	3193	1/1	0.82	0.34	86,86,86,86	0
55	MG	BA	1705	1/1	0.82	0.17	109,109,109,109	0
55	MG	DA	3146	1/1	0.82	0.19	33,33,33,33	0
55	MG	AA	3056	1/1	0.82	0.21	55,55,55,55	0
55	MG	DA	3314	1/1	0.82	0.15	70,70,70,70	0
55	MG	AA	3038	1/1	0.82	0.28	68,68,68,68	0
56	OHX	AA	3554	7/7	0.82	0.08	138,143,153,173	1
55	MG	DA	3270	1/1	0.82	0.62	73,73,73,73	0
56	OHX	DA	3253	7/7	0.82	0.11	141,144,160,190	1
55	MG	DA	3041	1/1	0.82	0.33	79,79,79,79	0
55	MG	DA	3278	1/1	0.82	0.37	84,84,84,84	0
56	OHX	BA	1776	7/7	0.82	0.14	119,138,152,176	2
56	OHX	DA	3447	7/7	0.82	0.09	122,140,155,176	2
55	MG	CA	1716	1/1	0.82	0.34	79,79,79,79	0
56	OHX	DA	3470	7/7	0.82	0.07	152,169,191,193	1
55	MG	DA	3047	1/1	0.82	0.24	79,79,79,79	0
56	OHX	DA	3475	7/7	0.82	0.11	126,139,148,175	1
56	OHX	BA	1788	7/7	0.82	0.12	123,136,147,176	1
55	MG	DA	3330	1/1	0.82	0.30	81,81,81,81	0
55	MG	DA	3333	1/1	0.82	0.27	84,84,84,84	0
55	MG	AA	3156	1/1	0.82	0.14	80,80,80,80	0
56	OHX	AA	3417	7/7	0.82	0.15	90,102,131,147	3
56	OHX	AA	3420	7/7	0.82	0.14	112,125,135,178	2
55	MG	CA	1639	1/1	0.82	0.49	69,69,69,69	0
55	MG	CB	101	1/1	0.82	0.16	105,105,105,105	0
55	MG	CA	1622	1/1	0.82	0.24	89,89,89,89	0
56	OHX	D3	101	7/7	0.82	0.09	129,139,156,171	2
56	OHX	AA	3481	7/7	0.83	0.14	88,92,119,127	2
55	MG	CA	1707	1/1	0.83	0.22	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	BA	1766	7/7	0.83	0.13	108,139,151,181	2
55	MG	DA	3038	1/1	0.83	0.24	77,77,77,77	0
55	MG	BA	1672	1/1	0.83	0.27	82,82,82,82	0
56	OHX	BA	1780	7/7	0.83	0.09	115,123,136,153	1
56	OHX	DA	3105	7/7	0.83	0.10	134,136,144,206	1
56	OHX	AA	3502	7/7	0.83	0.07	128,135,148,184	1
55	MG	AA	3316	1/1	0.83	0.14	79,79,79,79	0
56	OHX	DA	3176	7/7	0.83	0.09	162,165,176,192	1
55	MG	BA	1675	1/1	0.83	0.40	87,87,87,87	0
56	OHX	DA	3226	7/7	0.83	0.14	120,131,144,175	1
55	MG	CA	1715	1/1	0.83	0.13	80,80,80,80	0
55	MG	AA	3275	1/1	0.83	0.41	71,71,71,71	0
56	OHX	DA	3258	7/7	0.83	0.10	103,111,118,148	1
55	MG	CA	1718	1/1	0.83	0.12	84,84,84,84	0
55	MG	BA	1701	1/1	0.83	0.20	68,68,68,68	0
56	OHX	BR	101	7/7	0.83	0.07	132,137,152,164	1
56	OHX	BB	114	7/7	0.83	0.11	176,178,180,206	1
56	OHX	AA	3524	7/7	0.83	0.10	115,120,140,187	1
56	OHX	DA	3463	7/7	0.83	0.08	142,149,156,188	1
55	MG	BA	1608	1/1	0.83	0.18	89,89,89,89	0
56	OHX	DA	3472	7/7	0.83	0.08	162,171,176,223	1
56	OHX	CA	1767	7/7	0.83	0.12	110,139,162,203	1
55	MG	BA	1610	1/1	0.83	0.21	75,75,75,75	0
55	MG	AA	3155	1/1	0.83	0.12	79,79,79,79	0
55	MG	AA	3324	1/1	0.83	0.23	84,84,84,84	0
55	MG	AA	3141	1/1	0.83	0.22	80,80,80,80	0
56	OHX	CA	1787	7/7	0.83	0.13	117,122,135,155	1
56	OHX	AA	3544	7/7	0.83	0.08	118,127,137,169	1
56	OHX	DB	216	7/7	0.83	0.11	123,138,155,204	1
55	MG	BD	101	1/1	0.83	0.19	103,103,103,103	0
55	MG	AA	3211	1/1	0.83	0.22	58,58,58,58	0
55	MG	AA	3297	1/1	0.83	0.07	80,80,80,80	0
56	OHX	CA	1806	7/7	0.83	0.09	138,150,153,181	1
55	MG	AA	3284	1/1	0.83	0.25	68,68,68,68	0
55	MG	CA	1644	1/1	0.84	0.18	89,89,89,89	0
55	MG	BA	1648	1/1	0.84	0.27	86,86,86,86	0
56	OHX	AA	3511	7/7	0.84	0.09	133,137,167,178	2
55	MG	AA	3307	1/1	0.84	0.20	72,72,72,72	0
56	OHX	AA	3514	7/7	0.84	0.09	126,137,144,183	1
55	MG	CA	1656	1/1	0.84	0.35	94,94,94,94	0
55	MG	CA	1657	1/1	0.84	0.25	81,81,81,81	0
56	OHX	CA	1808	7/7	0.84	0.07	163,164,177,210	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AB	204	1/1	0.84	0.34	80,80,80,80	0
55	MG	AB	205	1/1	0.84	0.23	68,68,68,68	0
55	MG	AA	3309	1/1	0.84	0.37	77,77,77,77	0
56	OHX	CA	1815	7/7	0.84	0.09	158,163,177,221	1
55	MG	AA	3245	1/1	0.84	0.22	70,70,70,70	0
55	MG	AA	3059	1/1	0.84	0.26	77,77,77,77	0
55	MG	CA	1667	1/1	0.84	0.35	78,78,78,78	0
55	MG	AA	3287	1/1	0.84	0.29	66,66,66,66	0
55	MG	AA	3314	1/1	0.84	0.20	63,63,63,63	0
55	MG	DA	3317	1/1	0.84	0.30	85,85,85,85	0
56	OHX	AA	3552	7/7	0.84	0.13	96,106,128,164	1
55	MG	AA	3052	1/1	0.84	0.24	71,71,71,71	0
55	MG	DA	3020	1/1	0.84	0.30	60,60,60,60	0
56	OHX	AB	216	7/7	0.84	0.12	106,124,147,185	1
55	MG	AA	3262	1/1	0.84	0.27	62,62,62,62	0
55	MG	DA	3233	1/1	0.84	0.20	65,65,65,65	0
55	MG	CA	1679	1/1	0.84	0.12	87,87,87,87	0
55	MG	AA	3044	1/1	0.84	0.29	42,42,42,42	0
55	MG	AA	3144	1/1	0.84	0.27	43,43,43,43	0
55	MG	AA	3325	1/1	0.84	0.45	75,75,75,75	0
56	OHX	BA	1781	7/7	0.84	0.10	115,133,141,174	1
55	MG	AA	3181	1/1	0.84	0.44	71,71,71,71	0
55	MG	DB	203	1/1	0.84	0.15	121,121,121,121	0
56	OHX	BA	1791	7/7	0.84	0.09	122,123,136,173	1
55	MG	BA	1690	1/1	0.84	0.12	81,81,81,81	0
55	MG	AA	3075	1/1	0.84	0.19	78,78,78,78	0
56	OHX	DA	3474	7/7	0.84	0.16	120,126,143,173	1
56	OHX	AA	3447	7/7	0.84	0.09	110,120,136,163	1
55	MG	AA	3357	1/1	0.84	0.22	69,69,69,69	0
55	MG	BB	112	1/1	0.84	0.10	80,80,80,80	0
55	MG	AA	3131	1/1	0.84	0.41	62,62,62,62	0
55	MG	BC	102	1/1	0.84	0.28	65,65,65,65	0
55	MG	DA	3066	1/1	0.84	0.25	77,77,77,77	0
56	OHX	BD	104	7/7	0.84	0.13	94,101,103,107	3
55	MG	CA	1701	1/1	0.84	0.22	109,109,109,109	0
55	MG	BA	1642	1/1	0.84	0.24	69,69,69,69	0
56	OHX	AA	3498	7/7	0.84	0.09	120,126,136,160	2
55	MG	DA	3085	1/1	0.84	0.33	53,53,53,53	0
55	MG	AA	3243	1/1	0.84	0.36	62,62,62,62	0
55	MG	BA	1643	1/1	0.85	0.10	67,67,67,67	0
55	MG	AA	3110	1/1	0.85	0.20	76,76,76,76	0
55	MG	BA	1607	1/1	0.85	0.17	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3318	1/1	0.85	0.18	75,75,75,75	0
56	OHX	AA	3540	7/7	0.85	0.09	104,109,137,150	2
55	MG	DA	3299	1/1	0.85	0.30	67,67,67,67	0
55	MG	AA	3168	1/1	0.85	0.27	36,36,36,36	0
56	OHX	AA	3454	7/7	0.85	0.09	103,116,132,145	1
56	OHX	CA	1775	7/7	0.85	0.09	139,154,159,200	1
55	MG	DA	3142	1/1	0.85	0.30	76,76,76,76	0
55	MG	CA	1618	1/1	0.85	0.09	82,82,82,82	0
55	MG	BA	1656	1/1	0.85	0.34	73,73,73,73	0
55	MG	AA	3172	1/1	0.85	0.33	71,71,71,71	0
56	OHX	DA	3455	7/7	0.85	0.09	139,144,150,194	1
56	OHX	AA	3488	7/7	0.85	0.08	155,156,163,203	1
56	OHX	DA	3468	7/7	0.85	0.09	143,146,150,189	1
56	OHX	CA	1789	7/7	0.85	0.08	152,164,170,204	1
55	MG	AA	3174	1/1	0.85	0.08	91,91,91,91	0
56	OHX	AA	3494	7/7	0.85	0.08	112,122,130,153	1
55	MG	CA	1690	1/1	0.85	0.21	93,93,93,93	0
55	MG	CA	1668	1/1	0.85	0.34	80,80,80,80	0
55	MG	DA	3272	1/1	0.85	0.10	57,57,57,57	0
55	MG	DA	3318	1/1	0.85	0.09	110,110,110,110	0
56	OHX	DA	3481	7/7	0.85	0.09	136,140,149,177	1
55	MG	CC	103	1/1	0.85	0.29	97,97,97,97	0
55	MG	CA	1692	1/1	0.85	0.35	104,104,104,104	0
55	MG	DA	3192	1/1	0.85	0.31	60,60,60,60	0
56	OHX	DB	215	7/7	0.85	0.09	147,149,158,191	1
55	MG	DA	3196	1/1	0.85	0.34	54,54,54,54	0
55	MG	AA	3012	1/1	0.85	0.25	45,45,45,45	0
55	MG	AA	3281	1/1	0.85	0.16	93,93,93,93	0
55	MG	DA	3067	1/1	0.85	0.12	82,82,82,82	0
56	OHX	CC	108	7/7	0.85	0.09	130,137,148,169	1
55	MG	CA	1625	1/1	0.85	0.25	87,87,87,87	0
55	MG	DB	205	1/1	0.86	0.18	64,64,64,64	0
55	MG	DB	206	1/1	0.86	0.40	81,81,81,81	0
56	OHX	AA	3548	7/7	0.86	0.08	125,128,143,177	1
55	MG	DB	207	1/1	0.86	0.19	70,70,70,70	0
55	MG	CA	1637	1/1	0.86	0.33	69,69,69,69	0
55	MG	CA	1666	1/1	0.86	0.24	75,75,75,75	0
56	OHX	AA	3559	7/7	0.86	0.08	123,137,143,179	1
55	MG	CC	101	1/1	0.86	0.28	79,79,79,79	0
55	MG	A1	201	1/1	0.86	0.38	62,62,62,62	0
55	MG	BS	101	1/1	0.86	0.17	81,81,81,81	0
56	OHX	AB	219	7/7	0.86	0.10	112,116,126,139	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	A1	204	7/7	0.86	0.11	107,117,147,182	3
55	MG	AA	3102	1/1	0.86	0.19	52,52,52,52	0
55	MG	CA	1673	1/1	0.86	0.27	76,76,76,76	0
56	OHX	DA	3109	7/7	0.86	0.10	99,116,138,153	1
56	OHX	DA	3111	7/7	0.86	0.09	118,129,134,197	1
56	OHX	BA	1772	7/7	0.86	0.09	165,176,177,219	1
55	MG	DA	3203	1/1	0.86	0.23	69,69,69,69	0
56	OHX	DA	3173	7/7	0.86	0.10	157,163,175,202	1
55	MG	AA	3160	1/1	0.86	0.25	69,69,69,69	0
56	OHX	DA	3220	7/7	0.86	0.13	141,154,156,201	1
55	MG	AA	3081	1/1	0.86	0.24	81,81,81,81	0
55	MG	DA	3017	1/1	0.86	0.38	66,66,66,66	0
56	OHX	BA	1782	7/7	0.86	0.08	137,145,154,180	1
56	OHX	BA	1783	7/7	0.86	0.09	121,130,148,178	1
56	OHX	BA	1785	7/7	0.86	0.07	117,124,136,144	2
56	OHX	DA	3407	7/7	0.86	0.10	124,134,145,191	1
55	MG	DA	3216	1/1	0.86	0.33	71,71,71,71	0
55	MG	DA	3232	1/1	0.86	0.40	63,63,63,63	0
56	OHX	DA	3437	7/7	0.86	0.10	113,120,134,160	1
55	MG	AA	3231	1/1	0.86	0.30	57,57,57,57	0
56	OHX	AA	3499	7/7	0.86	0.12	107,112,120,152	1
56	OHX	DA	3450	7/7	0.86	0.09	133,139,150,199	1
56	OHX	DA	3452	7/7	0.86	0.10	99,118,125,155	1
55	MG	DA	3235	1/1	0.86	0.29	66,66,66,66	0
56	OHX	DA	3454	7/7	0.86	0.07	136,143,163,191	1
55	MG	DA	3101	1/1	0.86	0.18	59,59,59,59	0
56	OHX	BA	1798	7/7	0.86	0.09	135,136,153,212	1
56	OHX	DA	3465	7/7	0.86	0.08	123,136,143,165	1
56	OHX	DA	3467	7/7	0.86	0.09	133,139,156,192	1
56	OHX	BA	1799	7/7	0.86	0.07	170,176,182,227	1
55	MG	DA	3102	1/1	0.86	0.25	76,76,76,76	0
56	OHX	BA	1810	7/7	0.86	0.11	138,141,150,186	1
55	MG	AA	3119	1/1	0.86	0.17	86,86,86,86	0
55	MG	DA	3113	1/1	0.86	0.23	73,73,73,73	0
55	MG	AA	3170	1/1	0.86	0.40	69,69,69,69	0
56	OHX	AA	3513	7/7	0.86	0.12	120,125,139,159	2
55	MG	CA	1610	1/1	0.86	0.27	87,87,87,87	0
55	MG	DA	3037	1/1	0.86	0.36	73,73,73,73	0
55	MG	BA	1689	1/1	0.86	0.12	80,80,80,80	0
56	OHX	DA	3484	7/7	0.86	0.10	109,123,139,168	1
56	OHX	DA	3488	7/7	0.86	0.17	87,112,131,159	1
55	MG	AA	3084	1/1	0.86	0.09	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	OHX	DA	3490	7/7	0.86	0.12	103,106,122,159	3
56	OHX	AA	3527	7/7	0.86	0.06	147,148,161,187	1
56	OHX	AA	3528	7/7	0.86	0.21	119,125,142,174	1
55	MG	AA	3138	1/1	0.86	0.17	78,78,78,78	0
55	MG	DA	3043	1/1	0.86	0.33	73,73,73,73	0
55	MG	BA	1645	1/1	0.86	0.11	76,76,76,76	0
55	MG	DA	3177	1/1	0.86	0.32	61,61,61,61	0
55	MG	DB	202	1/1	0.86	0.15	98,98,98,98	0
55	MG	DA	3178	1/1	0.86	0.34	58,58,58,58	0
56	OHX	D5	102	7/7	0.86	0.10	114,129,141,158	1
56	OHX	DA	3091	7/7	0.87	0.12	103,121,134,170	1
56	OHX	BA	1765	7/7	0.87	0.16	91,107,120,150	3
55	MG	BA	1604	1/1	0.87	0.17	69,69,69,69	0
55	MG	AA	3074	1/1	0.87	0.24	90,90,90,90	0
55	MG	AA	3124	1/1	0.87	0.26	88,88,88,88	0
55	MG	AA	3147	1/1	0.87	0.33	49,49,49,49	0
55	MG	AA	3161	1/1	0.87	0.21	57,57,57,57	0
55	MG	AA	3224	1/1	0.87	0.13	79,79,79,79	0
56	OHX	AA	3495	7/7	0.87	0.10	106,114,133,188	1
55	MG	BA	1652	1/1	0.87	0.36	68,68,68,68	0
55	MG	BA	1615	1/1	0.87	0.29	78,78,78,78	0
55	MG	BA	1616	1/1	0.87	0.18	101,101,101,101	0
55	MG	DA	3059	1/1	0.87	0.24	40,40,40,40	0
55	MG	BA	1621	1/1	0.87	0.26	77,77,77,77	0
55	MG	BA	1667	1/1	0.87	0.37	73,73,73,73	0
55	MG	DA	3208	1/1	0.87	0.36	61,61,61,61	0
56	OHX	AA	3509	7/7	0.87	0.11	91,109,142,150	3
55	MG	AA	3100	1/1	0.87	0.30	58,58,58,58	0
56	OHX	DA	3439	7/7	0.87	0.10	127,146,152,174	1
56	OHX	DA	3440	7/7	0.87	0.07	142,144,161,189	1
55	MG	CA	1632	1/1	0.87	0.36	56,56,56,56	0
55	MG	DA	3211	1/1	0.87	0.30	57,57,57,57	0
55	MG	AA	3166	1/1	0.87	0.28	41,41,41,41	0
55	MG	DA	3228	1/1	0.87	0.36	58,58,58,58	0
56	OHX	BL	201	7/7	0.87	0.08	145,153,159,202	1
55	MG	DA	3231	1/1	0.87	0.21	50,50,50,50	0
55	MG	AA	3195	1/1	0.87	0.30	58,58,58,58	0
55	MG	DA	3090	1/1	0.87	0.24	54,54,54,54	0
55	MG	AA	3233	1/1	0.87	0.24	82,82,82,82	0
55	MG	DA	3097	1/1	0.87	0.34	67,67,67,67	0
55	MG	DA	3100	1/1	0.87	0.28	87,87,87,87	0
56	OHX	AA	3536	7/7	0.87	0.12	99,110,129,173	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CC	106	1/1	0.87	0.35	75,75,75,75	0
55	MG	DA	3331	1/1	0.87	0.09	69,69,69,69	0
55	MG	CA	1684	1/1	0.87	0.32	82,82,82,82	0
55	MG	AO	201	1/1	0.87	0.25	66,66,66,66	0
56	OHX	DA	3477	7/7	0.87	0.07	153,157,164,211	1
56	OHX	AA	3543	7/7	0.87	0.07	145,150,162,204	1
55	MG	AA	3130	1/1	0.87	0.28	43,43,43,43	0
56	OHX	AA	3545	7/7	0.87	0.12	92,105,127,145	2
55	MG	DA	3114	1/1	0.87	0.26	37,37,37,37	0
55	MG	DB	204	1/1	0.87	0.15	76,76,76,76	0
55	MG	A3	101	1/1	0.87	0.37	71,71,71,71	0
55	MG	DA	3131	1/1	0.87	0.23	72,72,72,72	0
55	MG	BA	1712	1/1	0.87	0.11	74,74,74,74	0
55	MG	DE	301	1/1	0.87	0.32	52,52,52,52	0
55	MG	BA	1713	1/1	0.87	0.28	81,81,81,81	0
55	MG	DA	3277	1/1	0.87	0.14	89,89,89,89	0
55	MG	BA	1714	1/1	0.87	0.28	83,83,83,83	0
55	MG	BA	1601	1/1	0.87	0.28	57,57,57,57	0
55	MG	CA	1694	1/1	0.87	0.32	89,89,89,89	0
56	OHX	BA	1743	7/7	0.87	0.18	79,96,129,159	2
55	MG	AA	3208	1/1	0.87	0.27	62,62,62,62	0
56	OHX	BA	1754	7/7	0.87	0.10	136,144,152,183	1
56	OHX	DA	3103	7/7	0.88	0.13	94,102,107,128	2
55	MG	AA	3099	1/1	0.88	0.27	60,60,60,60	0
56	OHX	AA	3500	7/7	0.88	0.09	118,131,153,193	1
55	MG	AA	3111	1/1	0.88	0.18	69,69,69,69	0
56	OHX	AA	3503	7/7	0.88	0.13	99,108,119,150	1
55	MG	DA	3315	1/1	0.88	0.34	78,78,78,78	0
56	OHX	DA	3165	7/7	0.88	0.08	123,135,143,168	1
55	MG	BA	1640	1/1	0.88	0.13	71,71,71,71	0
55	MG	CA	1646	1/1	0.88	0.23	79,79,79,79	0
56	OHX	AA	3508	7/7	0.88	0.07	192,206,214,236	1
55	MG	DA	3106	1/1	0.88	0.29	80,80,80,80	0
55	MG	AA	3140	1/1	0.88	0.27	70,70,70,70	0
55	MG	CA	1650	1/1	0.88	0.32	66,66,66,66	0
55	MG	AA	3234	1/1	0.88	0.19	68,68,68,68	0
56	OHX	BA	1797	7/7	0.88	0.12	117,130,138,173	1
55	MG	DA	3029	1/1	0.88	0.23	70,70,70,70	0
55	MG	DA	3120	1/1	0.88	0.24	52,52,52,52	0
55	MG	DA	3328	1/1	0.88	0.20	99,99,99,99	0
56	OHX	DA	3436	7/7	0.88	0.08	121,133,143,171	1
55	MG	BW	201	1/1	0.88	0.32	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	AA	3526	7/7	0.88	0.12	87,90,101,128	1
55	MG	BA	1687	1/1	0.88	0.25	96,96,96,96	0
55	MG	CA	1659	1/1	0.88	0.17	116,116,116,116	0
56	OHX	DA	3446	7/7	0.88	0.09	118,121,142,162	1
55	MG	AA	3308	1/1	0.88	0.22	63,63,63,63	0
56	OHX	DA	3448	7/7	0.88	0.07	134,147,163,206	1
55	MG	AA	3125	1/1	0.88	0.18	63,63,63,63	0
56	OHX	BC	106	7/7	0.88	0.10	119,120,134,160	1
55	MG	DA	3275	1/1	0.88	0.32	53,53,53,53	0
55	MG	AA	3063	1/1	0.88	0.27	45,45,45,45	0
55	MG	BA	1619	1/1	0.88	0.25	64,64,64,64	0
55	MG	AA	3117	1/1	0.88	0.15	90,90,90,90	0
55	MG	BA	1622	1/1	0.88	0.21	92,92,92,92	0
56	OHX	DA	3466	7/7	0.88	0.12	116,124,134,165	2
56	OHX	CA	1782	7/7	0.88	0.08	134,137,147,160	1
55	MG	AA	3068	1/1	0.88	0.11	92,92,92,92	0
56	OHX	DA	3469	7/7	0.88	0.08	116,119,133,163	1
56	OHX	AA	3408	7/7	0.88	0.10	107,111,135,163	1
56	OHX	AA	3412	7/7	0.88	0.08	119,122,141,174	1
55	MG	AA	3250	1/1	0.88	0.26	55,55,55,55	0
55	MG	CA	1670	1/1	0.88	0.18	95,95,95,95	0
56	OHX	AA	3436	7/7	0.88	0.13	90,93,119,164	1
56	OHX	DA	3476	7/7	0.88	0.09	126,136,143,174	1
55	MG	BA	1629	1/1	0.88	0.24	79,79,79,79	0
56	OHX	CA	1798	7/7	0.88	0.07	116,126,129,163	1
55	MG	BA	1668	1/1	0.88	0.26	64,64,64,64	0
56	OHX	CA	1802	7/7	0.88	0.09	130,138,148,200	1
55	MG	AA	3252	1/1	0.88	0.35	52,52,52,52	0
56	OHX	AA	3455	7/7	0.88	0.08	173,192,201,215	1
56	OHX	DA	3486	7/7	0.88	0.10	123,132,147,175	1
55	MG	AA	3132	1/1	0.88	0.47	48,48,48,48	0
56	OHX	AA	3459	7/7	0.88	0.12	91,107,133,162	1
55	MG	CA	1721	1/1	0.88	0.15	80,80,80,80	0
55	MG	DA	3202	1/1	0.88	0.22	65,65,65,65	0
55	MG	AA	3259	1/1	0.88	0.12	60,60,60,60	0
56	OHX	CK	201	7/7	0.88	0.10	143,148,155,179	1
55	MG	BA	1674	1/1	0.88	0.19	67,67,67,67	0
55	MG	DA	3078	1/1	0.88	0.29	42,42,42,42	0
55	MG	AA	3134	1/1	0.88	0.33	48,48,48,48	0
55	MG	DA	3086	1/1	0.88	0.34	51,51,51,51	0
55	MG	AA	3070	1/1	0.88	0.22	56,56,56,56	0
55	MG	CC	105	1/1	0.88	0.30	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	1714	1/1	0.89	0.21	84,84,84,84	0
56	OHX	AA	3549	7/7	0.89	0.14	96,102,109,128	2
55	MG	AA	3239	1/1	0.89	0.37	52,52,52,52	0
55	MG	AA	3289	1/1	0.89	0.33	61,61,61,61	0
56	OHX	DA	3255	7/7	0.89	0.12	93,104,107,143	1
56	OHX	AA	3553	7/7	0.89	0.09	160,165,172,209	1
56	OHX	DA	3362	7/7	0.89	0.11	83,98,103,158	1
56	OHX	DA	3399	7/7	0.89	0.10	104,107,123,144	2
56	OHX	BD	102	7/7	0.89	0.08	170,180,207,224	1
55	MG	BB	110	1/1	0.89	0.06	80,80,80,80	0
56	OHX	CA	1754	7/7	0.89	0.10	116,125,134,168	1
55	MG	DA	3334	1/1	0.89	0.23	75,75,75,75	0
56	OHX	CA	1759	7/7	0.89	0.09	125,133,140,148	1
56	OHX	DA	3438	7/7	0.89	0.07	120,135,146,170	1
56	OHX	AA	3560	7/7	0.89	0.10	132,136,153,192	1
55	MG	BA	1624	1/1	0.89	0.35	79,79,79,79	0
56	OHX	AB	213	7/7	0.89	0.11	88,108,129,159	3
55	MG	DA	3204	1/1	0.89	0.27	58,58,58,58	0
56	OHX	CA	1783	7/7	0.89	0.14	113,117,137,164	1
55	MG	AA	3076	1/1	0.89	0.12	81,81,81,81	0
55	MG	AA	3151	1/1	0.89	0.23	46,46,46,46	0
56	OHX	A1	203	7/7	0.89	0.12	97,103,123,154	1
55	MG	AA	3247	1/1	0.89	0.23	66,66,66,66	0
56	OHX	BA	1737	7/7	0.89	0.10	120,131,149,172	1
55	MG	CB	102	1/1	0.89	0.10	80,80,80,80	0
56	OHX	DA	3462	7/7	0.89	0.09	154,157,165,208	1
55	MG	DA	3046	1/1	0.89	0.25	78,78,78,78	0
55	MG	BA	1697	1/1	0.89	0.18	74,74,74,74	0
56	OHX	BA	1761	7/7	0.89	0.08	136,147,154,197	1
56	OHX	AA	3367	7/7	0.89	0.14	69,72,90,147	3
55	MG	DA	3129	1/1	0.89	0.17	68,68,68,68	0
56	OHX	AA	3519	7/7	0.89	0.10	103,114,126,154	1
55	MG	AA	3066	1/1	0.89	0.27	62,62,62,62	0
56	OHX	CA	1809	7/7	0.89	0.07	150,160,169,213	1
56	OHX	AA	3521	7/7	0.89	0.10	103,107,119,167	2
55	MG	AA	3109	1/1	0.89	0.28	38,38,38,38	0
55	MG	DA	3050	1/1	0.89	0.31	74,74,74,74	0
55	MG	CA	1698	1/1	0.89	0.43	86,86,86,86	0
55	MG	AA	3235	1/1	0.89	0.17	57,57,57,57	0
56	OHX	DA	3478	7/7	0.89	0.10	106,110,128,170	1
55	MG	CA	1653	1/1	0.89	0.20	75,75,75,75	0
55	MG	AA	3087	1/1	0.89	0.13	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	1676	1/1	0.89	0.26	78,78,78,78	0
55	MG	DA	3250	1/1	0.89	0.21	64,64,64,64	0
56	OHX	AA	3537	7/7	0.89	0.08	164,173,184,214	1
56	OHX	DA	3485	7/7	0.89	0.06	131,137,152,172	1
56	OHX	BA	1793	7/7	0.89	0.12	129,132,141,164	1
55	MG	DA	3164	1/1	0.89	0.29	63,63,63,63	0
55	MG	CA	1655	1/1	0.89	0.27	70,70,70,70	0
55	MG	DA	3015	1/1	0.89	0.21	56,56,56,56	0
56	OHX	DB	209	7/7	0.89	0.11	130,143,158,186	1
55	MG	AE	301	1/1	0.89	0.32	51,51,51,51	0
56	OHX	DB	214	7/7	0.89	0.07	145,149,169,184	1
56	OHX	DA	3118	7/7	0.89	0.11	99,101,123,146	3
55	MG	DA	3183	1/1	0.89	0.14	99,99,99,99	0
55	MG	AA	3258	1/1	0.89	0.20	39,39,39,39	0
56	OHX	BA	1807	7/7	0.89	0.07	133,136,150,177	1
55	MG	DA	3023	1/1	0.89	0.27	70,70,70,70	0
56	OHX	DA	3174	7/7	0.89	0.10	100,112,120,180	1
56	OHX	D1	201	7/7	0.89	0.09	110,112,135,162	1
56	OHX	BA	1811	7/7	0.89	0.11	110,118,135,147	1
55	MG	AA	3237	1/1	0.89	0.29	62,62,62,62	0
55	MG	AA	3323	1/1	0.90	0.23	58,58,58,58	0
56	OHX	DA	3254	7/7	0.90	0.09	126,129,138,165	1
55	MG	DA	3011	1/1	0.90	0.14	84,84,84,84	0
55	MG	DA	3297	1/1	0.90	0.19	70,70,70,70	0
55	MG	CA	1620	1/1	0.90	0.27	63,63,63,63	0
55	MG	AA	3294	1/1	0.90	0.16	36,36,36,36	0
56	OHX	DA	3405	7/7	0.90	0.10	129,133,151,175	1
55	MG	AA	3036	1/1	0.90	0.31	48,48,48,48	0
55	MG	AA	3094	1/1	0.90	0.39	48,48,48,48	0
56	OHX	CA	1751	7/7	0.90	0.10	102,126,129,174	1
56	OHX	DA	3433	7/7	0.90	0.17	104,114,132,147	1
55	MG	AA	3159	1/1	0.90	0.47	81,81,81,81	0
56	OHX	AA	3485	7/7	0.90	0.11	103,114,131,163	1
56	OHX	CA	1757	7/7	0.90	0.10	117,123,150,175	1
55	MG	DA	3110	1/1	0.90	0.33	60,60,60,60	0
56	OHX	AA	3489	7/7	0.90	0.08	136,140,156,178	1
55	MG	AA	3263	1/1	0.90	0.23	39,39,39,39	0
55	MG	DA	3222	1/1	0.90	0.25	83,83,83,83	0
56	OHX	CA	1777	7/7	0.90	0.10	157,162,168,202	1
56	OHX	AB	215	7/7	0.90	0.10	110,123,130,165	1
55	MG	DA	3031	1/1	0.90	0.18	77,77,77,77	0
56	OHX	AA	3496	7/7	0.90	0.09	107,119,130,176	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	1706	1/1	0.90	0.30	85,85,85,85	0
55	MG	AA	3005	1/1	0.90	0.21	48,48,48,48	0
55	MG	DA	3119	1/1	0.90	0.23	38,38,38,38	0
56	OHX	DA	3457	7/7	0.90	0.07	149,156,166,200	1
56	OHX	DA	3458	7/7	0.90	0.07	173,175,178,215	1
56	OHX	DA	3460	7/7	0.90	0.10	111,124,134,174	1
56	OHX	A3	102	7/7	0.90	0.09	106,109,134,147	2
55	MG	BB	109	1/1	0.90	0.14	80,80,80,80	0
56	OHX	CA	1790	7/7	0.90	0.11	99,111,123,147	2
55	MG	DA	3128	1/1	0.90	0.29	75,75,75,75	0
55	MG	BA	1666	1/1	0.90	0.35	81,81,81,81	0
55	MG	AA	3128	1/1	0.90	0.27	53,53,53,53	0
55	MG	DA	3324	1/1	0.90	0.31	66,66,66,66	0
55	MG	AA	3142	1/1	0.90	0.36	75,75,75,75	0
55	MG	BA	1702	1/1	0.90	0.23	84,84,84,84	0
55	MG	AA	3001	1/1	0.90	0.28	32,32,32,32	0
56	OHX	BA	1775	7/7	0.90	0.09	113,130,145,176	1
55	MG	AA	3278	1/1	0.90	0.13	73,73,73,73	0
55	MG	DA	3265	1/1	0.90	0.15	73,73,73,73	0
55	MG	CA	1638	1/1	0.90	0.30	59,59,59,59	0
55	MG	AB	206	1/1	0.90	0.29	77,77,77,77	0
56	OHX	AA	3515	7/7	0.90	0.12	93,97,116,159	2
55	MG	AA	3167	1/1	0.90	0.16	51,51,51,51	0
55	MG	CA	1602	1/1	0.90	0.30	58,58,58,58	0
55	MG	AA	3214	1/1	0.90	0.27	41,41,41,41	0
56	OHX	DA	3483	7/7	0.90	0.10	103,116,126,199	1
56	OHX	BA	1787	7/7	0.90	0.08	124,129,137,172	1
55	MG	AA	3023	1/1	0.90	0.21	35,35,35,35	0
56	OHX	BA	1790	7/7	0.90	0.07	163,166,178,211	1
55	MG	AA	3033	1/1	0.90	0.25	39,39,39,39	0
55	MG	AA	3045	1/1	0.90	0.14	33,33,33,33	0
55	MG	AA	3107	1/1	0.90	0.30	51,51,51,51	0
55	MG	DA	3280	1/1	0.90	0.36	63,63,63,63	0
55	MG	DA	3282	1/1	0.90	0.28	69,69,69,69	0
56	OHX	BA	1796	7/7	0.90	0.09	119,126,142,152	1
55	MG	AA	3255	1/1	0.90	0.18	47,47,47,47	0
55	MG	DA	3285	1/1	0.90	0.33	57,57,57,57	0
55	MG	DA	3193	1/1	0.90	0.23	43,43,43,43	0
55	MG	AA	3319	1/1	0.90	0.13	63,63,63,63	0
55	MG	AA	3175	1/1	0.90	0.15	46,46,46,46	0
56	OHX	BA	1808	7/7	0.90	0.07	121,129,141,156	1
55	MG	AA	3292	1/1	0.90	0.36	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	AA	3445	7/7	0.90	0.09	118,124,140,177	1
55	MG	DA	3002	1/1	0.90	0.32	46,46,46,46	0
55	MG	AA	3197	1/1	0.91	0.20	57,57,57,57	0
55	MG	CA	1677	1/1	0.91	0.32	73,73,73,73	0
55	MG	CA	1636	1/1	0.91	0.17	82,82,82,82	0
55	MG	AA	3266	1/1	0.91	0.36	62,62,62,62	0
55	MG	AA	3154	1/1	0.91	0.16	52,52,52,52	0
55	MG	AA	3203	1/1	0.91	0.30	72,72,72,72	0
56	OHX	DA	3172	7/7	0.91	0.32	95,104,112,142	1
55	MG	AA	3303	1/1	0.91	0.15	77,77,77,77	0
55	MG	DA	3001	1/1	0.91	0.19	39,39,39,39	0
55	MG	AA	3093	1/1	0.91	0.33	35,35,35,35	0
56	OHX	DA	3217	7/7	0.91	0.08	144,149,153,189	1
55	MG	CA	1642	1/1	0.91	0.33	69,69,69,69	0
56	OHX	DA	3221	7/7	0.91	0.08	120,130,140,174	1
55	MG	BA	1627	1/1	0.91	0.15	58,58,58,58	0
55	MG	CA	1603	1/1	0.91	0.19	62,62,62,62	0
56	OHX	AA	3516	7/7	0.91	0.12	90,98,116,166	1
56	OHX	AA	3517	7/7	0.91	0.08	125,127,137,177	1
55	MG	AA	3105	1/1	0.91	0.31	65,65,65,65	0
55	MG	CA	1647	1/1	0.91	0.27	70,70,70,70	0
55	MG	AA	3242	1/1	0.91	0.24	43,43,43,43	0
55	MG	DA	3024	1/1	0.91	0.23	63,63,63,63	0
55	MG	DA	3026	1/1	0.91	0.22	55,55,55,55	0
55	MG	AA	3143	1/1	0.91	0.10	87,87,87,87	0
55	MG	CA	1651	1/1	0.91	0.11	73,73,73,73	0
56	OHX	DA	3409	7/7	0.91	0.11	103,117,129,162	1
55	MG	CA	1695	1/1	0.91	0.09	94,94,94,94	0
55	MG	BA	1710	1/1	0.91	0.14	113,113,113,113	0
56	OHX	DA	3427	7/7	0.91	0.06	134,147,151,184	1
55	MG	DA	3271	1/1	0.91	0.34	59,59,59,59	0
56	OHX	DA	3434	7/7	0.91	0.09	127,134,154,190	1
56	OHX	DA	3435	7/7	0.91	0.19	86,99,124,155	1
56	OHX	BA	1812	7/7	0.91	0.06	170,174,180,213	1
55	MG	AA	3280	1/1	0.91	0.30	61,61,61,61	0
55	MG	DA	3273	1/1	0.91	0.19	41,41,41,41	0
55	MG	BA	1679	1/1	0.91	0.24	60,60,60,60	0
55	MG	AE	302	1/1	0.91	0.09	74,74,74,74	0
55	MG	AA	3158	1/1	0.91	0.32	49,49,49,49	0
56	OHX	DA	3442	7/7	0.91	0.06	135,142,161,190	1
56	OHX	DA	3444	7/7	0.91	0.09	123,132,145,175	1
56	OHX	AA	3392	7/7	0.91	0.11	81,92,124,181	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	AA	3398	7/7	0.91	0.10	90,95,125,158	1
56	OHX	BD	103	7/7	0.91	0.07	108,110,116,155	1
55	MG	BF	301	1/1	0.91	0.20	79,79,79,79	0
56	OHX	CA	1747	7/7	0.91	0.10	129,134,147,212	1
55	MG	AA	3029	1/1	0.91	0.31	59,59,59,59	0
56	OHX	CA	1753	7/7	0.91	0.15	82,120,146,173	3
55	MG	A1	202	1/1	0.91	0.14	75,75,75,75	0
56	OHX	AA	3547	7/7	0.91	0.10	80,87,107,118	1
55	MG	AA	3220	1/1	0.91	0.21	38,38,38,38	0
56	OHX	CA	1758	7/7	0.91	0.07	150,162,166,191	1
56	OHX	DA	3461	7/7	0.91	0.08	171,173,180,211	1
55	MG	DA	3283	1/1	0.91	0.37	86,86,86,86	0
56	OHX	CA	1765	7/7	0.91	0.06	169,177,182,233	1
56	OHX	DA	3464	7/7	0.91	0.08	117,129,143,171	1
55	MG	AA	3176	1/1	0.91	0.32	46,46,46,46	0
55	MG	DA	3179	1/1	0.91	0.24	46,46,46,46	0
55	MG	AA	3317	1/1	0.91	0.22	55,55,55,55	0
55	MG	AA	3049	1/1	0.91	0.10	66,66,66,66	0
56	OHX	AA	3555	7/7	0.91	0.10	82,85,105,128	1
55	MG	DA	3289	1/1	0.91	0.27	84,84,84,84	0
55	MG	AA	3050	1/1	0.91	0.32	45,45,45,45	0
55	MG	DA	3052	1/1	0.91	0.33	42,42,42,42	0
56	OHX	AA	3569	7/7	0.91	0.06	134,142,144,168	1
56	OHX	AB	210	7/7	0.91	0.07	101,108,128,154	1
56	OHX	AA	3473	7/7	0.91	0.06	104,114,132,167	1
56	OHX	AA	3475	7/7	0.91	0.07	132,134,145,192	1
56	OHX	AA	3478	7/7	0.91	0.08	147,161,167,217	1
56	OHX	CA	1794	7/7	0.91	0.10	102,115,122,149	1
55	MG	AA	3227	1/1	0.91	0.17	61,61,61,61	0
55	MG	DA	3055	1/1	0.91	0.14	54,54,54,54	0
55	MG	AA	3189	1/1	0.91	0.26	63,63,63,63	0
56	OHX	CA	1801	7/7	0.91	0.07	137,140,148,200	1
55	MG	CA	1671	1/1	0.91	0.28	78,78,78,78	0
55	MG	BA	1693	1/1	0.91	0.15	68,68,68,68	0
56	OHX	AW	101	7/7	0.91	0.10	112,118,129,149	1
55	MG	AA	3149	1/1	0.91	0.28	58,58,58,58	0
55	MG	DA	3300	1/1	0.91	0.26	63,63,63,63	0
56	OHX	BA	1744	7/7	0.91	0.10	134,144,157,183	1
56	OHX	DA	3491	7/7	0.91	0.07	104,107,129,176	1
55	MG	DA	3069	1/1	0.91	0.06	63,63,63,63	0
56	OHX	BA	1751	7/7	0.91	0.12	101,112,132,168	2
55	MG	AA	3260	1/1	0.91	0.34	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	BA	1757	7/7	0.91	0.12	86,113,131,156	4
55	MG	DA	3074	1/1	0.91	0.28	40,40,40,40	0
56	OHX	BA	1763	7/7	0.91	0.10	123,136,140,184	1
55	MG	DA	3206	1/1	0.91	0.16	52,52,52,52	0
55	MG	DA	3308	1/1	0.91	0.20	60,60,60,60	0
55	MG	DA	3309	1/1	0.91	0.17	68,68,68,68	0
56	OHX	BA	1774	7/7	0.91	0.08	104,121,130,163	1
55	MG	AA	3073	1/1	0.91	0.22	68,68,68,68	0
56	OHX	AA	3501	7/7	0.91	0.07	104,117,124,169	1
57	PAR	CA	1722	42/42	0.91	0.08	72,88,95,97	0
56	OHX	AA	3482	7/7	0.92	0.15	85,96,105,135	1
55	MG	AA	3146	1/1	0.92	0.31	36,36,36,36	0
56	OHX	CD	101	7/7	0.92	0.07	166,174,199,220	1
56	OHX	BA	1758	7/7	0.92	0.07	153,155,160,202	1
55	MG	AA	3337	1/1	0.92	0.23	73,73,73,73	0
55	MG	BA	1676	1/1	0.92	0.28	78,78,78,78	0
55	MG	DA	3152	1/1	0.92	0.21	57,57,57,57	0
56	OHX	AA	3491	7/7	0.92	0.10	96,99,117,169	1
55	MG	AA	3221	1/1	0.92	0.17	41,41,41,41	0
55	MG	AA	3003	1/1	0.92	0.23	39,39,39,39	0
55	MG	AA	3098	1/1	0.92	0.15	29,29,29,29	0
55	MG	DA	3175	1/1	0.92	0.28	53,53,53,53	0
55	MG	AA	3041	1/1	0.92	0.17	59,59,59,59	0
56	OHX	BA	1779	7/7	0.92	0.09	129,134,141,170	1
55	MG	BA	1682	1/1	0.92	0.07	68,68,68,68	0
55	MG	AA	3080	1/1	0.92	0.09	63,63,63,63	0
55	MG	DA	3040	1/1	0.92	0.16	66,66,66,66	0
56	OHX	DA	3218	7/7	0.92	0.28	96,106,121,133	1
55	MG	AB	203	1/1	0.92	0.20	58,58,58,58	0
55	MG	DA	3042	1/1	0.92	0.23	74,74,74,74	0
55	MG	AA	3265	1/1	0.92	0.37	62,62,62,62	0
55	MG	BA	1634	1/1	0.92	0.10	73,73,73,73	0
56	OHX	DA	3245	7/7	0.92	0.09	95,128,139,165	1
55	MG	CA	1648	1/1	0.92	0.35	70,70,70,70	0
55	MG	AA	3015	1/1	0.92	0.18	44,44,44,44	0
55	MG	AA	3179	1/1	0.92	0.17	39,39,39,39	0
55	MG	AA	3053	1/1	0.92	0.21	77,77,77,77	0
55	MG	B1	101	1/1	0.92	0.13	96,96,96,96	0
55	MG	AA	3069	1/1	0.92	0.25	54,54,54,54	0
56	OHX	DA	3376	7/7	0.92	0.13	38,106,133,165	3
55	MG	AA	3085	1/1	0.92	0.21	74,74,74,74	0
55	MG	AA	3034	1/1	0.92	0.30	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3057	1/1	0.92	0.25	58,58,58,58	0
56	OHX	DA	3408	7/7	0.92	0.10	122,131,146,182	1
55	MG	DA	3207	1/1	0.92	0.25	37,37,37,37	0
55	MG	CA	1604	1/1	0.92	0.10	72,72,72,72	0
56	OHX	DA	3415	7/7	0.92	0.07	128,140,160,189	1
56	OHX	DA	3417	7/7	0.92	0.07	145,152,156,188	1
56	OHX	DA	3420	7/7	0.92	0.09	116,120,125,152	1
56	OHX	BA	1801	7/7	0.92	0.07	129,138,143,174	1
56	OHX	DA	3424	7/7	0.92	0.09	124,129,137,157	2
55	MG	AA	3088	1/1	0.92	0.20	66,66,66,66	0
56	OHX	DA	3429	7/7	0.92	0.08	118,130,143,180	1
56	OHX	DA	3432	7/7	0.92	0.06	116,131,140,173	1
56	OHX	BA	1806	7/7	0.92	0.11	110,117,124,159	1
55	MG	AA	3312	1/1	0.92	0.18	71,71,71,71	0
55	MG	AA	3035	1/1	0.92	0.12	38,38,38,38	0
56	OHX	AA	3522	7/7	0.92	0.12	74,93,104,150	2
55	MG	AA	3019	1/1	0.92	0.23	42,42,42,42	0
55	MG	DA	3070	1/1	0.92	0.22	69,69,69,69	0
55	MG	CA	1612	1/1	0.92	0.17	95,95,95,95	0
55	MG	AA	3204	1/1	0.92	0.28	45,45,45,45	0
55	MG	AA	3091	1/1	0.92	0.14	85,85,85,85	0
55	MG	CB	103	1/1	0.92	0.06	80,80,80,80	0
55	MG	BA	1650	1/1	0.92	0.18	85,85,85,85	0
55	MG	BA	1651	1/1	0.92	0.27	76,76,76,76	0
55	MG	DA	3089	1/1	0.92	0.48	54,54,54,54	0
55	MG	DA	3240	1/1	0.92	0.28	64,64,64,64	0
55	MG	AA	3165	1/1	0.92	0.24	79,79,79,79	0
55	MG	DA	3092	1/1	0.92	0.17	74,74,74,74	0
55	MG	AA	3286	1/1	0.92	0.33	83,83,83,83	0
55	MG	DA	3252	1/1	0.92	0.34	81,81,81,81	0
55	MG	BA	1611	1/1	0.92	0.24	47,47,47,47	0
56	OHX	DA	3456	7/7	0.92	0.07	133,142,150,207	1
55	MG	AA	3210	1/1	0.92	0.28	43,43,43,43	0
55	MG	DA	3264	1/1	0.92	0.16	78,78,78,78	0
55	MG	BA	1661	1/1	0.92	0.23	61,61,61,61	0
56	OHX	AA	3404	7/7	0.92	0.09	108,112,133,175	1
55	MG	BA	1662	1/1	0.92	0.18	56,56,56,56	0
56	OHX	AA	3409	7/7	0.92	0.13	99,110,115,152	1
56	OHX	CA	1769	7/7	0.92	0.09	141,144,170,199	1
56	OHX	CA	1773	7/7	0.92	0.08	123,130,144,181	1
55	MG	BA	1663	1/1	0.92	0.48	80,80,80,80	0
55	MG	AA	3057	1/1	0.92	0.17	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	CA	1776	7/7	0.92	0.08	112,115,132,151	1
55	MG	DA	3009	1/1	0.92	0.28	50,50,50,50	0
56	OHX	CA	1780	7/7	0.92	0.06	138,146,156,182	1
56	OHX	CA	1781	7/7	0.92	0.09	153,161,166,239	1
56	OHX	AA	3433	7/7	0.92	0.10	77,91,106,131	2
55	MG	AA	3290	1/1	0.92	0.31	66,66,66,66	0
56	OHX	AA	3439	7/7	0.92	0.09	114,122,140,194	1
56	OHX	AA	3563	7/7	0.92	0.07	128,136,143,179	1
56	OHX	AA	3564	7/7	0.92	0.10	94,114,124,148	1
56	OHX	AA	3443	7/7	0.92	0.10	110,114,126,149	2
55	MG	AA	3006	1/1	0.92	0.24	40,40,40,40	0
55	MG	DA	3116	1/1	0.92	0.23	62,62,62,62	0
56	OHX	AA	3448	7/7	0.92	0.06	141,143,155,200	1
56	OHX	CA	1792	7/7	0.92	0.06	189,191,192,232	1
56	OHX	AA	3449	7/7	0.92	0.10	102,118,124,165	1
55	MG	DA	3013	1/1	0.92	0.26	40,40,40,40	0
55	MG	CA	1680	1/1	0.92	0.28	78,78,78,78	0
55	MG	BA	1618	1/1	0.92	0.20	71,71,71,71	0
56	OHX	DA	3487	7/7	0.92	0.10	106,108,129,150	1
55	MG	BA	1671	1/1	0.92	0.35	68,68,68,68	0
56	OHX	AA	3457	7/7	0.92	0.12	86,94,124,185	1
55	MG	DA	3021	1/1	0.92	0.23	62,62,62,62	0
56	OHX	AA	3460	7/7	0.92	0.08	131,133,148,193	1
56	OHX	CA	1807	7/7	0.92	0.09	109,119,124,150	1
55	MG	DA	3281	1/1	0.92	0.10	65,65,65,65	0
55	MG	AA	3061	1/1	0.92	0.29	59,59,59,59	0
56	OHX	CA	1810	7/7	0.92	0.10	113,132,142,167	1
55	MG	DA	3137	1/1	0.92	0.26	51,51,51,51	0
56	OHX	BA	1745	7/7	0.92	0.10	119,123,132,169	1
56	OHX	BA	1747	7/7	0.92	0.10	117,129,140,148	1
56	OHX	BA	1748	7/7	0.92	0.08	124,127,141,171	1
56	OHX	BA	1749	7/7	0.92	0.10	112,116,136,168	1
55	MG	BA	1620	1/1	0.92	0.25	73,73,73,73	0
56	OHX	CV	101	7/7	0.92	0.07	174,182,196,223	1
55	MG	DA	3025	1/1	0.92	0.12	59,59,59,59	0
56	OHX	BA	1752	7/7	0.92	0.06	168,174,177,207	1
55	MG	DA	3012	1/1	0.93	0.17	44,44,44,44	0
55	MG	DA	3080	1/1	0.93	0.21	43,43,43,43	0
55	MG	AA	3020	1/1	0.93	0.32	42,42,42,42	0
55	MG	DA	3014	1/1	0.93	0.21	55,55,55,55	0
56	OHX	AB	214	7/7	0.93	0.08	125,133,135,173	1
56	OHX	DA	3385	7/7	0.93	0.09	78,128,134,201	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	DA	3398	7/7	0.93	0.07	119,127,142,162	1
55	MG	AA	3086	1/1	0.93	0.31	73,73,73,73	0
55	MG	AA	3267	1/1	0.93	0.17	37,37,37,37	0
56	OHX	CA	1756	7/7	0.93	0.11	99,109,123,147	2
56	OHX	AB	217	7/7	0.93	0.17	100,108,115,151	1
55	MG	CA	1696	1/1	0.93	0.27	74,74,74,74	0
55	MG	CA	1697	1/1	0.93	0.20	66,66,66,66	0
56	OHX	DA	3414	7/7	0.93	0.10	126,128,140,174	1
55	MG	DA	3312	1/1	0.93	0.19	81,81,81,81	0
56	OHX	DA	3416	7/7	0.93	0.11	112,112,142,167	1
55	MG	BA	1631	1/1	0.93	0.09	85,85,85,85	0
55	MG	AA	3229	1/1	0.93	0.25	65,65,65,65	0
56	OHX	CA	1772	7/7	0.93	0.07	142,144,153,197	1
55	MG	AA	3103	1/1	0.93	0.30	50,50,50,50	0
56	OHX	DA	3425	7/7	0.93	0.07	125,134,139,188	1
55	MG	AA	3072	1/1	0.93	0.29	73,73,73,73	0
56	OHX	BA	1738	7/7	0.93	0.08	112,124,136,189	1
56	OHX	DA	3430	7/7	0.93	0.08	176,181,185,214	1
56	OHX	DA	3431	7/7	0.93	0.06	139,144,155,180	1
55	MG	DA	3104	1/1	0.93	0.32	64,64,64,64	0
55	MG	CA	1703	1/1	0.93	0.25	84,84,84,84	0
55	MG	AF	302	1/1	0.93	0.19	83,83,83,83	0
55	MG	AA	3058	1/1	0.93	0.09	61,61,61,61	0
55	MG	DA	3032	1/1	0.93	0.05	38,38,38,38	0
55	MG	AA	3021	1/1	0.93	0.24	35,35,35,35	0
55	MG	DA	3034	1/1	0.93	0.26	69,69,69,69	0
55	MG	AA	3108	1/1	0.93	0.14	54,54,54,54	0
55	MG	CA	1709	1/1	0.93	0.22	76,76,76,76	0
55	MG	AA	3060	1/1	0.93	0.19	89,89,89,89	0
56	OHX	BA	1756	7/7	0.93	0.07	153,171,174,206	1
56	OHX	DA	3443	7/7	0.93	0.08	113,124,137,188	1
55	MG	BA	1684	1/1	0.93	0.19	67,67,67,67	0
55	MG	AA	3022	1/1	0.93	0.22	28,28,28,28	0
55	MG	AA	3201	1/1	0.93	0.30	35,35,35,35	0
56	OHX	AA	3510	7/7	0.93	0.10	98,106,123,159	1
55	MG	AA	3013	1/1	0.93	0.26	27,27,27,27	0
55	MG	DA	3139	1/1	0.93	0.37	54,54,54,54	0
56	OHX	BA	1770	7/7	0.93	0.08	114,115,121,163	1
56	OHX	CA	1800	7/7	0.93	0.05	165,167,172,220	1
56	OHX	BA	1771	7/7	0.93	0.17	101,104,120,152	2
55	MG	DA	3140	1/1	0.93	0.20	55,55,55,55	0
55	MG	AA	3040	1/1	0.93	0.27	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3113	1/1	0.93	0.18	88,88,88,88	0
55	MG	AA	3115	1/1	0.93	0.32	57,57,57,57	0
56	OHX	BA	1777	7/7	0.93	0.07	176,178,192,246	1
55	MG	AA	3011	1/1	0.93	0.22	44,44,44,44	0
55	MG	AA	3031	1/1	0.93	0.18	40,40,40,40	0
55	MG	D0	201	1/1	0.93	0.12	51,51,51,51	0
55	MG	D7	101	1/1	0.93	0.37	69,69,69,69	0
55	MG	DA	3274	1/1	0.93	0.31	69,69,69,69	0
55	MG	AA	3169	1/1	0.93	0.39	47,47,47,47	0
56	OHX	AA	3395	7/7	0.93	0.12	100,109,130,162	1
55	MG	AA	3018	1/1	0.93	0.24	49,49,49,49	0
55	MG	DA	3154	1/1	0.93	0.18	60,60,60,60	0
55	MG	DA	3051	1/1	0.93	0.33	39,39,39,39	0
55	MG	DA	3161	1/1	0.93	0.26	41,41,41,41	0
55	MG	AA	3293	1/1	0.93	0.15	72,72,72,72	0
55	MG	AA	3171	1/1	0.93	0.17	59,59,59,59	0
56	OHX	AA	3419	7/7	0.93	0.08	102,113,133,143	3
56	OHX	DA	3087	7/7	0.93	0.09	102,119,134,177	1
55	MG	BA	1659	1/1	0.93	0.30	43,43,43,43	0
55	MG	DA	3056	1/1	0.93	0.23	48,48,48,48	0
55	MG	AA	3339	1/1	0.93	0.30	58,58,58,58	0
55	MG	AA	3004	1/1	0.93	0.26	32,32,32,32	0
55	MG	DA	3286	1/1	0.93	0.13	77,77,77,77	0
55	MG	AA	3356	1/1	0.93	0.33	70,70,70,70	0
55	MG	DA	3184	1/1	0.93	0.28	37,37,37,37	0
55	MG	DA	3185	1/1	0.93	0.29	49,49,49,49	0
56	OHX	DA	3163	7/7	0.93	0.10	124,127,154,166	1
55	MG	DA	3063	1/1	0.93	0.40	59,59,59,59	0
56	OHX	DA	3169	7/7	0.93	0.07	110,124,136,172	1
56	OHX	DA	3171	7/7	0.93	0.12	95,116,127,171	1
55	MG	AA	3121	1/1	0.93	0.20	65,65,65,65	0
55	MG	AA	3223	1/1	0.93	0.18	43,43,43,43	0
56	OHX	BA	1809	7/7	0.93	0.06	159,162,164,206	1
55	MG	CA	1607	1/1	0.93	0.18	86,86,86,86	0
55	MG	DA	3198	1/1	0.93	0.30	44,44,44,44	0
55	MG	CA	1688	1/1	0.93	0.14	79,79,79,79	0
55	MG	AA	3123	1/1	0.93	0.15	65,65,65,65	0
55	MG	BA	1669	1/1	0.93	0.22	68,68,68,68	0
56	OHX	AA	3558	7/7	0.93	0.07	92,100,110,168	1
56	OHX	DA	3224	7/7	0.93	0.11	104,110,126,166	1
56	OHX	AA	3462	7/7	0.93	0.10	105,108,119,142	2
56	OHX	AA	3466	7/7	0.93	0.07	98,120,132,157	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	DA	3248	7/7	0.93	0.08	110,118,139,156	1
55	MG	AA	3225	1/1	0.93	0.45	52,52,52,52	0
56	OHX	AA	3474	7/7	0.93	0.08	113,120,132,160	1
55	MG	AA	3305	1/1	0.94	0.39	66,66,66,66	0
55	MG	AF	301	1/1	0.94	0.09	74,74,74,74	0
56	OHX	BA	1767	7/7	0.94	0.07	151,158,165,212	1
55	MG	AA	3191	1/1	0.94	0.07	39,39,39,39	0
55	MG	DA	3088	1/1	0.94	0.26	47,47,47,47	0
55	MG	AA	3192	1/1	0.94	0.23	34,34,34,34	0
56	OHX	BA	1773	7/7	0.94	0.08	135,139,146,167	1
55	MG	AA	3133	1/1	0.94	0.28	45,45,45,45	0
55	MG	AA	3097	1/1	0.94	0.16	50,50,50,50	0
56	OHX	DA	3170	7/7	0.94	0.10	114,125,135,172	1
55	MG	DA	3093	1/1	0.94	0.16	46,46,46,46	0
55	MG	DA	3095	1/1	0.94	0.16	58,58,58,58	0
55	MG	DA	3316	1/1	0.94	0.18	51,51,51,51	0
55	MG	CA	1645	1/1	0.94	0.28	58,58,58,58	0
55	MG	BA	1644	1/1	0.94	0.21	62,62,62,62	0
56	OHX	DA	3215	7/7	0.94	0.10	97,115,127,150	3
55	MG	DA	3319	1/1	0.94	0.32	69,69,69,69	0
56	OHX	AA	3504	7/7	0.94	0.14	101,103,116,145	2
55	MG	AA	3002	1/1	0.94	0.24	34,34,34,34	0
56	OHX	BA	1784	7/7	0.94	0.17	94,101,111,137	1
55	MG	DA	3321	1/1	0.94	0.16	56,56,56,56	0
55	MG	DA	3219	1/1	0.94	0.17	62,62,62,62	0
55	MG	A7	101	1/1	0.94	0.25	56,56,56,56	0
55	MG	AA	3199	1/1	0.94	0.23	75,75,75,75	0
55	MG	AA	3276	1/1	0.94	0.23	76,76,76,76	0
55	MG	AA	3153	1/1	0.94	0.29	40,40,40,40	0
55	MG	DA	3107	1/1	0.94	0.20	42,42,42,42	0
55	MG	CA	1652	1/1	0.94	0.08	69,69,69,69	0
55	MG	DA	3329	1/1	0.94	0.28	60,60,60,60	0
55	MG	DA	3236	1/1	0.94	0.31	62,62,62,62	0
55	MG	BA	1605	1/1	0.94	0.10	81,81,81,81	0
55	MG	DA	3332	1/1	0.94	0.24	78,78,78,78	0
55	MG	DA	3238	1/1	0.94	0.17	67,67,67,67	0
56	OHX	DA	3391	7/7	0.94	0.08	117,125,144,183	1
55	MG	BA	1606	1/1	0.94	0.20	70,70,70,70	0
55	MG	AA	3047	1/1	0.94	0.26	65,65,65,65	0
56	OHX	DA	3400	7/7	0.94	0.07	113,116,126,149	1
56	OHX	BA	1803	7/7	0.94	0.07	211,214,221,256	1
55	MG	CA	1705	1/1	0.94	0.31	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3007	1/1	0.94	0.32	43,43,43,43	0
55	MG	AA	3139	1/1	0.94	0.20	47,47,47,47	0
56	OHX	DA	3410	7/7	0.94	0.06	107,112,124,146	1
55	MG	DA	3036	1/1	0.94	0.10	47,47,47,47	0
55	MG	DA	3123	1/1	0.94	0.24	38,38,38,38	0
55	MG	DA	3125	1/1	0.94	0.22	54,54,54,54	0
55	MG	DA	3260	1/1	0.94	0.23	68,68,68,68	0
55	MG	DA	3261	1/1	0.94	0.31	53,53,53,53	0
56	OHX	DA	3419	7/7	0.94	0.16	82,93,100,126	2
56	OHX	AA	3532	7/7	0.94	0.07	136,144,160,202	1
56	OHX	AA	3535	7/7	0.94	0.19	94,101,108,146	1
55	MG	BA	1658	1/1	0.94	0.27	47,47,47,47	0
56	OHX	AA	3362	7/7	0.94	0.09	104,116,120,168	1
55	MG	AA	3206	1/1	0.94	0.17	37,37,37,37	0
56	OHX	DA	3428	7/7	0.94	0.11	93,108,120,163	1
56	OHX	AA	3383	7/7	0.94	0.14	91,96,109,133	1
56	OHX	AA	3384	7/7	0.94	0.13	96,100,107,136	1
55	MG	DA	3130	1/1	0.94	0.08	48,48,48,48	0
55	MG	CA	1710	1/1	0.94	0.19	78,78,78,78	0
56	OHX	CA	1743	7/7	0.94	0.09	101,120,132,162	1
55	MG	DA	3268	1/1	0.94	0.20	44,44,44,44	0
55	MG	DA	3269	1/1	0.94	0.29	52,52,52,52	0
55	MG	DA	3133	1/1	0.94	0.17	51,51,51,51	0
55	MG	CA	1711	1/1	0.94	0.33	57,57,57,57	0
55	MG	AA	3207	1/1	0.94	0.36	44,44,44,44	0
56	OHX	AA	3414	7/7	0.94	0.11	92,104,120,143	1
56	OHX	AA	3550	7/7	0.94	0.06	118,128,136,169	1
56	OHX	AA	3416	7/7	0.94	0.08	108,113,125,155	1
55	MG	AA	3173	1/1	0.94	0.34	65,65,65,65	0
56	OHX	CA	1762	7/7	0.94	0.09	148,151,154,182	1
56	OHX	CA	1764	7/7	0.94	0.09	113,122,135,168	1
55	MG	AA	3101	1/1	0.94	0.20	47,47,47,47	0
55	MG	DA	3143	1/1	0.94	0.18	38,38,38,38	0
56	OHX	CA	1768	7/7	0.94	0.07	123,135,145,174	1
56	OHX	DA	3449	7/7	0.94	0.07	147,154,162,185	1
56	OHX	AA	3425	7/7	0.94	0.07	158,168,177,207	1
56	OHX	CA	1771	7/7	0.94	0.11	105,107,134,145	1
56	OHX	AA	3556	7/7	0.94	0.10	82,96,111,154	1
56	OHX	AA	3557	7/7	0.94	0.19	89,102,113,146	1
55	MG	BA	1664	1/1	0.94	0.22	54,54,54,54	0
56	OHX	AA	3435	7/7	0.94	0.08	83,103,126,156	2
55	MG	AA	3246	1/1	0.94	0.23	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3126	1/1	0.94	0.20	54,54,54,54	0
56	OHX	AA	3442	7/7	0.94	0.06	97,106,127,148	1
56	OHX	AA	3565	7/7	0.94	0.07	97,104,114,159	1
55	MG	AA	3248	1/1	0.94	0.20	28,28,28,28	0
55	MG	AA	3025	1/1	0.94	0.22	37,37,37,37	0
56	OHX	AB	208	7/7	0.94	0.10	95,117,137,155	2
56	OHX	AA	3446	7/7	0.94	0.05	148,150,154,190	1
55	MG	AA	3177	1/1	0.94	0.18	46,46,46,46	0
55	MG	AA	3065	1/1	0.94	0.11	46,46,46,46	0
55	MG	AA	3253	1/1	0.94	0.17	49,49,49,49	0
55	MG	AA	3219	1/1	0.94	0.20	65,65,65,65	0
55	MG	DA	3054	1/1	0.94	0.16	56,56,56,56	0
55	MG	AA	3026	1/1	0.94	0.23	43,43,43,43	0
56	OHX	CA	1793	7/7	0.94	0.07	142,146,153,194	1
55	MG	AA	3257	1/1	0.94	0.25	64,64,64,64	0
56	OHX	CA	1795	7/7	0.94	0.07	115,125,132,165	1
56	OHX	AO	203	7/7	0.94	0.15	83,92,110,152	1
55	MG	AA	3027	1/1	0.94	0.14	35,35,35,35	0
55	MG	AA	3299	1/1	0.94	0.23	41,41,41,41	0
55	MG	DA	3290	1/1	0.94	0.14	37,37,37,37	0
55	MG	AA	3182	1/1	0.94	0.25	66,66,66,66	0
56	OHX	BA	1731	7/7	0.94	0.11	99,107,129,161	1
56	OHX	AA	3463	7/7	0.94	0.08	94,102,127,154	1
56	OHX	AA	3465	7/7	0.94	0.10	82,99,109,148	1
56	OHX	BA	1742	7/7	0.94	0.08	149,155,172,201	1
55	MG	AA	3184	1/1	0.94	0.21	35,35,35,35	0
56	OHX	AA	3468	7/7	0.94	0.08	110,120,137,165	1
56	OHX	AA	3472	7/7	0.94	0.10	95,115,124,169	1
55	MG	CA	1633	1/1	0.94	0.35	46,46,46,46	0
55	MG	CA	1634	1/1	0.94	0.34	64,64,64,64	0
55	MG	DA	3186	1/1	0.94	0.21	34,34,34,34	0
56	OHX	AA	3476	7/7	0.94	0.09	88,98,119,157	1
55	MG	AA	3187	1/1	0.94	0.19	40,40,40,40	0
55	MG	AA	3028	1/1	0.94	0.22	35,35,35,35	0
55	MG	DA	3003	1/1	0.94	0.15	43,43,43,43	0
55	MG	DA	3005	1/1	0.94	0.17	41,41,41,41	0
55	MG	DA	3008	1/1	0.94	0.12	43,43,43,43	0
55	MG	DA	3077	1/1	0.94	0.33	52,52,52,52	0
56	OHX	BA	1759	7/7	0.94	0.07	173,177,187,214	1
56	OHX	AA	3486	7/7	0.94	0.07	95,110,127,153	1
56	OHX	DA	3081	7/7	0.94	0.14	99,102,113,145	1
56	OHX	DA	3083	7/7	0.94	0.09	104,111,120,146	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	BA	1762	7/7	0.94	0.08	121,131,144,180	1
55	MG	AA	3304	1/1	0.94	0.13	55,55,55,55	0
56	OHX	BA	1764	7/7	0.94	0.09	147,152,158,209	1
58	ZN	CG	301	1/1	0.94	0.19	116,116,116,116	0
56	OHX	DA	3348	7/7	0.95	0.08	97,115,128,140	1
56	OHX	AA	3432	7/7	0.95	0.07	129,136,142,160	1
56	OHX	DA	3372	7/7	0.95	0.11	90,96,108,138	1
56	OHX	CA	1763	7/7	0.95	0.07	142,143,157,189	1
55	MG	AA	3077	1/1	0.95	0.27	39,39,39,39	0
56	OHX	DA	3388	7/7	0.95	0.10	108,118,139,160	1
56	OHX	AA	3434	7/7	0.95	0.14	98,102,107,132	1
56	OHX	DA	3392	7/7	0.95	0.07	115,117,129,183	1
56	OHX	DA	3393	7/7	0.95	0.06	133,134,150,191	1
56	OHX	DA	3394	7/7	0.95	0.08	127,139,150,223	0
56	OHX	DA	3396	7/7	0.95	0.12	96,99,105,140	1
55	MG	AA	3194	1/1	0.95	0.33	56,56,56,56	0
55	MG	AA	3104	1/1	0.95	0.29	62,62,62,62	0
56	OHX	AA	3437	7/7	0.95	0.09	76,82,94,136	1
56	OHX	DA	3402	7/7	0.95	0.07	122,136,148,204	1
56	OHX	DA	3404	7/7	0.95	0.10	107,121,131,166	1
56	OHX	CA	1770	7/7	0.95	0.06	143,153,167,200	1
56	OHX	DA	3406	7/7	0.95	0.11	88,107,111,147	3
55	MG	BA	1632	1/1	0.95	0.15	73,73,73,73	0
56	OHX	AA	3441	7/7	0.95	0.06	113,135,152,175	1
55	MG	AA	3114	1/1	0.95	0.32	62,62,62,62	0
55	MG	CA	1702	1/1	0.95	0.23	59,59,59,59	0
56	OHX	DA	3411	7/7	0.95	0.09	104,112,132,163	1
56	OHX	BA	1760	7/7	0.95	0.08	109,109,121,147	1
56	OHX	AA	3525	7/7	0.95	0.06	118,124,140,179	1
55	MG	DA	3108	1/1	0.95	0.31	56,56,56,56	0
56	OHX	CA	1778	7/7	0.95	0.06	148,157,164,202	1
55	MG	AA	3261	1/1	0.95	0.16	53,53,53,53	0
55	MG	DA	3006	1/1	0.95	0.15	63,63,63,63	0
55	MG	DA	3007	1/1	0.95	0.21	43,43,43,43	0
56	OHX	DA	3421	7/7	0.95	0.08	96,112,124,166	1
55	MG	AA	3164	1/1	0.95	0.17	45,45,45,45	0
55	MG	DA	3115	1/1	0.95	0.18	44,44,44,44	0
56	OHX	AA	3534	7/7	0.95	0.06	103,124,138,161	2
56	OHX	DA	3426	7/7	0.95	0.07	118,125,141,168	1
55	MG	CA	1613	1/1	0.95	0.23	73,73,73,73	0
55	MG	BA	1609	1/1	0.95	0.13	65,65,65,65	0
55	MG	AA	3032	1/1	0.95	0.40	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3152	1/1	0.95	0.33	50,50,50,50	0
55	MG	BA	1694	1/1	0.95	0.23	60,60,60,60	0
55	MG	AA	3180	1/1	0.95	0.31	42,42,42,42	0
56	OHX	AA	3461	7/7	0.95	0.07	102,110,120,148	1
56	OHX	AA	3542	7/7	0.95	0.10	92,98,124,157	1
55	MG	AA	3017	1/1	0.95	0.19	26,26,26,26	0
55	MG	DA	3016	1/1	0.95	0.34	51,51,51,51	0
56	OHX	AA	3464	7/7	0.95	0.09	105,115,140,175	1
55	MG	AA	3268	1/1	0.95	0.14	38,38,38,38	0
55	MG	DA	3018	1/1	0.95	0.15	47,47,47,47	0
55	MG	AA	3024	1/1	0.95	0.24	45,45,45,45	0
56	OHX	AA	3470	7/7	0.95	0.06	116,126,152,171	1
56	OHX	CA	1803	7/7	0.95	0.06	137,147,156,198	1
55	MG	AA	3008	1/1	0.95	0.26	32,32,32,32	0
55	MG	DA	3213	1/1	0.95	0.26	57,57,57,57	0
56	OHX	DA	3445	7/7	0.95	0.07	121,130,142,174	1
55	MG	AA	3273	1/1	0.95	0.30	60,60,60,60	0
56	OHX	BA	1789	7/7	0.95	0.06	132,137,146,191	1
55	MG	BA	1646	1/1	0.95	0.20	48,48,48,48	0
55	MG	DA	3141	1/1	0.95	0.22	64,64,64,64	0
55	MG	DA	3227	1/1	0.95	0.17	44,44,44,44	0
56	OHX	DA	3451	7/7	0.95	0.11	103,107,114,153	1
56	OHX	AA	3479	7/7	0.95	0.06	94,103,125,176	3
55	MG	CA	1717	1/1	0.95	0.24	64,64,64,64	0
55	MG	D5	101	1/1	0.95	0.14	43,43,43,43	0
55	MG	DA	3229	1/1	0.95	0.26	45,45,45,45	0
56	OHX	AA	3483	7/7	0.95	0.10	106,109,118,158	2
56	OHX	AA	3562	7/7	0.95	0.13	100,110,119,157	1
55	MG	DA	3230	1/1	0.95	0.09	51,51,51,51	0
56	OHX	BA	1800	7/7	0.95	0.07	127,133,145,177	1
55	MG	AA	3274	1/1	0.95	0.05	36,36,36,36	0
56	OHX	BA	1802	7/7	0.95	0.07	100,117,125,149	1
56	OHX	AA	3376	7/7	0.95	0.12	96,107,117,142	1
55	MG	DA	3028	1/1	0.95	0.19	44,44,44,44	0
55	MG	BC	101	1/1	0.95	0.21	62,62,62,62	0
56	OHX	AA	3385	7/7	0.95	0.09	73,87,109,139	2
55	MG	AA	3030	1/1	0.95	0.23	36,36,36,36	0
56	OHX	DA	3094	7/7	0.95	0.06	110,121,124,149	1
56	OHX	DA	3099	7/7	0.95	0.10	104,109,114,163	1
56	OHX	AA	3394	7/7	0.95	0.08	113,123,125,181	1
56	OHX	DA	3471	7/7	0.95	0.08	112,124,129,160	1
55	MG	AA	3016	1/1	0.95	0.30	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	1658	1/1	0.95	0.16	65,65,65,65	0
56	OHX	AA	3399	7/7	0.95	0.09	97,111,117,147	1
56	OHX	AA	3401	7/7	0.95	0.07	101,105,125,153	1
55	MG	AA	3145	1/1	0.95	0.21	27,27,27,27	0
56	OHX	AA	3405	7/7	0.95	0.09	100,103,111,158	1
56	OHX	DA	3159	7/7	0.95	0.09	75,86,105,131	3
55	MG	AA	3254	1/1	0.95	0.34	43,43,43,43	0
55	MG	DA	3155	1/1	0.95	0.22	58,58,58,58	0
56	OHX	DA	3166	7/7	0.95	0.07	159,166,176,197	1
55	MG	DA	3241	1/1	0.95	0.06	47,47,47,47	0
55	MG	AA	3046	1/1	0.95	0.14	50,50,50,50	0
55	MG	CC	102	1/1	0.95	0.35	69,69,69,69	0
56	OHX	A6	101	7/7	0.95	0.09	112,127,141,158	2
56	OHX	CA	1733	7/7	0.95	0.12	109,120,127,147	1
56	OHX	CA	1735	7/7	0.95	0.08	146,153,168,212	0
56	OHX	CA	1738	7/7	0.95	0.09	120,123,126,168	1
56	OHX	DA	3214	7/7	0.95	0.08	82,92,98,133	2
56	OHX	CA	1739	7/7	0.95	0.09	140,150,165,188	1
56	OHX	CA	1741	7/7	0.95	0.09	101,122,129,156	2
55	MG	CA	1693	1/1	0.95	0.13	55,55,55,55	0
56	OHX	DB	210	7/7	0.95	0.08	119,127,150,173	2
56	OHX	DB	211	7/7	0.95	0.07	105,121,145,156	2
56	OHX	DB	212	7/7	0.95	0.07	144,152,161,194	1
56	OHX	CA	1745	7/7	0.95	0.08	117,120,127,165	1
55	MG	BA	1653	1/1	0.95	0.26	64,64,64,64	0
56	OHX	CA	1749	7/7	0.95	0.08	124,137,161,188	2
56	OHX	CA	1750	7/7	0.95	0.12	110,113,130,151	1
55	MG	CA	1663	1/1	0.95	0.10	65,65,65,65	0
56	OHX	BA	1740	7/7	0.95	0.11	107,110,122,131	1
56	OHX	DA	3246	7/7	0.95	0.11	89,97,107,138	1
56	OHX	AA	3421	7/7	0.95	0.10	78,84,91,130	1
56	OHX	AA	3423	7/7	0.95	0.07	100,115,121,157	1
55	MG	AA	3213	1/1	0.95	0.10	60,60,60,60	0
56	OHX	AA	3428	7/7	0.95	0.06	114,120,124,169	1
56	OHX	D8	101	7/7	0.95	0.09	140,149,164,175	1
57	PAR	BA	1715	42/42	0.95	0.08	61,73,83,89	0
56	OHX	BA	1746	7/7	0.95	0.13	95,103,110,146	1
56	OHX	AA	3430	7/7	0.95	0.06	119,125,132,176	1
56	OHX	CA	1814	7/7	0.96	0.05	149,152,161,212	1
55	MG	BA	1678	1/1	0.96	0.21	44,44,44,44	0
55	MG	DA	3149	1/1	0.96	0.14	53,53,53,53	0
55	MG	AA	3320	1/1	0.96	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3042	1/1	0.96	0.14	42,42,42,42	0
56	OHX	AA	3406	7/7	0.96	0.12	93,96,102,133	1
56	OHX	CA	1731	7/7	0.96	0.09	90,118,129,156	1
55	MG	AA	3116	1/1	0.96	0.23	63,63,63,63	0
55	MG	AE	303	1/1	0.96	0.14	36,36,36,36	0
56	OHX	BA	1753	7/7	0.96	0.08	103,110,125,169	1
55	MG	DA	3058	1/1	0.96	0.24	70,70,70,70	0
56	OHX	DA	3082	7/7	0.96	0.09	92,102,108,132	1
56	OHX	BA	1755	7/7	0.96	0.08	123,128,136,161	1
55	MG	BA	1614	1/1	0.96	0.17	73,73,73,73	0
55	MG	DA	3225	1/1	0.96	0.36	55,55,55,55	0
55	MG	AA	3217	1/1	0.96	0.07	66,66,66,66	0
56	OHX	CA	1748	7/7	0.96	0.07	137,145,152,186	1
55	MG	BC	103	1/1	0.96	0.34	70,70,70,70	0
55	MG	AA	3232	1/1	0.96	0.12	62,62,62,62	0
55	MG	AA	3251	1/1	0.96	0.24	75,75,75,75	0
56	OHX	CA	1752	7/7	0.96	0.08	139,147,150,191	1
55	MG	AA	3064	1/1	0.96	0.38	52,52,52,52	0
55	MG	BA	1665	1/1	0.96	0.13	53,53,53,53	0
56	OHX	AA	3426	7/7	0.96	0.06	104,117,127,168	3
55	MG	DA	3180	1/1	0.96	0.23	45,45,45,45	0
56	OHX	AA	3493	7/7	0.96	0.07	102,115,123,140	1
55	MG	DA	3234	1/1	0.96	0.17	41,41,41,41	0
56	OHX	AA	3431	7/7	0.96	0.08	101,115,120,168	1
56	OHX	CA	1761	7/7	0.96	0.06	133,143,154,174	1
55	MG	AA	3205	1/1	0.96	0.08	42,42,42,42	0
55	MG	AA	3271	1/1	0.96	0.40	63,63,63,63	0
55	MG	DA	3121	1/1	0.96	0.48	78,78,78,78	0
55	MG	AA	3150	1/1	0.96	0.14	53,53,53,53	0
56	OHX	CA	1766	7/7	0.96	0.07	116,126,135,171	1
55	MG	DA	3292	1/1	0.96	0.13	51,51,51,51	0
55	MG	AA	3009	1/1	0.96	0.13	29,29,29,29	0
56	OHX	AA	3438	7/7	0.96	0.06	113,130,139,188	1
56	OHX	AA	3561	7/7	0.96	0.10	86,92,112,144	2
55	MG	DA	3189	1/1	0.96	0.32	56,56,56,56	0
56	OHX	DA	3459	7/7	0.96	0.12	85,104,120,156	1
55	MG	DA	3190	1/1	0.96	0.44	44,44,44,44	0
55	MG	DA	3126	1/1	0.96	0.37	63,63,63,63	0
55	MG	CA	1606	1/1	0.96	0.10	70,70,70,70	0
55	MG	AA	3014	1/1	0.96	0.20	33,33,33,33	0
56	OHX	AA	3568	7/7	0.96	0.09	101,109,114,153	1
56	OHX	DA	3243	7/7	0.96	0.10	74,100,112,145	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3194	1/1	0.96	0.18	48,48,48,48	0
55	MG	AA	3136	1/1	0.96	0.17	42,42,42,42	0
56	OHX	CA	1779	7/7	0.96	0.06	125,132,137,172	1
56	OHX	AB	209	7/7	0.96	0.09	98,103,137,147	3
55	MG	CA	1635	1/1	0.96	0.13	51,51,51,51	0
56	OHX	AB	211	7/7	0.96	0.06	124,127,142,178	1
56	OHX	AB	212	7/7	0.96	0.07	91,105,122,151	3
56	OHX	DA	3257	7/7	0.96	0.08	107,112,124,148	1
55	MG	AA	3241	1/1	0.96	0.20	52,52,52,52	0
55	MG	DA	3045	1/1	0.96	0.16	61,61,61,61	0
56	OHX	DA	3355	7/7	0.96	0.07	109,111,119,148	2
56	OHX	AA	3452	7/7	0.96	0.12	92,103,111,136	1
56	OHX	DA	3365	7/7	0.96	0.07	100,119,136,159	2
56	OHX	DA	3366	7/7	0.96	0.08	87,100,130,154	2
56	OHX	DA	3367	7/7	0.96	0.09	100,113,133,149	1
56	OHX	AA	3366	7/7	0.96	0.08	79,94,104,141	1
56	OHX	DA	3375	7/7	0.96	0.07	129,138,149,173	1
55	MG	DA	3305	1/1	0.96	0.21	48,48,48,48	0
56	OHX	DA	3377	7/7	0.96	0.09	91,105,111,146	2
56	OHX	DA	3383	7/7	0.96	0.07	110,119,138,151	2
56	OHX	AA	3369	7/7	0.96	0.07	76,100,116,143	1
56	OHX	AA	3371	7/7	0.96	0.10	65,79,88,136	2
56	OHX	AO	202	7/7	0.96	0.07	93,104,115,140	1
56	OHX	AA	3518	7/7	0.96	0.07	106,114,121,148	1
55	MG	DA	3306	1/1	0.96	0.34	86,86,86,86	0
56	OHX	AA	3380	7/7	0.96	0.09	86,90,110,143	1
56	OHX	CA	1796	7/7	0.96	0.06	150,159,170,195	1
55	MG	AA	3082	1/1	0.96	0.18	57,57,57,57	0
55	MG	CA	1611	1/1	0.96	0.18	81,81,81,81	0
55	MG	AA	3183	1/1	0.96	0.20	59,59,59,59	0
56	OHX	BA	1805	7/7	0.96	0.10	98,103,107,150	1
56	OHX	DA	3403	7/7	0.96	0.09	99,105,122,140	1
56	OHX	BA	1725	7/7	0.96	0.09	95,114,126,182	1
55	MG	CN	201	1/1	0.96	0.10	79,79,79,79	0
56	OHX	BA	1732	7/7	0.96	0.07	128,131,145,175	2
56	OHX	BA	1733	7/7	0.96	0.10	98,108,118,146	1
56	OHX	CA	1805	7/7	0.96	0.05	128,130,148,187	1
55	MG	AA	3067	1/1	0.96	0.10	50,50,50,50	0
56	OHX	DO	201	7/7	0.96	0.07	112,117,125,146	1
55	MG	AA	3228	1/1	0.96	0.26	53,53,53,53	0
56	OHX	AA	3467	7/7	0.96	0.11	72,88,95,139	1
56	OHX	AA	3396	7/7	0.96	0.12	93,107,119,142	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	BG	302	7/7	0.96	0.06	138,141,145,177	1
56	OHX	AA	3469	7/7	0.96	0.07	103,113,128,153	1
55	MG	BA	1654	1/1	0.96	0.25	64,64,64,64	0
56	OHX	AA	3531	7/7	0.96	0.05	225,229,234,256	1
56	OHX	BA	1741	7/7	0.97	0.07	95,110,126,148	1
56	OHX	AA	3378	7/7	0.97	0.15	77,88,108,118	1
56	OHX	DA	3168	7/7	0.97	0.07	129,143,154,181	1
55	MG	AA	3037	1/1	0.97	0.18	55,55,55,55	0
56	OHX	AA	3381	7/7	0.97	0.06	127,136,147,180	1
56	OHX	AA	3444	7/7	0.97	0.10	79,89,101,122	2
55	MG	AA	3202	1/1	0.97	0.10	30,30,30,30	0
55	MG	AA	3190	1/1	0.97	0.10	43,43,43,43	0
55	MG	DA	3027	1/1	0.97	0.10	78,78,78,78	0
56	OHX	AA	3386	7/7	0.97	0.09	75,83,104,131	1
56	OHX	AA	3387	7/7	0.97	0.06	110,123,134,164	1
56	OHX	AA	3450	7/7	0.97	0.06	97,112,128,161	2
55	MG	BA	1641	1/1	0.97	0.13	54,54,54,54	0
55	MG	BA	1660	1/1	0.97	0.32	52,52,52,52	0
55	MG	AA	3240	1/1	0.97	0.30	56,56,56,56	0
55	MG	AA	3298	1/1	0.97	0.17	45,45,45,45	0
55	MG	DA	3262	1/1	0.97	0.19	59,59,59,59	0
55	MG	DA	3263	1/1	0.97	0.20	55,55,55,55	0
56	OHX	AA	3458	7/7	0.97	0.08	96,103,139,158	1
55	MG	BA	1626	1/1	0.97	0.25	47,47,47,47	0
55	MG	AA	3272	1/1	0.97	0.27	29,29,29,29	0
55	MG	AA	3196	1/1	0.97	0.27	43,43,43,43	0
56	OHX	BC	107	7/7	0.97	0.07	126,137,143,151	1
55	MG	AA	3010	1/1	0.97	0.24	39,39,39,39	0
55	MG	DA	3098	1/1	0.97	0.20	63,63,63,63	0
56	OHX	AA	3566	7/7	0.97	0.05	171,177,185,204	1
56	OHX	CA	1728	7/7	0.97	0.07	104,119,138,150	2
55	MG	DA	3301	1/1	0.97	0.18	60,60,60,60	0
55	MG	AA	3288	1/1	0.97	0.25	55,55,55,55	0
56	OHX	CA	1734	7/7	0.97	0.07	145,147,151,167	1
56	OHX	DA	3354	7/7	0.97	0.09	88,99,121,135	1
55	MG	DA	3182	1/1	0.97	0.16	52,52,52,52	0
56	OHX	DA	3357	7/7	0.97	0.07	100,118,130,150	1
56	OHX	DA	3359	7/7	0.97	0.06	99,118,131,143	1
56	OHX	CA	1736	7/7	0.97	0.07	163,166,178,209	0
56	OHX	BA	1768	7/7	0.97	0.09	87,95,105,130	2
56	OHX	BA	1769	7/7	0.97	0.05	159,168,172,218	1
56	OHX	CA	1740	7/7	0.97	0.06	125,134,139,166	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	DA	3369	7/7	0.97	0.08	89,100,105,125	1
56	OHX	DA	3370	7/7	0.97	0.12	94,102,123,149	1
55	MG	DA	3135	1/1	0.97	0.18	42,42,42,42	0
56	OHX	DA	3373	7/7	0.97	0.09	93,104,119,171	1
56	OHX	DA	3374	7/7	0.97	0.07	127,131,139,156	1
55	MG	AA	3198	1/1	0.97	0.15	34,34,34,34	0
56	OHX	CA	1744	7/7	0.97	0.07	128,134,150,164	1
55	MG	DA	3138	1/1	0.97	0.15	43,43,43,43	0
56	OHX	DA	3379	7/7	0.97	0.07	116,134,147,164	1
56	OHX	DA	3382	7/7	0.97	0.10	67,85,95,136	2
56	OHX	CA	1746	7/7	0.97	0.07	112,115,128,150	1
56	OHX	DA	3384	7/7	0.97	0.06	89,92,105,143	2
55	MG	AA	3264	1/1	0.97	0.27	51,51,51,51	0
56	OHX	DA	3387	7/7	0.97	0.05	108,115,125,151	1
56	OHX	AA	3471	7/7	0.97	0.06	80,105,117,155	1
56	OHX	DA	3390	7/7	0.97	0.06	117,127,135,170	1
55	MG	CA	1669	1/1	0.97	0.29	48,48,48,48	0
55	MG	A5	101	1/1	0.97	0.23	43,43,43,43	0
55	MG	AA	3244	1/1	0.97	0.21	41,41,41,41	0
55	MG	DA	3019	1/1	0.97	0.17	41,41,41,41	0
56	OHX	DA	3395	7/7	0.97	0.10	102,109,124,139	1
56	OHX	AA	3427	7/7	0.97	0.07	131,132,136,155	1
55	MG	DA	3144	1/1	0.97	0.33	44,44,44,44	0
56	OHX	AA	3429	7/7	0.97	0.12	84,97,102,156	1
56	OHX	CC	109	7/7	0.97	0.05	112,114,129,153	3
56	OHX	DA	3401	7/7	0.97	0.07	108,115,120,150	1
56	OHX	CC	110	7/7	0.97	0.06	103,121,132,150	4
55	MG	BA	1617	1/1	0.97	0.28	60,60,60,60	0
56	OHX	AA	3363	7/7	0.97	0.07	89,101,119,137	1
55	MG	AA	3122	1/1	0.97	0.18	57,57,57,57	0
56	OHX	AA	3533	7/7	0.97	0.09	79,94,100,134	1
55	MG	DA	3147	1/1	0.97	0.18	55,55,55,55	0
55	MG	DA	3022	1/1	0.97	0.32	63,63,63,63	0
55	MG	AA	3095	1/1	0.97	0.22	42,42,42,42	0
56	OHX	AA	3374	7/7	0.97	0.09	32,70,109,140	3
56	OHX	BA	1728	7/7	0.97	0.07	140,147,157,166	1
56	OHX	BA	1730	7/7	0.97	0.07	106,118,135,150	1
56	OHX	AA	3487	7/7	0.97	0.07	73,82,95,140	2
56	OHX	AA	3375	7/7	0.97	0.07	83,101,103,143	1
55	MG	DA	3150	1/1	0.97	0.10	46,46,46,46	0
56	OHX	BA	1735	7/7	0.97	0.07	120,129,137,168	1
56	OHX	AA	3490	7/7	0.97	0.13	85,93,105,125	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	DA	3132	7/7	0.97	0.05	185,187,192,225	1
56	OHX	DA	3134	7/7	0.97	0.07	114,120,126,150	1
56	OHX	DA	3422	7/7	0.97	0.07	92,100,111,154	1
56	OHX	DA	3136	7/7	0.97	0.07	95,108,117,144	1
56	OHX	AA	3377	7/7	0.97	0.08	77,87,106,151	2
56	OHX	AA	3440	7/7	0.97	0.07	83,91,111,141	1
58	ZN	CQ	101	1/1	0.97	0.06	120,120,120,120	0
55	MG	AA	3185	1/1	0.98	0.23	35,35,35,35	0
55	MG	DA	3247	1/1	0.98	0.31	48,48,48,48	0
56	OHX	DA	3249	7/7	0.98	0.06	93,103,118,149	1
55	MG	DA	3156	1/1	0.98	0.10	73,73,73,73	0
56	OHX	BA	1734	7/7	0.98	0.07	92,99,114,146	1
55	MG	BA	1707	1/1	0.98	0.08	63,63,63,63	0
56	OHX	BA	1736	7/7	0.98	0.05	112,121,128,152	1
55	MG	DA	3188	1/1	0.98	0.21	38,38,38,38	0
55	MG	AA	3186	1/1	0.98	0.15	57,57,57,57	0
56	OHX	DA	3339	7/7	0.98	0.08	91,96,120,132	0
56	OHX	BA	1739	7/7	0.98	0.07	109,119,131,155	1
55	MG	DA	3079	1/1	0.98	0.12	49,49,49,49	0
56	OHX	AA	3336	7/7	0.98	0.12	67,91,105,145	0
56	OHX	DA	3356	7/7	0.98	0.06	85,97,114,129	2
56	OHX	AA	3388	7/7	0.98	0.05	106,112,125,156	1
56	OHX	DA	3358	7/7	0.98	0.06	107,117,135,165	2
56	OHX	AA	3390	7/7	0.98	0.07	48,74,93,125	2
56	OHX	DA	3360	7/7	0.98	0.14	72,81,91,113	1
56	OHX	DA	3361	7/7	0.98	0.08	68,94,122,134	3
56	OHX	AA	3348	7/7	0.98	0.06	75,81,98,100	3
56	OHX	DA	3364	7/7	0.98	0.08	75,93,104,118	1
56	OHX	AA	3477	7/7	0.98	0.07	81,92,107,133	2
56	OHX	AA	3353	7/7	0.98	0.08	71,99,117,132	1
56	OHX	CA	1760	7/7	0.98	0.04	145,148,151,188	1
56	OHX	DA	3368	7/7	0.98	0.08	86,101,103,132	2
56	OHX	AA	3354	7/7	0.98	0.06	96,105,128,164	0
56	OHX	AA	3355	7/7	0.98	0.07	88,95,127,131	3
56	OHX	DA	3371	7/7	0.98	0.05	119,121,131,160	1
56	OHX	AA	3397	7/7	0.98	0.06	96,102,109,143	1
56	OHX	AA	3359	7/7	0.98	0.05	91,110,118,137	1
56	OHX	DA	3064	7/7	0.98	0.06	87,100,123,131	3
56	OHX	DA	3068	7/7	0.98	0.06	102,127,131,147	0
56	OHX	DA	3071	7/7	0.98	0.07	107,121,146,184	0
56	OHX	DA	3073	7/7	0.98	0.06	89,101,109,132	1
56	OHX	DA	3378	7/7	0.98	0.06	153,156,169,185	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	AA	3361	7/7	0.98	0.07	76,81,111,125	3
56	OHX	DA	3380	7/7	0.98	0.06	108,123,139,150	1
56	OHX	DA	3381	7/7	0.98	0.06	111,118,134,167	1
56	OHX	AA	3400	7/7	0.98	0.07	64,77,80,123	1
55	MG	BA	1698	1/1	0.98	0.32	54,54,54,54	0
56	OHX	DA	3084	7/7	0.98	0.06	132,139,149,176	1
56	OHX	AB	207	7/7	0.98	0.06	89,93,105,113	1
56	OHX	DA	3386	7/7	0.98	0.07	108,110,132,139	1
56	OHX	AA	3402	7/7	0.98	0.07	73,86,98,123	1
56	OHX	AA	3403	7/7	0.98	0.07	59,89,94,139	1
56	OHX	DA	3389	7/7	0.98	0.07	82,85,99,113	1
55	MG	AA	3216	1/1	0.98	0.24	33,33,33,33	0
56	OHX	AA	3365	7/7	0.98	0.07	86,102,111,118	3
55	MG	AA	3315	1/1	0.98	0.11	50,50,50,50	0
55	MG	AA	3163	1/1	0.98	0.33	34,34,34,34	0
56	OHX	AA	3368	7/7	0.98	0.06	104,115,121,140	1
56	OHX	BA	1814	7/7	0.98	0.06	88,100,109,173	0
56	OHX	AA	3410	7/7	0.98	0.08	91,99,106,125	1
56	OHX	DA	3397	7/7	0.98	0.05	104,119,125,149	1
56	OHX	AA	3411	7/7	0.98	0.05	107,117,135,154	0
56	OHX	AA	3453	7/7	0.98	0.10	72,88,95,134	2
55	MG	DA	3195	1/1	0.98	0.04	46,46,46,46	0
56	OHX	AA	3413	7/7	0.98	0.06	94,104,121,143	1
56	OHX	DA	3157	7/7	0.98	0.09	76,87,96,121	1
56	OHX	BC	105	7/7	0.98	0.06	129,141,151,159	1
56	OHX	DA	3162	7/7	0.98	0.05	128,132,141,207	0
56	OHX	AE	304	7/7	0.98	0.15	73,87,113,116	2
56	OHX	AA	3370	7/7	0.98	0.07	74,85,99,119	1
56	OHX	DB	208	7/7	0.98	0.06	120,124,144,144	2
56	OHX	AA	3415	7/7	0.98	0.07	90,93,100,146	1
55	MG	A0	201	1/1	0.98	0.12	52,52,52,52	0
56	OHX	AA	3373	7/7	0.98	0.05	84,96,108,141	1
56	OHX	CA	1724	7/7	0.98	0.10	88,111,121,131	0
56	OHX	CA	1726	7/7	0.98	0.08	89,98,100,124	1
56	OHX	AA	3418	7/7	0.98	0.06	96,110,119,135	1
56	OHX	CA	1791	7/7	0.98	0.06	100,118,129,154	1
56	OHX	CA	1729	7/7	0.98	0.08	104,115,126,154	1
56	OHX	CA	1730	7/7	0.98	0.06	132,134,143,167	0
55	MG	DA	3197	1/1	0.98	0.17	49,49,49,49	0
56	OHX	DA	3418	7/7	0.98	0.07	87,98,117,139	3
56	OHX	CA	1732	7/7	0.98	0.07	112,117,126,152	1
55	MG	AA	3218	1/1	0.98	0.25	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	BA	1723	7/7	0.98	0.08	93,106,124,143	1
56	OHX	BA	1724	7/7	0.98	0.06	114,121,136,156	0
55	MG	AA	3188	1/1	0.98	0.09	29,29,29,29	0
56	OHX	BA	1726	7/7	0.98	0.05	134,139,145,195	0
56	OHX	BA	1727	7/7	0.98	0.07	116,137,148,161	1
55	MG	BA	1623	1/1	0.98	0.25	39,39,39,39	0
58	ZN	BG	301	1/1	0.98	0.17	84,84,84,84	0
58	ZN	BQ	101	1/1	0.98	0.07	135,135,135,135	0
56	OHX	BA	1729	7/7	0.98	0.06	110,115,135,137	1
56	OHX	AA	3424	7/7	0.98	0.06	84,93,116,147	1
56	OHX	BA	1720	7/7	0.99	0.06	95,108,133,161	2
56	OHX	BA	1721	7/7	0.99	0.06	109,115,141,157	1
56	OHX	BA	1722	7/7	0.99	0.04	114,116,123,159	0
56	OHX	AA	3332	7/7	0.99	0.08	40,73,95,99	2
56	OHX	AA	3407	7/7	0.99	0.06	53,82,90,103	2
56	OHX	AA	3333	7/7	0.99	0.05	99,103,122,123	0
56	OHX	AA	3335	7/7	0.99	0.09	62,76,78,127	0
55	MG	AA	3283	1/1	0.99	0.04	21,21,21,21	0
56	OHX	AA	3338	7/7	0.99	0.05	66,87,106,113	2
56	OHX	AA	3340	7/7	0.99	0.06	84,93,95,126	0
56	OHX	AA	3341	7/7	0.99	0.09	77,80,88,124	1
56	OHX	AA	3342	7/7	0.99	0.06	65,86,103,114	1
56	OHX	AA	3344	7/7	0.99	0.05	86,92,112,118	1
56	OHX	AA	3345	7/7	0.99	0.06	87,112,122,135	0
56	OHX	AA	3346	7/7	0.99	0.06	73,81,101,124	2
56	OHX	AA	3382	7/7	0.99	0.05	65,73,84,93	0
56	OHX	AA	3347	7/7	0.99	0.04	74,77,98,102	2
55	MG	AA	3238	1/1	0.99	0.40	47,47,47,47	0
56	OHX	CA	1723	7/7	0.99	0.12	84,100,111,141	0
56	OHX	AA	3349	7/7	0.99	0.04	94,104,124,143	0
56	OHX	CA	1725	7/7	0.99	0.04	108,111,122,123	1
56	OHX	AA	3422	7/7	0.99	0.06	63,104,126,147	2
56	OHX	CA	1727	7/7	0.99	0.04	114,118,131,143	0
56	OHX	DA	3062	7/7	0.99	0.06	70,95,103,114	1
56	OHX	AA	3350	7/7	0.99	0.06	95,103,113,148	1
56	OHX	DA	3065	7/7	0.99	0.05	55,92,111,137	1
56	OHX	AA	3351	7/7	0.99	0.09	60,68,78,99	3
56	OHX	AA	3352	7/7	0.99	0.05	80,86,96,122	1
56	OHX	AA	3389	7/7	0.99	0.07	80,93,103,143	0
56	OHX	DA	3075	7/7	0.99	0.05	89,91,114,123	1
56	OHX	DA	3335	7/7	0.99	0.07	87,96,112,126	0
56	OHX	DA	3337	7/7	0.99	0.08	74,80,86,97	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	DA	3338	7/7	0.99	0.07	72,79,93,112	0
55	MG	DA	3167	1/1	0.99	0.10	61,61,61,61	0
56	OHX	DA	3340	7/7	0.99	0.04	86,102,124,126	1
56	OHX	DA	3341	7/7	0.99	0.07	87,105,126,140	0
56	OHX	DA	3412	7/7	0.99	0.05	93,110,113,161	1
56	OHX	DA	3342	7/7	0.99	0.05	79,85,102,102	2
56	OHX	DA	3343	7/7	0.99	0.06	93,113,122,129	0
56	OHX	DA	3344	7/7	0.99	0.07	93,104,111,114	1
56	OHX	DA	3345	7/7	0.99	0.07	89,96,107,130	0
56	OHX	DA	3347	7/7	0.99	0.05	89,99,108,134	0
56	OHX	AA	3391	7/7	0.99	0.07	69,80,102,109	3
56	OHX	DA	3349	7/7	0.99	0.05	103,105,113,143	0
56	OHX	DA	3350	7/7	0.99	0.05	90,99,110,132	1
56	OHX	DA	3351	7/7	0.99	0.05	87,96,108,109	1
56	OHX	DA	3352	7/7	0.99	0.06	105,120,129,149	0
56	OHX	DA	3353	7/7	0.99	0.05	102,117,129,132	1
55	MG	BA	1603	1/1	0.99	0.09	40,40,40,40	0
56	OHX	AA	3393	7/7	0.99	0.07	50,81,89,115	2
55	MG	DA	3004	1/1	0.99	0.12	32,32,32,32	0
56	OHX	CA	1737	7/7	0.99	0.04	103,118,125,148	1
56	OHX	AA	3358	7/7	0.99	0.07	79,81,92,113	1
55	MG	DA	3122	1/1	0.99	0.30	30,30,30,30	0
56	OHX	AA	3360	7/7	0.99	0.05	88,94,111,129	2
55	MG	DA	3187	1/1	0.99	0.26	55,55,55,55	0
56	OHX	CA	1742	7/7	0.99	0.05	153,166,169,174	1
56	OHX	DA	3363	7/7	0.99	0.05	95,105,122,123	2
55	MG	AA	3212	1/1	0.99	0.17	33,33,33,33	0
55	MG	AA	3129	1/1	0.99	0.07	43,43,43,43	0
56	OHX	AA	3364	7/7	0.99	0.06	72,81,97,125	1
56	OHX	AA	3327	7/7	0.99	0.09	38,70,106,113	0
56	OHX	AA	3329	7/7	0.99	0.05	73,97,104,113	0
56	OHX	AA	3330	7/7	0.99	0.09	81,85,101,147	0
56	OHX	AA	3331	7/7	0.99	0.08	93,94,108,145	0
56	OHX	BA	1716	7/7	0.99	0.09	73,86,99,116	0
56	OHX	BA	1717	7/7	0.99	0.06	81,90,105,119	0
56	OHX	DA	3160	7/7	0.99	0.05	79,114,122,124	0
56	OHX	BA	1718	7/7	0.99	0.11	68,82,103,130	2
56	OHX	BA	1719	7/7	0.99	0.06	85,102,114,124	1
56	OHX	DA	3212	7/7	1.00	0.05	64,77,91,94	1
56	OHX	AA	3328	7/7	1.00	0.05	67,76,86,89	1
56	OHX	AA	3326	7/7	1.00	0.06	75,76,87,119	0
56	OHX	AA	3379	7/7	1.00	0.09	20,47,62,138	0

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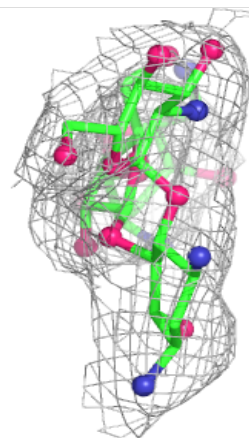
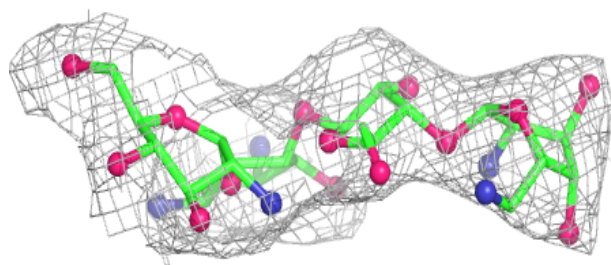
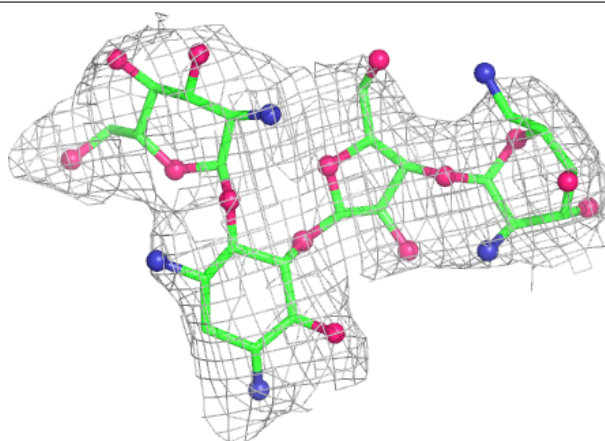
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	DA	3336	7/7	1.00	0.04	86,95,105,106	0
56	OHX	AF	303	7/7	1.00	0.08	46,54,72,103	0
56	OHX	DF	301	7/7	1.00	0.06	53,80,83,83	1
56	OHX	DA	3061	7/7	1.00	0.04	81,86,92,106	0
56	OHX	DA	3346	7/7	1.00	0.04	107,113,126,132	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

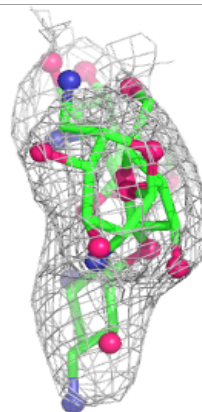
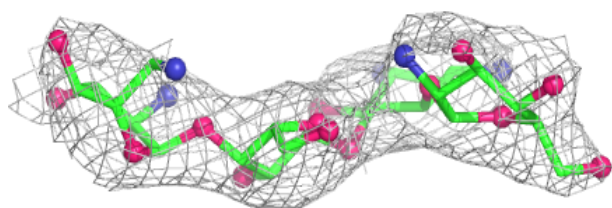
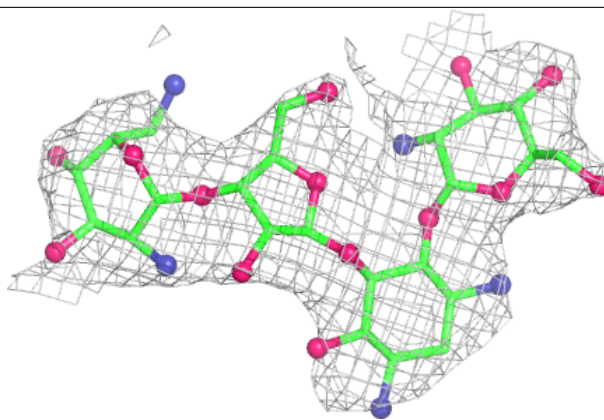
Electron density around PAR CA 1722:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PAR BA 1715:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.