wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:17 PM GMT

PDB ID	:	4V8E
Title	:	Crystal structure analysis of ribosomal decoding (near-cognate tRNA-tyr complex).
Authors	:	Jenner, L.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on	:	2011-12-07
Resolution	:	3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

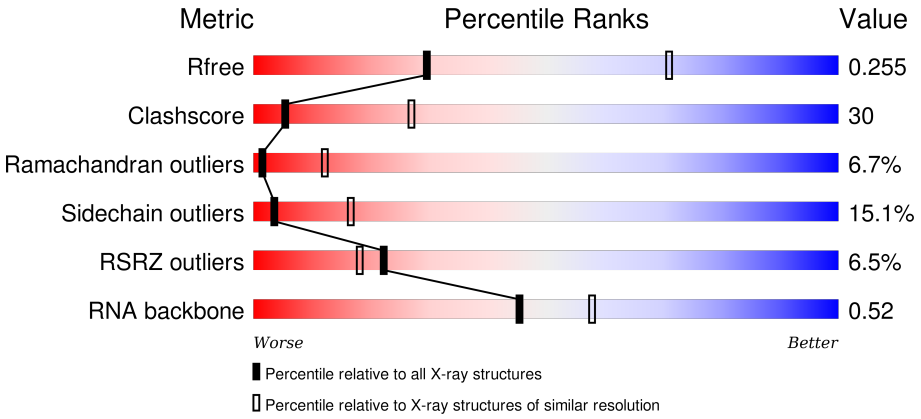
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)
RNA backbone	2183	1005 (3.82-2.78)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	2% 36% 47% 17%
1	CA	2912	2% 33% 49% 17%
2	AB	122	2% 43% 45% 11%
2	CB	122	% 30% 49% 20%

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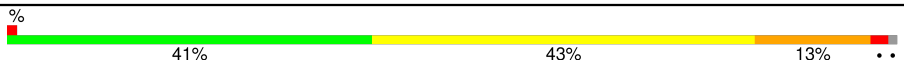
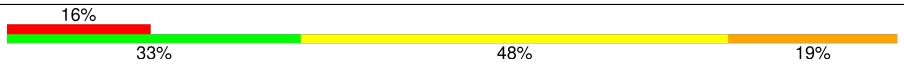
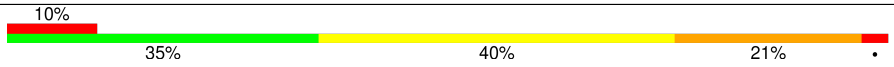
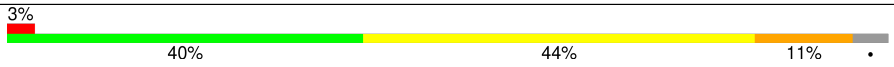
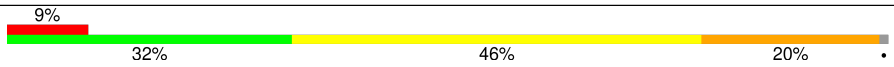
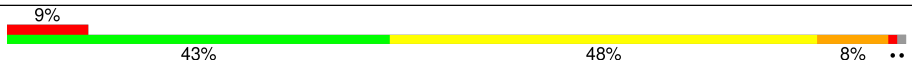
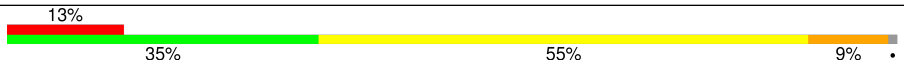
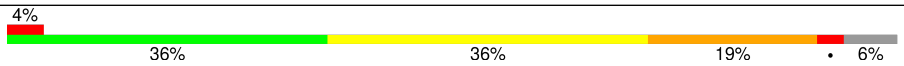
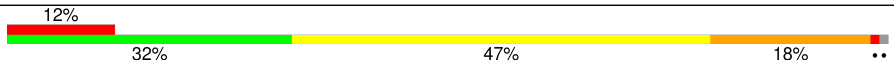
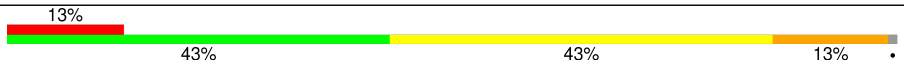
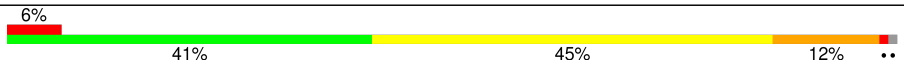
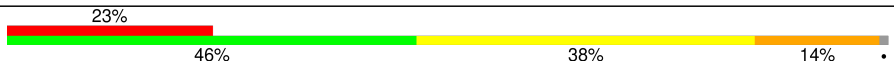
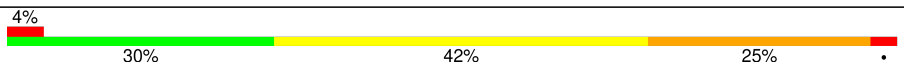
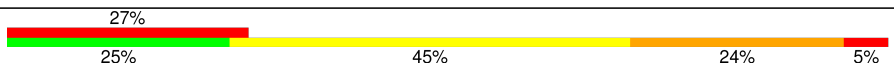
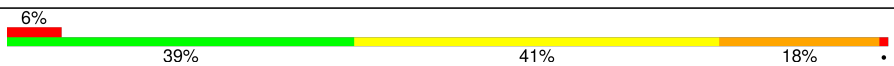
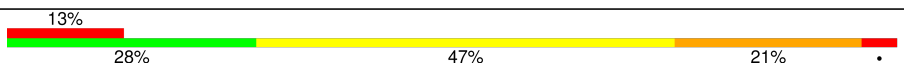
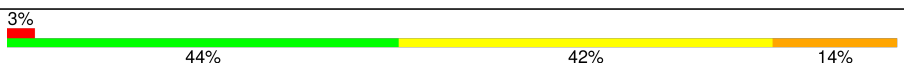
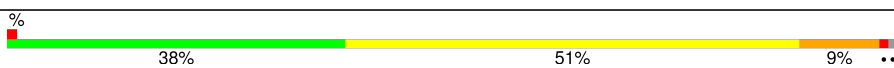
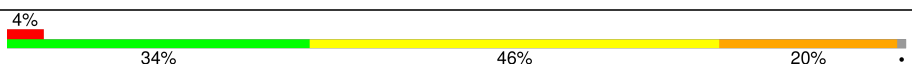
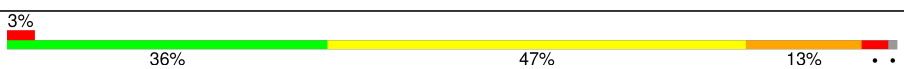
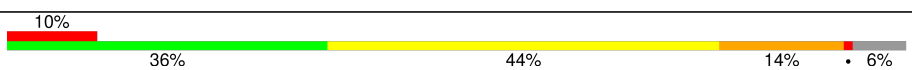
Mol	Chain	Length	Quality of chain
3	AD	276	
3	CD	276	
4	AE	206	
4	CE	206	
5	AF	210	
5	CF	210	
6	AG	182	
6	CG	182	
7	AH	180	
7	CH	180	
8	AK	148	
8	CK	148	
9	AM	140	
9	CM	140	
10	AN	122	
10	CN	122	
11	AO	150	
11	CO	150	
12	AP	141	
12	CP	141	
13	A0	118	
13	C0	118	
14	AQ	112	
14	CQ	112	
15	AR	146	

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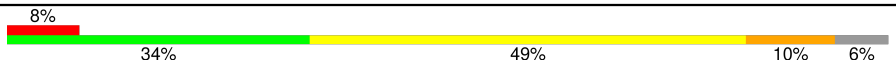
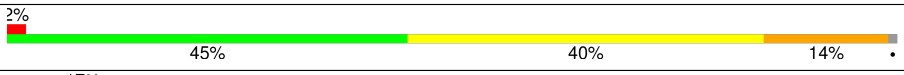
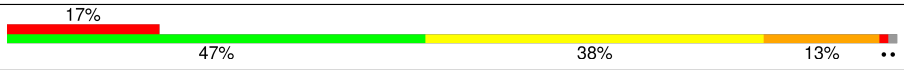
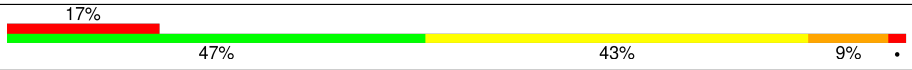
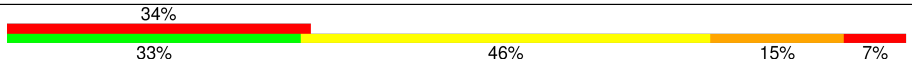
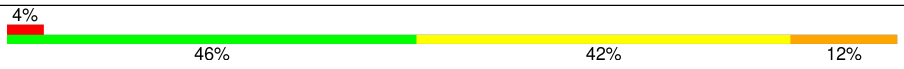
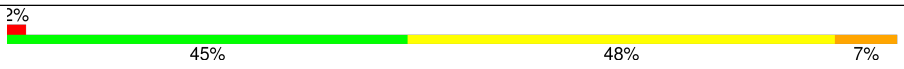
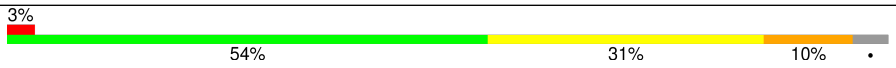
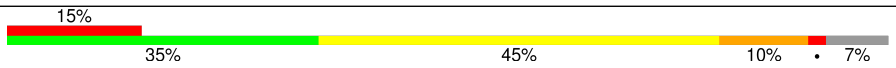
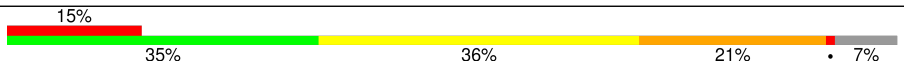
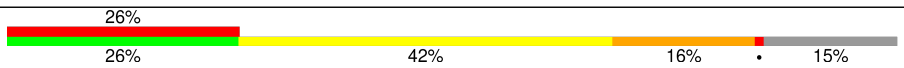
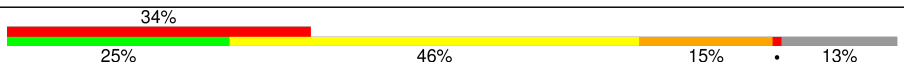
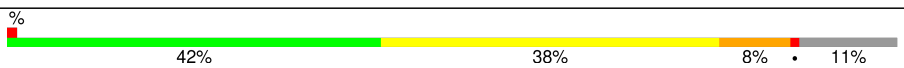
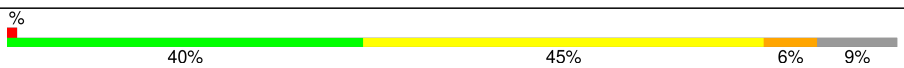
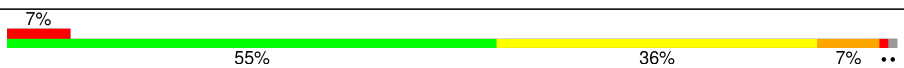
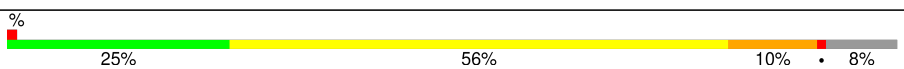
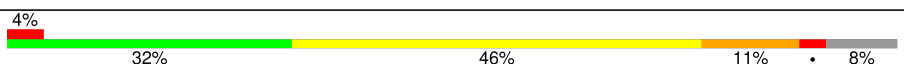
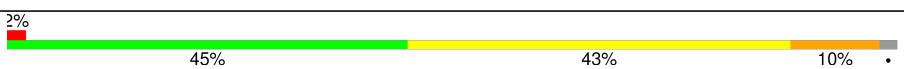
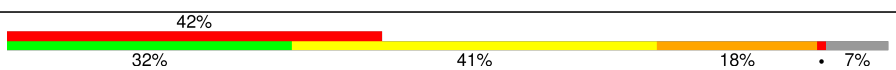
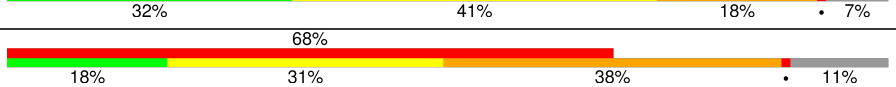
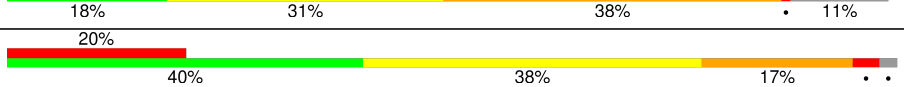
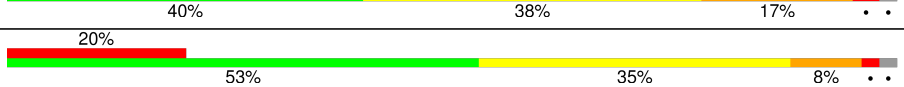
Mol	Chain	Length	Quality of chain
15	CR	146	
16	A1	118	
16	C1	118	
17	A2	101	
17	C2	101	
18	AS	113	
18	CS	113	
19	AT	96	
19	CT	96	
20	AU	110	
20	CU	110	
21	AV	206	
21	CV	206	
22	A3	85	
22	C3	85	
23	AZ	98	
23	CZ	98	
24	AW	72	
24	CW	72	
25	AX	60	
25	CX	60	
26	A4	71	
26	C4	71	
27	A5	60	
27	C5	60	

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Mol	Chain	Length	Quality of chain
28	A6	54	80% 7% 52% 17% 7% 17%
28	C6	54	48% 17% 44% 22% 17%
29	A7	49	2% 53% 31% 8% 8%
29	C7	49	41% 41% 10% 8%
30	A8	65	2% 32% 43% 15% 8%
30	C8	65	3% 22% 45% 20% 6% 8%
31	BA	1506	% 29% 52% 18%
31	DA	1506	% 28% 53% 19%
32	BE	256	8% 38% 41% 13% 7%
32	DE	256	13% 33% 46% 13% 7%
33	BF	239	7% 40% 38% 7% 14%
33	DF	239	21% 40% 38% 8% 14%
34	BG	208	% 52% 37% 10%
34	DG	208	2% 41% 47% 12%
35	BH	162	3% 46% 38% 9% 7%
35	DH	162	2% 37% 48% 9% 7%
36	BI	101	% 53% 40% 7%
36	DI	101	48% 47% 6%
37	BJ	156	13% 45% 47% 7%
37	DJ	156	4% 49% 44% 7%
38	BK	138	% 44% 44% 12%
38	DK	138	50% 43% 7%
39	BL	128	10% 45% 49% 5%
39	DL	128	5% 32% 53% 14%
40	BM	105	7% 36% 50% 9% 6%

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Mol	Chain	Length	Quality of chain
40	DM	105	11% 35% 50% 8% 6%
41	BN	129	12% 46% 39% 8% 8%
41	DN	129	11% 50% 34% 8% 8%
42	BO	132	5% 57% 29% 8% 5%
42	DO	132	9% 33% 45% 15% 5%
43	BP	126	2% 44% 36% 10% 8%
43	DP	126	3% 34% 43% 14% 7%
44	BQ	61	36% 46% 13% 5%
44	DQ	61	16% 38% 46% 8% 5%
45	BR	89	52% 42% 6%
45	DR	89	57% 35% 7%
46	BS	88	% 42% 39% 15% 5%
46	DS	88	51% 40% 5% 5%
47	BT	105	% 43% 44% 8% 5%
47	DT	105	3% 50% 41% 5%
48	BU	88	5% 44% 38% 18%
48	DU	88	9% 42% 32% 8% 18%
49	BV	93	8% 42% 34% 8% 16%
49	DV	93	5% 24% 48% 10% 16%
50	BW	106	10% 39% 47% 8% 7%
50	DW	106	4% 43% 42% 8% 7%
51	BX	27	44% 44% 7%
51	DX	27	33% 52% 7%
52	BB	85	15% 12% 36% 49%
52	BD	85	6% 21% 45% 33%

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Mol	Chain	Length	Quality of chain
52	DB	85	13% 11% 34% 54%
52	DD	85	2% 19% 48% 32%
53	BC	77	44% 39% 17%
53	DC	77	45% 39% 16%
54	B1	16	6% 50% 19% 25% 6%
54	D1	16	31% 38% 25% 6%

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	A1	201	-	-	-	X
55	MG	AA	3002	-	-	-	X
55	MG	AA	3004	-	-	-	X
55	MG	AA	3006	-	-	-	X
55	MG	AA	3016	-	-	-	X
55	MG	AA	3019	-	-	-	X
55	MG	AA	3020	-	-	-	X
55	MG	AA	3024	-	-	-	X
55	MG	AA	3025	-	-	-	X
55	MG	AA	3027	-	-	-	X
55	MG	AA	3029	-	-	-	X
55	MG	AA	3031	-	-	-	X
55	MG	AA	3032	-	-	-	X
55	MG	AA	3039	-	-	-	X
55	MG	AA	3040	-	-	-	X
55	MG	AA	3049	-	-	-	X
55	MG	AA	3050	-	-	-	X
55	MG	AA	3057	-	-	-	X
55	MG	AA	3062	-	-	-	X
55	MG	AA	3064	-	-	-	X
55	MG	AA	3065	-	-	-	X
55	MG	AA	3068	-	-	-	X
55	MG	AA	3069	-	-	-	X
55	MG	AA	3070	-	-	-	X
55	MG	AA	3072	-	-	-	X
55	MG	AA	3080	-	-	-	X
55	MG	AA	3081	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	3082	-	-	-	X
55	MG	AA	3084	-	-	-	X
55	MG	AA	3090	-	-	-	X
55	MG	AA	3096	-	-	-	X
55	MG	AA	3100	-	-	-	X
55	MG	AA	3106	-	-	-	X
55	MG	AA	3109	-	-	-	X
55	MG	AA	3110	-	-	-	X
55	MG	AA	3111	-	-	-	X
55	MG	AA	3112	-	-	-	X
55	MG	AA	3116	-	-	-	X
55	MG	AA	3118	-	-	-	X
55	MG	AA	3121	-	-	-	X
55	MG	AA	3126	-	-	-	X
55	MG	AA	3142	-	-	-	X
55	MG	AA	3143	-	-	-	X
55	MG	AA	3146	-	-	-	X
55	MG	AA	3151	-	-	-	X
55	MG	AA	3157	-	-	-	X
55	MG	AA	3158	-	-	-	X
55	MG	AA	3171	-	-	-	X
55	MG	AA	3172	-	-	-	X
55	MG	AA	3173	-	-	-	X
55	MG	AA	3175	-	-	-	X
55	MG	AA	3177	-	-	-	X
55	MG	AA	3178	-	-	-	X
55	MG	AA	3188	-	-	-	X
55	MG	AA	3189	-	-	-	X
55	MG	AA	3195	-	-	-	X
55	MG	AA	3197	-	-	-	X
55	MG	AA	3210	-	-	-	X
55	MG	AA	3212	-	-	-	X
55	MG	AA	3213	-	-	-	X
55	MG	AA	3221	-	-	-	X
55	MG	AA	3231	-	-	-	X
55	MG	AA	3235	-	-	-	X
55	MG	AA	3241	-	-	-	X
55	MG	AA	3244	-	-	-	X
55	MG	AA	3250	-	-	-	X
55	MG	AA	3252	-	-	-	X
55	MG	AA	3255	-	-	-	X
55	MG	AA	3261	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	3268	-	-	-	X
55	MG	AA	3275	-	-	-	X
55	MG	AA	3343	-	-	-	X
55	MG	AA	3345	-	-	-	X
55	MG	AA	3352	-	-	-	X
55	MG	AA	3353	-	-	-	X
55	MG	AA	3354	-	-	-	X
55	MG	AA	3355	-	-	-	X
55	MG	AA	3374	-	-	-	X
55	MG	AA	3376	-	-	-	X
55	MG	AA	3377	-	-	-	X
55	MG	AA	3379	-	-	-	X
55	MG	AA	3380	-	-	-	X
55	MG	AA	3381	-	-	-	X
55	MG	AA	3383	-	-	-	X
55	MG	AA	3384	-	-	-	X
55	MG	AA	3386	-	-	-	X
55	MG	AA	3387	-	-	-	X
55	MG	AA	3393	-	-	-	X
55	MG	AA	3397	-	-	-	X
55	MG	AA	3408	-	-	-	X
55	MG	AA	3412	-	-	-	X
55	MG	AA	3414	-	-	-	X
55	MG	AA	3415	-	-	-	X
55	MG	AB	202	-	-	-	X
55	MG	AE	301	-	-	-	X
55	MG	AO	202	-	-	-	X
55	MG	BA	1602	-	-	-	X
55	MG	BA	1605	-	-	-	X
55	MG	BA	1608	-	-	-	X
55	MG	BA	1611	-	-	-	X
55	MG	BA	1616	-	-	-	X
55	MG	BA	1620	-	-	-	X
55	MG	BA	1624	-	-	-	X
55	MG	BA	1632	-	-	-	X
55	MG	BA	1635	-	-	-	X
55	MG	BA	1636	-	-	-	X
55	MG	BA	1645	-	-	-	X
55	MG	BA	1654	-	-	-	X
55	MG	BA	1699	-	-	-	X
55	MG	BA	1705	-	-	-	X
55	MG	BA	1709	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	BA	1718	-	-	-	X
55	MG	BA	1719	-	-	-	X
55	MG	BA	1725	-	-	-	X
55	MG	BA	1735	-	-	-	X
55	MG	BA	1737	-	-	-	X
55	MG	BA	1743	-	-	-	X
55	MG	BA	1754	-	-	-	X
55	MG	BQ	101	-	-	-	X
55	MG	CA	3002	-	-	-	X
55	MG	CA	3004	-	-	-	X
55	MG	CA	3006	-	-	-	X
55	MG	CA	3009	-	-	-	X
55	MG	CA	3010	-	-	-	X
55	MG	CA	3015	-	-	-	X
55	MG	CA	3018	-	-	-	X
55	MG	CA	3032	-	-	-	X
55	MG	CA	3033	-	-	-	X
55	MG	CA	3034	-	-	-	X
55	MG	CA	3035	-	-	-	X
55	MG	CA	3036	-	-	-	X
55	MG	CA	3049	-	-	-	X
55	MG	CA	3050	-	-	-	X
55	MG	CA	3051	-	-	-	X
55	MG	CA	3061	-	-	-	X
55	MG	CA	3065	-	-	-	X
55	MG	CA	3066	-	-	-	X
55	MG	CA	3067	-	-	-	X
55	MG	CA	3068	-	-	-	X
55	MG	CA	3069	-	-	-	X
55	MG	CA	3071	-	-	-	X
55	MG	CA	3072	-	-	-	X
55	MG	CA	3081	-	-	-	X
55	MG	CA	3083	-	-	-	X
55	MG	CA	3084	-	-	-	X
55	MG	CA	3090	-	-	-	X
55	MG	CA	3099	-	-	-	X
55	MG	CA	3104	-	-	-	X
55	MG	CA	3105	-	-	-	X
55	MG	CA	3108	-	-	-	X
55	MG	CA	3109	-	-	-	X
55	MG	CA	3113	-	-	-	X
55	MG	CA	3120	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	CA	3121	-	-	-	X
55	MG	CA	3122	-	-	-	X
55	MG	CA	3123	-	-	-	X
55	MG	CA	3127	-	-	-	X
55	MG	CA	3130	-	-	-	X
55	MG	CA	3131	-	-	-	X
55	MG	CA	3134	-	-	-	X
55	MG	CA	3138	-	-	-	X
55	MG	CA	3139	-	-	-	X
55	MG	CA	3142	-	-	-	X
55	MG	CA	3145	-	-	-	X
55	MG	CA	3147	-	-	-	X
55	MG	CA	3153	-	-	-	X
55	MG	CA	3160	-	-	-	X
55	MG	CA	3172	-	-	-	X
55	MG	CA	3175	-	-	-	X
55	MG	CA	3176	-	-	-	X
55	MG	CA	3178	-	-	-	X
55	MG	CA	3181	-	-	-	X
55	MG	CA	3192	-	-	-	X
55	MG	CA	3193	-	-	-	X
55	MG	CA	3214	-	-	-	X
55	MG	CA	3216	-	-	-	X
55	MG	CA	3218	-	-	-	X
55	MG	CA	3220	-	-	-	X
55	MG	CA	3231	-	-	-	X
55	MG	CA	3261	-	-	-	X
55	MG	CA	3264	-	-	-	X
55	MG	CA	3265	-	-	-	X
55	MG	CA	3440	-	-	-	X
55	MG	CA	3444	-	-	-	X
55	MG	CA	3446	-	-	-	X
55	MG	CA	3448	-	-	-	X
55	MG	CA	3449	-	-	-	X
55	MG	CA	3453	-	-	-	X
55	MG	CA	3454	-	-	-	X
55	MG	CA	3455	-	-	-	X
55	MG	CA	3471	-	-	-	X
55	MG	CA	3472	-	-	-	X
55	MG	CE	301	-	-	-	X
55	MG	DA	1601	-	-	-	X
55	MG	DA	1603	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	1604	-	-	-	X
55	MG	DA	1605	-	-	-	X
55	MG	DA	1610	-	-	-	X
55	MG	DA	1614	-	-	-	X
55	MG	DA	1617	-	-	-	X
55	MG	DA	1619	-	-	-	X
55	MG	DA	1632	-	-	-	X
55	MG	DA	1641	-	-	-	X
55	MG	DA	1643	-	-	-	X
55	MG	DA	1649	-	-	-	X
55	MG	DA	1650	-	-	-	X
55	MG	DA	1652	-	-	-	X
55	MG	DA	1657	-	-	-	X
55	MG	DA	1659	-	-	-	X
55	MG	DA	1663	-	-	-	X
55	MG	DA	1668	-	-	-	X
55	MG	DA	1669	-	-	-	X
55	MG	DA	1674	-	-	-	X
55	MG	DA	1675	-	-	-	X
55	MG	DA	1676	-	-	-	X
55	MG	DA	1688	-	-	-	X
55	MG	DA	1720	-	-	-	X
55	MG	DC	101	-	-	-	X
56	OHX	AA	3147	-	-	-	X
56	OHX	AA	3292	-	-	-	X
56	OHX	AA	3312	-	-	-	X
56	OHX	AA	3342	-	-	-	X
56	OHX	AA	3359	-	-	-	X
56	OHX	AA	3361	-	-	-	X
56	OHX	AA	3362	-	-	-	X
56	OHX	AA	3399	-	-	-	X
56	OHX	AA	3417	-	-	-	X
56	OHX	AA	3419	-	-	-	X
56	OHX	AA	3420	-	-	-	X
56	OHX	AA	3422	-	-	-	X
56	OHX	AA	3424	-	-	-	X
56	OHX	AA	3426	-	-	-	X
56	OHX	AA	3434	-	-	-	X
56	OHX	AA	3441	-	-	-	X
56	OHX	AA	3452	-	-	-	X
56	OHX	AA	3456	-	-	-	X
56	OHX	AA	3458	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	OHX	AA	3488	-	-	-	X
56	OHX	AA	3568	-	-	X	-
56	OHX	AB	207	-	-	-	X
56	OHX	AB	209	-	-	-	X
56	OHX	AB	216	-	-	-	X
56	OHX	AB	218	-	-	-	X
56	OHX	BA	1667	-	-	-	X
56	OHX	BA	1673	-	-	X	-
56	OHX	BA	1674	-	-	-	X
56	OHX	BA	1684	-	-	X	-
56	OHX	BA	1686	-	-	-	X
56	OHX	BA	1755	-	-	-	X
56	OHX	BA	1757	-	-	-	X
56	OHX	BA	1764	-	-	-	X
56	OHX	BA	1790	-	-	-	X
56	OHX	BA	1791	-	-	-	X
56	OHX	BB	107	-	-	-	X
56	OHX	BD	104	-	-	-	X
56	OHX	C6	101	-	-	X	-
56	OHX	CA	3232	-	-	-	X
56	OHX	CA	3234	-	-	-	X
56	OHX	CA	3236	-	-	-	X
56	OHX	CA	3244	-	-	-	X
56	OHX	CA	3247	-	-	-	X
56	OHX	CA	3252	-	-	-	X
56	OHX	CA	3271	-	-	-	X
56	OHX	CA	3272	-	-	-	X
56	OHX	CA	3273	-	-	-	X
56	OHX	CA	3281	-	-	-	X
56	OHX	CA	3286	-	-	-	X
56	OHX	CA	3292	-	-	-	X
56	OHX	CA	3293	-	-	-	X
56	OHX	CA	3343	-	-	-	X
56	OHX	CA	3348	-	-	-	X
56	OHX	CA	3350	-	-	-	X
56	OHX	CA	3399	-	-	-	X
56	OHX	CA	3435	-	-	-	X
56	OHX	CA	3461	-	-	-	X
56	OHX	DA	1718	-	-	-	X
56	OHX	DA	1728	-	-	-	X
56	OHX	DA	1731	-	-	X	-
56	OHX	DA	1732	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	OHX	DA	1760	-	-	X	-
56	OHX	DA	1767	-	-	X	-
56	OHX	DA	1791	-	-	-	X
56	OHX	DC	107	-	-	X	-

2 Entry composition

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

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

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

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

There are 14 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 54 is a RNA chain called MRNA.

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	BA	115	Total Mg 115 115	0	0
55	CA	274	Total Mg 274 274	0	0
55	C5	1	Total Mg 1 1	0	0
55	AB	6	Total Mg 6 6	0	0
55	B1	1	Total Mg 1 1	0	0
55	DN	1	Total Mg 1 1	0	0
55	DC	6	Total Mg 6 6	0	0
55	BB	5	Total Mg 5 5	0	0
55	AE	3	Total Mg 3 3	0	0
55	DL	1	Total Mg 1 1	0	0
55	C0	1	Total Mg 1 1	0	0
55	AA	331	Total Mg 331 331	0	0
55	BQ	1	Total Mg 1 1	0	0
55	A5	1	Total Mg 1 1	0	0
55	BC	5	Total Mg 5 5	0	0
55	A1	1	Total Mg 1 1	0	0
55	BN	1	Total Mg 1 1	0	0
55	C7	1	Total Mg 1 1	0	0
55	DA	119	Total Mg 119 119	0	0
55	AO	3	Total Mg 3 3	0	0
55	A0	1	Total Mg 1 1	0	0
55	D1	1	Total Mg 1 1	0	0

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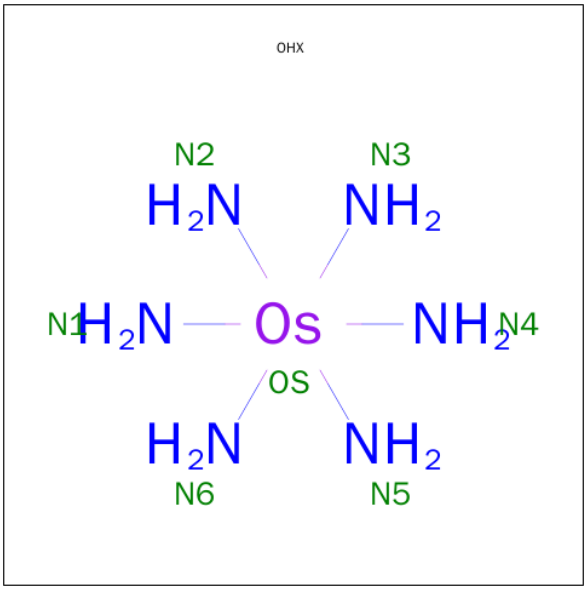
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	CB	7	Total Mg 7 7	0	0
55	BS	1	Total Mg 1 1	0	0
55	BD	1	Total Mg 1 1	0	0
55	CE	1	Total Mg 1 1	0	0
55	A3	1	Total Mg 1 1	0	0
55	AF	2	Total Mg 2 2	0	0
55	DB	2	Total Mg 2 2	0	0

- Molecule 56 is osmium (III) hexammine (three-letter code: OHX) (formula: $H_{12}N_6Os$).



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

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

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

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

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

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

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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		
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		
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		
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		
56	BA	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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

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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
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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		
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		
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 7 6 1	0	0
56	DA	1	Total N Os 7 6 1	0	0
56	DA	1	Total N Os 7 6 1	0	0
56	DG	1	Total N Os 7 6 1	0	0
56	DK	1	Total N Os 7 6 1	0	0
56	DR	1	Total N Os 7 6 1	0	0
56	DV	1	Total N Os 7 6 1	0	0
56	DB	1	Total N Os 7 6 1	0	0
56	DB	1	Total N Os 7 6 1	0	0
56	DB	1	Total N Os 7 6 1	0	0
56	DC	1	Total N Os 7 6 1	0	0
56	DC	1	Total N Os 7 6 1	0	0
56	DC	1	Total N Os 7 6 1	0	0
56	DC	1	Total N Os 7 6 1	0	0
56	DD	1	Total N Os 7 6 1	0	0

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

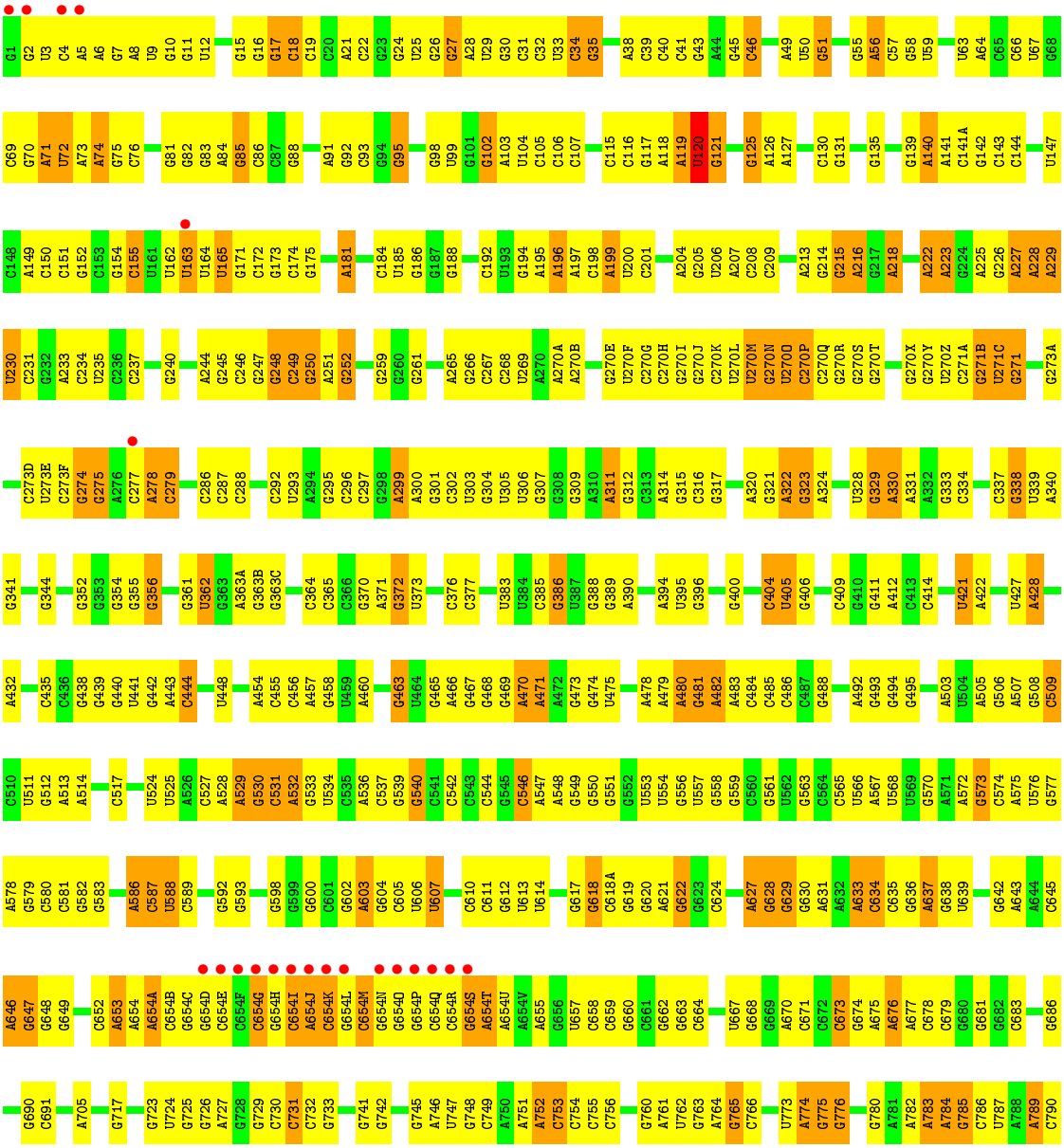
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	DG	1	Total Zn 1 1	0	0
57	BG	1	Total Zn 1 1	0	0
57	BQ	1	Total Zn 1 1	0	0
57	DQ	1	Total Zn 1 1	0	0

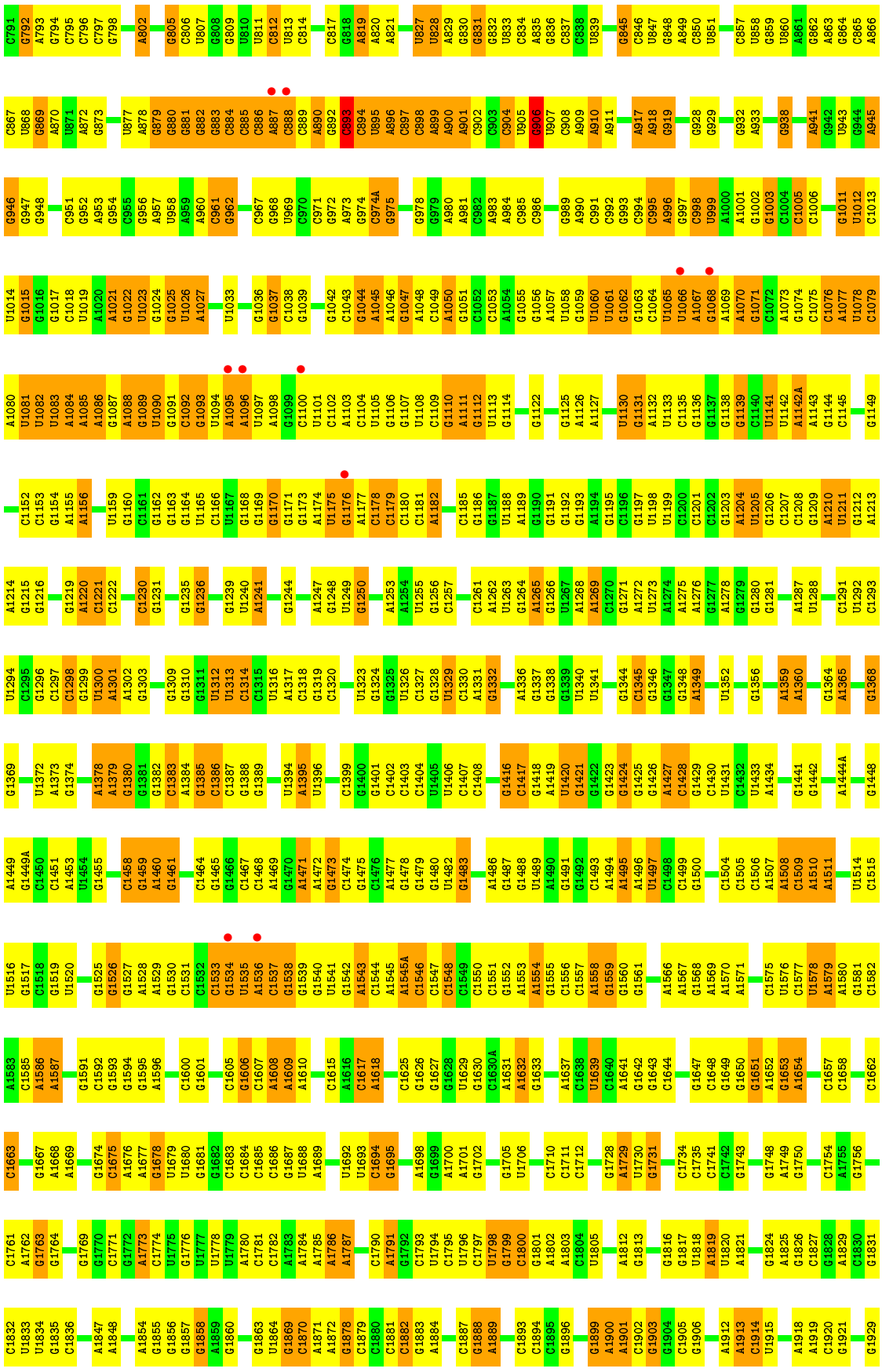
3 Residue-property plots (i)

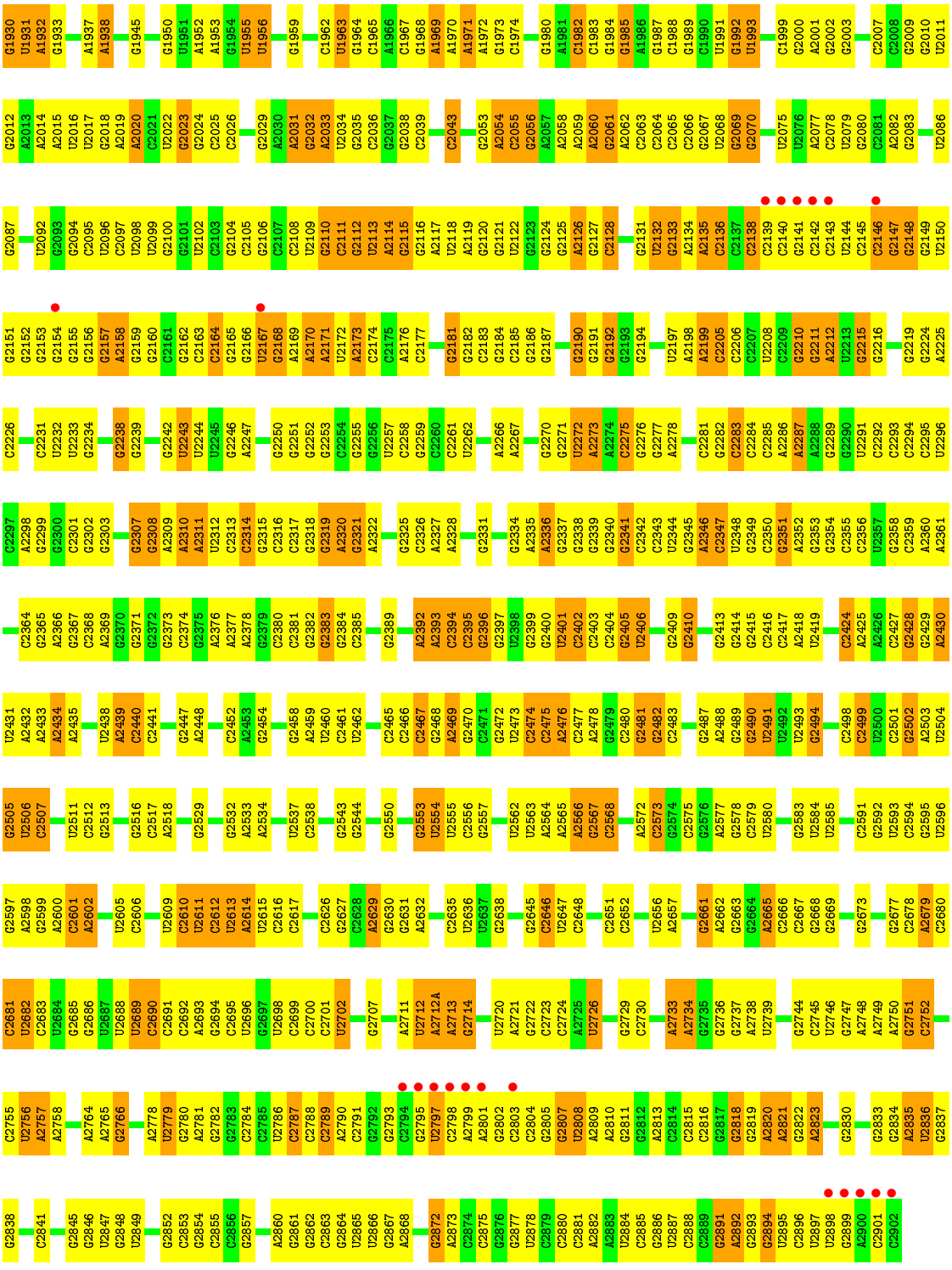
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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)

Chain AA: 2% 36% 47% 17%

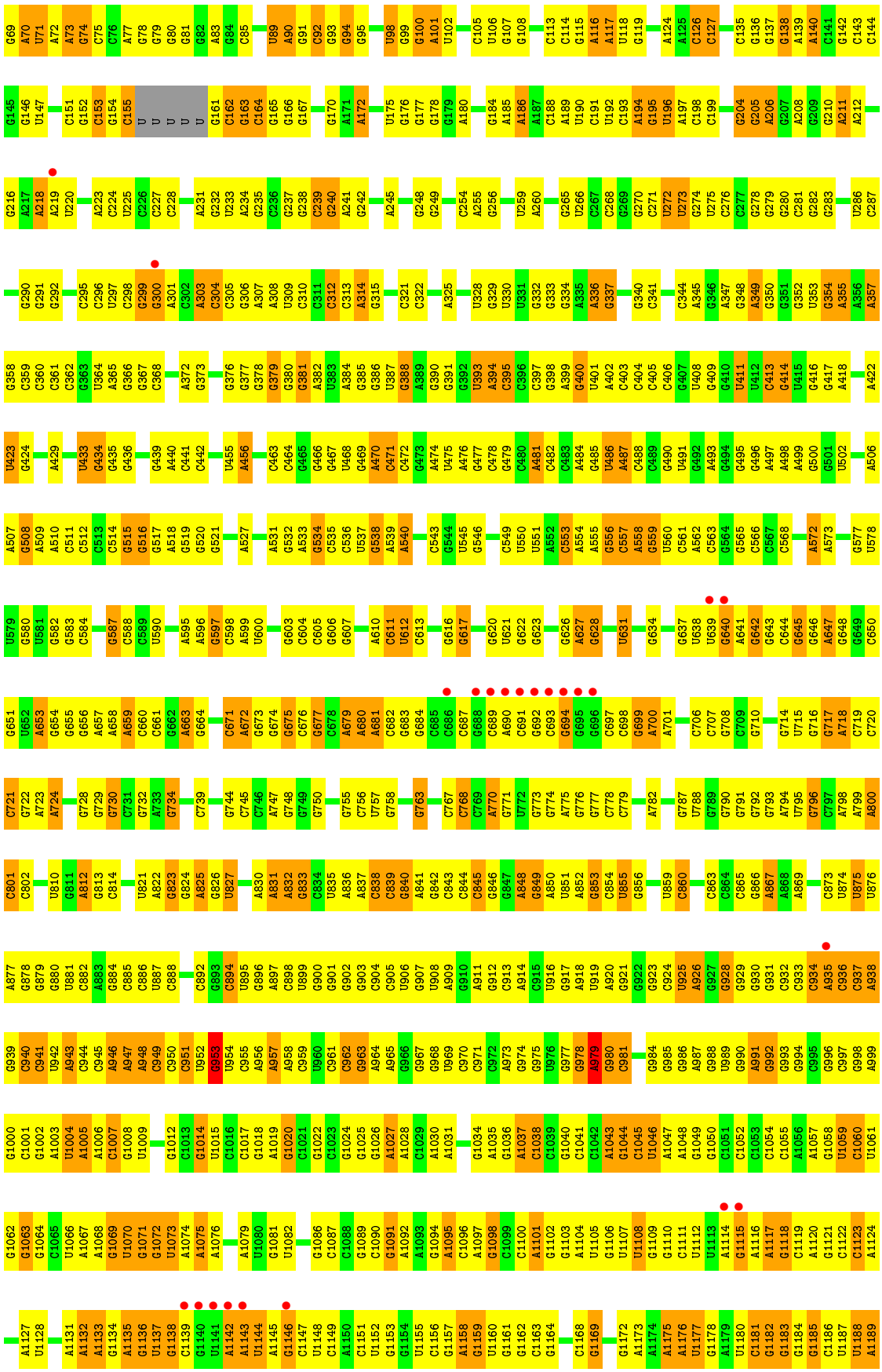


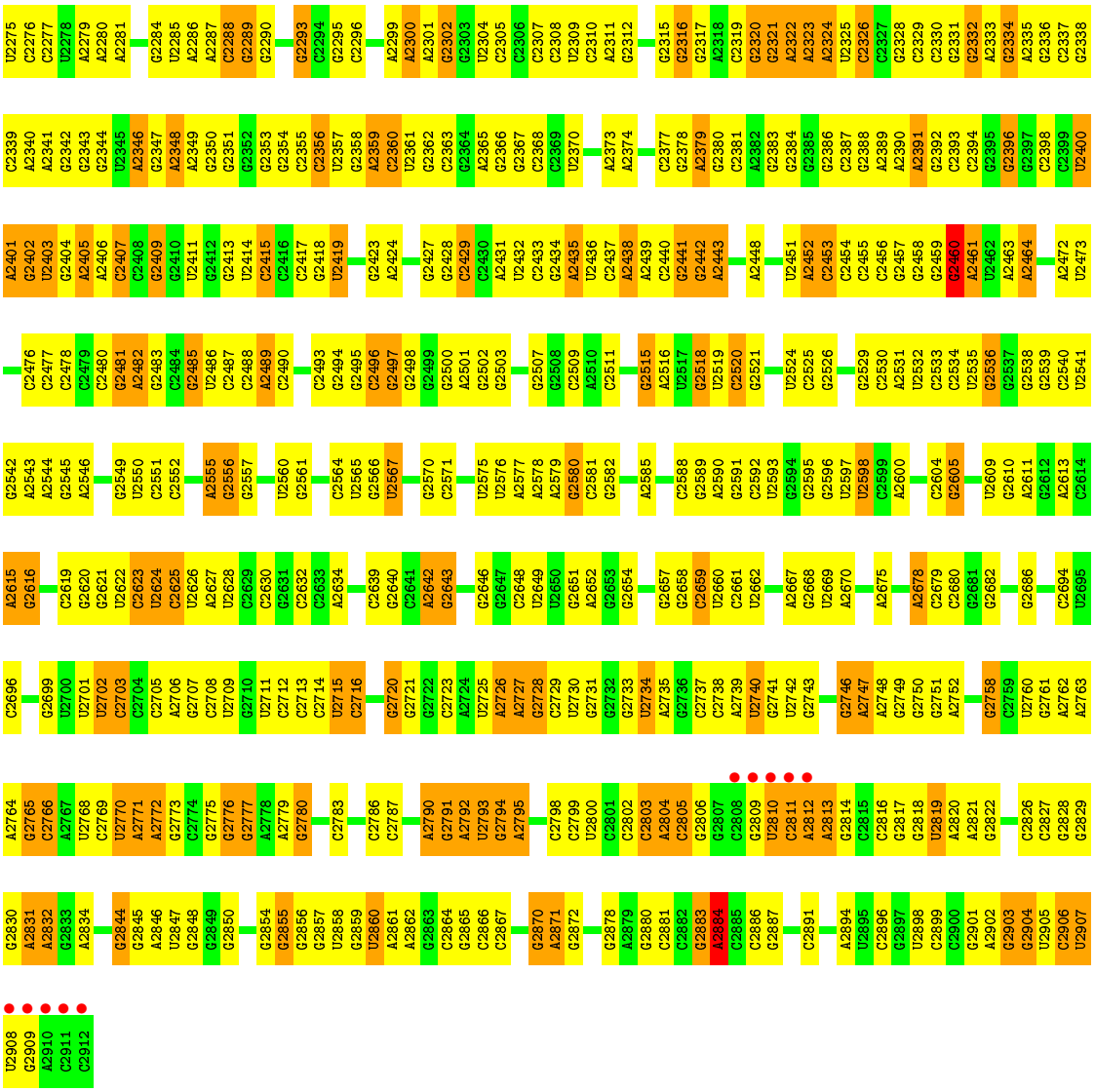




- Molecule 1: RNA (2912-MER)

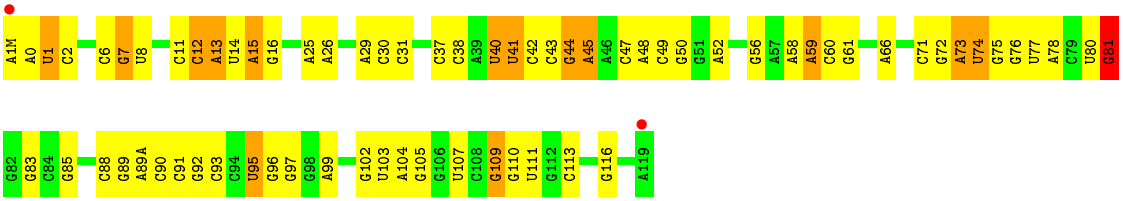
Chain CA:





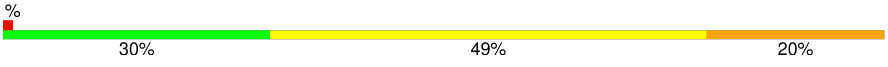
• Molecule 2: 5S RIBOSOMAL RNA

Chain AB:



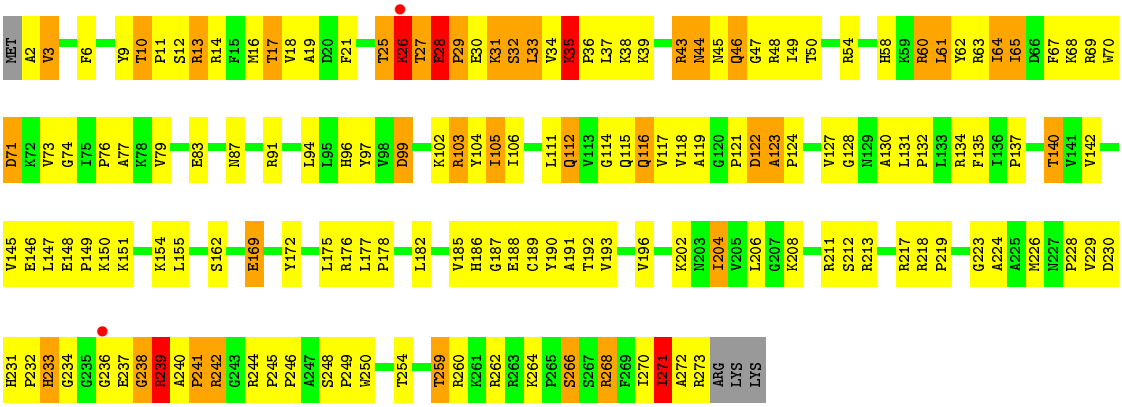
• Molecule 2: 5S RIBOSOMAL RNA

Chain CB:



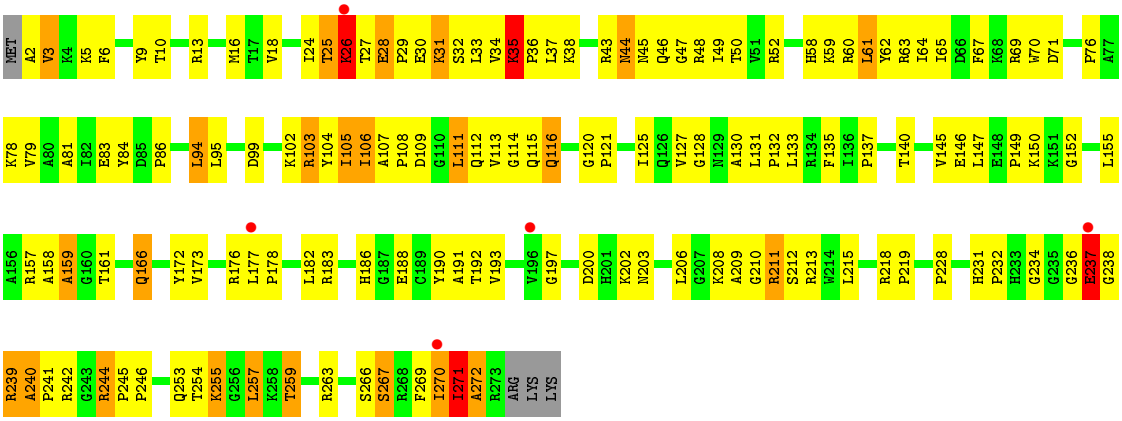
- Molecule 3: 50S ribosomal protein L2

Chain AD:



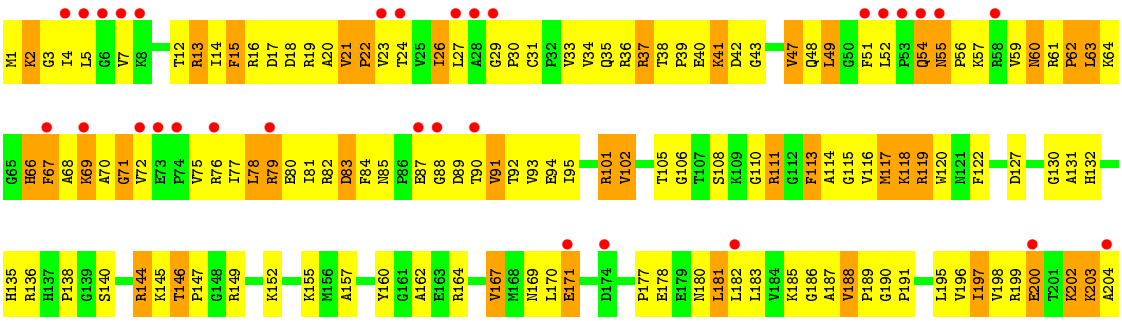
- Molecule 3: 50S ribosomal protein L2

Chain CD:



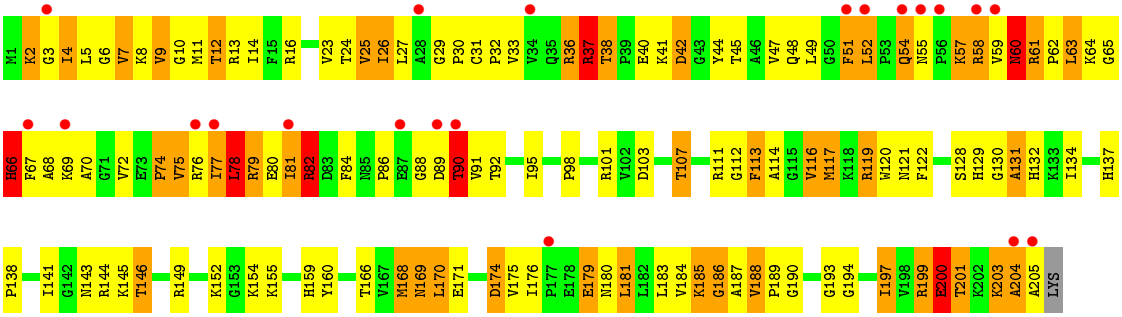
- Molecule 4: 50S ribosomal protein L3

Chain AE:



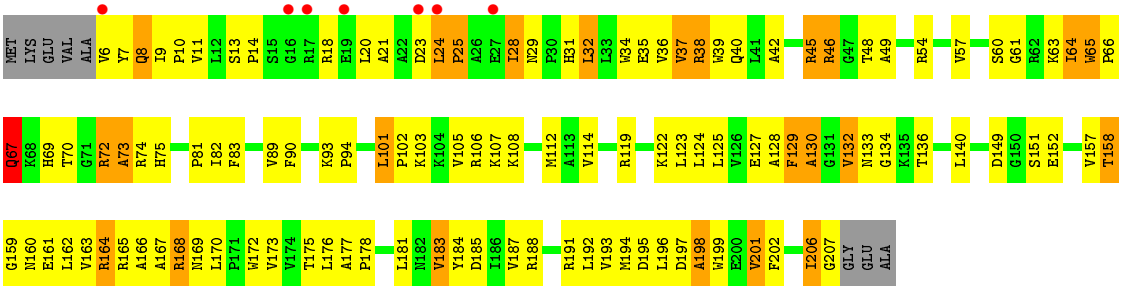
• Molecule 4: 50S ribosomal protein L3

Chain CE:



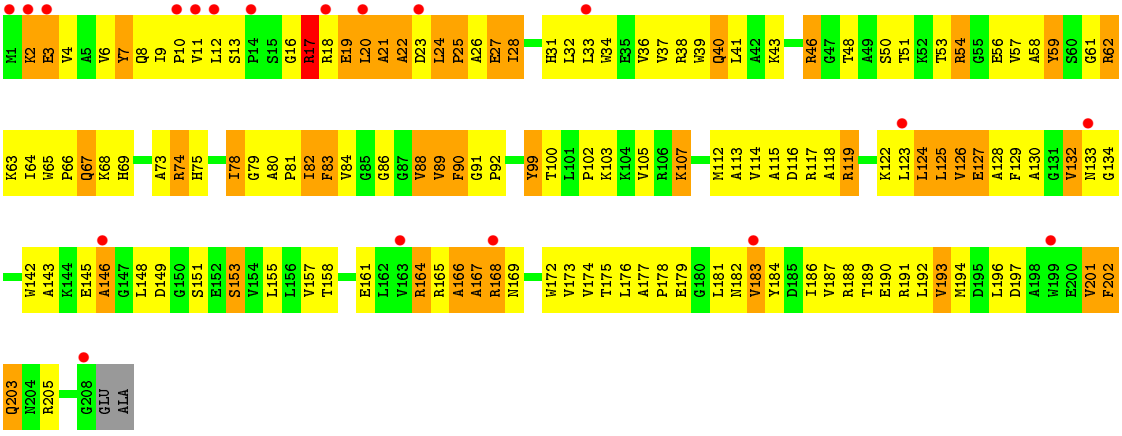
• Molecule 5: 50S ribosomal protein L4

Chain AF:



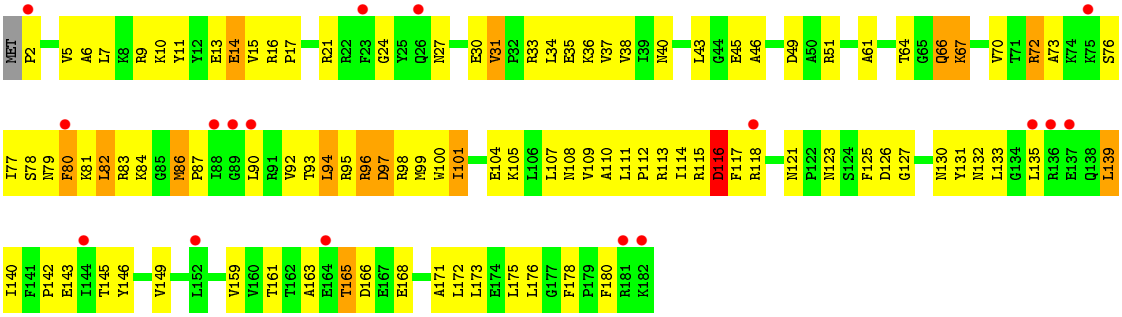
• Molecule 5: 50S ribosomal protein L4

Chain CF:



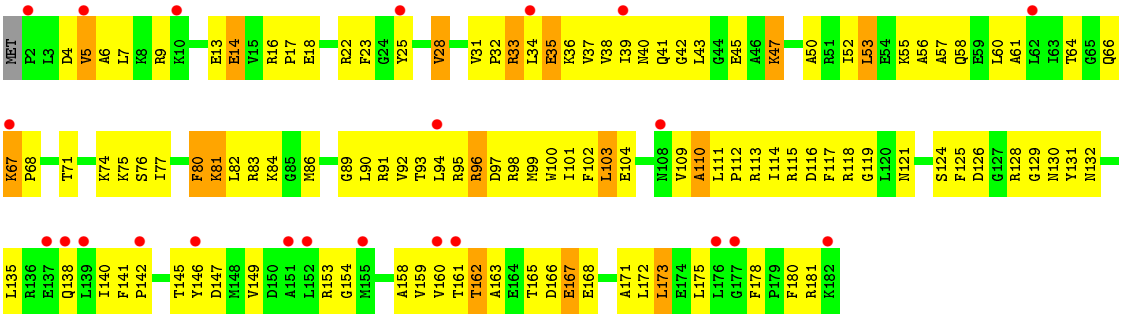
• Molecule 6: 50S ribosomal protein L5

Chain AG:



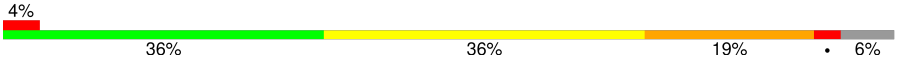
• Molecule 6: 50S ribosomal protein L5

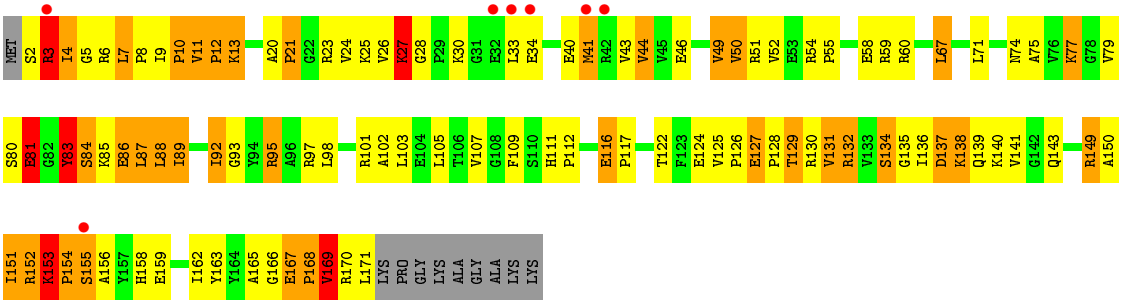
Chain CG:



• Molecule 7: 50S ribosomal protein L6

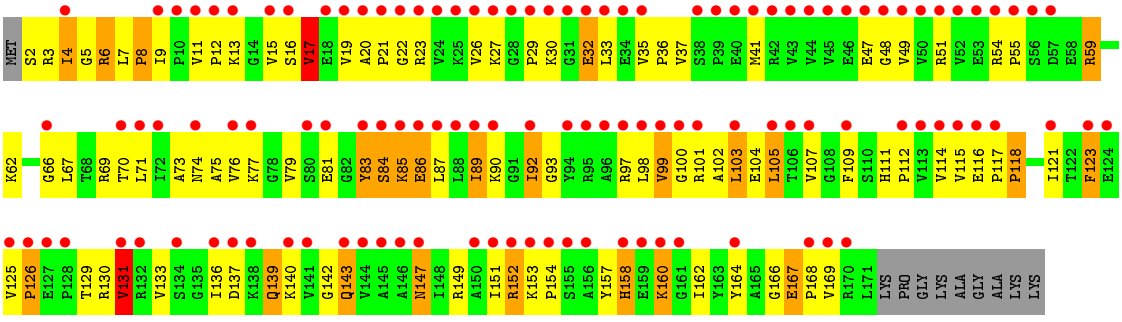
Chain AH:





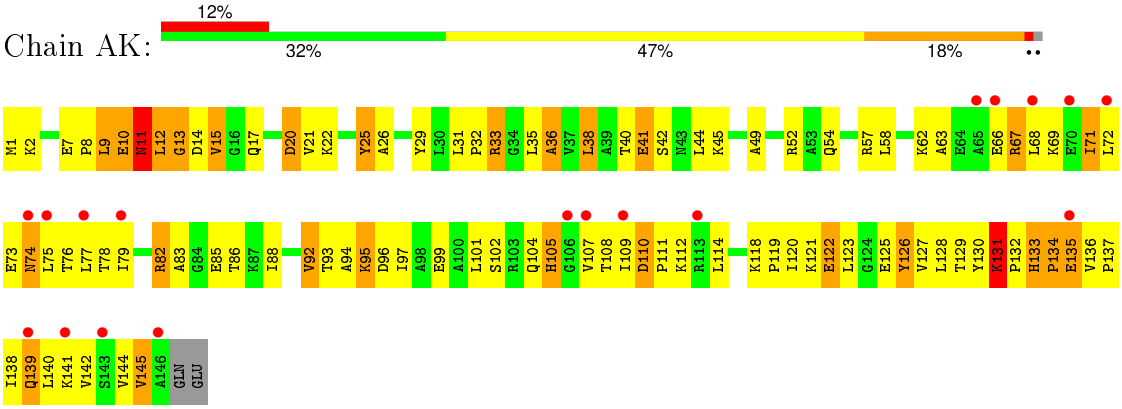
• Molecule 7: 50S ribosomal protein L6

Chain CH:



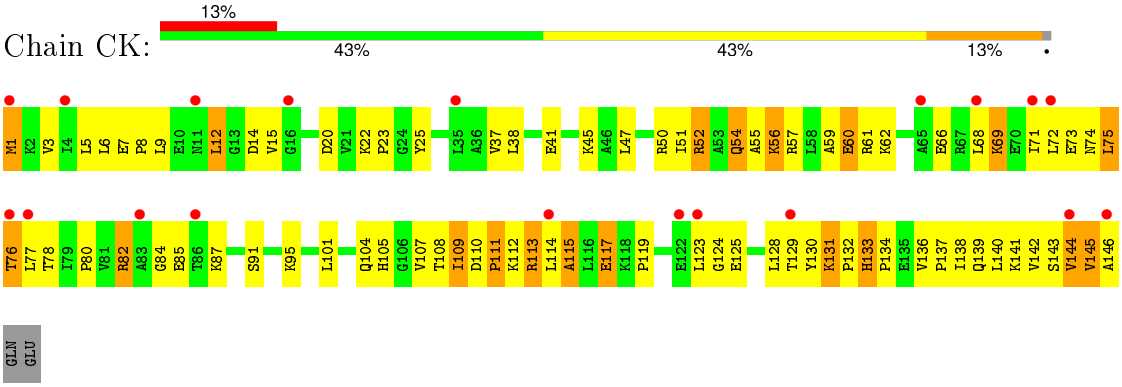
- Molecule 8: 50S ribosomal protein L9

Chain AK:



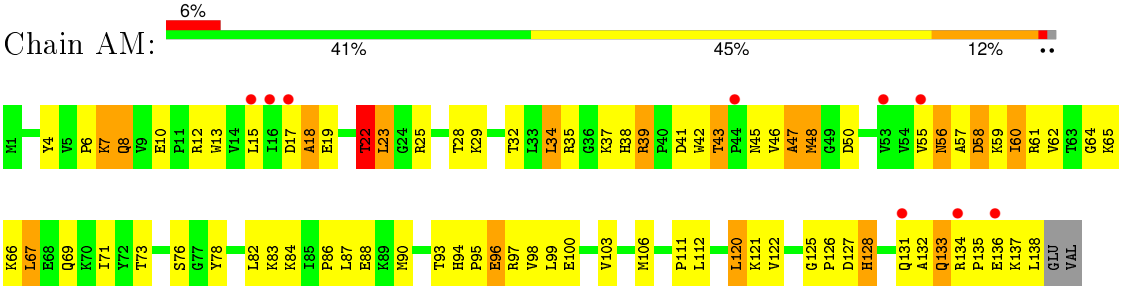
- Molecule 8: 50S ribosomal protein L9

Chain CK:



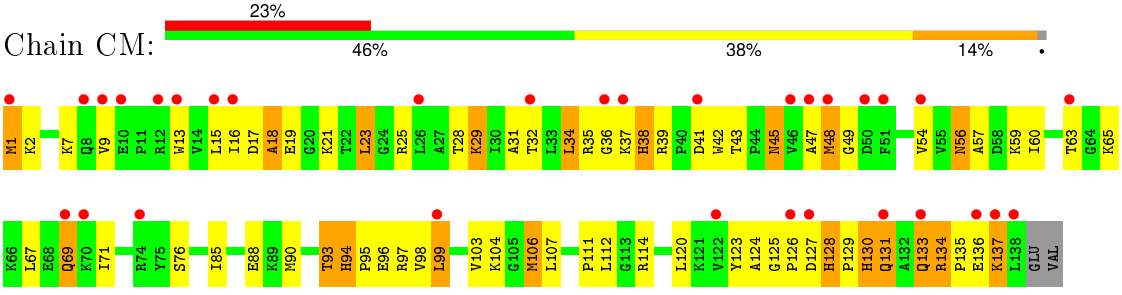
- Molecule 9: 50S ribosomal protein L13

Chain AM:



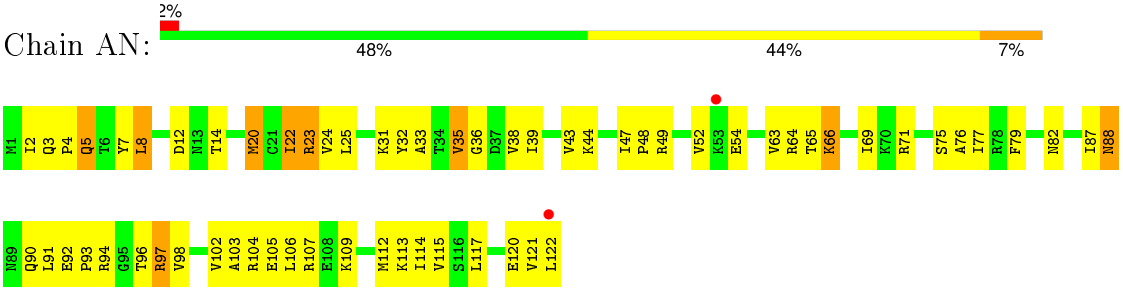
- Molecule 9: 50S ribosomal protein L13

Chain CM:



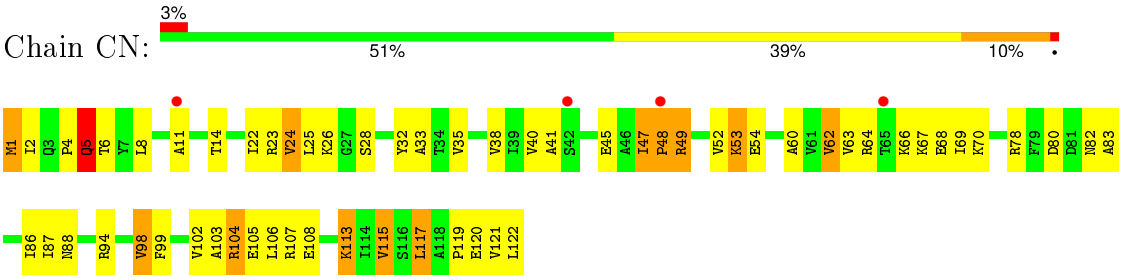
- Molecule 10: 50S ribosomal protein L14

Chain AN:



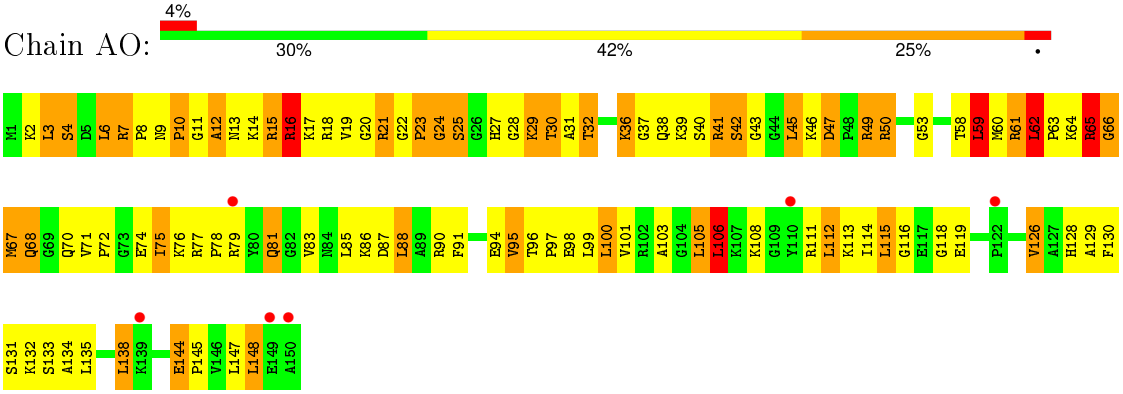
• Molecule 10: 50S ribosomal protein L14

Chain CN:



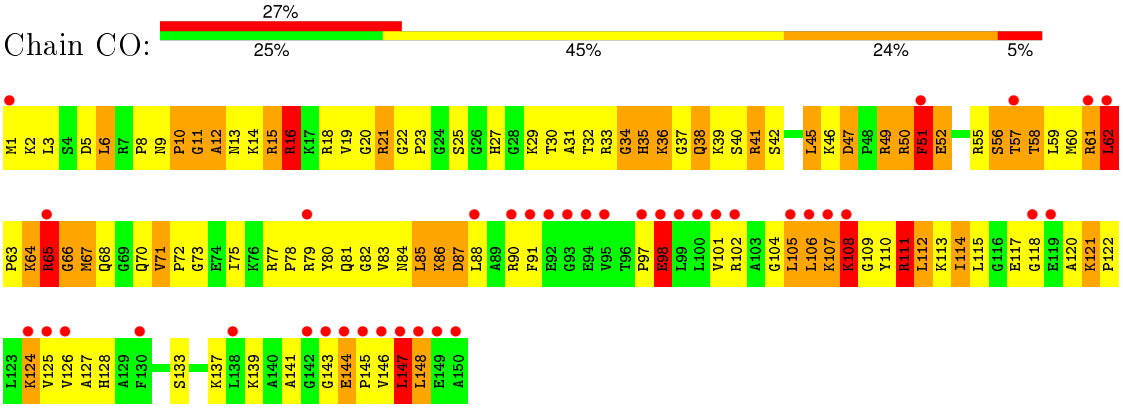
• Molecule 11: 50S ribosomal protein L15

Chain AO:



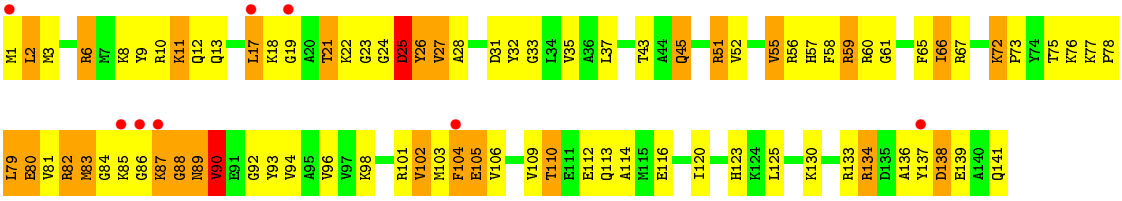
• Molecule 11: 50S ribosomal protein L15

Chain CO:



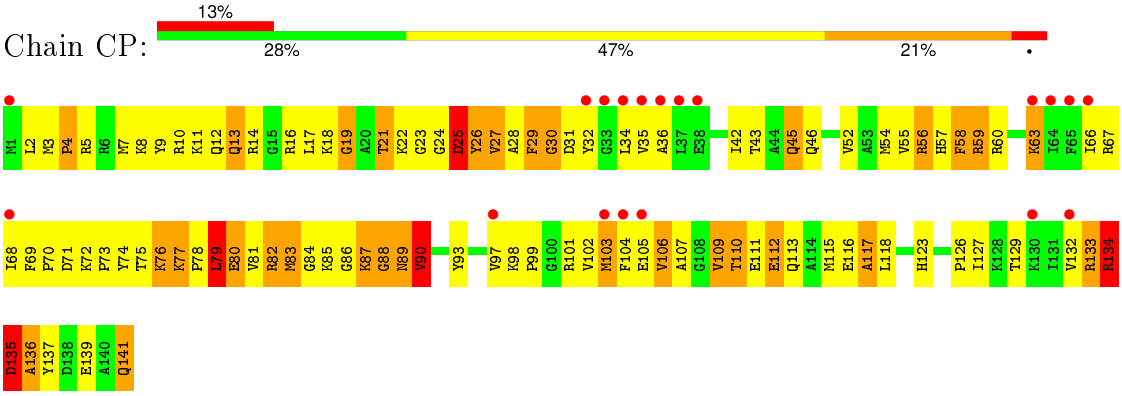
• Molecule 12: 50S ribosomal protein L16

Chain AP:



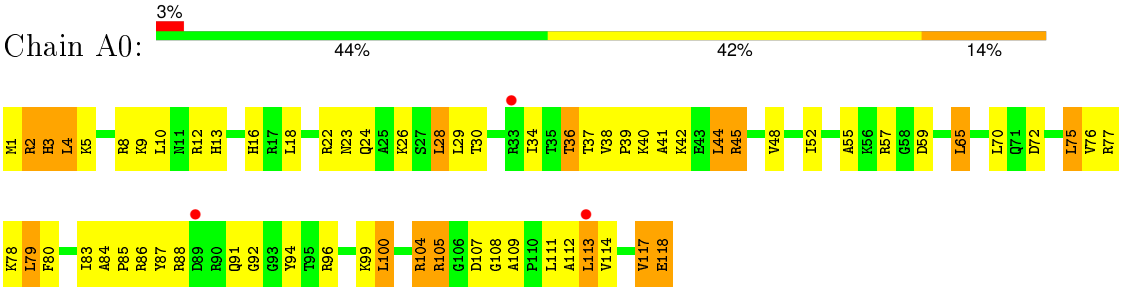
• Molecule 12: 50S ribosomal protein L16

Chain CP:



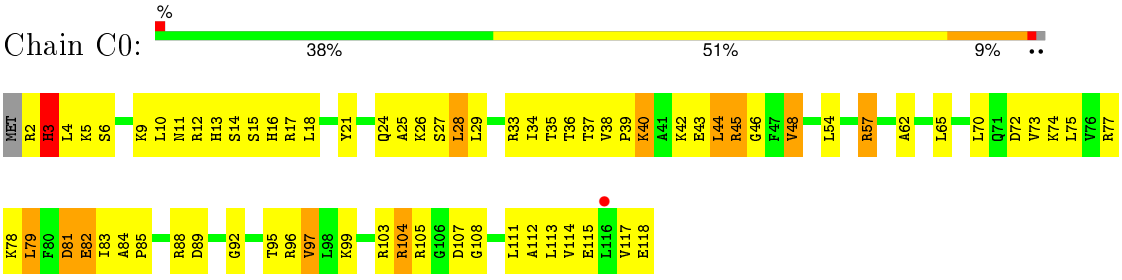
• Molecule 13: 50S ribosomal protein L17

Chain A0:



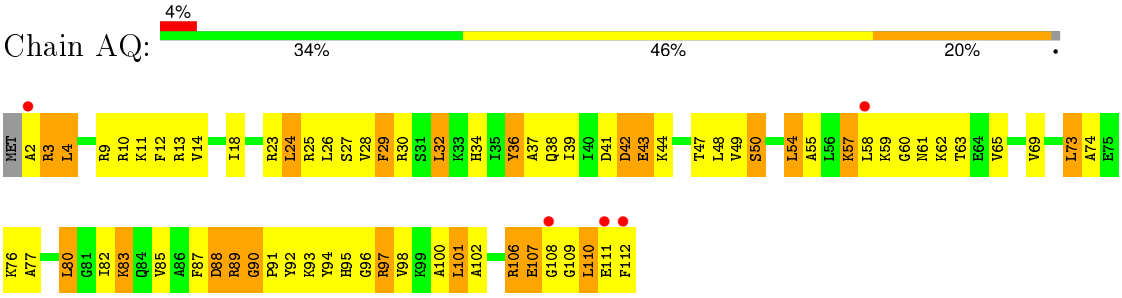
• Molecule 13: 50S ribosomal protein L17

Chain C0:



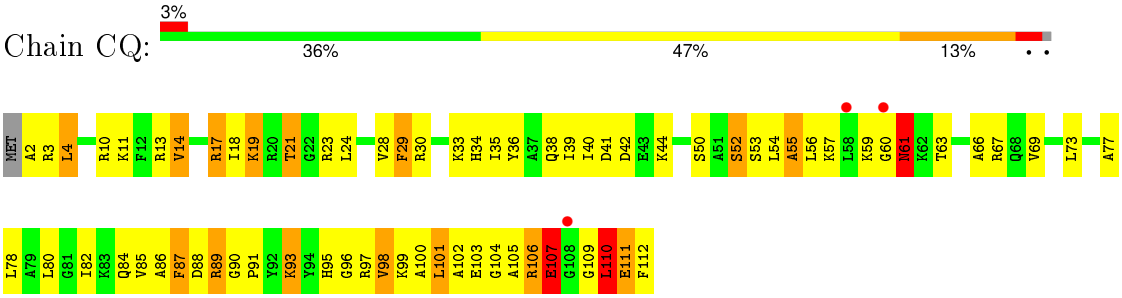
• Molecule 14: 50S ribosomal protein L18

Chain AQ:



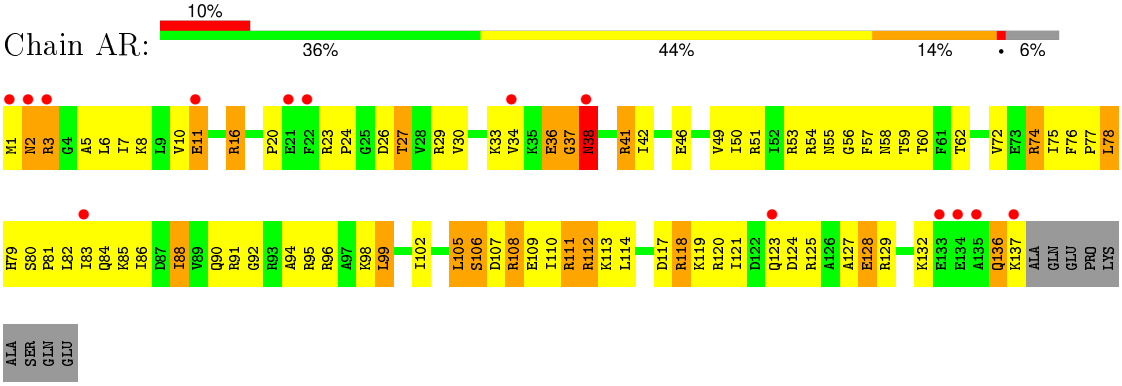
- Molecule 14: 50S ribosomal protein L18

Chain CQ:



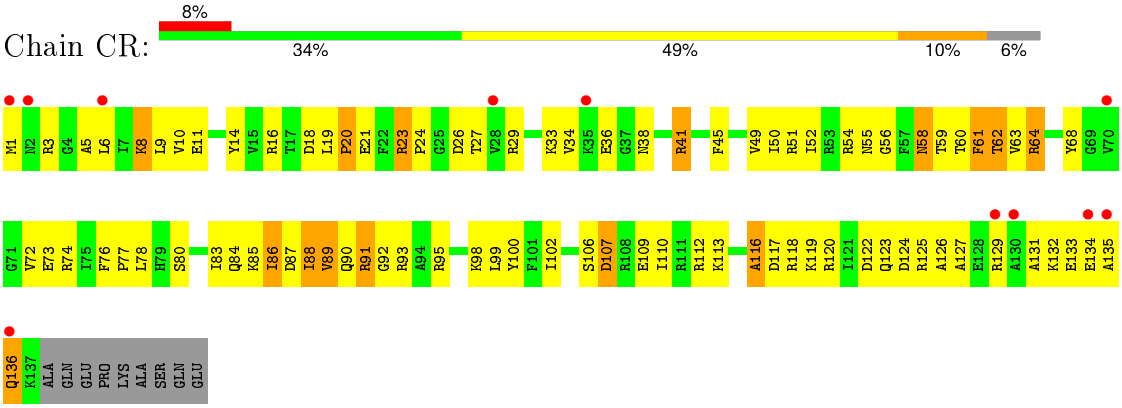
- Molecule 15: 50S ribosomal protein L19

Chain AR:



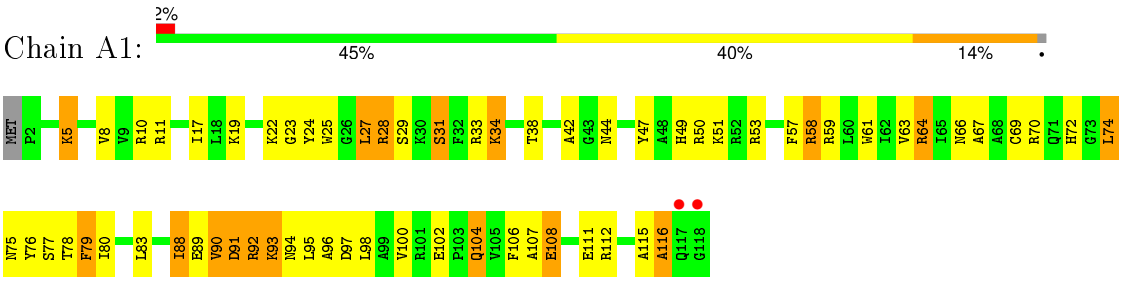
- Molecule 15: 50S ribosomal protein L19

Chain CR:



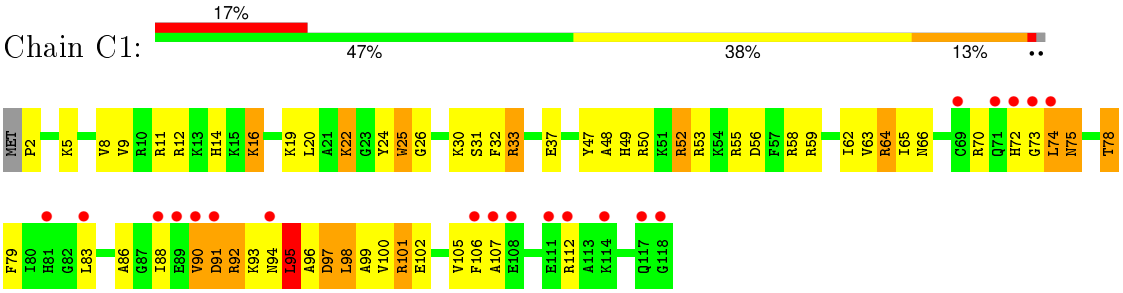
- Molecule 16: 50S ribosomal protein L20

Chain A1:



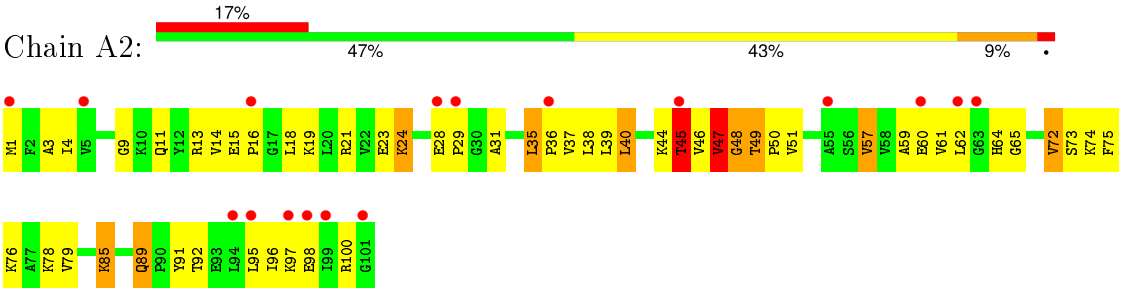
- Molecule 16: 50S ribosomal protein L20

Chain C1:



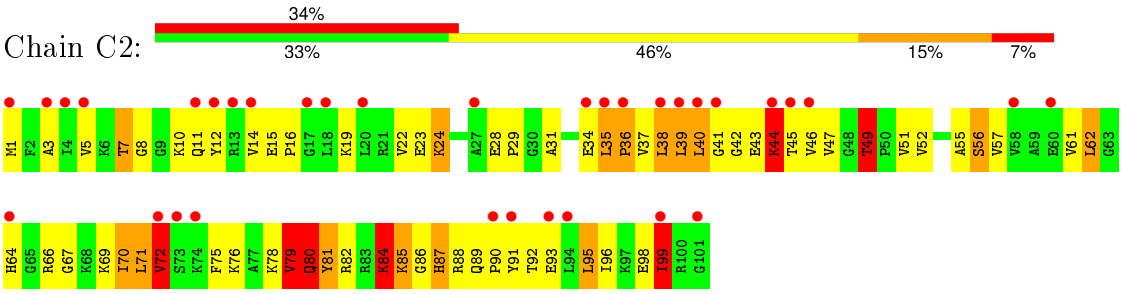
• Molecule 17: 50S ribosomal protein L21

Chain A2:



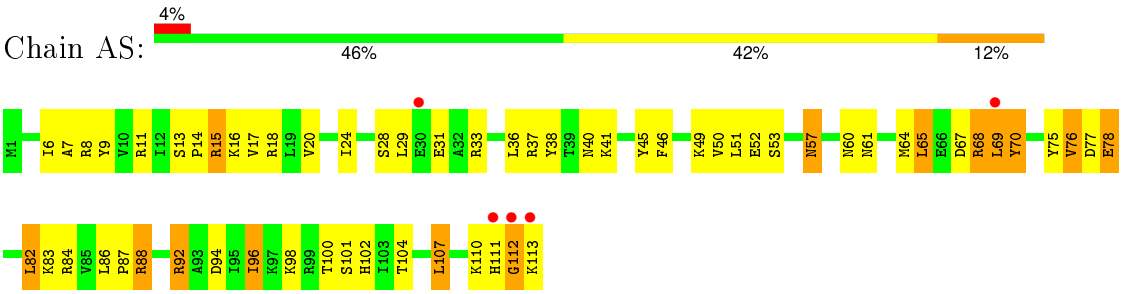
• Molecule 17: 50S ribosomal protein L21

Chain C2:



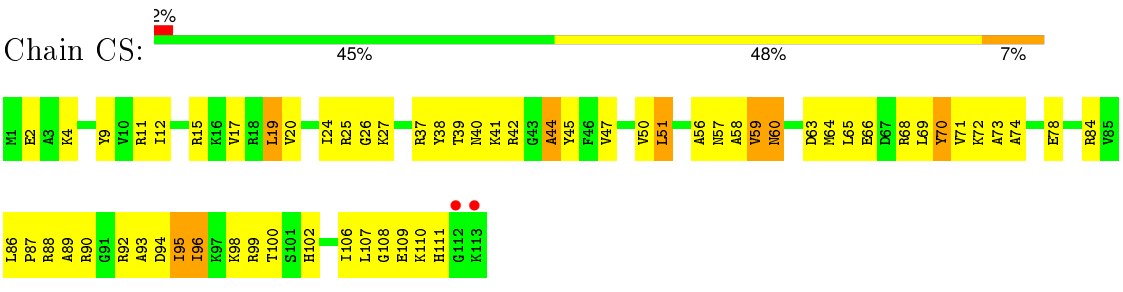
• Molecule 18: 50S ribosomal protein L22

Chain AS:



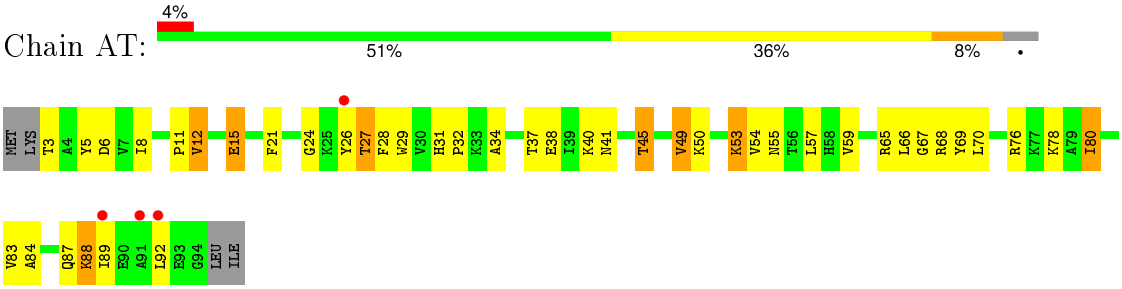
• Molecule 18: 50S ribosomal protein L22

Chain CS:



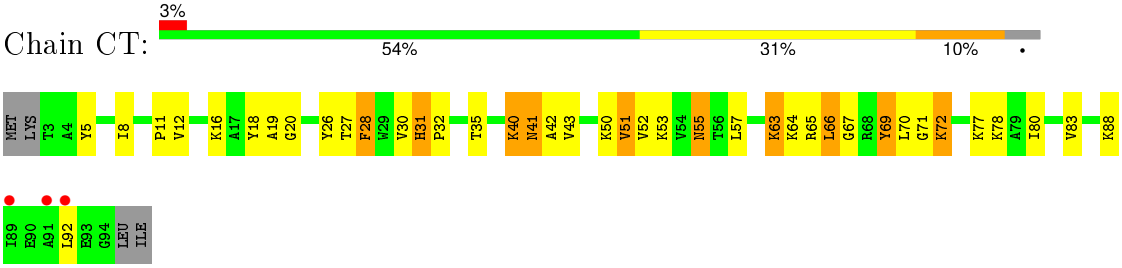
• Molecule 19: 50S ribosomal protein L23

Chain AT:



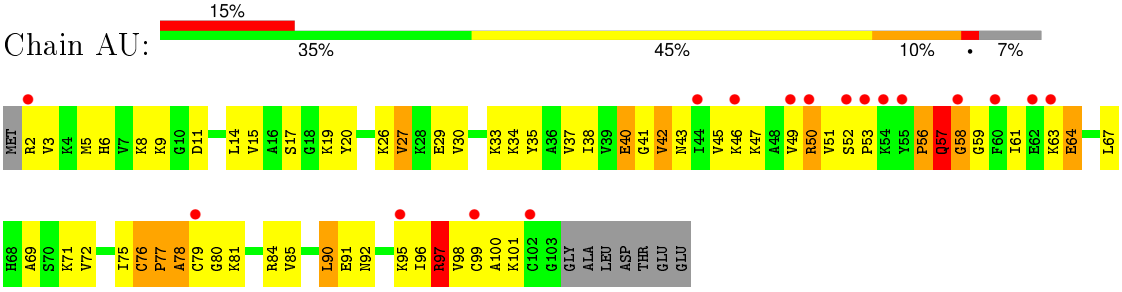
• Molecule 19: 50S ribosomal protein L23

Chain CT:



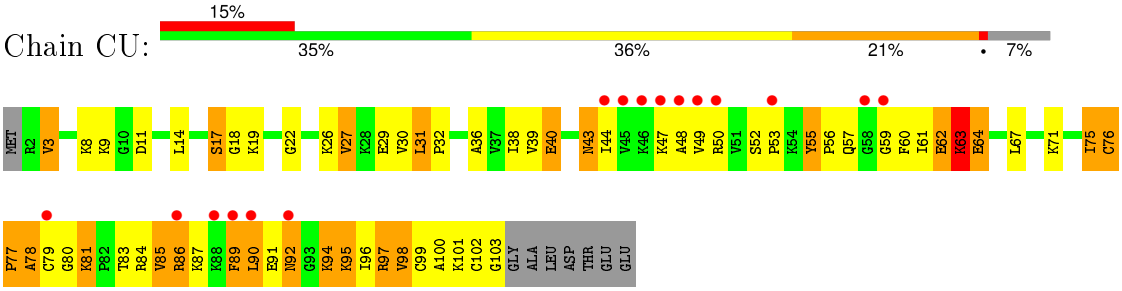
• Molecule 20: 50S ribosomal protein L24

Chain AU:



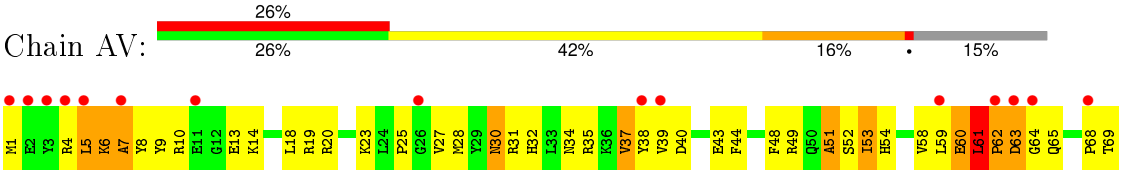
• Molecule 20: 50S ribosomal protein L24

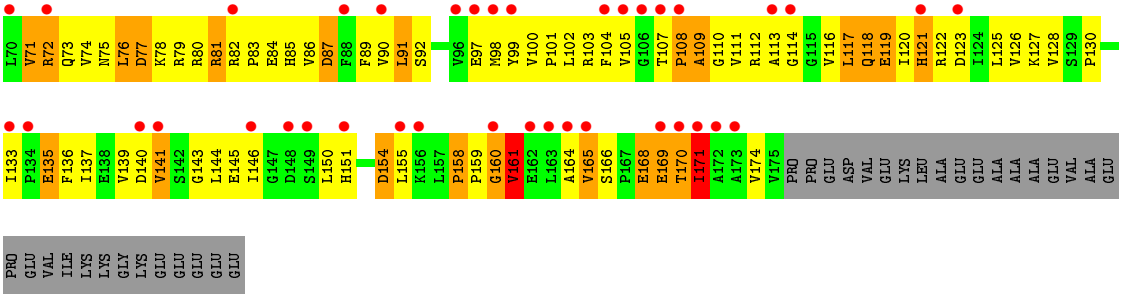
Chain CU:



• Molecule 21: 50S ribosomal protein L25

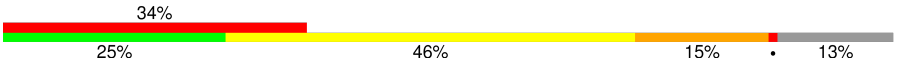
Chain AV:

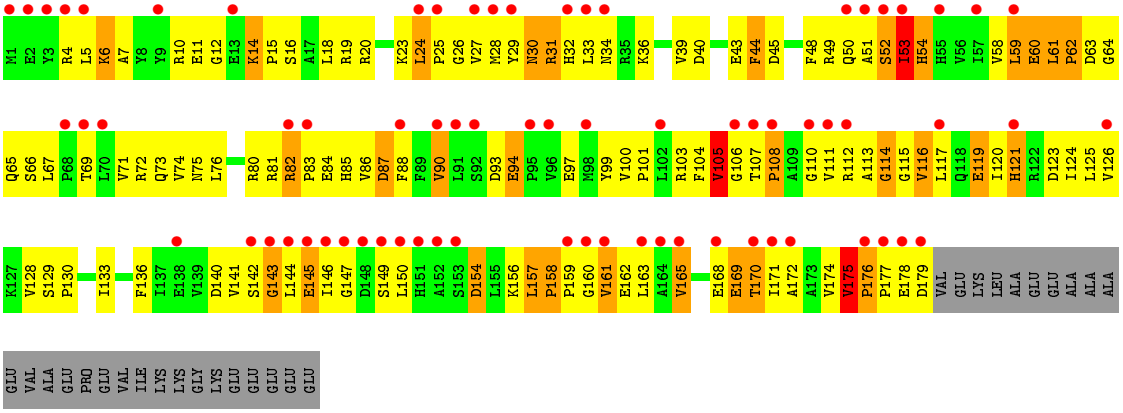




• Molecule 21: 50S ribosomal protein L25

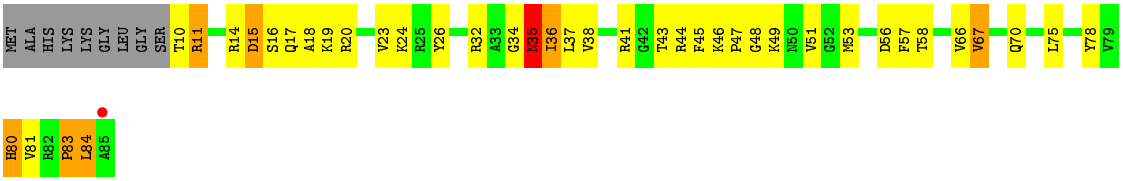
Chain CV:





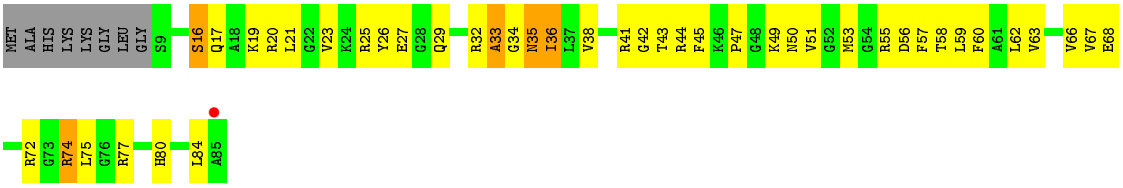
• Molecule 22: 50S ribosomal protein L27

Chain A3:



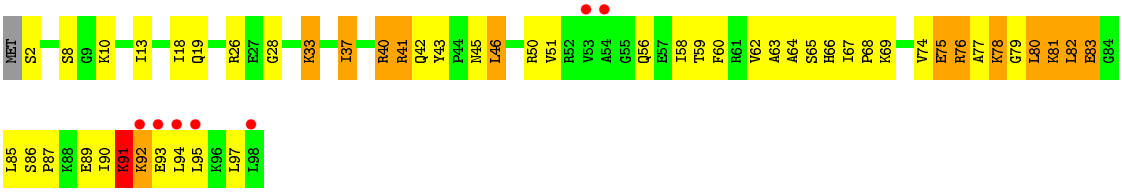
• Molecule 22: 50S ribosomal protein L27

Chain C3:

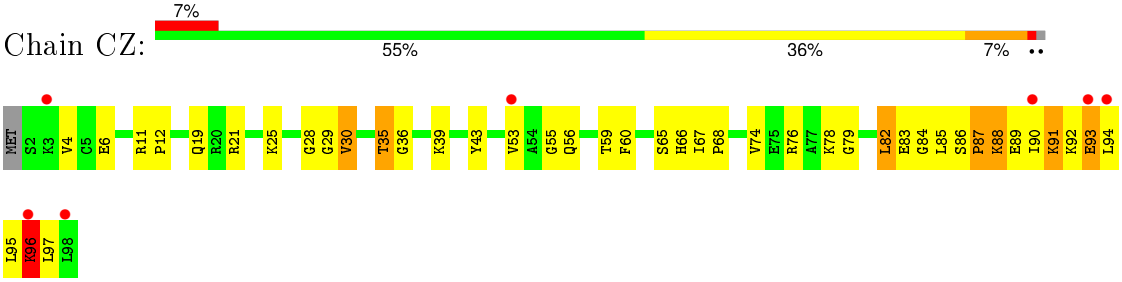


• Molecule 23: 50S ribosomal protein L28

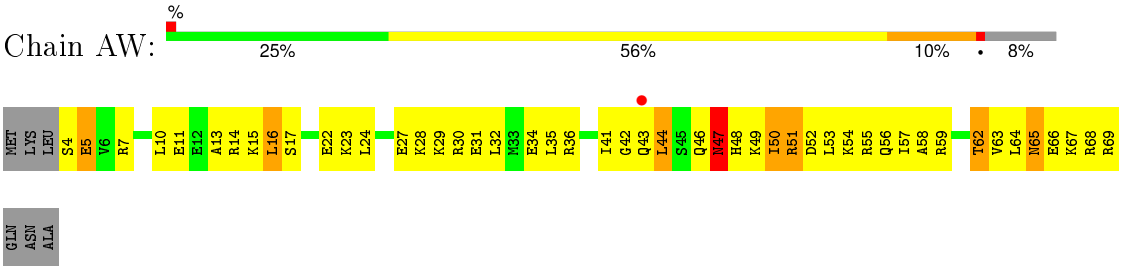
Chain AZ:



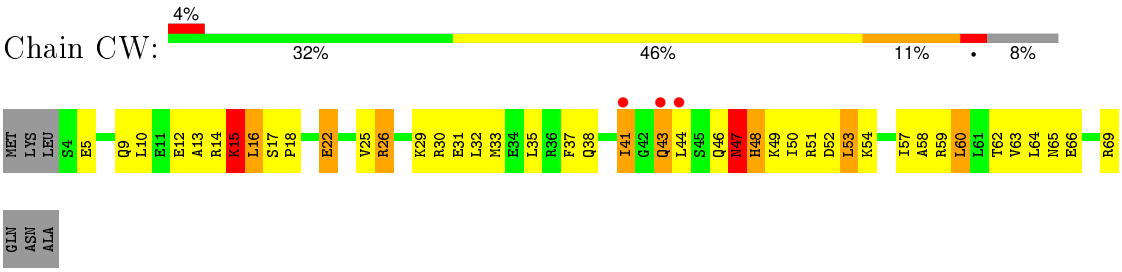
• Molecule 23: 50S ribosomal protein L28



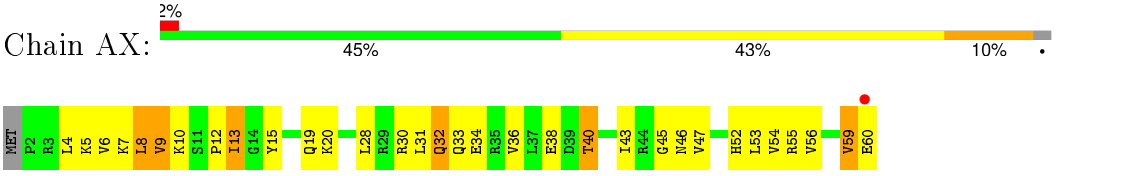
• Molecule 24: 50S ribosomal protein L29



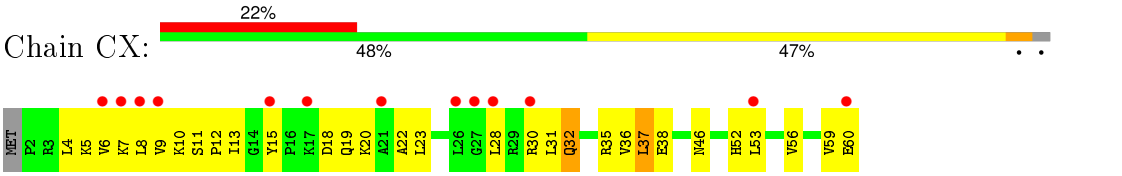
• Molecule 24: 50S ribosomal protein L29



• Molecule 25: 50S ribosomal protein L30

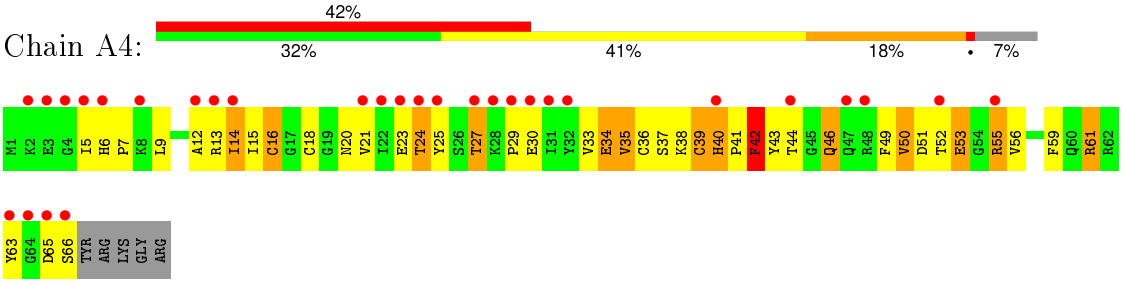


• Molecule 25: 50S ribosomal protein L30



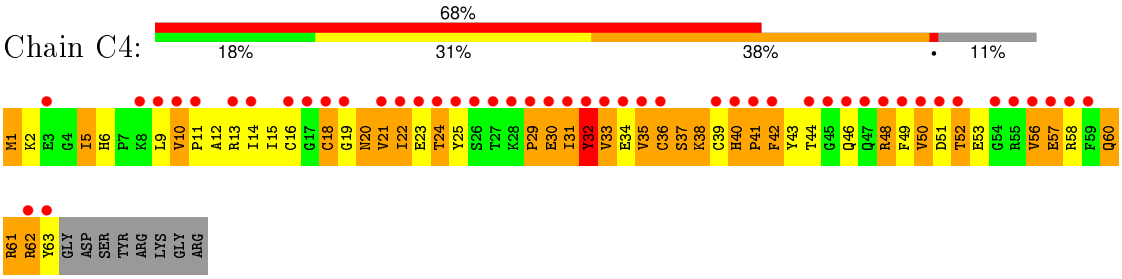
- Molecule 26: 50S ribosomal protein L31

Chain A4:



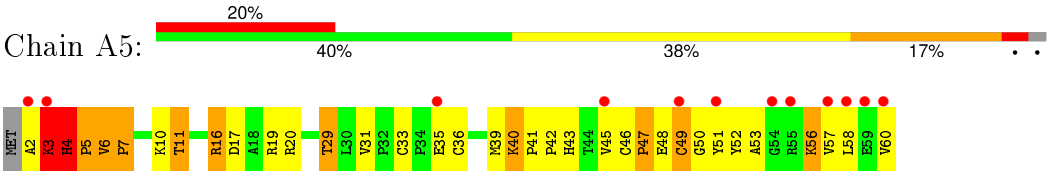
- Molecule 26: 50S ribosomal protein L31

Chain C4:



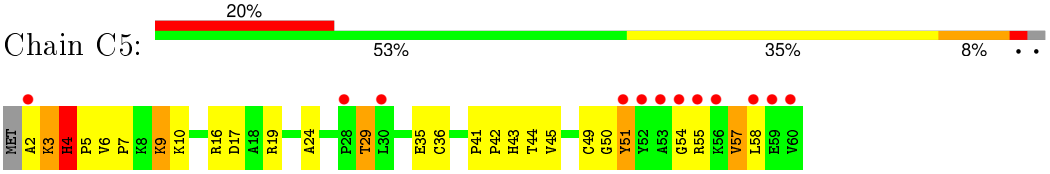
- Molecule 27: 50S ribosomal protein L32

Chain A5:



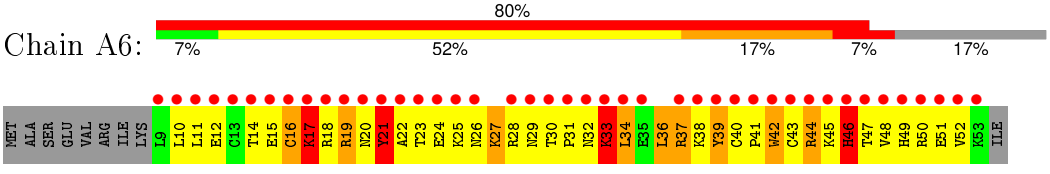
- Molecule 27: 50S ribosomal protein L32

Chain C5:



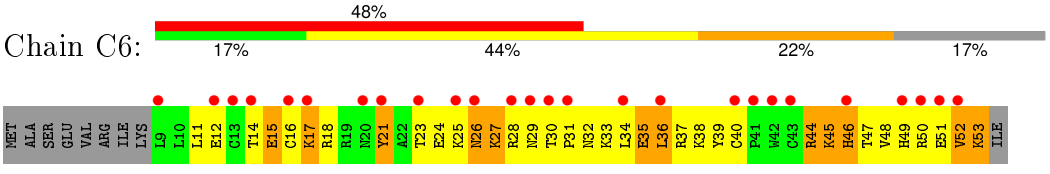
- Molecule 28: 50S ribosomal protein L33

Chain A6:



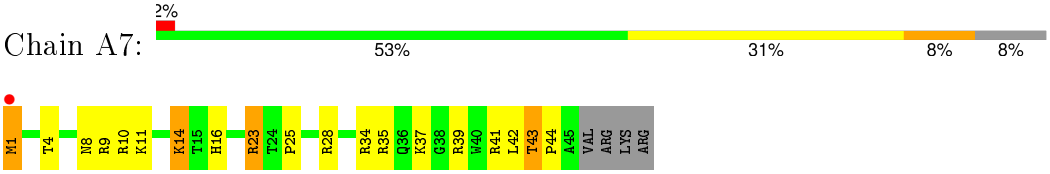
- Molecule 28: 50S ribosomal protein L33

Chain C6:



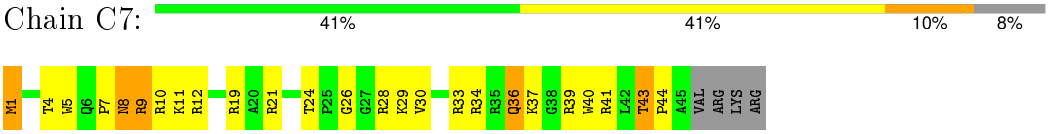
- Molecule 29: 50S ribosomal protein L34

Chain A7:



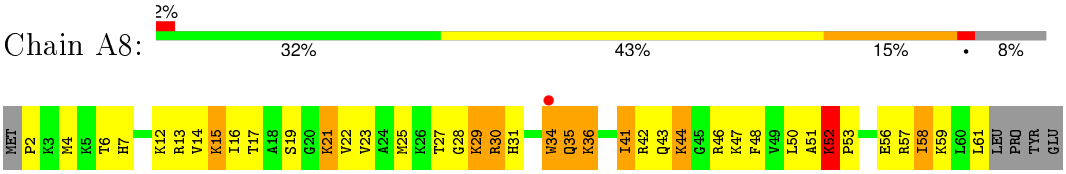
• Molecule 29: 50S ribosomal protein L34

Chain C7:



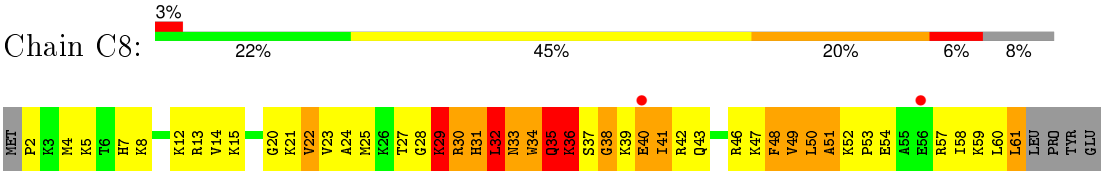
• Molecule 30: 50S ribosomal protein L35

Chain A8:



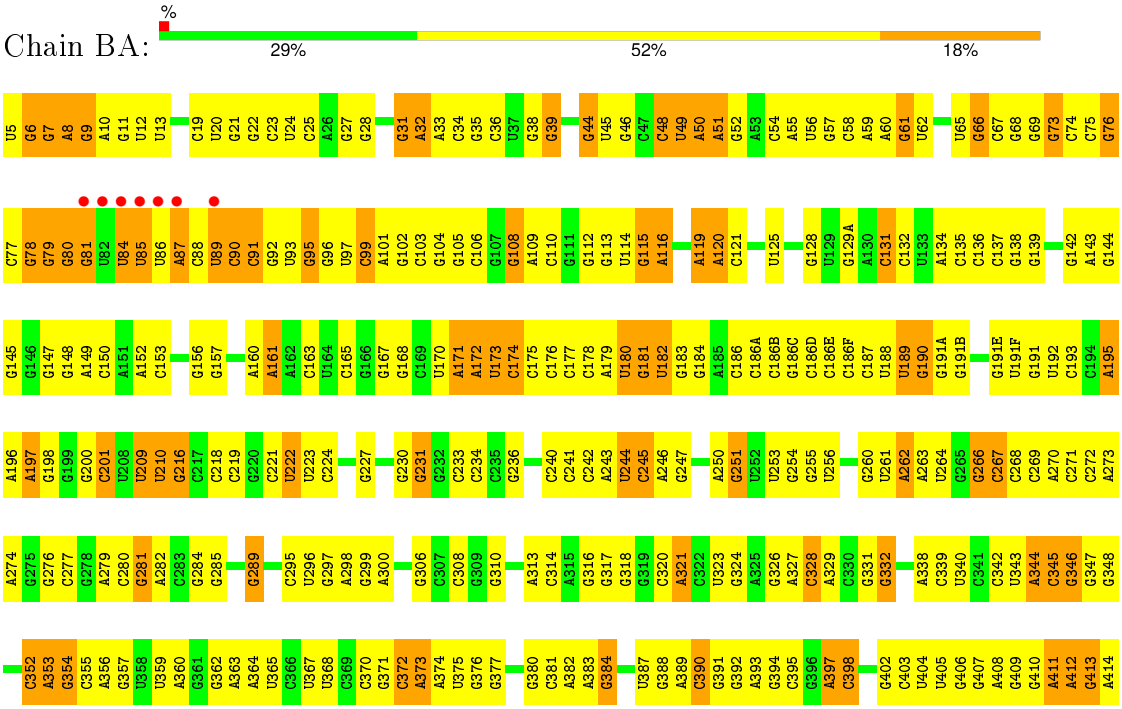
• Molecule 30: 50S ribosomal protein L35

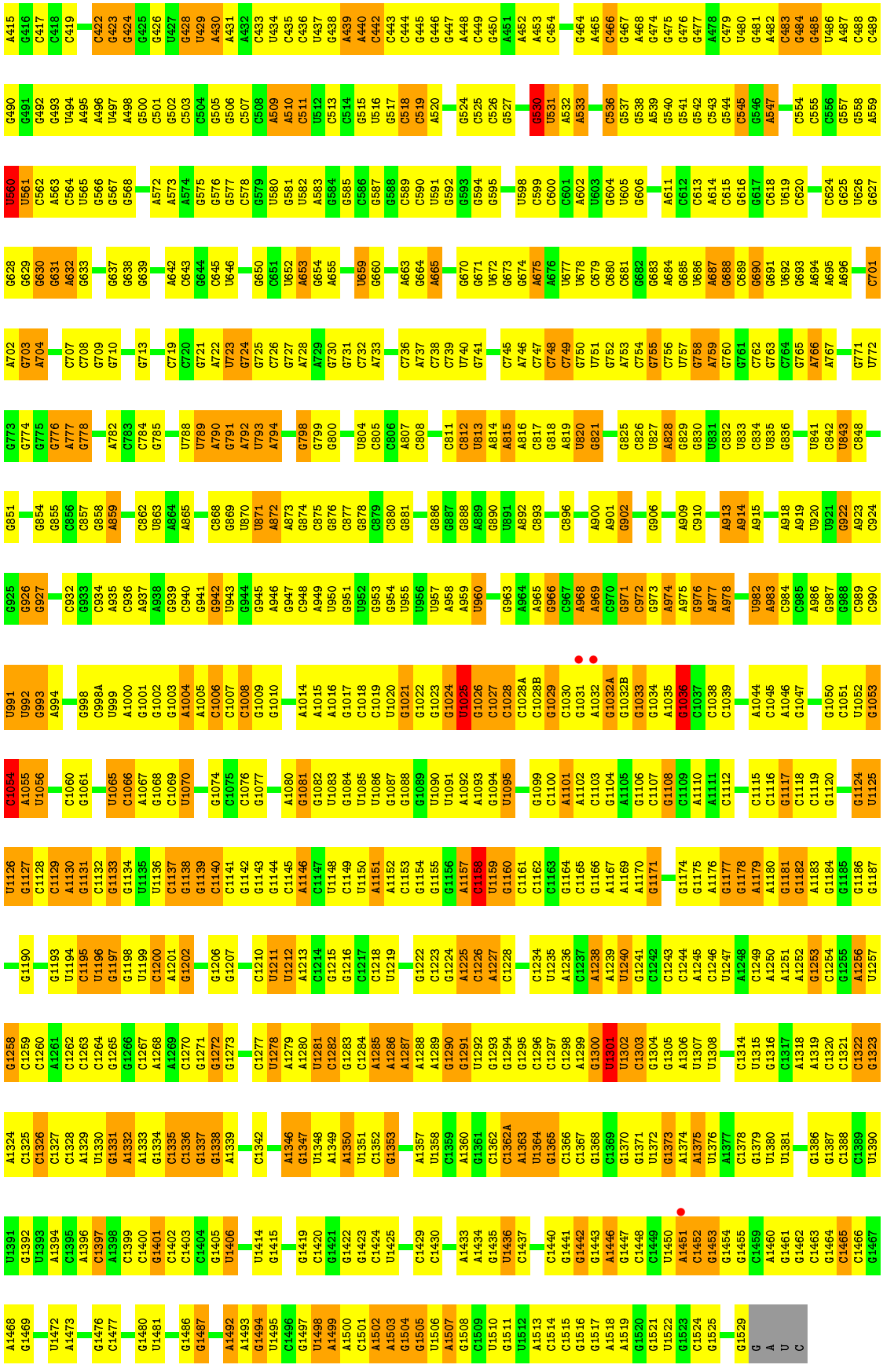
Chain C8:



• Molecule 31: 16S ribosomal RNA

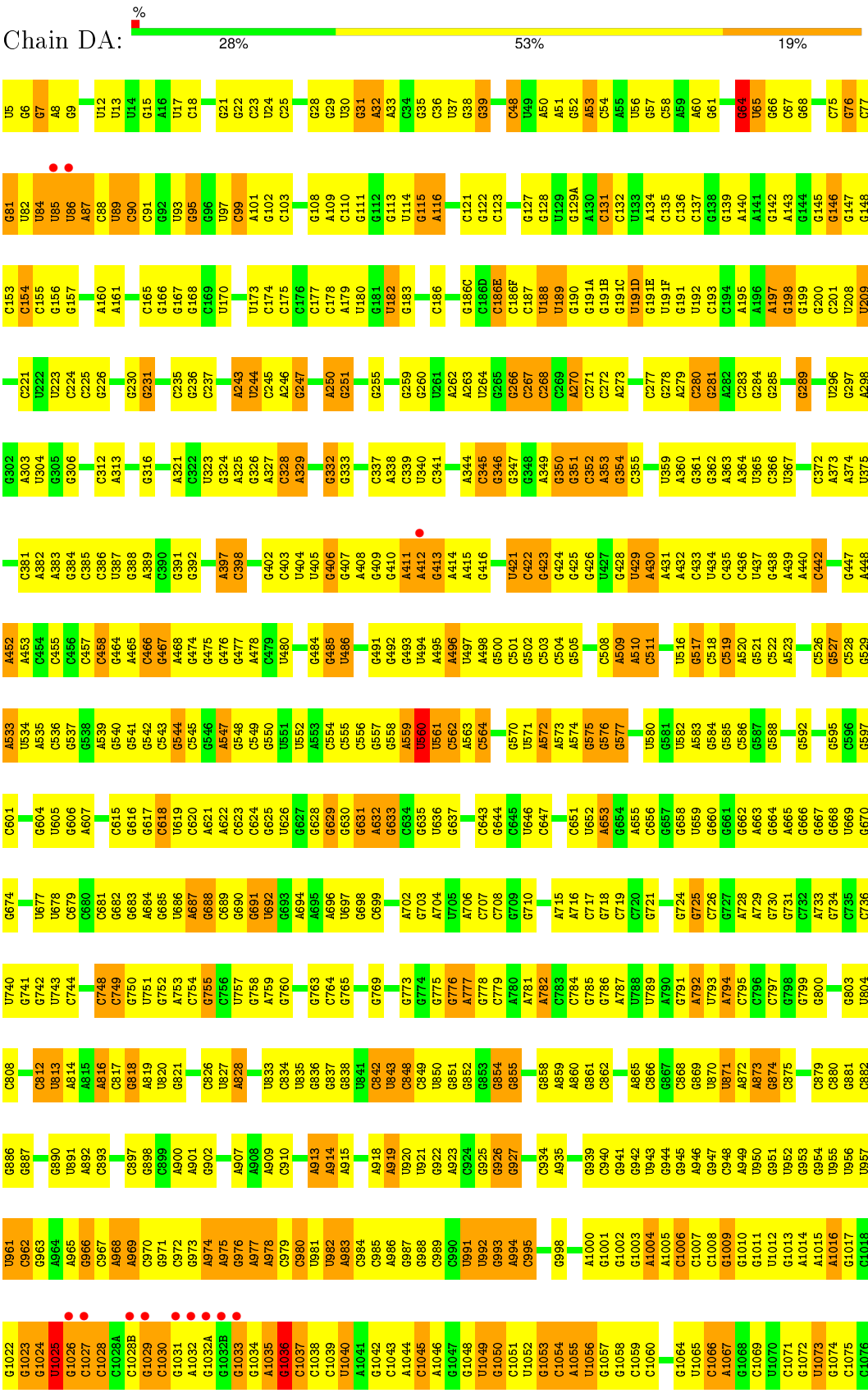
Chain BA:

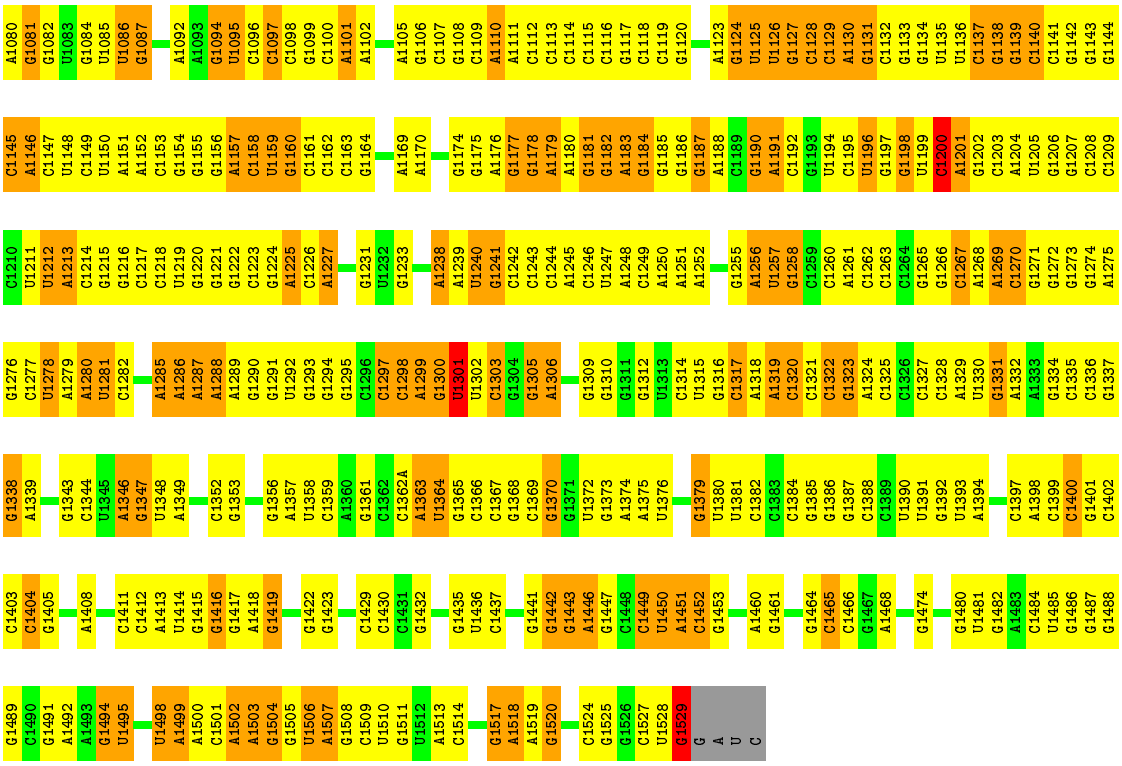




- Molecule 31: 16S ribosomal RNA

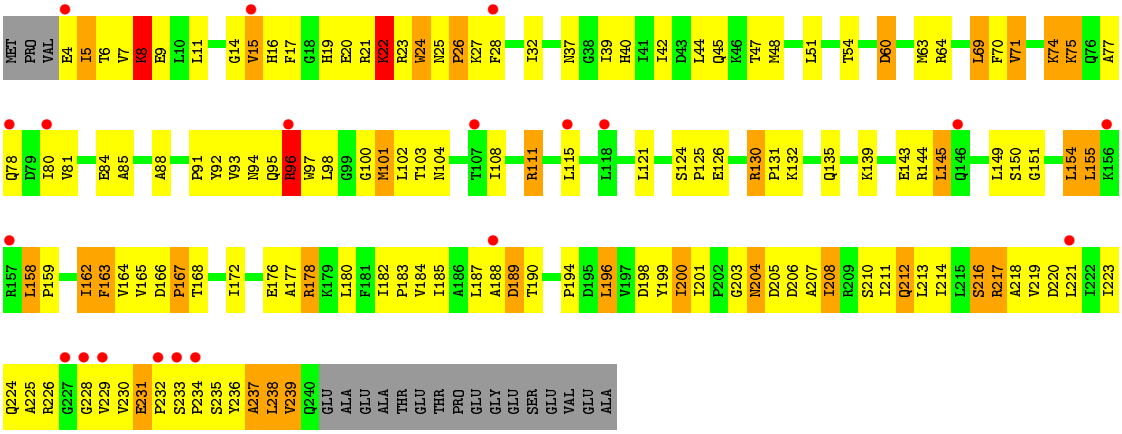
Chain DA:





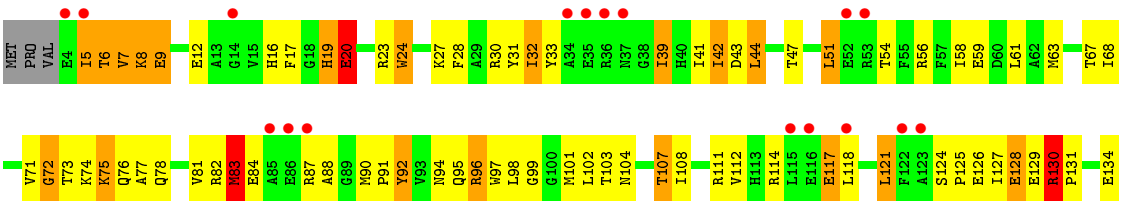
• Molecule 32: 30S RIBOSOMAL PROTEIN S2

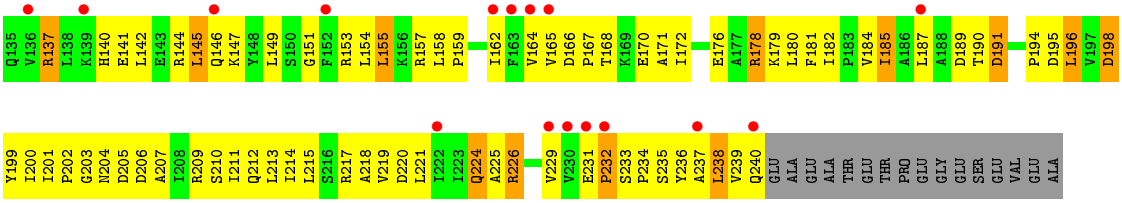
Chain BE:



• Molecule 32: 30S RIBOSOMAL PROTEIN S2

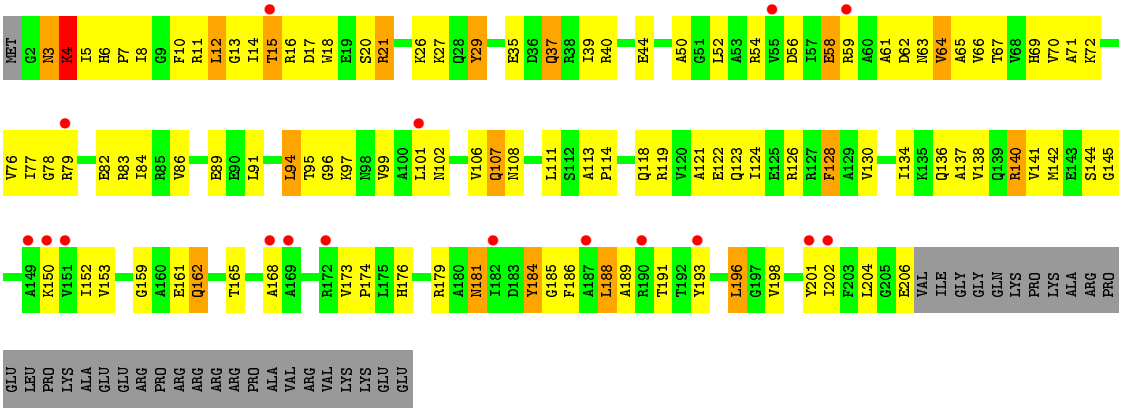
Chain DE:





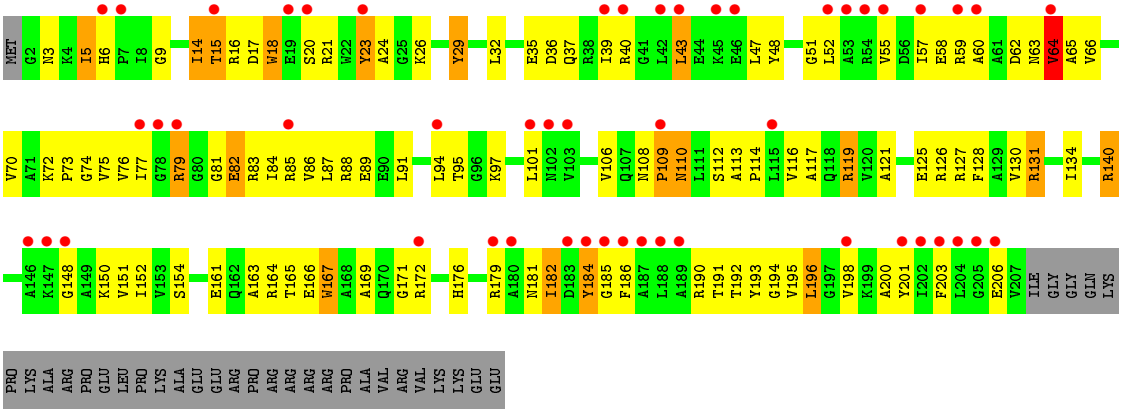
• Molecule 33: 30S RIBOSOMAL PROTEIN S3

Chain BF:



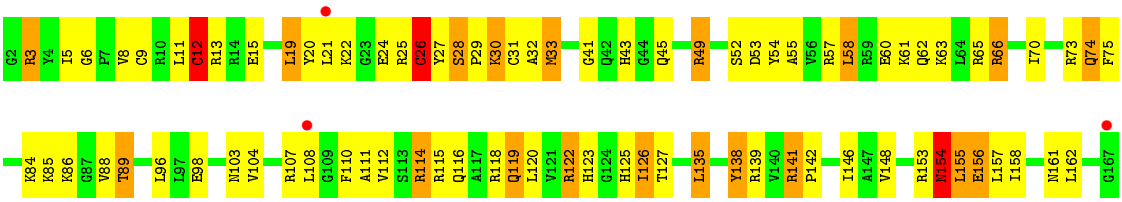
• Molecule 33: 30S RIBOSOMAL PROTEIN S3

Chain DF:

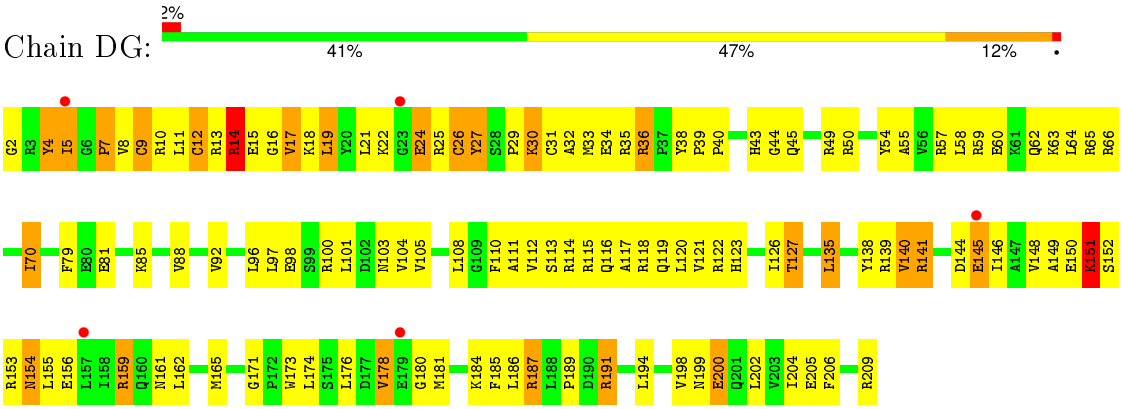


• Molecule 34: 30S RIBOSOMAL PROTEIN S4

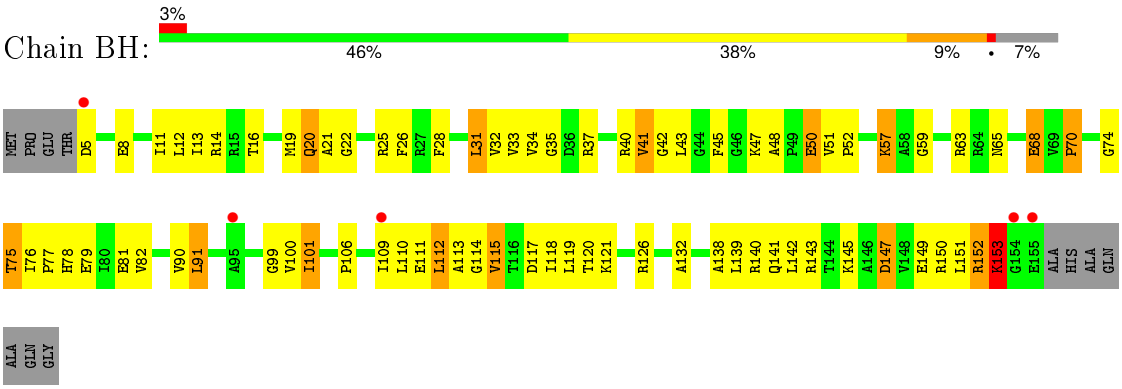
Chain BG:



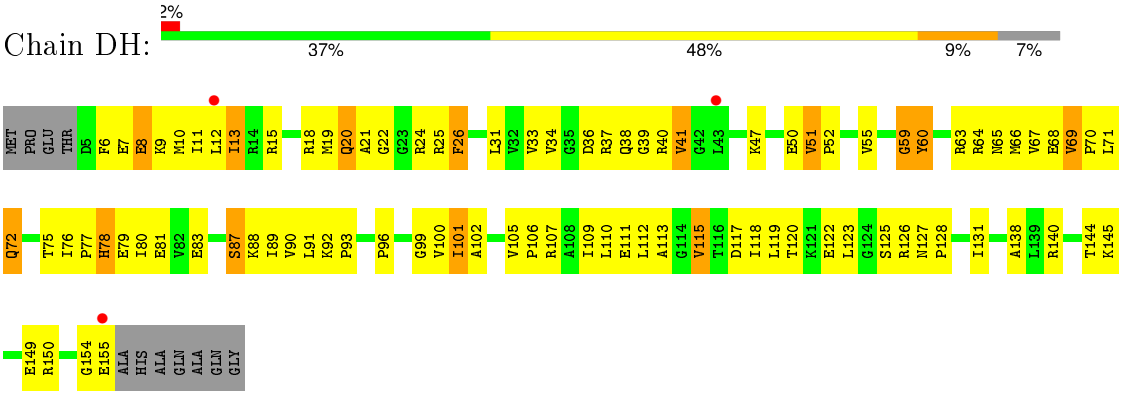
• Molecule 34: 30S RIBOSOMAL PROTEIN S4



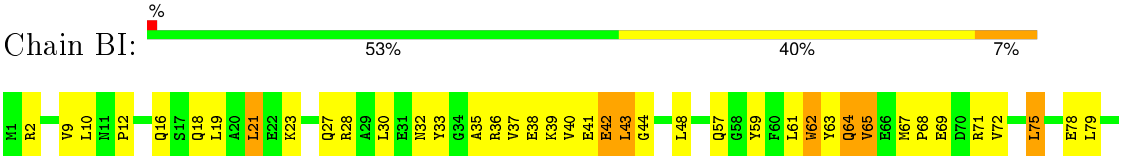
• Molecule 35: 30S RIBOSOMAL PROTEIN S5

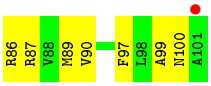


• Molecule 35: 30S RIBOSOMAL PROTEIN S5



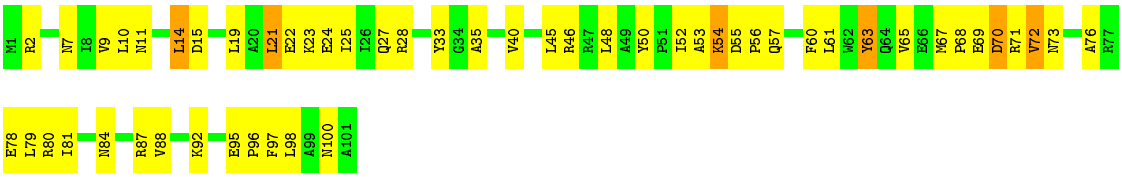
• Molecule 36: 30S RIBOSOMAL PROTEIN S6





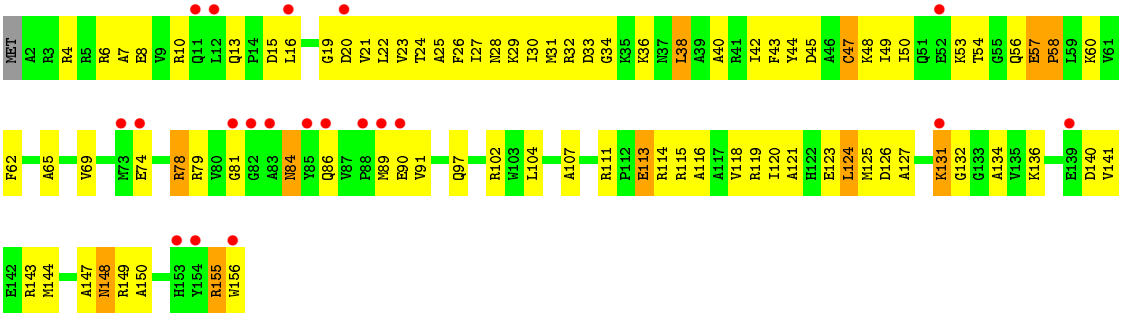
• Molecule 36: 30S RIBOSOMAL PROTEIN S6

Chain DI:



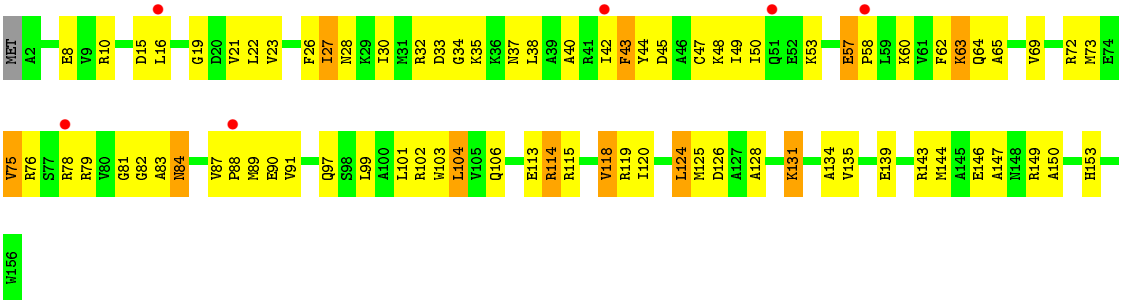
• Molecule 37: 30S RIBOSOMAL PROTEIN S7

Chain BJ:



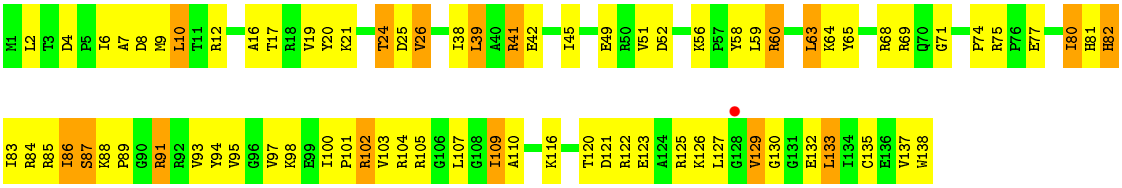
• Molecule 37: 30S RIBOSOMAL PROTEIN S7

Chain DJ:



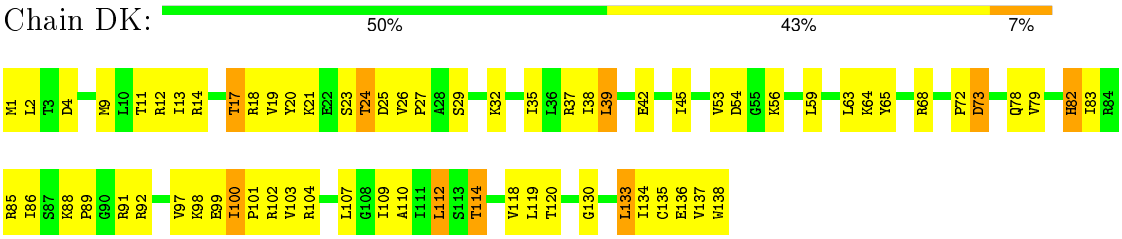
• Molecule 38: 30S RIBOSOMAL PROTEIN S8

Chain BK:



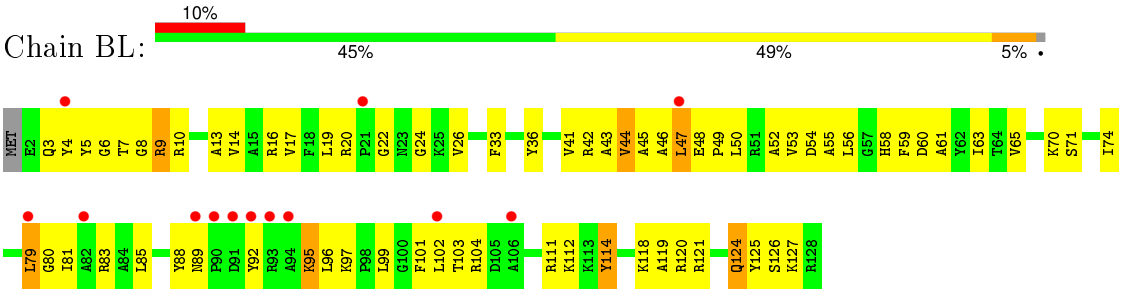
• Molecule 38: 30S RIBOSOMAL PROTEIN S8

Chain DK:



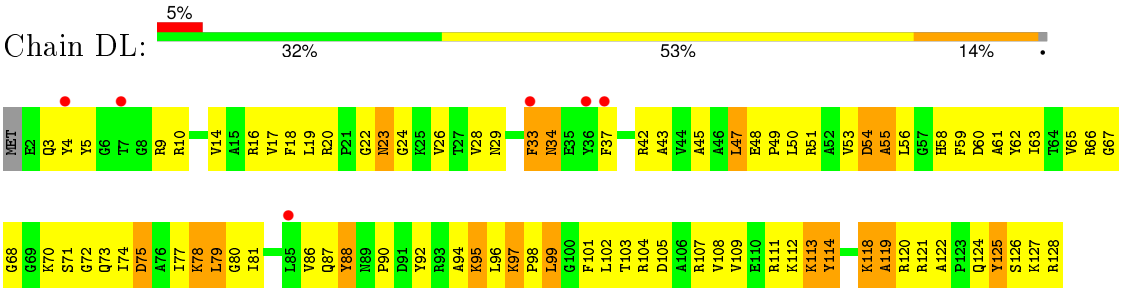
• Molecule 39: 30S RIBOSOMAL PROTEIN S9

Chain BL:



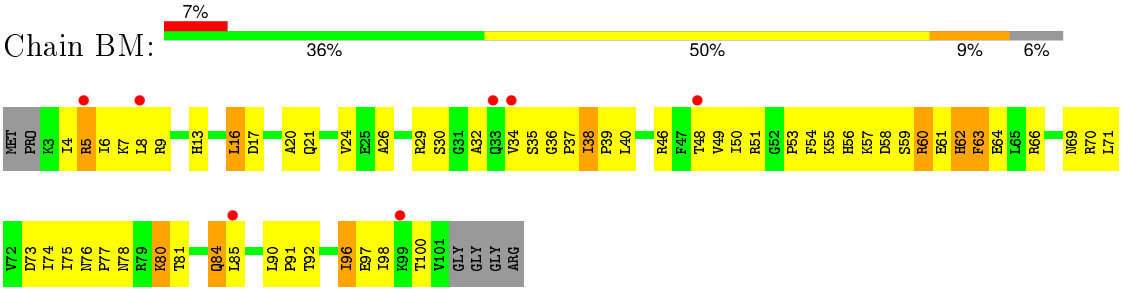
• Molecule 39: 30S RIBOSOMAL PROTEIN S9

Chain DL:



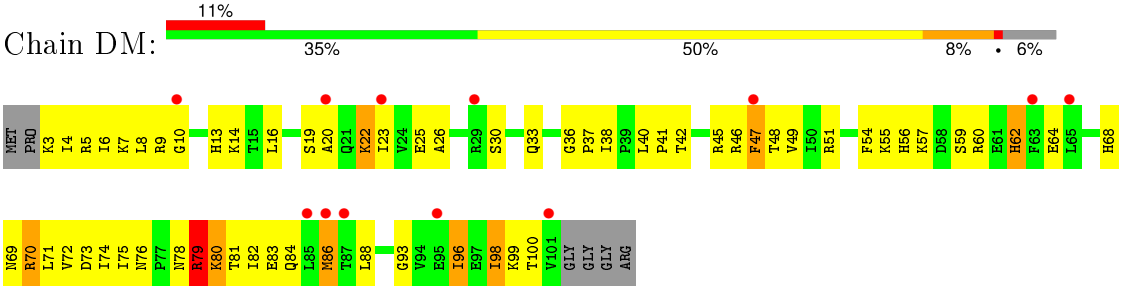
• Molecule 40: 30S RIBOSOMAL PROTEIN S10

Chain BM:



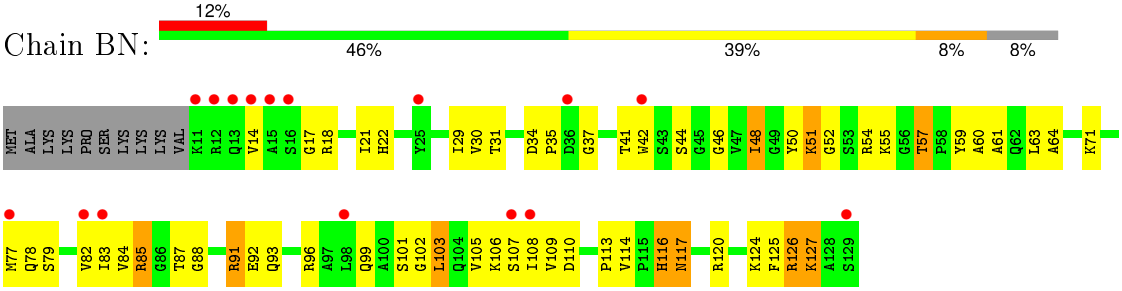
• Molecule 40: 30S RIBOSOMAL PROTEIN S10

Chain DM:



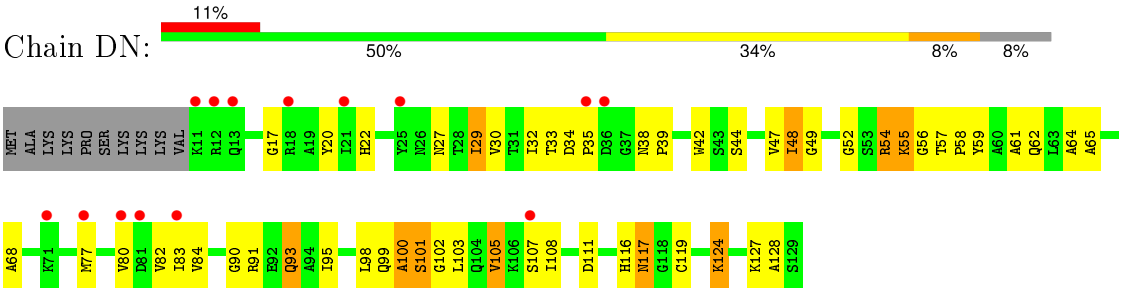
• Molecule 41: 30S RIBOSOMAL PROTEIN S11

Chain BN:



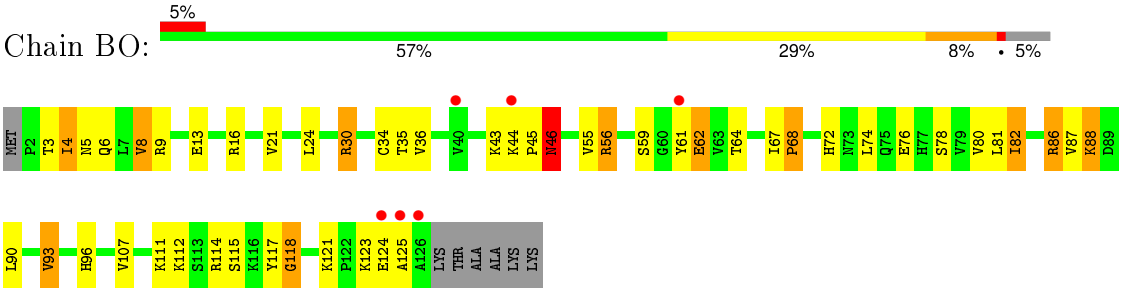
- Molecule 41: 30S RIBOSOMAL PROTEIN S11

Chain DN:



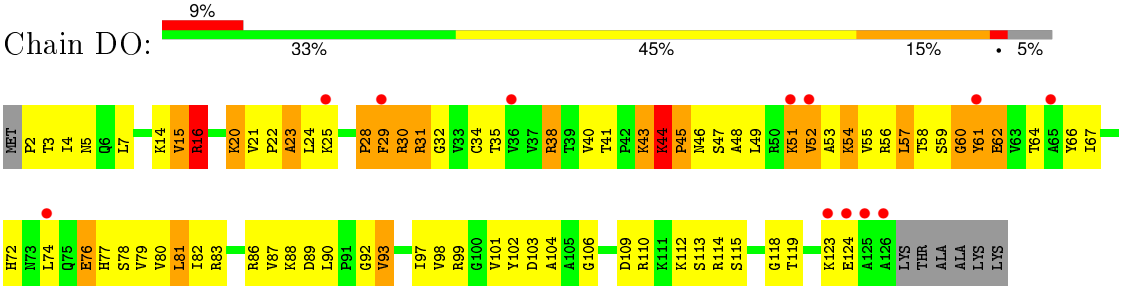
- Molecule 42: 30S RIBOSOMAL PROTEIN S12

Chain BO:



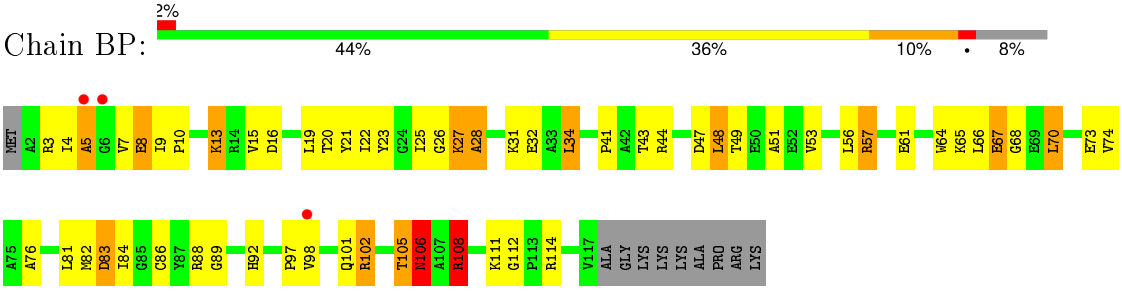
- Molecule 42: 30S RIBOSOMAL PROTEIN S12

Chain DO:



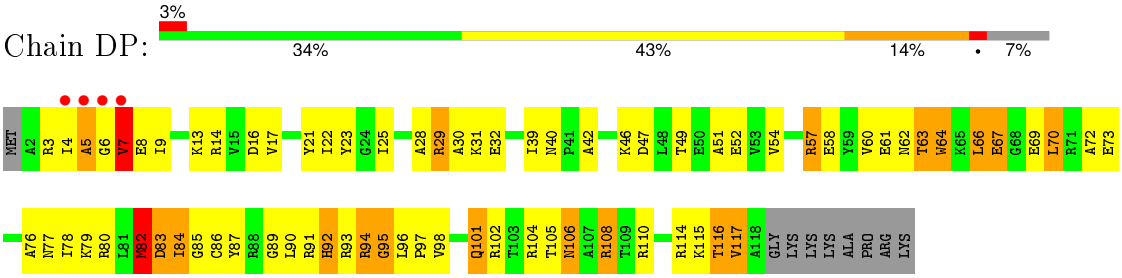
- Molecule 43: 30S RIBOSOMAL PROTEIN S13

Chain BP:



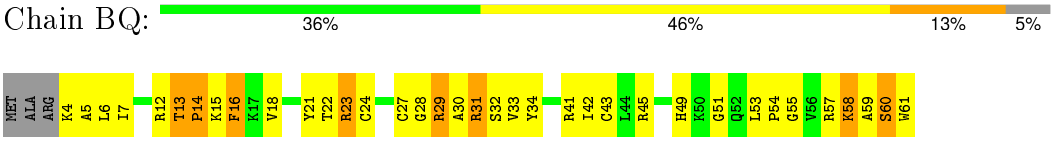
- Molecule 43: 30S RIBOSOMAL PROTEIN S13

Chain DP:



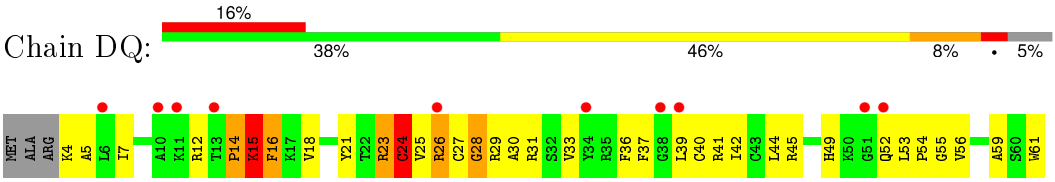
- Molecule 44: 30S RIBOSOMAL PROTEIN S14

Chain BQ:



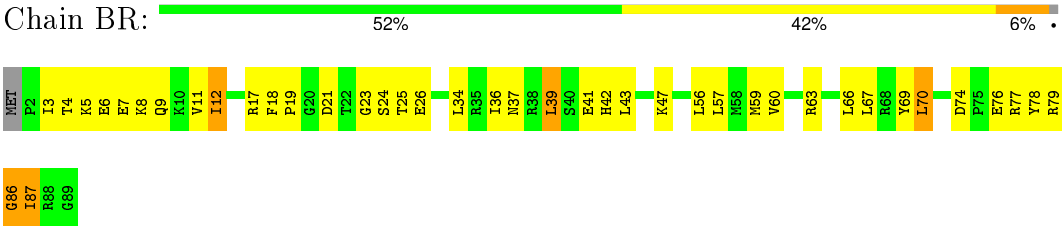
- Molecule 44: 30S RIBOSOMAL PROTEIN S14

Chain DQ:



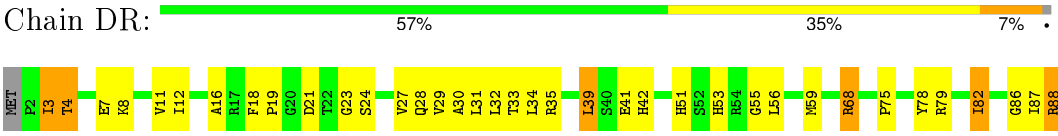
- Molecule 45: 30S RIBOSOMAL PROTEIN S15

Chain BR:



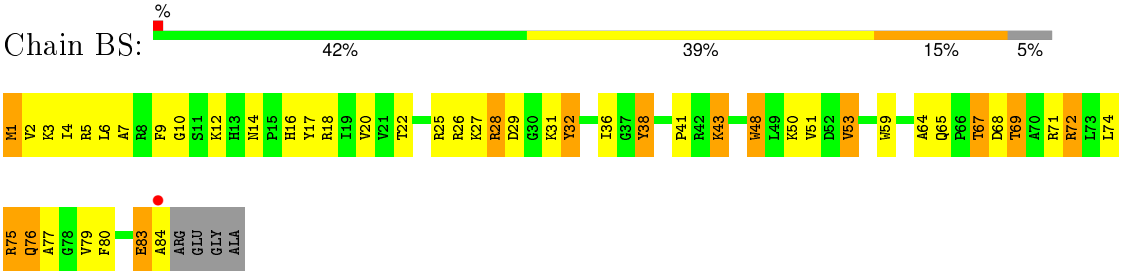
- Molecule 45: 30S RIBOSOMAL PROTEIN S15

Chain DR:



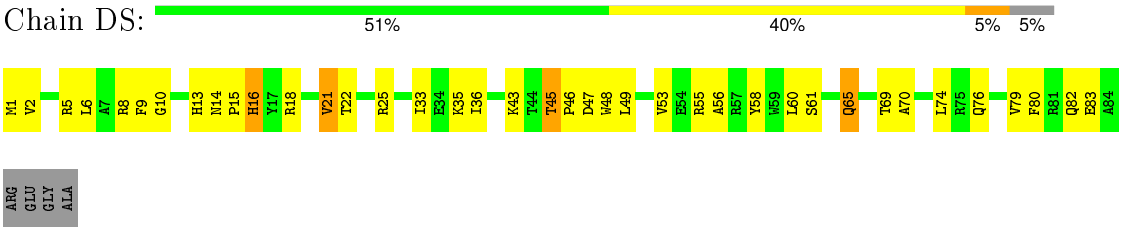
- Molecule 46: 30S RIBOSOMAL PROTEIN S16

Chain BS:



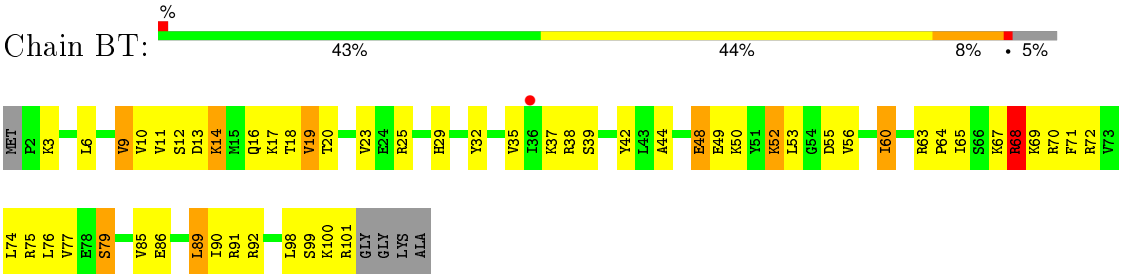
- Molecule 46: 30S RIBOSOMAL PROTEIN S16

Chain DS:



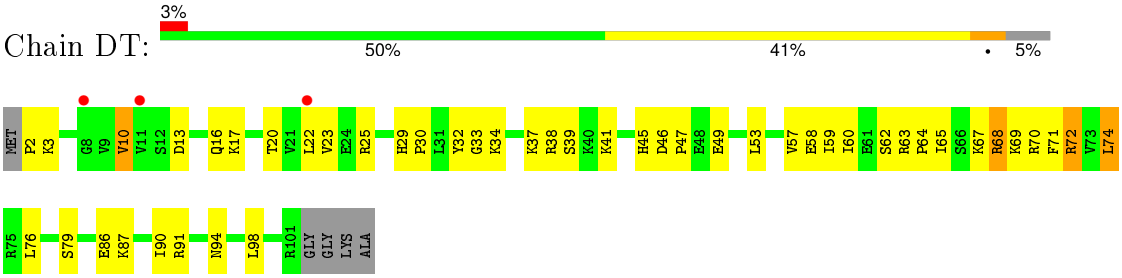
• Molecule 47: 30S RIBOSOMAL PROTEIN S17

Chain BT:



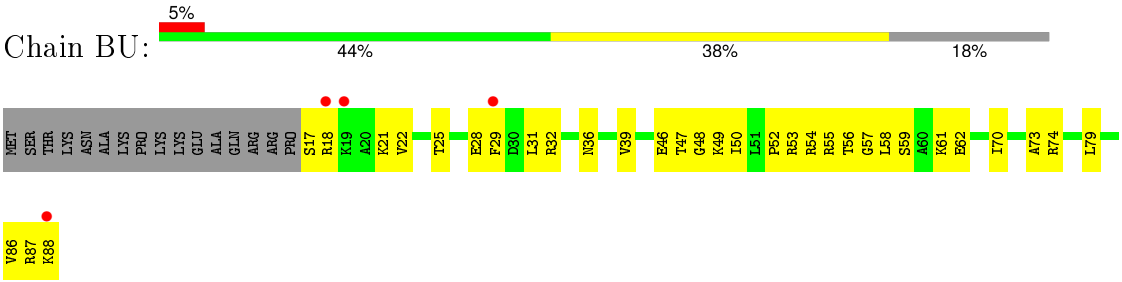
• Molecule 47: 30S RIBOSOMAL PROTEIN S17

Chain DT:



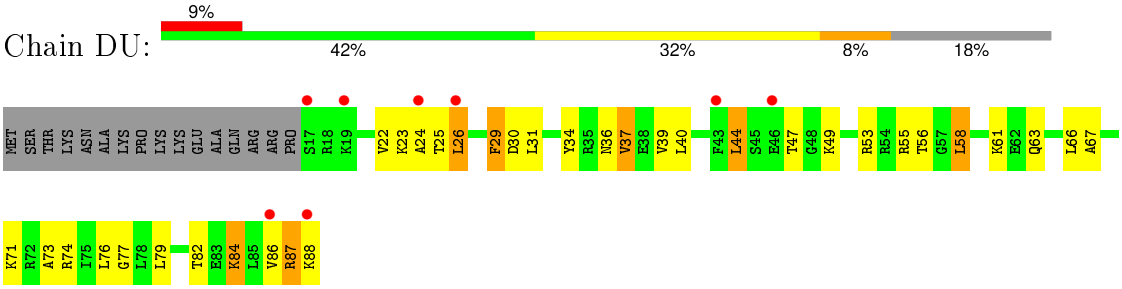
• Molecule 48: 30S RIBOSOMAL PROTEIN S18

Chain BU:



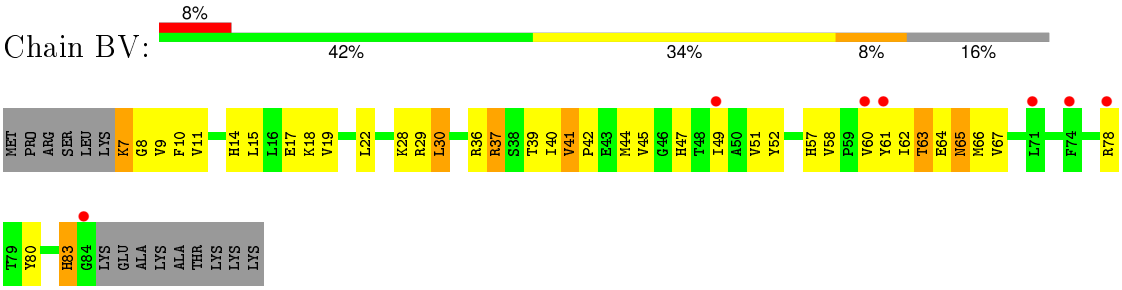
• Molecule 48: 30S RIBOSOMAL PROTEIN S18

Chain DU:



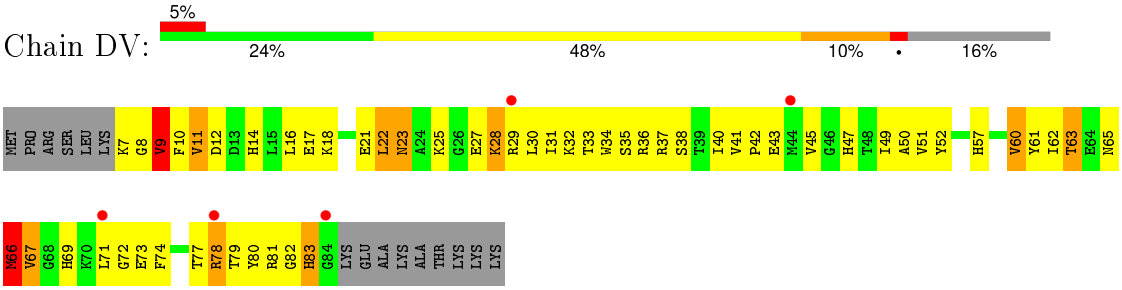
• Molecule 49: 30S RIBOSOMAL PROTEIN S19

Chain BV:



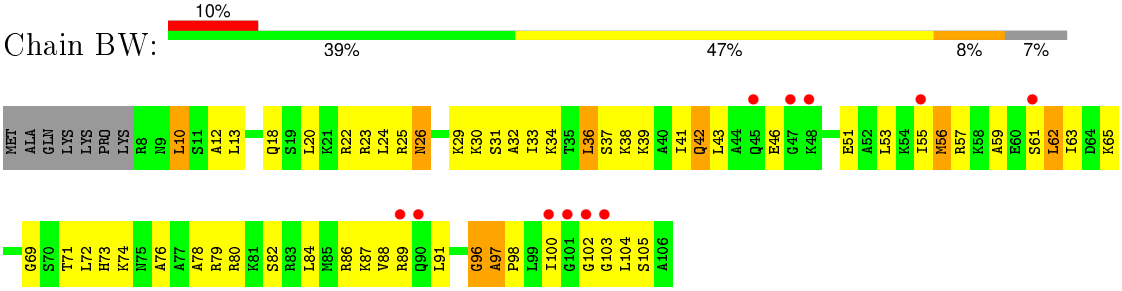
• Molecule 49: 30S RIBOSOMAL PROTEIN S19

Chain DV:



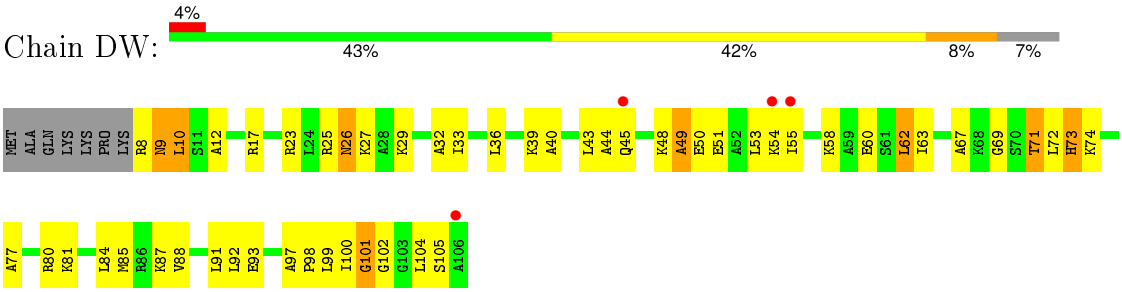
• Molecule 50: 30S RIBOSOMAL PROTEIN S20

Chain BW:



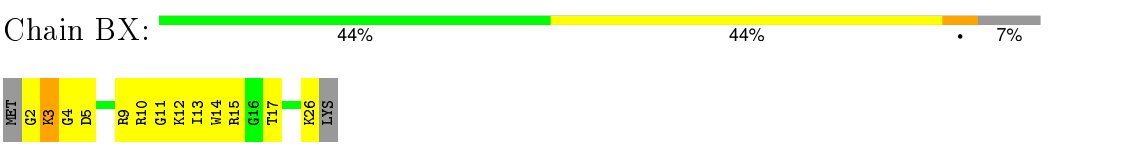
• Molecule 50: 30S RIBOSOMAL PROTEIN S20

Chain DW:



• Molecule 51: 30S RIBOSOMAL PROTEIN THX

Chain BX:

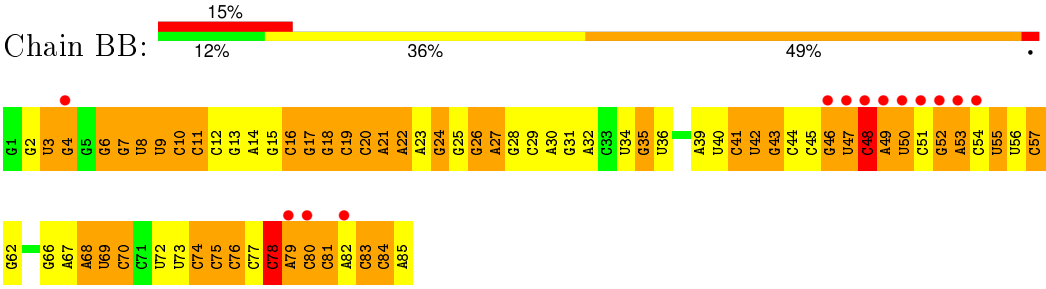


• Molecule 51: 30S RIBOSOMAL PROTEIN THX

Chain DX:

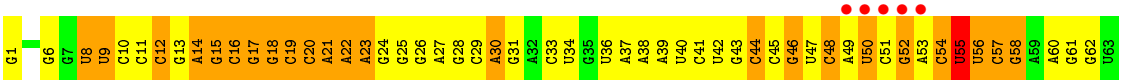
• Molecule 52: TRNA-TYR

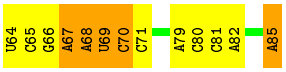
Chain BB:



• Molecule 52: TRNA-TYR

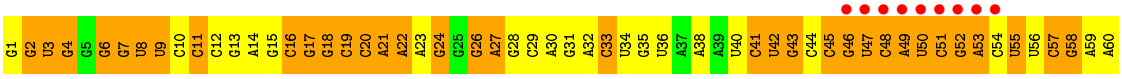
Chain BD:

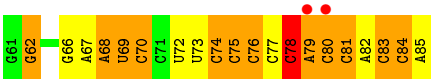




• Molecule 52: TRNA-TYR

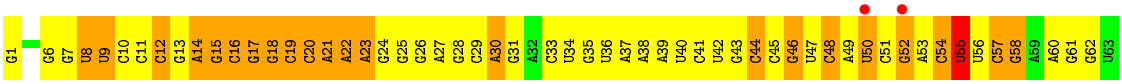
Chain DB:

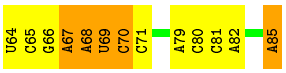




• Molecule 52: TRNA-TYR

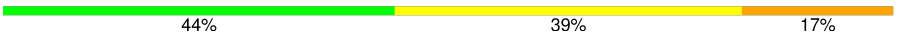
Chain DD:





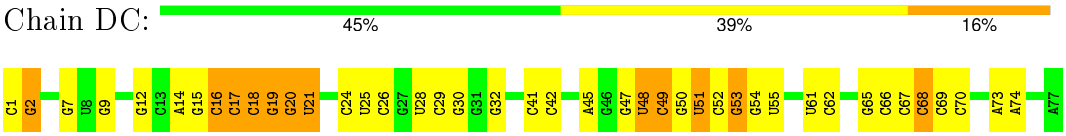
• Molecule 53: TRNA-FMET

Chain BC:



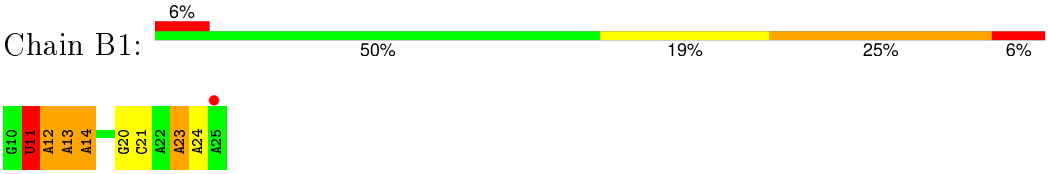
• Molecule 53: TRNA-FMET

Chain DC:



- Molecule 54: MRNA

Chain B1:



- Molecule 54: MRNA

Chain D1:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.25Å 450.87Å 622.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	256.19 – 3.30 256.19 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (256.19-3.30) 92.8 (256.19-3.20)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_810)	Depositor
R, R_{free}	0.206 , 0.259 0.205 , 0.255	Depositor DCC
R_{free} test set	1826 reflections (0.22%)	DCC
Wilson B-factor (Å^2)	90.6	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 91.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 962434 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	303952	wwPDB-VP
Average B, all atoms (Å^2)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MIA, ZN, OHX, 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	0.34	0/70233	0.73	38/109643 (0.0%)
1	CA	0.30	1/70122 (0.0%)	0.70	35/109469 (0.0%)
2	AB	0.32	0/2928	0.79	11/4568 (0.2%)
2	CB	0.27	0/2928	0.70	1/4568 (0.0%)
3	AD	0.30	0/2165	0.56	0/2919
3	CD	0.28	0/2165	0.50	0/2919
4	AE	0.27	0/1601	0.53	0/2160
4	CE	0.26	0/1601	0.51	0/2160
5	AF	0.27	0/1620	0.49	0/2194
5	CF	0.25	0/1662	0.54	0/2249
6	AG	0.23	0/1499	0.45	0/2016
6	CG	0.21	0/1499	0.42	0/2016
7	AH	0.27	0/1332	0.51	0/1802
7	CH	0.23	0/1332	0.47	0/1802
8	AK	0.24	0/1151	0.50	0/1558
8	CK	0.22	0/1151	0.50	0/1558
9	AM	0.26	0/1131	0.48	0/1525
9	CM	0.23	0/1131	0.45	0/1525
10	AN	0.26	0/943	0.47	0/1269
10	CN	0.25	0/943	0.45	0/1269
11	AO	0.27	0/1162	0.60	1/1544 (0.1%)
11	CO	0.24	0/1162	0.47	0/1544
12	AP	0.27	0/1143	0.45	0/1527
12	CP	0.23	0/1143	0.43	0/1527
13	A0	0.25	0/982	0.48	0/1312
13	C0	0.24	0/974	0.44	0/1302
14	AQ	0.25	0/892	0.47	0/1187
14	CQ	0.24	0/892	0.47	0/1187
15	AR	0.27	0/1155	0.50	0/1542
15	CR	0.24	0/1155	0.44	0/1542
16	A1	0.27	0/982	0.50	0/1306
16	C1	0.24	0/982	0.41	0/1306

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

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

All (1) bond length outliers are listed below:

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

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

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

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

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

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

The worst 5 of 14995 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:2320:G:C8	1:CA:2324:A:C2	1.85	1.64
1:CA:216:G:N2	1:CA:218:A:H61	1.09	1.47
1:AA:2308:G:N1	1:AA:2311:A:N1	1.63	1.43
1:CA:216:G:H21	1:CA:218:A:N6	0.92	1.42
1:AA:2308:G:N2	1:AA:2311:A:H2	1.02	1.42

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BA:85:U:O2'	7:CH:100:GLY:O[3_555]	1.93	0.27

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	AD	270/276 (98%)	218 (81%)	35 (13%)	17 (6%)	2 13
3	CD	270/276 (98%)	218 (81%)	40 (15%)	12 (4%)	3 22
4	AE	203/206 (98%)	141 (70%)	39 (19%)	23 (11%)	0 3
4	CE	203/206 (98%)	131 (64%)	46 (23%)	26 (13%)	0 2
5	AF	200/210 (95%)	168 (84%)	23 (12%)	9 (4%)	3 21
5	CF	206/210 (98%)	144 (70%)	35 (17%)	27 (13%)	0 2
6	AG	179/182 (98%)	147 (82%)	25 (14%)	7 (4%)	4 25
6	CG	179/182 (98%)	144 (80%)	27 (15%)	8 (4%)	3 21
7	AH	168/180 (93%)	123 (73%)	20 (12%)	25 (15%)	0 1
7	CH	168/180 (93%)	111 (66%)	41 (24%)	16 (10%)	1 6
8	AK	144/148 (97%)	99 (69%)	31 (22%)	14 (10%)	1 5
8	CK	144/148 (97%)	104 (72%)	32 (22%)	8 (6%)	2 16
9	AM	136/140 (97%)	108 (79%)	17 (12%)	11 (8%)	1 8
9	CM	136/140 (97%)	106 (78%)	23 (17%)	7 (5%)	2 19
10	AN	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	11 47
10	CN	120/122 (98%)	107 (89%)	9 (8%)	4 (3%)	5 30
11	AO	148/150 (99%)	93 (63%)	35 (24%)	20 (14%)	0 2
11	CO	148/150 (99%)	91 (62%)	32 (22%)	25 (17%)	0 1
12	AP	139/141 (99%)	101 (73%)	21 (15%)	17 (12%)	0 2
12	CP	139/141 (99%)	95 (68%)	24 (17%)	20 (14%)	0 1
13	A0	116/118 (98%)	96 (83%)	15 (13%)	5 (4%)	3 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	C0	115/118 (98%)	97 (84%)	12 (10%)	6 (5%)	2 18
14	AQ	109/112 (97%)	86 (79%)	14 (13%)	9 (8%)	1 8
14	CQ	109/112 (97%)	72 (66%)	24 (22%)	13 (12%)	0 3
15	AR	135/146 (92%)	107 (79%)	22 (16%)	6 (4%)	3 22
15	CR	135/146 (92%)	112 (83%)	15 (11%)	8 (6%)	2 15
16	A1	115/118 (98%)	96 (84%)	13 (11%)	6 (5%)	2 18
16	C1	115/118 (98%)	89 (77%)	16 (14%)	10 (9%)	1 7
17	A2	99/101 (98%)	85 (86%)	9 (9%)	5 (5%)	2 19
17	C2	99/101 (98%)	73 (74%)	14 (14%)	12 (12%)	0 3
18	AS	111/113 (98%)	97 (87%)	13 (12%)	1 (1%)	21 60
18	CS	111/113 (98%)	99 (89%)	9 (8%)	3 (3%)	6 35
19	AT	90/96 (94%)	84 (93%)	5 (6%)	1 (1%)	17 57
19	CT	90/96 (94%)	73 (81%)	14 (16%)	3 (3%)	5 30
20	AU	100/110 (91%)	76 (76%)	13 (13%)	11 (11%)	0 4
20	CU	100/110 (91%)	62 (62%)	27 (27%)	11 (11%)	0 4
21	AV	173/206 (84%)	113 (65%)	40 (23%)	20 (12%)	0 3
21	CV	177/206 (86%)	112 (63%)	40 (23%)	25 (14%)	0 1
22	A3	74/85 (87%)	62 (84%)	7 (10%)	5 (7%)	1 12
22	C3	75/85 (88%)	59 (79%)	13 (17%)	3 (4%)	4 24
23	AZ	95/98 (97%)	76 (80%)	13 (14%)	6 (6%)	2 13
23	CZ	95/98 (97%)	76 (80%)	9 (10%)	10 (10%)	1 4
24	AW	64/72 (89%)	57 (89%)	4 (6%)	3 (5%)	3 20
24	CW	64/72 (89%)	52 (81%)	7 (11%)	5 (8%)	1 9
25	AX	57/60 (95%)	52 (91%)	5 (9%)	0	100 100
25	CX	57/60 (95%)	52 (91%)	5 (9%)	0	100 100
26	A4	64/71 (90%)	39 (61%)	13 (20%)	12 (19%)	0 1
26	C4	61/71 (86%)	23 (38%)	20 (33%)	18 (30%)	0 0
27	A5	57/60 (95%)	42 (74%)	9 (16%)	6 (10%)	1 4
27	C5	57/60 (95%)	47 (82%)	8 (14%)	2 (4%)	4 29
28	A6	43/54 (80%)	23 (54%)	13 (30%)	7 (16%)	0 1
28	C6	43/54 (80%)	23 (54%)	11 (26%)	9 (21%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
29	A7	43/49 (88%)	41 (95%)	2 (5%)	0	100 100
29	C7	43/49 (88%)	40 (93%)	3 (7%)	0	100 100
30	A8	58/65 (89%)	47 (81%)	8 (14%)	3 (5%)	2 18
30	C8	58/65 (89%)	41 (71%)	6 (10%)	11 (19%)	0 1
32	BE	235/256 (92%)	181 (77%)	38 (16%)	16 (7%)	1 12
32	DE	235/256 (92%)	177 (75%)	40 (17%)	18 (8%)	1 9
33	BF	203/239 (85%)	161 (79%)	36 (18%)	6 (3%)	5 33
33	DF	204/239 (85%)	163 (80%)	35 (17%)	6 (3%)	6 34
34	BG	206/208 (99%)	179 (87%)	19 (9%)	8 (4%)	4 25
34	DG	206/208 (99%)	159 (77%)	35 (17%)	12 (6%)	2 15
35	BH	149/162 (92%)	127 (85%)	16 (11%)	6 (4%)	4 24
35	DH	149/162 (92%)	132 (89%)	15 (10%)	2 (1%)	15 52
36	BI	99/101 (98%)	89 (90%)	7 (7%)	3 (3%)	5 33
36	DI	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	9 43
37	BJ	153/156 (98%)	128 (84%)	21 (14%)	4 (3%)	7 36
37	DJ	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	15 52
38	BK	136/138 (99%)	116 (85%)	16 (12%)	4 (3%)	6 34
38	DK	136/138 (99%)	116 (85%)	15 (11%)	5 (4%)	4 27
39	BL	125/128 (98%)	95 (76%)	25 (20%)	5 (4%)	4 24
39	DL	125/128 (98%)	97 (78%)	21 (17%)	7 (6%)	2 16
40	BM	97/105 (92%)	83 (86%)	13 (13%)	1 (1%)	19 58
40	DM	97/105 (92%)	82 (84%)	14 (14%)	1 (1%)	19 58
41	BN	117/129 (91%)	99 (85%)	12 (10%)	6 (5%)	2 19
41	DN	117/129 (91%)	103 (88%)	8 (7%)	6 (5%)	2 19
42	BO	123/132 (93%)	100 (81%)	17 (14%)	6 (5%)	3 19
42	DO	123/132 (93%)	94 (76%)	17 (14%)	12 (10%)	1 5
43	BP	114/126 (90%)	82 (72%)	22 (19%)	10 (9%)	1 7
43	DP	115/126 (91%)	85 (74%)	18 (16%)	12 (10%)	1 4
44	BQ	56/61 (92%)	40 (71%)	10 (18%)	6 (11%)	0 4
44	DQ	56/61 (92%)	41 (73%)	8 (14%)	7 (12%)	0 2
45	BR	86/89 (97%)	76 (88%)	8 (9%)	2 (2%)	8 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
45	DR	86/89 (97%)	77 (90%)	8 (9%)	1 (1%)	16 54
46	BS	82/88 (93%)	60 (73%)	20 (24%)	2 (2%)	7 38
46	DS	82/88 (93%)	70 (85%)	11 (13%)	1 (1%)	16 54
47	BT	98/105 (93%)	82 (84%)	13 (13%)	3 (3%)	5 32
47	DT	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	9 43
48	BU	70/88 (80%)	59 (84%)	10 (14%)	1 (1%)	14 50
48	DU	70/88 (80%)	57 (81%)	12 (17%)	1 (1%)	14 50
49	BV	76/93 (82%)	59 (78%)	14 (18%)	3 (4%)	4 25
49	DV	76/93 (82%)	55 (72%)	17 (22%)	4 (5%)	2 17
50	BW	97/106 (92%)	78 (80%)	16 (16%)	3 (3%)	5 32
50	DW	97/106 (92%)	82 (84%)	9 (9%)	6 (6%)	2 14
51	BX	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	3 23
51	DX	23/27 (85%)	21 (91%)	0	2 (9%)	1 7
All	All	11319/12052 (94%)	8877 (78%)	1684 (15%)	758 (7%)	1 12

5 of 758 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	AD	214/218 (98%)	172 (80%)	42 (20%)	1 7
3	CD	214/218 (98%)	187 (87%)	27 (13%)	5 24
4	AE	165/166 (99%)	137 (83%)	28 (17%)	2 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	CE	165/166 (99%)	125 (76%)	40 (24%)	1 3
5	AF	161/166 (97%)	137 (85%)	24 (15%)	4 17
5	CF	165/166 (99%)	137 (83%)	28 (17%)	2 12
6	AG	155/156 (99%)	136 (88%)	19 (12%)	6 25
6	CG	155/156 (99%)	139 (90%)	16 (10%)	9 34
7	AH	142/148 (96%)	112 (79%)	30 (21%)	1 6
7	CH	142/148 (96%)	123 (87%)	19 (13%)	5 21
8	AK	122/124 (98%)	98 (80%)	24 (20%)	1 7
8	CK	122/124 (98%)	104 (85%)	18 (15%)	4 17
9	AM	117/119 (98%)	98 (84%)	19 (16%)	3 14
9	CM	117/119 (98%)	95 (81%)	22 (19%)	2 8
10	AN	100/100 (100%)	92 (92%)	8 (8%)	15 49
10	CN	100/100 (100%)	88 (88%)	12 (12%)	6 27
11	AO	116/116 (100%)	84 (72%)	32 (28%)	0 2
11	CO	116/116 (100%)	84 (72%)	32 (28%)	0 2
12	AP	111/111 (100%)	91 (82%)	20 (18%)	2 10
12	CP	111/111 (100%)	88 (79%)	23 (21%)	1 6
13	A0	101/101 (100%)	83 (82%)	18 (18%)	2 10
13	C0	100/101 (99%)	84 (84%)	16 (16%)	3 14
14	AQ	87/88 (99%)	70 (80%)	17 (20%)	2 7
14	CQ	87/88 (99%)	72 (83%)	15 (17%)	2 12
15	AR	120/127 (94%)	103 (86%)	17 (14%)	4 19
15	CR	120/127 (94%)	105 (88%)	15 (12%)	6 24
16	A1	93/94 (99%)	79 (85%)	14 (15%)	3 16
16	C1	93/94 (99%)	80 (86%)	13 (14%)	4 20
17	A2	82/82 (100%)	69 (84%)	13 (16%)	3 14
17	C2	82/82 (100%)	62 (76%)	20 (24%)	1 3
18	AS	92/92 (100%)	73 (79%)	19 (21%)	1 6
18	CS	92/92 (100%)	80 (87%)	12 (13%)	5 22
19	AT	74/78 (95%)	65 (88%)	9 (12%)	6 26
19	CT	74/78 (95%)	64 (86%)	10 (14%)	5 21

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	DI	90/90 (100%)	80 (89%)	10 (11%)	8 31
37	BJ	126/127 (99%)	106 (84%)	20 (16%)	3 14
37	DJ	126/127 (99%)	109 (86%)	17 (14%)	5 21
38	BK	119/119 (100%)	99 (83%)	20 (17%)	2 13
38	DK	119/119 (100%)	105 (88%)	14 (12%)	6 27
39	BL	98/99 (99%)	85 (87%)	13 (13%)	5 21
39	DL	98/99 (99%)	82 (84%)	16 (16%)	3 14
40	BM	89/92 (97%)	76 (85%)	13 (15%)	4 18
40	DM	89/92 (97%)	80 (90%)	9 (10%)	9 35
41	BN	90/99 (91%)	78 (87%)	12 (13%)	5 21
41	DN	90/99 (91%)	83 (92%)	7 (8%)	16 50
42	BO	104/109 (95%)	92 (88%)	12 (12%)	7 29
42	DO	104/109 (95%)	85 (82%)	19 (18%)	2 9
43	BP	94/101 (93%)	80 (85%)	14 (15%)	4 17
43	DP	94/101 (93%)	82 (87%)	12 (13%)	5 23
44	BQ	48/50 (96%)	42 (88%)	6 (12%)	6 24
44	DQ	48/50 (96%)	44 (92%)	4 (8%)	14 47
45	BR	79/80 (99%)	74 (94%)	5 (6%)	22 60
45	DR	79/80 (99%)	72 (91%)	7 (9%)	12 43
46	BS	72/74 (97%)	60 (83%)	12 (17%)	3 13
46	DS	72/74 (97%)	66 (92%)	6 (8%)	14 47
47	BT	95/97 (98%)	84 (88%)	11 (12%)	7 29
47	DT	95/97 (98%)	88 (93%)	7 (7%)	17 52
48	BU	63/77 (82%)	61 (97%)	2 (3%)	46 79
48	DU	63/77 (82%)	54 (86%)	9 (14%)	4 19
49	BV	67/80 (84%)	55 (82%)	12 (18%)	2 10
49	DV	67/80 (84%)	55 (82%)	12 (18%)	2 10
50	BW	76/82 (93%)	68 (90%)	8 (10%)	8 33
50	DW	76/82 (93%)	68 (90%)	8 (10%)	8 33
51	BX	20/22 (91%)	19 (95%)	1 (5%)	30 68
51	DX	20/22 (91%)	19 (95%)	1 (5%)	30 68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9565/9996 (96%)	8122 (85%)	1443 (15%)	3 16

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

Mol	Chain	Res	Type
41	BN	93	GLN
4	CE	203	LYS
39	DL	79	LEU
43	BP	32	GLU
50	BW	10	LEU

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

Mol	Chain	Res	Type
42	BO	6	GLN
5	CF	169	ASN
41	DN	93	GLN
43	BP	101	GLN
50	BW	42	GLN

5.3.3 RNA

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

5 of 2136 RNA backbone outliers are listed below:

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

5 of 234 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	BB	78	C
1	CA	936	C
52	DB	6	G
52	BD	17	G
1	CA	126	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	BB	38	52	21,31,32	0.43	0	26,44,47	2.04	6 (23%)
52	MIA	BD	38	52	21,31,32	0.47	0	26,44,47	2.67	5 (19%)
52	MIA	DB	38	52	21,31,32	0.62	0	26,44,47	2.51	6 (23%)
52	MIA	DD	38	52	21,31,32	0.48	0	26,44,47	2.24	6 (23%)

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

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

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

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	BD	38	MIA	C12-N6-C6	-5.15	117.02	123.42
52	DD	38	MIA	C12-N6-C6	-4.55	117.76	123.42
52	BB	38	MIA	C12-N6-C6	-3.96	118.49	123.42
52	BB	38	MIA	C4-C5-N7	-3.46	106.29	109.48
52	DB	38	MIA	C4-C5-N7	-3.43	106.33	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
56	OHX	A1	202	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	A1	203	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	A3	102	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	A6	101	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3138	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3147	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3154	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3160	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3263	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3287	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3288	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3289	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3290	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3291	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3292	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3293	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3294	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3295	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3296	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3297	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3298	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3299	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3300	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3301	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3302	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3303	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3304	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3305	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3306	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3307	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3308	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3309	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3310	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3311	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3312	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3313	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3314	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3315	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3316	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3317	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3318	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3319	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3320	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
56	OHX	AA	3321	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3322	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3323	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3324	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3325	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3326	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3327	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3328	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3329	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3330	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3331	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3332	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3333	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3334	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3335	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3336	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3337	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3338	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3339	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3340	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3341	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3342	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3359	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3360	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3361	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3362	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3363	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3364	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3365	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3366	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3367	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3368	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3369	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3370	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3371	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3372	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3373	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3399	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3400	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3401	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3402	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3403	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3404	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	OHX	AA	3405	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3406	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3407	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3417	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3418	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3419	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3420	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3421	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3422	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3423	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3424	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3425	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3426	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3427	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3428	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3429	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3430	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3431	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3432	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3433	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3434	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3435	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3436	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3437	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3438	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3439	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3440	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3441	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3442	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3443	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3444	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3445	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3446	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3447	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3448	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3449	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3450	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3451	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3452	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3453	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3454	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3455	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3456	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
56	OHX	AA	3457	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3458	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3459	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3460	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3461	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3462	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3463	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3464	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3465	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3466	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3467	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3468	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3469	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3470	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3471	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3472	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3473	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3474	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3475	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3476	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3477	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3478	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3479	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3480	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3481	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3482	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3483	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3484	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3485	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3486	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3487	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3488	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3489	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3490	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3491	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3492	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3493	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3494	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3495	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3496	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3497	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3498	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3499	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	OHX	AA	3500	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3501	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3502	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3503	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3504	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3505	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3506	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3507	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3508	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3509	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3510	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3511	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3512	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3513	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3514	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3515	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3516	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3517	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3518	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3519	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3520	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3521	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3522	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3523	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3524	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3525	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3526	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3527	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3528	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3529	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3530	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3531	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3532	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3533	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3534	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3535	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3536	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3537	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3538	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3539	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3540	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3541	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3542	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
56	OHX	AA	3543	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3544	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3545	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3546	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3547	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3548	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3549	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3550	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3551	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3552	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3553	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3554	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3555	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3556	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3557	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3558	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3559	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3560	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3561	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3562	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3563	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3564	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3565	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3566	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3567	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3568	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3569	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	207	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	208	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	209	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	210	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	211	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	212	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	213	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	214	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	215	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	216	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	217	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	218	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	219	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AE	304	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AF	303	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AO	204	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
56	OHX	AO	205	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AW	101	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1656	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1657	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1659	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1661	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1662	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1663	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1664	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1665	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1666	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1667	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1668	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1669	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1670	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1671	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1672	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1673	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1674	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1675	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1676	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1677	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1678	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1679	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1680	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1681	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1682	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1683	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1684	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1685	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1686	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1687	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1688	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1689	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1690	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1691	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1692	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1693	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1694	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1695	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1696	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1755	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1756	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	OHX	BA	1757	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1758	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1759	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1760	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1761	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1762	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1763	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1764	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1765	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1766	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1767	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1768	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1769	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1770	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1771	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1772	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1773	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1774	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1775	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1776	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1777	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1778	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1779	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1780	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1781	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1782	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1783	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1784	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1785	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1786	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1787	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1788	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1789	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1790	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1791	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1792	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1793	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1794	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1795	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1796	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1797	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1798	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1799	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	OHX	BA	1800	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1801	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1802	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1803	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1804	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1805	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1806	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1807	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1808	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1809	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1810	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1811	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1812	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1813	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1814	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1815	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1816	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BB	106	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BB	107	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BC	106	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BC	107	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BD	102	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BD	103	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BD	104	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BG	302	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BR	101	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	C1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	C3	101	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	C5	102	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	C6	101	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3232	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3233	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3234	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3235	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3236	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3237	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3238	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3239	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3240	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3241	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3242	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3243	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3244	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	OHX	CA	3245	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3246	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3247	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3248	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3249	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3250	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3251	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3252	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3253	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3254	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3255	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3256	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3269	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3270	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3271	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3272	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3273	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3274	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3275	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3276	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3277	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3278	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3279	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3280	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3281	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3282	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3283	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3284	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3285	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3286	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3287	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3288	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3289	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3290	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3291	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3292	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3293	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3294	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3295	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3296	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3297	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3298	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3299	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	OHX	CA	3300	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3301	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3302	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3303	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3304	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3305	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3306	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3307	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3308	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3309	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3310	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3311	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3312	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3313	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3314	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3315	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3316	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3317	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3318	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3319	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3320	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3321	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3322	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3323	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3324	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3325	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3326	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3327	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3328	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3329	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3330	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3331	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3332	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3333	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3334	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3335	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3336	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3337	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3338	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3339	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3340	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3341	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3342	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
56	OHX	CA	3343	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3344	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3345	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3346	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3347	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3348	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3349	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3350	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3351	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3352	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3353	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3354	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3355	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3356	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3357	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3358	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3359	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3360	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3361	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3362	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3363	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3364	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3365	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3366	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3367	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3368	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3369	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3370	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3371	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3372	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3373	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3374	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3375	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3376	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3377	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3378	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3379	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3380	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3381	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3382	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3383	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3384	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3385	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	OHX	CA	3386	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3387	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3388	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3389	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3390	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3391	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3392	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3393	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3394	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3395	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3396	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3397	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3398	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3399	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3400	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3401	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3402	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3403	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3404	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3405	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3406	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3407	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3408	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3409	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3410	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3411	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3412	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3413	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3414	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3415	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3416	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3417	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3418	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3419	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3420	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3421	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3422	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3423	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3424	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3425	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3426	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3427	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3428	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
56	OHX	CA	3429	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3430	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3431	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3432	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3433	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3434	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3435	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3436	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3437	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3438	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3450	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3461	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3462	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3463	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3464	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3465	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3466	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3467	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3468	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3469	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3470	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3481	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3482	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3483	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3484	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3485	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3486	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3487	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3488	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3489	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3490	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3491	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3492	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	208	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	209	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	210	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	211	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	212	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	213	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	214	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	215	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	216	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	217	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	OHX	CB	218	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	219	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	220	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CF	301	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CO	201	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1718	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1719	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1721	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1722	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1723	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1724	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1726	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1727	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1728	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1729	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1730	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1731	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1732	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1733	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1734	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1735	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1736	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1737	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1738	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1739	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1740	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1741	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1742	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1743	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1744	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1745	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1746	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1747	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1748	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1749	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1750	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1751	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1752	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1753	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1754	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1755	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1756	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1757	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	OHX	DA	1758	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1759	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1760	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1761	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1762	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1763	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1764	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1765	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1766	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1767	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1768	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1769	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1770	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1771	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1772	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1773	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1774	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1775	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1776	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1777	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1778	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1779	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1780	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1781	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1782	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1783	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1784	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1785	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1786	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1787	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1788	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1789	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1790	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1791	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1792	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1793	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1794	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1795	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1796	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1797	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1798	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1799	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1800	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
56	OHX	DA	1801	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1802	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1803	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1804	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1805	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1806	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1807	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1808	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1809	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1810	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1811	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1812	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DB	103	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DB	104	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DB	105	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DC	107	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DC	108	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DC	109	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DC	110	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DD	101	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DG	302	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DK	201	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DR	101	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DV	101	-	0,6,6	0.00	-	0,15,15	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	A1	202	-	-	0/0/0/0	0/0/0/0
56	OHX	A1	203	-	-	0/0/0/0	0/0/0/0
56	OHX	A3	102	-	-	0/0/0/0	0/0/0/0
56	OHX	A6	101	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3138	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3147	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3154	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3160	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3263	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3287	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3288	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3289	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	AA	3290	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3291	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3292	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3293	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3294	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3295	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3296	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3297	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3298	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3299	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3300	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3301	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3302	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3303	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3304	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3305	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3306	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3307	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3308	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3309	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3310	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3311	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3312	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3313	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3314	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3315	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3316	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3317	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3318	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3319	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3320	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3321	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3322	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3323	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3324	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3325	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3326	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3327	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3328	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3329	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3330	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3331	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	AA	3332	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3333	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3334	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3335	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3336	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3337	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3338	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3339	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3340	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3341	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3342	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3359	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3360	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3361	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3362	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3363	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3364	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3365	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3366	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3367	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3368	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3369	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3370	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3371	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3372	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3373	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3399	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3400	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3401	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3402	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3403	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3404	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3405	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3406	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3407	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3417	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3418	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3419	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3420	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3421	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3422	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3423	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	AA	3424	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3425	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3426	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3427	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3428	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3429	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3430	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3431	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3432	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3433	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3434	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3435	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3436	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3437	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3438	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3439	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3440	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3441	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3442	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3443	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3444	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3445	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3446	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3447	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3448	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3449	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3450	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3451	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3452	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3453	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3454	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3455	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3456	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3457	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3458	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3459	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3460	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3461	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3462	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3463	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3464	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3465	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	AA	3466	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3467	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3468	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3469	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3470	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3471	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3472	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3473	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3474	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3475	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3476	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3477	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3478	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3479	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3480	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3481	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3482	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3483	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3484	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3485	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3486	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3487	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3488	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3489	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3490	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3491	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3492	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3493	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3494	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3495	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3496	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3497	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3498	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3499	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3500	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3501	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3502	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3503	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3504	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3505	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3506	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3507	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	AA	3508	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3509	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3510	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3511	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3512	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3513	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3514	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3515	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3516	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3517	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3518	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3519	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3520	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3521	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3522	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3523	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3524	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3525	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3526	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3527	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3528	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3529	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3530	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3531	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3532	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3533	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3534	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3535	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3536	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3537	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3538	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3539	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3540	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3541	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3542	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3543	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3544	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3545	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3546	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3547	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3548	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3549	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	AA	3550	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3551	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3552	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3553	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3554	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3555	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3556	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3557	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3558	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3559	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3560	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3561	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3562	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3563	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3564	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3565	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3566	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3567	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3568	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3569	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	207	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	208	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	209	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	210	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	211	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	212	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	213	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	214	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	215	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	216	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	217	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	218	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	219	-	-	0/0/0/0	0/0/0/0
56	OHX	AE	304	-	-	0/0/0/0	0/0/0/0
56	OHX	AF	303	-	-	0/0/0/0	0/0/0/0
56	OHX	AO	204	-	-	0/0/0/0	0/0/0/0
56	OHX	AO	205	-	-	0/0/0/0	0/0/0/0
56	OHX	AW	101	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1656	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1657	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1659	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1661	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	BA	1662	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1663	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1664	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1665	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1666	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1667	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1668	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1669	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1670	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1671	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1672	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1673	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1674	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1675	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1676	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1677	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1678	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1679	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1680	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1681	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1682	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1683	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1684	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1685	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1686	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1687	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1688	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1689	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1690	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1691	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1692	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1693	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1694	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1695	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1696	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1755	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1756	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1757	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1758	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1759	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1760	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1761	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	BA	1762	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1763	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1764	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1765	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1766	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1767	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1768	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1769	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1770	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1771	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1772	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1773	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1774	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1775	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1776	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1777	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1778	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1779	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1780	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1781	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1782	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1783	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1784	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1785	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1786	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1787	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1788	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1789	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1790	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1791	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1792	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1793	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1794	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1795	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1796	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1797	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1798	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1799	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1800	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1801	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1802	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1803	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	BA	1804	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1805	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1806	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1807	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1808	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1809	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1810	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1811	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1812	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1813	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1814	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1815	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1816	-	-	0/0/0/0	0/0/0/0
56	OHX	BB	106	-	-	0/0/0/0	0/0/0/0
56	OHX	BB	107	-	-	0/0/0/0	0/0/0/0
56	OHX	BC	106	-	-	0/0/0/0	0/0/0/0
56	OHX	BC	107	-	-	0/0/0/0	0/0/0/0
56	OHX	BD	102	-	-	0/0/0/0	0/0/0/0
56	OHX	BD	103	-	-	0/0/0/0	0/0/0/0
56	OHX	BD	104	-	-	0/0/0/0	0/0/0/0
56	OHX	BG	302	-	-	0/0/0/0	0/0/0/0
56	OHX	BR	101	-	-	0/0/0/0	0/0/0/0
56	OHX	C1	201	-	-	0/0/0/0	0/0/0/0
56	OHX	C3	101	-	-	0/0/0/0	0/0/0/0
56	OHX	C5	102	-	-	0/0/0/0	0/0/0/0
56	OHX	C6	101	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3232	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3233	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3234	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3235	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3236	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3237	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3238	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3239	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3240	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3241	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3242	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3243	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3244	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3245	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3246	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3247	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	CA	3248	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3249	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3250	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3251	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3252	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3253	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3254	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3255	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3256	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3269	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3270	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3271	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3272	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3273	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3274	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3275	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3276	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3277	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3278	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3279	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3280	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3281	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3282	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3283	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3284	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3285	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3286	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3287	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3288	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3289	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3290	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3291	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3292	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3293	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3294	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3295	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3296	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3297	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3298	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3299	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3300	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3301	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	CA	3302	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3303	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3304	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3305	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3306	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3307	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3308	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3309	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3310	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3311	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3312	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3313	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3314	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3315	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3316	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3317	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3318	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3319	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3320	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3321	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3322	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3323	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3324	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3325	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3326	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3327	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3328	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3329	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3330	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3331	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3332	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3333	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3334	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3335	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3336	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3337	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3338	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3339	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3340	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3341	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3342	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3343	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	CA	3344	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3345	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3346	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3347	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3348	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3349	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3350	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3351	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3352	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3353	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3354	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3355	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3356	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3357	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3358	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3359	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3360	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3361	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3362	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3363	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3364	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3365	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3366	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3367	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3368	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3369	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3370	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3371	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3372	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3373	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3374	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3375	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3376	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3377	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3378	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3379	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3380	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3381	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3382	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3383	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3384	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3385	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	CA	3386	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3387	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3388	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3389	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3390	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3391	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3392	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3393	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3394	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3395	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3396	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3397	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3398	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3399	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3400	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3401	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3402	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3403	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3404	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3405	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3406	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3407	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3408	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3409	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3410	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3411	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3412	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3413	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3414	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3415	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3416	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3417	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3418	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3419	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3420	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3421	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3422	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3423	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3424	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3425	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3426	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3427	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	CA	3428	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3429	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3430	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3431	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3432	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3433	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3434	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3435	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3436	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3437	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3438	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3450	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3461	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3462	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3463	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3464	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3465	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3466	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3467	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3468	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3469	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3470	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3481	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3482	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3483	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3484	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3485	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3486	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3487	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3488	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3489	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3490	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3491	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3492	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	208	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	209	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	210	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	211	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	212	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	213	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	214	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	215	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	CB	216	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	217	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	218	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	219	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	220	-	-	0/0/0/0	0/0/0/0
56	OHX	CF	301	-	-	0/0/0/0	0/0/0/0
56	OHX	CO	201	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1718	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1719	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1721	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1722	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1723	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1724	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1726	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1727	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1728	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1729	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1730	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1731	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1732	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1733	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1734	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1735	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1736	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1737	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1738	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1739	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1740	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1741	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1742	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1743	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1744	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1745	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1746	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1747	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1748	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1749	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1750	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1751	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1752	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1753	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1754	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	DA	1755	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1756	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1757	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1758	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1759	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1760	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1761	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1762	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1763	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1764	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1765	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1766	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1767	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1768	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1769	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1770	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1771	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1772	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1773	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1774	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1775	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1776	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1777	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1778	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1779	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1780	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1781	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1782	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1783	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1784	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1785	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1786	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1787	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1788	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1789	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1790	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1791	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1792	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1793	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1794	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1795	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1796	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	DA	1797	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1798	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1799	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1800	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1801	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1802	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1803	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1804	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1805	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1806	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1807	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1808	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1809	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1810	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1811	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1812	-	-	0/0/0/0	0/0/0/0
56	OHX	DB	103	-	-	0/0/0/0	0/0/0/0
56	OHX	DB	104	-	-	0/0/0/0	0/0/0/0
56	OHX	DB	105	-	-	0/0/0/0	0/0/0/0
56	OHX	DC	107	-	-	0/0/0/0	0/0/0/0
56	OHX	DC	108	-	-	0/0/0/0	0/0/0/0
56	OHX	DC	109	-	-	0/0/0/0	0/0/0/0
56	OHX	DC	110	-	-	0/0/0/0	0/0/0/0
56	OHX	DD	101	-	-	0/0/0/0	0/0/0/0
56	OHX	DG	302	-	-	0/0/0/0	0/0/0/0
56	OHX	DK	201	-	-	0/0/0/0	0/0/0/0
56	OHX	DR	101	-	-	0/0/0/0	0/0/0/0
56	OHX	DV	101	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

233 monomers are involved in 316 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	A6	101	OHX	3	0
56	AA	3154	OHX	2	0
56	AA	3291	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	AA	3292	OHX	1	0
56	AA	3294	OHX	2	0
56	AA	3299	OHX	1	0
56	AA	3300	OHX	1	0
56	AA	3305	OHX	1	0
56	AA	3311	OHX	1	0
56	AA	3312	OHX	1	0
56	AA	3313	OHX	1	0
56	AA	3318	OHX	1	0
56	AA	3320	OHX	1	0
56	AA	3322	OHX	1	0
56	AA	3325	OHX	1	0
56	AA	3329	OHX	1	0
56	AA	3330	OHX	1	0
56	AA	3333	OHX	1	0
56	AA	3338	OHX	1	0
56	AA	3362	OHX	1	0
56	AA	3368	OHX	1	0
56	AA	3370	OHX	1	0
56	AA	3373	OHX	1	0
56	AA	3399	OHX	2	0
56	AA	3402	OHX	1	0
56	AA	3407	OHX	1	0
56	AA	3418	OHX	1	0
56	AA	3419	OHX	1	0
56	AA	3420	OHX	1	0
56	AA	3421	OHX	3	0
56	AA	3424	OHX	2	0
56	AA	3425	OHX	1	0
56	AA	3426	OHX	2	0
56	AA	3429	OHX	1	0
56	AA	3430	OHX	1	0
56	AA	3431	OHX	1	0
56	AA	3433	OHX	1	0
56	AA	3434	OHX	1	0
56	AA	3438	OHX	2	0
56	AA	3446	OHX	1	0
56	AA	3447	OHX	1	0
56	AA	3449	OHX	1	0
56	AA	3450	OHX	3	0
56	AA	3452	OHX	2	0
56	AA	3455	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	AA	3456	OHX	1	0
56	AA	3458	OHX	3	0
56	AA	3460	OHX	1	0
56	AA	3461	OHX	1	0
56	AA	3473	OHX	2	0
56	AA	3475	OHX	1	0
56	AA	3478	OHX	1	0
56	AA	3480	OHX	1	0
56	AA	3485	OHX	1	0
56	AA	3487	OHX	1	0
56	AA	3489	OHX	1	0
56	AA	3491	OHX	1	0
56	AA	3499	OHX	1	0
56	AA	3508	OHX	1	0
56	AA	3510	OHX	1	0
56	AA	3512	OHX	1	0
56	AA	3513	OHX	1	0
56	AA	3514	OHX	1	0
56	AA	3518	OHX	1	0
56	AA	3526	OHX	1	0
56	AA	3531	OHX	2	0
56	AA	3533	OHX	2	0
56	AA	3534	OHX	1	0
56	AA	3536	OHX	2	0
56	AA	3538	OHX	1	0
56	AA	3556	OHX	1	0
56	AA	3557	OHX	1	0
56	AA	3559	OHX	1	0
56	AA	3560	OHX	2	0
56	AA	3562	OHX	1	0
56	AA	3566	OHX	1	0
56	AA	3567	OHX	1	0
56	AA	3568	OHX	5	0
56	AB	212	OHX	1	0
56	AB	217	OHX	2	0
56	AB	219	OHX	1	0
56	AF	303	OHX	1	0
56	AO	205	OHX	1	0
56	BA	1661	OHX	1	0
56	BA	1666	OHX	3	0
56	BA	1670	OHX	1	0
56	BA	1671	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	BA	1672	OHX	1	0
56	BA	1673	OHX	5	0
56	BA	1675	OHX	1	0
56	BA	1678	OHX	1	0
56	BA	1683	OHX	1	0
56	BA	1684	OHX	7	0
56	BA	1688	OHX	1	0
56	BA	1693	OHX	1	0
56	BA	1695	OHX	1	0
56	BA	1755	OHX	1	0
56	BA	1756	OHX	1	0
56	BA	1760	OHX	2	0
56	BA	1762	OHX	1	0
56	BA	1768	OHX	1	0
56	BA	1772	OHX	1	0
56	BA	1774	OHX	1	0
56	BA	1775	OHX	2	0
56	BA	1778	OHX	1	0
56	BA	1782	OHX	1	0
56	BA	1783	OHX	1	0
56	BA	1786	OHX	1	0
56	BA	1795	OHX	2	0
56	BA	1797	OHX	2	0
56	BA	1798	OHX	1	0
56	BA	1800	OHX	1	0
56	BA	1804	OHX	2	0
56	BA	1805	OHX	1	0
56	BA	1812	OHX	2	0
56	BA	1813	OHX	1	0
56	BB	106	OHX	1	0
56	BC	106	OHX	2	0
56	BD	102	OHX	1	0
56	BG	302	OHX	2	0
56	C5	102	OHX	1	0
56	C6	101	OHX	4	0
56	CA	3232	OHX	1	0
56	CA	3233	OHX	1	0
56	CA	3234	OHX	3	0
56	CA	3236	OHX	1	0
56	CA	3240	OHX	1	0
56	CA	3244	OHX	1	0
56	CA	3247	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	CA	3269	OHX	1	0
56	CA	3270	OHX	2	0
56	CA	3272	OHX	1	0
56	CA	3274	OHX	1	0
56	CA	3275	OHX	1	0
56	CA	3276	OHX	1	0
56	CA	3278	OHX	2	0
56	CA	3279	OHX	2	0
56	CA	3281	OHX	1	0
56	CA	3283	OHX	1	0
56	CA	3293	OHX	1	0
56	CA	3296	OHX	1	0
56	CA	3300	OHX	2	0
56	CA	3304	OHX	1	0
56	CA	3305	OHX	1	0
56	CA	3310	OHX	1	0
56	CA	3316	OHX	1	0
56	CA	3320	OHX	1	0
56	CA	3321	OHX	1	0
56	CA	3324	OHX	1	0
56	CA	3326	OHX	1	0
56	CA	3327	OHX	1	0
56	CA	3331	OHX	1	0
56	CA	3332	OHX	3	0
56	CA	3333	OHX	1	0
56	CA	3350	OHX	1	0
56	CA	3351	OHX	1	0
56	CA	3354	OHX	1	0
56	CA	3362	OHX	1	0
56	CA	3363	OHX	1	0
56	CA	3365	OHX	1	0
56	CA	3375	OHX	1	0
56	CA	3376	OHX	1	0
56	CA	3377	OHX	2	0
56	CA	3383	OHX	1	0
56	CA	3384	OHX	1	0
56	CA	3396	OHX	1	0
56	CA	3399	OHX	1	0
56	CA	3403	OHX	1	0
56	CA	3411	OHX	1	0
56	CA	3415	OHX	1	0
56	CA	3416	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	CA	3418	OHX	1	0
56	CA	3425	OHX	1	0
56	CA	3428	OHX	1	0
56	CA	3432	OHX	1	0
56	CA	3435	OHX	1	0
56	CA	3462	OHX	1	0
56	CA	3468	OHX	1	0
56	CA	3481	OHX	1	0
56	CA	3484	OHX	1	0
56	CA	3486	OHX	2	0
56	CA	3487	OHX	1	0
56	CA	3490	OHX	1	0
56	CA	3492	OHX	1	0
56	CB	209	OHX	1	0
56	CB	211	OHX	1	0
56	CB	212	OHX	1	0
56	CB	217	OHX	1	0
56	DA	1718	OHX	1	0
56	DA	1719	OHX	1	0
56	DA	1721	OHX	2	0
56	DA	1724	OHX	1	0
56	DA	1727	OHX	1	0
56	DA	1730	OHX	1	0
56	DA	1731	OHX	4	0
56	DA	1733	OHX	1	0
56	DA	1734	OHX	3	0
56	DA	1737	OHX	1	0
56	DA	1740	OHX	1	0
56	DA	1742	OHX	1	0
56	DA	1745	OHX	1	0
56	DA	1748	OHX	1	0
56	DA	1749	OHX	1	0
56	DA	1751	OHX	1	0
56	DA	1752	OHX	1	0
56	DA	1754	OHX	1	0
56	DA	1755	OHX	1	0
56	DA	1756	OHX	1	0
56	DA	1759	OHX	1	0
56	DA	1760	OHX	7	0
56	DA	1762	OHX	1	0
56	DA	1764	OHX	2	0
56	DA	1767	OHX	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	DA	1768	OHX	1	0
56	DA	1770	OHX	2	0
56	DA	1775	OHX	1	0
56	DA	1779	OHX	1	0
56	DA	1783	OHX	2	0
56	DA	1787	OHX	2	0
56	DA	1792	OHX	1	0
56	DA	1795	OHX	1	0
56	DA	1800	OHX	1	0
56	DA	1808	OHX	1	0
56	DA	1812	OHX	1	0
56	DB	103	OHX	1	0
56	DC	107	OHX	6	0
56	DC	108	OHX	1	0
56	DC	109	OHX	1	0
56	DC	110	OHX	2	0
56	DD	101	OHX	1	0
56	DG	302	OHX	2	0
56	DK	201	OHX	1	0
56	DV	101	OHX	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.19	51 (1%) 71 65	45, 76, 209, 243	0
1	CA	2907/2912 (99%)	-0.37	44 (1%) 76 71	58, 92, 230, 245	0
2	AB	122/122 (100%)	-0.33	2 (1%) 74 69	73, 95, 116, 177	0
2	CB	122/122 (100%)	-0.58	1 (0%) 87 84	92, 127, 146, 198	0
3	AD	272/276 (98%)	0.01	2 (0%) 89 86	39, 66, 84, 105	0
3	CD	272/276 (98%)	0.19	5 (1%) 71 65	55, 78, 96, 128	0
4	AE	205/206 (99%)	0.78	32 (15%) 3 2	51, 86, 130, 142	0
4	CE	205/206 (99%)	0.55	21 (10%) 9 7	64, 100, 148, 165	0
5	AF	202/210 (96%)	0.11	7 (3%) 48 40	47, 81, 118, 130	0
5	CF	208/210 (99%)	0.44	19 (9%) 11 9	62, 106, 160, 184	0
6	AG	181/182 (99%)	0.67	17 (9%) 11 9	84, 107, 138, 149	0
6	CG	181/182 (99%)	0.71	23 (12%) 5 4	120, 141, 164, 171	0
7	AH	170/180 (94%)	0.36	7 (4%) 41 34	86, 112, 130, 157	0
7	CH	170/180 (94%)	3.43	118 (69%) 0 0	155, 198, 220, 229	0
8	AK	146/148 (98%)	0.60	18 (12%) 5 4	79, 131, 147, 150	0
8	CK	146/148 (98%)	0.64	19 (13%) 5 3	84, 130, 152, 158	0
9	AM	138/140 (98%)	0.51	9 (6%) 22 18	66, 87, 124, 136	0
9	CM	138/140 (98%)	1.20	32 (23%) 1 1	83, 114, 140, 156	0
10	AN	122/122 (100%)	0.24	2 (1%) 74 69	57, 78, 93, 101	0
10	CN	122/122 (100%)	0.35	4 (3%) 50 43	75, 95, 111, 124	0
11	AO	150/150 (100%)	0.03	6 (4%) 42 34	48, 88, 117, 160	0
11	CO	150/150 (100%)	1.20	40 (26%) 1 1	45, 108, 146, 178	0
12	AP	141/141 (100%)	0.43	8 (5%) 27 22	58, 83, 105, 127	0
12	CP	141/141 (100%)	0.69	19 (13%) 4 3	58, 109, 140, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	A0	118/118 (100%)	0.45	3 (2%) 61 54	61, 81, 103, 113	0
13	C0	117/118 (99%)	0.05	1 (0%) 85 82	69, 87, 106, 121	0
14	AQ	111/112 (99%)	0.39	5 (4%) 37 30	70, 92, 117, 131	0
14	CQ	111/112 (99%)	-0.13	3 (2%) 58 51	86, 123, 147, 162	0
15	AR	137/146 (93%)	0.83	14 (10%) 9 7	73, 93, 143, 170	0
15	CR	137/146 (93%)	0.30	11 (8%) 15 12	84, 104, 163, 183	0
16	A1	117/118 (99%)	0.10	2 (1%) 73 67	52, 75, 108, 139	0
16	C1	117/118 (99%)	0.85	20 (17%) 2 2	67, 106, 143, 162	0
17	A2	101/101 (100%)	0.99	17 (16%) 2 2	53, 98, 122, 141	0
17	C2	101/101 (100%)	1.64	34 (33%) 0 1	67, 129, 142, 151	0
18	AS	113/113 (100%)	0.49	5 (4%) 38 31	54, 73, 104, 156	0
18	CS	113/113 (100%)	0.05	2 (1%) 71 65	64, 80, 114, 158	0
19	AT	92/96 (95%)	0.18	4 (4%) 39 32	57, 71, 95, 107	0
19	CT	92/96 (95%)	0.22	3 (3%) 50 43	74, 88, 113, 127	0
20	AU	102/110 (92%)	0.86	17 (16%) 2 2	74, 101, 152, 162	0
20	CU	102/110 (92%)	0.68	16 (15%) 3 2	95, 118, 166, 181	0
21	AV	175/206 (84%)	1.73	53 (30%) 1 1	87, 126, 188, 191	0
21	CV	179/206 (86%)	1.84	71 (39%) 0 1	122, 160, 208, 216	0
22	A3	76/85 (89%)	0.06	1 (1%) 79 74	59, 77, 91, 132	0
22	C3	77/85 (90%)	-0.04	1 (1%) 79 74	83, 95, 117, 147	0
23	AZ	97/98 (98%)	0.21	7 (7%) 18 15	58, 78, 126, 156	0
23	CZ	97/98 (98%)	0.37	7 (7%) 18 15	68, 86, 132, 155	0
24	AW	66/72 (91%)	0.40	1 (1%) 76 71	63, 84, 98, 125	0
24	CW	66/72 (91%)	0.43	3 (4%) 37 30	84, 107, 130, 139	0
25	AX	59/60 (98%)	0.19	1 (1%) 73 67	63, 83, 112, 130	0
25	CX	59/60 (98%)	1.08	13 (22%) 1 1	80, 110, 141, 162	0
26	A4	66/71 (92%)	2.14	30 (45%) 0 0	120, 156, 173, 179	0
26	C4	63/71 (88%)	3.45	48 (76%) 0 0	146, 185, 194, 199	0
27	A5	59/60 (98%)	1.38	12 (20%) 1 1	49, 88, 168, 171	0
27	C5	59/60 (98%)	0.60	12 (20%) 1 1	65, 92, 173, 187	0
28	A6	45/54 (83%)	5.66	43 (95%) 0 0	124, 151, 168, 177	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	C6	45/54 (83%)	2.95	26 (57%) 0 0	141, 169, 183, 186	0
29	A7	45/49 (91%)	-0.28	1 (2%) 65 59	47, 55, 69, 78	0
29	C7	45/49 (91%)	-0.24	0 100 100	56, 66, 77, 100	0
30	A8	60/65 (92%)	0.28	1 (1%) 73 67	55, 73, 90, 114	0
30	C8	60/65 (92%)	0.55	2 (3%) 50 43	78, 90, 112, 137	0
31	BA	1502/1506 (99%)	-0.44	10 (0%) 89 86	58, 107, 187, 244	0
31	DA	1502/1506 (99%)	-0.55	12 (0%) 87 84	71, 119, 189, 244	0
32	BE	237/256 (92%)	0.68	20 (8%) 14 11	111, 144, 182, 193	0
32	DE	237/256 (92%)	0.68	33 (13%) 4 3	126, 161, 196, 211	0
33	BF	205/239 (85%)	0.61	17 (8%) 14 11	96, 119, 152, 160	0
33	DF	206/239 (86%)	1.21	50 (24%) 1 1	127, 147, 175, 180	0
34	BG	208/208 (100%)	-0.06	3 (1%) 78 73	92, 116, 136, 147	0
34	DG	208/208 (100%)	-0.02	5 (2%) 62 55	93, 111, 132, 145	0
35	BH	151/162 (93%)	0.22	5 (3%) 50 43	81, 105, 127, 161	0
35	DH	151/162 (93%)	0.01	3 (1%) 68 62	104, 121, 142, 165	0
36	BI	101/101 (100%)	-0.08	1 (0%) 84 80	81, 108, 122, 145	0
36	DI	101/101 (100%)	0.33	0 100 100	81, 106, 124, 149	0
37	BJ	155/156 (99%)	0.71	20 (12%) 5 3	106, 121, 149, 158	0
37	DJ	155/156 (99%)	0.41	6 (3%) 43 36	113, 131, 153, 164	0
38	BK	138/138 (100%)	-0.08	1 (0%) 89 86	89, 110, 123, 129	0
38	DK	138/138 (100%)	-0.06	0 100 100	104, 125, 136, 146	0
39	BL	127/128 (99%)	0.51	13 (10%) 9 7	87, 142, 160, 169	0
39	DL	127/128 (99%)	0.14	6 (4%) 35 29	117, 155, 168, 174	0
40	BM	99/105 (94%)	0.48	7 (7%) 19 15	91, 142, 170, 174	0
40	DM	99/105 (94%)	0.47	12 (12%) 6 4	124, 159, 175, 179	0
41	BN	119/129 (92%)	0.94	16 (13%) 4 3	72, 104, 133, 161	0
41	DN	119/129 (92%)	0.74	14 (11%) 6 5	91, 112, 139, 167	0
42	BO	125/132 (94%)	0.37	6 (4%) 34 28	69, 83, 112, 158	0
42	DO	125/132 (94%)	0.70	12 (9%) 10 9	93, 110, 134, 166	0
43	BP	116/126 (92%)	0.18	3 (2%) 59 53	92, 128, 145, 153	0
43	DP	117/126 (92%)	0.28	4 (3%) 49 42	106, 156, 169, 171	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	BQ	58/61 (95%)	-0.04	0 100 100	91, 108, 122, 129	0
44	DQ	58/61 (95%)	0.95	10 (17%) 2 2	126, 140, 157, 160	0
45	BR	88/89 (98%)	-0.29	0 100 100	80, 100, 121, 125	0
45	DR	88/89 (98%)	-0.08	0 100 100	85, 112, 133, 140	0
46	BS	84/88 (95%)	-0.12	1 (1%) 81 76	100, 118, 139, 175	0
46	DS	84/88 (95%)	-0.10	0 100 100	96, 107, 127, 158	0
47	BT	100/105 (95%)	-0.21	1 (1%) 84 80	93, 112, 125, 133	0
47	DT	100/105 (95%)	0.10	3 (3%) 54 47	94, 114, 135, 143	0
48	BU	72/88 (81%)	0.17	4 (5%) 28 22	88, 106, 139, 164	0
48	DU	72/88 (81%)	0.42	8 (11%) 7 6	97, 114, 155, 169	0
49	BV	78/93 (83%)	0.34	7 (8%) 12 9	109, 130, 147, 152	0
49	DV	78/93 (83%)	0.37	5 (6%) 23 19	145, 163, 182, 185	0
50	BW	99/106 (93%)	0.37	11 (11%) 7 6	105, 124, 155, 160	0
50	DW	99/106 (93%)	0.25	4 (4%) 42 34	95, 117, 153, 163	0
51	BX	25/27 (92%)	-0.57	0 100 100	102, 117, 137, 154	0
51	DX	25/27 (92%)	-0.43	0 100 100	122, 143, 158, 168	0
52	BB	84/85 (98%)	0.62	13 (15%) 3 2	82, 123, 154, 169	0
52	BD	84/85 (98%)	-0.19	5 (5%) 25 20	75, 137, 217, 227	0
52	DB	84/85 (98%)	0.62	11 (13%) 5 3	93, 128, 156, 171	0
52	DD	84/85 (98%)	-0.46	2 (2%) 62 55	84, 137, 217, 225	0
53	BC	77/77 (100%)	-0.34	0 100 100	77, 114, 139, 153	0
53	DC	77/77 (100%)	-0.74	0 100 100	88, 122, 150, 157	0
54	B1	16/16 (100%)	0.08	1 (6%) 23 19	76, 104, 156, 163	0
54	D1	16/16 (100%)	-0.44	0 100 100	85, 109, 157, 165	0
All	All	21100/21658 (97%)	0.15	1361 (6%) 22 18	39, 105, 182, 245	0

The worst 5 of 1361 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	CH	99	VAL	16.3
1	CA	690	A	15.4
1	CA	691	C	13.3
42	BO	126	ALA	13.2
1	CA	689	C	12.8

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
52	MIA	DB	38	29/30	0.90	0.21	-	84,93,111,126	0
52	MIA	BB	38	29/30	0.95	0.18	-	68,83,97,106	0
52	MIA	BD	38	29/30	0.85	0.26	-	116,135,182,198	0
52	MIA	DD	38	29/30	0.88	0.20	-	120,140,186,205	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
55	MG	CA	3138	1/1	0.99	0.45	43.09	53,53,53,53	0
55	MG	AA	3002	1/1	0.94	0.44	41.79	41,41,41,41	0
55	MG	AA	3177	1/1	0.96	0.44	41.43	37,37,37,37	0
55	MG	AA	3178	1/1	0.96	0.44	40.05	39,39,39,39	0
55	MG	CA	3147	1/1	0.94	0.35	36.53	51,51,51,51	0
55	MG	AA	3241	1/1	0.94	0.32	36.52	60,60,60,60	0
55	MG	AA	3158	1/1	0.97	0.42	32.61	50,50,50,50	0
55	MG	CA	3216	1/1	0.90	0.39	29.79	91,91,91,91	0
55	MG	AA	3384	1/1	0.95	0.42	28.99	59,59,59,59	0
55	MG	AA	3024	1/1	0.77	0.38	27.43	63,63,63,63	0
55	MG	AA	3050	1/1	0.90	0.32	27.38	60,60,60,60	0
55	MG	AA	3175	1/1	0.95	0.37	26.89	39,39,39,39	0
55	MG	CA	3139	1/1	0.97	0.29	26.69	56,56,56,56	0
55	MG	CA	3105	1/1	0.91	0.47	26.03	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	AA	3268	1/1	0.90	0.45	26.02	73,73,73,73	0
55	MG	AA	3121	1/1	0.82	0.42	26.01	53,53,53,53	0
55	MG	CA	3104	1/1	0.89	0.42	25.66	41,41,41,41	0
55	MG	AA	3355	1/1	0.98	0.48	24.97	36,36,36,36	0
55	MG	AA	3172	1/1	0.97	0.43	24.94	38,38,38,38	0
55	MG	BA	1645	1/1	0.88	0.38	24.44	51,51,51,51	0
55	MG	DA	1657	1/1	0.92	0.42	23.94	70,70,70,70	0
55	MG	BA	1620	1/1	0.93	0.44	23.78	70,70,70,70	0
55	MG	CA	3134	1/1	0.91	0.34	23.55	65,65,65,65	0
55	MG	BA	1611	1/1	0.80	0.35	23.44	84,84,84,84	0
55	MG	CA	3034	1/1	0.59	0.36	23.26	91,91,91,91	0
55	MG	AA	3109	1/1	0.87	0.47	22.89	47,47,47,47	0
55	MG	AA	3343	1/1	0.99	0.43	22.53	34,34,34,34	0
55	MG	DA	1674	1/1	0.81	0.30	22.40	99,99,99,99	0
55	MG	AA	3065	1/1	0.94	0.39	22.35	49,49,49,49	0
55	MG	BA	1699	1/1	0.55	0.43	22.32	79,79,79,79	0
55	MG	CA	3108	1/1	0.97	0.31	22.18	52,52,52,52	0
55	MG	BA	1602	1/1	0.84	0.43	21.96	75,75,75,75	0
55	MG	AA	3261	1/1	0.90	0.38	21.39	64,64,64,64	0
55	MG	AA	3231	1/1	0.82	0.48	21.37	66,66,66,66	0
55	MG	DA	1720	1/1	0.31	0.48	21.06	105,105,105,105	0
55	MG	AA	3142	1/1	0.98	0.56	20.86	45,45,45,45	0
55	MG	AA	3116	1/1	0.88	0.31	20.85	45,45,45,45	0
55	MG	DA	1676	1/1	0.87	0.41	20.75	83,83,83,83	0
55	MG	AA	3100	1/1	0.76	0.38	20.04	108,108,108,108	0
55	MG	AA	3379	1/1	0.87	0.43	19.54	55,55,55,55	0
55	MG	AA	3354	1/1	0.76	0.39	19.42	57,57,57,57	0
55	MG	CA	3145	1/1	0.96	0.43	19.41	74,74,74,74	0
55	MG	AA	3106	1/1	0.92	0.44	19.37	70,70,70,70	0
55	MG	AA	3345	1/1	0.98	0.41	19.04	47,47,47,47	0
55	MG	AA	3006	1/1	0.99	0.49	18.61	45,45,45,45	0
55	MG	DA	1675	1/1	0.81	0.37	17.91	92,92,92,92	0
55	MG	CA	3142	1/1	0.84	0.33	17.79	71,71,71,71	0
55	MG	CA	3214	1/1	0.86	0.28	17.77	65,65,65,65	0
55	MG	AA	3252	1/1	0.94	0.38	17.69	47,47,47,47	0
55	MG	CA	3181	1/1	0.95	0.33	17.37	62,62,62,62	0
55	MG	AA	3157	1/1	0.92	0.47	17.18	49,49,49,49	0
55	MG	AA	3387	1/1	0.97	0.35	17.07	42,42,42,42	0
55	MG	BA	1725	1/1	0.98	0.46	17.06	69,69,69,69	0
55	MG	AA	3081	1/1	0.92	0.39	16.87	56,56,56,56	0
55	MG	CA	3193	1/1	0.89	0.33	16.72	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	CA	3066	1/1	0.95	0.38	16.62	56,56,56,56	0
55	MG	AA	3096	1/1	0.94	0.32	16.55	71,71,71,71	0
55	MG	AA	3004	1/1	0.97	0.45	16.49	37,37,37,37	0
55	MG	CA	3264	1/1	0.91	0.36	16.43	49,49,49,49	0
55	MG	AA	3062	1/1	0.98	0.37	16.20	73,73,73,73	0
55	MG	AA	3151	1/1	0.93	0.35	16.16	62,62,62,62	0
55	MG	CA	3261	1/1	0.98	0.41	15.95	48,48,48,48	0
55	MG	AA	3275	1/1	0.81	0.42	15.85	64,64,64,64	0
55	MG	AA	3210	1/1	0.99	0.49	15.65	41,41,41,41	0
55	MG	AA	3040	1/1	0.98	0.46	15.36	47,47,47,47	0
55	MG	AA	3049	1/1	0.94	0.35	15.29	64,64,64,64	0
55	MG	AA	3016	1/1	0.97	0.36	14.97	39,39,39,39	0
55	MG	DA	1659	1/1	0.80	0.25	14.72	89,89,89,89	0
55	MG	AA	3143	1/1	0.98	0.43	14.68	46,46,46,46	0
55	MG	DA	1603	1/1	0.96	0.40	14.66	71,71,71,71	0
55	MG	AA	3197	1/1	0.99	0.35	14.64	50,50,50,50	0
55	MG	DA	1652	1/1	0.93	0.42	14.63	52,52,52,52	0
55	MG	CA	3099	1/1	0.92	0.34	14.51	51,51,51,51	0
55	MG	CA	3130	1/1	0.95	0.43	14.38	58,58,58,58	0
55	MG	CA	3068	1/1	0.98	0.35	14.06	44,44,44,44	0
55	MG	CA	3065	1/1	0.95	0.36	14.04	55,55,55,55	0
55	MG	BA	1754	1/1	0.93	0.38	13.68	61,61,61,61	0
55	MG	AA	3412	1/1	0.98	0.42	13.67	39,39,39,39	0
55	MG	CA	3449	1/1	0.99	0.46	13.60	54,54,54,54	0
55	MG	AA	3235	1/1	0.94	0.34	13.53	50,50,50,50	0
55	MG	CA	3018	1/1	0.97	0.33	13.52	55,55,55,55	0
55	MG	AA	3110	1/1	0.98	0.50	13.41	48,48,48,48	0
55	MG	CA	3084	1/1	0.91	0.38	13.40	60,60,60,60	0
55	MG	CA	3067	1/1	0.97	0.28	13.31	49,49,49,49	0
55	MG	CA	3160	1/1	0.93	0.39	13.30	49,49,49,49	0
55	MG	AA	3057	1/1	0.92	0.41	13.28	72,72,72,72	0
55	MG	AA	3189	1/1	0.98	0.39	13.03	42,42,42,42	0
55	MG	AA	3408	1/1	0.97	0.44	12.96	47,47,47,47	0
55	MG	AA	3118	1/1	0.94	0.29	12.88	53,53,53,53	0
55	MG	CA	3122	1/1	0.99	0.33	12.81	40,40,40,40	0
55	MG	DA	1619	1/1	0.91	0.37	12.79	98,98,98,98	0
55	MG	DC	101	1/1	0.97	0.31	12.73	85,85,85,85	0
55	MG	CA	3009	1/1	0.96	0.31	12.61	39,39,39,39	0
55	MG	AA	3212	1/1	0.97	0.41	12.49	35,35,35,35	0
55	MG	AA	3039	1/1	0.96	0.33	12.38	40,40,40,40	0
55	MG	CA	3109	1/1	0.93	0.29	12.37	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	BQ	101	1/1	0.86	0.54	12.32	96,96,96,96	0
55	MG	AA	3195	1/1	0.96	0.38	12.31	43,43,43,43	0
55	MG	AA	3126	1/1	0.94	0.34	12.20	85,85,85,85	0
55	MG	AA	3025	1/1	0.99	0.30	11.91	59,59,59,59	0
55	MG	CA	3113	1/1	0.94	0.32	11.79	61,61,61,61	0
55	MG	DA	1649	1/1	0.85	0.28	11.78	87,87,87,87	0
55	MG	CA	3004	1/1	0.98	0.28	11.64	49,49,49,49	0
55	MG	DA	1669	1/1	0.91	0.36	11.63	64,64,64,64	0
55	MG	AA	3383	1/1	0.90	0.32	11.56	46,46,46,46	0
55	MG	BA	1719	1/1	0.97	0.43	11.44	51,51,51,51	0
55	MG	AA	3072	1/1	0.95	0.28	11.31	65,65,65,65	0
55	MG	AA	3374	1/1	0.93	0.34	10.85	29,29,29,29	0
55	MG	CA	3453	1/1	0.96	0.29	10.53	58,58,58,58	0
55	MG	DA	1617	1/1	0.63	0.23	10.50	115,115,115,115	0
55	MG	AA	3111	1/1	0.96	0.37	10.48	35,35,35,35	0
55	MG	CA	3051	1/1	0.96	0.33	10.31	69,69,69,69	0
55	MG	CA	3069	1/1	0.97	0.23	10.24	69,69,69,69	0
55	MG	CA	3440	1/1	0.95	0.36	10.17	54,54,54,54	0
55	MG	AA	3414	1/1	0.93	0.29	10.14	57,57,57,57	0
55	MG	AA	3027	1/1	0.97	0.37	10.02	42,42,42,42	0
55	MG	DA	1604	1/1	0.90	0.44	9.85	82,82,82,82	0
55	MG	AA	3221	1/1	0.61	0.25	9.65	68,68,68,68	0
55	MG	BA	1743	1/1	0.98	0.38	9.58	69,69,69,69	0
55	MG	CA	3033	1/1	0.83	0.26	9.58	71,71,71,71	0
55	MG	AA	3084	1/1	0.89	0.33	9.49	58,58,58,58	0
55	MG	CA	3471	1/1	0.96	0.32	9.48	57,57,57,57	0
55	MG	CA	3192	1/1	0.77	0.27	9.21	87,87,87,87	0
55	MG	CA	3049	1/1	0.96	0.31	9.21	62,62,62,62	0
55	MG	CA	3032	1/1	0.96	0.29	9.03	70,70,70,70	0
55	MG	AA	3377	1/1	0.95	0.33	8.89	51,51,51,51	0
55	MG	DA	1688	1/1	0.76	0.34	8.80	101,101,101,101	0
55	MG	CA	3083	1/1	0.93	0.35	8.63	44,44,44,44	0
55	MG	AA	3068	1/1	0.75	0.26	8.62	61,61,61,61	0
55	MG	CA	3071	1/1	0.95	0.25	8.55	51,51,51,51	0
55	MG	CA	3090	1/1	0.98	0.32	8.48	55,55,55,55	0
55	MG	DA	1663	1/1	0.92	0.27	8.38	66,66,66,66	0
55	MG	BA	1624	1/1	0.97	0.29	8.08	70,70,70,70	0
55	MG	BA	1636	1/1	0.89	0.27	8.05	61,61,61,61	0
55	MG	CA	3220	1/1	0.77	0.30	8.05	85,85,85,85	0
55	MG	CA	3455	1/1	0.74	0.41	8.04	97,97,97,97	0
55	MG	AA	3146	1/1	0.97	0.32	8.03	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	BA	1616	1/1	0.95	0.29	7.98	61,61,61,61	0
55	MG	AA	3188	1/1	0.93	0.31	7.88	40,40,40,40	0
55	MG	AA	3069	1/1	0.95	0.44	7.87	62,62,62,62	0
55	MG	DA	1610	1/1	0.97	0.24	7.83	96,96,96,96	0
56	OHX	BA	1790	7/7	0.90	0.22	7.34	96,123,133,185	1
55	MG	CA	3172	1/1	0.94	0.33	7.32	86,86,86,86	0
55	MG	AA	3173	1/1	0.95	0.32	7.25	52,52,52,52	0
55	MG	DA	1601	1/1	0.95	0.23	7.22	87,87,87,87	0
55	MG	CA	3036	1/1	0.84	0.25	7.04	87,87,87,87	0
55	MG	CA	3231	1/1	0.91	0.34	6.99	89,89,89,89	0
55	MG	CA	3123	1/1	0.92	0.28	6.86	36,36,36,36	0
55	MG	CA	3175	1/1	0.85	0.37	6.86	64,64,64,64	0
56	OHX	BD	104	7/7	0.93	0.24	6.84	82,85,90,147	2
55	MG	BA	1705	1/1	0.80	0.30	6.75	63,63,63,63	0
55	MG	DA	1641	1/1	0.68	0.42	6.70	130,130,130,130	0
55	MG	CA	3127	1/1	0.97	0.27	6.66	53,53,53,53	0
55	MG	AA	3070	1/1	0.92	0.21	6.65	52,52,52,52	0
56	OHX	CA	3273	7/7	0.99	0.20	6.58	58,69,86,110	0
55	MG	CE	301	1/1	0.84	0.37	6.52	56,56,56,56	0
55	MG	DA	1614	1/1	0.88	0.24	6.52	91,91,91,91	0
55	MG	BA	1718	1/1	0.78	0.23	6.34	78,78,78,78	0
55	MG	BA	1709	1/1	0.95	0.31	6.33	100,100,100,100	0
55	MG	AA	3171	1/1	0.96	0.23	6.25	48,48,48,48	0
55	MG	BA	1632	1/1	0.89	0.28	6.22	108,108,108,108	0
55	MG	CA	3035	1/1	0.93	0.24	6.20	92,92,92,92	0
55	MG	AA	3250	1/1	0.92	0.35	6.12	56,56,56,56	0
55	MG	CA	3446	1/1	0.95	0.30	6.11	47,47,47,47	0
55	MG	AA	3415	1/1	0.95	0.26	6.02	52,52,52,52	0
55	MG	A1	201	1/1	0.82	0.28	5.89	71,71,71,71	0
55	MG	AA	3386	1/1	0.93	0.23	5.88	42,42,42,42	0
55	MG	AA	3380	1/1	0.92	0.28	5.79	66,66,66,66	0
55	MG	AA	3032	1/1	0.94	0.30	5.77	41,41,41,41	0
55	MG	AA	3080	1/1	0.96	0.42	5.67	55,55,55,55	0
55	MG	DA	1643	1/1	0.72	0.34	5.65	136,136,136,136	0
55	MG	CA	3444	1/1	0.94	0.27	5.64	52,52,52,52	0
55	MG	AB	202	1/1	0.86	0.22	5.56	72,72,72,72	0
55	MG	CA	3010	1/1	0.94	0.21	5.47	47,47,47,47	0
55	MG	CA	3061	1/1	0.86	0.29	5.43	64,64,64,64	0
55	MG	AA	3353	1/1	0.91	0.25	5.25	39,39,39,39	0
55	MG	AO	202	1/1	0.97	0.30	5.15	55,55,55,55	0
55	MG	AA	3393	1/1	0.98	0.20	5.15	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	CA	3050	1/1	0.99	0.27	5.14	65,65,65,65	0
55	MG	BA	1735	1/1	0.93	0.21	5.13	48,48,48,48	0
55	MG	CA	3121	1/1	0.91	0.35	5.12	55,55,55,55	0
55	MG	CA	3120	1/1	0.97	0.36	5.01	48,48,48,48	0
56	OHX	AA	3420	7/7	0.99	0.22	4.98	63,69,102,115	0
56	OHX	CA	3292	7/7	0.98	0.20	4.96	69,105,113,146	0
56	OHX	CA	3236	7/7	0.99	0.20	4.93	81,104,120,146	0
55	MG	CA	3176	1/1	0.94	0.33	4.85	67,67,67,67	0
56	OHX	CA	3252	7/7	0.87	0.18	4.84	108,118,136,203	1
55	MG	CA	3006	1/1	0.98	0.20	4.84	47,47,47,47	0
55	MG	CA	3265	1/1	0.92	0.22	4.83	55,55,55,55	0
56	OHX	CA	3350	7/7	0.93	0.15	4.75	112,134,144,175	1
55	MG	CA	3218	1/1	0.86	0.26	4.72	83,83,83,83	0
55	MG	CA	3072	1/1	0.90	0.33	4.69	43,43,43,43	0
55	MG	AA	3031	1/1	0.95	0.25	4.69	35,35,35,35	0
55	MG	AA	3244	1/1	0.89	0.22	4.68	49,49,49,49	0
56	OHX	AA	3417	7/7	1.00	0.21	4.56	68,72,82,103	0
55	MG	CA	3081	1/1	0.95	0.31	4.48	63,63,63,63	0
55	MG	BA	1737	1/1	0.90	0.26	4.45	46,46,46,46	0
55	MG	DA	1632	1/1	0.76	0.27	4.44	83,83,83,83	0
56	OHX	BA	1755	7/7	0.99	0.19	4.40	72,74,97,109	0
55	MG	AA	3019	1/1	0.94	0.48	4.38	72,72,72,72	0
55	MG	AA	3213	1/1	0.96	0.23	4.32	49,49,49,49	0
55	MG	BA	1654	1/1	0.99	0.35	4.32	47,47,47,47	0
56	OHX	AA	3399	7/7	1.00	0.20	4.28	42,51,73,98	0
56	OHX	BA	1667	7/7	0.88	0.17	4.22	118,130,146,200	1
55	MG	AA	3064	1/1	0.89	0.21	4.14	66,66,66,66	0
56	OHX	AA	3426	7/7	0.99	0.21	4.14	70,84,89,118	0
56	OHX	DA	1728	7/7	0.95	0.18	4.05	78,116,123,162	0
55	MG	DA	1668	1/1	0.97	0.23	4.01	86,86,86,86	0
56	OHX	CA	3244	7/7	0.94	0.17	4.00	94,113,121,172	1
56	OHX	CA	3348	7/7	0.88	0.23	3.97	104,111,132,178	1
56	OHX	DA	1791	7/7	0.95	0.15	3.90	103,104,121,153	1
55	MG	DA	1605	1/1	0.98	0.26	3.88	63,63,63,63	0
56	OHX	AA	3458	7/7	0.94	0.23	3.88	34,48,113,148	3
55	MG	CA	3002	1/1	0.93	0.33	3.87	50,50,50,50	0
55	MG	AA	3381	1/1	0.91	0.30	3.80	59,59,59,59	0
56	OHX	AA	3452	7/7	0.96	0.22	3.78	61,75,91,137	2
55	MG	AE	301	1/1	0.99	0.32	3.77	52,52,52,52	0
56	OHX	AA	3422	7/7	0.99	0.18	3.77	74,81,107,116	0
56	OHX	AA	3434	7/7	0.99	0.17	3.75	62,71,94,101	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	BA	1605	1/1	0.96	0.19	3.75	104,104,104,104	0
55	MG	DA	1650	1/1	0.88	0.20	3.71	67,67,67,67	0
56	OHX	DA	1732	7/7	0.94	0.17	3.70	134,143,157,195	0
55	MG	AA	3376	1/1	0.96	0.34	3.65	33,33,33,33	0
55	MG	BA	1608	1/1	0.92	0.26	3.62	55,55,55,55	0
56	OHX	CA	3343	7/7	0.96	0.16	3.61	109,118,132,184	1
55	MG	CA	3178	1/1	0.82	0.28	3.48	52,52,52,52	0
56	OHX	BA	1764	7/7	0.97	0.17	3.39	88,94,120,157	0
56	OHX	AA	3419	7/7	0.99	0.18	3.38	67,75,91,95	0
56	OHX	CA	3232	7/7	0.99	0.21	3.34	72,77,83,137	0
55	MG	CA	3472	1/1	0.96	0.20	3.34	59,59,59,59	0
56	OHX	CA	3272	7/7	1.00	0.20	3.30	54,70,84,85	1
55	MG	AA	3029	1/1	0.97	0.30	3.18	38,38,38,38	0
55	MG	CA	3015	1/1	0.97	0.27	3.16	54,54,54,54	0
56	OHX	AA	3361	7/7	0.98	0.20	3.11	51,71,83,107	0
55	MG	CA	3153	1/1	0.94	0.23	3.08	56,56,56,56	0
56	OHX	AA	3292	7/7	0.99	0.17	3.06	50,75,88,112	0
56	OHX	AA	3359	7/7	1.00	0.18	3.06	61,75,93,113	0
55	MG	AA	3255	1/1	0.90	0.20	3.04	64,64,64,64	0
55	MG	AA	3090	1/1	0.94	0.17	2.98	85,85,85,85	0
56	OHX	AA	3456	7/7	0.98	0.20	2.92	59,75,90,132	2
55	MG	AA	3112	1/1	0.94	0.26	2.91	47,47,47,47	0
56	OHX	CA	3234	7/7	0.98	0.15	2.90	77,91,119,122	2
55	MG	CA	3131	1/1	0.97	0.34	2.84	65,65,65,65	0
56	OHX	CA	3281	7/7	0.99	0.19	2.84	101,105,126,132	0
55	MG	BA	1635	1/1	0.81	0.23	2.80	96,96,96,96	0
56	OHX	AA	3424	7/7	0.99	0.18	2.69	92,97,108,112	0
55	MG	AA	3020	1/1	0.95	0.38	2.62	44,44,44,44	0
56	OHX	AA	3362	7/7	0.98	0.20	2.61	40,81,119,136	1
56	OHX	AA	3488	7/7	0.92	0.19	2.52	86,101,105,150	1
55	MG	CA	3454	1/1	0.99	0.29	2.51	51,51,51,51	0
56	OHX	AA	3147	7/7	0.92	0.19	2.51	89,98,103,163	1
56	OHX	BB	107	7/7	0.91	0.23	2.50	71,92,103,147	3
56	OHX	CA	3461	7/7	0.99	0.20	2.45	38,55,94,109	0
56	OHX	CA	3435	7/7	0.84	0.18	2.41	105,108,131,192	1
56	OHX	CA	3271	7/7	0.99	0.23	2.39	67,82,101,115	0
56	OHX	AB	207	7/7	0.98	0.14	2.38	89,99,126,152	1
56	OHX	CA	3399	7/7	0.89	0.18	2.35	97,104,115,165	2
55	MG	CA	3448	1/1	0.88	0.17	2.34	63,63,63,63	0
55	MG	AA	3397	1/1	0.68	0.18	2.33	80,80,80,80	0
56	OHX	AB	218	7/7	0.94	0.17	2.30	128,132,146,199	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	OHX	CA	3247	7/7	0.96	0.17	2.30	95,104,117,152	1
56	OHX	AA	3312	7/7	0.91	0.17	2.26	64,87,123,173	1
56	OHX	AB	216	7/7	0.93	0.20	2.25	88,124,141,184	1
56	OHX	DA	1718	7/7	0.99	0.19	2.17	73,98,100,135	0
56	OHX	AB	209	7/7	0.96	0.18	2.16	63,88,125,152	2
56	OHX	AA	3342	7/7	0.98	0.18	2.14	78,85,104,123	1
56	OHX	BA	1674	7/7	0.88	0.17	2.12	117,122,137,199	1
56	OHX	CA	3293	7/7	0.96	0.16	2.11	100,117,128,163	0
56	OHX	BA	1791	7/7	0.97	0.17	2.09	82,106,122,150	2
56	OHX	AA	3441	7/7	0.98	0.17	2.07	84,93,115,140	0
55	MG	AA	3352	1/1	0.97	0.21	2.04	41,41,41,41	0
56	OHX	BA	1686	7/7	0.70	0.17	2.03	141,143,153,230	1
56	OHX	BA	1757	7/7	0.99	0.18	2.03	57,66,87,98	2
56	OHX	CA	3286	7/7	0.99	0.15	2.02	87,94,108,115	0
55	MG	AA	3082	1/1	0.89	0.20	2.01	50,50,50,50	0
56	OHX	AA	3451	7/7	0.98	0.18	1.97	75,85,92,125	1
55	MG	CA	3008	1/1	0.90	0.23	1.96	52,52,52,52	0
56	OHX	AA	3514	7/7	0.95	0.18	1.93	84,93,104,149	1
56	OHX	CA	3368	7/7	0.95	0.14	1.91	108,126,135,177	1
55	MG	CA	3075	1/1	0.96	0.21	1.90	45,45,45,45	0
56	OHX	DA	1774	7/7	0.86	0.15	1.90	131,135,155,208	1
56	OHX	BA	1789	7/7	0.97	0.17	1.82	108,112,133,182	1
56	OHX	CA	3314	7/7	0.98	0.16	1.81	84,93,97,114	1
56	OHX	AA	3365	7/7	0.90	0.22	1.79	90,106,114,161	2
56	OHX	AA	3433	7/7	0.99	0.17	1.75	63,65,104,122	1
56	OHX	DA	1762	7/7	0.96	0.16	1.74	107,112,122,180	1
56	OHX	AA	3288	7/7	0.99	0.20	1.71	76,85,101,127	1
56	OHX	AA	3154	7/7	0.95	0.17	1.67	76,89,110,133	1
56	OHX	CA	3395	7/7	0.94	0.17	1.64	106,111,125,156	1
56	OHX	CA	3324	7/7	0.98	0.19	1.63	65,83,94,110	2
56	OHX	DA	1753	7/7	0.89	0.18	1.62	120,124,134,196	1
56	OHX	AA	3512	7/7	0.91	0.18	1.60	99,114,126,166	2
56	OHX	BA	1805	7/7	0.93	0.17	1.59	90,105,122,143	3
56	OHX	CA	3277	7/7	0.99	0.17	1.57	73,81,99,107	1
56	OHX	AB	215	7/7	0.94	0.18	1.55	105,114,120,153	1
56	OHX	DA	1778	7/7	0.91	0.15	1.53	142,148,154,267	0
56	OHX	AA	3418	7/7	0.99	0.20	1.48	39,61,82,95	0
56	OHX	BA	1806	7/7	0.89	0.20	1.47	97,127,142,180	2
55	MG	CA	3022	1/1	0.96	0.17	1.46	55,55,55,55	0
56	OHX	CA	3386	7/7	0.95	0.15	1.45	110,116,134,181	1
56	OHX	AB	208	7/7	0.96	0.16	1.44	113,119,131,170	1
56	OHX	AA	3370	7/7	0.91	0.21	1.44	115,126,140,200	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	CB	203	1/1	0.95	0.14	1.43	111,111,111,111	0
56	OHX	AA	3366	7/7	0.94	0.20	1.43	85,90,106,173	1
56	OHX	DA	1755	7/7	0.93	0.16	1.43	103,120,143,191	1
56	OHX	CA	3278	7/7	0.98	0.15	1.42	81,96,114,120	0
56	OHX	AA	3423	7/7	0.99	0.21	1.39	44,66,84,86	1
56	OHX	AA	3427	7/7	0.99	0.19	1.38	29,70,88,108	0
56	OHX	BA	1780	7/7	0.99	0.16	1.36	94,102,115,117	1
56	OHX	BA	1669	7/7	0.78	0.18	1.35	124,127,142,200	1
56	OHX	CA	3255	7/7	0.99	0.13	1.35	103,107,122,145	1
56	OHX	AA	3400	7/7	0.98	0.19	1.35	69,80,83,116	1
56	OHX	AA	3435	7/7	0.99	0.18	1.34	61,70,93,100	3
56	OHX	AA	3474	7/7	0.95	0.18	1.33	51,85,127,151	2
56	OHX	AA	3368	7/7	0.96	0.18	1.33	76,83,98,126	1
56	OHX	CA	3269	7/7	0.89	0.18	1.32	98,100,123,153	2
56	OHX	CA	3287	7/7	0.98	0.17	1.31	69,74,104,109	3
56	OHX	AA	3428	7/7	0.99	0.19	1.29	67,79,86,113	0
56	OHX	BC	107	7/7	0.97	0.16	1.27	105,124,134,145	1
56	OHX	CA	3280	7/7	0.99	0.18	1.26	82,87,100,129	0
56	OHX	CA	3346	7/7	0.97	0.15	1.26	99,104,119,151	1
56	OHX	BA	1759	7/7	0.98	0.19	1.26	78,93,120,156	0
56	OHX	CB	212	7/7	0.93	0.15	1.23	101,120,135,155	1
56	OHX	CA	3335	7/7	0.96	0.15	1.23	96,110,125,200	0
56	OHX	CA	3373	7/7	0.92	0.17	1.21	113,122,129,160	1
56	OHX	AA	3289	7/7	1.00	0.19	1.17	53,58,81,93	0
55	MG	AF	301	1/1	0.92	0.28	1.17	83,83,83,83	0
56	OHX	CA	3305	7/7	0.99	0.16	1.17	70,83,99,129	1
57	ZN	BG	301	1/1	0.97	0.30	1.13	79,79,79,79	0
56	OHX	CB	217	7/7	0.93	0.22	1.13	128,135,146,182	1
56	OHX	AA	3475	7/7	0.96	0.17	1.12	67,93,111,167	1
56	OHX	CA	3429	7/7	0.87	0.16	1.12	127,129,142,209	1
56	OHX	CA	3276	7/7	0.99	0.17	1.09	81,100,117,133	0
56	OHX	CA	3302	7/7	0.93	0.20	1.09	79,86,104,139	1
56	OHX	AA	3369	7/7	0.92	0.18	1.08	80,102,119,165	1
56	OHX	CA	3318	7/7	0.92	0.18	1.08	34,112,130,183	1
56	OHX	AA	3290	7/7	0.98	0.18	1.08	10,72,91,128	0
56	OHX	AF	303	7/7	1.00	0.21	1.06	45,52,58,77	0
56	OHX	AA	3299	7/7	0.98	0.17	1.05	54,81,94,118	1
55	MG	AA	3390	1/1	0.95	0.20	1.03	46,46,46,46	0
56	OHX	DC	110	7/7	0.98	0.14	1.00	78,91,106,144	4
56	OHX	AA	3430	7/7	0.99	0.17	0.99	63,78,92,111	1
56	OHX	AA	3480	7/7	0.97	0.18	0.96	90,100,124,135	1
56	OHX	AA	3523	7/7	0.89	0.17	0.92	109,114,123,180	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	OHX	DA	1743	7/7	0.97	0.14	0.91	109,113,118,148	1
56	OHX	CA	3311	7/7	0.98	0.17	0.91	79,95,105,127	1
56	OHX	BA	1767	7/7	0.97	0.17	0.89	92,119,140,142	0
55	MG	AA	3038	1/1	0.88	0.25	0.89	46,46,46,46	0
56	OHX	AA	3320	7/7	0.99	0.19	0.89	69,81,96,121	1
56	OHX	BA	1756	7/7	0.99	0.20	0.86	59,79,107,108	0
56	OHX	BA	1760	7/7	0.99	0.15	0.85	71,106,126,148	0
56	OHX	CA	3297	7/7	0.99	0.14	0.85	84,94,129,142	1
56	OHX	AA	3308	7/7	0.98	0.17	0.83	66,73,104,120	2
56	OHX	DA	1733	7/7	0.98	0.15	0.82	146,151,163,202	0
56	OHX	CA	3485	7/7	0.98	0.15	0.82	88,102,109,144	1
56	OHX	AA	3440	7/7	0.99	0.18	0.82	59,88,102,124	0
56	OHX	DC	109	7/7	0.96	0.15	0.81	88,92,104,159	3
56	OHX	CA	3299	7/7	0.98	0.15	0.81	99,105,124,141	1
56	OHX	AA	3454	7/7	0.98	0.17	0.80	68,93,112,112	1
55	MG	AE	302	1/1	0.86	0.21	0.79	71,71,71,71	0
56	OHX	DA	1782	7/7	0.90	0.16	0.78	117,128,138,207	1
56	OHX	AA	3464	7/7	0.96	0.14	0.78	117,125,139,188	0
56	OHX	CA	3237	7/7	0.98	0.15	0.75	109,109,122,166	0
56	OHX	CA	3375	7/7	0.95	0.15	0.74	103,118,131,145	1
56	OHX	BA	1770	7/7	0.97	0.16	0.71	102,113,126,149	1
55	MG	CA	3021	1/1	0.95	0.17	0.70	60,60,60,60	0
55	MG	CB	202	1/1	0.85	0.17	0.70	99,99,99,99	0
56	OHX	CA	3256	7/7	0.99	0.16	0.70	88,101,112,126	1
56	OHX	AA	3492	7/7	0.95	0.17	0.70	79,89,95,107	3
56	OHX	BA	1664	7/7	0.94	0.15	0.69	108,126,142,197	1
56	OHX	CA	3233	7/7	0.98	0.16	0.69	74,85,95,121	0
56	OHX	CA	3275	7/7	0.99	0.15	0.65	56,80,112,114	1
56	OHX	CA	3462	7/7	0.97	0.16	0.63	71,82,94,110	1
56	OHX	AA	3569	7/7	0.90	0.16	0.62	116,117,125,191	1
56	OHX	CA	3328	7/7	0.91	0.16	0.61	50,117,131,206	0
55	MG	CA	3460	1/1	0.92	0.27	0.60	72,72,72,72	0
56	OHX	CA	3289	7/7	0.99	0.14	0.59	69,83,106,125	0
55	MG	CA	3267	1/1	0.89	0.15	0.57	65,65,65,65	0
56	OHX	AA	3425	7/7	1.00	0.19	0.55	45,61,75,79	0
56	OHX	AA	3552	7/7	0.90	0.18	0.53	105,122,135,199	1
56	OHX	CA	3428	7/7	0.93	0.13	0.53	123,134,138,182	1
56	OHX	AA	3317	7/7	0.97	0.16	0.53	79,88,118,156	1
56	OHX	CA	3243	7/7	0.98	0.12	0.49	121,128,140,172	0
56	OHX	AA	3564	7/7	0.91	0.17	0.47	102,105,128,167	1
56	OHX	BA	1777	7/7	0.96	0.14	0.47	114,118,140,171	1
56	OHX	CA	3283	7/7	0.99	0.16	0.46	81,83,86,120	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	OHX	DA	1726	7/7	0.98	0.17	0.46	87,101,123,159	0
56	OHX	CA	3282	7/7	0.99	0.15	0.45	79,83,97,109	0
56	OHX	CA	3378	7/7	0.95	0.12	0.44	128,141,148,178	1
56	OHX	CA	3309	7/7	0.96	0.17	0.43	92,108,125,150	1
56	OHX	BC	106	7/7	0.97	0.15	0.43	110,133,144,147	1
56	OHX	AO	205	7/7	0.93	0.18	0.42	83,89,107,180	1
56	OHX	DD	101	7/7	0.88	0.14	0.42	155,165,187,227	0
56	OHX	AA	3513	7/7	0.95	0.16	0.40	80,88,116,153	1
56	OHX	AA	3323	7/7	0.98	0.15	0.39	72,87,96,117	1
56	OHX	CB	216	7/7	0.89	0.13	0.36	117,132,146,206	1
56	OHX	DA	1799	7/7	0.93	0.13	0.36	122,127,139,209	1
56	OHX	CA	3336	7/7	0.98	0.13	0.35	114,127,138,191	0
56	OHX	CA	3409	7/7	0.87	0.17	0.32	97,100,119,183	1
56	OHX	AA	3301	7/7	0.99	0.15	0.32	88,89,93,110	1
56	OHX	DA	1744	7/7	0.98	0.14	0.31	103,108,120,148	1
57	ZN	DG	301	1/1	0.98	0.28	0.31	122,122,122,122	0
56	OHX	BA	1774	7/7	0.97	0.16	0.31	80,98,111,147	1
56	OHX	DA	1722	7/7	0.99	0.15	0.30	84,90,106,116	0
56	OHX	CF	301	7/7	1.00	0.18	0.30	54,58,79,92	0
56	OHX	AA	3431	7/7	0.99	0.16	0.30	74,81,100,115	0
56	OHX	AA	3565	7/7	0.92	0.19	0.30	117,122,134,195	1
55	MG	CA	3028	1/1	0.87	0.14	0.30	73,73,73,73	0
56	OHX	CA	3315	7/7	0.98	0.15	0.29	90,101,110,160	1
56	OHX	BA	1693	7/7	0.96	0.15	0.26	112,112,134,152	1
56	OHX	AA	3479	7/7	0.95	0.15	0.24	106,122,142,174	1
56	OHX	CA	3351	7/7	0.97	0.14	0.24	102,107,134,173	1
56	OHX	AA	3510	7/7	0.89	0.18	0.21	92,103,113,152	2
56	OHX	AA	3485	7/7	0.95	0.14	0.20	104,114,127,171	1
56	OHX	BA	1815	7/7	0.95	0.15	0.19	110,125,133,172	1
56	OHX	BA	1802	7/7	0.97	0.14	0.19	107,121,133,185	1
56	OHX	CA	3288	7/7	0.98	0.16	0.18	87,95,104,133	0
56	OHX	AA	3532	7/7	0.88	0.20	0.17	89,105,116,172	1
56	OHX	AB	217	7/7	0.93	0.17	0.16	85,105,116,146	1
56	OHX	BA	1690	7/7	0.90	0.13	0.15	118,127,134,188	1
56	OHX	DA	1723	7/7	0.99	0.15	0.14	107,111,116,151	0
56	OHX	BA	1761	7/7	0.99	0.15	0.13	102,104,115,161	0
56	OHX	DA	1727	7/7	0.99	0.14	0.12	114,126,131,160	0
56	OHX	CA	3416	7/7	0.94	0.16	0.08	114,117,128,182	1
56	OHX	AA	3511	7/7	0.97	0.12	0.08	133,145,154,207	0
56	OHX	CA	3239	7/7	0.99	0.16	0.08	66,92,107,113	1
56	OHX	DA	1737	7/7	0.97	0.14	0.07	87,110,131,158	1
55	MG	A0	201	1/1	0.99	0.21	0.05	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	OHX	BA	1688	7/7	0.98	0.13	0.05	107,112,123,154	1
56	OHX	BA	1768	7/7	0.98	0.12	0.05	128,139,147,175	0
56	OHX	AA	3461	7/7	0.98	0.18	0.04	60,78,98,143	1
56	OHX	DA	1787	7/7	0.91	0.13	0.04	95,113,121,162	2
55	MG	CA	3019	1/1	0.89	0.19	0.03	46,46,46,46	0
55	MG	AA	3395	1/1	0.96	0.20	0.02	40,40,40,40	0
56	OHX	DA	1729	7/7	0.98	0.14	0.00	104,108,118,152	1
56	OHX	AA	3547	7/7	0.91	0.17	0.00	69,84,101,157	2
56	OHX	BA	1766	7/7	0.98	0.17	-0.02	89,96,106,129	1
56	OHX	DA	1804	7/7	0.96	0.16	-0.02	107,115,128,173	1
56	OHX	CA	3270	7/7	0.99	0.16	-0.03	73,87,105,117	0
56	OHX	AA	3300	7/7	0.96	0.15	-0.03	67,91,120,167	1
56	OHX	BA	1678	7/7	0.95	0.15	-0.04	115,118,134,165	1
56	OHX	AA	3536	7/7	0.84	0.25	-0.04	116,124,157,192	1
56	OHX	CA	3310	7/7	0.99	0.14	-0.04	74,88,107,129	1
55	MG	CA	3073	1/1	0.93	0.18	-0.05	54,54,54,54	0
56	OHX	BA	1804	7/7	0.89	0.17	-0.05	134,142,150,227	1
56	OHX	CA	3371	7/7	0.90	0.15	-0.07	67,90,123,162	1
56	OHX	AA	3407	7/7	0.94	0.15	-0.07	108,117,126,165	1
56	OHX	DA	1812	7/7	0.74	0.13	-0.08	149,158,168,252	1
56	OHX	AA	3360	7/7	0.99	0.17	-0.08	58,67,70,97	1
56	OHX	CA	3246	7/7	0.96	0.16	-0.08	113,116,120,151	1
56	OHX	BA	1763	7/7	0.99	0.15	-0.08	94,115,123,136	0
56	OHX	AA	3367	7/7	0.96	0.14	-0.09	121,129,147,173	1
55	MG	DA	1655	1/1	0.88	0.15	-0.09	78,78,78,78	0
56	OHX	AA	3500	7/7	0.97	0.13	-0.10	94,114,122,159	1
56	OHX	BA	1816	7/7	0.93	0.14	-0.10	127,130,142,194	1
56	OHX	CA	3433	7/7	0.91	0.17	-0.11	121,129,144,183	1
56	OHX	DA	1719	7/7	0.99	0.16	-0.12	79,99,112,124	0
56	OHX	AA	3444	7/7	0.99	0.16	-0.12	80,103,116,131	1
56	OHX	AA	3291	7/7	0.99	0.17	-0.12	68,75,102,108	3
56	OHX	BA	1788	7/7	0.97	0.14	-0.13	118,118,132,157	1
56	OHX	AA	3498	7/7	0.97	0.16	-0.15	92,94,127,136	1
56	OHX	CA	3241	7/7	0.99	0.14	-0.16	90,96,101,122	1
56	OHX	CA	3463	7/7	0.97	0.15	-0.17	107,129,139,156	1
56	OHX	CA	3323	7/7	0.98	0.13	-0.19	107,111,118,169	0
56	OHX	CA	3377	7/7	0.94	0.15	-0.20	90,95,111,135	2
56	OHX	CA	3312	7/7	0.99	0.15	-0.21	85,101,114,134	1
56	OHX	BA	1696	7/7	0.99	0.15	-0.24	47,75,99,113	0
56	OHX	AA	3316	7/7	0.98	0.14	-0.24	80,95,97,136	0
56	OHX	BA	1666	7/7	0.87	0.15	-0.25	117,122,134,158	2
56	OHX	BA	1685	7/7	0.87	0.12	-0.26	198,199,207,267	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	OHX	AA	3483	7/7	0.90	0.15	-0.26	124,141,146,196	1
56	OHX	CA	3341	7/7	0.96	0.14	-0.29	74,100,107,145	2
55	MG	BA	1634	1/1	0.91	0.20	-0.30	74,74,74,74	0
56	OHX	CA	3357	7/7	0.98	0.15	-0.30	86,98,106,151	1
56	OHX	CA	3274	7/7	0.99	0.16	-0.30	67,83,114,118	0
56	OHX	AA	3468	7/7	0.97	0.14	-0.31	99,111,119,167	1
56	OHX	DA	1785	7/7	0.94	0.13	-0.32	110,114,129,164	1
56	OHX	CA	3322	7/7	0.98	0.13	-0.32	104,117,127,154	1
56	OHX	AA	3304	7/7	0.94	0.13	-0.32	109,115,135,200	1
56	OHX	AA	3471	7/7	0.97	0.16	-0.33	98,107,114,163	1
56	OHX	CA	3301	7/7	0.98	0.15	-0.33	55,85,123,136	3
56	OHX	CA	3320	7/7	0.98	0.13	-0.34	140,142,153,174	0
56	OHX	CB	218	7/7	0.82	0.12	-0.35	141,159,166,235	1
56	OHX	AA	3555	7/7	0.94	0.16	-0.36	112,114,124,192	1
56	OHX	AA	3449	7/7	0.98	0.17	-0.37	64,74,89,112	2
56	OHX	AA	3478	7/7	0.97	0.16	-0.38	77,90,100,131	1
56	OHX	AA	3293	7/7	0.99	0.16	-0.39	54,82,88,102	2
56	OHX	CA	3370	7/7	0.94	0.13	-0.39	116,120,142,180	1
56	OHX	CA	3345	7/7	0.97	0.13	-0.40	91,108,114,146	1
56	OHX	AA	3531	7/7	0.95	0.11	-0.41	119,124,135,185	1
56	OHX	BA	1813	7/7	0.96	0.13	-0.41	128,130,137,174	1
56	OHX	A1	202	7/7	0.98	0.17	-0.41	85,95,114,146	1
56	OHX	AA	3518	7/7	0.98	0.16	-0.42	67,73,103,130	1
56	OHX	CB	220	7/7	0.92	0.13	-0.42	133,142,154,201	0
56	OHX	CA	3235	7/7	0.98	0.16	-0.44	43,79,99,118	0
56	OHX	CA	3319	7/7	0.98	0.15	-0.46	87,97,106,138	1
56	OHX	AA	3263	7/7	0.98	0.16	-0.47	76,102,114,143	1
56	OHX	AA	3295	7/7	0.98	0.15	-0.47	84,98,116,152	0
56	OHX	DA	1781	7/7	0.92	0.12	-0.48	107,126,135,195	1
56	OHX	BA	1803	7/7	0.93	0.15	-0.49	101,126,136,190	1
56	OHX	CA	3332	7/7	0.99	0.15	-0.49	70,82,93,103	1
56	OHX	AA	3326	7/7	0.98	0.15	-0.50	83,94,100,118	1
56	OHX	CA	3437	7/7	0.94	0.13	-0.50	98,105,117,166	2
56	OHX	CA	3304	7/7	0.93	0.13	-0.52	113,122,141,181	2
56	OHX	CA	3482	7/7	0.96	0.12	-0.52	84,120,131,181	0
56	OHX	AA	3287	7/7	0.99	0.15	-0.52	75,88,103,129	2
56	OHX	AA	3296	7/7	0.99	0.12	-0.52	115,120,123,158	0
56	OHX	AA	3517	7/7	0.97	0.17	-0.53	88,111,115,145	1
56	OHX	DC	107	7/7	0.90	0.11	-0.53	131,132,141,177	1
56	OHX	BA	1795	7/7	0.97	0.12	-0.54	109,127,134,173	1
56	OHX	DA	1745	7/7	0.92	0.14	-0.55	115,123,143,223	0
56	OHX	DA	1736	7/7	0.95	0.13	-0.56	130,135,157,193	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	OHX	DA	1735	7/7	0.97	0.11	-0.56	110,115,118,170	1
56	OHX	AA	3309	7/7	0.99	0.17	-0.56	64,84,90,112	1
56	OHX	BA	1769	7/7	0.98	0.15	-0.57	102,107,127,145	0
56	OHX	CA	3295	7/7	0.98	0.15	-0.58	102,105,117,137	1
56	OHX	BA	1687	7/7	0.98	0.16	-0.58	94,99,108,140	1
56	OHX	CA	3337	7/7	0.96	0.13	-0.58	109,124,136,185	0
56	OHX	BA	1778	7/7	0.96	0.14	-0.59	99,120,131,182	0
56	OHX	CA	3436	7/7	0.92	0.14	-0.59	115,121,137,192	1
56	OHX	DA	1739	7/7	0.98	0.12	-0.60	98,110,124,155	1
56	OHX	CA	3450	7/7	0.98	0.12	-0.62	112,125,137,206	0
56	OHX	CA	3465	7/7	0.96	0.11	-0.63	131,136,147,181	1
56	OHX	AA	3311	7/7	0.98	0.15	-0.63	97,106,117,155	1
56	OHX	CA	3331	7/7	0.97	0.14	-0.64	101,112,120,147	1
56	OHX	AA	3373	7/7	0.94	0.17	-0.65	75,103,110,155	1
56	OHX	AA	3533	7/7	0.94	0.15	-0.66	98,103,114,150	2
56	OHX	AA	3443	7/7	0.99	0.16	-0.66	69,76,84,127	1
56	OHX	AA	3327	7/7	0.98	0.13	-0.66	107,115,135,188	1
55	MG	AA	3233	1/1	0.95	0.13	-0.67	59,59,59,59	0
56	OHX	DA	1793	7/7	0.95	0.10	-0.67	146,150,161,207	1
56	OHX	AA	3297	7/7	0.99	0.15	-0.68	87,98,102,106	1
56	OHX	AA	3405	7/7	0.97	0.12	-0.69	103,111,138,161	1
56	OHX	AB	219	7/7	0.95	0.15	-0.69	104,111,125,162	1
56	OHX	CA	3347	7/7	0.97	0.13	-0.71	86,102,110,148	1
56	OHX	CA	3321	7/7	0.98	0.13	-0.72	111,119,144,156	0
56	OHX	AA	3466	7/7	0.99	0.14	-0.73	89,94,108,128	1
56	OHX	AE	304	7/7	1.00	0.16	-0.74	74,87,107,110	1
56	OHX	AA	3542	7/7	0.93	0.13	-0.74	118,127,135,189	1
56	OHX	CA	3403	7/7	0.94	0.14	-0.75	88,108,114,167	1
56	OHX	AA	3305	7/7	0.96	0.17	-0.76	83,97,103,135	1
56	OHX	CA	3325	7/7	0.97	0.14	-0.76	108,122,148,156	1
56	OHX	AA	3459	7/7	0.99	0.14	-0.77	71,92,105,129	1
56	OHX	AA	3307	7/7	0.98	0.15	-0.78	85,90,103,127	1
56	OHX	CA	3388	7/7	0.96	0.12	-0.78	112,116,127,180	1
56	OHX	CA	3481	7/7	0.97	0.15	-0.78	35,87,114,138	2
56	OHX	AB	211	7/7	0.99	0.14	-0.79	74,85,113,121	0
56	OHX	DA	1770	7/7	0.95	0.12	-0.79	136,142,156,217	1
56	OHX	AA	3324	7/7	0.96	0.15	-0.81	92,110,118,165	1
56	OHX	CA	3327	7/7	0.99	0.14	-0.81	76,83,103,129	1
56	OHX	AA	3554	7/7	0.86	0.13	-0.82	116,128,150,205	1
56	OHX	CA	3356	7/7	0.97	0.14	-0.82	96,109,118,157	1
57	ZN	DQ	101	1/1	0.98	0.14	-0.82	123,123,123,123	0
56	OHX	CA	3491	7/7	0.91	0.13	-0.83	92,108,117,175	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	OHX	DA	1769	7/7	0.94	0.11	-0.84	133,140,147,188	1
56	OHX	BD	103	7/7	0.96	0.14	-0.84	86,95,103,174	1
56	OHX	AA	3539	7/7	0.91	0.13	-0.84	116,125,136,193	1
56	OHX	AO	204	7/7	0.99	0.14	-0.85	83,94,106,121	1
55	MG	C0	201	1/1	0.97	0.16	-0.85	61,61,61,61	0
56	OHX	AA	3568	7/7	0.95	0.13	-0.86	78,93,100,118	1
56	OHX	AA	3470	7/7	0.98	0.15	-0.86	107,109,130,160	1
56	OHX	AA	3337	7/7	0.96	0.14	-0.86	97,106,127,177	1
56	OHX	CA	3384	7/7	0.96	0.12	-0.89	118,124,135,184	1
56	OHX	CA	3349	7/7	0.97	0.12	-0.90	115,117,131,178	1
56	OHX	CO	201	7/7	0.98	0.13	-0.90	104,109,121,141	1
56	OHX	DC	108	7/7	0.93	0.10	-0.91	120,132,142,180	1
56	OHX	A6	101	7/7	0.94	0.14	-0.92	113,122,137,155	1
56	OHX	CA	3376	7/7	0.93	0.14	-0.92	113,130,136,172	1
56	OHX	DA	1740	7/7	0.97	0.12	-0.93	139,153,162,184	0
56	OHX	CB	208	7/7	0.99	0.13	-0.93	105,109,142,147	0
56	OHX	BA	1810	7/7	0.98	0.13	-0.93	106,108,121,152	1
56	OHX	BA	1692	7/7	0.89	0.12	-0.95	126,131,140,209	1
56	OHX	CA	3392	7/7	0.95	0.11	-0.96	126,132,142,192	1
56	OHX	AA	3437	7/7	0.99	0.14	-0.96	81,95,107,131	0
56	OHX	CA	3397	7/7	0.87	0.10	-0.96	128,138,154,219	1
56	OHX	AA	3138	7/7	0.91	0.15	-0.96	88,92,127,173	1
56	OHX	BA	1812	7/7	0.91	0.13	-0.96	151,164,170,231	1
56	OHX	CA	3245	7/7	0.94	0.12	-0.97	99,120,129,189	1
56	OHX	BA	1799	7/7	0.97	0.11	-0.97	158,163,176,213	1
56	OHX	CA	3483	7/7	0.98	0.14	-0.97	84,93,103,136	1
56	OHX	DA	1754	7/7	0.98	0.12	-0.98	98,102,118,156	1
56	OHX	BA	1785	7/7	0.97	0.14	-0.98	109,122,129,170	1
56	OHX	CA	3431	7/7	0.91	0.13	-0.98	105,117,132,179	1
56	OHX	C6	101	7/7	0.94	0.11	-0.98	132,145,157,184	1
56	OHX	AA	3160	7/7	0.96	0.11	-0.98	116,121,130,182	1
56	OHX	DA	1783	7/7	0.86	0.12	-0.99	123,123,145,185	1
56	OHX	AA	3445	7/7	0.99	0.15	-0.99	75,87,109,120	1
56	OHX	AA	3332	7/7	0.98	0.15	-1.00	77,106,123,134	1
56	OHX	DA	1763	7/7	0.92	0.10	-1.00	154,159,173,250	0
56	OHX	CB	214	7/7	0.94	0.12	-1.00	129,139,146,186	1
56	OHX	AA	3318	7/7	0.98	0.16	-1.00	92,102,113,133	1
56	OHX	DA	1767	7/7	0.98	0.09	-1.02	120,124,135,184	1
56	OHX	BA	1656	7/7	0.85	0.10	-1.02	160,162,176,267	0
56	OHX	BA	1671	7/7	0.97	0.08	-1.03	127,131,133,210	1
56	OHX	CA	3417	7/7	0.93	0.10	-1.04	151,167,187,222	1
55	MG	DN	201	1/1	0.91	0.12	-1.04	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	OHX	AA	3432	7/7	0.99	0.15	-1.04	72,98,103,107	0
56	OHX	BA	1673	7/7	0.91	0.13	-1.05	117,123,127,191	1
55	MG	CA	3043	1/1	0.87	0.11	-1.05	82,82,82,82	0
56	OHX	CA	3396	7/7	0.92	0.13	-1.05	135,136,150,198	1
56	OHX	CA	3303	7/7	0.99	0.12	-1.05	92,96,123,138	0
56	OHX	AA	3457	7/7	0.99	0.15	-1.07	73,83,101,131	1
56	OHX	AA	3439	7/7	0.99	0.15	-1.08	69,82,92,115	1
56	OHX	C1	201	7/7	0.95	0.14	-1.09	102,111,123,165	1
56	OHX	AA	3526	7/7	0.86	0.15	-1.11	120,129,136,176	1
56	OHX	AA	3506	7/7	0.94	0.14	-1.11	97,110,123,157	1
56	OHX	DA	1764	7/7	0.98	0.09	-1.12	115,121,127,171	1
56	OHX	DA	1803	7/7	0.96	0.10	-1.15	135,141,144,207	1
56	OHX	CA	3306	7/7	0.94	0.12	-1.15	98,106,119,148	1
56	OHX	AA	3508	7/7	0.95	0.11	-1.16	122,129,136,204	1
56	OHX	AA	3463	7/7	0.99	0.15	-1.17	77,89,96,134	1
56	OHX	AW	101	7/7	0.97	0.15	-1.18	103,112,128,156	1
56	OHX	DK	201	7/7	0.95	0.09	-1.18	137,138,149,200	1
56	OHX	CA	3414	7/7	0.95	0.09	-1.18	155,156,163,215	1
56	OHX	CA	3374	7/7	0.94	0.12	-1.20	106,124,128,169	1
56	OHX	BA	1691	7/7	0.89	0.11	-1.20	148,150,156,215	1
56	OHX	DA	1808	7/7	0.91	0.14	-1.21	119,124,131,178	1
55	MG	BA	1626	1/1	0.90	0.13	-1.21	81,81,81,81	0
56	OHX	BA	1798	7/7	0.96	0.12	-1.21	140,143,151,221	1
56	OHX	AA	3556	7/7	0.87	0.11	-1.23	212,217,223,266	1
56	OHX	DA	1801	7/7	0.94	0.11	-1.23	141,143,154,216	1
56	OHX	AA	3363	7/7	0.99	0.14	-1.27	90,99,133,145	1
56	OHX	BA	1665	7/7	0.98	0.14	-1.28	82,92,111,128	1
56	OHX	AA	3429	7/7	0.99	0.14	-1.28	69,73,84,102	1
56	OHX	BA	1808	7/7	0.97	0.17	-1.28	84,90,96,110	2
56	OHX	CA	3394	7/7	0.97	0.13	-1.30	97,100,116,155	1
56	OHX	AA	3455	7/7	0.99	0.17	-1.31	56,75,100,119	2
56	OHX	BA	1661	7/7	0.95	0.12	-1.31	108,124,128,170	1
56	OHX	AA	3535	7/7	0.90	0.13	-1.32	104,112,123,191	1
56	OHX	AA	3465	7/7	0.97	0.12	-1.32	85,99,124,159	1
56	OHX	CA	3418	7/7	0.96	0.12	-1.34	115,119,129,166	1
56	OHX	AA	3401	7/7	0.96	0.12	-1.35	93,112,116,173	1
56	OHX	AA	3340	7/7	0.97	0.10	-1.37	159,167,171,209	0
56	OHX	AA	3557	7/7	0.98	0.16	-1.38	75,87,101,114	1
56	OHX	CA	3421	7/7	0.88	0.14	-1.39	113,126,135,198	1
56	OHX	DA	1761	7/7	0.97	0.11	-1.39	130,132,145,205	0
56	OHX	AA	3489	7/7	0.98	0.14	-1.39	72,78,92,128	1
56	OHX	AA	3339	7/7	0.96	0.11	-1.40	151,155,164,211	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	OHX	DA	1805	7/7	0.89	0.09	-1.40	155,158,165,245	1
56	OHX	BA	1670	7/7	0.95	0.10	-1.40	135,143,147,201	1
56	OHX	CA	3354	7/7	0.99	0.15	-1.41	78,88,98,105	1
56	OHX	AA	3503	7/7	0.97	0.12	-1.41	99,121,138,179	1
56	OHX	CA	3430	7/7	0.96	0.11	-1.42	96,106,114,197	1
56	OHX	CA	3339	7/7	0.98	0.12	-1.44	100,105,127,171	1
55	MG	BN	201	1/1	0.96	0.12	-1.44	80,80,80,80	0
56	OHX	CA	3240	7/7	0.98	0.12	-1.47	96,99,103,148	1
56	OHX	AA	3560	7/7	0.94	0.14	-1.49	102,104,127,184	1
56	OHX	AA	3551	7/7	0.94	0.10	-1.49	141,143,149,194	1
56	OHX	DA	1760	7/7	0.96	0.11	-1.50	142,145,152,204	1
56	OHX	BD	102	7/7	0.88	0.10	-1.53	153,174,197,228	0
56	OHX	CA	3363	7/7	0.96	0.12	-1.53	94,99,114,167	1
56	OHX	DG	302	7/7	0.94	0.09	-1.55	133,142,147,197	1
56	OHX	CA	3340	7/7	0.94	0.13	-1.56	115,122,140,168	1
56	OHX	CB	211	7/7	0.97	0.10	-1.56	122,128,152,168	1
56	OHX	AA	3504	7/7	0.96	0.12	-1.56	112,118,129,179	1
56	OHX	CA	3410	7/7	0.94	0.11	-1.56	114,125,132,190	1
56	OHX	CA	3248	7/7	0.96	0.10	-1.58	116,128,134,203	1
56	OHX	CA	3468	7/7	0.95	0.11	-1.58	115,126,133,180	1
56	OHX	CA	3425	7/7	0.90	0.13	-1.59	101,110,125,187	1
56	OHX	DR	101	7/7	0.96	0.11	-1.59	135,141,146,189	1
56	OHX	AA	3329	7/7	0.98	0.12	-1.60	85,90,103,133	1
56	OHX	CA	3489	7/7	0.93	0.14	-1.61	91,101,112,140	1
56	OHX	AA	3537	7/7	0.86	0.11	-1.61	171,189,202,242	1
56	OHX	CA	3366	7/7	0.94	0.10	-1.62	140,148,168,207	0
56	OHX	CA	3391	7/7	0.96	0.10	-1.64	140,144,157,182	1
56	OHX	BA	1681	7/7	0.92	0.11	-1.64	153,163,173,229	1
56	OHX	AA	3330	7/7	0.97	0.13	-1.66	102,112,122,166	1
56	OHX	AA	3321	7/7	0.98	0.11	-1.66	97,109,121,173	1
56	OHX	DA	1768	7/7	0.95	0.10	-1.67	121,132,163,218	0
56	OHX	CA	3407	7/7	0.83	0.12	-1.69	142,149,155,227	1
56	OHX	AA	3313	7/7	0.95	0.16	-1.70	96,112,122,174	0
56	OHX	DA	1807	7/7	0.95	0.10	-1.71	117,126,135,195	1
56	OHX	AA	3553	7/7	0.94	0.12	-1.71	113,118,133,183	1
56	OHX	AA	3549	7/7	0.98	0.12	-1.71	97,102,111,165	1
56	OHX	BR	101	7/7	0.95	0.10	-1.74	117,129,143,169	1
56	OHX	DA	1792	7/7	0.96	0.11	-1.77	110,118,129,172	1
56	OHX	DA	1811	7/7	0.95	0.06	-1.79	137,141,149,222	1
56	OHX	AA	3561	7/7	0.95	0.10	-1.82	152,158,173,226	1
56	OHX	CB	219	7/7	0.89	0.09	-1.82	145,151,161,232	1
56	OHX	AA	3314	7/7	0.98	0.14	-1.83	81,93,123,149	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	OHX	AA	3335	7/7	0.99	0.12	-1.85	94,101,113,136	1
56	OHX	DA	1752	7/7	0.94	0.12	-1.85	107,121,128,186	1
56	OHX	CA	3484	7/7	0.96	0.12	-1.87	104,113,129,146	1
56	OHX	DA	1746	7/7	0.99	0.09	-1.88	126,134,146,189	1
56	OHX	DA	1779	7/7	0.94	0.09	-1.90	144,146,155,215	1
56	OHX	CA	3488	7/7	0.98	0.08	-1.91	113,123,127,179	1
56	OHX	BA	1793	7/7	0.96	0.10	-1.93	95,105,117,163	1
55	MG	CA	3474	1/1	0.96	0.12	-1.97	70,70,70,70	0
56	OHX	BA	1668	7/7	0.96	0.10	-1.97	116,121,137,182	1
56	OHX	AA	3302	7/7	0.96	0.14	-1.99	88,114,124,193	1
56	OHX	DA	1734	7/7	0.99	0.10	-2.00	102,105,122,149	1
56	OHX	AA	3548	7/7	0.96	0.11	-2.01	113,118,133,172	1
56	OHX	CA	3334	7/7	0.97	0.11	-2.03	110,115,136,183	0
56	OHX	DA	1772	7/7	0.96	0.09	-2.03	131,135,143,214	1
56	OHX	AA	3494	7/7	0.96	0.15	-2.05	59,86,128,185	1
56	OHX	BG	302	7/7	0.99	0.09	-2.11	128,137,145,186	1
56	OHX	BA	1809	7/7	0.95	0.10	-2.11	141,153,160,232	0
56	OHX	AA	3534	7/7	0.92	0.12	-2.13	136,141,145,222	1
56	OHX	CA	3367	7/7	0.94	0.09	-2.14	129,137,147,194	1
56	OHX	BA	1814	7/7	0.97	0.11	-2.18	101,109,125,174	1
56	OHX	DA	1789	7/7	0.96	0.06	-2.20	176,179,184,242	1
56	OHX	CA	3424	7/7	0.97	0.08	-2.20	141,145,151,214	1
56	OHX	CA	3393	7/7	0.94	0.12	-2.24	93,114,121,181	1
56	OHX	AA	3472	7/7	0.98	0.12	-2.26	120,126,137,153	1
56	OHX	BA	1794	7/7	0.94	0.11	-2.29	118,138,149,184	1
56	OHX	BA	1683	7/7	0.98	0.09	-2.30	124,130,146,183	1
56	OHX	BA	1682	7/7	0.97	0.12	-2.31	119,124,130,186	1
56	OHX	CA	3254	7/7	0.98	0.08	-2.32	167,174,181,211	0
56	OHX	CA	3422	7/7	0.91	0.11	-2.33	126,137,143,193	1
55	MG	CA	3026	1/1	0.96	0.10	-2.35	58,58,58,58	0
56	OHX	BA	1775	7/7	0.98	0.10	-2.35	111,114,129,169	1
56	OHX	BA	1786	7/7	0.98	0.11	-2.38	93,97,101,149	1
56	OHX	CA	3401	7/7	0.96	0.09	-2.42	136,149,158,185	1
56	OHX	AA	3322	7/7	0.97	0.12	-2.46	89,98,107,146	1
56	OHX	CA	3398	7/7	0.95	0.10	-2.51	129,132,142,192	1
56	OHX	BA	1765	7/7	0.99	0.12	-2.54	111,119,130,164	0
56	OHX	BA	1679	7/7	0.95	0.12	-2.54	116,125,129,189	1
56	OHX	AA	3310	7/7	0.99	0.12	-2.55	94,104,125,156	0
57	ZN	BQ	102	1/1	0.99	0.09	-2.58	130,130,130,130	0
56	OHX	AA	3371	7/7	0.96	0.14	-2.78	93,107,117,177	1
56	OHX	AA	3509	7/7	0.93	0.14	-2.93	92,96,122,175	1
56	OHX	DA	1784	7/7	0.88	0.10	-2.98	150,153,166,225	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	OHX	BA	1684	7/7	0.96	0.11	-2.98	109,118,126,149	1
56	OHX	CA	3438	7/7	0.96	0.10	-3.00	97,104,116,167	1
56	OHX	BA	1773	7/7	0.98	0.10	-3.03	101,102,110,142	1
56	OHX	CA	3382	7/7	0.96	0.10	-3.16	129,131,148,199	1
56	OHX	AA	3524	7/7	0.94	0.13	-3.19	111,120,128,172	1
56	OHX	AA	3507	7/7	0.96	0.12	-3.20	101,111,128,158	1
56	OHX	DA	1773	7/7	0.93	0.10	-3.26	122,126,137,197	1
56	OHX	CA	3362	7/7	0.97	0.08	-3.34	129,136,141,186	1
55	MG	CA	3228	1/1	0.83	0.09	-3.34	65,65,65,65	0
56	OHX	BA	1801	7/7	0.95	0.08	-3.37	118,138,142,207	1
56	OHX	AA	3520	7/7	0.97	0.11	-3.41	127,132,145,185	1
56	OHX	AA	3294	7/7	0.99	0.12	-3.42	94,100,117,120	0
56	OHX	AA	3563	7/7	0.96	0.10	-3.45	124,125,134,183	1
56	OHX	DA	1800	7/7	0.95	0.08	-3.47	137,140,150,220	1
56	OHX	CA	3381	7/7	0.96	0.11	-3.54	102,112,121,159	1
56	OHX	BA	1675	7/7	0.95	0.08	-3.56	120,128,140,197	1
56	OHX	DA	1766	7/7	0.98	0.10	-3.65	118,124,133,175	1
55	MG	AA	3194	1/1	0.97	0.12	-3.67	26,26,26,26	0
56	OHX	DA	1796	7/7	0.95	0.11	-3.67	134,139,149,195	1
56	OHX	DA	1777	7/7	0.93	0.09	-3.68	150,152,155,232	1
56	OHX	CA	3406	7/7	0.97	0.08	-3.77	151,161,169,211	1
56	OHX	BA	1672	7/7	0.89	0.11	-3.81	156,159,170,224	1
56	OHX	AA	3538	7/7	0.97	0.12	-3.89	88,94,114,159	1
56	OHX	CA	3352	7/7	0.97	0.09	-4.01	133,145,147,191	1
56	OHX	DA	1771	7/7	0.97	0.11	-4.58	97,105,129,152	1
56	OHX	CA	3380	7/7	0.96	0.09	-4.69	106,119,130,170	1
56	OHX	AA	3325	7/7	0.97	0.11	-4.92	91,103,115,154	1
55	MG	AA	3085	1/1	0.93	0.11	-5.23	58,58,58,58	0
56	OHX	BA	1694	7/7	0.91	0.08	-5.25	159,161,173,226	1
56	OHX	CA	3364	7/7	0.96	0.10	-5.46	117,120,133,182	1
56	OHX	CA	3423	7/7	0.97	0.08	-5.82	123,126,136,189	1
55	MG	BA	1637	1/1	0.84	0.07	-5.91	83,83,83,83	0
56	OHX	DA	1806	7/7	0.94	0.07	-7.86	142,150,160,228	1
55	MG	CA	3012	1/1	0.94	0.27	-	53,53,53,53	0
55	MG	BA	1633	1/1	0.84	0.17	-	59,59,59,59	0
55	MG	AA	3035	1/1	0.80	0.57	-	64,64,64,64	0
55	MG	DA	1646	1/1	0.95	0.23	-	64,64,64,64	0
56	OHX	AA	3453	7/7	0.99	0.12	-	95,106,114,148	0
55	MG	AA	3152	1/1	0.93	0.35	-	56,56,56,56	0
56	OHX	CB	213	7/7	0.93	0.12	-	131,144,166,188	1
55	MG	AA	3283	1/1	0.98	0.33	-	55,55,55,55	0
55	MG	BA	1641	1/1	0.87	0.35	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	DA	1612	1/1	0.95	0.40	-	86,86,86,86	0
55	MG	DA	1627	1/1	0.94	0.51	-	77,77,77,77	0
55	MG	AA	3054	1/1	0.95	0.33	-	49,49,49,49	0
55	MG	BA	1711	1/1	0.78	0.50	-	94,94,94,94	0
55	MG	DA	1673	1/1	0.78	0.35	-	80,80,80,80	0
55	MG	DA	1691	1/1	0.93	0.38	-	54,54,54,54	0
55	MG	DA	1611	1/1	0.84	0.28	-	92,92,92,92	0
55	MG	AA	3018	1/1	0.98	0.40	-	43,43,43,43	0
56	OHX	BA	1772	7/7	0.95	0.14	-	106,118,144,175	0
55	MG	DL	201	1/1	0.92	0.48	-	92,92,92,92	0
55	MG	AA	3061	1/1	0.91	0.42	-	49,49,49,49	0
55	MG	BA	1732	1/1	0.97	0.47	-	52,52,52,52	0
55	MG	BD	101	1/1	0.91	0.30	-	93,93,93,93	0
55	MG	AA	3095	1/1	0.70	0.39	-	89,89,89,89	0
55	MG	DA	1662	1/1	0.86	0.36	-	73,73,73,73	0
56	OHX	AA	3567	7/7	0.91	0.14	-	103,106,118,172	1
56	OHX	BA	1676	7/7	0.95	0.11	-	143,151,156,210	1
55	MG	BA	1647	1/1	0.91	0.18	-	112,112,112,112	0
55	MG	CA	3459	1/1	0.93	0.29	-	56,56,56,56	0
55	MG	AA	3053	1/1	0.95	0.46	-	60,60,60,60	0
55	MG	BA	1703	1/1	0.72	0.50	-	108,108,108,108	0
55	MG	DA	1622	1/1	0.77	0.20	-	122,122,122,122	0
55	MG	AA	3216	1/1	0.84	0.44	-	71,71,71,71	0
56	OHX	CA	3359	7/7	0.91	0.14	-	115,123,136,171	2
55	MG	CA	3203	1/1	0.92	0.40	-	47,47,47,47	0
55	MG	AA	3101	1/1	0.94	0.44	-	63,63,63,63	0
55	MG	AA	3256	1/1	0.91	0.54	-	53,53,53,53	0
55	MG	DA	1642	1/1	0.79	0.45	-	112,112,112,112	0
56	OHX	AA	3546	7/7	0.94	0.16	-	98,103,119,179	1
55	MG	DA	1609	1/1	0.94	0.37	-	91,91,91,91	0
55	MG	AA	3239	1/1	0.95	0.28	-	44,44,44,44	0
56	OHX	CA	3308	7/7	0.97	0.17	-	88,90,121,161	0
55	MG	DA	1602	1/1	0.97	0.41	-	68,68,68,68	0
56	OHX	CA	3415	7/7	0.94	0.13	-	134,135,143,187	1
55	MG	AA	3098	1/1	0.91	0.30	-	77,77,77,77	0
56	OHX	AB	212	7/7	0.95	0.17	-	81,99,131,153	1
55	MG	CA	3257	1/1	0.97	0.30	-	60,60,60,60	0
55	MG	AA	3060	1/1	0.98	0.23	-	70,70,70,70	0
56	OHX	AA	3328	7/7	0.98	0.11	-	89,97,114,142	1
56	OHX	DA	1759	7/7	0.97	0.11	-	120,137,147,190	0
56	OHX	AA	3491	7/7	0.88	0.15	-	162,182,190,220	1
55	MG	AA	3028	1/1	0.88	0.38	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	OHX	DA	1797	7/7	0.97	0.06	-	149,152,159,218	1
55	MG	BA	1613	1/1	0.92	0.30	-	65,65,65,65	0
55	MG	AA	3243	1/1	0.96	0.39	-	51,51,51,51	0
55	MG	AA	3134	1/1	0.93	0.21	-	82,82,82,82	0
55	MG	BA	1606	1/1	0.84	0.42	-	92,92,92,92	0
55	MG	AA	3217	1/1	0.92	0.45	-	60,60,60,60	0
55	MG	CA	3137	1/1	0.83	0.43	-	74,74,74,74	0
56	OHX	CA	3353	7/7	0.97	0.15	-	81,96,110,140	1
55	MG	AA	3042	1/1	0.97	0.29	-	43,43,43,43	0
55	MG	BA	1623	1/1	0.98	0.30	-	67,67,67,67	0
55	MG	BA	1621	1/1	0.92	0.45	-	55,55,55,55	0
55	MG	AA	3389	1/1	0.90	0.36	-	44,44,44,44	0
55	MG	AA	3174	1/1	0.80	0.49	-	76,76,76,76	0
55	MG	CA	3197	1/1	0.89	0.40	-	79,79,79,79	0
56	OHX	AA	3438	7/7	0.99	0.17	-	51,64,72,96	2
56	OHX	AA	3484	7/7	0.90	0.20	-	76,100,111,147	2
55	MG	DA	1660	1/1	0.79	0.48	-	88,88,88,88	0
55	MG	CA	3125	1/1	0.95	0.20	-	52,52,52,52	0
56	OHX	CA	3467	7/7	0.93	0.12	-	131,146,152,199	1
56	OHX	CA	3385	7/7	0.95	0.11	-	115,124,135,193	1
56	OHX	DA	1794	7/7	0.84	0.14	-	124,130,139,205	1
56	OHX	DA	1731	7/7	0.97	0.10	-	129,139,145,172	1
55	MG	CA	3103	1/1	0.92	0.24	-	70,70,70,70	0
55	MG	AA	3269	1/1	0.95	0.41	-	72,72,72,72	0
55	MG	DA	1712	1/1	0.86	0.31	-	98,98,98,98	0
56	OHX	BA	1797	7/7	0.94	0.22	-	71,104,132,136	3
55	MG	CA	3095	1/1	0.82	0.26	-	54,54,54,54	0
55	MG	AA	3246	1/1	0.93	0.39	-	36,36,36,36	0
55	MG	AA	3236	1/1	0.86	0.40	-	40,40,40,40	0
55	MG	AA	3180	1/1	0.88	0.31	-	65,65,65,65	0
55	MG	AA	3119	1/1	0.86	0.37	-	64,64,64,64	0
56	OHX	AA	3303	7/7	0.98	0.13	-	93,102,117,145	1
56	OHX	AA	3298	7/7	0.98	0.21	-	71,88,99,110	1
55	MG	AA	3017	1/1	0.81	0.49	-	100,100,100,100	0
55	MG	DA	1713	1/1	0.87	0.41	-	79,79,79,79	0
55	MG	BA	1722	1/1	0.91	0.52	-	91,91,91,91	0
55	MG	AA	3163	1/1	0.92	0.35	-	61,61,61,61	0
56	OHX	AA	3306	7/7	0.90	0.12	-	134,139,151,214	1
56	OHX	BA	1807	7/7	0.98	0.09	-	135,141,150,224	0
55	MG	CA	3204	1/1	0.84	0.41	-	73,73,73,73	0
56	OHX	AA	3364	7/7	0.98	0.16	-	92,103,108,119	1
56	OHX	AA	3406	7/7	0.97	0.24	-	84,92,109,162	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	AF	302	1/1	0.91	0.30	-	81,81,81,81	0
55	MG	AA	3204	1/1	0.94	0.16	-	61,61,61,61	0
56	OHX	BA	1787	7/7	0.96	0.13	-	107,117,138,149	2
55	MG	BA	1729	1/1	0.92	0.53	-	73,73,73,73	0
56	OHX	C3	101	7/7	0.89	0.16	-	119,129,151,179	2
55	MG	DA	1654	1/1	0.90	0.36	-	61,61,61,61	0
55	MG	DA	1682	1/1	0.80	0.57	-	87,87,87,87	0
56	OHX	BA	1689	7/7	0.92	0.13	-	113,130,139,190	1
55	MG	CA	3053	1/1	0.88	0.16	-	99,99,99,99	0
55	MG	AA	3114	1/1	0.94	0.37	-	47,47,47,47	0
56	OHX	DA	1758	7/7	0.98	0.08	-	132,137,143,204	0
55	MG	AA	3023	1/1	0.93	0.50	-	52,52,52,52	0
55	MG	BA	1639	1/1	0.89	0.10	-	102,102,102,102	0
55	MG	AA	3176	1/1	0.98	0.20	-	60,60,60,60	0
56	OHX	DA	1809	7/7	0.95	0.09	-	124,126,139,221	1
55	MG	AA	3127	1/1	0.87	0.37	-	57,57,57,57	0
55	MG	BA	1631	1/1	0.76	0.30	-	78,78,78,78	0
56	OHX	CA	3387	7/7	0.92	0.16	-	111,127,150,170	2
55	MG	AA	3162	1/1	0.86	0.55	-	38,38,38,38	0
55	MG	AA	3047	1/1	0.98	0.37	-	54,54,54,54	0
55	MG	AB	203	1/1	0.91	0.46	-	71,71,71,71	0
56	OHX	AA	3497	7/7	0.97	0.15	-	94,106,111,138	2
55	MG	AA	3078	1/1	0.94	0.32	-	59,59,59,59	0
56	OHX	CA	3466	7/7	0.94	0.15	-	96,98,116,157	1
55	MG	DA	1679	1/1	0.88	0.28	-	69,69,69,69	0
55	MG	BA	1650	1/1	0.84	0.55	-	72,72,72,72	0
55	MG	CA	3079	1/1	0.78	0.29	-	73,73,73,73	0
55	MG	AA	3273	1/1	0.91	0.57	-	66,66,66,66	0
55	MG	DA	1606	1/1	0.93	0.19	-	84,84,84,84	0
56	OHX	CA	3251	7/7	0.98	0.13	-	88,107,125,141	1
55	MG	BA	1609	1/1	0.90	0.32	-	73,73,73,73	0
56	OHX	AA	3566	7/7	0.90	0.19	-	92,97,126,175	2
55	MG	DA	1635	1/1	0.83	0.41	-	96,96,96,96	0
56	OHX	AA	3447	7/7	0.97	0.15	-	91,102,120,163	1
55	MG	AA	3073	1/1	0.96	0.33	-	69,69,69,69	0
55	MG	CA	3445	1/1	0.96	0.23	-	38,38,38,38	0
55	MG	AA	3182	1/1	0.97	0.55	-	45,45,45,45	0
55	MG	AA	3398	1/1	0.94	0.40	-	51,51,51,51	0
55	MG	CA	3167	1/1	0.96	0.48	-	75,75,75,75	0
55	MG	CA	3442	1/1	0.93	0.21	-	61,61,61,61	0
56	OHX	DA	1798	7/7	0.94	0.09	-	128,133,140,212	1
55	MG	AA	3344	1/1	0.97	0.39	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	AA	3030	1/1	0.98	0.34	-	44,44,44,44	0
55	MG	DA	1694	1/1	0.83	0.38	-	104,104,104,104	0
55	MG	DA	1690	1/1	0.90	0.43	-	63,63,63,63	0
56	OHX	CA	3238	7/7	0.98	0.17	-	80,102,103,125	1
55	MG	AA	3009	1/1	0.71	0.42	-	89,89,89,89	0
55	MG	AA	3170	1/1	0.92	0.20	-	50,50,50,50	0
55	MG	AA	3086	1/1	0.93	0.38	-	95,95,95,95	0
55	MG	AA	3278	1/1	0.96	0.43	-	35,35,35,35	0
56	OHX	BA	1771	7/7	0.96	0.20	-	77,100,122,150	1
55	MG	DA	1670	1/1	0.85	0.40	-	64,64,64,64	0
55	MG	CA	3478	1/1	0.84	0.48	-	82,82,82,82	0
55	MG	DA	1685	1/1	0.97	0.17	-	59,59,59,59	0
55	MG	BA	1604	1/1	0.80	0.42	-	72,72,72,72	0
55	MG	CA	3144	1/1	0.98	0.34	-	54,54,54,54	0
55	MG	CA	3003	1/1	0.97	0.37	-	51,51,51,51	0
56	OHX	DA	1721	7/7	0.99	0.14	-	94,108,116,135	0
55	MG	AA	3264	1/1	0.79	0.42	-	76,76,76,76	0
55	MG	CA	3005	1/1	0.82	0.21	-	48,48,48,48	0
55	MG	CA	3063	1/1	0.94	0.25	-	70,70,70,70	0
55	MG	CA	3458	1/1	0.91	0.23	-	82,82,82,82	0
55	MG	CA	3154	1/1	0.92	0.32	-	46,46,46,46	0
56	OHX	AA	3446	7/7	0.99	0.15	-	68,90,101,115	2
56	OHX	DA	1741	7/7	0.97	0.14	-	97,116,128,170	1
56	OHX	AA	3522	7/7	0.84	0.17	-	118,131,145,201	1
55	MG	AA	3132	1/1	0.76	0.51	-	81,81,81,81	0
56	OHX	AA	3545	7/7	0.87	0.21	-	90,96,105,167	2
55	MG	CA	3056	1/1	0.92	0.49	-	79,79,79,79	0
55	MG	AA	3167	1/1	0.96	0.53	-	53,53,53,53	0
55	MG	AA	3092	1/1	0.79	0.17	-	73,73,73,73	0
56	OHX	DA	1730	7/7	0.97	0.15	-	102,111,123,157	0
55	MG	AA	3117	1/1	0.92	0.33	-	48,48,48,48	0
55	MG	CA	3070	1/1	0.93	0.24	-	44,44,44,44	0
55	MG	BB	103	1/1	0.90	0.35	-	91,91,91,91	0
55	MG	AA	3149	1/1	0.84	0.32	-	74,74,74,74	0
55	MG	CA	3017	1/1	0.91	0.21	-	92,92,92,92	0
56	OHX	BA	1776	7/7	0.99	0.13	-	102,114,119,153	1
55	MG	AA	3192	1/1	0.93	0.39	-	48,48,48,48	0
55	MG	AA	3144	1/1	0.91	0.55	-	71,71,71,71	0
55	MG	AA	3128	1/1	0.89	0.38	-	54,54,54,54	0
55	MG	AA	3254	1/1	0.92	0.33	-	42,42,42,42	0
55	MG	AA	3136	1/1	0.86	0.27	-	57,57,57,57	0
55	MG	DA	1636	1/1	0.89	0.31	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	CA	3447	1/1	0.84	0.46	-	58,58,58,58	0
55	MG	AA	3357	1/1	0.96	0.40	-	73,73,73,73	0
55	MG	AA	3161	1/1	0.96	0.32	-	50,50,50,50	0
55	MG	AA	3048	1/1	0.77	0.62	-	94,94,94,94	0
56	OHX	CA	3402	7/7	0.91	0.11	-	159,162,170,218	1
55	MG	AA	3281	1/1	0.90	0.52	-	70,70,70,70	0
55	MG	AO	203	1/1	0.91	0.28	-	56,56,56,56	0
56	OHX	DA	1738	7/7	0.98	0.10	-	115,122,137,171	1
56	OHX	BA	1657	7/7	0.82	0.19	-	116,125,141,215	1
55	MG	DC	103	1/1	0.65	0.29	-	96,96,96,96	0
55	MG	CA	3097	1/1	0.88	0.34	-	67,67,67,67	0
55	MG	DA	1618	1/1	0.93	0.26	-	105,105,105,105	0
55	MG	DA	1615	1/1	0.95	0.28	-	98,98,98,98	0
55	MG	AA	3041	1/1	0.95	0.24	-	49,49,49,49	0
55	MG	DA	1625	1/1	0.99	0.14	-	97,97,97,97	0
56	OHX	DB	105	7/7	0.88	0.20	-	88,91,103,175	5
55	MG	AO	201	1/1	0.90	0.40	-	80,80,80,80	0
56	OHX	DA	1780	7/7	0.98	0.09	-	127,131,138,167	1
55	MG	AA	3191	1/1	0.90	0.30	-	45,45,45,45	0
55	MG	BA	1607	1/1	0.92	0.39	-	93,93,93,93	0
55	MG	CA	3199	1/1	0.92	0.34	-	62,62,62,62	0
55	MG	B1	101	1/1	0.99	0.50	-	26,26,26,26	0
55	MG	CA	3157	1/1	0.90	0.31	-	76,76,76,76	0
55	MG	CA	3149	1/1	0.93	0.39	-	55,55,55,55	0
56	OHX	AA	3473	7/7	0.96	0.17	-	66,95,102,124	1
55	MG	BA	1702	1/1	0.82	0.27	-	62,62,62,62	0
55	MG	AA	3409	1/1	0.86	0.48	-	56,56,56,56	0
55	MG	CA	3219	1/1	0.94	0.54	-	79,79,79,79	0
55	MG	BA	1603	1/1	0.88	0.32	-	63,63,63,63	0
56	OHX	CA	3365	7/7	0.96	0.08	-	164,171,176,213	1
55	MG	AA	3242	1/1	0.98	0.36	-	37,37,37,37	0
56	OHX	CA	3298	7/7	0.97	0.14	-	90,98,134,148	0
55	MG	CA	3225	1/1	0.90	0.28	-	48,48,48,48	0
55	MG	DA	1613	1/1	0.87	0.25	-	87,87,87,87	0
55	MG	AA	3240	1/1	0.97	0.33	-	43,43,43,43	0
55	MG	AA	3148	1/1	0.97	0.37	-	65,65,65,65	0
56	OHX	BA	1762	7/7	0.99	0.17	-	72,94,107,136	0
56	OHX	AA	3558	7/7	0.97	0.11	-	95,121,125,156	1
55	MG	DA	1626	1/1	0.84	0.52	-	84,84,84,84	0
55	MG	AA	3093	1/1	0.92	0.47	-	91,91,91,91	0
55	MG	DA	1629	1/1	0.79	0.22	-	93,93,93,93	0
55	MG	AA	3253	1/1	0.93	0.39	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	CA	3112	1/1	0.94	0.35	-	41,41,41,41	0
55	MG	AA	3248	1/1	0.71	0.39	-	86,86,86,86	0
55	MG	AA	3181	1/1	0.92	0.46	-	61,61,61,61	0
55	MG	AA	3131	1/1	0.93	0.32	-	94,94,94,94	0
55	MG	AA	3051	1/1	0.99	0.35	-	49,49,49,49	0
55	MG	BA	1751	1/1	0.41	0.48	-	95,95,95,95	0
55	MG	AA	3228	1/1	0.94	0.28	-	67,67,67,67	0
55	MG	CA	3092	1/1	0.96	0.54	-	52,52,52,52	0
55	MG	BA	1715	1/1	0.94	0.36	-	74,74,74,74	0
56	OHX	BA	1782	7/7	0.97	0.14	-	133,144,159,198	0
56	OHX	CA	3408	7/7	0.95	0.09	-	136,139,143,209	1
55	MG	CA	3189	1/1	0.95	0.41	-	67,67,67,67	0
56	OHX	CA	3342	7/7	0.96	0.14	-	116,123,130,201	1
56	OHX	AB	213	7/7	0.97	0.18	-	85,93,130,132	3
55	MG	BA	1612	1/1	0.94	0.39	-	81,81,81,81	0
55	MG	CA	3168	1/1	0.88	0.40	-	72,72,72,72	0
55	MG	CA	3187	1/1	0.62	0.41	-	86,86,86,86	0
56	OHX	BA	1781	7/7	0.97	0.13	-	91,111,121,156	1
56	OHX	CA	3284	7/7	0.88	0.13	-	136,147,155,216	1
55	MG	CA	3180	1/1	0.88	0.32	-	75,75,75,75	0
56	OHX	CA	3316	7/7	0.99	0.10	-	119,122,129,158	0
55	MG	AA	3267	1/1	0.92	0.41	-	80,80,80,80	0
55	MG	DC	102	1/1	0.90	0.41	-	69,69,69,69	0
55	MG	DA	1725	1/1	0.65	0.41	-	87,87,87,87	0
55	MG	AA	3392	1/1	0.90	0.62	-	64,64,64,64	0
55	MG	AA	3391	1/1	0.90	0.28	-	59,59,59,59	0
56	OHX	DA	1751	7/7	0.95	0.19	-	66,109,137,183	2
55	MG	BB	104	1/1	0.74	0.50	-	87,87,87,87	0
56	OHX	AA	3502	7/7	0.98	0.11	-	97,102,112,146	1
56	OHX	BA	1663	7/7	0.97	0.10	-	132,137,143,190	1
55	MG	AA	3223	1/1	0.90	0.37	-	56,56,56,56	0
55	MG	CA	3226	1/1	0.87	0.45	-	65,65,65,65	0
55	MG	BC	105	1/1	0.80	0.47	-	87,87,87,87	0
56	OHX	AA	3334	7/7	0.98	0.17	-	66,79,94,105	1
55	MG	CA	3046	1/1	0.67	0.27	-	76,76,76,76	0
55	MG	CA	3102	1/1	0.96	0.46	-	67,67,67,67	0
56	OHX	DA	1757	7/7	0.94	0.12	-	123,127,134,157	1
56	OHX	CA	3294	7/7	0.98	0.14	-	91,93,107,125	1
55	MG	CA	3011	1/1	0.98	0.35	-	46,46,46,46	0
55	MG	AA	3249	1/1	0.88	0.41	-	58,58,58,58	0
56	OHX	AA	3462	7/7	0.99	0.15	-	75,85,103,106	1
55	MG	CA	3129	1/1	0.80	0.60	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	OHX	CA	3412	7/7	0.95	0.15	-	99,116,129,164	2
55	MG	CA	3212	1/1	0.93	0.46	-	75,75,75,75	0
55	MG	AA	3094	1/1	0.97	0.55	-	39,39,39,39	0
55	MG	BA	1734	1/1	0.83	0.45	-	70,70,70,70	0
55	MG	AA	3139	1/1	0.90	0.37	-	48,48,48,48	0
56	OHX	CA	3253	7/7	0.96	0.15	-	107,120,133,155	1
55	MG	DA	1633	1/1	0.90	0.51	-	74,74,74,74	0
55	MG	BA	1648	1/1	0.43	0.49	-	99,99,99,99	0
55	MG	BA	1712	1/1	0.83	0.56	-	95,95,95,95	0
55	MG	CA	3195	1/1	0.94	0.24	-	68,68,68,68	0
56	OHX	CB	215	7/7	0.89	0.14	-	108,133,144,220	1
55	MG	AA	3411	1/1	0.95	0.32	-	63,63,63,63	0
55	MG	DA	1620	1/1	0.92	0.50	-	79,79,79,79	0
56	OHX	DA	1742	7/7	0.99	0.10	-	117,127,141,176	1
55	MG	AA	3270	1/1	0.85	0.10	-	94,94,94,94	0
55	MG	CA	3016	1/1	0.96	0.23	-	55,55,55,55	0
55	MG	AA	3156	1/1	0.93	0.46	-	45,45,45,45	0
55	MG	CA	3156	1/1	0.89	0.37	-	84,84,84,84	0
55	MG	CA	3473	1/1	0.97	0.29	-	50,50,50,50	0
55	MG	AB	206	1/1	0.88	0.56	-	83,83,83,83	0
55	MG	DA	1696	1/1	0.57	0.21	-	112,112,112,112	0
55	MG	CA	3088	1/1	0.68	0.40	-	86,86,86,86	0
55	MG	CB	206	1/1	0.92	0.32	-	83,83,83,83	0
55	MG	BA	1741	1/1	0.93	0.48	-	73,73,73,73	0
56	OHX	CA	3307	7/7	0.97	0.12	-	92,104,131,164	0
55	MG	CA	3184	1/1	0.85	0.41	-	60,60,60,60	0
55	MG	D1	101	1/1	0.66	0.36	-	78,78,78,78	0
55	MG	BA	1615	1/1	0.82	0.26	-	113,113,113,113	0
55	MG	CA	3038	1/1	0.77	0.17	-	74,74,74,74	0
56	OHX	BA	1783	7/7	0.95	0.20	-	77,87,125,141	2
55	MG	DA	1665	1/1	0.85	0.48	-	70,70,70,70	0
55	MG	AA	3122	1/1	0.87	0.43	-	62,62,62,62	0
56	OHX	CA	3329	7/7	0.99	0.11	-	102,103,123,146	1
55	MG	AE	303	1/1	0.92	0.28	-	32,32,32,32	0
55	MG	DB	101	1/1	0.79	0.42	-	78,78,78,78	0
55	MG	BA	1710	1/1	0.68	0.51	-	97,97,97,97	0
55	MG	AA	3102	1/1	0.92	0.40	-	79,79,79,79	0
55	MG	AA	3227	1/1	0.86	0.40	-	63,63,63,63	0
55	MG	BA	1752	1/1	0.98	0.47	-	53,53,53,53	0
55	MG	AA	3123	1/1	0.94	0.24	-	72,72,72,72	0
56	OHX	DA	1765	7/7	0.88	0.23	-	117,133,141,227	1
55	MG	DA	1648	1/1	0.91	0.10	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	OHX	BA	1796	7/7	0.92	0.12	-	143,156,164,225	0
55	MG	BA	1750	1/1	0.89	0.42	-	72,72,72,72	0
55	MG	CA	3076	1/1	0.84	0.40	-	64,64,64,64	0
55	MG	DC	104	1/1	0.94	0.40	-	77,77,77,77	0
55	MG	AA	3277	1/1	0.96	0.48	-	46,46,46,46	0
55	MG	CA	3098	1/1	0.97	0.16	-	63,63,63,63	0
55	MG	DA	1705	1/1	0.87	0.47	-	108,108,108,108	0
55	MG	CA	3047	1/1	0.97	0.38	-	41,41,41,41	0
56	OHX	BA	1680	7/7	0.92	0.11	-	120,125,145,238	1
55	MG	AA	3074	1/1	0.91	0.36	-	73,73,73,73	0
55	MG	AA	3226	1/1	0.98	0.48	-	42,42,42,42	0
55	MG	CA	3085	1/1	0.72	0.32	-	102,102,102,102	0
55	MG	AA	3021	1/1	0.84	0.51	-	80,80,80,80	0
55	MG	AA	3280	1/1	0.88	0.40	-	77,77,77,77	0
55	MG	AA	3259	1/1	0.91	0.35	-	35,35,35,35	0
55	MG	CA	3205	1/1	0.84	0.31	-	63,63,63,63	0
55	MG	AA	3058	1/1	0.85	0.32	-	73,73,73,73	0
55	MG	CA	3159	1/1	0.86	0.33	-	75,75,75,75	0
55	MG	BB	102	1/1	0.93	0.27	-	85,85,85,85	0
55	MG	BA	1716	1/1	0.90	0.36	-	55,55,55,55	0
56	OHX	AA	3562	7/7	0.90	0.16	-	98,105,127,189	1
56	OHX	CA	3426	7/7	0.93	0.09	-	142,146,155,215	1
55	MG	AA	3120	1/1	0.88	0.27	-	71,71,71,71	0
55	MG	AA	3012	1/1	0.95	0.32	-	46,46,46,46	0
56	OHX	AA	3402	7/7	0.94	0.21	-	87,110,129,141	3
55	MG	AA	3155	1/1	0.91	0.13	-	85,85,85,85	0
56	OHX	CA	3344	7/7	0.95	0.17	-	96,110,117,162	1
55	MG	AA	3097	1/1	0.83	0.23	-	59,59,59,59	0
55	MG	CA	3054	1/1	0.96	0.30	-	54,54,54,54	0
55	MG	CA	3477	1/1	0.78	0.42	-	60,60,60,60	0
56	OHX	DA	1724	7/7	0.98	0.14	-	84,106,133,148	1
55	MG	BA	1746	1/1	0.59	0.40	-	82,82,82,82	0
55	MG	CA	3115	1/1	0.91	0.37	-	63,63,63,63	0
56	OHX	DA	1756	7/7	0.95	0.10	-	145,145,160,212	1
55	MG	CA	3041	1/1	0.95	0.25	-	73,73,73,73	0
55	MG	AA	3388	1/1	0.99	0.43	-	41,41,41,41	0
55	MG	AA	3285	1/1	0.84	0.50	-	80,80,80,80	0
56	OHX	AB	214	7/7	0.95	0.16	-	110,118,132,162	1
56	OHX	C5	102	7/7	0.96	0.14	-	114,118,133,165	1
55	MG	AA	3005	1/1	0.94	0.41	-	43,43,43,43	0
55	MG	AA	3247	1/1	0.88	0.35	-	81,81,81,81	0
56	OHX	AA	3448	7/7	0.98	0.14	-	87,90,112,131	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	OHX	AA	3482	7/7	0.97	0.12	-	105,118,127,177	1
56	OHX	AA	3467	7/7	0.98	0.12	-	100,105,117,133	1
55	MG	CA	3201	1/1	0.81	0.51	-	79,79,79,79	0
55	MG	AA	3007	1/1	0.97	0.26	-	31,31,31,31	0
55	MG	BA	1720	1/1	0.79	0.51	-	58,58,58,58	0
56	OHX	AA	3515	7/7	0.95	0.14	-	100,121,139,211	1
55	MG	DA	1672	1/1	0.89	0.31	-	83,83,83,83	0
55	MG	AA	3257	1/1	0.90	0.41	-	57,57,57,57	0
55	MG	AA	3010	1/1	0.94	0.26	-	40,40,40,40	0
55	MG	CB	201	1/1	0.93	0.24	-	77,77,77,77	0
55	MG	CA	3150	1/1	0.94	0.35	-	55,55,55,55	0
55	MG	CA	3140	1/1	0.82	0.37	-	59,59,59,59	0
55	MG	DA	1630	1/1	0.76	0.34	-	95,95,95,95	0
55	MG	AA	3207	1/1	0.94	0.47	-	57,57,57,57	0
55	MG	AA	3237	1/1	0.94	0.34	-	45,45,45,45	0
55	MG	AA	3115	1/1	0.99	0.32	-	51,51,51,51	0
55	MG	AA	3141	1/1	0.92	0.55	-	44,44,44,44	0
56	OHX	CA	3317	7/7	0.97	0.10	-	116,126,142,180	1
56	OHX	A3	102	7/7	0.98	0.14	-	90,98,113,134	2
55	MG	BA	1638	1/1	0.98	0.33	-	57,57,57,57	0
55	MG	CA	3266	1/1	0.93	0.33	-	64,64,64,64	0
55	MG	AA	3229	1/1	0.90	0.50	-	59,59,59,59	0
55	MG	CA	3198	1/1	0.73	0.30	-	118,118,118,118	0
56	OHX	BA	1662	7/7	0.94	0.14	-	105,117,141,193	1
55	MG	BA	1713	1/1	0.84	0.27	-	59,59,59,59	0
55	MG	BA	1618	1/1	0.64	0.39	-	63,63,63,63	0
56	OHX	CB	210	7/7	0.96	0.15	-	104,124,140,171	1
55	MG	DA	1651	1/1	0.98	0.45	-	62,62,62,62	0
56	OHX	CA	3434	7/7	0.92	0.14	-	96,110,126,177	1
55	MG	BA	1717	1/1	0.94	0.45	-	51,51,51,51	0
55	MG	AA	3225	1/1	0.96	0.30	-	63,63,63,63	0
55	MG	BA	1630	1/1	0.94	0.12	-	90,90,90,90	0
55	MG	CA	3116	1/1	0.96	0.39	-	69,69,69,69	0
56	OHX	CA	3249	7/7	0.98	0.17	-	86,90,104,128	1
55	MG	BA	1649	1/1	0.94	0.28	-	74,74,74,74	0
55	MG	AA	3125	1/1	0.90	0.34	-	92,92,92,92	0
55	MG	DC	105	1/1	0.83	0.51	-	54,54,54,54	0
55	MG	CA	3179	1/1	0.78	0.12	-	73,73,73,73	0
55	MG	BA	1727	1/1	0.76	0.43	-	70,70,70,70	0
56	OHX	AA	3315	7/7	0.99	0.13	-	89,99,111,137	1
56	OHX	DA	1776	7/7	0.97	0.10	-	114,116,125,160	1
55	MG	AA	3103	1/1	0.86	0.11	-	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	CA	3057	1/1	0.78	0.36	-	95,95,95,95	0
56	OHX	CA	3379	7/7	0.93	0.11	-	134,137,155,207	1
55	MG	AA	3033	1/1	0.98	0.37	-	48,48,48,48	0
56	OHX	AA	3544	7/7	0.91	0.18	-	103,105,124,176	1
56	OHX	BA	1792	7/7	0.95	0.09	-	150,163,168,209	1
55	MG	CA	3045	1/1	0.94	0.62	-	91,91,91,91	0
56	OHX	AA	3490	7/7	0.92	0.16	-	94,113,129,158	1
56	OHX	AA	3501	7/7	0.98	0.16	-	101,109,129,149	1
56	OHX	AA	3469	7/7	0.97	0.12	-	79,91,98,161	1
55	MG	BA	1658	1/1	0.84	0.41	-	71,71,71,71	0
55	MG	DA	1703	1/1	0.97	0.46	-	73,73,73,73	0
55	MG	AA	3071	1/1	0.97	0.60	-	68,68,68,68	0
55	MG	CA	3158	1/1	0.95	0.41	-	56,56,56,56	0
55	MG	CA	3206	1/1	0.78	0.46	-	90,90,90,90	0
55	MG	BA	1721	1/1	0.86	0.39	-	70,70,70,70	0
55	MG	DA	1717	1/1	0.79	0.26	-	100,100,100,100	0
55	MG	DB	102	1/1	0.92	0.25	-	102,102,102,102	0
56	OHX	CA	3369	7/7	0.98	0.15	-	97,113,121,158	1
55	MG	AA	3129	1/1	0.92	0.32	-	83,83,83,83	0
55	MG	BA	1619	1/1	0.96	0.27	-	50,50,50,50	0
55	MG	CA	3059	1/1	0.85	0.41	-	63,63,63,63	0
55	MG	DA	1644	1/1	0.93	0.14	-	149,149,149,149	0
56	OHX	BB	106	7/7	0.96	0.13	-	164,167,173,198	1
55	MG	DA	1666	1/1	0.94	0.44	-	62,62,62,62	0
56	OHX	CA	3400	7/7	0.95	0.13	-	116,133,145,220	1
56	OHX	AA	3529	7/7	0.94	0.17	-	90,106,115,167	1
55	MG	CA	3194	1/1	0.95	0.25	-	63,63,63,63	0
55	MG	AA	3203	1/1	0.98	0.32	-	50,50,50,50	0
56	OHX	CA	3326	7/7	0.99	0.12	-	97,110,130,136	2
55	MG	BA	1730	1/1	0.74	0.55	-	73,73,73,73	0
56	OHX	BA	1659	7/7	0.94	0.16	-	114,130,135,179	1
55	MG	AA	3015	1/1	0.70	0.43	-	76,76,76,76	0
55	MG	AA	3215	1/1	0.89	0.52	-	50,50,50,50	0
55	MG	CA	3163	1/1	0.96	0.40	-	80,80,80,80	0
55	MG	AA	3130	1/1	0.89	0.33	-	75,75,75,75	0
55	MG	DA	1634	1/1	0.73	0.10	-	118,118,118,118	0
55	MG	DA	1689	1/1	0.93	0.39	-	87,87,87,87	0
55	MG	CA	3111	1/1	0.98	0.41	-	30,30,30,30	0
55	MG	AA	3014	1/1	0.97	0.45	-	44,44,44,44	0
55	MG	AA	3260	1/1	0.82	0.52	-	58,58,58,58	0
55	MG	CA	3479	1/1	0.90	0.47	-	64,64,64,64	0
55	MG	CA	3013	1/1	0.91	0.20	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	BA	1748	1/1	0.78	0.24	-	66,66,66,66	0
55	MG	BA	1617	1/1	0.88	0.48	-	71,71,71,71	0
55	MG	BA	1708	1/1	0.88	0.42	-	77,77,77,77	0
56	OHX	DA	1802	7/7	0.97	0.12	-	120,122,140,196	1
55	MG	AA	3099	1/1	0.90	0.30	-	65,65,65,65	0
55	MG	BA	1747	1/1	0.85	0.39	-	74,74,74,74	0
55	MG	CA	3229	1/1	0.86	0.39	-	80,80,80,80	0
55	MG	CA	3106	1/1	0.97	0.27	-	61,61,61,61	0
55	MG	CA	3077	1/1	0.85	0.24	-	57,57,57,57	0
55	MG	BA	1707	1/1	0.88	0.31	-	70,70,70,70	0
55	MG	AB	205	1/1	0.91	0.33	-	50,50,50,50	0
55	MG	CA	3260	1/1	0.89	0.24	-	71,71,71,71	0
55	MG	CA	3025	1/1	0.96	0.18	-	83,83,83,83	0
55	MG	CA	3086	1/1	0.87	0.39	-	68,68,68,68	0
55	MG	BB	101	1/1	0.93	0.49	-	70,70,70,70	0
55	MG	BA	1614	1/1	0.87	0.36	-	73,73,73,73	0
56	OHX	CA	3411	7/7	0.94	0.11	-	117,123,138,184	1
55	MG	CA	3044	1/1	0.90	0.16	-	74,74,74,74	0
55	MG	AA	3238	1/1	0.90	0.55	-	50,50,50,50	0
55	MG	C7	101	1/1	0.89	0.39	-	54,54,54,54	0
55	MG	AA	3218	1/1	0.85	0.39	-	82,82,82,82	0
56	OHX	CB	209	7/7	0.95	0.17	-	117,133,147,190	1
55	MG	AA	3211	1/1	0.97	0.52	-	62,62,62,62	0
55	MG	DA	1639	1/1	0.96	0.45	-	70,70,70,70	0
55	MG	BA	1643	1/1	0.91	0.11	-	78,78,78,78	0
55	MG	DA	1711	1/1	0.93	0.23	-	107,107,107,107	0
56	OHX	AA	3486	7/7	0.96	0.17	-	127,135,138,199	1
56	OHX	CA	3358	7/7	0.93	0.11	-	128,130,147,230	1
55	MG	CA	3166	1/1	0.97	0.51	-	58,58,58,58	0
55	MG	CA	3143	1/1	0.93	0.37	-	60,60,60,60	0
55	MG	CA	3055	1/1	0.98	0.28	-	66,66,66,66	0
55	MG	CA	3052	1/1	0.98	0.39	-	66,66,66,66	0
56	OHX	AA	3521	7/7	0.98	0.13	-	87,94,107,160	1
55	MG	A5	101	1/1	0.95	0.24	-	41,41,41,41	0
55	MG	BA	1642	1/1	0.94	0.23	-	102,102,102,102	0
55	MG	CA	3185	1/1	0.87	0.46	-	75,75,75,75	0
55	MG	AA	3140	1/1	0.94	0.24	-	41,41,41,41	0
55	MG	CA	3174	1/1	0.94	0.48	-	52,52,52,52	0
56	OHX	CA	3427	7/7	0.92	0.10	-	114,126,136,203	1
56	OHX	CA	3242	7/7	0.99	0.14	-	95,107,117,129	1
56	OHX	CA	3404	7/7	0.93	0.10	-	149,155,166,217	1
55	MG	AA	3091	1/1	0.81	0.20	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	CA	3014	1/1	0.98	0.30	-	76,76,76,76	0
55	MG	CA	3215	1/1	0.73	0.30	-	137,137,137,137	0
55	MG	AA	3003	1/1	0.95	0.34	-	39,39,39,39	0
55	MG	AA	3013	1/1	0.92	0.42	-	41,41,41,41	0
55	MG	AA	3107	1/1	0.76	0.44	-	79,79,79,79	0
56	OHX	CA	3420	7/7	0.84	0.14	-	131,141,152,216	1
56	OHX	BA	1677	7/7	0.88	0.12	-	141,145,154,220	1
55	MG	CA	3148	1/1	0.92	0.29	-	57,57,57,57	0
55	MG	AA	3079	1/1	0.78	0.40	-	88,88,88,88	0
55	MG	CA	3258	1/1	0.93	0.35	-	56,56,56,56	0
55	MG	CA	3202	1/1	0.79	0.49	-	79,79,79,79	0
55	MG	DA	1697	1/1	0.91	0.40	-	72,72,72,72	0
55	MG	DC	106	1/1	0.85	0.55	-	91,91,91,91	0
55	MG	DA	1640	1/1	0.87	0.35	-	83,83,83,83	0
55	MG	AA	3351	1/1	0.97	0.38	-	53,53,53,53	0
55	MG	AA	3056	1/1	0.90	0.21	-	36,36,36,36	0
55	MG	AA	3416	1/1	0.93	0.40	-	74,74,74,74	0
55	MG	AA	3251	1/1	0.91	0.36	-	49,49,49,49	0
55	MG	DA	1715	1/1	0.64	0.28	-	89,89,89,89	0
56	OHX	AA	3403	7/7	0.92	0.19	-	109,110,128,178	1
55	MG	BA	1655	1/1	0.94	0.23	-	60,60,60,60	0
55	MG	BA	1651	1/1	0.95	0.10	-	90,90,90,90	0
55	MG	CA	3133	1/1	0.98	0.35	-	48,48,48,48	0
55	MG	CA	3087	1/1	0.85	0.14	-	70,70,70,70	0
55	MG	CA	3128	1/1	0.96	0.16	-	72,72,72,72	0
55	MG	BA	1753	1/1	0.93	0.46	-	67,67,67,67	0
56	OHX	AA	3404	7/7	0.96	0.23	-	74,98,116,164	1
56	OHX	CA	3389	7/7	0.98	0.11	-	101,110,123,155	1
55	MG	CA	3451	1/1	0.90	0.33	-	46,46,46,46	0
56	OHX	AA	3550	7/7	0.94	0.16	-	111,121,131,187	1
56	OHX	AA	3338	7/7	0.98	0.14	-	82,93,108,126	1
55	MG	CA	3107	1/1	0.83	0.24	-	82,82,82,82	0
55	MG	CA	3060	1/1	0.84	0.23	-	75,75,75,75	0
55	MG	CA	3221	1/1	0.93	0.43	-	69,69,69,69	0
56	OHX	DA	1810	7/7	0.94	0.14	-	134,135,143,197	1
55	MG	DA	1707	1/1	0.83	0.45	-	85,85,85,85	0
55	MG	AA	3183	1/1	0.93	0.43	-	88,88,88,88	0
56	OHX	CA	3355	7/7	0.97	0.12	-	108,110,119,149	1
55	MG	BA	1704	1/1	0.83	0.24	-	88,88,88,88	0
55	MG	DA	1695	1/1	0.78	0.51	-	76,76,76,76	0
55	MG	AA	3214	1/1	0.98	0.32	-	46,46,46,46	0
56	OHX	AA	3442	7/7	0.99	0.17	-	70,87,119,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	DA	1621	1/1	0.78	0.32	-	98,98,98,98	0
56	OHX	AA	3527	7/7	0.94	0.10	-	130,134,147,188	1
55	MG	CA	3031	1/1	0.85	0.10	-	53,53,53,53	0
55	MG	BA	1653	1/1	0.94	0.35	-	63,63,63,63	0
55	MG	BA	1698	1/1	0.92	0.50	-	62,62,62,62	0
55	MG	CA	3183	1/1	0.87	0.38	-	93,93,93,93	0
55	MG	CA	3029	1/1	0.92	0.28	-	76,76,76,76	0
55	MG	CA	3452	1/1	0.92	0.18	-	51,51,51,51	0
56	OHX	CA	3372	7/7	0.98	0.14	-	112,137,145,182	0
55	MG	CA	3119	1/1	0.83	0.28	-	61,61,61,61	0
55	MG	AA	3150	1/1	0.81	0.41	-	68,68,68,68	0
55	MG	CA	3151	1/1	0.93	0.37	-	76,76,76,76	0
55	MG	DA	1684	1/1	0.90	0.52	-	79,79,79,79	0
55	MG	CA	3040	1/1	0.85	0.44	-	70,70,70,70	0
56	OHX	AA	3528	7/7	0.93	0.14	-	112,118,137,160	2
56	OHX	BA	1784	7/7	0.96	0.14	-	122,129,148,203	0
55	MG	CA	3110	1/1	0.69	0.39	-	85,85,85,85	0
55	MG	AA	3046	1/1	0.88	0.50	-	68,68,68,68	0
55	MG	CA	3126	1/1	0.95	0.30	-	54,54,54,54	0
56	OHX	CA	3490	7/7	0.97	0.14	-	102,105,118,156	1
56	OHX	CA	3470	7/7	0.91	0.13	-	113,126,137,181	1
55	MG	CA	3062	1/1	0.85	0.14	-	78,78,78,78	0
55	MG	BA	1744	1/1	0.74	0.19	-	90,90,90,90	0
55	MG	CA	3118	1/1	0.98	0.40	-	69,69,69,69	0
55	MG	BA	1723	1/1	0.86	0.30	-	82,82,82,82	0
55	MG	DA	1624	1/1	0.68	0.10	-	73,73,73,73	0
55	MG	AA	3245	1/1	0.83	0.27	-	68,68,68,68	0
55	MG	DA	1700	1/1	0.98	0.47	-	70,70,70,70	0
56	OHX	CA	3361	7/7	0.98	0.10	-	113,119,132,166	1
55	MG	CA	3439	1/1	0.92	0.33	-	63,63,63,63	0
55	MG	CA	3082	1/1	0.84	0.42	-	62,62,62,62	0
55	MG	BA	1738	1/1	0.98	0.17	-	41,41,41,41	0
55	MG	DA	1698	1/1	0.68	0.50	-	95,95,95,95	0
55	MG	CA	3213	1/1	0.69	0.23	-	121,121,121,121	0
55	MG	BA	1742	1/1	0.88	0.46	-	86,86,86,86	0
55	MG	DA	1667	1/1	0.83	0.42	-	68,68,68,68	0
55	MG	AA	3137	1/1	0.64	0.49	-	51,51,51,51	0
55	MG	CA	3186	1/1	0.90	0.23	-	75,75,75,75	0
55	MG	DA	1704	1/1	0.94	0.44	-	73,73,73,73	0
55	MG	BA	1736	1/1	0.94	0.51	-	64,64,64,64	0
55	MG	BA	1627	1/1	0.77	0.40	-	80,80,80,80	0
55	MG	DA	1692	1/1	0.94	0.50	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	DA	1702	1/1	0.79	0.19	-	122,122,122,122	0
55	MG	AA	3026	1/1	0.81	0.44	-	92,92,92,92	0
55	MG	AA	3159	1/1	0.87	0.29	-	65,65,65,65	0
56	OHX	DB	104	7/7	0.82	0.16	-	129,133,143,205	2
55	MG	BA	1726	1/1	0.93	0.33	-	61,61,61,61	0
55	MG	DA	1686	1/1	0.88	0.28	-	73,73,73,73	0
56	OHX	CA	3419	7/7	0.83	0.13	-	153,156,164,238	1
55	MG	CA	3027	1/1	0.64	0.35	-	81,81,81,81	0
55	MG	BC	104	1/1	0.90	0.53	-	57,57,57,57	0
55	MG	AA	3043	1/1	0.98	0.38	-	46,46,46,46	0
55	MG	AA	3113	1/1	0.98	0.39	-	32,32,32,32	0
55	MG	AA	3396	1/1	0.91	0.47	-	71,71,71,71	0
55	MG	CA	3224	1/1	0.95	0.29	-	77,77,77,77	0
55	MG	DA	1661	1/1	0.77	0.41	-	76,76,76,76	0
56	OHX	CA	3492	7/7	0.97	0.15	-	97,102,115,126	1
55	MG	AA	3077	1/1	0.83	0.29	-	73,73,73,73	0
55	MG	BA	1640	1/1	0.93	0.35	-	73,73,73,73	0
56	OHX	CA	3330	7/7	0.98	0.10	-	102,106,115,169	0
56	OHX	A1	203	7/7	0.89	0.19	-	100,107,140,182	3
55	MG	BA	1714	1/1	0.97	0.29	-	56,56,56,56	0
55	MG	AA	3413	1/1	0.95	0.30	-	57,57,57,57	0
56	OHX	AA	3516	7/7	0.95	0.14	-	101,109,121,183	1
55	MG	AA	3022	1/1	0.96	0.34	-	15,15,15,15	0
56	OHX	AA	3450	7/7	0.97	0.18	-	65,94,112,113	3
55	MG	BS	101	1/1	0.82	0.32	-	93,93,93,93	0
55	MG	DA	1706	1/1	0.75	0.17	-	100,100,100,100	0
55	MG	BA	1739	1/1	0.92	0.44	-	70,70,70,70	0
55	MG	AB	201	1/1	0.91	0.39	-	73,73,73,73	0
55	MG	AA	3209	1/1	0.89	0.35	-	57,57,57,57	0
56	OHX	AA	3559	7/7	0.91	0.10	-	124,133,143,186	1
56	OHX	AA	3476	7/7	0.95	0.14	-	102,122,137,175	1
55	MG	AA	3410	1/1	0.98	0.46	-	61,61,61,61	0
55	MG	AA	3185	1/1	0.98	0.45	-	36,36,36,36	0
55	MG	CA	3164	1/1	0.74	0.47	-	97,97,97,97	0
55	MG	AA	3356	1/1	0.88	0.56	-	58,58,58,58	0
55	MG	DA	1664	1/1	0.95	0.47	-	31,31,31,31	0
56	OHX	AA	3496	7/7	0.96	0.17	-	117,124,142,215	0
55	MG	CA	3132	1/1	0.93	0.25	-	80,80,80,80	0
56	OHX	CA	3390	7/7	0.92	0.10	-	117,128,152,209	1
55	MG	DA	1608	1/1	0.94	0.21	-	78,78,78,78	0
55	MG	AA	3187	1/1	0.90	0.54	-	86,86,86,86	0
55	MG	AA	3193	1/1	0.89	0.19	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	CA	3124	1/1	0.98	0.31	-	44,44,44,44	0
55	MG	AA	3186	1/1	0.91	0.37	-	49,49,49,49	0
56	OHX	DB	103	7/7	0.95	0.10	-	166,171,179,191	1
55	MG	AA	3284	1/1	0.77	0.36	-	66,66,66,66	0
55	MG	AA	3063	1/1	0.95	0.34	-	76,76,76,76	0
55	MG	AA	3008	1/1	0.95	0.39	-	42,42,42,42	0
55	MG	AA	3286	1/1	0.89	0.53	-	68,68,68,68	0
55	MG	CA	3161	1/1	0.96	0.28	-	71,71,71,71	0
55	MG	BB	105	1/1	0.91	0.51	-	63,63,63,63	0
55	MG	BA	1733	1/1	0.95	0.51	-	60,60,60,60	0
55	MG	BA	1731	1/1	0.98	0.40	-	57,57,57,57	0
55	MG	CA	3074	1/1	0.88	0.32	-	64,64,64,64	0
55	MG	CA	3093	1/1	0.91	0.32	-	81,81,81,81	0
55	MG	DA	1607	1/1	0.97	0.35	-	82,82,82,82	0
56	OHX	DA	1748	7/7	0.97	0.11	-	95,111,122,149	1
55	MG	AA	3164	1/1	0.87	0.27	-	70,70,70,70	0
55	MG	CA	3223	1/1	0.79	0.39	-	88,88,88,88	0
55	MG	AA	3232	1/1	0.90	0.42	-	75,75,75,75	0
55	MG	AA	3045	1/1	0.91	0.41	-	65,65,65,65	0
56	OHX	DA	1795	7/7	0.97	0.11	-	112,118,132,167	1
55	MG	AA	3222	1/1	0.89	0.52	-	64,64,64,64	0
56	OHX	DA	1750	7/7	0.96	0.13	-	127,137,146,202	1
55	MG	BA	1728	1/1	0.86	0.46	-	90,90,90,90	0
55	MG	AA	3124	1/1	0.86	0.44	-	70,70,70,70	0
55	MG	AA	3168	1/1	0.95	0.30	-	89,89,89,89	0
55	MG	CA	3173	1/1	0.97	0.33	-	53,53,53,53	0
55	MG	BA	1749	1/1	0.90	0.49	-	88,88,88,88	0
55	MG	AA	3196	1/1	0.99	0.38	-	36,36,36,36	0
55	MG	AA	3271	1/1	0.82	0.14	-	39,39,39,39	0
55	MG	AA	3083	1/1	0.94	0.29	-	88,88,88,88	0
56	OHX	BA	1695	7/7	0.87	0.10	-	129,147,158,217	1
55	MG	AA	3208	1/1	0.75	0.37	-	65,65,65,65	0
55	MG	AA	3037	1/1	0.90	0.48	-	63,63,63,63	0
56	OHX	AA	3331	7/7	0.90	0.27	-	72,87,130,163	3
56	OHX	AA	3477	7/7	0.96	0.14	-	108,119,125,208	1
55	MG	CA	3171	1/1	0.92	0.36	-	82,82,82,82	0
55	MG	AA	3034	1/1	0.87	0.43	-	56,56,56,56	0
56	OHX	CA	3487	7/7	0.96	0.08	-	135,139,147,210	1
55	MG	AA	3282	1/1	0.79	0.37	-	69,69,69,69	0
55	MG	DA	1693	1/1	0.96	0.51	-	54,54,54,54	0
56	OHX	AA	3499	7/7	0.96	0.14	-	101,113,131,183	1
55	MG	AA	3001	1/1	0.96	0.41	-	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	AA	3179	1/1	0.93	0.52	-	60,60,60,60	0
55	MG	AA	3066	1/1	0.97	0.36	-	83,83,83,83	0
56	OHX	DA	1749	7/7	0.94	0.18	-	91,120,126,173	1
55	MG	AA	3089	1/1	0.89	0.55	-	84,84,84,84	0
55	MG	BA	1625	1/1	0.90	0.46	-	65,65,65,65	0
56	OHX	CA	3300	7/7	0.98	0.16	-	66,75,91,101	1
55	MG	BA	1724	1/1	0.91	0.38	-	59,59,59,59	0
55	MG	CA	3064	1/1	0.94	0.22	-	89,89,89,89	0
55	MG	CA	3475	1/1	0.97	0.20	-	55,55,55,55	0
55	MG	CA	3191	1/1	0.91	0.46	-	72,72,72,72	0
55	MG	CA	3091	1/1	0.84	0.42	-	74,74,74,74	0
56	OHX	AA	3336	7/7	0.95	0.11	-	146,153,168,218	0
55	MG	CA	3007	1/1	0.98	0.25	-	45,45,45,45	0
55	MG	AA	3276	1/1	0.94	0.41	-	69,69,69,69	0
55	MG	AA	3394	1/1	0.98	0.47	-	43,43,43,43	0
55	MG	CA	3170	1/1	0.93	0.21	-	65,65,65,65	0
55	MG	BA	1601	1/1	0.73	0.22	-	81,81,81,81	0
55	MG	AA	3274	1/1	0.93	0.59	-	89,89,89,89	0
55	MG	CB	207	1/1	0.85	0.47	-	76,76,76,76	0
55	MG	CA	3136	1/1	0.62	0.42	-	91,91,91,91	0
56	OHX	AA	3436	7/7	0.99	0.11	-	78,91,117,117	0
56	OHX	AA	3519	7/7	0.93	0.10	-	140,146,150,214	1
55	MG	AA	3076	1/1	0.80	0.42	-	72,72,72,72	0
55	MG	AA	3190	1/1	0.64	0.40	-	69,69,69,69	0
55	MG	AA	3108	1/1	0.77	0.32	-	82,82,82,82	0
56	OHX	CA	3285	7/7	0.98	0.12	-	94,107,126,147	1
56	OHX	AA	3540	7/7	0.93	0.14	-	109,134,164,188	2
56	OHX	CA	3279	7/7	0.99	0.13	-	80,89,109,118	0
55	MG	DA	1658	1/1	0.96	0.46	-	64,64,64,64	0
55	MG	AA	3272	1/1	0.97	0.50	-	50,50,50,50	0
55	MG	AA	3348	1/1	0.86	0.41	-	46,46,46,46	0
56	OHX	CA	3313	7/7	0.99	0.12	-	103,112,124,157	0
55	MG	AA	3199	1/1	0.79	0.64	-	76,76,76,76	0
55	MG	CA	3208	1/1	0.94	0.35	-	70,70,70,70	0
55	MG	DA	1701	1/1	0.72	0.41	-	90,90,90,90	0
56	OHX	CA	3250	7/7	0.94	0.14	-	106,109,126,164	1
55	MG	CA	3146	1/1	0.93	0.38	-	77,77,77,77	0
56	OHX	AA	3505	7/7	0.95	0.19	-	86,108,110,156	1
55	MG	CA	3200	1/1	0.87	0.36	-	56,56,56,56	0
55	MG	DA	1645	1/1	0.84	0.47	-	91,91,91,91	0
55	MG	AA	3206	1/1	0.86	0.52	-	64,64,64,64	0
55	MG	AA	3265	1/1	0.95	0.27	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	OHX	AA	3319	7/7	0.98	0.16	-	87,95,122,151	1
55	MG	CA	3141	1/1	0.88	0.46	-	77,77,77,77	0
55	MG	DA	1716	1/1	0.86	0.33	-	85,85,85,85	0
56	OHX	CA	3291	7/7	0.99	0.13	-	86,105,118,139	0
55	MG	BC	101	1/1	0.88	0.52	-	69,69,69,69	0
56	OHX	DA	1788	7/7	0.96	0.12	-	96,113,128,168	1
55	MG	CA	3078	1/1	0.95	0.35	-	76,76,76,76	0
55	MG	BA	1697	1/1	0.95	0.40	-	37,37,37,37	0
55	MG	BA	1652	1/1	0.91	0.33	-	63,63,63,63	0
55	MG	AA	3234	1/1	0.83	0.14	-	56,56,56,56	0
55	MG	AA	3220	1/1	0.71	0.48	-	64,64,64,64	0
55	MG	BA	1644	1/1	0.87	0.51	-	94,94,94,94	0
55	MG	BA	1740	1/1	0.97	0.45	-	61,61,61,61	0
55	MG	CA	3030	1/1	0.95	0.31	-	89,89,89,89	0
55	MG	DA	1638	1/1	0.94	0.18	-	89,89,89,89	0
55	MG	AA	3165	1/1	0.59	0.57	-	84,84,84,84	0
55	MG	AA	3135	1/1	0.80	0.30	-	67,67,67,67	0
56	OHX	AA	3541	7/7	0.92	0.21	-	102,114,134,158	2
56	OHX	CA	3413	7/7	0.91	0.15	-	121,130,144,215	1
56	OHX	CA	3486	7/7	0.92	0.17	-	87,109,129,181	2
55	MG	CA	3230	1/1	0.87	0.49	-	79,79,79,79	0
55	MG	CA	3177	1/1	0.94	0.33	-	57,57,57,57	0
55	MG	AA	3350	1/1	0.89	0.43	-	80,80,80,80	0
55	MG	CA	3263	1/1	0.94	0.28	-	69,69,69,69	0
55	MG	DA	1681	1/1	0.72	0.32	-	100,100,100,100	0
55	MG	CA	3094	1/1	0.92	0.54	-	79,79,79,79	0
55	MG	DA	1616	1/1	0.93	0.39	-	88,88,88,88	0
56	OHX	CA	3383	7/7	0.94	0.14	-	111,116,132,194	1
55	MG	DA	1677	1/1	0.91	0.34	-	76,76,76,76	0
55	MG	AA	3224	1/1	0.80	0.55	-	68,68,68,68	0
55	MG	DA	1709	1/1	0.93	0.50	-	80,80,80,80	0
56	OHX	AA	3333	7/7	0.91	0.19	-	91,114,128,179	2
55	MG	CA	3020	1/1	0.89	0.29	-	70,70,70,70	0
55	MG	BA	1706	1/1	0.97	0.42	-	79,79,79,79	0
55	MG	CA	3023	1/1	0.92	0.23	-	85,85,85,85	0
56	OHX	BA	1800	7/7	0.98	0.13	-	106,107,118,143	1
55	MG	CA	3135	1/1	0.90	0.44	-	45,45,45,45	0
55	MG	AA	3349	1/1	0.97	0.44	-	61,61,61,61	0
56	OHX	DV	101	7/7	0.93	0.09	-	162,169,185,231	1
55	MG	DA	1683	1/1	0.88	0.47	-	71,71,71,71	0
55	MG	BA	1610	1/1	0.85	0.31	-	92,92,92,92	0
56	OHX	DA	1775	7/7	0.89	0.11	-	133,145,148,215	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	DA	1687	1/1	0.95	0.16	-	63,63,63,63	0
55	MG	AA	3347	1/1	0.79	0.46	-	70,70,70,70	0
55	MG	CA	3001	1/1	0.96	0.26	-	46,46,46,46	0
55	MG	CB	205	1/1	0.87	0.42	-	74,74,74,74	0
55	MG	CA	3207	1/1	0.83	0.29	-	68,68,68,68	0
55	MG	CA	3188	1/1	0.90	0.45	-	60,60,60,60	0
56	OHX	AA	3487	7/7	0.96	0.13	-	95,110,116,167	1
55	MG	AA	3088	1/1	0.95	0.17	-	60,60,60,60	0
55	MG	DA	1708	1/1	0.55	0.46	-	87,87,87,87	0
55	MG	BA	1628	1/1	0.70	0.36	-	80,80,80,80	0
55	MG	CA	3268	1/1	0.88	0.12	-	52,52,52,52	0
56	OHX	CA	3290	7/7	0.99	0.13	-	94,101,123,130	0
55	MG	A3	101	1/1	0.94	0.44	-	60,60,60,60	0
55	MG	CA	3210	1/1	0.91	0.56	-	74,74,74,74	0
55	MG	DA	1637	1/1	0.91	0.54	-	106,106,106,106	0
55	MG	CA	3165	1/1	0.95	0.45	-	57,57,57,57	0
55	MG	AA	3145	1/1	0.86	0.44	-	56,56,56,56	0
56	OHX	CA	3360	7/7	0.95	0.10	-	116,124,135,193	1
55	MG	BC	103	1/1	0.91	0.43	-	62,62,62,62	0
55	MG	CA	3209	1/1	0.93	0.35	-	85,85,85,85	0
55	MG	CA	3162	1/1	0.94	0.48	-	65,65,65,65	0
55	MG	CA	3080	1/1	0.97	0.09	-	57,57,57,57	0
55	MG	AA	3198	1/1	0.96	0.30	-	54,54,54,54	0
55	MG	CA	3117	1/1	0.89	0.23	-	69,69,69,69	0
55	MG	AA	3378	1/1	0.90	0.34	-	47,47,47,47	0
56	OHX	AA	3525	7/7	0.96	0.13	-	100,109,122,187	1
55	MG	CA	3089	1/1	0.94	0.27	-	60,60,60,60	0
56	OHX	AA	3495	7/7	0.97	0.17	-	86,93,120,158	1
56	OHX	AA	3543	7/7	0.95	0.10	-	113,117,131,189	1
55	MG	BA	1646	1/1	0.77	0.40	-	95,95,95,95	0
55	MG	AA	3184	1/1	0.95	0.34	-	38,38,38,38	0
55	MG	AA	3166	1/1	0.84	0.48	-	66,66,66,66	0
56	OHX	BA	1779	7/7	0.99	0.13	-	102,112,125,152	1
55	MG	AA	3105	1/1	0.64	0.44	-	124,124,124,124	0
55	MG	AA	3059	1/1	0.78	0.58	-	85,85,85,85	0
55	MG	CA	3096	1/1	0.90	0.36	-	64,64,64,64	0
55	MG	AA	3230	1/1	0.91	0.23	-	66,66,66,66	0
55	MG	AA	3346	1/1	0.97	0.26	-	42,42,42,42	0
56	OHX	CA	3464	7/7	0.94	0.16	-	78,109,122,137	3
55	MG	CA	3058	1/1	0.94	0.39	-	50,50,50,50	0
55	MG	BA	1701	1/1	0.98	0.32	-	57,57,57,57	0
56	OHX	BA	1811	7/7	0.97	0.13	-	88,104,115,154	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	CA	3476	1/1	0.96	0.35	-	52,52,52,52	0
55	MG	CB	204	1/1	0.75	0.38	-	73,73,73,73	0
56	OHX	AA	3341	7/7	0.99	0.13	-	75,103,114,126	1
55	MG	CA	3227	1/1	0.93	0.34	-	79,79,79,79	0
55	MG	CA	3024	1/1	0.96	0.18	-	48,48,48,48	0
55	MG	CA	3101	1/1	0.90	0.38	-	59,59,59,59	0
55	MG	AA	3385	1/1	0.97	0.46	-	34,34,34,34	0
55	MG	AA	3153	1/1	0.94	0.67	-	64,64,64,64	0
55	MG	BC	102	1/1	0.49	0.21	-	68,68,68,68	0
55	MG	C5	101	1/1	0.91	0.22	-	50,50,50,50	0
55	MG	CA	3114	1/1	0.83	0.45	-	57,57,57,57	0
55	MG	BA	1660	1/1	0.91	0.25	-	97,97,97,97	0
55	MG	AA	3052	1/1	0.77	0.47	-	85,85,85,85	0
55	MG	AA	3219	1/1	0.98	0.34	-	48,48,48,48	0
55	MG	CA	3480	1/1	0.91	0.23	-	72,72,72,72	0
55	MG	CA	3217	1/1	0.82	0.37	-	58,58,58,58	0
55	MG	DA	1710	1/1	0.61	0.20	-	103,103,103,103	0
55	MG	CA	3259	1/1	0.96	0.24	-	65,65,65,65	0
55	MG	CA	3457	1/1	0.31	0.33	-	66,66,66,66	0
56	OHX	CA	3469	7/7	0.97	0.09	-	89,110,121,162	1
55	MG	DA	1678	1/1	0.84	0.15	-	118,118,118,118	0
56	OHX	DA	1747	7/7	0.95	0.15	-	109,122,155,200	1
56	OHX	CA	3296	7/7	0.98	0.14	-	65,90,108,135	2
55	MG	AA	3055	1/1	0.93	0.39	-	65,65,65,65	0
55	MG	AA	3205	1/1	0.96	0.17	-	40,40,40,40	0
55	MG	CA	3456	1/1	0.84	0.21	-	66,66,66,66	0
56	OHX	BA	1758	7/7	0.99	0.17	-	69,88,100,119	0
56	OHX	AA	3460	7/7	0.99	0.15	-	87,98,107,140	0
55	MG	CA	3042	1/1	0.76	0.27	-	67,67,67,67	0
55	MG	DA	1714	1/1	0.76	0.33	-	97,97,97,97	0
55	MG	DA	1699	1/1	0.98	0.35	-	78,78,78,78	0
55	MG	CA	3169	1/1	0.87	0.23	-	71,71,71,71	0
56	OHX	AA	3530	7/7	0.90	0.17	-	101,121,143,206	1
55	MG	AA	3266	1/1	0.88	0.29	-	78,78,78,78	0
55	MG	BA	1622	1/1	0.91	0.13	-	123,123,123,123	0
55	MG	DA	1656	1/1	0.92	0.36	-	68,68,68,68	0
55	MG	CA	3190	1/1	0.96	0.14	-	60,60,60,60	0
55	MG	CA	3441	1/1	0.78	0.34	-	99,99,99,99	0
55	MG	CA	3196	1/1	0.82	0.52	-	92,92,92,92	0
55	MG	DA	1623	1/1	0.81	0.47	-	124,124,124,124	0
55	MG	DA	1628	1/1	0.61	0.47	-	78,78,78,78	0
55	MG	CA	3182	1/1	0.95	0.46	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
55	MG	CA	3048	1/1	0.96	0.34	-	44,44,44,44	0
55	MG	DA	1671	1/1	0.93	0.22	-	64,64,64,64	0
55	MG	AA	3087	1/1	0.67	0.52	-	83,83,83,83	0
56	OHX	AA	3372	7/7	0.97	0.14	-	93,103,121,167	1
55	MG	AB	204	1/1	0.95	0.61	-	68,68,68,68	0
55	MG	CA	3037	1/1	0.79	0.35	-	89,89,89,89	0
55	MG	CA	3152	1/1	0.93	0.37	-	54,54,54,54	0
55	MG	CA	3100	1/1	0.97	0.43	-	63,63,63,63	0
55	MG	DA	1680	1/1	0.90	0.27	-	72,72,72,72	0
55	MG	AA	3382	1/1	0.97	0.43	-	36,36,36,36	0
56	OHX	CA	3338	7/7	0.97	0.18	-	95,103,117,121	1
55	MG	AA	3358	1/1	0.96	0.30	-	51,51,51,51	0
55	MG	AA	3067	1/1	0.88	0.17	-	97,97,97,97	0
55	MG	BA	1629	1/1	0.88	0.23	-	112,112,112,112	0
55	MG	AA	3375	1/1	0.99	0.37	-	31,31,31,31	0
55	MG	AA	3201	1/1	0.91	0.34	-	45,45,45,45	0
56	OHX	AA	3481	7/7	0.96	0.16	-	95,108,126,156	2
55	MG	AA	3104	1/1	0.89	0.54	-	68,68,68,68	0
55	MG	AA	3036	1/1	0.99	0.38	-	36,36,36,36	0
56	OHX	AB	210	7/7	0.92	0.21	-	83,107,129,146	3
55	MG	DA	1631	1/1	0.78	0.47	-	111,111,111,111	0
56	OHX	DA	1786	7/7	0.83	0.14	-	143,151,161,223	1
55	MG	DA	1647	1/1	0.98	0.40	-	90,90,90,90	0
55	MG	AA	3044	1/1	0.73	0.53	-	72,72,72,72	0
55	MG	CA	3155	1/1	0.87	0.17	-	58,58,58,58	0
55	MG	BA	1745	1/1	0.95	0.54	-	83,83,83,83	0
55	MG	CA	3211	1/1	0.91	0.15	-	116,116,116,116	0
55	MG	AA	3202	1/1	0.93	0.38	-	45,45,45,45	0
55	MG	AA	3075	1/1	0.93	0.52	-	44,44,44,44	0
56	OHX	CA	3432	7/7	0.91	0.13	-	119,135,143,173	1
55	MG	CA	3262	1/1	0.96	0.46	-	74,74,74,74	0
55	MG	DA	1653	1/1	0.90	0.50	-	73,73,73,73	0
55	MG	CA	3039	1/1	0.83	0.36	-	65,65,65,65	0
56	OHX	CA	3405	7/7	0.97	0.10	-	112,116,119,187	1
56	OHX	CA	3333	7/7	0.96	0.11	-	104,127,133,184	1
55	MG	CA	3443	1/1	0.92	0.42	-	49,49,49,49	0
55	MG	AA	3258	1/1	0.98	0.46	-	65,65,65,65	0
55	MG	AA	3133	1/1	0.92	0.22	-	54,54,54,54	0
55	MG	AA	3011	1/1	0.96	0.36	-	49,49,49,49	0
55	MG	AA	3169	1/1	0.86	0.53	-	76,76,76,76	0
55	MG	AA	3200	1/1	0.94	0.44	-	45,45,45,45	0
56	OHX	AA	3421	7/7	1.00	0.20	-	50,71,87,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	OHX	DA	1790	7/7	0.94	0.11	-	135,136,148,199	1
56	OHX	AA	3493	7/7	0.93	0.14	-	109,111,123,166	1
55	MG	AA	3262	1/1	0.93	0.38	-	52,52,52,52	0
55	MG	CA	3222	1/1	0.70	0.21	-	81,81,81,81	0
55	MG	AA	3279	1/1	0.86	0.39	-	81,81,81,81	0
55	MG	BA	1700	1/1	0.90	0.42	-	61,61,61,61	0

6.5 Other polymers

There are no such residues in this entry.