wwPDB X-ray Structure Validation Summary Report (i)

Sep 16, 2026 – 08:42 pm BST

PDB ID	:	5ON6 / pdb_00005on6
Title	:	Crystal structure of haemanthamine bound to the 80S ribosome
Authors	:	Pellegrino, S.; Meyer, M.; Yusupova, G.; Yusupov, M.
Deposited on	:	2017-08-03
Resolution	:	3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

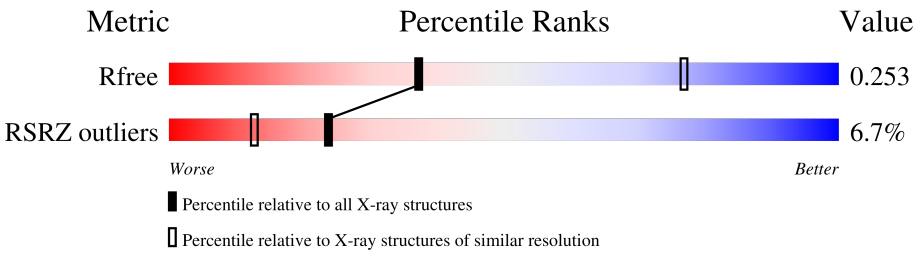
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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
85	MG	1	3744	-	-	-	X
85	MG	1	3955	-	-	-	X
85	MG	1	3965	-	-	-	X
85	MG	1	4030	-	-	-	X
85	MG	1	4152	-	-	-	X
85	MG	1	4171	-	-	-	X
85	MG	6	2061	-	-	-	X
85	MG	6	2076	-	-	-	X
85	MG	6	2085	-	-	-	X
85	MG	6	2092	-	-	-	X
85	MG	6	2110	-	-	-	X
85	MG	6	2185	-	-	-	X
85	MG	A	2066	-	-	-	X
85	MG	A	2068	-	-	-	X
85	MG	A	2070	-	-	-	X
85	MG	A	2078	-	-	-	X
85	MG	A	2100	-	-	-	X
85	MG	A	2110	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	A	2118	-	-	-	X
85	MG	A	2132	-	-	-	X
85	MG	A	2151	-	-	-	X
85	MG	A	2155	-	-	-	X
85	MG	AR	3776	-	-	-	X
85	MG	AR	3814	-	-	-	X

2 Entry composition (i)

There are 88 unique types of molecules in this entry. The entry contains 410383 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 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1	3149	67355	30086	12142	21978	3149	0	0	0
1	AR	3149	67355	30086	12142	21978	3149	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	3	121	2579	1152	461	845	121	0	0	0
2	AS	121	2579	1152	461	845	121	0	0	0

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	4	158	3353	1500	586	1109	158	0	0	0
3	AT	158	3353	1500	586	1109	158	0	0	0

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	j	252	1914	1191	388	334	1	0	0	0
4	CD	252	1914	1191	388	334	1	0	0	0

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	k	386	3075	1950	584	533	8	0	0	0
5	CE	386	3075	1950	584	533	8	0	0	0

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	l	361	2748	1729	522	494	3	0	0	0
6	CF	361	2748	1729	522	494	3	0	0	0

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	m	296	2375	1501	414	458	2	0	0	0
7	CG	296	2375	1501	414	458	2	0	0	0

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	n	156	1239	800	222	216	1	0	0	0
8	CH	156	1239	800	222	216	1	0	0	0

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	o	222	1784	1151	324	308	1	0	0	0
9	CI	222	1784	1151	324	308	1	0	0	0

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	p	233	1804	1151	323	327	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	CJ	233	1804	1151	323	327	3	0	0	0

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	q	191	1518	963	274	277	4	0	0	0
11	CK	191	1518	963	274	277	4	0	0	0

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	r	211	1705	1083	322	294	6	0	0	0
12	CL	211	1705	1083	322	294	6	0	0	0

- Molecule 13 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	s	169	1353	847	253	249	4	0	0	0
13	CM	169	1353	847	253	249	4	0	0	0

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	t	193	1543	962	315	266	0	0	0
14	CN	193	1543	962	315	266	0	0	0

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	u	136	1053	675	199	177	2	0	0	0
15	CO	136	1053	675	199	177	2	0	0	0

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	v	203	1720	1077	361	281	1	0	0	0
16	CP	203	1720	1077	361	281	1	0	0	0

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	w	197	1555	1003	289	262	1	0	0	0
17	CQ	197	1555	1003	289	262	1	0	0	0

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	x	183	1420	882	281	257	0	0	0
18	CR	183	1420	882	281	257	0	0	0

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	y	185	1441	908	290	241	2	0	0	0
19	CS	185	1441	908	290	241	2	0	0	0

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
20	z	188	1521	935	326	260	0	0	0
20	CT	188	1521	935	326	260	0	0	0

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	0	172	1445	930	267	244	4	0	0	0
21	CU	172	1445	930	267	244	4	0	0	0

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	2	159	1276	805	246	221	4	0	0	0
22	CV	159	1276	805	246	221	4	0	0	0

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
23	5	100	796	516	131	149	0	0	0
23	CW	100	796	516	131	149	0	0	0

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	lR	136	1003	628	189	179	7	0	0	0
24	CX	136	1003	628	189	179	7	0	0	0

- Molecule 25 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
25	6	1783	37990	16984	6723	12500	1783	0	0	0
25	A	1781	37948	16965	6715	12487	1781	0	0	0

- Molecule 26 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	7	98	699	443	137	118	1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	CY	98	699	443	137	118	1	0	0	0

- Molecule 27 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	8	121	964	620	169	173	2	0	0	0
27	CZ	121	964	620	169	173	2	0	0	0

- Molecule 28 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
28	9	126	993	625	192	176	0	0	0
28	DA	126	993	625	192	176	0	0	0

- Molecule 29 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
29	AA	135	1092	710	202	180	0	0	0
29	DB	135	1092	710	202	180	0	0	0

- Molecule 30 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	AB	148	1173	749	231	190	3	0	0	0
30	DC	148	1173	749	231	190	3	0	0	0

- Molecule 31 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
31	AC	58	462	289	100	73	0	0	0
31	DD	58	462	289	100	73	0	0	0

- Molecule 32 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	AD	97	743	479	124	139	1	0	0	0
32	DE	97	743	479	124	139	1	0	0	0

- Molecule 33 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	AE	109	876	556	167	152	1	0	0	0
33	DF	109	876	556	167	152	1	0	0	0

- Molecule 34 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	AF	127	1020	647	205	167	1	0	0	0
34	DG	127	1020	647	205	167	1	0	0	0

- Molecule 35 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	AG	106	850	540	165	144	1	0	0	0
35	DH	106	850	540	165	144	1	0	0	0

- Molecule 36 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	AH	112	880	545	179	152	4	0	0	0
36	DI	112	880	545	179	152	4	0	0	0

- Molecule 37 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	AI	119	969	615	186	167	1	0	0	0
37	DJ	119	969	615	186	167	1	0	0	0

- Molecule 38 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	AJ	99	771	481	156	132	2	0	0	0
38	DK	99	771	481	156	132	2	0	0	0

- Molecule 39 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	AK	87	681	414	148	114	5	0	0	0
39	DL	87	681	414	148	114	5	0	0	0

- Molecule 40 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
40	AL	77	612	391	115	106	0	0	0
40	DM	77	612	391	115	106	0	0	0

- Molecule 41 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	AM	50	436	272	97	65	2	0	0	0
41	DN	50	436	272	97	65	2	0	0	0

- Molecule 42 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	AN	52	417	259	86	67	5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	DO	52	417	259	86	67	5	0	0	0

- Molecule 43 is a protein called 60S ribosomal protein L41-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	AO	25	233	142	63	27	1	0	0	0
43	DP	25	233	142	63	27	1	0	0	0

- Molecule 44 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	AP	105	847	534	170	138	5	0	0	0
44	DQ	105	847	534	170	138	5	0	0	0

- Molecule 45 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	AQ	91	694	429	138	121	6	0	0	0
45	DR	91	694	429	138	121	6	0	0	0

- Molecule 46 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
46	i	159	1104	652	221	231	0	0	0

- Molecule 47 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
47	m2	150	750	450	150	150	0	0	0

- Molecule 48 is a protein called Suppressor protein STM1,Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
48	sM	104	680	403	140	137	0	0	0

- Molecule 49 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	p0	143	1076	686	192	195	3	0	0	0

- Molecule 50 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	B	206	1577	1014	278	283	2	0	0	0
			Total	C	N	O	S			
50	s0	206	1583	1017	281	283	2	0	0	0

- Molecule 51 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	C	214	1709	1084	310	311	4	0	0	0
			Total	C	N	O	S			
51	s1	216	1722	1091	312	315	4	0	0	0

- Molecule 52 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	D	217	1635	1047	289	297	2	0	0	0
			Total	C	N	O	S			
52	s2	217	1635	1047	289	297	2	0	0	0

- Molecule 53 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	E	223	1734	1101	313	314	6	0	0	0
			Total	C	N	O	S			
53	s3	223	1734	1101	313	314	6	0	0	0

- Molecule 54 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	F	260	2068	1316	389	360	3	0	0	0
54	s4	260	2068	1316	389	360	3	0	0	0

- Molecule 55 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	G	206	1609	1007	300	299	3	0	0	0
55	s5	206	1609	1007	300	299	3	0	0	0

- Molecule 56 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
56	H	226	1799	1129	346	321	3	0	0	0
56	s6	218	1755	1102	337	313	3	0	0	0

- Molecule 57 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
57	I	184	1481	951	265	265	0	0	0
57	s7	186	1491	957	267	267	0	0	0

- Molecule 58 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
58	J	188	1489	925	298	264	2	0	0	0
58	s8	188	1489	925	298	264	2	0	0	0

- Molecule 59 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
59	K	185	1494	943	289	261	1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
59	s9	185	1494	943	289	261	1	0	0	0

- Molecule 60 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
60	L	96	772	499	126	145	2	0	0	0
			Total	C	N	O	S			
60	c0	96	760	489	125	144	2	0	0	0

- Molecule 61 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
61	M	155	1213	774	230	206	3	0	0	0
			Total	C	N	O	S			
61	c1	146	1168	747	221	197	3	0	0	0

- Molecule 62 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
62	N	124	890	560	156	172	2	0	0	0
			Total	C	N	O	S			
62	c2	124	890	560	156	172	2	0	0	0

- Molecule 63 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
63	O	150	1192	759	224	207	2	0	0	0
			Total	C	N	O	S			
63	c3	150	1192	759	224	207	2	0	0	0

- Molecule 64 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
64	P	127	891	545	182	163	1	0	0	0
			Total	C	N	O	S			
64	c4	128	949	582	188	176	3	0	0	0

- Molecule 65 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
65	Q	124	977	622	182	166	7	0	0	0
65	c5	135	1039	658	196	178	7	0	0	0

- Molecule 66 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
66	R	141	1105	708	203	194	0	0	0
66	c6	142	1111	711	204	196	0	0	0

- Molecule 67 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
67	S	120	926	577	177	170	2	0	0	0
67	c7	117	906	563	174	167	2	0	0	0

- Molecule 68 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
68	T	145	1192	743	237	210	2	0	0	0
68	c8	145	1192	743	237	210	2	0	0	0

- Molecule 69 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
69	U	143	1112	694	208	208	2	0	0	0
69	c9	143	1112	694	208	208	2	0	0	0

- Molecule 70 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
70	V	107	855	539	156	159	1	0	0	0
70	d0	110	882	554	161	166	1	0	0	0

- Molecule 71 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
71	W	87	684	420	125	137	2	0	0	0
71	d1	87	684	420	125	137	2	0	0	0

- Molecule 72 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
72	X	129	1021	650	188	180	3	0	0	0
72	d2	129	1021	650	188	180	3	0	0	0

- Molecule 73 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
73	Y	144	1121	708	220	191	2	0	0	0
73	d3	144	1121	708	220	191	2	0	0	0

- Molecule 74 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
74	Z	134	1073	676	208	189	0	0	0
74	d4	134	1073	676	208	189	0	0	0

- Molecule 75 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
75	a	70	563	360	104	99	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
75	d5	69	558	357	103	98	0	0	0

- Molecule 76 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
76	b	97	769	475	160	129	5	0	0	0
76	d6	97	769	475	160	129	5	0	0	0

- Molecule 77 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
77	c	81	610	382	110	113	5	0	0	0
77	d7	81	610	382	110	113	5	0	0	0

- Molecule 78 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
78	d	63	497	306	99	91	1	0	0	0
78	d8	63	497	306	99	91	1	0	0	0

- Molecule 79 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
79	e	53	442	274	92	72	4	0	0	0
79	d9	53	442	274	92	72	4	0	0	0

- Molecule 80 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
80	f	60	475	299	98	77	1	0	0	0
80	e0	62	491	309	101	80	1	0	0	0

- Molecule 81 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
81	g	71	566	362	106	94	4	0	0	0

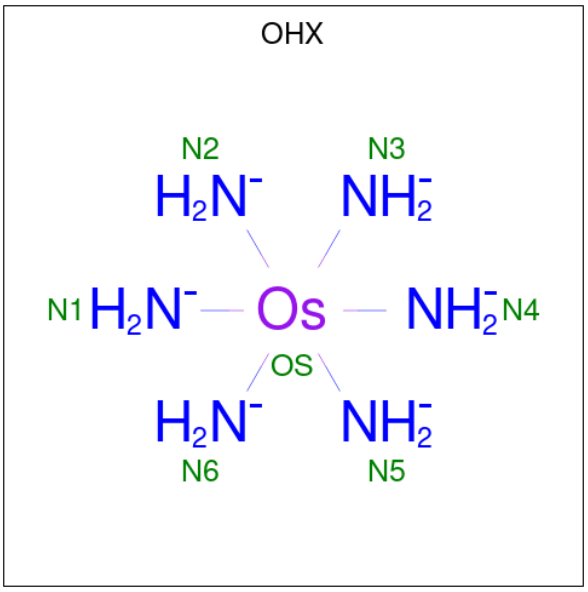
- Molecule 82 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
82	h	318	2441	1544	419	470	8	0	0	0
			Total	C	N	O	S			
82	sR	318	2442	1544	418	472	8	0	0	0

- Molecule 83 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
83	e1	51	397	249	73	71	4	0	0	0

- Molecule 84 is osmium (III) hexammine (CCD ID: OHX) (formula: $H_{12}N_6Os$).



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84	1	1	7	6	1	0	0
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84	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
84	1	1	7	6	1	0	0
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84	1	1	7	6	1	0	0
			Total	N	Os		
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84	1	1	7	6	1	0	0
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84	1	1	7	6	1	0	0
			Total	N	Os		
84	1	1	7	6	1	0	0
			Total	N	Os		
84	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	1	1	7	6	1	0	0
			Total	N	Os		
84	1	1	7	6	1	0	0
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84	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	1	1	7	6	1	0	0
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84	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	1	1	Total N Os 7 6 1	0	0
84	1	1	Total N Os 7 6 1	0	0
84	1	1	Total N Os 7 6 1	0	0
84	1	1	Total N Os 7 6 1	0	0
84	1	1	Total Os 1 1	0	0
84	1	1	Total N Os 7 6 1	0	0
84	1	1	Total N Os 7 6 1	0	0
84	3	1	Total N Os 7 6 1	0	0
84	3	1	Total N Os 7 6 1	0	0
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84	4	1	Total N Os 7 6 1	0	0
84	4	1	Total N Os 7 6 1	0	0
84	4	1	Total N Os 7 6 1	0	0
84	4	1	Total N Os 7 6 1	0	0
84	4	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	k	1	7	6	1	0	0
84	l	1	7	6	1	0	0
84	r	1	7	6	1	0	0
84	v	1	7	6	1	0	0
84	x	1	7	6	1	0	0
84	x	1	7	6	1	0	0
84	y	1	7	6	1	0	0
84	z	1	7	6	1	0	0
84	2	1	7	6	1	0	0
84	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
84	6	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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84	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	6	1	7	6	1	0	0
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84	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
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84	6	1	7	6	1	0	0
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84	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
84	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
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			Total	N	Os		
84	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
84	6	1	7	6	1	0	0
			Total	N	Os		
84	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
84	AC	1	7	6	1	0	0
			Total	N	Os		
84	AG	1	7	6	1	0	0
			Total	N	Os		
84	AH	1	7	6	1	0	0
			Total	N	Os		
84	AK	1	7	6	1	0	0
			Total	N	Os		
84	AM	1	7	6	1	0	0
			Total	N	Os		
84	AP	1	7	6	1	0	0
			Total	N	Os		
84	AR	1	7	6	1	0	0
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			Total	N	Os		
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			Total	N	Os		
84	AR	1	7	6	1	0	0
			Total	N	Os		
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	AR	1	7	6	1	0	0
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	AR	1	7	6	1	0	0
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84	AR	1	7	6	1	0	0
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
84	AR	1	7	6	1	0	0
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84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	AR	1	7	6	1	0	0
			Total	N	Os		
84	AR	1	7	6	1	0	0
			Total	N	Os		
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84	AR	1	7	6	1	0	0
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84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	AR	1	7	6	1	0	0
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84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	AR	1	7	6	1	0	0
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84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
84	AR	1	7	6	1	0	0
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84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
84	AR	1	7	6	1	0	0
			Total	N	Os		
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
84	AR	1	7	6	1	0	0
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84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	AR	1	7	6	1	0	0
			Total	N	Os		
84	AR	1	7	6	1	0	0
			Total	N	Os		
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	AR	1	7	6	1	0	0
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			Total	N	Os		
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84	AR	1	7	6	1	0	0
			Total	N	Os		
84	AR	1	7	6	1	0	0
			Total	N	Os		
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
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			Total	N	Os		
84	AR	1	7	6	1	0	0
			Total	N	Os		
84	AS	1	7	6	1	0	0
			Total	N	Os		
84	AS	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	AS	1	7	6	1	0	0
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84	AS	1	7	6	1	0	0
84	AS	1	7	6	1	0	0
84	AS	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
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84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	AT	1	7	6	1	0	0
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84	AT	1	7	6	1	0	0
			Total	N	Os		
84	AT	1	7	6	1	0	0
			Total	N	Os		
84	AT	1	7	6	1	0	0
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84	CE	1	7	6	1	0	0
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84	CE	1	7	6	1	0	0
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84	CF	1	7	6	1	0	0
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84	CG	1	7	6	1	0	0
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84	CG	1	7	6	1	0	0
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84	CK	1	7	6	1	0	0
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84	CL	1	7	6	1	0	0
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84	CM	1	7	6	1	0	0
			Total	N	Os		
84	CP	1	7	6	1	0	0
			Total	N	Os		
84	CV	1	7	6	1	0	0
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84	CX	1	7	6	1	0	0
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84	CX	1	7	6	1	0	0
			Total	N	Os		
84	DD	1	7	6	1	0	0
			Total	N	Os		
84	DH	1	7	6	1	0	0
			Total	N	Os		
84	DQ	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	A	1	7	6	1	0	0
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84	A	1	7	6	1	0	0
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84	A	1	7	6	1	0	0
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			Total	N	Os		
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			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	A	1	7	6	1	0	0
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			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	A	1	7	6	1	0	0
			Total	N	Os		
84	J	1	7	6	1	0	0
			Total	N	Os		
84	K	1	7	6	1	0	0
			Total	N	Os		
84	M	1	7	6	1	0	0
			Total	N	Os		
84	O	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	Q	1	7	6	1	0	0
84	T	1	7	6	1	0	0
84	e	1	7	6	1	0	0
84	h	1	7	6	1	0	0
84	s8	1	7	6	1	0	0
84	c1	1	7	6	1	0	0
84	c3	1	7	6	1	0	0
84	c4	1	7	6	1	0	0
84	c5	1	7	6	1	0	0
84	c8	1	7	6	1	0	0
84	d9	1	7	6	1	0	0
84	sR	1	7	6	1	0	0

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
85	1	498	498	498	0	0
85	3	13	13	13	0	0
85	4	25	25	25	0	0
85	j	2	2	2	0	0
85	k	3	3	3	0	0
85	l	3	3	3	0	0
85	n	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	o	2	Total 2	Mg 2	0	0
85	r	1	Total 1	Mg 1	0	0
85	s	1	Total 1	Mg 1	0	0
85	t	3	Total 3	Mg 3	0	0
85	v	3	Total 3	Mg 3	0	0
85	w	2	Total 2	Mg 2	0	0
85	x	7	Total 7	Mg 7	0	0
85	z	1	Total 1	Mg 1	0	0
85	lR	1	Total 1	Mg 1	0	0
85	6	146	Total 146	Mg 146	0	0
85	AB	7	Total 7	Mg 7	0	0
85	AF	2	Total 2	Mg 2	0	0
85	AG	1	Total 1	Mg 1	0	0
85	AH	1	Total 1	Mg 1	0	0
85	AK	1	Total 1	Mg 1	0	0
85	AP	1	Total 1	Mg 1	0	0
85	AR	515	Total 515	Mg 515	0	0
85	AS	20	Total 20	Mg 20	0	0
85	AT	14	Total 14	Mg 14	0	0
85	CD	2	Total 2	Mg 2	0	0
85	CE	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
85	CF	1	1	1	0	0
85	CG	2	2	2	0	0
85	CI	1	1	1	0	0
85	CJ	1	1	1	0	0
85	CK	1	1	1	0	0
85	CL	1	1	1	0	0
85	CM	2	2	2	0	0
85	CO	1	1	1	0	0
85	CP	4	4	4	0	0
85	CQ	4	4	4	0	0
85	CR	5	5	5	0	0
85	CU	1	1	1	0	0
85	CX	2	2	2	0	0
85	DA	2	2	2	0	0
85	DC	4	4	4	0	0
85	DE	1	1	1	0	0
85	DH	2	2	2	0	0
85	DI	2	2	2	0	0
85	DL	1	1	1	0	0
85	DO	1	1	1	0	0
85	DQ	2	2	2	0	0

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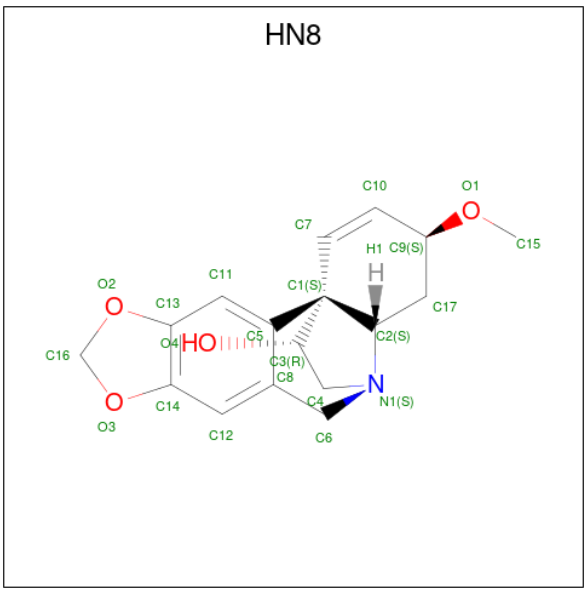
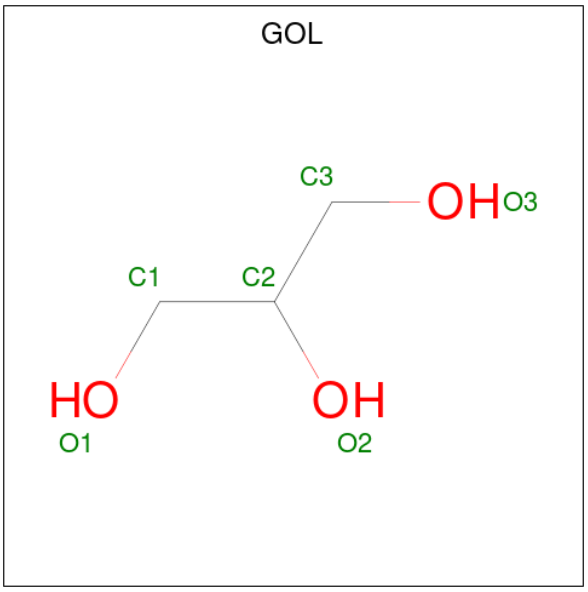
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
85	sM	2	2	2	0	0
85	A	116	116	116	0	0
85	D	1	1	1	0	0
85	F	1	1	1	0	0
85	H	1	1	1	0	0
85	T	1	1	1	0	0
85	U	1	1	1	0	0
85	V	1	1	1	0	0
85	Y	1	1	1	0	0
85	b	1	1	1	0	0
85	s4	1	1	1	0	0
85	s6	1	1	1	0	0
85	s8	1	1	1	0	0
85	c1	1	1	1	0	0
85	c6	1	1	1	0	0
85	c8	1	1	1	0	0
85	c9	1	1	1	0	0
85	d3	2	2	2	0	0
85	d4	1	1	1	0	0
85	d5	1	1	1	0	0
85	d6	2	2	2	0	0

- Molecule 86 is Haemanthamine (CCD ID: HN8) (formula: $C_{17}H_{19}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
86	1	1	22	17	1	4	0	0
			Total	C	N	O		
86	AR	1	22	17	1	4	0	0

- Molecule 87 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
87	v	1	6	3	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
87	6	1	6	3	3	0	0
			Total	C	O		
87	AR	1	6	3	3	0	0
			Total	C	O		
87	AR	1	6	3	3	0	0
			Total	C	O		
87	A	1	6	3	3	0	0

- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
88	AK	1	1	1	0	0
			Total	Zn		
88	AN	1	1	1	0	0
			Total	Zn		
88	AP	1	1	1	0	0
			Total	Zn		
88	AQ	1	1	1	0	0
			Total	Zn		
88	DL	1	1	1	0	0
			Total	Zn		
88	DO	1	1	1	0	0
			Total	Zn		
88	DQ	1	1	1	0	0
			Total	Zn		
88	DR	1	1	1	0	0
			Total	Zn		
88	b	1	1	1	0	0
			Total	Zn		
88	c	1	1	1	0	0
			Total	Zn		
88	e	1	1	1	0	0
			Total	Zn		
88	g	1	1	1	0	0
			Total	Zn		
88	d6	1	1	1	0	0
			Total	Zn		
88	d7	1	1	1	0	0
			Total	Zn		
88	d9	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
88	e1	1	1	1	0	0

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	303.13Å 286.50Å 435.66Å 90.00° 98.87° 90.00°	Depositor
Resolution (Å)	99.84 – 3.10 99.84 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (99.84-3.10) 99.5 (99.84-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 3.13Å)	Xtriage
Refinement program	PHENIX dev_2450	Depositor
R, R_{free}	0.222 , 0.252 0.223 , 0.253	Depositor DCC
R_{free} test set	26196 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å^2)	67.3	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 76.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	410383	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

4.6 Ligand geometry (i)

Of 2548 ligands modelled in this entry, 1 is modelled with single atom and 1477 are monoatomic - leaving 1070 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	$\#\|Z\| > 2$
84	OHX	6	2001	-	0,6,6	-	-	-		
84	OHX	1	3652	-	0,6,6	-	-	-		
84	OHX	AR	3558	-	0,6,6	-	-	-		
84	OHX	1	3429	-	0,6,6	-	-	-		
84	OHX	6	1974	-	0,6,6	-	-	-		
84	OHX	6	2029	-	0,6,6	-	-	-		
84	OHX	AR	3704	-	0,6,6	-	-	-		
84	OHX	AS	211	-	0,6,6	-	-	-		
84	OHX	A	1918	-	0,6,6	-	-	-		
84	OHX	A	1983	-	0,6,6	-	-	-		
84	OHX	AR	3502	-	0,6,6	-	-	-		
84	OHX	AR	3640	85	0,6,6	-	-	-		
84	OHX	AR	3555	-	0,6,6	-	-	-		
84	OHX	1	3679	-	0,6,6	-	-	-		
84	OHX	AR	3635	-	0,6,6	-	-	-		
84	OHX	1	3585	85	0,6,6	-	-	-		
84	OHX	AT	207	-	0,6,6	-	-	-		
84	OHX	AR	3700	-	0,6,6	-	-	-		
84	OHX	sR	401	-	0,6,6	-	-	-		
84	OHX	AR	3512	-	0,6,6	-	-	-		
84	OHX	6	1936	-	0,6,6	-	-	-		
84	OHX	c1	201	-	0,6,6	-	-	-		
84	OHX	6	1918	-	0,6,6	-	-	-		
84	OHX	c4	201	-	0,6,6	-	-	-		
84	OHX	1	3582	-	0,6,6	-	-	-		
84	OHX	1	3547	-	0,6,6	-	-	-		
84	OHX	AR	3503	-	0,6,6	-	-	-		
84	OHX	AR	3455	-	0,6,6	-	-	-		
84	OHX	A	2020	-	0,6,6	-	-	-		
84	OHX	AR	3489	87,85	0,6,6	-	-	-		
84	OHX	6	1906	-	0,6,6	-	-	-		
84	OHX	AR	3415	-	0,6,6	-	-	-		
84	OHX	A	2028	-	0,6,6	-	-	-		
84	OHX	A	2015	-	0,6,6	-	-	-		
84	OHX	1	3636	-	0,6,6	-	-	-		
84	OHX	4	205	-	0,6,6	-	-	-		
84	OHX	AR	3515	-	0,6,6	-	-	-		
84	OHX	1	3569	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	AR	3577	-	0,6,6	-	-	-		
84	OHX	AR	3699	-	0,6,6	-	-	-		
84	OHX	1	3464	85	0,6,6	-	-	-		
84	OHX	AR	3726	85	0,6,6	-	-	-		
84	OHX	3	202	-	0,6,6	-	-	-		
84	OHX	AR	3597	-	0,6,6	-	-	-		
84	OHX	A	1981	-	0,6,6	-	-	-		
84	OHX	1	3413	-	0,6,6	-	-	-		
84	OHX	AR	3513	-	0,6,6	-	-	-		
84	OHX	1	3635	-	0,6,6	-	-	-		
84	OHX	6	1952	-	0,6,6	-	-	-		
84	OHX	AS	209	-	0,6,6	-	-	-		
84	OHX	6	2021	-	0,6,6	-	-	-		
84	OHX	1	3708	-	0,6,6	-	-	-		
84	OHX	6	1902	-	0,6,6	-	-	-		
84	OHX	AR	3604	-	0,6,6	-	-	-		
84	OHX	A	1924	-	0,6,6	-	-	-		
84	OHX	A	1926	-	0,6,6	-	-	-		
84	OHX	A	1965	-	0,6,6	-	-	-		
84	OHX	1	3457	85	0,6,6	-	-	-		
84	OHX	AR	3684	-	0,6,6	-	-	-		
84	OHX	A	2040	-	0,6,6	-	-	-		
84	OHX	1	3668	-	0,6,6	-	-	-		
84	OHX	A	1949	-	0,6,6	-	-	-		
84	OHX	1	3451	85	0,6,6	-	-	-		
84	OHX	AR	3622	85	0,6,6	-	-	-		
84	OHX	1	3685	-	0,6,6	-	-	-		
84	OHX	AR	3628	-	0,6,6	-	-	-		
84	OHX	AR	3580	-	0,6,6	-	-	-		
84	OHX	AR	3593	-	0,6,6	-	-	-		
84	OHX	AR	3414	-	0,6,6	-	-	-		
84	OHX	6	1940	-	0,6,6	-	-	-		
84	OHX	1	3408	-	0,6,6	-	-	-		
84	OHX	r	301	-	0,6,6	-	-	-		
87	GOL	v	305	-	5,5,5	0.18	0	5,5,5	0.54	0
84	OHX	AR	3460	85	0,6,6	-	-	-		
84	OHX	1	3625	-	0,6,6	-	-	-		
84	OHX	AR	3686	-	0,6,6	-	-	-		
84	OHX	6	2046	-	0,6,6	-	-	-		
84	OHX	6	1983	-	0,6,6	-	-	-		
84	OHX	AR	3608	-	0,6,6	-	-	-		
84	OHX	1	3410	-	0,6,6	-	-	-		
84	OHX	1	3419	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	AR	3469	-	0,6,6	-	-	-		
84	OHX	1	3619	-	0,6,6	-	-	-		
84	OHX	6	1999	-	0,6,6	-	-	-		
84	OHX	T	201	-	0,6,6	-	-	-		
84	OHX	AR	3739	-	0,6,6	-	-	-		
84	OHX	6	1925	-	0,6,6	-	-	-		
84	OHX	AR	3733	-	0,6,6	-	-	-		
84	OHX	A	1977	-	0,6,6	-	-	-		
84	OHX	1	3666	-	0,6,6	-	-	-		
84	OHX	AR	3657	85	0,6,6	-	-	-		
84	OHX	1	3590	85	0,6,6	-	-	-		
84	OHX	AR	3643	85	0,6,6	-	-	-		
84	OHX	AR	3464	-	0,6,6	-	-	-		
84	OHX	AR	3639	-	0,6,6	-	-	-		
84	OHX	1	3485	-	0,6,6	-	-	-		
84	OHX	1	3601	-	0,6,6	-	-	-		
84	OHX	AR	3416	85	0,6,6	-	-	-		
84	OHX	AR	3439	-	0,6,6	-	-	-		
84	OHX	AR	3495	-	0,6,6	-	-	-		
84	OHX	AR	3696	84	0,6,6	-	-	-		
84	OHX	1	3466	-	0,6,6	-	-	-		
84	OHX	A	1932	-	0,6,6	-	-	-		
84	OHX	1	3718	-	0,6,6	-	-	-		
86	HN8	AR	4263	-	24,26,26	0.29	0	36,41,41	1.60	4 (11%)
84	OHX	1	3551	-	0,6,6	-	-	-		
84	OHX	1	3571	-	0,6,6	-	-	-		
84	OHX	AR	3741	-	0,6,6	-	-	-		
84	OHX	6	1987	-	0,6,6	-	-	-		
84	OHX	6	1914	-	0,6,6	-	-	-		
84	OHX	AR	3606	-	0,6,6	-	-	-		
84	OHX	AR	3609	-	0,6,6	-	-	-		
84	OHX	1	3492	85	0,6,6	-	-	-		
84	OHX	AR	3691	-	0,6,6	-	-	-		
84	OHX	AK	102	85	0,6,6	-	-	-		
84	OHX	6	1923	-	0,6,6	-	-	-		
84	OHX	AR	3511	-	0,6,6	-	-	-		
84	OHX	AR	3548	-	0,6,6	-	-	-		
84	OHX	AR	3454	-	0,6,6	-	-	-		
84	OHX	AR	3624	-	0,6,6	-	-	-		
84	OHX	AR	3642	-	0,6,6	-	-	-		
84	OHX	1	3561	-	0,6,6	-	-	-		
84	OHX	AR	3687	-	0,6,6	-	-	-		
84	OHX	6	1942	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	1	3659	-	0,6,6	-	-	-		
84	OHX	AR	3707	85	0,6,6	-	-	-		
84	OHX	1	3487	-	0,6,6	-	-	-		
84	OHX	AR	3560	-	0,6,6	-	-	-		
84	OHX	6	1973	-	0,6,6	-	-	-		
84	OHX	AR	3692	-	0,6,6	-	-	-		
84	OHX	AR	3715	-	0,6,6	-	-	-		
84	OHX	s8	301	-	0,6,6	-	-	-		
84	OHX	1	3509	85	0,6,6	-	-	-		
84	OHX	AR	3463	-	0,6,6	-	-	-		
84	OHX	AR	3404	-	0,6,6	-	-	-		
84	OHX	AR	3690	85	0,6,6	-	-	-		
84	OHX	AR	3638	-	0,6,6	-	-	-		
84	OHX	AR	3599	85	0,6,6	-	-	-		
84	OHX	A	1980	-	0,6,6	-	-	-		
84	OHX	AR	3538	-	0,6,6	-	-	-		
84	OHX	AR	3479	85	0,6,6	-	-	-		
84	OHX	A	2012	-	0,6,6	-	-	-		
84	OHX	v	301	-	0,6,6	-	-	-		
84	OHX	1	3434	-	0,6,6	-	-	-		
84	OHX	AR	3579	-	0,6,6	-	-	-		
84	OHX	6	1932	-	0,6,6	-	-	-		
84	OHX	1	3617	-	0,6,6	-	-	-		
84	OHX	A	1960	-	0,6,6	-	-	-		
84	OHX	1	3671	-	0,6,6	-	-	-		
84	OHX	1	3512	-	0,6,6	-	-	-		
84	OHX	6	2025	-	0,6,6	-	-	-		
84	OHX	A	2021	85	0,6,6	-	-	-		
84	OHX	1	3458	-	0,6,6	-	-	-		
84	OHX	1	3444	85	0,6,6	-	-	-		
84	OHX	AT	212	-	0,6,6	-	-	-		
84	OHX	AR	3522	-	0,6,6	-	-	-		
84	OHX	1	3428	-	0,6,6	-	-	-		
84	OHX	1	3544	-	0,6,6	-	-	-		
84	OHX	1	3448	85	0,6,6	-	-	-		
84	OHX	6	2002	-	0,6,6	-	-	-		
84	OHX	AR	3409	-	0,6,6	-	-	-		
84	OHX	1	3502	-	0,6,6	-	-	-		
84	OHX	A	1991	-	0,6,6	-	-	-		
84	OHX	AR	3703	-	0,6,6	-	-	-		
84	OHX	1	3491	-	0,6,6	-	-	-		
84	OHX	1	3647	85	0,6,6	-	-	-		
84	OHX	1	3658	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	AR	3598	-	0,6,6	-	-	-		
84	OHX	1	3678	-	0,6,6	-	-	-		
84	OHX	AR	3658	85	0,6,6	-	-	-		
84	OHX	1	3450	85	0,6,6	-	-	-		
84	OHX	AR	3481	-	0,6,6	-	-	-		
84	OHX	3	209	-	0,6,6	-	-	-		
84	OHX	2	201	-	0,6,6	-	-	-		
84	OHX	6	2042	-	0,6,6	-	-	-		
84	OHX	1	3426	85	0,6,6	-	-	-		
84	OHX	6	1996	-	0,6,6	-	-	-		
84	OHX	A	1911	-	0,6,6	-	-	-		
84	OHX	1	3613	-	0,6,6	-	-	-		
84	OHX	1	3573	85	0,6,6	-	-	-		
84	OHX	6	2045	-	0,6,6	-	-	-		
84	OHX	AR	3585	-	0,6,6	-	-	-		
84	OHX	CG	301	-	0,6,6	-	-	-		
84	OHX	AR	3623	-	0,6,6	-	-	-		
84	OHX	6	1984	-	0,6,6	-	-	-		
84	OHX	6	2016	85	0,6,6	-	-	-		
84	OHX	AR	3615	-	0,6,6	-	-	-		
84	OHX	1	3634	-	0,6,6	-	-	-		
84	OHX	AR	3559	-	0,6,6	-	-	-		
84	OHX	6	1943	-	0,6,6	-	-	-		
84	OHX	AR	3570	85	0,6,6	-	-	-		
84	OHX	AR	3529	85	0,6,6	-	-	-		
84	OHX	AR	3729	-	0,6,6	-	-	-		
84	OHX	A	2017	-	0,6,6	-	-	-		
84	OHX	6	2005	-	0,6,6	-	-	-		
84	OHX	1	3446	-	0,6,6	-	-	-		
84	OHX	AS	203	-	0,6,6	-	-	-		
84	OHX	6	1975	-	0,6,6	-	-	-		
84	OHX	A	1933	-	0,6,6	-	-	-		
84	OHX	A	1945	-	0,6,6	-	-	-		
84	OHX	A	1910	-	0,6,6	-	-	-		
84	OHX	AR	3582	85	0,6,6	-	-	-		
84	OHX	AR	3418	-	0,6,6	-	-	-		
84	OHX	AR	3539	-	0,6,6	-	-	-		
84	OHX	AR	3421	-	0,6,6	-	-	-		
84	OHX	AR	3547	-	0,6,6	-	-	-		
84	OHX	AS	202	-	0,6,6	-	-	-		
84	OHX	A	1903	-	0,6,6	-	-	-		
84	OHX	A	2014	-	0,6,6	-	-	-		
84	OHX	6	1905	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	1	3555	-	0,6,6	-	-	-		
84	OHX	A	2026	-	0,6,6	-	-	-		
84	OHX	AR	3470	-	0,6,6	-	-	-		
84	OHX	1	3524	-	0,6,6	-	-	-		
84	OHX	4	204	-	0,6,6	-	-	-		
84	OHX	6	1919	-	0,6,6	-	-	-		
84	OHX	6	2041	-	0,6,6	-	-	-		
84	OHX	6	2039	-	0,6,6	-	-	-		
84	OHX	AR	3680	-	0,6,6	-	-	-		
84	OHX	A	1920	-	0,6,6	-	-	-		
84	OHX	3	201	-	0,6,6	-	-	-		
84	OHX	1	3660	-	0,6,6	-	-	-		
84	OHX	AT	213	-	0,6,6	-	-	-		
84	OHX	AR	3706	-	0,6,6	-	-	-		
84	OHX	l	401	-	0,6,6	-	-	-		
84	OHX	AR	3591	-	0,6,6	-	-	-		
84	OHX	1	3577	85	0,6,6	-	-	-		
84	OHX	6	2023	-	0,6,6	-	-	-		
84	OHX	6	2032	-	0,6,6	-	-	-		
84	OHX	A	2001	-	0,6,6	-	-	-		
84	OHX	AR	3583	-	0,6,6	-	-	-		
84	OHX	1	3721	-	0,6,6	-	-	-		
84	OHX	AR	3457	-	0,6,6	-	-	-		
84	OHX	1	3477	-	0,6,6	-	-	-		
84	OHX	1	3644	-	0,6,6	-	-	-		
84	OHX	AR	3483	-	0,6,6	-	-	-		
84	OHX	A	1941	-	0,6,6	-	-	-		
84	OHX	AR	3427	-	0,6,6	-	-	-		
84	OHX	1	3505	-	0,6,6	-	-	-		
84	OHX	1	3533	-	0,6,6	-	-	-		
84	OHX	1	3605	-	0,6,6	-	-	-		
84	OHX	1	3437	85	0,6,6	-	-	-		
84	OHX	1	3592	-	0,6,6	-	-	-		
84	OHX	A	1982	-	0,6,6	-	-	-		
84	OHX	6	1980	-	0,6,6	-	-	-		
84	OHX	1	3442	-	0,6,6	-	-	-		
84	OHX	1	3649	-	0,6,6	-	-	-		
84	OHX	6	1981	-	0,6,6	-	-	-		
84	OHX	AR	3619	-	0,6,6	-	-	-		
84	OHX	AR	3743	-	0,6,6	-	-	-		
84	OHX	1	3719	-	0,6,6	-	-	-		
84	OHX	AR	3736	-	0,6,6	-	-	-		
84	OHX	A	2043	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	1	3656	-	0,6,6	-	-	-		
84	OHX	1	3452	-	0,6,6	-	-	-		
84	OHX	AR	3618	-	0,6,6	-	-	-		
84	OHX	AR	3467	-	0,6,6	-	-	-		
84	OHX	AR	3685	-	0,6,6	-	-	-		
84	OHX	1	3545	-	0,6,6	-	-	-		
84	OHX	A	1985	-	0,6,6	-	-	-		
84	OHX	AR	3740	-	0,6,6	-	-	-		
84	OHX	1	3529	-	0,6,6	-	-	-		
84	OHX	AR	3725	-	0,6,6	-	-	-		
84	OHX	A	1935	-	0,6,6	-	-	-		
84	OHX	AR	3592	-	0,6,6	-	-	-		
84	OHX	1	3405	-	0,6,6	-	-	-		
84	OHX	6	1941	-	0,6,6	-	-	-		
84	OHX	6	1986	-	0,6,6	-	-	-		
84	OHX	1	3595	-	0,6,6	-	-	-		
84	OHX	6	2049	-	0,6,6	-	-	-		
84	OHX	AR	3456	-	0,6,6	-	-	-		
84	OHX	4	214	-	0,6,6	-	-	-		
84	OHX	6	1921	-	0,6,6	-	-	-		
84	OHX	A	1901	-	0,6,6	-	-	-		
84	OHX	1	3469	-	0,6,6	-	-	-		
84	OHX	AR	3487	-	0,6,6	-	-	-		
84	OHX	1	3642	85	0,6,6	-	-	-		
84	OHX	1	3702	-	0,6,6	-	-	-		
84	OHX	1	3700	-	0,6,6	-	-	-		
84	OHX	AR	3533	-	0,6,6	-	-	-		
84	OHX	A	1998	-	0,6,6	-	-	-		
84	OHX	6	1971	-	0,6,6	-	-	-		
84	OHX	AR	3567	-	0,6,6	-	-	-		
84	OHX	AR	3462	85	0,6,6	-	-	-		
84	OHX	1	3580	-	0,6,6	-	-	-		
84	OHX	AR	3450	-	0,6,6	-	-	-		
84	OHX	1	3593	-	0,6,6	-	-	-		
84	OHX	6	2038	-	0,6,6	-	-	-		
84	OHX	1	3532	-	0,6,6	-	-	-		
84	OHX	AR	3532	-	0,6,6	-	-	-		
84	OHX	6	1957	-	0,6,6	-	-	-		
84	OHX	AR	3434	85	0,6,6	-	-	-		
84	OHX	1	3425	-	0,6,6	-	-	-		
84	OHX	1	3677	85	0,6,6	-	-	-		
84	OHX	1	3711	-	0,6,6	-	-	-		
84	OHX	1	3695	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	1	3586	-	0,6,6	-	-	-		
84	OHX	6	2010	-	0,6,6	-	-	-		
84	OHX	A	2018	-	0,6,6	-	-	-		
84	OHX	1	3707	-	0,6,6	-	-	-		
84	OHX	1	3602	85	0,6,6	-	-	-		
84	OHX	A	1997	-	0,6,6	-	-	-		
84	OHX	6	2000	-	0,6,6	-	-	-		
84	OHX	AR	3516	-	0,6,6	-	-	-		
84	OHX	A	1906	85	0,6,6	-	-	-		
84	OHX	AR	3433	-	0,6,6	-	-	-		
84	OHX	AR	3683	-	0,6,6	-	-	-		
84	OHX	1	3705	-	0,6,6	-	-	-		
84	OHX	1	3515	-	0,6,6	-	-	-		
84	OHX	AR	3712	85	0,6,6	-	-	-		
84	OHX	AR	3468	-	0,6,6	-	-	-		
84	OHX	AR	3493	85	0,6,6	-	-	-		
84	OHX	AS	201	-	0,6,6	-	-	-		
84	OHX	1	3470	-	0,6,6	-	-	-		
84	OHX	6	1998	-	0,6,6	-	-	-		
84	OHX	6	2047	-	0,6,6	-	-	-		
84	OHX	AR	3652	-	0,6,6	-	-	-		
84	OHX	AR	3737	-	0,6,6	-	-	-		
84	OHX	3	208	-	0,6,6	-	-	-		
84	OHX	6	2043	85	0,6,6	-	-	-		
84	OHX	1	3454	-	0,6,6	-	-	-		
84	OHX	6	1916	-	0,6,6	-	-	-		
84	OHX	1	3597	-	0,6,6	-	-	-		
84	OHX	x	201	85	0,6,6	-	-	-		
84	OHX	AR	3661	-	0,6,6	-	-	-		
84	OHX	1	3471	-	0,6,6	-	-	-		
84	OHX	AR	3745	-	0,6,6	-	-	-		
84	OHX	AS	205	85	0,6,6	-	-	-		
84	OHX	A	1970	-	0,6,6	-	-	-		
84	OHX	A	1989	-	0,6,6	-	-	-		
84	OHX	A	1948	-	0,6,6	-	-	-		
84	OHX	AR	3526	85	0,6,6	-	-	-		
84	OHX	1	3484	-	0,6,6	-	-	-		
84	OHX	AR	3561	-	0,6,6	-	-	-		
84	OHX	A	1914	-	0,6,6	-	-	-		
84	OHX	4	201	-	0,6,6	-	-	-		
84	OHX	A	1999	-	0,6,6	-	-	-		
84	OHX	A	1976	-	0,6,6	-	-	-		
84	OHX	1	3436	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	1	3546	-	0,6,6	-	-	-		
84	OHX	A	1959	-	0,6,6	-	-	-		
84	OHX	A	2032	-	0,6,6	-	-	-		
84	OHX	1	3430	-	0,6,6	-	-	-		
84	OHX	AR	3573	-	0,6,6	-	-	-		
84	OHX	A	1964	-	0,6,6	-	-	-		
84	OHX	AR	3716	-	0,6,6	-	-	-		
84	OHX	1	3528	-	0,6,6	-	-	-		
84	OHX	AR	3572	-	0,6,6	-	-	-		
84	OHX	A	1978	-	0,6,6	-	-	-		
84	OHX	AR	3705	-	0,6,6	-	-	-		
84	OHX	AR	3675	85	0,6,6	-	-	-		
84	OHX	A	2007	-	0,6,6	-	-	-		
84	OHX	6	2011	85	0,6,6	-	-	-		
84	OHX	1	3575	-	0,6,6	-	-	-		
84	OHX	1	3536	-	0,6,6	-	-	-		
84	OHX	AT	209	-	0,6,6	-	-	-		
84	OHX	1	3490	-	0,6,6	-	-	-		
84	OHX	CP	501	-	0,6,6	-	-	-		
87	GOL	AR	4261	1	5,5,5	0.14	0	5,5,5	0.33	0
84	OHX	6	1970	-	0,6,6	-	-	-		
84	OHX	A	1925	-	0,6,6	-	-	-		
84	OHX	AR	3422	-	0,6,6	-	-	-		
84	OHX	1	3465	-	0,6,6	-	-	-		
84	OHX	6	1948	85	0,6,6	-	-	-		
84	OHX	AR	3722	-	0,6,6	-	-	-		
84	OHX	AR	3486	-	0,6,6	-	-	-		
84	OHX	AR	3447	-	0,6,6	-	-	-		
84	OHX	6	2033	-	0,6,6	-	-	-		
84	OHX	AR	3461	-	0,6,6	-	-	-		
84	OHX	A	2000	-	0,6,6	-	-	-		
84	OHX	1	3661	-	0,6,6	-	-	-		
84	OHX	1	3431	-	0,6,6	-	-	-		
84	OHX	AR	3655	-	0,6,6	-	-	-		
84	OHX	AR	3641	-	0,6,6	-	-	-		
84	OHX	6	1993	-	0,6,6	-	-	-		
84	OHX	DQ	201	85	0,6,6	-	-	-		
84	OHX	1	3724	85	0,6,6	-	-	-		
84	OHX	AR	3474	-	0,6,6	-	-	-		
84	OHX	1	3531	-	0,6,6	-	-	-		
84	OHX	6	2018	-	0,6,6	-	-	-		
84	OHX	AR	3701	-	0,6,6	-	-	-		
84	OHX	AR	3413	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	A	2009	-	0,6,6	-	-	-		
87	GOL	A	2160	-	5,5,5	0.10	0	5,5,5	0.29	0
84	OHX	1	3489	85	0,6,6	-	-	-		
84	OHX	AR	3621	85	0,6,6	-	-	-		
84	OHX	6	1937	-	0,6,6	-	-	-		
84	OHX	AR	3552	-	0,6,6	-	-	-		
84	OHX	1	3713	85	0,6,6	-	-	-		
84	OHX	6	1979	-	0,6,6	-	-	-		
84	OHX	AR	3562	85	0,6,6	-	-	-		
84	OHX	1	3557	-	0,6,6	-	-	-		
84	OHX	A	1950	-	0,6,6	-	-	-		
84	OHX	A	1954	-	0,6,6	-	-	-		
84	OHX	AR	3505	-	0,6,6	-	-	-		
84	OHX	1	3650	-	0,6,6	-	-	-		
84	OHX	1	3603	85	0,6,6	-	-	-		
84	OHX	6	1992	-	0,6,6	-	-	-		
84	OHX	6	2007	-	0,6,6	-	-	-		
84	OHX	AR	3540	-	0,6,6	-	-	-		
84	OHX	AR	3603	-	0,6,6	-	-	-		
84	OHX	1	3558	-	0,6,6	-	-	-		
84	OHX	6	1922	-	0,6,6	-	-	-		
84	OHX	AR	3553	85	0,6,6	-	-	-		
84	OHX	1	3684	-	0,6,6	-	-	-		
84	OHX	6	1927	-	0,6,6	-	-	-		
84	OHX	AR	3645	-	0,6,6	-	-	-		
84	OHX	AR	3649	-	0,6,6	-	-	-		
84	OHX	AR	3670	-	0,6,6	-	-	-		
84	OHX	AT	204	-	0,6,6	-	-	-		
84	OHX	AR	3719	-	0,6,6	-	-	-		
84	OHX	6	1907	-	0,6,6	-	-	-		
84	OHX	AR	3476	85	0,6,6	-	-	-		
84	OHX	AR	3565	-	0,6,6	-	-	-		
84	OHX	A	1975	-	0,6,6	-	-	-		
84	OHX	1	3692	-	0,6,6	-	-	-		
84	OHX	A	2035	-	0,6,6	-	-	-		
84	OHX	AR	3666	-	0,6,6	-	-	-		
84	OHX	1	3483	-	0,6,6	-	-	-		
84	OHX	1	3663	-	0,6,6	-	-	-		
84	OHX	AR	3682	-	0,6,6	-	-	-		
84	OHX	3	204	-	0,6,6	-	-	-		
84	OHX	1	3513	85	0,6,6	-	-	-		
84	OHX	AR	3485	-	0,6,6	-	-	-		
84	OHX	CF	402	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	1	3427	-	0,6,6	-	-	-		
84	OHX	1	3506	-	0,6,6	-	-	-		
84	OHX	AR	3498	-	0,6,6	-	-	-		
84	OHX	6	1912	-	0,6,6	-	-	-		
84	OHX	1	3566	-	0,6,6	-	-	-		
84	OHX	AR	3504	-	0,6,6	-	-	-		
84	OHX	AR	3672	-	0,6,6	-	-	-		
84	OHX	AT	217	-	0,6,6	-	-	-		
84	OHX	1	3706	-	0,6,6	-	-	-		
84	OHX	AR	3534	-	0,6,6	-	-	-		
84	OHX	A	1909	-	0,6,6	-	-	-		
84	OHX	AR	3676	-	0,6,6	-	-	-		
84	OHX	AR	3478	-	0,6,6	-	-	-		
84	OHX	AS	207	-	0,6,6	-	-	-		
84	OHX	A	1946	85	0,6,6	-	-	-		
84	OHX	1	3620	85	0,6,6	-	-	-		
84	OHX	M	201	-	0,6,6	-	-	-		
84	OHX	1	3640	-	0,6,6	-	-	-		
84	OHX	6	2051	-	0,6,6	-	-	-		
84	OHX	AR	3542	-	0,6,6	-	-	-		
84	OHX	1	3662	-	0,6,6	-	-	-		
84	OHX	AR	3631	-	0,6,6	-	-	-		
84	OHX	6	1989	-	0,6,6	-	-	-		
84	OHX	AR	3420	-	0,6,6	-	-	-		
84	OHX	1	3445	-	0,6,6	-	-	-		
84	OHX	A	2003	-	0,6,6	-	-	-		
84	OHX	AR	3734	-	0,6,6	-	-	-		
84	OHX	A	1984	-	0,6,6	-	-	-		
84	OHX	1	3459	-	0,6,6	-	-	-		
84	OHX	A	1942	85	0,6,6	-	-	-		
84	OHX	A	1913	-	0,6,6	-	-	-		
84	OHX	1	3657	85	0,6,6	-	-	-		
84	OHX	6	2030	-	0,6,6	-	-	-		
84	OHX	AT	215	-	0,6,6	-	-	-		
84	OHX	AR	3627	-	0,6,6	-	-	-		
84	OHX	A	2022	-	0,6,6	-	-	-		
84	OHX	A	2005	-	0,6,6	-	-	-		
84	OHX	1	3421	-	0,6,6	-	-	-		
84	OHX	6	1991	-	0,6,6	-	-	-		
84	OHX	AR	3632	-	0,6,6	-	-	-		
84	OHX	AR	3407	85	0,6,6	-	-	-		
84	OHX	AR	3443	-	0,6,6	-	-	-		
84	OHX	AR	3711	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	AR	3602	-	0,6,6	-	-	-		
84	OHX	AR	3586	-	0,6,6	-	-	-		
84	OHX	4	215	-	0,6,6	-	-	-		
84	OHX	4	209	-	0,6,6	-	-	-		
84	OHX	6	1978	-	0,6,6	-	-	-		
84	OHX	1	3630	-	0,6,6	-	-	-		
84	OHX	A	1931	-	0,6,6	-	-	-		
84	OHX	1	3503	-	0,6,6	-	-	-		
84	OHX	A	1928	-	0,6,6	-	-	-		
84	OHX	AR	3451	-	0,6,6	-	-	-		
84	OHX	A	2019	-	0,6,6	-	-	-		
84	OHX	O	201	-	0,6,6	-	-	-		
84	OHX	1	3472	85	0,6,6	-	-	-		
84	OHX	4	211	-	0,6,6	-	-	-		
84	OHX	AR	3440	-	0,6,6	-	-	-		
84	OHX	AR	3709	-	0,6,6	-	-	-		
84	OHX	6	1988	-	0,6,6	-	-	-		
84	OHX	1	3587	-	0,6,6	-	-	-		
84	OHX	A	1973	-	0,6,6	-	-	-		
84	OHX	1	3651	-	0,6,6	-	-	-		
84	OHX	AR	3448	-	0,6,6	-	-	-		
84	OHX	AR	3601	-	0,6,6	-	-	-		
84	OHX	A	2041	-	0,6,6	-	-	-		
84	OHX	6	1915	-	0,6,6	-	-	-		
84	OHX	A	1966	-	0,6,6	-	-	-		
84	OHX	A	1972	-	0,6,6	-	-	-		
84	OHX	A	1987	-	0,6,6	-	-	-		
84	OHX	A	1971	-	0,6,6	-	-	-		
84	OHX	AR	3728	-	0,6,6	-	-	-		
84	OHX	AR	3730	-	0,6,6	-	-	-		
84	OHX	1	3423	-	0,6,6	-	-	-		
84	OHX	CM	201	-	0,6,6	-	-	-		
84	OHX	6	1956	-	0,6,6	-	-	-		
84	OHX	1	3474	-	0,6,6	-	-	-		
84	OHX	AT	202	-	0,6,6	-	-	-		
84	OHX	1	3689	-	0,6,6	-	-	-		
84	OHX	A	2004	-	0,6,6	-	-	-		
84	OHX	AR	3634	-	0,6,6	-	-	-		
84	OHX	AR	3496	-	0,6,6	-	-	-		
84	OHX	AT	214	-	0,6,6	-	-	-		
84	OHX	AR	3488	-	0,6,6	-	-	-		
84	OHX	6	1968	-	0,6,6	-	-	-		
84	OHX	AR	3482	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	AR	3549	-	0,6,6	-	-	-		
84	OHX	6	1985	85	0,6,6	-	-	-		
84	OHX	A	1979	-	0,6,6	-	-	-		
84	OHX	1	3525	-	0,6,6	-	-	-		
84	OHX	AR	3581	-	0,6,6	-	-	-		
84	OHX	6	2024	-	0,6,6	-	-	-		
84	OHX	AR	3521	-	0,6,6	-	-	-		
84	OHX	6	1961	-	0,6,6	-	-	-		
84	OHX	1	3637	-	0,6,6	-	-	-		
84	OHX	AR	3524	-	0,6,6	-	-	-		
84	OHX	1	3481	85	0,6,6	-	-	-		
84	OHX	AR	3536	-	0,6,6	-	-	-		
84	OHX	AT	210	-	0,6,6	-	-	-		
84	OHX	AR	3519	-	0,6,6	-	-	-		
84	OHX	CL	301	85	0,6,6	-	-	-		
84	OHX	A	2010	-	0,6,6	-	-	-		
84	OHX	1	3520	-	0,6,6	-	-	-		
84	OHX	CV	201	-	0,6,6	-	-	-		
84	OHX	A	2036	-	0,6,6	-	-	-		
84	OHX	A	2023	-	0,6,6	-	-	-		
84	OHX	A	1958	-	0,6,6	-	-	-		
84	OHX	AR	3458	85	0,6,6	-	-	-		
84	OHX	A	2034	-	0,6,6	-	-	-		
84	OHX	6	1946	85	0,6,6	-	-	-		
84	OHX	AR	3431	-	0,6,6	-	-	-		
84	OHX	e	101	-	0,6,6	-	-	-		
84	OHX	AR	3459	-	0,6,6	-	-	-		
84	OHX	AR	3575	-	0,6,6	-	-	-		
84	OHX	AR	3544	-	0,6,6	-	-	-		
84	OHX	AR	3531	85	0,6,6	-	-	-		
84	OHX	AR	3742	-	0,6,6	-	-	-		
84	OHX	A	1919	-	0,6,6	-	-	-		
84	OHX	4	212	-	0,6,6	-	-	-		
84	OHX	1	3672	-	0,6,6	-	-	-		
84	OHX	6	1965	-	0,6,6	-	-	-		
84	OHX	6	2003	-	0,6,6	-	-	-		
84	OHX	A	1921	85	0,6,6	-	-	-		
84	OHX	1	3607	-	0,6,6	-	-	-		
84	OHX	1	3606	85	0,6,6	-	-	-		
84	OHX	AR	3594	-	0,6,6	-	-	-		
84	OHX	AT	203	-	0,6,6	-	-	-		
84	OHX	A	1927	-	0,6,6	-	-	-		
84	OHX	AR	3626	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	AR	3510	-	0,6,6	-	-	-		
84	OHX	1	3507	85	0,6,6	-	-	-		
84	OHX	AR	3541	-	0,6,6	-	-	-		
84	OHX	6	2012	-	0,6,6	-	-	-		
84	OHX	6	2052	-	0,6,6	-	-	-		
84	OHX	AR	3629	-	0,6,6	-	-	-		
84	OHX	A	1951	-	0,6,6	-	-	-		
84	OHX	1	3447	-	0,6,6	-	-	-		
84	OHX	AR	3588	85	0,6,6	-	-	-		
84	OHX	1	3478	-	0,6,6	-	-	-		
86	HN8	1	4223	-	24,26,26	0.28	0	36,41,41	1.03	2 (5%)
84	OHX	1	3535	-	0,6,6	-	-	-		
84	OHX	1	3680	-	0,6,6	-	-	-		
84	OHX	1	3675	-	0,6,6	-	-	-		
84	OHX	AR	3426	-	0,6,6	-	-	-		
84	OHX	AR	3656	-	0,6,6	-	-	-		
84	OHX	AR	3663	-	0,6,6	-	-	-		
84	OHX	A	1953	-	0,6,6	-	-	-		
84	OHX	AR	3668	85	0,6,6	-	-	-		
84	OHX	1	3714	-	0,6,6	-	-	-		
84	OHX	1	3693	-	0,6,6	-	-	-		
84	OHX	1	3417	-	0,6,6	-	-	-		
84	OHX	6	1909	-	0,6,6	-	-	-		
84	OHX	6	1972	-	0,6,6	-	-	-		
84	OHX	AR	3616	-	0,6,6	-	-	-		
84	OHX	AR	3714	85	0,6,6	-	-	-		
84	OHX	AR	3744	-	0,6,6	-	-	-		
87	GOL	AR	4262	84	5,5,5	0.26	0	5,5,5	0.53	0
84	OHX	4	216	-	0,6,6	-	-	-		
84	OHX	AR	3566	85	0,6,6	-	-	-		
84	OHX	1	3480	85	0,6,6	-	-	-		
84	OHX	1	3540	85	0,6,6	-	-	-		
84	OHX	CG	302	-	0,6,6	-	-	-		
84	OHX	A	1944	-	0,6,6	-	-	-		
84	OHX	AR	3568	-	0,6,6	-	-	-		
84	OHX	1	3703	-	0,6,6	-	-	-		
84	OHX	1	3501	-	0,6,6	-	-	-		
84	OHX	1	3537	85	0,6,6	-	-	-		
84	OHX	1	3648	-	0,6,6	-	-	-		
84	OHX	1	3633	-	0,6,6	-	-	-		
84	OHX	1	3641	-	0,6,6	-	-	-		
84	OHX	1	3522	85	0,6,6	-	-	-		
84	OHX	1	3670	85	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	6	1977	85	0,6,6	-	-	-		
84	OHX	AR	3612	85	0,6,6	-	-	-		
84	OHX	AR	3625	-	0,6,6	-	-	-		
84	OHX	AR	3723	-	0,6,6	-	-	-		
84	OHX	1	3565	-	0,6,6	-	-	-		
84	OHX	6	2015	-	0,6,6	-	-	-		
84	OHX	1	3596	-	0,6,6	-	-	-		
84	OHX	1	3432	-	0,6,6	-	-	-		
84	OHX	AR	3517	-	0,6,6	-	-	-		
84	OHX	AR	3674	85	0,6,6	-	-	-		
84	OHX	A	2030	-	0,6,6	-	-	-		
84	OHX	1	3576	-	0,6,6	-	-	-		
84	OHX	1	3441	-	0,6,6	-	-	-		
84	OHX	AR	3438	-	0,6,6	-	-	-		
84	OHX	K	201	-	0,6,6	-	-	-		
84	OHX	AR	3590	85	0,6,6	-	-	-		
84	OHX	1	3608	-	0,6,6	-	-	-		
84	OHX	AR	3543	-	0,6,6	-	-	-		
84	OHX	AS	210	85	0,6,6	-	-	-		
84	OHX	AR	3551	-	0,6,6	-	-	-		
84	OHX	CX	202	-	0,6,6	-	-	-		
84	OHX	6	1904	-	0,6,6	-	-	-		
84	OHX	AR	3569	-	0,6,6	-	-	-		
84	OHX	1	3494	-	0,6,6	-	-	-		
84	OHX	1	3530	-	0,6,6	-	-	-		
84	OHX	AH	201	-	0,6,6	-	-	-		
84	OHX	AR	3727	-	0,6,6	-	-	-		
84	OHX	1	3610	-	0,6,6	-	-	-		
84	OHX	1	3418	-	0,6,6	-	-	-		
84	OHX	AR	3644	-	0,6,6	-	-	-		
84	OHX	1	3631	-	0,6,6	-	-	-		
84	OHX	1	3455	-	0,6,6	-	-	-		
84	OHX	1	3422	85	0,6,6	-	-	-		
84	OHX	AR	3665	-	0,6,6	-	-	-		
84	OHX	AR	3735	-	0,6,6	-	-	-		
84	OHX	A	1955	-	0,6,6	-	-	-		
84	OHX	1	3655	-	0,6,6	-	-	-		
84	OHX	1	3614	-	0,6,6	-	-	-		
84	OHX	1	3701	-	0,6,6	-	-	-		
84	OHX	6	1938	-	0,6,6	-	-	-		
84	OHX	1	3632	-	0,6,6	-	-	-		
84	OHX	A	1936	85	0,6,6	-	-	-		
84	OHX	1	3482	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	1	3412	-	0,6,6	-	-	-		
84	OHX	1	3424	85	0,6,6	-	-	-		
84	OHX	1	3584	-	0,6,6	-	-	-		
84	OHX	1	3699	-	0,6,6	-	-	-		
84	OHX	6	2020	-	0,6,6	-	-	-		
84	OHX	AR	3731	-	0,6,6	-	-	-		
84	OHX	A	1930	-	0,6,6	-	-	-		
84	OHX	A	1993	-	0,6,6	-	-	-		
84	OHX	AR	3506	-	0,6,6	-	-	-		
84	OHX	AR	3499	-	0,6,6	-	-	-		
84	OHX	AR	3527	85	0,6,6	-	-	-		
84	OHX	AR	3650	-	0,6,6	-	-	-		
84	OHX	1	3467	-	0,6,6	-	-	-		
84	OHX	6	1969	85	0,6,6	-	-	-		
84	OHX	6	1976	-	0,6,6	-	-	-		
84	OHX	1	3698	-	0,6,6	-	-	-		
84	OHX	A	1937	-	0,6,6	-	-	-		
84	OHX	1	3420	-	0,6,6	-	-	-		
84	OHX	1	3594	-	0,6,6	-	-	-		
84	OHX	1	3604	-	0,6,6	-	-	-		
84	OHX	AR	3449	-	0,6,6	-	-	-		
84	OHX	6	1963	-	0,6,6	-	-	-		
84	OHX	AR	3595	-	0,6,6	-	-	-		
84	OHX	AT	206	-	0,6,6	-	-	-		
84	OHX	6	2050	-	0,6,6	-	-	-		
84	OHX	1	3407	-	0,6,6	-	-	-		
84	OHX	AR	3405	-	0,6,6	-	-	-		
84	OHX	6	1924	85	0,6,6	-	-	-		
84	OHX	1	3645	-	0,6,6	-	-	-		
84	OHX	AR	3497	-	0,6,6	-	-	-		
84	OHX	A	1992	-	0,6,6	-	-	-		
84	OHX	1	3646	-	0,6,6	-	-	-		
84	OHX	6	1903	-	0,6,6	-	-	-		
84	OHX	6	2035	85	0,6,6	-	-	-		
84	OHX	1	3414	-	0,6,6	-	-	-		
84	OHX	1	3550	-	0,6,6	-	-	-		
84	OHX	1	3456	-	0,6,6	-	-	-		
84	OHX	AR	3508	-	0,6,6	-	-	-		
84	OHX	6	1953	-	0,6,6	-	-	-		
84	OHX	AR	3702	-	0,6,6	-	-	-		
84	OHX	AR	3613	85	0,6,6	-	-	-		
84	OHX	AT	201	-	0,6,6	-	-	-		
84	OHX	A	1907	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	1	3440	-	0,6,6	-	-	-		
84	OHX	AR	3465	85	0,6,6	-	-	-		
84	OHX	1	3688	-	0,6,6	-	-	-		
84	OHX	AR	3477	84	0,6,6	-	-	-		
84	OHX	1	3510	-	0,6,6	-	-	-		
84	OHX	1	3600	-	0,6,6	-	-	-		
84	OHX	AR	3664	-	0,6,6	-	-	-		
84	OHX	AT	205	-	0,6,6	-	-	-		
84	OHX	A	1902	-	0,6,6	-	-	-		
84	OHX	1	3720	-	0,6,6	-	-	-		
84	OHX	A	2027	-	0,6,6	-	-	-		
84	OHX	A	2029	-	0,6,6	-	-	-		
84	OHX	1	3629	-	0,6,6	-	-	-		
84	OHX	A	1990	-	0,6,6	-	-	-		
84	OHX	A	2025	-	0,6,6	-	-	-		
84	OHX	k	401	-	0,6,6	-	-	-		
84	OHX	1	3496	-	0,6,6	-	-	-		
84	OHX	AR	3724	-	0,6,6	-	-	-		
84	OHX	1	3439	85	0,6,6	-	-	-		
84	OHX	A	1962	-	0,6,6	-	-	-		
84	OHX	1	3495	-	0,6,6	-	-	-		
84	OHX	1	3559	-	0,6,6	-	-	-		
84	OHX	AT	211	-	0,6,6	-	-	-		
84	OHX	6	2004	-	0,6,6	-	-	-		
84	OHX	A	2031	-	0,6,6	-	-	-		
84	OHX	6	1967	85	0,6,6	-	-	-		
84	OHX	1	3526	-	0,6,6	-	-	-		
84	OHX	AR	3406	-	0,6,6	-	-	-		
84	OHX	1	3579	-	0,6,6	-	-	-		
84	OHX	c5	201	-	0,6,6	-	-	-		
84	OHX	6	1954	-	0,6,6	-	-	-		
84	OHX	1	3624	-	0,6,6	-	-	-		
84	OHX	1	3519	-	0,6,6	-	-	-		
84	OHX	1	3704	-	0,6,6	-	-	-		
84	OHX	1	3562	-	0,6,6	-	-	-		
84	OHX	AR	3732	-	0,6,6	-	-	-		
84	OHX	AR	3717	85	0,6,6	-	-	-		
84	OHX	AR	3402	-	0,6,6	-	-	-		
84	OHX	AR	3660	-	0,6,6	-	-	-		
84	OHX	1	3438	-	0,6,6	-	-	-		
84	OHX	AR	3681	-	0,6,6	-	-	-		
84	OHX	AR	3494	85	0,6,6	-	-	-		
84	OHX	1	3518	85	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	1	3618	-	0,6,6	-	-	-		
84	OHX	1	3638	-	0,6,6	-	-	-		
84	OHX	1	3667	-	0,6,6	-	-	-		
84	OHX	6	1990	-	0,6,6	-	-	-		
84	OHX	1	3538	-	0,6,6	-	-	-		
84	OHX	6	1926	-	0,6,6	-	-	-		
84	OHX	AR	3600	-	0,6,6	-	-	-		
84	OHX	AR	3673	-	0,6,6	-	-	-		
84	OHX	6	1962	-	0,6,6	-	-	-		
84	OHX	1	3543	85	0,6,6	-	-	-		
84	OHX	4	213	-	0,6,6	-	-	-		
84	OHX	AS	208	-	0,6,6	-	-	-		
84	OHX	1	3674	-	0,6,6	-	-	-		
84	OHX	A	1923	-	0,6,6	-	-	-		
84	OHX	1	3686	-	0,6,6	-	-	-		
84	OHX	1	3697	84	0,6,6	-	-	-		
84	OHX	AR	3708	-	0,6,6	-	-	-		
84	OHX	AR	3694	-	0,6,6	-	-	-		
84	OHX	1	3433	-	0,6,6	-	-	-		
84	OHX	1	3653	85	0,6,6	-	-	-		
84	OHX	1	3541	85	0,6,6	-	-	-		
84	OHX	AR	3617	-	0,6,6	-	-	-		
84	OHX	A	1917	-	0,6,6	-	-	-		
84	OHX	AR	3442	-	0,6,6	-	-	-		
84	OHX	AR	3671	85	0,6,6	-	-	-		
84	OHX	AR	3678	-	0,6,6	-	-	-		
84	OHX	1	3493	-	0,6,6	-	-	-		
84	OHX	AR	3432	-	0,6,6	-	-	-		
84	OHX	A	1915	-	0,6,6	-	-	-		
84	OHX	A	2039	-	0,6,6	-	-	-		
84	OHX	1	3643	85	0,6,6	-	-	-		
84	OHX	AR	3620	-	0,6,6	-	-	-		
84	OHX	1	3570	-	0,6,6	-	-	-		
84	OHX	1	3409	-	0,6,6	-	-	-		
84	OHX	1	3553	-	0,6,6	-	-	-		
84	OHX	AR	3679	-	0,6,6	-	-	-		
84	OHX	A	2013	-	0,6,6	-	-	-		
84	OHX	1	3511	-	0,6,6	-	-	-		
84	OHX	AR	3490	85	0,6,6	-	-	-		
84	OHX	6	2027	-	0,6,6	-	-	-		
84	OHX	AR	3473	-	0,6,6	-	-	-		
84	OHX	AR	3545	85	0,6,6	-	-	-		
84	OHX	1	3616	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	GOL	6	2199	-	5,5,5	0.10	0	5,5,5	0.33	0
84	OHX	AR	3419	-	0,6,6	-	-	-		
84	OHX	AR	3480	-	0,6,6	-	-	-		
84	OHX	6	1994	-	0,6,6	-	-	-		
84	OHX	1	3687	-	0,6,6	-	-	-		
84	OHX	AR	3425	-	0,6,6	-	-	-		
84	OHX	AR	3578	-	0,6,6	-	-	-		
84	OHX	1	3612	-	0,6,6	-	-	-		
84	OHX	1	3628	-	0,6,6	-	-	-		
84	OHX	AR	3429	85	0,6,6	-	-	-		
84	OHX	AR	3713	-	0,6,6	-	-	-		
84	OHX	6	1928	85	0,6,6	-	-	-		
84	OHX	1	3564	-	0,6,6	-	-	-		
84	OHX	AS	206	-	0,6,6	-	-	-		
84	OHX	6	1950	-	0,6,6	-	-	-		
84	OHX	A	1963	-	0,6,6	-	-	-		
84	OHX	1	3514	-	0,6,6	-	-	-		
84	OHX	c8	201	-	0,6,6	-	-	-		
84	OHX	A	2024	-	0,6,6	-	-	-		
84	OHX	6	1939	-	0,6,6	-	-	-		
84	OHX	AR	3453	-	0,6,6	-	-	-		
84	OHX	4	208	85	0,6,6	-	-	-		
84	OHX	AR	3430	-	0,6,6	-	-	-		
84	OHX	1	3508	-	0,6,6	-	-	-		
84	OHX	AR	3523	-	0,6,6	-	-	-		
84	OHX	1	3568	-	0,6,6	-	-	-		
84	OHX	CF	401	-	0,6,6	-	-	-		
84	OHX	AR	3491	-	0,6,6	-	-	-		
84	OHX	1	3460	-	0,6,6	-	-	-		
84	OHX	AR	3424	-	0,6,6	-	-	-		
84	OHX	6	2026	-	0,6,6	-	-	-		
84	OHX	AR	3695	-	0,6,6	-	-	-		
84	OHX	AR	3435	-	0,6,6	-	-	-		
84	OHX	A	1908	-	0,6,6	-	-	-		
84	OHX	1	3449	-	0,6,6	-	-	-		
84	OHX	A	1929	-	0,6,6	-	-	-		
84	OHX	AR	3689	-	0,6,6	-	-	-		
84	OHX	6	1955	-	0,6,6	-	-	-		
84	OHX	A	1904	-	0,6,6	-	-	-		
84	OHX	1	3609	-	0,6,6	-	-	-		
84	OHX	AR	3698	-	0,6,6	-	-	-		
84	OHX	1	3665	-	0,6,6	-	-	-		
84	OHX	A	1905	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	AR	3530	-	0,6,6	-	-	-		
84	OHX	6	1917	-	0,6,6	-	-	-		
84	OHX	AR	3408	-	0,6,6	-	-	-		
84	OHX	AS	204	85	0,6,6	-	-	-		
84	OHX	6	1964	-	0,6,6	-	-	-		
84	OHX	AR	3564	-	0,6,6	-	-	-		
84	OHX	1	3654	-	0,6,6	-	-	-		
84	OHX	1	3664	85	0,6,6	-	-	-		
84	OHX	6	2031	-	0,6,6	-	-	-		
84	OHX	AR	3471	-	0,6,6	-	-	-		
84	OHX	AR	3475	-	0,6,6	-	-	-		
84	OHX	1	3499	-	0,6,6	-	-	-		
84	OHX	6	1949	-	0,6,6	-	-	-		
84	OHX	1	3479	-	0,6,6	-	-	-		
84	OHX	AR	3445	-	0,6,6	-	-	-		
84	OHX	6	1982	-	0,6,6	-	-	-		
84	OHX	1	3539	84	0,6,6	-	-	-		
84	OHX	A	1974	-	0,6,6	-	-	-		
84	OHX	c3	201	-	0,6,6	-	-	-		
84	OHX	1	3622	-	0,6,6	-	-	-		
84	OHX	1	3497	-	0,6,6	-	-	-		
84	OHX	6	2014	-	0,6,6	-	-	-		
84	OHX	AR	3528	-	0,6,6	-	-	-		
84	OHX	AR	3607	-	0,6,6	-	-	-		
84	OHX	1	3521	-	0,6,6	-	-	-		
84	OHX	6	2013	-	0,6,6	-	-	-		
84	OHX	6	2028	85	0,6,6	-	-	-		
84	OHX	1	3549	-	0,6,6	-	-	-		
84	OHX	1	3591	-	0,6,6	-	-	-		
84	OHX	AR	3563	-	0,6,6	-	-	-		
84	OHX	AR	3518	-	0,6,6	-	-	-		
84	OHX	h	401	-	0,6,6	-	-	-		
84	OHX	3	203	85	0,6,6	-	-	-		
84	OHX	AR	3574	-	0,6,6	-	-	-		
84	OHX	1	3588	85	0,6,6	-	-	-		
84	OHX	A	1995	-	0,6,6	-	-	-		
84	OHX	1	3462	-	0,6,6	-	-	-		
84	OHX	1	3416	-	0,6,6	-	-	-		
84	OHX	AR	3411	-	0,6,6	-	-	-		
84	OHX	AR	3589	-	0,6,6	-	-	-		
84	OHX	AR	3667	-	0,6,6	-	-	-		
84	OHX	AR	3401	-	0,6,6	-	-	-		
84	OHX	A	2006	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	1	3406	-	0,6,6	-	-	-		
84	OHX	1	3443	-	0,6,6	-	-	-		
84	OHX	y	201	-	0,6,6	-	-	-		
84	OHX	AR	3693	-	0,6,6	-	-	-		
84	OHX	AP	502	85	0,6,6	-	-	-		
84	OHX	1	3669	-	0,6,6	-	-	-		
84	OHX	AG	201	-	0,6,6	-	-	-		
84	OHX	AR	3710	-	0,6,6	-	-	-		
84	OHX	DD	101	-	0,6,6	-	-	-		
84	OHX	1	3681	-	0,6,6	-	-	-		
84	OHX	1	3560	-	0,6,6	-	-	-		
84	OHX	6	1930	-	0,6,6	-	-	-		
84	OHX	6	1958	-	0,6,6	-	-	-		
84	OHX	AR	3738	-	0,6,6	-	-	-		
84	OHX	A	1967	-	0,6,6	-	-	-		
84	OHX	AR	3633	-	0,6,6	-	-	-		
84	OHX	1	3402	-	0,6,6	-	-	-		
84	OHX	1	3468	-	0,6,6	-	-	-		
84	OHX	4	210	-	0,6,6	-	-	-		
84	OHX	x	202	-	0,6,6	-	-	-		
84	OHX	AR	3554	-	0,6,6	-	-	-		
84	OHX	A	1986	-	0,6,6	-	-	-		
84	OHX	1	3463	-	0,6,6	-	-	-		
84	OHX	CE	402	-	0,6,6	-	-	-		
84	OHX	Q	201	-	0,6,6	-	-	-		
84	OHX	4	207	-	0,6,6	-	-	-		
84	OHX	AR	3677	-	0,6,6	-	-	-		
84	OHX	1	3556	-	0,6,6	-	-	-		
84	OHX	AR	3437	85	0,6,6	-	-	-		
84	OHX	AR	3596	-	0,6,6	-	-	-		
84	OHX	DH	201	-	0,6,6	-	-	-		
84	OHX	A	2038	-	0,6,6	-	-	-		
84	OHX	AR	3576	-	0,6,6	-	-	-		
84	OHX	AT	216	-	0,6,6	-	-	-		
84	OHX	AR	3410	-	0,6,6	-	-	-		
84	OHX	1	3453	85	0,6,6	-	-	-		
84	OHX	AR	3452	-	0,6,6	-	-	-		
84	OHX	1	3694	-	0,6,6	-	-	-		
84	OHX	AR	3403	-	0,6,6	-	-	-		
84	OHX	AR	3654	-	0,6,6	-	-	-		
84	OHX	6	1908	-	0,6,6	-	-	-		
84	OHX	AR	3535	-	0,6,6	-	-	-		
84	OHX	6	2048	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	1	3567	-	0,6,6	-	-	-		
84	OHX	AR	3718	-	0,6,6	-	-	-		
84	OHX	1	3581	-	0,6,6	-	-	-		
84	OHX	A	2002	-	0,6,6	-	-	-		
84	OHX	6	1931	-	0,6,6	-	-	-		
84	OHX	AR	3423	-	0,6,6	-	-	-		
84	OHX	AR	3514	85	0,6,6	-	-	-		
84	OHX	6	1934	-	0,6,6	-	-	-		
84	OHX	AR	3653	-	0,6,6	-	-	-		
84	OHX	AR	3546	-	0,6,6	-	-	-		
84	OHX	A	1916	-	0,6,6	-	-	-		
84	OHX	1	3572	-	0,6,6	-	-	-		
84	OHX	1	3723	1	0,6,6	-	-	-		
84	OHX	A	1947	-	0,6,6	-	-	-		
84	OHX	1	3626	-	0,6,6	-	-	-		
84	OHX	6	1945	-	0,6,6	-	-	-		
84	OHX	AR	3417	85	0,6,6	-	-	-		
84	OHX	1	3517	-	0,6,6	-	-	-		
84	OHX	6	1966	-	0,6,6	-	-	-		
84	OHX	AR	3614	-	0,6,6	-	-	-		
84	OHX	1	3578	85	0,6,6	-	-	-		
84	OHX	AR	3636	-	0,6,6	-	-	-		
84	OHX	A	2016	-	0,6,6	-	-	-		
84	OHX	A	1943	-	0,6,6	-	-	-		
84	OHX	1	3461	-	0,6,6	-	-	-		
84	OHX	AR	3412	-	0,6,6	-	-	-		
84	OHX	AR	3500	-	0,6,6	-	-	-		
84	OHX	A	1912	-	0,6,6	-	-	-		
84	OHX	6	1997	-	0,6,6	-	-	-		
84	OHX	1	3690	-	0,6,6	-	-	-		
84	OHX	AR	3630	-	0,6,6	-	-	-		
84	OHX	AR	3662	85	0,6,6	-	-	-		
84	OHX	AR	3611	-	0,6,6	-	-	-		
84	OHX	6	1951	-	0,6,6	-	-	-		
84	OHX	A	1940	-	0,6,6	-	-	-		
84	OHX	A	1938	-	0,6,6	-	-	-		
84	OHX	6	1995	-	0,6,6	-	-	-		
84	OHX	A	1957	85	0,6,6	-	-	-		
84	OHX	1	3621	-	0,6,6	-	-	-		
84	OHX	A	2008	-	0,6,6	-	-	-		
84	OHX	AR	3651	-	0,6,6	-	-	-		
84	OHX	1	3552	-	0,6,6	-	-	-		
84	OHX	4	202	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	6	1929	-	0,6,6	-	-	-		
84	OHX	AR	3525	85	0,6,6	-	-	-		
84	OHX	A	2011	85	0,6,6	-	-	-		
84	OHX	6	2006	-	0,6,6	-	-	-		
84	OHX	1	3523	-	0,6,6	-	-	-		
84	OHX	A	1961	-	0,6,6	-	-	-		
84	OHX	1	3709	-	0,6,6	-	-	-		
84	OHX	AR	3550	85	0,6,6	-	-	-		
84	OHX	1	3403	-	0,6,6	-	-	-		
84	OHX	4	206	-	0,6,6	-	-	-		
84	OHX	6	1960	-	0,6,6	-	-	-		
84	OHX	AR	3428	-	0,6,6	-	-	-		
84	OHX	A	1939	-	0,6,6	-	-	-		
84	OHX	AR	3507	-	0,6,6	-	-	-		
84	OHX	AR	3484	-	0,6,6	-	-	-		
84	OHX	AR	3492	-	0,6,6	-	-	-		
84	OHX	1	3696	-	0,6,6	-	-	-		
84	OHX	1	3404	85	0,6,6	-	-	-		
84	OHX	1	3476	-	0,6,6	-	-	-		
84	OHX	AR	3688	-	0,6,6	-	-	-		
84	OHX	A	1968	-	0,6,6	-	-	-		
84	OHX	1	3583	-	0,6,6	-	-	-		
84	OHX	A	2037	-	0,6,6	-	-	-		
84	OHX	6	2034	-	0,6,6	-	-	-		
84	OHX	AR	3587	-	0,6,6	-	-	-		
84	OHX	6	2017	-	0,6,6	-	-	-		
84	OHX	1	3682	-	0,6,6	-	-	-		
84	OHX	AM	101	85	0,6,6	-	-	-		
84	OHX	d9	101	-	0,6,6	-	-	-		
84	OHX	1	3486	85	0,6,6	-	-	-		
84	OHX	A	1996	-	0,6,6	-	-	-		
84	OHX	1	3498	-	0,6,6	-	-	-		
84	OHX	AR	3466	-	0,6,6	-	-	-		
84	OHX	3	205	-	0,6,6	-	-	-		
84	OHX	A	1988	-	0,6,6	-	-	-		
84	OHX	AR	3446	-	0,6,6	-	-	-		
84	OHX	AR	3571	-	0,6,6	-	-	-		
84	OHX	1	3504	-	0,6,6	-	-	-		
84	OHX	AR	3610	-	0,6,6	-	-	-		
84	OHX	AR	3669	-	0,6,6	-	-	-		
84	OHX	1	3534	-	0,6,6	-	-	-		
84	OHX	AR	3584	-	0,6,6	-	-	-		
84	OHX	1	3554	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	AR	3637	-	0,6,6	-	-	-		
84	OHX	A	1922	-	0,6,6	-	-	-		
84	OHX	1	3516	85	0,6,6	-	-	-		
84	OHX	AR	3520	-	0,6,6	-	-	-		
84	OHX	CE	401	-	0,6,6	-	-	-		
84	OHX	AR	3721	85	0,6,6	-	-	-		
84	OHX	6	1959	-	0,6,6	-	-	-		
84	OHX	AR	3659	-	0,6,6	-	-	-		
84	OHX	1	3542	-	0,6,6	-	-	-		
84	OHX	AR	3436	-	0,6,6	-	-	-		
84	OHX	A	1956	-	0,6,6	-	-	-		
84	OHX	6	1910	-	0,6,6	-	-	-		
84	OHX	z	201	-	0,6,6	-	-	-		
84	OHX	1	3639	-	0,6,6	-	-	-		
84	OHX	6	1901	-	0,6,6	-	-	-		
84	OHX	6	1920	-	0,6,6	-	-	-		
84	OHX	6	2009	-	0,6,6	-	-	-		
84	OHX	6	2037	-	0,6,6	-	-	-		
84	OHX	AR	3509	85	0,6,6	-	-	-		
84	OHX	1	3623	-	0,6,6	-	-	-		
84	OHX	6	2040	-	0,6,6	-	-	-		
84	OHX	6	1947	-	0,6,6	-	-	-		
84	OHX	1	3615	-	0,6,6	-	-	-		
84	OHX	A	2042	-	0,6,6	-	-	-		
84	OHX	AR	3647	85	0,6,6	-	-	-		
84	OHX	1	3475	-	0,6,6	-	-	-		
84	OHX	1	3627	-	0,6,6	-	-	-		
84	OHX	6	1911	85	0,6,6	-	-	-		
84	OHX	AR	3605	-	0,6,6	-	-	-		
84	OHX	1	3716	-	0,6,6	-	-	-		
84	OHX	A	2033	-	0,6,6	-	-	-		
84	OHX	1	3691	-	0,6,6	-	-	-		
84	OHX	1	3548	-	0,6,6	-	-	-		
84	OHX	6	1913	-	0,6,6	-	-	-		
84	OHX	6	2036	-	0,6,6	-	-	-		
84	OHX	6	2044	-	0,6,6	-	-	-		
84	OHX	AR	3441	85	0,6,6	-	-	-		
84	OHX	6	2022	-	0,6,6	-	-	-		
84	OHX	AR	3697	-	0,6,6	-	-	-		
84	OHX	6	1944	-	0,6,6	-	-	-		
84	OHX	1	3715	-	0,6,6	-	-	-		
84	OHX	1	3574	-	0,6,6	-	-	-		
84	OHX	AR	3646	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	AR	3444	-	0,6,6	-	-	-		
84	OHX	4	203	-	0,6,6	-	-	-		
84	OHX	3	207	-	0,6,6	-	-	-		
84	OHX	CX	201	-	0,6,6	-	-	-		
84	OHX	A	1934	-	0,6,6	-	-	-		
84	OHX	A	1969	-	0,6,6	-	-	-		
84	OHX	1	3717	-	0,6,6	-	-	-		
84	OHX	1	3435	-	0,6,6	-	-	-		
84	OHX	1	3411	-	0,6,6	-	-	-		
84	OHX	6	2019	-	0,6,6	-	-	-		
84	OHX	AR	3556	-	0,6,6	-	-	-		
84	OHX	AR	3472	-	0,6,6	-	-	-		
84	OHX	1	3401	-	0,6,6	-	-	-		
84	OHX	1	3599	-	0,6,6	-	-	-		
84	OHX	3	206	-	0,6,6	-	-	-		
84	OHX	AR	3557	-	0,6,6	-	-	-		
84	OHX	AC	101	-	0,6,6	-	-	-		
84	OHX	A	1994	-	0,6,6	-	-	-		
84	OHX	1	3563	85	0,6,6	-	-	-		
84	OHX	1	3598	-	0,6,6	-	-	-		
84	OHX	1	3488	-	0,6,6	-	-	-		
84	OHX	1	3500	85	0,6,6	-	-	-		
84	OHX	1	3710	85	0,6,6	-	-	-		
84	OHX	1	3676	-	0,6,6	-	-	-		
84	OHX	6	1933	85	0,6,6	-	-	-		
84	OHX	1	3527	-	0,6,6	-	-	-		
84	OHX	1	3611	-	0,6,6	-	-	-		
84	OHX	1	3673	-	0,6,6	-	-	-		
84	OHX	6	1935	-	0,6,6	-	-	-		
84	OHX	AR	3720	-	0,6,6	-	-	-		
84	OHX	6	2008	-	0,6,6	-	-	-		
84	OHX	AT	208	85	0,6,6	-	-	-		
84	OHX	A	1952	-	0,6,6	-	-	-		
84	OHX	1	3415	-	0,6,6	-	-	-		
84	OHX	AR	3501	-	0,6,6	-	-	-		
84	OHX	AR	3537	-	0,6,6	-	-	-		
84	OHX	AR	3648	-	0,6,6	-	-	-		
84	OHX	1	3589	85	0,6,6	-	-	-		
84	OHX	1	3683	-	0,6,6	-	-	-		
84	OHX	1	3473	-	0,6,6	-	-	-		
84	OHX	1	3712	-	0,6,6	-	-	-		
84	OHX	CK	201	-	0,6,6	-	-	-		
84	OHX	J	301	-	0,6,6	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	HN8	AR	4263	-	-	0/2/48/48	0/6/5/5
87	GOL	6	2199	-	-	0/4/4/4	-
87	GOL	AR	4261	1	-	2/4/4/4	-
87	GOL	A	2160	-	-	0/4/4/4	-
87	GOL	AR	4262	84	-	1/4/4/4	-
86	HN8	1	4223	-	-	0/2/48/48	0/6/5/5
87	GOL	v	305	-	-	2/4/4/4	-

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
86	AR	4263	HN8	C5-C1-C3	-5.16	100.15	106.09
86	AR	4263	HN8	C5-C1-C2	-5.00	102.67	106.70
86	AR	4263	HN8	C5-C1-C7	4.00	116.29	114.53
86	1	4223	HN8	C5-C1-C7	3.71	116.17	114.53
86	AR	4263	HN8	C3-C1-C2	2.87	107.05	102.28

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	v	305	GOL	O1-C1-C2-C3
87	AR	4261	GOL	C1-C2-C3-O3
87	v	305	GOL	O1-C1-C2-O2
87	AR	4261	GOL	O2-C2-C3-O3
87	AR	4262	GOL	C1-C2-C3-O3

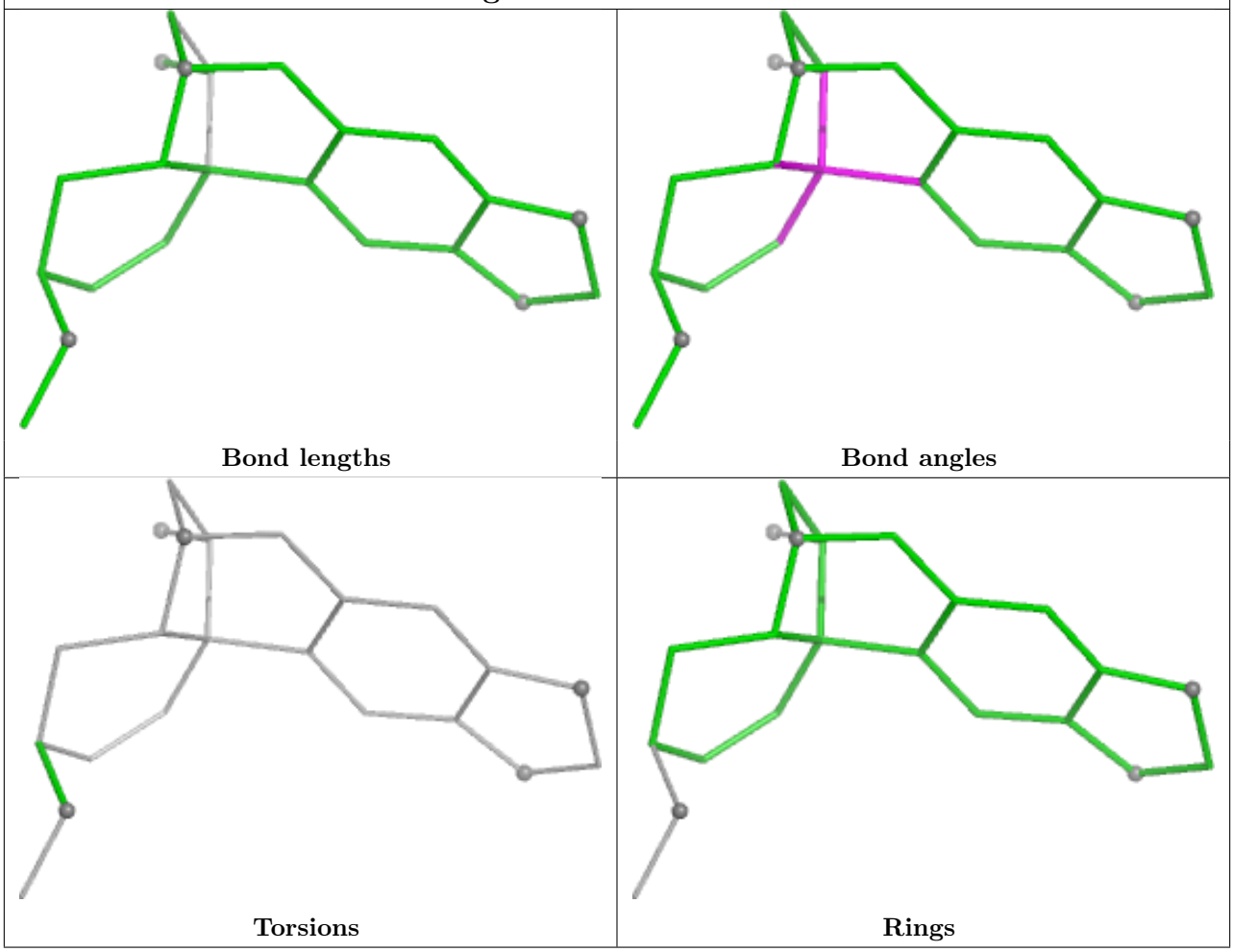
There are no ring outliers.

No monomer is involved in short contacts.

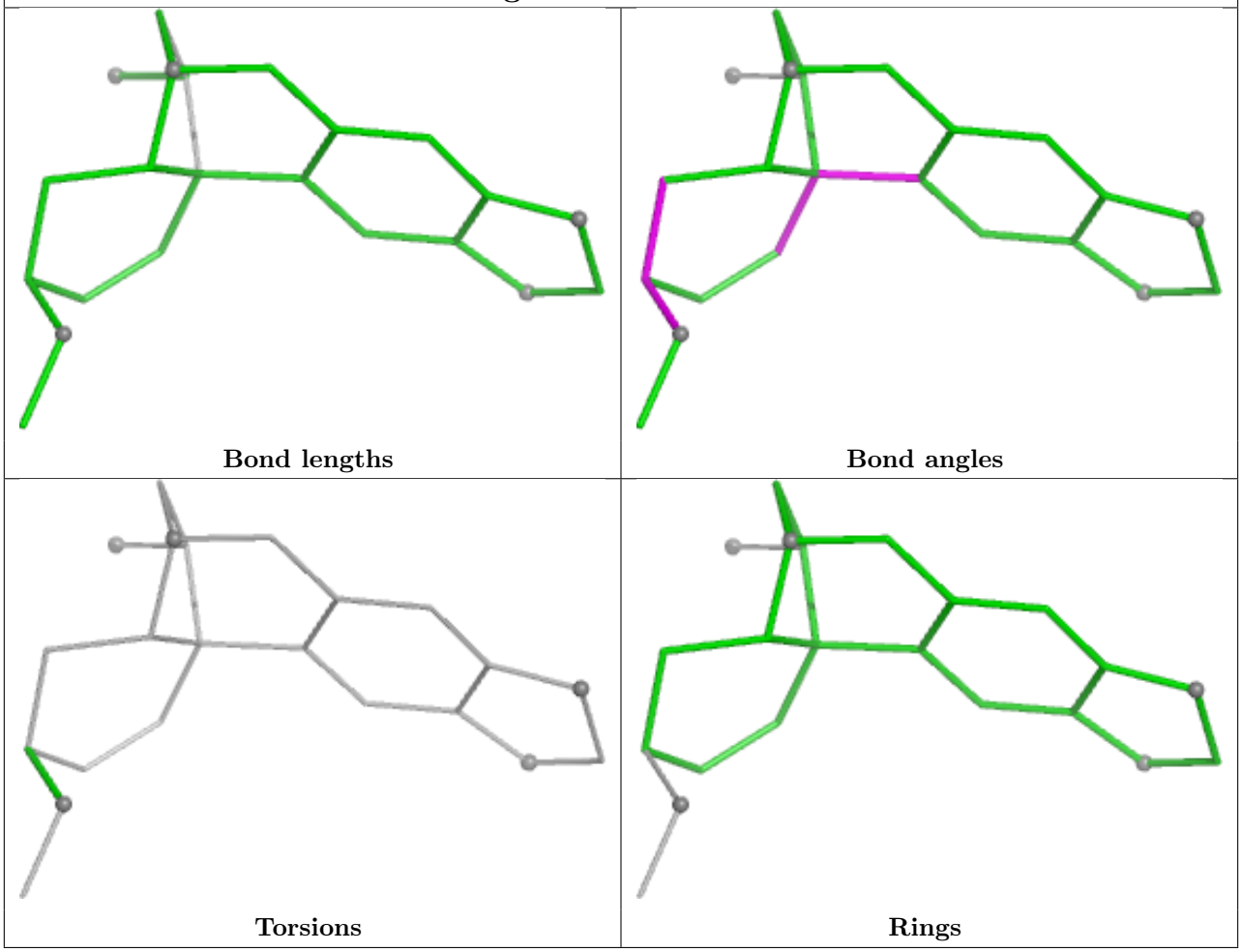
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HN8 AR 4263



Ligand HN8 1 4223



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	sM	2
25	A	1
47	m2	1
5	CE	1
50	s0	1
54	s4	1

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	85:SER	C	119:UNK	N	44.14
1	sM	139:UNK	C	155:UNK	N	37.59
1	A	1716:C	O3'	1717:G	P	4.52
1	m2	23:UNK	C	28:UNK	N	3.62
1	CE	168:LYS	C	169:THR	N	1.19

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	1	3149/3396 (92%)	0.16	105 (3%)	49	29	26, 47, 129, 223	0
1	AR	3149/3396 (92%)	0.22	135 (4%)	40	22	25, 49, 123, 225	0
2	3	121/121 (100%)	-0.00	1 (0%)	82	65	35, 63, 75, 82	0
2	AS	121/121 (100%)	0.04	2 (1%)	69	48	34, 52, 66, 73	0
3	4	158/158 (100%)	0.21	5 (3%)	50	30	34, 51, 91, 138	0
3	AT	158/158 (100%)	0.32	10 (6%)	26	14	34, 60, 99, 128	0
4	CD	252/252 (100%)	0.51	14 (5%)	30	16	33, 52, 74, 82	0
4	j	252/252 (100%)	0.41	6 (2%)	59	38	31, 46, 64, 77	0
5	CE	386/386 (100%)	0.14	5 (1%)	75	56	25, 41, 55, 95	0
5	k	386/386 (100%)	0.19	4 (1%)	79	61	25, 48, 62, 80	0
6	CF	361/361 (100%)	0.32	6 (1%)	69	48	31, 47, 65, 88	0
6	l	361/361 (100%)	0.25	5 (1%)	73	53	27, 44, 62, 71	0
7	CG	296/296 (100%)	0.46	18 (6%)	27	15	39, 57, 83, 104	0
7	m	296/296 (100%)	0.40	11 (3%)	45	25	46, 69, 89, 115	0
8	CH	156/175 (89%)	0.16	2 (1%)	75	56	37, 46, 68, 84	0
8	n	156/175 (89%)	0.12	1 (0%)	85	70	36, 43, 66, 86	0
9	CI	222/222 (100%)	0.21	6 (2%)	56	35	27, 35, 78, 133	0
9	o	222/222 (100%)	0.14	3 (1%)	73	53	29, 38, 73, 123	0
10	CJ	233/233 (100%)	0.90	31 (13%)	7	4	70, 82, 123, 144	0
10	p	233/233 (100%)	0.76	12 (5%)	33	17	56, 70, 105, 116	0
11	CK	191/191 (100%)	0.23	4 (2%)	63	42	35, 45, 66, 82	0
11	q	191/191 (100%)	0.33	4 (2%)	63	42	42, 53, 66, 86	0
12	CL	211/220 (95%)	0.36	7 (3%)	49	29	39, 59, 80, 93	0
12	r	211/220 (95%)	0.31	6 (2%)	55	34	33, 46, 81, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	CM	169/169 (100%)	0.50	8 (4%) 36 19	40, 61, 75, 83	0
13	s	169/169 (100%)	0.75	7 (4%) 41 23	55, 77, 90, 96	0
14	CN	193/193 (100%)	0.45	8 (4%) 41 23	41, 62, 101, 119	0
14	t	193/193 (100%)	0.34	5 (2%) 57 36	33, 53, 95, 125	0
15	CO	136/136 (100%)	0.32	8 (5%) 28 15	34, 40, 63, 71	0
15	u	136/136 (100%)	0.37	6 (4%) 39 21	37, 43, 60, 68	0
16	CP	203/203 (100%)	0.42	1 (0%) 87 73	38, 55, 67, 71	0
16	v	203/203 (100%)	0.33	0 100 100	33, 44, 57, 64	0
17	CQ	197/197 (100%)	0.24	9 (4%) 37 20	25, 30, 60, 66	0
17	w	197/197 (100%)	0.18	4 (2%) 65 44	28, 34, 55, 60	0
18	CR	183/183 (100%)	0.68	24 (13%) 7 4	31, 39, 137, 167	0
18	x	183/183 (100%)	0.53	17 (9%) 14 8	32, 40, 105, 140	0
19	CS	185/185 (100%)	0.25	3 (1%) 70 49	32, 46, 56, 60	0
19	y	185/185 (100%)	0.31	3 (1%) 70 49	33, 43, 63, 87	0
20	CT	188/188 (100%)	0.77	17 (9%) 15 8	48, 63, 158, 169	0
20	z	188/188 (100%)	0.70	13 (6%) 23 12	48, 64, 150, 167	0
21	0	172/172 (100%)	0.25	3 (1%) 69 48	35, 41, 55, 65	0
21	CU	172/172 (100%)	0.21	5 (2%) 53 32	30, 37, 50, 57	0
22	2	159/159 (100%)	0.36	2 (1%) 75 56	34, 45, 87, 97	0
22	CV	159/159 (100%)	0.35	6 (3%) 44 25	31, 41, 74, 84	0
23	5	100/100 (100%)	0.85	8 (8%) 18 10	79, 93, 105, 123	0
23	CW	100/100 (100%)	0.74	4 (4%) 42 23	77, 87, 98, 119	0
24	CX	136/136 (100%)	0.14	3 (2%) 62 41	29, 38, 57, 59	0
24	lR	136/136 (100%)	0.18	2 (1%) 72 52	31, 43, 56, 62	0
25	6	1783/1800 (99%)	0.63	116 (6%) 25 13	41, 78, 169, 233	0
25	A	1781/1800 (98%)	0.72	123 (6%) 23 12	49, 87, 186, 250	0
26	7	98/98 (100%)	1.53	33 (33%) 1 0	43, 59, 150, 157	0
26	CY	98/98 (100%)	1.26	22 (22%) 2 1	38, 53, 145, 177	0
27	8	121/121 (100%)	0.44	3 (2%) 58 37	44, 57, 77, 117	0
27	CZ	121/121 (100%)	0.72	9 (7%) 20 11	48, 64, 85, 100	0
28	9	126/126 (100%)	0.21	3 (2%) 59 38	40, 55, 64, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	DA	126/126 (100%)	0.40	4 (3%) 50 30	40, 57, 73, 82	0
29	AA	135/135 (100%)	0.51	1 (0%) 84 68	69, 83, 94, 104	0
29	DB	135/135 (100%)	0.76	7 (5%) 33 17	81, 95, 110, 120	0
30	AB	148/148 (100%)	0.40	5 (3%) 48 28	27, 46, 73, 86	0
30	DC	148/148 (100%)	0.45	3 (2%) 65 44	30, 51, 71, 77	0
31	AC	58/58 (100%)	0.67	5 (8%) 16 9	32, 52, 102, 122	0
31	DD	58/58 (100%)	0.44	1 (1%) 69 48	38, 51, 80, 88	0
32	AD	97/97 (100%)	0.64	6 (6%) 26 14	67, 77, 99, 110	0
32	DE	97/97 (100%)	0.86	10 (10%) 12 6	71, 83, 105, 109	0
33	AE	109/109 (100%)	0.53	3 (2%) 55 34	42, 56, 95, 106	0
33	DF	109/109 (100%)	0.43	4 (3%) 45 25	41, 52, 92, 111	0
34	AF	127/127 (100%)	0.19	2 (1%) 70 49	25, 40, 52, 69	0
34	DG	127/127 (100%)	0.19	3 (2%) 59 38	24, 43, 55, 77	0
35	AG	106/106 (100%)	0.31	4 (3%) 44 25	31, 36, 61, 72	0
35	DH	106/106 (100%)	0.25	2 (1%) 66 45	28, 35, 64, 87	0
36	AH	112/112 (100%)	0.80	7 (6%) 26 14	43, 63, 104, 114	0
36	DI	112/112 (100%)	0.97	12 (10%) 11 6	46, 68, 113, 125	0
37	AI	119/119 (100%)	0.55	7 (5%) 28 15	46, 61, 70, 77	0
37	DJ	119/119 (100%)	0.69	7 (5%) 28 15	51, 67, 81, 88	0
38	AJ	99/99 (100%)	0.50	5 (5%) 33 18	52, 61, 93, 113	0
38	DK	99/99 (100%)	0.62	7 (7%) 22 12	59, 70, 92, 110	0
39	AK	87/87 (100%)	0.52	5 (5%) 29 16	32, 36, 63, 86	0
39	DL	87/87 (100%)	0.69	5 (5%) 29 16	36, 42, 77, 113	0
40	AL	77/77 (100%)	0.65	2 (2%) 57 36	67, 79, 101, 108	0
40	DM	77/77 (100%)	0.76	4 (5%) 33 17	76, 88, 107, 115	0
41	AM	50/50 (100%)	0.53	0 100 100	42, 45, 52, 62	0
41	DN	50/50 (100%)	0.70	3 (6%) 27 15	45, 49, 59, 70	0
42	AN	52/52 (100%)	0.18	1 (1%) 66 45	37, 43, 61, 69	0
42	DO	52/52 (100%)	0.07	2 (3%) 44 25	32, 35, 48, 62	0
43	AO	25/25 (100%)	0.85	1 (4%) 42 23	52, 54, 59, 59	0
43	DP	25/25 (100%)	0.63	1 (4%) 42 23	43, 46, 59, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	AP	105/105 (100%)	0.51	4 (3%) 44 25	34, 50, 74, 103	0
44	DQ	105/105 (100%)	0.31	5 (4%) 35 19	37, 50, 65, 97	0
45	AQ	91/91 (100%)	0.33	0 100 100	40, 50, 67, 80	0
45	DR	91/91 (100%)	0.55	1 (1%) 78 59	39, 53, 69, 79	0
46	i	159/272 (58%)	1.40	42 (26%) 1 1	70, 90, 143, 148	0
47	m2	0/150	-	-	-	-
48	sM	63/104 (60%)	1.35	13 (20%) 2 1	62, 91, 108, 114	0
49	p0	143/311 (45%)	1.10	14 (9%) 13 7	89, 108, 172, 179	0
50	B	206/206 (100%)	1.01	22 (10%) 11 6	93, 110, 125, 146	0
50	s0	206/206 (100%)	0.79	16 (7%) 19 10	77, 97, 115, 120	0
51	C	214/216 (99%)	1.29	31 (14%) 6 3	93, 121, 142, 150	0
51	s1	216/216 (100%)	0.68	15 (6%) 23 12	68, 83, 110, 129	0
52	D	217/217 (100%)	0.84	11 (5%) 33 18	68, 87, 108, 125	0
52	s2	217/217 (100%)	0.74	15 (6%) 23 12	57, 76, 92, 106	0
53	E	223/223 (100%)	1.06	24 (10%) 11 6	74, 91, 118, 137	0
53	s3	223/223 (100%)	1.35	33 (14%) 5 3	75, 103, 134, 148	0
54	F	260/260 (100%)	1.01	24 (9%) 14 8	63, 87, 97, 121	0
54	s4	260/260 (100%)	0.75	11 (4%) 40 22	53, 84, 98, 128	0
55	G	206/206 (100%)	1.45	50 (24%) 2 1	92, 112, 131, 141	0
55	s5	206/206 (100%)	1.13	26 (12%) 8 4	74, 95, 114, 122	0
56	H	226/226 (100%)	1.01	24 (10%) 11 6	61, 94, 116, 143	0
56	s6	218/226 (96%)	0.91	18 (8%) 17 9	52, 83, 111, 124	0
57	I	184/186 (98%)	1.16	19 (10%) 12 6	87, 119, 148, 156	0
57	s7	186/186 (100%)	1.17	22 (11%) 9 5	77, 112, 147, 152	0
58	J	188/199 (94%)	0.78	14 (7%) 20 11	53, 70, 111, 126	0
58	s8	188/199 (94%)	0.87	15 (7%) 18 10	49, 73, 124, 140	0
59	K	185/185 (100%)	1.02	22 (11%) 9 5	77, 95, 129, 158	0
59	s9	185/185 (100%)	0.71	9 (4%) 35 18	67, 85, 116, 151	0
60	L	96/105 (91%)	1.27	18 (18%) 3 1	81, 102, 129, 139	0
60	c0	96/105 (91%)	1.55	26 (27%) 1 1	96, 126, 139, 147	0
61	M	155/155 (100%)	1.21	24 (15%) 5 2	56, 70, 126, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
61	c1	146/155 (94%)	0.97	15 (10%) 12 6	55, 70, 104, 131	0
62	N	124/124 (100%)	1.34	19 (15%) 5 3	133, 140, 152, 160	0
62	c2	124/124 (100%)	1.57	32 (25%) 1 1	161, 169, 184, 190	0
63	O	150/150 (100%)	0.89	10 (6%) 24 13	64, 85, 100, 104	0
63	c3	150/150 (100%)	0.90	13 (8%) 16 9	59, 78, 96, 111	0
64	P	127/128 (99%)	1.52	32 (25%) 1 1	66, 119, 135, 138	0
64	c4	128/128 (100%)	0.77	6 (4%) 36 19	57, 81, 91, 94	0
65	Q	124/141 (87%)	0.93	14 (11%) 10 5	75, 89, 126, 146	0
65	c5	135/141 (95%)	1.20	22 (16%) 4 2	82, 97, 118, 131	0
66	R	141/142 (99%)	1.34	21 (14%) 5 3	81, 107, 115, 120	0
66	c6	142/142 (100%)	1.32	26 (18%) 3 1	67, 91, 106, 127	0
67	S	120/125 (96%)	1.16	20 (16%) 4 2	90, 109, 134, 138	0
67	c7	117/125 (93%)	1.05	12 (10%) 12 6	78, 97, 122, 130	0
68	T	145/145 (100%)	0.88	10 (6%) 23 12	71, 99, 129, 140	0
68	c8	145/145 (100%)	0.73	8 (5%) 30 16	79, 91, 116, 127	0
69	U	143/143 (100%)	1.03	11 (7%) 19 10	84, 102, 119, 133	0
69	c9	143/143 (100%)	0.63	3 (2%) 63 42	71, 86, 106, 119	0
70	V	107/110 (97%)	2.02	49 (45%) 0 0	73, 109, 141, 145	0
70	d0	110/110 (100%)	1.58	30 (27%) 1 1	70, 111, 154, 172	0
71	W	87/87 (100%)	0.83	4 (4%) 37 20	90, 96, 115, 124	0
71	d1	87/87 (100%)	0.50	1 (1%) 78 59	75, 83, 110, 121	0
72	X	129/129 (100%)	0.81	3 (2%) 61 39	68, 81, 88, 101	0
72	d2	129/129 (100%)	0.56	0 100 100	57, 70, 81, 97	0
73	Y	144/144 (100%)	0.86	13 (9%) 15 8	57, 62, 73, 88	0
73	d3	144/144 (100%)	0.63	10 (6%) 23 12	46, 52, 66, 78	0
74	Z	134/134 (100%)	1.03	19 (14%) 6 3	69, 97, 114, 125	0
74	d4	134/134 (100%)	0.92	12 (8%) 15 8	62, 88, 103, 122	0
75	a	70/70 (100%)	1.42	16 (22%) 2 1	111, 123, 138, 139	0
75	d5	69/70 (98%)	0.96	2 (2%) 53 32	93, 113, 124, 127	0
76	b	97/97 (100%)	1.39	17 (17%) 4 2	67, 83, 135, 138	0
76	d6	97/97 (100%)	0.80	5 (5%) 33 17	51, 63, 95, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
77	c	81/81 (100%)	0.98	7 (8%) 16 9	82, 95, 127, 134	0
77	d7	81/81 (100%)	0.82	7 (8%) 16 9	72, 87, 126, 132	0
78	d	63/63 (100%)	1.48	12 (19%) 3 1	104, 121, 132, 134	0
78	d8	63/63 (100%)	1.26	6 (9%) 14 7	91, 107, 121, 125	0
79	d9	53/53 (100%)	1.20	9 (16%) 4 2	71, 82, 120, 128	0
79	e	53/53 (100%)	0.86	1 (1%) 66 45	75, 80, 96, 104	0
80	e0	62/62 (100%)	0.96	8 (12%) 7 4	59, 83, 113, 125	0
80	f	60/62 (96%)	0.82	5 (8%) 17 9	63, 92, 131, 134	0
81	g	71/71 (100%)	1.54	23 (32%) 1 0	105, 124, 144, 150	0
82	h	318/318 (100%)	0.94	25 (7%) 18 10	97, 115, 135, 147	0
82	sR	318/318 (100%)	1.28	52 (16%) 4 2	99, 121, 140, 157	0
83	e1	51/51 (100%)	1.51	14 (27%) 1 1	145, 157, 165, 167	0
All	All	33004/34167 (96%)	0.59	2199 (6%) 24 13	24, 66, 132, 250	0

The worst 5 of 2199 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	CY	81	PRO	12.2
55	G	152	GLY	8.2
3	AT	81	U	7.5
1	AR	3275	U	7.4
26	7	88	ASP	7.1

5.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	A	2094	1/1	-0.18	0.40	110,110,110,110	0
85	MG	1	4140	1/1	-0.07	0.37	187,187,187,187	0
85	MG	A	2110	1/1	0.01	0.45	116,116,116,116	0
85	MG	6	2076	1/1	0.07	0.41	105,105,105,105	0
85	MG	1	4152	1/1	0.11	0.49	111,111,111,111	0
85	MG	AR	3814	1/1	0.18	0.42	105,105,105,105	0
85	MG	t	202	1/1	0.27	0.35	101,101,101,101	0
85	MG	A	2146	1/1	0.29	0.32	120,120,120,120	0
85	MG	6	2168	1/1	0.34	0.30	132,132,132,132	0
85	MG	1	3965	1/1	0.43	0.43	94,94,94,94	0
85	MG	1	4030	1/1	0.44	0.43	72,72,72,72	0
85	MG	6	2061	1/1	0.46	0.41	100,100,100,100	0
85	MG	A	2089	1/1	0.47	0.34	90,90,90,90	0
85	MG	6	2153	1/1	0.49	0.39	97,97,97,97	0
85	MG	AR	4030	1/1	0.53	0.20	59,59,59,59	0
85	MG	A	2104	1/1	0.53	0.19	137,137,137,137	0
85	MG	A	2139	1/1	0.57	0.26	64,64,64,64	0
85	MG	A	2124	1/1	0.57	0.40	68,68,68,68	0
85	MG	A	2095	1/1	0.58	0.27	96,96,96,96	0
85	MG	AR	4119	1/1	0.58	0.31	91,91,91,91	0
85	MG	A	2092	1/1	0.59	0.38	91,91,91,91	0
85	MG	AR	4050	1/1	0.59	0.35	91,91,91,91	0
85	MG	A	2132	1/1	0.60	0.43	98,98,98,98	0
85	MG	AR	4156	1/1	0.61	0.39	72,72,72,72	0
85	MG	CR	203	1/1	0.61	0.27	95,95,95,95	0
85	MG	6	2118	1/1	0.62	0.35	93,93,93,93	0
85	MG	A	2057	1/1	0.62	0.38	70,70,70,70	0
85	MG	AR	3817	1/1	0.62	0.30	112,112,112,112	0
85	MG	6	2158	1/1	0.63	0.30	74,74,74,74	0
85	MG	A	2118	1/1	0.63	0.44	80,80,80,80	0
85	MG	AR	4137	1/1	0.63	0.35	79,79,79,79	0
85	MG	6	2115	1/1	0.64	0.29	85,85,85,85	0
85	MG	A	2070	1/1	0.65	0.46	79,79,79,79	0
85	MG	A	2081	1/1	0.65	0.30	66,66,66,66	0
84	OHX	AR	3686	7/7	0.65	0.24	156,156,156,157	0
85	MG	6	2086	1/1	0.65	0.32	82,82,82,82	0
85	MG	AR	4117	1/1	0.65	0.25	64,64,64,64	0
85	MG	6	2072	1/1	0.65	0.24	40,40,40,40	0
85	MG	A	2100	1/1	0.65	0.53	92,92,92,92	0
85	MG	AR	4171	1/1	0.66	0.31	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	4068	1/1	0.66	0.23	99,99,99,99	0
85	MG	A	2103	1/1	0.66	0.37	73,73,73,73	0
85	MG	1	4171	1/1	0.66	0.41	85,85,85,85	0
85	MG	AR	3977	1/1	0.66	0.31	41,41,41,41	0
85	MG	A	2072	1/1	0.66	0.36	66,66,66,66	0
85	MG	6	2194	1/1	0.66	0.32	108,108,108,108	0
85	MG	AR	4151	1/1	0.66	0.14	148,148,148,148	0
85	MG	AR	4153	1/1	0.66	0.33	88,88,88,88	0
85	MG	1	3790	1/1	0.66	0.24	43,43,43,43	0
84	OHX	AR	3733	7/7	0.67	0.20	187,188,188,188	0
85	MG	6	2185	1/1	0.67	0.41	89,89,89,89	0
84	OHX	AR	3664	7/7	0.67	0.23	180,180,181,181	0
85	MG	A	2062	1/1	0.67	0.36	65,65,65,65	0
85	MG	H	301	1/1	0.67	0.26	83,83,83,83	0
85	MG	A	2122	1/1	0.68	0.33	86,86,86,86	0
85	MG	6	2092	1/1	0.68	0.46	93,93,93,93	0
85	MG	1	3772	1/1	0.68	0.15	35,35,35,35	0
85	MG	6	2059	1/1	0.68	0.35	70,70,70,70	0
85	MG	6	2090	1/1	0.68	0.23	49,49,49,49	0
85	MG	A	2121	1/1	0.68	0.19	62,62,62,62	0
85	MG	6	2160	1/1	0.69	0.31	85,85,85,85	0
85	MG	A	2114	1/1	0.69	0.33	76,76,76,76	0
85	MG	AR	4160	1/1	0.69	0.19	78,78,78,78	0
85	MG	1	3750	1/1	0.69	0.17	55,55,55,55	0
84	OHX	AR	3737	7/7	0.69	0.25	158,158,158,159	0
85	MG	1	4161	1/1	0.70	0.18	69,69,69,69	0
84	OHX	6	2040	7/7	0.70	0.20	184,184,185,185	0
85	MG	6	2069	1/1	0.70	0.28	65,65,65,65	0
85	MG	A	2087	1/1	0.70	0.21	78,78,78,78	0
85	MG	1	3952	1/1	0.70	0.33	77,77,77,77	0
85	MG	6	2174	1/1	0.70	0.19	58,58,58,58	0
85	MG	6	2056	1/1	0.70	0.27	77,77,77,77	0
85	MG	1	3948	1/1	0.71	0.21	73,73,73,73	0
85	MG	6	2134	1/1	0.71	0.31	80,80,80,80	0
85	MG	A	2115	1/1	0.71	0.30	83,83,83,83	0
85	MG	6	2175	1/1	0.71	0.20	118,118,118,118	0
85	MG	6	2054	1/1	0.71	0.30	49,49,49,49	0
85	MG	6	2191	1/1	0.71	0.27	87,87,87,87	0
85	MG	1	3958	1/1	0.71	0.13	44,44,44,44	0
85	MG	AR	4125	1/1	0.71	0.37	82,82,82,82	0
85	MG	3	212	1/1	0.71	0.34	62,62,62,62	0
85	MG	6	2162	1/1	0.71	0.17	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	A	2107	1/1	0.71	0.26	80,80,80,80	0
87	GOL	6	2199	6/6	0.71	0.24	49,49,49,49	0
85	MG	6	2133	1/1	0.72	0.21	61,61,61,61	0
85	MG	1	3853	1/1	0.72	0.34	48,48,48,48	0
85	MG	A	2127	1/1	0.72	0.28	83,83,83,83	0
85	MG	3	220	1/1	0.72	0.23	68,68,68,68	0
85	MG	1	4219	1/1	0.72	0.27	98,98,98,98	0
85	MG	A	2096	1/1	0.72	0.34	62,62,62,62	0
85	MG	A	2046	1/1	0.72	0.31	67,67,67,67	0
85	MG	A	2050	1/1	0.72	0.33	67,67,67,67	0
85	MG	1	4056	1/1	0.73	0.24	51,51,51,51	0
85	MG	AR	4072	1/1	0.73	0.23	70,70,70,70	0
85	MG	6	2119	1/1	0.73	0.32	74,74,74,74	0
85	MG	6	2159	1/1	0.73	0.14	82,82,82,82	0
85	MG	6	2183	1/1	0.73	0.38	71,71,71,71	0
85	MG	1	4087	1/1	0.73	0.23	59,59,59,59	0
85	MG	d5	201	1/1	0.73	0.17	71,71,71,71	0
85	MG	1	3803	1/1	0.73	0.16	41,41,41,41	0
85	MG	1	3908	1/1	0.74	0.30	62,62,62,62	0
85	MG	A	2082	1/1	0.74	0.22	61,61,61,61	0
85	MG	6	2192	1/1	0.74	0.34	74,74,74,74	0
85	MG	AR	4074	1/1	0.74	0.20	77,77,77,77	0
85	MG	AR	4184	1/1	0.74	0.22	69,69,69,69	0
85	MG	AR	4240	1/1	0.74	0.26	70,70,70,70	0
84	OHX	1	3709	7/7	0.74	0.25	157,158,158,158	0
85	MG	A	2130	1/1	0.74	0.20	74,74,74,74	0
85	MG	1	4174	1/1	0.74	0.39	55,55,55,55	0
84	OHX	1	3714	7/7	0.74	0.22	146,147,147,148	0
85	MG	AR	4126	1/1	0.74	0.37	83,83,83,83	0
84	OHX	CF	401	7/7	0.74	0.23	146,146,147,147	0
85	MG	6	2104	1/1	0.74	0.28	70,70,70,70	0
84	OHX	1	3717	7/7	0.74	0.22	144,144,144,145	0
85	MG	A	2084	1/1	0.75	0.28	72,72,72,72	0
85	MG	AT	226	1/1	0.75	0.15	63,63,63,63	0
84	OHX	1	401	7/7	0.75	0.22	143,143,144,144	0
85	MG	DE	201	1/1	0.75	0.15	72,72,72,72	0
84	OHX	1	3668	7/7	0.75	0.34	124,124,124,124	0
84	OHX	AR	3705	7/7	0.75	0.29	141,142,142,142	0
85	MG	1	3819	1/1	0.75	0.37	27,27,27,27	0
85	MG	AR	3776	1/1	0.75	0.42	76,76,76,76	0
85	MG	AR	4116	1/1	0.75	0.19	99,99,99,99	0
85	MG	1	4150	1/1	0.75	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	A	2150	1/1	0.75	0.34	86,86,86,86	0
85	MG	A	2080	1/1	0.75	0.34	65,65,65,65	0
84	OHX	AR	3728	7/7	0.75	0.25	151,152,152,152	0
85	MG	6	2112	1/1	0.75	0.39	46,46,46,46	0
85	MG	6	2113	1/1	0.76	0.34	77,77,77,77	0
85	MG	AR	3991	1/1	0.76	0.21	98,98,98,98	0
85	MG	1	4079	1/1	0.76	0.24	97,97,97,97	0
84	OHX	AR	3739	7/7	0.76	0.24	148,149,149,150	0
85	MG	6	2074	1/1	0.76	0.34	62,62,62,62	0
85	MG	1	3955	1/1	0.76	0.41	51,51,51,51	0
84	OHX	AR	3717	7/7	0.76	0.26	144,144,144,144	0
85	MG	A	2091	1/1	0.76	0.36	71,71,71,71	0
85	MG	6	2140	1/1	0.76	0.26	69,69,69,69	0
84	OHX	1	3708	7/7	0.76	0.26	134,134,134,134	0
85	MG	DI	202	1/1	0.76	0.31	56,56,56,56	0
85	MG	6	2154	1/1	0.76	0.18	54,54,54,54	0
85	MG	6	2195	1/1	0.76	0.31	35,35,35,35	0
85	MG	A	2151	1/1	0.76	0.45	52,52,52,52	0
85	MG	A	2155	1/1	0.76	0.42	75,75,75,75	0
85	MG	1	4012	1/1	0.76	0.21	50,50,50,50	0
84	OHX	1	3687	7/7	0.76	0.23	149,149,150,150	0
84	OHX	1	3695	7/7	0.76	0.22	154,154,155,155	0
85	MG	A	2105	1/1	0.77	0.25	94,94,94,94	0
84	OHX	c4	201	7/7	0.77	0.25	152,152,153,153	0
85	MG	AR	3780	1/1	0.77	0.19	88,88,88,88	0
85	MG	1	3744	1/1	0.77	0.47	83,83,83,83	0
84	OHX	6	2039	7/7	0.77	0.28	132,133,133,134	0
85	MG	AR	3903	1/1	0.77	0.31	39,39,39,39	0
84	OHX	1	3718	7/7	0.77	0.23	149,149,149,149	0
84	OHX	AR	3740	7/7	0.77	0.24	161,161,161,162	0
85	MG	A	2085	1/1	0.77	0.22	63,63,63,63	0
85	MG	AR	4021	1/1	0.77	0.27	82,82,82,82	0
85	MG	6	2120	1/1	0.77	0.32	69,69,69,69	0
84	OHX	AR	3734	7/7	0.77	0.24	148,148,148,149	0
84	OHX	CF	402	7/7	0.77	0.25	145,146,146,146	0
85	MG	A	2093	1/1	0.77	0.20	100,100,100,100	0
85	MG	6	2186	1/1	0.77	0.21	107,107,107,107	0
84	OHX	A	2037	7/7	0.77	0.23	153,154,154,155	0
85	MG	4	234	1/1	0.77	0.25	44,44,44,44	0
84	OHX	A	2038	7/7	0.77	0.23	146,147,147,147	0
85	MG	c6	201	1/1	0.77	0.25	89,89,89,89	0
84	OHX	A	2040	7/7	0.77	0.22	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	4122	1/1	0.77	0.15	68,68,68,68	0
88	ZN	d7	101	1/1	0.77	0.20	143,143,143,143	0
85	MG	1	4104	1/1	0.78	0.14	53,53,53,53	0
84	OHX	AR	3726	7/7	0.78	0.35	118,118,118,118	0
85	MG	6	2110	1/1	0.78	0.42	54,54,54,54	0
85	MG	A	2055	1/1	0.78	0.33	71,71,71,71	0
85	MG	A	2056	1/1	0.78	0.30	65,65,65,65	0
85	MG	A	2131	1/1	0.78	0.21	64,64,64,64	0
85	MG	3	218	1/1	0.78	0.33	54,54,54,54	0
85	MG	1	3729	1/1	0.78	0.29	90,90,90,90	0
85	MG	AR	4163	1/1	0.78	0.15	62,62,62,62	0
85	MG	AR	3824	1/1	0.78	0.23	77,77,77,77	0
85	MG	A	2078	1/1	0.78	0.40	54,54,54,54	0
85	MG	AR	3828	1/1	0.78	0.36	60,60,60,60	0
84	OHX	z	201	7/7	0.78	0.19	155,156,157,157	0
85	MG	1	4070	1/1	0.78	0.16	68,68,68,68	0
84	OHX	6	2046	7/7	0.78	0.25	151,152,152,152	0
84	OHX	1	3691	7/7	0.78	0.15	201,201,201,201	0
85	MG	DI	201	1/1	0.78	0.17	68,68,68,68	0
84	OHX	AM	101	7/7	0.79	0.33	121,121,121,121	0
84	OHX	AR	3732	7/7	0.79	0.25	146,146,147,147	0
85	MG	1	3989	1/1	0.79	0.27	55,55,55,55	0
85	MG	1	4006	1/1	0.79	0.20	47,47,47,47	0
84	OHX	CM	201	7/7	0.79	0.20	150,150,151,151	0
84	OHX	A	2002	7/7	0.79	0.25	147,148,149,149	0
84	OHX	1	3716	7/7	0.79	0.23	138,138,139,139	0
84	OHX	AR	3719	7/7	0.79	0.25	133,133,133,133	0
85	MG	x	206	1/1	0.79	0.16	35,35,35,35	0
85	MG	A	2059	1/1	0.79	0.37	53,53,53,53	0
85	MG	1	3848	1/1	0.79	0.33	60,60,60,60	0
85	MG	A	2064	1/1	0.79	0.36	65,65,65,65	0
85	MG	A	2120	1/1	0.79	0.31	85,85,85,85	0
85	MG	A	2065	1/1	0.79	0.35	57,57,57,57	0
85	MG	A	2068	1/1	0.79	0.44	84,84,84,84	0
85	MG	A	2069	1/1	0.79	0.30	58,58,58,58	0
84	OHX	AR	3720	7/7	0.79	0.24	152,152,152,152	0
85	MG	1	4088	1/1	0.79	0.19	44,44,44,44	0
85	MG	1	3879	1/1	0.79	0.32	45,45,45,45	0
85	MG	AR	3792	1/1	0.79	0.31	43,43,43,43	0
85	MG	AR	3812	1/1	0.79	0.14	32,32,32,32	0
84	OHX	A	2042	7/7	0.79	0.17	172,173,173,174	0
84	OHX	AR	3722	7/7	0.79	0.26	140,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	1	3696	7/7	0.79	0.26	146,146,147,147	0
85	MG	6	2075	1/1	0.79	0.31	76,76,76,76	0
85	MG	A	2088	1/1	0.79	0.26	59,59,59,59	0
85	MG	AR	3829	1/1	0.79	0.20	66,66,66,66	0
85	MG	AR	3841	1/1	0.79	0.35	54,54,54,54	0
85	MG	1	3743	1/1	0.79	0.32	79,79,79,79	0
87	GOL	AR	4261	6/6	0.79	0.21	48,48,48,48	0
88	ZN	c	101	1/1	0.79	0.16	145,145,145,145	0
85	MG	6	2085	1/1	0.79	0.40	75,75,75,75	0
85	MG	1	3818	1/1	0.80	0.28	39,39,39,39	0
85	MG	1	3980	1/1	0.80	0.39	73,73,73,73	0
85	MG	AR	4098	1/1	0.80	0.16	46,46,46,46	0
85	MG	6	2130	1/1	0.80	0.20	66,66,66,66	0
84	OHX	AR	3652	7/7	0.80	0.33	112,112,113,113	0
85	MG	1	4003	1/1	0.80	0.24	79,79,79,79	0
85	MG	1	3823	1/1	0.80	0.24	41,41,41,41	0
84	OHX	AR	3716	7/7	0.80	0.23	143,143,143,143	0
85	MG	A	2117	1/1	0.80	0.22	71,71,71,71	0
85	MG	A	2066	1/1	0.80	0.42	79,79,79,79	0
85	MG	1	4217	1/1	0.80	0.38	58,58,58,58	0
84	OHX	6	2024	7/7	0.80	0.21	151,152,152,153	0
85	MG	3	210	1/1	0.80	0.35	59,59,59,59	0
85	MG	1	4045	1/1	0.80	0.12	39,39,39,39	0
85	MG	A	2075	1/1	0.80	0.37	74,74,74,74	0
84	OHX	AR	3729	7/7	0.80	0.29	120,120,120,121	0
85	MG	6	2102	1/1	0.80	0.36	45,45,45,45	0
85	MG	1	3752	1/1	0.80	0.30	57,57,57,57	0
85	MG	A	2134	1/1	0.80	0.22	70,70,70,70	0
85	MG	AR	3962	1/1	0.80	0.26	93,93,93,93	0
85	MG	AR	3976	1/1	0.80	0.38	81,81,81,81	0
85	MG	A	2148	1/1	0.80	0.30	64,64,64,64	0
85	MG	AR	4217	1/1	0.80	0.22	80,80,80,80	0
85	MG	AR	4219	1/1	0.80	0.16	67,67,67,67	0
84	OHX	AR	3741	7/7	0.80	0.15	207,208,208,208	0
85	MG	1	3778	1/1	0.80	0.31	49,49,49,49	0
85	MG	V	201	1/1	0.80	0.30	70,70,70,70	0
84	OHX	6	2038	7/7	0.80	0.24	148,148,148,148	0
85	MG	AR	4024	1/1	0.80	0.20	53,53,53,53	0
84	OHX	AR	3694	7/7	0.80	0.23	146,147,147,147	0
85	MG	6	2188	1/1	0.80	0.24	66,66,66,66	0
87	GOL	A	2160	6/6	0.80	0.20	60,60,60,60	0
85	MG	A	2044	1/1	0.80	0.28	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	4131	1/1	0.80	0.15	48,48,48,48	0
84	OHX	A	2015	7/7	0.81	0.19	169,170,171,172	0
84	OHX	A	2023	7/7	0.81	0.22	144,145,145,145	0
85	MG	AS	217	1/1	0.81	0.19	44,44,44,44	0
85	MG	AR	4080	1/1	0.81	0.21	32,32,32,32	0
85	MG	CE	404	1/1	0.81	0.13	27,27,27,27	0
85	MG	CL	302	1/1	0.81	0.28	68,68,68,68	0
85	MG	AR	4091	1/1	0.81	0.31	35,35,35,35	0
85	MG	A	2128	1/1	0.81	0.29	78,78,78,78	0
84	OHX	x	202	7/7	0.81	0.23	144,144,145,145	0
84	OHX	1	3676	7/7	0.81	0.20	149,150,150,150	0
84	OHX	6	2021	7/7	0.81	0.18	181,181,182,182	0
85	MG	1	4111	1/1	0.81	0.27	44,44,44,44	0
85	MG	A	2135	1/1	0.81	0.41	55,55,55,55	0
85	MG	6	2187	1/1	0.81	0.21	82,82,82,82	0
84	OHX	1	3686	7/7	0.81	0.19	156,156,157,157	0
85	MG	A	2053	1/1	0.81	0.31	57,57,57,57	0
84	OHX	6	2032	7/7	0.81	0.30	131,131,132,132	0
84	OHX	1	3700	7/7	0.81	0.23	148,148,149,149	0
85	MG	6	2098	1/1	0.81	0.40	68,68,68,68	0
85	MG	A	2159	1/1	0.81	0.42	64,64,64,64	0
85	MG	AR	4011	1/1	0.81	0.20	58,58,58,58	0
85	MG	AR	4015	1/1	0.81	0.17	45,45,45,45	0
85	MG	Y	201	1/1	0.81	0.14	61,61,61,61	0
84	OHX	1	3642	7/7	0.81	0.25	135,135,136,136	0
84	OHX	CG	302	7/7	0.81	0.22	147,147,147,148	0
85	MG	6	2105	1/1	0.81	0.43	64,64,64,64	0
84	OHX	AR	3711	7/7	0.81	0.20	144,144,145,145	0
85	MG	A	2111	1/1	0.81	0.34	90,90,90,90	0
84	OHX	1	3632	7/7	0.81	0.18	156,156,156,156	0
85	MG	AR	4218	1/1	0.81	0.15	54,54,54,54	0
84	OHX	4	214	7/7	0.82	0.21	140,140,140,140	0
85	MG	1	3953	1/1	0.82	0.14	46,46,46,46	0
85	MG	6	2117	1/1	0.82	0.20	65,65,65,65	0
85	MG	AR	4194	1/1	0.82	0.13	53,53,53,53	0
84	OHX	1	3627	7/7	0.82	0.19	141,142,142,143	0
85	MG	1	3737	1/1	0.82	0.41	57,57,57,57	0
85	MG	1	3964	1/1	0.82	0.24	68,68,68,68	0
85	MG	AR	3833	1/1	0.82	0.17	49,49,49,49	0
85	MG	AR	4250	1/1	0.82	0.44	59,59,59,59	0
84	OHX	1	3672	7/7	0.82	0.20	147,147,147,148	0
85	MG	AS	219	1/1	0.82	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	AR	3745	7/7	0.82	0.28	128,128,128,128	0
85	MG	AR	3948	1/1	0.82	0.24	40,40,40,40	0
85	MG	CE	407	1/1	0.82	0.40	41,41,41,41	0
85	MG	4	233	1/1	0.82	0.12	48,48,48,48	0
85	MG	1	3985	1/1	0.82	0.20	50,50,50,50	0
85	MG	6	2145	1/1	0.82	0.10	59,59,59,59	0
84	OHX	AR	3718	7/7	0.82	0.17	166,167,167,167	0
85	MG	1	3751	1/1	0.82	0.18	40,40,40,40	0
85	MG	AR	4013	1/1	0.82	0.23	65,65,65,65	0
84	OHX	6	2045	7/7	0.82	0.24	141,141,142,142	0
85	MG	A	2047	1/1	0.82	0.35	55,55,55,55	0
84	OHX	1	3656	7/7	0.82	0.22	143,143,143,144	0
85	MG	A	2052	1/1	0.82	0.32	53,53,53,53	0
84	OHX	6	2048	7/7	0.82	0.17	173,174,174,174	0
85	MG	AR	4026	1/1	0.82	0.28	60,60,60,60	0
85	MG	1	4042	1/1	0.82	0.23	48,48,48,48	0
85	MG	AR	4044	1/1	0.82	0.24	60,60,60,60	0
84	OHX	6	2002	7/7	0.82	0.24	132,133,133,134	0
85	MG	A	2138	1/1	0.82	0.26	66,66,66,66	0
85	MG	1	4053	1/1	0.82	0.17	74,74,74,74	0
84	OHX	AR	3641	7/7	0.82	0.24	133,133,133,133	0
84	OHX	6	2006	7/7	0.82	0.23	151,151,152,152	0
84	OHX	A	2026	7/7	0.82	0.29	123,123,124,124	0
85	MG	1	3820	1/1	0.82	0.36	65,65,65,65	0
84	OHX	A	2034	7/7	0.82	0.13	231,232,232,232	0
85	MG	1	3846	1/1	0.82	0.31	39,39,39,39	0
84	OHX	1	3702	7/7	0.82	0.12	219,219,219,219	0
84	OHX	1	3694	7/7	0.82	0.30	116,116,117,117	0
85	MG	1	3874	1/1	0.82	0.32	49,49,49,49	0
85	MG	c1	202	1/1	0.82	0.28	67,67,67,67	0
84	OHX	1	3719	7/7	0.82	0.27	120,120,121,121	0
85	MG	AR	3766	1/1	0.82	0.20	96,96,96,96	0
84	OHX	6	2033	7/7	0.82	0.21	150,151,151,152	0
85	MG	AR	3779	1/1	0.82	0.23	73,73,73,73	0
84	OHX	c3	201	7/7	0.82	0.19	155,156,156,157	0
85	MG	1	3951	1/1	0.82	0.30	69,69,69,69	0
85	MG	AR	3796	1/1	0.82	0.35	64,64,64,64	0
85	MG	CG	304	1/1	0.83	0.14	56,56,56,56	0
85	MG	A	2102	1/1	0.83	0.35	58,58,58,58	0
84	OHX	A	2041	7/7	0.83	0.28	139,139,140,140	0
85	MG	AR	3756	1/1	0.83	0.36	36,36,36,36	0
85	MG	AR	4046	1/1	0.83	0.12	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	3759	1/1	0.83	0.26	34,34,34,34	0
84	OHX	1	3698	7/7	0.83	0.18	162,163,163,163	0
84	OHX	K	201	7/7	0.83	0.27	137,137,138,138	0
85	MG	6	2123	1/1	0.83	0.20	69,69,69,69	0
85	MG	6	2125	1/1	0.83	0.29	75,75,75,75	0
85	MG	A	2049	1/1	0.83	0.40	54,54,54,54	0
84	OHX	s8	301	7/7	0.83	0.18	167,167,168,168	0
84	OHX	1	3659	7/7	0.83	0.23	140,140,140,141	0
85	MG	1	3897	1/1	0.83	0.20	46,46,46,46	0
84	OHX	6	2010	7/7	0.83	0.21	154,155,155,155	0
85	MG	1	3927	1/1	0.83	0.09	42,42,42,42	0
84	OHX	1	3721	7/7	0.83	0.27	127,127,127,128	0
84	OHX	1	3712	7/7	0.83	0.24	133,133,133,133	0
84	OHX	AR	3651	7/7	0.83	0.21	150,151,151,151	0
85	MG	AR	3830	1/1	0.83	0.27	42,42,42,42	0
84	OHX	AR	3725	7/7	0.83	0.18	165,165,165,165	0
85	MG	AR	3840	1/1	0.83	0.17	47,47,47,47	0
84	OHX	A	1993	7/7	0.83	0.21	151,151,152,152	0
84	OHX	4	216	7/7	0.83	0.24	126,126,126,126	0
84	OHX	AR	3663	7/7	0.83	0.21	147,148,148,148	0
85	MG	A	2140	1/1	0.83	0.44	82,82,82,82	0
85	MG	A	2144	1/1	0.83	0.33	69,69,69,69	0
84	OHX	1	3701	7/7	0.83	0.23	139,139,140,140	0
85	MG	AR	3966	1/1	0.83	0.32	38,38,38,38	0
85	MG	AR	4185	1/1	0.83	0.15	38,38,38,38	0
85	MG	AR	3968	1/1	0.83	0.19	30,30,30,30	0
85	MG	A	2153	1/1	0.83	0.42	51,51,51,51	0
85	MG	1	3971	1/1	0.83	0.17	35,35,35,35	0
85	MG	1	4211	1/1	0.83	0.23	42,42,42,42	0
85	MG	AR	3984	1/1	0.83	0.30	50,50,50,50	0
85	MG	AR	4220	1/1	0.83	0.15	44,44,44,44	0
84	OHX	A	2025	7/7	0.83	0.16	173,173,173,173	0
84	OHX	1	3655	7/7	0.83	0.22	138,138,138,139	0
85	MG	AR	4255	1/1	0.83	0.51	57,57,57,57	0
84	OHX	A	2029	7/7	0.83	0.17	184,184,184,184	0
84	OHX	1	3705	7/7	0.83	0.24	131,131,132,132	0
85	MG	AS	221	1/1	0.83	0.16	60,60,60,60	0
84	OHX	AR	3695	7/7	0.83	0.26	122,122,123,123	0
84	OHX	6	1989	7/7	0.83	0.23	143,144,144,145	0
84	OHX	6	2042	7/7	0.83	0.23	151,151,151,151	0
84	OHX	AS	211	7/7	0.84	0.22	141,141,142,142	0
84	OHX	AT	213	7/7	0.84	0.24	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	1	3665	7/7	0.84	0.24	129,129,129,129	0
84	OHX	1	3673	7/7	0.84	0.23	133,133,133,133	0
84	OHX	AR	3654	7/7	0.84	0.23	137,137,138,138	0
84	OHX	AR	3658	7/7	0.84	0.28	122,123,123,123	0
85	MG	3	211	1/1	0.84	0.15	38,38,38,38	0
85	MG	6	2124	1/1	0.84	0.19	66,66,66,66	0
84	OHX	A	1985	7/7	0.84	0.21	140,140,141,141	0
84	OHX	AR	3659	7/7	0.84	0.23	136,136,137,137	0
84	OHX	AR	3721	7/7	0.84	0.20	139,139,140,140	0
84	OHX	6	2023	7/7	0.84	0.19	161,161,162,162	0
85	MG	AR	3853	1/1	0.84	0.28	43,43,43,43	0
85	MG	6	2138	1/1	0.84	0.27	73,73,73,73	0
85	MG	1	4000	1/1	0.84	0.14	43,43,43,43	0
85	MG	A	2106	1/1	0.84	0.31	58,58,58,58	0
85	MG	AR	3957	1/1	0.84	0.21	55,55,55,55	0
85	MG	AS	220	1/1	0.84	0.20	68,68,68,68	0
85	MG	6	2144	1/1	0.84	0.30	74,74,74,74	0
85	MG	A	2112	1/1	0.84	0.32	86,86,86,86	0
85	MG	AS	228	1/1	0.84	0.24	84,84,84,84	0
85	MG	4	237	1/1	0.84	0.13	38,38,38,38	0
85	MG	AT	229	1/1	0.84	0.26	55,55,55,55	0
85	MG	6	2146	1/1	0.84	0.31	80,80,80,80	0
85	MG	t	201	1/1	0.84	0.08	51,51,51,51	0
85	MG	1	3797	1/1	0.84	0.27	79,79,79,79	0
85	MG	6	2155	1/1	0.84	0.42	58,58,58,58	0
84	OHX	1	3690	7/7	0.84	0.24	122,123,123,123	0
85	MG	1	3808	1/1	0.84	0.36	43,43,43,43	0
84	OHX	AR	3667	7/7	0.84	0.17	146,147,147,147	0
85	MG	AR	4014	1/1	0.84	0.21	57,57,57,57	0
84	OHX	AR	3727	7/7	0.84	0.15	187,188,188,188	0
84	OHX	AR	3668	7/7	0.84	0.23	131,132,132,132	0
84	OHX	AR	3675	7/7	0.84	0.22	138,139,139,139	0
85	MG	1	3828	1/1	0.84	0.33	30,30,30,30	0
84	OHX	6	2027	7/7	0.84	0.22	146,147,147,148	0
85	MG	AR	4037	1/1	0.84	0.29	70,70,70,70	0
84	OHX	6	1997	7/7	0.84	0.25	132,132,133,133	0
85	MG	A	2143	1/1	0.84	0.21	106,106,106,106	0
84	OHX	6	2050	7/7	0.84	0.18	159,159,160,160	0
85	MG	6	2080	1/1	0.84	0.29	69,69,69,69	0
84	OHX	AR	3735	7/7	0.84	0.26	129,129,129,129	0
85	MG	6	2189	1/1	0.84	0.19	63,63,63,63	0
84	OHX	AR	3702	7/7	0.84	0.22	139,139,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	6	2088	1/1	0.84	0.21	82,82,82,82	0
84	OHX	1	3653	7/7	0.84	0.22	133,133,133,133	0
85	MG	A	2157	1/1	0.84	0.45	75,75,75,75	0
84	OHX	O	201	7/7	0.84	0.17	158,159,159,160	0
85	MG	AF	202	1/1	0.84	0.17	28,28,28,28	0
85	MG	1	3924	1/1	0.84	0.36	60,60,60,60	0
85	MG	1	4149	1/1	0.84	0.16	54,54,54,54	0
85	MG	b	101	1/1	0.84	0.25	65,65,65,65	0
85	MG	AR	3765	1/1	0.84	0.25	71,71,71,71	0
85	MG	A	2073	1/1	0.84	0.40	50,50,50,50	0
84	OHX	AR	3706	7/7	0.84	0.19	155,155,155,156	0
84	OHX	AR	3710	7/7	0.84	0.22	137,137,137,138	0
85	MG	1	4158	1/1	0.84	0.08	47,47,47,47	0
85	MG	AR	4148	1/1	0.84	0.18	43,43,43,43	0
84	OHX	x	201	7/7	0.84	0.35	110,110,110,110	0
85	MG	AR	3788	1/1	0.84	0.26	28,28,28,28	0
85	MG	1	3726	1/1	0.85	0.29	54,54,54,54	0
84	OHX	AR	3730	7/7	0.85	0.15	176,176,176,176	0
85	MG	1	3731	1/1	0.85	0.29	36,36,36,36	0
84	OHX	6	2007	7/7	0.85	0.20	145,146,146,146	0
84	OHX	1	3596	7/7	0.85	0.18	143,144,144,144	0
84	OHX	AR	3657	7/7	0.85	0.25	114,114,115,115	0
84	OHX	6	2018	7/7	0.85	0.15	189,189,189,189	0
84	OHX	1	3613	7/7	0.85	0.27	120,120,121,121	0
84	OHX	1	3658	7/7	0.85	0.21	142,143,143,143	0
85	MG	1	3766	1/1	0.85	0.18	73,73,73,73	0
84	OHX	3	209	7/7	0.85	0.20	152,152,152,152	0
85	MG	1	4124	1/1	0.85	0.13	48,48,48,48	0
85	MG	A	2071	1/1	0.85	0.36	64,64,64,64	0
84	OHX	AR	3665	7/7	0.85	0.23	133,133,133,133	0
84	OHX	4	213	7/7	0.85	0.27	117,117,117,117	0
84	OHX	AS	209	7/7	0.85	0.20	140,140,140,140	0
85	MG	1	3801	1/1	0.85	0.28	37,37,37,37	0
84	OHX	1	3703	7/7	0.85	0.24	131,131,132,132	0
84	OHX	AR	3670	7/7	0.85	0.21	143,143,144,144	0
85	MG	AR	4060	1/1	0.85	0.29	70,70,70,70	0
85	MG	1	3814	1/1	0.85	0.20	77,77,77,77	0
85	MG	AR	4069	1/1	0.85	0.21	26,26,26,26	0
85	MG	1	3816	1/1	0.85	0.20	44,44,44,44	0
84	OHX	AT	217	7/7	0.85	0.24	128,128,128,128	0
85	MG	AR	4077	1/1	0.85	0.11	40,40,40,40	0
85	MG	1	4210	1/1	0.85	0.13	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	CE	402	7/7	0.85	0.21	138,139,139,139	0
85	MG	1	4213	1/1	0.85	0.29	50,50,50,50	0
84	OHX	1	3641	7/7	0.85	0.20	141,141,141,141	0
84	OHX	AR	3680	7/7	0.85	0.22	141,141,142,142	0
84	OHX	6	2034	7/7	0.85	0.18	155,155,155,155	0
84	OHX	6	2036	7/7	0.85	0.28	135,135,136,136	0
84	OHX	A	1969	7/7	0.85	0.23	144,144,145,145	0
84	OHX	1	3707	7/7	0.85	0.26	125,125,126,126	0
84	OHX	1	3664	7/7	0.85	0.27	124,124,124,124	0
84	OHX	1	3692	7/7	0.85	0.32	113,113,113,113	0
84	OHX	A	2012	7/7	0.85	0.22	139,140,140,140	0
85	MG	1	3900	1/1	0.85	0.34	42,42,42,42	0
85	MG	A	2109	1/1	0.85	0.23	60,60,60,60	0
84	OHX	6	2041	7/7	0.85	0.22	143,144,145,145	0
84	OHX	A	2017	7/7	0.85	0.21	158,159,160,160	0
85	MG	AR	4161	1/1	0.85	0.11	39,39,39,39	0
85	MG	AR	4162	1/1	0.85	0.18	56,56,56,56	0
84	OHX	AR	3708	7/7	0.85	0.24	138,138,139,139	0
85	MG	1	3941	1/1	0.85	0.29	78,78,78,78	0
85	MG	1	3942	1/1	0.85	0.25	32,32,32,32	0
85	MG	1	3945	1/1	0.85	0.20	57,57,57,57	0
84	OHX	1	3711	7/7	0.85	0.25	119,120,120,120	0
85	MG	AR	4202	1/1	0.85	0.43	29,29,29,29	0
85	MG	AR	4213	1/1	0.85	0.24	53,53,53,53	0
85	MG	A	2126	1/1	0.85	0.40	64,64,64,64	0
85	MG	AR	4214	1/1	0.85	0.11	55,55,55,55	0
85	MG	AR	3771	1/1	0.85	0.16	42,42,42,42	0
84	OHX	6	1962	7/7	0.85	0.22	136,137,137,137	0
84	OHX	6	1972	7/7	0.85	0.20	142,143,143,144	0
84	OHX	A	2032	7/7	0.85	0.17	154,154,155,155	0
84	OHX	6	2047	7/7	0.85	0.20	161,162,162,162	0
85	MG	AR	4246	1/1	0.85	0.20	22,22,22,22	0
84	OHX	6	1975	7/7	0.85	0.23	120,120,120,120	0
84	OHX	1	3616	7/7	0.85	0.20	146,146,147,147	0
84	OHX	A	2039	7/7	0.85	0.18	166,167,168,168	0
84	OHX	6	2052	7/7	0.85	0.25	143,144,144,144	0
85	MG	6	2087	1/1	0.85	0.16	56,56,56,56	0
85	MG	AR	3821	1/1	0.85	0.12	42,42,42,42	0
85	MG	1	3978	1/1	0.85	0.24	46,46,46,46	0
85	MG	AS	231	1/1	0.85	0.24	56,56,56,56	0
85	MG	AR	3827	1/1	0.85	0.22	58,58,58,58	0
84	OHX	1	3644	7/7	0.85	0.15	166,167,167,167	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	AR	3597	7/7	0.85	0.19	150,151,151,151	0
85	MG	6	2096	1/1	0.85	0.35	68,68,68,68	0
84	OHX	AR	3610	7/7	0.85	0.20	137,138,138,138	0
85	MG	D	301	1/1	0.85	0.30	58,58,58,58	0
84	OHX	AR	3638	7/7	0.85	0.31	119,119,119,119	0
85	MG	CP	502	1/1	0.85	0.26	45,45,45,45	0
85	MG	6	2103	1/1	0.85	0.37	69,69,69,69	0
84	OHX	1	3650	7/7	0.85	0.25	128,128,128,128	0
85	MG	s6	301	1/1	0.85	0.31	77,77,77,77	0
84	OHX	AR	3646	7/7	0.85	0.28	108,108,108,108	0
85	MG	AR	3913	1/1	0.85	0.30	26,26,26,26	0
85	MG	AR	3914	1/1	0.85	0.24	32,32,32,32	0
85	MG	AR	3915	1/1	0.85	0.34	28,28,28,28	0
84	OHX	1	3626	7/7	0.85	0.23	124,124,124,124	0
85	MG	AR	3951	1/1	0.85	0.32	29,29,29,29	0
85	MG	1	4017	1/1	0.85	0.12	101,101,101,101	0
85	MG	1	4029	1/1	0.85	0.10	47,47,47,47	0
85	MG	s	300	1/1	0.86	0.25	70,70,70,70	0
84	OHX	AR	3644	7/7	0.86	0.27	126,127,127,127	0
85	MG	AR	4062	1/1	0.86	0.12	42,42,42,42	0
85	MG	1	3973	1/1	0.86	0.15	37,37,37,37	0
84	OHX	AR	3709	7/7	0.86	0.32	110,111,111,111	0
84	OHX	1	3679	7/7	0.86	0.23	131,131,132,132	0
84	OHX	1	3640	7/7	0.86	0.24	124,124,124,125	0
84	OHX	A	1971	7/7	0.86	0.19	149,150,151,151	0
84	OHX	1	3669	7/7	0.86	0.18	131,131,131,131	0
85	MG	A	2077	1/1	0.86	0.37	48,48,48,48	0
85	MG	6	2066	1/1	0.86	0.28	74,74,74,74	0
84	OHX	1	3671	7/7	0.86	0.20	149,150,150,150	0
85	MG	AR	4107	1/1	0.86	0.20	78,78,78,78	0
85	MG	6	2070	1/1	0.86	0.38	73,73,73,73	0
84	OHX	AR	3656	7/7	0.86	0.22	134,134,134,134	0
85	MG	1	4009	1/1	0.86	0.27	42,42,42,42	0
84	OHX	6	2026	7/7	0.86	0.19	146,146,147,147	0
85	MG	1	4016	1/1	0.86	0.26	39,39,39,39	0
84	OHX	A	2013	7/7	0.86	0.23	132,133,133,133	0
85	MG	AR	4134	1/1	0.86	0.18	44,44,44,44	0
85	MG	AR	3767	1/1	0.86	0.34	35,35,35,35	0
85	MG	1	3813	1/1	0.86	0.21	61,61,61,61	0
84	OHX	1	3651	7/7	0.86	0.23	130,130,131,131	0
84	OHX	6	2005	7/7	0.86	0.28	126,126,127,127	0
84	OHX	A	2022	7/7	0.86	0.15	167,167,167,167	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	4046	1/1	0.86	0.24	37,37,37,37	0
85	MG	6	2091	1/1	0.86	0.35	61,61,61,61	0
84	OHX	AR	3660	7/7	0.86	0.24	123,123,124,124	0
85	MG	AR	3807	1/1	0.86	0.21	25,25,25,25	0
85	MG	AR	4169	1/1	0.86	0.10	46,46,46,46	0
84	OHX	y	201	7/7	0.86	0.25	128,129,129,129	0
85	MG	1	4057	1/1	0.86	0.20	26,26,26,26	0
84	OHX	6	2051	7/7	0.86	0.15	172,172,172,173	0
85	MG	AR	4189	1/1	0.86	0.45	32,32,32,32	0
84	OHX	A	2027	7/7	0.86	0.18	159,160,161,161	0
84	OHX	1	3620	7/7	0.86	0.27	118,118,118,118	0
84	OHX	AR	3666	7/7	0.86	0.21	130,131,131,131	0
85	MG	1	4099	1/1	0.86	0.14	44,44,44,44	0
84	OHX	AH	201	7/7	0.86	0.26	129,129,129,130	0
85	MG	1	4110	1/1	0.86	0.10	30,30,30,30	0
85	MG	1	3857	1/1	0.86	0.23	56,56,56,56	0
85	MG	1	3867	1/1	0.86	0.30	35,35,35,35	0
85	MG	AR	4239	1/1	0.86	0.14	39,39,39,39	0
85	MG	1	3873	1/1	0.86	0.11	48,48,48,48	0
85	MG	AR	3844	1/1	0.86	0.22	27,27,27,27	0
85	MG	AR	3851	1/1	0.86	0.13	38,38,38,38	0
84	OHX	6	2035	7/7	0.86	0.22	142,142,143,143	0
85	MG	AR	4257	1/1	0.86	0.23	51,51,51,51	0
85	MG	AR	3854	1/1	0.86	0.30	48,48,48,48	0
85	MG	AR	3862	1/1	0.86	0.23	56,56,56,56	0
84	OHX	6	2008	7/7	0.86	0.18	136,136,136,136	0
85	MG	1	3880	1/1	0.86	0.26	31,31,31,31	0
84	OHX	AR	3600	7/7	0.86	0.27	119,119,119,119	0
84	OHX	AR	3677	7/7	0.86	0.30	110,111,111,111	0
84	OHX	AR	3678	7/7	0.86	0.22	137,137,137,138	0
85	MG	A	2142	1/1	0.86	0.14	80,80,80,80	0
84	OHX	AR	3736	7/7	0.86	0.24	132,132,132,133	0
85	MG	AT	231	1/1	0.86	0.27	52,52,52,52	0
84	OHX	6	2037	7/7	0.86	0.22	137,137,138,138	0
84	OHX	AR	3631	7/7	0.86	0.15	175,176,177,177	0
84	OHX	AR	3692	7/7	0.86	0.15	170,171,171,171	0
85	MG	6	2143	1/1	0.86	0.21	75,75,75,75	0
85	MG	AR	3974	1/1	0.86	0.38	81,81,81,81	0
84	OHX	AR	3637	7/7	0.86	0.19	129,129,129,129	0
84	OHX	AR	3742	7/7	0.86	0.25	128,129,129,129	0
84	OHX	1	3667	7/7	0.86	0.22	127,127,128,128	0
85	MG	6	2150	1/1	0.86	0.17	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	4002	1/1	0.86	0.35	28,28,28,28	0
85	MG	AR	4003	1/1	0.86	0.33	45,45,45,45	0
84	OHX	AR	3700	7/7	0.86	0.19	135,135,135,135	0
84	OHX	AR	3701	7/7	0.86	0.28	128,128,128,128	0
85	MG	1	3954	1/1	0.86	0.26	46,46,46,46	0
84	OHX	AR	3639	7/7	0.86	0.18	138,139,139,139	0
84	OHX	AR	3640	7/7	0.86	0.26	126,126,126,126	0
85	MG	c8	202	1/1	0.86	0.34	79,79,79,79	0
85	MG	c9	201	1/1	0.86	0.11	79,79,79,79	0
84	OHX	6	2014	7/7	0.86	0.24	129,129,129,130	0
85	MG	6	2161	1/1	0.86	0.20	58,58,58,58	0
84	OHX	AR	3707	7/7	0.86	0.27	129,129,130,130	0
87	GOL	AR	4262	6/6	0.86	0.21	48,48,48,48	0
85	MG	1	3966	1/1	0.86	0.19	69,69,69,69	0
85	MG	6	2171	1/1	0.86	0.18	56,56,56,56	0
85	MG	4	241	1/1	0.86	0.36	45,45,45,45	0
84	OHX	6	2004	7/7	0.87	0.18	157,157,158,158	0
84	OHX	A	2021	7/7	0.87	0.24	133,133,134,134	0
85	MG	1	4044	1/1	0.87	0.10	47,47,47,47	0
85	MG	AR	4056	1/1	0.87	0.17	44,44,44,44	0
84	OHX	AR	3636	7/7	0.87	0.23	133,133,134,134	0
84	OHX	4	215	7/7	0.87	0.24	137,138,138,138	0
85	MG	AR	4063	1/1	0.87	0.18	54,54,54,54	0
85	MG	AR	3748	1/1	0.87	0.27	44,44,44,44	0
85	MG	6	2081	1/1	0.87	0.26	55,55,55,55	0
85	MG	AR	4071	1/1	0.87	0.09	39,39,39,39	0
84	OHX	1	3629	7/7	0.87	0.19	148,148,148,149	0
85	MG	AR	3761	1/1	0.87	0.16	31,31,31,31	0
85	MG	AR	4076	1/1	0.87	0.18	48,48,48,48	0
84	OHX	AR	3682	7/7	0.87	0.20	144,144,144,145	0
84	OHX	AR	3685	7/7	0.87	0.27	120,121,121,121	0
85	MG	AR	4086	1/1	0.87	0.23	42,42,42,42	0
85	MG	AR	4087	1/1	0.87	0.28	63,63,63,63	0
84	OHX	A	2028	7/7	0.87	0.19	157,157,158,158	0
85	MG	AR	3769	1/1	0.87	0.26	59,59,59,59	0
84	OHX	1	3688	7/7	0.87	0.25	129,130,130,130	0
85	MG	AR	3772	1/1	0.87	0.26	37,37,37,37	0
85	MG	A	2083	1/1	0.87	0.27	68,68,68,68	0
85	MG	1	3861	1/1	0.87	0.16	34,34,34,34	0
84	OHX	A	2031	7/7	0.87	0.17	159,160,161,161	0
85	MG	1	4091	1/1	0.87	0.17	47,47,47,47	0
84	OHX	AR	3690	7/7	0.87	0.26	117,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	A	2033	7/7	0.87	0.21	146,146,147,147	0
84	OHX	1	3631	7/7	0.87	0.25	116,116,117,117	0
84	OHX	A	2036	7/7	0.87	0.10	252,253,253,253	0
85	MG	AR	4139	1/1	0.87	0.16	46,46,46,46	0
85	MG	AR	4142	1/1	0.87	0.12	46,46,46,46	0
85	MG	1	4121	1/1	0.87	0.17	64,64,64,64	0
85	MG	1	3887	1/1	0.87	0.45	42,42,42,42	0
85	MG	A	2099	1/1	0.87	0.40	71,71,71,71	0
84	OHX	AR	3693	7/7	0.87	0.33	131,131,131,131	0
85	MG	AR	4155	1/1	0.87	0.21	34,34,34,34	0
84	OHX	1	3598	7/7	0.87	0.25	127,127,127,127	0
84	OHX	1	3605	7/7	0.87	0.20	129,130,130,130	0
84	OHX	6	2016	7/7	0.87	0.28	120,120,121,121	0
85	MG	1	3925	1/1	0.87	0.12	46,46,46,46	0
84	OHX	AR	3650	7/7	0.87	0.26	118,118,118,118	0
84	OHX	1	3674	7/7	0.87	0.21	136,136,137,137	0
84	OHX	A	2043	7/7	0.87	0.17	155,156,156,157	0
84	OHX	AR	3703	7/7	0.87	0.22	136,136,136,136	0
84	OHX	1	3666	7/7	0.87	0.29	117,118,118,118	0
85	MG	AR	4188	1/1	0.87	0.53	31,31,31,31	0
84	OHX	1	3723	7/7	0.87	0.28	113,113,113,113	0
84	OHX	AR	3655	7/7	0.87	0.20	129,129,130,130	0
84	OHX	3	205	7/7	0.87	0.17	127,128,128,128	0
85	MG	AR	4209	1/1	0.87	0.15	74,74,74,74	0
84	OHX	6	1979	7/7	0.87	0.22	135,135,136,136	0
84	OHX	1	3612	7/7	0.87	0.27	122,122,122,122	0
85	MG	AR	3890	1/1	0.87	0.27	29,29,29,29	0
85	MG	AR	3897	1/1	0.87	0.35	51,51,51,51	0
85	MG	6	2142	1/1	0.87	0.21	83,83,83,83	0
84	OHX	6	2030	7/7	0.87	0.26	118,118,118,119	0
85	MG	AR	4237	1/1	0.87	0.12	39,39,39,39	0
84	OHX	6	1992	7/7	0.87	0.21	137,137,138,138	0
84	OHX	A	1946	7/7	0.87	0.17	165,166,166,167	0
85	MG	AR	3934	1/1	0.87	0.27	32,32,32,32	0
84	OHX	AR	3579	7/7	0.87	0.24	130,130,130,130	0
85	MG	A	2136	1/1	0.87	0.32	74,74,74,74	0
85	MG	3	221	1/1	0.87	0.16	34,34,34,34	0
85	MG	4	228	1/1	0.87	0.20	54,54,54,54	0
84	OHX	A	1970	7/7	0.87	0.29	132,132,133,133	0
84	OHX	AR	3587	7/7	0.87	0.22	126,126,126,126	0
84	OHX	A	1977	7/7	0.87	0.19	153,154,154,155	0
84	OHX	AR	3596	7/7	0.87	0.20	121,121,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AS	223	1/1	0.87	0.29	41,41,41,41	0
85	MG	AS	226	1/1	0.87	0.14	67,67,67,67	0
84	OHX	1	3710	7/7	0.87	0.20	136,137,137,137	0
84	OHX	A	1996	7/7	0.87	0.19	139,140,140,141	0
85	MG	AT	218	1/1	0.87	0.19	30,30,30,30	0
85	MG	AR	3980	1/1	0.87	0.28	40,40,40,40	0
85	MG	A	2156	1/1	0.87	0.30	45,45,45,45	0
84	OHX	A	1997	7/7	0.87	0.21	139,140,140,140	0
85	MG	AR	3986	1/1	0.87	0.13	56,56,56,56	0
85	MG	x	203	1/1	0.87	0.32	63,63,63,63	0
85	MG	AR	3996	1/1	0.87	0.22	56,56,56,56	0
85	MG	U	201	1/1	0.87	0.42	76,76,76,76	0
85	MG	6	2169	1/1	0.87	0.21	49,49,49,49	0
84	OHX	6	1998	7/7	0.87	0.17	146,146,147,147	0
85	MG	AR	4006	1/1	0.87	0.26	47,47,47,47	0
85	MG	CR	201	1/1	0.87	0.29	29,29,29,29	0
84	OHX	A	2006	7/7	0.87	0.20	149,150,150,150	0
84	OHX	A	2011	7/7	0.87	0.16	149,149,150,150	0
85	MG	6	2178	1/1	0.87	0.24	57,57,57,57	0
84	OHX	AR	3604	7/7	0.87	0.15	158,159,159,159	0
84	OHX	1	3592	7/7	0.87	0.24	117,117,117,117	0
87	GOL	v	305	6/6	0.87	0.15	38,38,38,38	0
84	OHX	A	2014	7/7	0.87	0.23	127,128,128,128	0
85	MG	6	2067	1/1	0.87	0.25	45,45,45,45	0
85	MG	AR	4028	1/1	0.87	0.11	41,41,41,41	0
85	MG	1	4022	1/1	0.87	0.18	53,53,53,53	0
85	MG	A	2051	1/1	0.87	0.32	67,67,67,67	0
84	OHX	AR	3674	7/7	0.87	0.24	130,130,130,131	0
84	OHX	A	1991	7/7	0.88	0.19	157,157,158,158	0
84	OHX	AR	3713	7/7	0.88	0.13	178,178,179,179	0
85	MG	DL	102	1/1	0.88	0.24	39,39,39,39	0
85	MG	sM	201	1/1	0.88	0.19	41,41,41,41	0
85	MG	6	2177	1/1	0.88	0.22	68,68,68,68	0
84	OHX	6	2029	7/7	0.88	0.18	152,153,153,154	0
84	OHX	1	3615	7/7	0.88	0.24	133,133,133,134	0
85	MG	6	2184	1/1	0.88	0.16	83,83,83,83	0
84	OHX	A	2000	7/7	0.88	0.21	140,141,141,141	0
85	MG	1	3767	1/1	0.88	0.21	60,60,60,60	0
84	OHX	6	1999	7/7	0.88	0.22	138,139,139,140	0
84	OHX	6	2001	7/7	0.88	0.24	119,120,120,120	0
84	OHX	A	2007	7/7	0.88	0.14	200,200,201,201	0
84	OHX	1	3567	7/7	0.88	0.23	128,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	1	3680	7/7	0.88	0.28	122,122,122,122	0
84	OHX	AR	3606	7/7	0.88	0.27	113,113,114,114	0
85	MG	6	2065	1/1	0.88	0.35	40,40,40,40	0
85	MG	AB	202	1/1	0.88	0.11	29,29,29,29	0
85	MG	AB	204	1/1	0.88	0.16	52,52,52,52	0
85	MG	1	3804	1/1	0.88	0.26	35,35,35,35	0
85	MG	AH	202	1/1	0.88	0.17	58,58,58,58	0
85	MG	1	4015	1/1	0.88	0.28	67,67,67,67	0
84	OHX	AR	3723	7/7	0.88	0.19	146,146,147,147	0
85	MG	1	3812	1/1	0.88	0.36	64,64,64,64	0
84	OHX	1	3685	7/7	0.88	0.23	121,121,121,121	0
84	OHX	AR	3611	7/7	0.88	0.23	126,126,126,126	0
85	MG	AR	4090	1/1	0.88	0.22	57,57,57,57	0
84	OHX	A	2018	7/7	0.88	0.18	155,155,156,156	0
85	MG	AR	4094	1/1	0.88	0.34	43,43,43,43	0
85	MG	A	2079	1/1	0.88	0.37	58,58,58,58	0
84	OHX	AR	3619	7/7	0.88	0.21	122,123,123,124	0
84	OHX	AR	3623	7/7	0.88	0.19	138,139,139,139	0
85	MG	AR	4109	1/1	0.88	0.12	39,39,39,39	0
84	OHX	AR	3676	7/7	0.88	0.25	122,122,123,123	0
84	OHX	AR	3624	7/7	0.88	0.16	150,150,151,151	0
84	OHX	AR	3628	7/7	0.88	0.17	147,148,148,148	0
85	MG	A	2086	1/1	0.88	0.15	66,66,66,66	0
84	OHX	1	3636	7/7	0.88	0.24	126,126,126,126	0
84	OHX	AR	3681	7/7	0.88	0.18	140,140,140,141	0
85	MG	1	3851	1/1	0.88	0.20	34,34,34,34	0
85	MG	1	3852	1/1	0.88	0.22	38,38,38,38	0
85	MG	1	4080	1/1	0.88	0.09	35,35,35,35	0
85	MG	AR	3801	1/1	0.88	0.17	32,32,32,32	0
85	MG	AR	4140	1/1	0.88	0.20	44,44,44,44	0
85	MG	AR	4141	1/1	0.88	0.11	37,37,37,37	0
85	MG	6	2093	1/1	0.88	0.30	47,47,47,47	0
85	MG	1	4084	1/1	0.88	0.10	32,32,32,32	0
84	OHX	AR	3632	7/7	0.88	0.25	117,117,118,118	0
84	OHX	AR	3683	7/7	0.88	0.23	126,127,127,127	0
84	OHX	1	3584	7/7	0.88	0.27	114,114,114,114	0
84	OHX	1	3621	7/7	0.88	0.20	125,126,126,126	0
84	OHX	AR	3689	7/7	0.88	0.22	118,118,119,119	0
85	MG	6	2106	1/1	0.88	0.33	50,50,50,50	0
84	OHX	A	2035	7/7	0.88	0.29	130,131,131,131	0
84	OHX	6	1960	7/7	0.88	0.21	118,118,118,118	0
85	MG	AR	4166	1/1	0.88	0.09	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	4167	1/1	0.88	0.10	71,71,71,71	0
84	OHX	1	3689	7/7	0.88	0.20	140,140,141,141	0
84	OHX	6	2015	7/7	0.88	0.21	135,135,136,136	0
85	MG	AR	4180	1/1	0.88	0.22	48,48,48,48	0
85	MG	1	4130	1/1	0.88	0.13	45,45,45,45	0
84	OHX	6	2044	7/7	0.88	0.19	140,141,141,141	0
85	MG	1	3899	1/1	0.88	0.27	39,39,39,39	0
85	MG	1	4148	1/1	0.88	0.11	53,53,53,53	0
84	OHX	1	3704	7/7	0.88	0.26	116,117,117,117	0
85	MG	1	3902	1/1	0.88	0.32	35,35,35,35	0
85	MG	AR	3864	1/1	0.88	0.27	40,40,40,40	0
84	OHX	AR	3699	7/7	0.88	0.23	117,117,117,117	0
84	OHX	1	3609	7/7	0.88	0.23	119,120,120,120	0
85	MG	6	2132	1/1	0.88	0.30	42,42,42,42	0
85	MG	1	4159	1/1	0.88	0.17	43,43,43,43	0
84	OHX	AR	3647	7/7	0.88	0.26	126,126,127,127	0
85	MG	6	2137	1/1	0.88	0.19	82,82,82,82	0
85	MG	AR	4234	1/1	0.88	0.27	32,32,32,32	0
85	MG	AR	3922	1/1	0.88	0.21	31,31,31,31	0
84	OHX	AR	3649	7/7	0.88	0.19	144,144,144,144	0
85	MG	AR	3935	1/1	0.88	0.34	49,49,49,49	0
85	MG	AR	3941	1/1	0.88	0.31	36,36,36,36	0
85	MG	A	2141	1/1	0.88	0.18	101,101,101,101	0
85	MG	1	4172	1/1	0.88	0.23	67,67,67,67	0
85	MG	AR	4253	1/1	0.88	0.21	41,41,41,41	0
85	MG	AR	4254	1/1	0.88	0.29	56,56,56,56	0
85	MG	1	3931	1/1	0.88	0.19	32,32,32,32	0
85	MG	1	3936	1/1	0.88	0.32	61,61,61,61	0
85	MG	AR	3960	1/1	0.88	0.11	41,41,41,41	0
84	OHX	1	3706	7/7	0.88	0.21	136,137,137,138	0
84	OHX	Q	201	7/7	0.88	0.15	165,165,165,165	0
85	MG	1	3944	1/1	0.88	0.17	32,32,32,32	0
84	OHX	AR	3704	7/7	0.88	0.23	133,133,133,133	0
84	OHX	6	2022	7/7	0.88	0.20	153,154,154,155	0
84	OHX	6	2049	7/7	0.88	0.16	170,171,171,171	0
84	OHX	6	1987	7/7	0.88	0.22	137,137,138,138	0
85	MG	F	301	1/1	0.88	0.28	64,64,64,64	0
85	MG	AR	3981	1/1	0.88	0.17	33,33,33,33	0
85	MG	AT	223	1/1	0.88	0.29	45,45,45,45	0
85	MG	6	2156	1/1	0.88	0.09	101,101,101,101	0
85	MG	AT	228	1/1	0.88	0.12	47,47,47,47	0
84	OHX	1	3556	7/7	0.88	0.23	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	1	3563	7/7	0.88	0.25	114,114,115,115	0
85	MG	CD	301	1/1	0.88	0.20	34,34,34,34	0
85	MG	CD	302	1/1	0.88	0.13	36,36,36,36	0
85	MG	AR	3994	1/1	0.88	0.17	25,25,25,25	0
85	MG	1	3734	1/1	0.88	0.28	43,43,43,43	0
85	MG	3	222	1/1	0.88	0.37	52,52,52,52	0
85	MG	4	220	1/1	0.88	0.43	64,64,64,64	0
85	MG	CM	202	1/1	0.88	0.26	62,62,62,62	0
85	MG	6	2165	1/1	0.88	0.15	51,51,51,51	0
85	MG	CP	505	1/1	0.88	0.13	71,71,71,71	0
84	OHX	1	3693	7/7	0.88	0.24	118,118,118,118	0
85	MG	4	229	1/1	0.88	0.22	54,54,54,54	0
84	OHX	6	2028	7/7	0.88	0.28	123,124,124,124	0
85	MG	1	3984	1/1	0.89	0.18	70,70,70,70	0
84	OHX	AR	3738	7/7	0.89	0.17	141,142,142,142	0
85	MG	1	3988	1/1	0.89	0.18	34,34,34,34	0
85	MG	CX	204	1/1	0.89	0.11	46,46,46,46	0
85	MG	DA	201	1/1	0.89	0.19	48,48,48,48	0
85	MG	DC	201	1/1	0.89	0.10	30,30,30,30	0
84	OHX	AR	3612	7/7	0.89	0.30	111,111,111,111	0
85	MG	4	235	1/1	0.89	0.20	70,70,70,70	0
84	OHX	AR	3617	7/7	0.89	0.23	123,123,123,123	0
84	OHX	1	3720	7/7	0.89	0.19	128,128,129,129	0
85	MG	l	403	1/1	0.89	0.15	37,37,37,37	0
85	MG	n	201	1/1	0.89	0.10	43,43,43,43	0
85	MG	o	302	1/1	0.89	0.14	39,39,39,39	0
84	OHX	AR	3662	7/7	0.89	0.27	111,111,112,112	0
84	OHX	AR	3621	7/7	0.89	0.20	135,135,136,136	0
85	MG	1	3815	1/1	0.89	0.18	40,40,40,40	0
85	MG	1	4013	1/1	0.89	0.14	52,52,52,52	0
85	MG	1	4014	1/1	0.89	0.12	57,57,57,57	0
84	OHX	1	3648	7/7	0.89	0.21	119,120,120,120	0
84	OHX	1	3657	7/7	0.89	0.22	123,123,124,124	0
85	MG	AB	201	1/1	0.89	0.10	34,34,34,34	0
84	OHX	1	3649	7/7	0.89	0.26	113,113,113,113	0
85	MG	6	2060	1/1	0.89	0.25	47,47,47,47	0
84	OHX	AT	214	7/7	0.89	0.21	131,131,131,132	0
85	MG	1	4028	1/1	0.89	0.10	46,46,46,46	0
84	OHX	AT	215	7/7	0.89	0.20	137,138,138,138	0
84	OHX	AT	216	7/7	0.89	0.24	132,132,132,132	0
85	MG	AR	4079	1/1	0.89	0.19	34,34,34,34	0
84	OHX	3	208	7/7	0.89	0.25	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	1	3602	7/7	0.89	0.24	128,128,128,129	0
84	OHX	AR	3635	7/7	0.89	0.20	137,138,138,138	0
85	MG	6	2073	1/1	0.89	0.35	48,48,48,48	0
84	OHX	AR	3673	7/7	0.89	0.24	125,125,125,125	0
85	MG	A	2074	1/1	0.89	0.28	55,55,55,55	0
85	MG	1	4051	1/1	0.89	0.12	44,44,44,44	0
84	OHX	CG	301	7/7	0.89	0.18	142,143,143,144	0
85	MG	AR	4102	1/1	0.89	0.29	30,30,30,30	0
84	OHX	1	3713	7/7	0.89	0.20	138,138,138,139	0
85	MG	AR	4108	1/1	0.89	0.15	36,36,36,36	0
84	OHX	AR	3714	7/7	0.89	0.22	132,132,133,133	0
85	MG	6	2083	1/1	0.89	0.34	63,63,63,63	0
84	OHX	1	3639	7/7	0.89	0.20	132,132,132,132	0
85	MG	1	3871	1/1	0.89	0.25	30,30,30,30	0
84	OHX	A	1959	7/7	0.89	0.20	137,138,139,139	0
85	MG	1	4081	1/1	0.89	0.16	29,29,29,29	0
84	OHX	J	301	7/7	0.89	0.15	157,157,158,158	0
85	MG	1	3876	1/1	0.89	0.23	37,37,37,37	0
84	OHX	6	1986	7/7	0.89	0.19	147,148,148,148	0
84	OHX	1	3643	7/7	0.89	0.29	114,114,114,114	0
85	MG	6	2095	1/1	0.89	0.28	41,41,41,41	0
85	MG	1	4093	1/1	0.89	0.25	57,57,57,57	0
84	OHX	6	2012	7/7	0.89	0.21	136,136,137,137	0
85	MG	AR	4145	1/1	0.89	0.19	70,70,70,70	0
85	MG	AR	4146	1/1	0.89	0.09	34,34,34,34	0
85	MG	A	2097	1/1	0.89	0.35	53,53,53,53	0
84	OHX	AR	3552	7/7	0.89	0.22	114,114,114,114	0
85	MG	1	4109	1/1	0.89	0.20	66,66,66,66	0
84	OHX	AR	3643	7/7	0.89	0.20	120,121,121,121	0
84	OHX	A	1989	7/7	0.89	0.16	154,155,155,155	0
84	OHX	d9	101	7/7	0.89	0.18	153,153,154,154	0
85	MG	AR	3836	1/1	0.89	0.23	48,48,48,48	0
85	MG	6	2107	1/1	0.89	0.42	43,43,43,43	0
84	OHX	6	2013	7/7	0.89	0.23	121,122,122,122	0
85	MG	6	2111	1/1	0.89	0.35	61,61,61,61	0
85	MG	AR	4165	1/1	0.89	0.20	43,43,43,43	0
85	MG	AR	3849	1/1	0.89	0.28	35,35,35,35	0
84	OHX	1	3601	7/7	0.89	0.26	112,112,112,112	0
84	OHX	AR	3724	7/7	0.89	0.22	130,130,131,131	0
85	MG	1	4138	1/1	0.89	0.11	33,33,33,33	0
85	MG	AR	3855	1/1	0.89	0.23	33,33,33,33	0
85	MG	AR	3859	1/1	0.89	0.37	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	A	2119	1/1	0.89	0.25	57,57,57,57	0
85	MG	6	2116	1/1	0.89	0.21	62,62,62,62	0
84	OHX	AR	3593	7/7	0.89	0.24	113,114,114,114	0
85	MG	AR	3868	1/1	0.89	0.26	25,25,25,25	0
85	MG	AR	3877	1/1	0.89	0.24	22,22,22,22	0
85	MG	AR	4196	1/1	0.89	0.12	43,43,43,43	0
85	MG	AR	3889	1/1	0.89	0.27	35,35,35,35	0
85	MG	1	3930	1/1	0.89	0.15	40,40,40,40	0
85	MG	AR	4210	1/1	0.89	0.32	54,54,54,54	0
84	OHX	1	3675	7/7	0.89	0.17	140,141,141,141	0
85	MG	AR	3898	1/1	0.89	0.33	28,28,28,28	0
85	MG	AR	3901	1/1	0.89	0.28	29,29,29,29	0
84	OHX	AR	3687	7/7	0.89	0.24	121,121,122,122	0
85	MG	1	4151	1/1	0.89	0.14	41,41,41,41	0
85	MG	A	2137	1/1	0.89	0.24	58,58,58,58	0
84	OHX	6	1993	7/7	0.89	0.20	134,135,135,135	0
85	MG	AR	4225	1/1	0.89	0.15	34,34,34,34	0
84	OHX	6	2017	7/7	0.89	0.19	135,135,136,136	0
84	OHX	AR	3691	7/7	0.89	0.25	116,116,116,117	0
84	OHX	6	1994	7/7	0.89	0.14	170,170,170,170	0
85	MG	1	3760	1/1	0.89	0.25	27,27,27,27	0
85	MG	1	3762	1/1	0.89	0.23	30,30,30,30	0
85	MG	AR	3946	1/1	0.89	0.13	59,59,59,59	0
85	MG	AR	4251	1/1	0.89	0.33	59,59,59,59	0
85	MG	A	2149	1/1	0.89	0.12	60,60,60,60	0
84	OHX	6	2019	7/7	0.89	0.18	140,140,141,141	0
85	MG	1	4180	1/1	0.89	0.27	45,45,45,45	0
85	MG	A	2152	1/1	0.89	0.35	43,43,43,43	0
85	MG	AR	3953	1/1	0.89	0.10	34,34,34,34	0
85	MG	AR	3955	1/1	0.89	0.10	34,34,34,34	0
85	MG	1	4183	1/1	0.89	0.09	44,44,44,44	0
85	MG	1	4207	1/1	0.89	0.19	36,36,36,36	0
84	OHX	AR	3608	7/7	0.89	0.22	131,131,132,132	0
84	OHX	1	3699	7/7	0.89	0.18	130,131,131,131	0
85	MG	1	3776	1/1	0.89	0.24	43,43,43,43	0
85	MG	1	4215	1/1	0.89	0.33	27,27,27,27	0
84	OHX	AR	3698	7/7	0.89	0.21	123,123,123,124	0
85	MG	1	3786	1/1	0.89	0.12	40,40,40,40	0
85	MG	AR	3978	1/1	0.89	0.26	49,49,49,49	0
85	MG	AT	220	1/1	0.89	0.16	53,53,53,53	0
84	OHX	6	2043	7/7	0.89	0.20	145,145,146,146	0
85	MG	1	3791	1/1	0.89	0.23	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3793	1/1	0.89	0.12	37,37,37,37	0
85	MG	3	216	1/1	0.89	0.30	58,58,58,58	0
85	MG	AR	3990	1/1	0.89	0.08	39,39,39,39	0
84	OHX	A	2019	7/7	0.89	0.16	176,176,176,176	0
85	MG	3	219	1/1	0.89	0.27	56,56,56,56	0
85	MG	1	3976	1/1	0.89	0.11	61,61,61,61	0
85	MG	AR	3997	1/1	0.89	0.09	44,44,44,44	0
84	OHX	A	2020	7/7	0.89	0.18	147,148,148,148	0
85	MG	1	3979	1/1	0.89	0.12	39,39,39,39	0
85	MG	AR	4005	1/1	0.89	0.18	40,40,40,40	0
85	MG	1	3802	1/1	0.89	0.18	86,86,86,86	0
85	MG	AT	224	1/1	0.90	0.22	68,68,68,68	0
84	OHX	3	206	7/7	0.90	0.18	127,127,128,128	0
85	MG	AT	227	1/1	0.90	0.44	79,79,79,79	0
85	MG	AR	3992	1/1	0.90	0.34	67,67,67,67	0
85	MG	1	3830	1/1	0.90	0.17	44,44,44,44	0
85	MG	1	4021	1/1	0.90	0.24	44,44,44,44	0
85	MG	6	2176	1/1	0.90	0.20	93,93,93,93	0
85	MG	1	3835	1/1	0.90	0.30	30,30,30,30	0
85	MG	k	402	1/1	0.90	0.10	37,37,37,37	0
85	MG	6	2180	1/1	0.90	0.12	64,64,64,64	0
85	MG	1	4027	1/1	0.90	0.20	35,35,35,35	0
84	OHX	6	1977	7/7	0.90	0.18	150,151,151,152	0
84	OHX	CK	201	7/7	0.90	0.22	118,118,119,119	0
84	OHX	CL	301	7/7	0.90	0.24	121,122,122,122	0
85	MG	1	4039	1/1	0.90	0.17	40,40,40,40	0
85	MG	AR	4017	1/1	0.90	0.07	95,95,95,95	0
84	OHX	AR	3615	7/7	0.90	0.17	132,133,133,133	0
85	MG	AR	4023	1/1	0.90	0.11	31,31,31,31	0
84	OHX	1	3662	7/7	0.90	0.26	116,116,116,116	0
84	OHX	A	1953	7/7	0.90	0.19	146,147,147,147	0
85	MG	DC	203	1/1	0.90	0.12	47,47,47,47	0
85	MG	AR	4027	1/1	0.90	0.21	76,76,76,76	0
84	OHX	6	1980	7/7	0.90	0.21	116,116,116,116	0
85	MG	AR	4029	1/1	0.90	0.19	42,42,42,42	0
85	MG	1	3863	1/1	0.90	0.21	55,55,55,55	0
84	OHX	A	1966	7/7	0.90	0.20	131,131,132,132	0
85	MG	AR	4039	1/1	0.90	0.29	56,56,56,56	0
85	MG	A	2045	1/1	0.90	0.31	58,58,58,58	0
85	MG	AR	4041	1/1	0.90	0.10	34,34,34,34	0
85	MG	AR	4042	1/1	0.90	0.14	57,57,57,57	0
84	OHX	6	1984	7/7	0.90	0.16	150,150,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	1	3591	7/7	0.90	0.25	109,109,109,109	0
85	MG	6	2063	1/1	0.90	0.23	82,82,82,82	0
85	MG	1	4064	1/1	0.90	0.20	58,58,58,58	0
84	OHX	4	210	7/7	0.90	0.27	108,108,108,108	0
85	MG	1	4074	1/1	0.90	0.11	37,37,37,37	0
85	MG	AR	3749	1/1	0.90	0.18	42,42,42,42	0
84	OHX	6	2020	7/7	0.90	0.17	135,136,136,137	0
84	OHX	A	1978	7/7	0.90	0.17	143,144,144,145	0
85	MG	6	2071	1/1	0.90	0.34	45,45,45,45	0
84	OHX	A	1980	7/7	0.90	0.19	137,137,138,138	0
84	OHX	A	1983	7/7	0.90	0.19	142,142,143,143	0
85	MG	AR	4075	1/1	0.90	0.10	36,36,36,36	0
85	MG	1	4085	1/1	0.90	0.14	51,51,51,51	0
84	OHX	1	3634	7/7	0.90	0.21	132,132,132,133	0
84	OHX	1	3683	7/7	0.90	0.19	118,118,118,118	0
84	OHX	1	3684	7/7	0.90	0.19	141,141,141,141	0
85	MG	1	4092	1/1	0.90	0.25	54,54,54,54	0
85	MG	6	2082	1/1	0.90	0.27	54,54,54,54	0
84	OHX	1	3619	7/7	0.90	0.22	127,127,127,127	0
85	MG	AR	3783	1/1	0.90	0.17	44,44,44,44	0
85	MG	AR	3785	1/1	0.90	0.38	57,57,57,57	0
85	MG	1	4094	1/1	0.90	0.12	78,78,78,78	0
85	MG	AR	4099	1/1	0.90	0.10	41,41,41,41	0
85	MG	AR	4101	1/1	0.90	0.11	48,48,48,48	0
85	MG	AR	3790	1/1	0.90	0.27	22,22,22,22	0
84	OHX	A	1995	7/7	0.90	0.19	151,152,152,152	0
85	MG	AR	3795	1/1	0.90	0.31	49,49,49,49	0
85	MG	1	4101	1/1	0.90	0.17	38,38,38,38	0
85	MG	AR	4114	1/1	0.90	0.12	40,40,40,40	0
85	MG	1	3913	1/1	0.90	0.34	28,28,28,28	0
85	MG	1	4105	1/1	0.90	0.23	26,26,26,26	0
85	MG	AR	3811	1/1	0.90	0.12	50,50,50,50	0
85	MG	1	3923	1/1	0.90	0.16	51,51,51,51	0
85	MG	A	2090	1/1	0.90	0.17	57,57,57,57	0
85	MG	AR	4123	1/1	0.90	0.24	57,57,57,57	0
84	OHX	6	1996	7/7	0.90	0.15	154,154,155,155	0
84	OHX	1	3606	7/7	0.90	0.18	138,138,138,138	0
85	MG	AR	4127	1/1	0.90	0.10	77,77,77,77	0
85	MG	AR	4132	1/1	0.90	0.23	49,49,49,49	0
85	MG	1	4116	1/1	0.90	0.20	44,44,44,44	0
85	MG	1	3746	1/1	0.90	0.23	26,26,26,26	0
85	MG	1	4122	1/1	0.90	0.13	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	6	2099	1/1	0.90	0.27	51,51,51,51	0
85	MG	1	3928	1/1	0.90	0.17	34,34,34,34	0
84	OHX	A	1999	7/7	0.90	0.19	146,146,147,147	0
84	OHX	AR	3684	7/7	0.90	0.21	124,125,125,125	0
84	OHX	r	301	7/7	0.90	0.20	115,115,115,115	0
85	MG	1	3753	1/1	0.90	0.25	35,35,35,35	0
85	MG	AR	4149	1/1	0.90	0.19	66,66,66,66	0
84	OHX	A	2003	7/7	0.90	0.21	129,130,130,130	0
85	MG	AR	3843	1/1	0.90	0.13	30,30,30,30	0
85	MG	1	3761	1/1	0.90	0.27	41,41,41,41	0
84	OHX	AR	3517	7/7	0.90	0.17	145,146,146,146	0
85	MG	A	2113	1/1	0.90	0.28	73,73,73,73	0
84	OHX	AR	3527	7/7	0.90	0.24	112,112,112,112	0
84	OHX	AR	3688	7/7	0.90	0.18	136,136,137,137	0
85	MG	1	4156	1/1	0.90	0.13	44,44,44,44	0
84	OHX	AR	3531	7/7	0.90	0.23	115,115,115,115	0
85	MG	1	3774	1/1	0.90	0.28	43,43,43,43	0
84	OHX	1	3652	7/7	0.90	0.25	110,110,110,110	0
85	MG	1	4167	1/1	0.90	0.12	23,23,23,23	0
85	MG	1	4170	1/1	0.90	0.37	41,41,41,41	0
85	MG	AR	3875	1/1	0.90	0.23	45,45,45,45	0
84	OHX	AR	3563	7/7	0.90	0.20	122,122,123,123	0
84	OHX	1	3599	7/7	0.90	0.25	115,116,116,116	0
85	MG	1	3787	1/1	0.90	0.18	46,46,46,46	0
85	MG	AR	3891	1/1	0.90	0.33	69,69,69,69	0
85	MG	1	4175	1/1	0.90	0.21	39,39,39,39	0
84	OHX	AR	3648	7/7	0.90	0.20	130,131,131,131	0
84	OHX	AR	3586	7/7	0.90	0.23	119,119,120,120	0
85	MG	AR	4198	1/1	0.90	0.30	51,51,51,51	0
85	MG	1	4201	1/1	0.90	0.23	28,28,28,28	0
85	MG	AR	4204	1/1	0.90	0.09	38,38,38,38	0
85	MG	AR	3906	1/1	0.90	0.18	33,33,33,33	0
85	MG	AR	3912	1/1	0.90	0.28	23,23,23,23	0
84	OHX	6	2031	7/7	0.90	0.25	125,126,126,126	0
84	OHX	1	3501	7/7	0.90	0.15	126,126,127,127	0
85	MG	AR	4215	1/1	0.90	0.22	70,70,70,70	0
85	MG	1	3798	1/1	0.90	0.21	32,32,32,32	0
85	MG	AR	3917	1/1	0.90	0.28	42,42,42,42	0
85	MG	6	2141	1/1	0.90	0.10	52,52,52,52	0
85	MG	AR	3924	1/1	0.90	0.22	27,27,27,27	0
84	OHX	1	3552	7/7	0.90	0.14	150,150,151,151	0
84	OHX	6	1950	7/7	0.90	0.19	135,135,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	AR	3599	7/7	0.90	0.18	136,136,136,136	0
85	MG	AR	3942	1/1	0.90	0.42	31,31,31,31	0
84	OHX	1	3614	7/7	0.90	0.18	133,133,133,134	0
85	MG	AR	4244	1/1	0.90	0.30	45,45,45,45	0
85	MG	1	3806	1/1	0.90	0.29	51,51,51,51	0
85	MG	AR	4248	1/1	0.90	0.33	45,45,45,45	0
85	MG	6	2147	1/1	0.90	0.12	57,57,57,57	0
85	MG	1	3986	1/1	0.90	0.08	42,42,42,42	0
85	MG	6	2152	1/1	0.90	0.23	62,62,62,62	0
84	OHX	AT	210	7/7	0.90	0.22	119,119,120,120	0
84	OHX	AR	3601	7/7	0.90	0.20	127,127,128,128	0
85	MG	1	3993	1/1	0.90	0.22	42,42,42,42	0
85	MG	AR	4259	1/1	0.90	0.31	16,16,16,16	0
85	MG	AS	212	1/1	0.90	0.33	41,41,41,41	0
85	MG	s4	301	1/1	0.90	0.21	59,59,59,59	0
84	OHX	AR	3602	7/7	0.90	0.17	143,143,144,144	0
85	MG	6	2157	1/1	0.90	0.14	56,56,56,56	0
84	OHX	6	1961	7/7	0.90	0.22	128,129,129,130	0
84	OHX	A	2030	7/7	0.90	0.19	142,143,143,144	0
84	OHX	1	3604	7/7	0.90	0.24	116,116,117,117	0
84	OHX	AR	3661	7/7	0.90	0.25	112,112,112,113	0
84	OHX	AR	3607	7/7	0.90	0.23	113,113,113,113	0
85	MG	AS	229	1/1	0.90	0.20	46,46,46,46	0
84	OHX	6	1971	7/7	0.90	0.18	136,136,136,137	0
85	MG	4	231	1/1	0.90	0.15	58,58,58,58	0
84	OHX	1	3645	7/7	0.90	0.21	125,126,126,126	0
85	MG	AT	222	1/1	0.90	0.18	43,43,43,43	0
85	MG	6	2170	1/1	0.90	0.17	64,64,64,64	0
85	MG	AR	3896	1/1	0.91	0.35	36,36,36,36	0
84	OHX	AR	3598	7/7	0.91	0.23	117,118,118,118	0
84	OHX	1	3575	7/7	0.91	0.22	116,117,117,117	0
85	MG	6	2173	1/1	0.91	0.28	48,48,48,48	0
85	MG	AR	3902	1/1	0.91	0.33	42,42,42,42	0
85	MG	6	2068	1/1	0.91	0.43	61,61,61,61	0
84	OHX	1	3577	7/7	0.91	0.22	118,118,119,119	0
85	MG	AR	3909	1/1	0.91	0.36	25,25,25,25	0
84	OHX	1	3677	7/7	0.91	0.20	116,116,117,117	0
84	OHX	e	101	7/7	0.91	0.19	143,144,145,145	0
85	MG	AR	4129	1/1	0.91	0.17	26,26,26,26	0
85	MG	1	4137	1/1	0.91	0.16	55,55,55,55	0
85	MG	AR	4133	1/1	0.91	0.17	25,25,25,25	0
84	OHX	1	3551	7/7	0.91	0.20	118,118,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	4135	1/1	0.91	0.09	62,62,62,62	0
84	OHX	AR	3603	7/7	0.91	0.23	107,107,107,107	0
85	MG	1	3983	1/1	0.91	0.22	55,55,55,55	0
84	OHX	1	3507	7/7	0.91	0.21	113,113,114,114	0
84	OHX	AR	3605	7/7	0.91	0.22	128,128,128,129	0
84	OHX	1	3681	7/7	0.91	0.21	127,127,127,128	0
85	MG	AR	4144	1/1	0.91	0.10	41,41,41,41	0
85	MG	1	3842	1/1	0.91	0.25	25,25,25,25	0
85	MG	1	3727	1/1	0.91	0.28	37,37,37,37	0
85	MG	AR	3943	1/1	0.91	0.14	41,41,41,41	0
84	OHX	1	3724	7/7	0.91	0.21	113,113,113,113	0
84	OHX	1	3660	7/7	0.91	0.17	153,153,154,154	0
85	MG	AR	4152	1/1	0.91	0.13	38,38,38,38	0
85	MG	AR	3949	1/1	0.91	0.12	32,32,32,32	0
85	MG	6	2193	1/1	0.91	0.25	55,55,55,55	0
85	MG	1	3732	1/1	0.91	0.26	26,26,26,26	0
85	MG	1	4004	1/1	0.91	0.15	44,44,44,44	0
85	MG	6	2197	1/1	0.91	0.23	56,56,56,56	0
85	MG	AR	3958	1/1	0.91	0.27	38,38,38,38	0
85	MG	6	2198	1/1	0.91	0.34	49,49,49,49	0
85	MG	1	4169	1/1	0.91	0.12	30,30,30,30	0
84	OHX	1	3661	7/7	0.91	0.22	119,120,120,120	0
84	OHX	1	3622	7/7	0.91	0.14	153,154,154,154	0
85	MG	AR	3971	1/1	0.91	0.32	57,57,57,57	0
85	MG	AR	4170	1/1	0.91	0.06	32,32,32,32	0
85	MG	1	3740	1/1	0.91	0.17	30,30,30,30	0
85	MG	AR	4174	1/1	0.91	0.13	39,39,39,39	0
85	MG	1	3742	1/1	0.91	0.15	38,38,38,38	0
85	MG	AR	4181	1/1	0.91	0.15	50,50,50,50	0
85	MG	AR	4182	1/1	0.91	0.12	79,79,79,79	0
84	OHX	1	3623	7/7	0.91	0.24	114,114,115,115	0
84	OHX	AR	3524	7/7	0.91	0.18	118,119,119,119	0
84	OHX	4	209	7/7	0.91	0.20	113,113,113,113	0
85	MG	1	4186	1/1	0.91	0.26	25,25,25,25	0
85	MG	1	4194	1/1	0.91	0.28	22,22,22,22	0
84	OHX	AR	3528	7/7	0.91	0.21	108,108,108,108	0
84	OHX	A	2016	7/7	0.91	0.18	142,143,143,144	0
84	OHX	AR	3620	7/7	0.91	0.17	143,144,144,144	0
85	MG	1	4023	1/1	0.91	0.25	57,57,57,57	0
85	MG	AR	4205	1/1	0.91	0.16	59,59,59,59	0
85	MG	AR	4207	1/1	0.91	0.16	48,48,48,48	0
84	OHX	1	3624	7/7	0.91	0.17	136,136,136,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3884	1/1	0.91	0.17	29,29,29,29	0
85	MG	1	3755	1/1	0.91	0.28	36,36,36,36	0
85	MG	1	3894	1/1	0.91	0.29	22,22,22,22	0
84	OHX	AR	3622	7/7	0.91	0.18	130,131,131,131	0
84	OHX	AR	3712	7/7	0.91	0.26	109,109,109,109	0
85	MG	AR	3784	1/1	0.91	0.25	51,51,51,51	0
85	MG	AR	4008	1/1	0.91	0.10	26,26,26,26	0
84	OHX	AR	3538	7/7	0.91	0.17	123,123,124,124	0
85	MG	AR	4222	1/1	0.91	0.26	58,58,58,58	0
84	OHX	AR	3543	7/7	0.91	0.20	123,123,123,123	0
85	MG	AR	4229	1/1	0.91	0.35	34,34,34,34	0
85	MG	1	3906	1/1	0.91	0.13	42,42,42,42	0
84	OHX	AR	3626	7/7	0.91	0.20	122,123,123,123	0
85	MG	1	3909	1/1	0.91	0.30	25,25,25,25	0
85	MG	AR	4020	1/1	0.91	0.08	41,41,41,41	0
84	OHX	1	3539	7/7	0.91	0.19	119,119,119,119	0
85	MG	A	2123	1/1	0.91	0.30	55,55,55,55	0
85	MG	AR	4022	1/1	0.91	0.10	30,30,30,30	0
84	OHX	AR	3559	7/7	0.91	0.20	121,121,121,121	0
85	MG	6	2129	1/1	0.91	0.32	62,62,62,62	0
85	MG	1	4058	1/1	0.91	0.24	51,51,51,51	0
85	MG	AR	4252	1/1	0.91	0.31	50,50,50,50	0
85	MG	4	226	1/1	0.91	0.21	42,42,42,42	0
85	MG	1	4061	1/1	0.91	0.21	54,54,54,54	0
84	OHX	AR	3562	7/7	0.91	0.22	124,124,124,124	0
84	OHX	CX	202	7/7	0.91	0.21	117,118,118,118	0
85	MG	AR	3822	1/1	0.91	0.22	46,46,46,46	0
85	MG	1	3926	1/1	0.91	0.10	37,37,37,37	0
85	MG	AS	214	1/1	0.91	0.22	52,52,52,52	0
84	OHX	A	1935	7/7	0.91	0.18	140,140,141,141	0
85	MG	AS	218	1/1	0.91	0.11	33,33,33,33	0
84	OHX	AR	3633	7/7	0.91	0.22	124,125,125,125	0
84	OHX	AR	3634	7/7	0.91	0.22	112,112,113,113	0
84	OHX	A	1958	7/7	0.91	0.12	173,173,173,173	0
84	OHX	1	3594	7/7	0.91	0.19	131,131,132,132	0
85	MG	AR	3835	1/1	0.91	0.23	45,45,45,45	0
85	MG	AR	4058	1/1	0.91	0.20	61,61,61,61	0
85	MG	1	3795	1/1	0.91	0.24	26,26,26,26	0
84	OHX	A	1960	7/7	0.91	0.15	151,151,151,152	0
84	OHX	AR	3564	7/7	0.91	0.13	155,155,155,155	0
85	MG	AT	219	1/1	0.91	0.21	36,36,36,36	0
85	MG	6	2148	1/1	0.91	0.27	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	A	2154	1/1	0.91	0.36	45,45,45,45	0
84	OHX	AR	3575	7/7	0.91	0.24	119,120,120,120	0
85	MG	AR	3845	1/1	0.91	0.15	23,23,23,23	0
84	OHX	1	3628	7/7	0.91	0.15	144,145,145,145	0
85	MG	1	3949	1/1	0.91	0.23	44,44,44,44	0
84	OHX	1	3541	7/7	0.91	0.20	119,119,120,120	0
85	MG	x	205	1/1	0.91	0.29	33,33,33,33	0
84	OHX	1	3597	7/7	0.91	0.22	117,117,118,118	0
85	MG	AR	4078	1/1	0.91	0.29	60,60,60,60	0
85	MG	1	3805	1/1	0.91	0.22	29,29,29,29	0
84	OHX	AR	3592	7/7	0.91	0.25	114,114,114,114	0
85	MG	6	2058	1/1	0.91	0.24	45,45,45,45	0
85	MG	CE	406	1/1	0.91	0.12	25,25,25,25	0
85	MG	AR	3865	1/1	0.91	0.20	24,24,24,24	0
85	MG	1	3807	1/1	0.91	0.11	41,41,41,41	0
85	MG	CI	301	1/1	0.91	0.09	33,33,33,33	0
84	OHX	1	3545	7/7	0.91	0.18	120,120,120,120	0
84	OHX	1	3633	7/7	0.91	0.20	134,134,135,135	0
85	MG	AR	4095	1/1	0.91	0.14	25,25,25,25	0
85	MG	AR	3885	1/1	0.91	0.27	33,33,33,33	0
85	MG	AR	3886	1/1	0.91	0.28	30,30,30,30	0
85	MG	AR	4100	1/1	0.91	0.12	57,57,57,57	0
85	MG	6	2062	1/1	0.91	0.23	51,51,51,51	0
85	MG	1	4115	1/1	0.91	0.10	36,36,36,36	0
84	OHX	1	3572	7/7	0.91	0.24	118,119,119,119	0
85	MG	AR	3893	1/1	0.91	0.43	50,50,50,50	0
85	MG	AR	3804	1/1	0.92	0.22	27,27,27,27	0
84	OHX	1	3517	7/7	0.92	0.18	119,119,120,120	0
84	OHX	AR	3565	7/7	0.92	0.22	113,113,113,113	0
85	MG	AR	4051	1/1	0.92	0.20	40,40,40,40	0
85	MG	AR	4052	1/1	0.92	0.16	86,86,86,86	0
85	MG	1	4184	1/1	0.92	0.10	36,36,36,36	0
84	OHX	AR	3568	7/7	0.92	0.19	117,117,117,117	0
85	MG	AR	3816	1/1	0.92	0.11	39,39,39,39	0
85	MG	1	4190	1/1	0.92	0.35	25,25,25,25	0
85	MG	1	4192	1/1	0.92	0.30	21,21,21,21	0
85	MG	6	2114	1/1	0.92	0.25	46,46,46,46	0
84	OHX	AR	3569	7/7	0.92	0.15	137,137,137,138	0
85	MG	CF	403	1/1	0.92	0.09	34,34,34,34	0
85	MG	1	4200	1/1	0.92	0.29	22,22,22,22	0
84	OHX	AR	3669	7/7	0.92	0.11	175,176,176,176	0
85	MG	1	4206	1/1	0.92	0.16	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	AR	3571	7/7	0.92	0.22	125,125,125,125	0
85	MG	CM	203	1/1	0.92	0.30	55,55,55,55	0
84	OHX	AR	3671	7/7	0.92	0.28	113,113,113,113	0
85	MG	6	2121	1/1	0.92	0.22	41,41,41,41	0
85	MG	CQ	201	1/1	0.92	0.17	34,34,34,34	0
84	OHX	AR	3627	7/7	0.92	0.21	127,128,128,128	0
85	MG	1	4026	1/1	0.92	0.36	65,65,65,65	0
85	MG	CU	201	1/1	0.92	0.15	38,38,38,38	0
85	MG	1	3888	1/1	0.92	0.23	29,29,29,29	0
85	MG	AR	4085	1/1	0.92	0.12	35,35,35,35	0
85	MG	DA	202	1/1	0.92	0.17	45,45,45,45	0
85	MG	AR	3842	1/1	0.92	0.09	47,47,47,47	0
85	MG	1	3763	1/1	0.92	0.18	29,29,29,29	0
85	MG	AR	4089	1/1	0.92	0.11	62,62,62,62	0
85	MG	1	3764	1/1	0.92	0.20	41,41,41,41	0
84	OHX	1	3569	7/7	0.92	0.25	111,111,111,111	0
85	MG	1	4036	1/1	0.92	0.39	70,70,70,70	0
85	MG	1	4038	1/1	0.92	0.14	41,41,41,41	0
85	MG	sM	202	1/1	0.92	0.21	42,42,42,42	0
84	OHX	AR	3576	7/7	0.92	0.20	128,128,129,129	0
85	MG	1	4040	1/1	0.92	0.12	74,74,74,74	0
85	MG	6	2139	1/1	0.92	0.18	45,45,45,45	0
85	MG	AR	3856	1/1	0.92	0.34	27,27,27,27	0
85	MG	AR	3858	1/1	0.92	0.22	36,36,36,36	0
85	MG	AR	4104	1/1	0.92	0.17	66,66,66,66	0
84	OHX	1	3546	7/7	0.92	0.19	127,127,127,127	0
84	OHX	AR	3584	7/7	0.92	0.16	131,131,131,132	0
84	OHX	A	1947	7/7	0.92	0.20	129,129,130,130	0
85	MG	AR	4113	1/1	0.92	0.07	37,37,37,37	0
84	OHX	1	3574	7/7	0.92	0.23	116,116,117,117	0
85	MG	4	217	1/1	0.92	0.28	52,52,52,52	0
85	MG	1	3785	1/1	0.92	0.25	25,25,25,25	0
85	MG	4	221	1/1	0.92	0.23	51,51,51,51	0
85	MG	AR	3882	1/1	0.92	0.21	47,47,47,47	0
85	MG	AR	3883	1/1	0.92	0.25	32,32,32,32	0
85	MG	4	222	1/1	0.92	0.15	33,33,33,33	0
85	MG	1	3915	1/1	0.92	0.20	36,36,36,36	0
85	MG	4	227	1/1	0.92	0.11	52,52,52,52	0
85	MG	AR	4128	1/1	0.92	0.17	55,55,55,55	0
85	MG	1	4054	1/1	0.92	0.16	56,56,56,56	0
85	MG	AR	4130	1/1	0.92	0.11	31,31,31,31	0
85	MG	1	3919	1/1	0.92	0.24	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	1	3617	7/7	0.92	0.21	122,122,122,122	0
85	MG	4	232	1/1	0.92	0.10	37,37,37,37	0
84	OHX	AR	3590	7/7	0.92	0.23	113,113,113,113	0
84	OHX	AR	3591	7/7	0.92	0.22	112,112,112,112	0
85	MG	AR	3900	1/1	0.92	0.33	37,37,37,37	0
84	OHX	A	1964	7/7	0.92	0.21	122,122,123,123	0
85	MG	4	236	1/1	0.92	0.15	50,50,50,50	0
84	OHX	1	3654	7/7	0.92	0.19	136,136,136,137	0
84	OHX	6	1973	7/7	0.92	0.17	137,138,138,138	0
84	OHX	6	1974	7/7	0.92	0.20	121,121,122,122	0
84	OHX	1	3635	7/7	0.92	0.18	122,122,123,123	0
85	MG	6	2167	1/1	0.92	0.15	53,53,53,53	0
85	MG	1	3932	1/1	0.92	0.19	55,55,55,55	0
85	MG	1	4082	1/1	0.92	0.08	35,35,35,35	0
85	MG	1	3933	1/1	0.92	0.15	49,49,49,49	0
84	OHX	AG	201	7/7	0.92	0.23	114,115,115,115	0
85	MG	AR	3923	1/1	0.92	0.43	38,38,38,38	0
85	MG	1	3937	1/1	0.92	0.11	68,68,68,68	0
85	MG	AR	3930	1/1	0.92	0.30	29,29,29,29	0
85	MG	v	303	1/1	0.92	0.19	44,44,44,44	0
85	MG	w	201	1/1	0.92	0.14	37,37,37,37	0
85	MG	AR	3936	1/1	0.92	0.29	20,20,20,20	0
85	MG	AR	3938	1/1	0.92	0.33	34,34,34,34	0
85	MG	1	3939	1/1	0.92	0.16	39,39,39,39	0
85	MG	x	204	1/1	0.92	0.28	28,28,28,28	0
85	MG	A	2101	1/1	0.92	0.19	64,64,64,64	0
84	OHX	1	3550	7/7	0.92	0.20	115,115,115,116	0
84	OHX	A	1979	7/7	0.92	0.16	142,143,144,144	0
85	MG	x	208	1/1	0.92	0.14	46,46,46,46	0
84	OHX	6	1978	7/7	0.92	0.20	117,117,117,118	0
85	MG	AR	4178	1/1	0.92	0.19	24,24,24,24	0
85	MG	AR	4179	1/1	0.92	0.13	43,43,43,43	0
85	MG	A	2108	1/1	0.92	0.32	57,57,57,57	0
84	OHX	A	1981	7/7	0.92	0.11	194,195,195,195	0
84	OHX	AR	3506	7/7	0.92	0.18	112,112,112,112	0
84	OHX	1	3638	7/7	0.92	0.18	122,123,123,123	0
84	OHX	6	2011	7/7	0.92	0.19	146,146,147,147	0
84	OHX	1	3536	7/7	0.92	0.23	109,109,109,109	0
85	MG	1	4107	1/1	0.92	0.09	40,40,40,40	0
84	OHX	1	3537	7/7	0.92	0.22	115,115,115,116	0
84	OHX	A	1994	7/7	0.92	0.18	142,143,144,144	0
84	OHX	6	1985	7/7	0.92	0.20	130,130,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	4113	1/1	0.92	0.29	57,57,57,57	0
85	MG	AR	3973	1/1	0.92	0.14	40,40,40,40	0
85	MG	AR	4203	1/1	0.92	0.10	29,29,29,29	0
85	MG	6	2196	1/1	0.92	0.40	48,48,48,48	0
84	OHX	AR	3537	7/7	0.92	0.15	131,132,132,132	0
85	MG	1	3962	1/1	0.92	0.13	39,39,39,39	0
85	MG	1	3963	1/1	0.92	0.17	45,45,45,45	0
85	MG	AR	3979	1/1	0.92	0.19	41,41,41,41	0
84	OHX	1	3588	7/7	0.92	0.19	128,128,128,128	0
84	OHX	c5	201	7/7	0.92	0.13	161,161,161,161	0
84	OHX	c8	201	7/7	0.92	0.15	146,147,147,148	0
84	OHX	1	3589	7/7	0.92	0.26	113,113,113,113	0
85	MG	AR	3747	1/1	0.92	0.16	23,23,23,23	0
84	OHX	AR	3546	7/7	0.92	0.20	123,124,124,124	0
84	OHX	A	2001	7/7	0.92	0.20	136,137,137,138	0
85	MG	AR	3750	1/1	0.92	0.17	27,27,27,27	0
85	MG	AR	4223	1/1	0.92	0.16	61,61,61,61	0
85	MG	AR	4224	1/1	0.92	0.16	47,47,47,47	0
85	MG	AR	3995	1/1	0.92	0.23	65,65,65,65	0
85	MG	AR	4227	1/1	0.92	0.20	22,22,22,22	0
85	MG	AR	3753	1/1	0.92	0.14	26,26,26,26	0
85	MG	AR	4230	1/1	0.92	0.26	18,18,18,18	0
85	MG	1	3834	1/1	0.92	0.22	22,22,22,22	0
85	MG	A	2145	1/1	0.92	0.11	92,92,92,92	0
85	MG	AR	3998	1/1	0.92	0.27	40,40,40,40	0
85	MG	AR	4000	1/1	0.92	0.18	25,25,25,25	0
85	MG	AR	4001	1/1	0.92	0.14	38,38,38,38	0
85	MG	1	4145	1/1	0.92	0.17	42,42,42,42	0
85	MG	AR	3760	1/1	0.92	0.19	53,53,53,53	0
85	MG	1	3728	1/1	0.92	0.33	52,52,52,52	0
85	MG	AR	3762	1/1	0.92	0.19	24,24,24,24	0
85	MG	1	3836	1/1	0.92	0.23	36,36,36,36	0
85	MG	1	3841	1/1	0.92	0.29	29,29,29,29	0
84	OHX	1	3485	7/7	0.92	0.17	120,121,121,121	0
84	OHX	AS	210	7/7	0.92	0.20	115,115,116,116	0
85	MG	A	2158	1/1	0.92	0.31	67,67,67,67	0
85	MG	1	4154	1/1	0.92	0.09	46,46,46,46	0
85	MG	AR	4016	1/1	0.92	0.16	33,33,33,33	0
84	OHX	A	2004	7/7	0.92	0.17	139,139,140,140	0
85	MG	AR	4019	1/1	0.92	0.23	45,45,45,45	0
85	MG	1	3987	1/1	0.92	0.45	65,65,65,65	0
85	MG	AS	215	1/1	0.92	0.24	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3849	1/1	0.92	0.23	23,23,23,23	0
84	OHX	A	2005	7/7	0.92	0.19	131,132,132,132	0
85	MG	6	2094	1/1	0.92	0.18	37,37,37,37	0
85	MG	1	4165	1/1	0.92	0.20	24,24,24,24	0
84	OHX	AR	3613	7/7	0.92	0.23	112,112,112,112	0
84	OHX	1	3488	7/7	0.92	0.19	109,109,109,110	0
85	MG	AS	224	1/1	0.92	0.13	55,55,55,55	0
85	MG	AS	225	1/1	0.92	0.14	58,58,58,58	0
84	OHX	AR	3561	7/7	0.92	0.22	110,110,110,111	0
85	MG	d6	101	1/1	0.92	0.23	49,49,49,49	0
84	OHX	AR	3618	7/7	0.92	0.21	113,113,114,114	0
84	OHX	1	3610	7/7	0.92	0.16	130,130,131,131	0
85	MG	AR	4032	1/1	0.92	0.16	48,48,48,48	0
85	MG	1	3865	1/1	0.92	0.19	45,45,45,45	0
85	MG	AR	3797	1/1	0.92	0.15	31,31,31,31	0
84	OHX	1	3593	7/7	0.92	0.13	166,167,167,167	0
85	MG	AR	3803	1/1	0.92	0.17	35,35,35,35	0
85	MG	AS	216	1/1	0.93	0.32	23,23,23,23	0
85	MG	1	3920	1/1	0.93	0.09	41,41,41,41	0
85	MG	1	3921	1/1	0.93	0.14	57,57,57,57	0
84	OHX	6	1970	7/7	0.93	0.19	126,126,127,127	0
85	MG	6	2064	1/1	0.93	0.27	53,53,53,53	0
84	OHX	1	3558	7/7	0.93	0.15	134,134,135,135	0
85	MG	1	3770	1/1	0.93	0.18	29,29,29,29	0
84	OHX	1	3559	7/7	0.93	0.13	143,143,143,144	0
85	MG	1	4096	1/1	0.93	0.23	27,27,27,27	0
85	MG	1	4098	1/1	0.93	0.10	47,47,47,47	0
85	MG	AR	4025	1/1	0.93	0.15	31,31,31,31	0
85	MG	1	3773	1/1	0.93	0.17	38,38,38,38	0
85	MG	AR	3782	1/1	0.93	0.14	36,36,36,36	0
84	OHX	AT	207	7/7	0.93	0.17	117,117,117,117	0
85	MG	1	4103	1/1	0.93	0.18	60,60,60,60	0
84	OHX	AT	208	7/7	0.93	0.24	114,114,114,114	0
85	MG	AT	221	1/1	0.93	0.34	52,52,52,52	0
84	OHX	6	2009	7/7	0.93	0.18	126,127,127,128	0
85	MG	AR	4034	1/1	0.93	0.10	60,60,60,60	0
85	MG	1	4106	1/1	0.93	0.33	67,67,67,67	0
85	MG	1	3781	1/1	0.93	0.20	33,33,33,33	0
85	MG	AR	4040	1/1	0.93	0.10	43,43,43,43	0
85	MG	6	2077	1/1	0.93	0.34	39,39,39,39	0
84	OHX	AT	212	7/7	0.93	0.17	128,128,128,128	0
84	OHX	AR	3573	7/7	0.93	0.17	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	1	3586	7/7	0.93	0.17	121,122,122,122	0
85	MG	AR	4047	1/1	0.93	0.20	54,54,54,54	0
85	MG	AR	4048	1/1	0.93	0.16	34,34,34,34	0
85	MG	AR	3802	1/1	0.93	0.08	40,40,40,40	0
85	MG	1	3788	1/1	0.93	0.30	45,45,45,45	0
85	MG	1	4114	1/1	0.93	0.16	52,52,52,52	0
84	OHX	1	3678	7/7	0.93	0.22	117,117,118,118	0
85	MG	AR	4057	1/1	0.93	0.21	41,41,41,41	0
85	MG	AR	3809	1/1	0.93	0.26	37,37,37,37	0
85	MG	AR	4059	1/1	0.93	0.15	47,47,47,47	0
84	OHX	AR	3577	7/7	0.93	0.14	156,157,158,158	0
85	MG	CO	201	1/1	0.93	0.12	44,44,44,44	0
85	MG	AR	4061	1/1	0.93	0.11	50,50,50,50	0
85	MG	CP	504	1/1	0.93	0.15	46,46,46,46	0
85	MG	1	4119	1/1	0.93	0.11	35,35,35,35	0
85	MG	AR	3813	1/1	0.93	0.15	55,55,55,55	0
85	MG	AR	4064	1/1	0.93	0.21	38,38,38,38	0
85	MG	CR	202	1/1	0.93	0.13	29,29,29,29	0
85	MG	1	3792	1/1	0.93	0.19	37,37,37,37	0
85	MG	AR	3815	1/1	0.93	0.12	32,32,32,32	0
84	OHX	1	3561	7/7	0.93	0.16	124,124,125,125	0
84	OHX	AR	3580	7/7	0.93	0.18	117,118,118,118	0
84	OHX	AR	3583	7/7	0.93	0.20	113,114,114,114	0
84	OHX	1	3663	7/7	0.93	0.17	111,111,111,111	0
85	MG	DC	202	1/1	0.93	0.23	48,48,48,48	0
85	MG	1	3800	1/1	0.93	0.15	45,45,45,45	0
84	OHX	AR	3585	7/7	0.93	0.20	117,117,117,117	0
84	OHX	1	3547	7/7	0.93	0.17	120,121,121,121	0
85	MG	1	4141	1/1	0.93	0.26	64,64,64,64	0
85	MG	6	2101	1/1	0.93	0.30	53,53,53,53	0
85	MG	DQ	204	1/1	0.93	0.11	32,32,32,32	0
85	MG	AR	3831	1/1	0.93	0.17	44,44,44,44	0
84	OHX	1	3540	7/7	0.93	0.20	111,111,111,111	0
84	OHX	AR	3588	7/7	0.93	0.22	112,112,112,113	0
85	MG	AR	4088	1/1	0.93	0.27	25,25,25,25	0
85	MG	1	3959	1/1	0.93	0.19	66,66,66,66	0
85	MG	AR	3838	1/1	0.93	0.18	27,27,27,27	0
85	MG	A	2048	1/1	0.93	0.23	52,52,52,52	0
84	OHX	1	3519	7/7	0.93	0.19	116,116,116,116	0
84	OHX	CP	501	7/7	0.93	0.18	126,126,126,127	0
84	OHX	6	1982	7/7	0.93	0.14	147,147,148,148	0
85	MG	6	2108	1/1	0.93	0.34	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	6	2109	1/1	0.93	0.33	56,56,56,56	0
85	MG	A	2054	1/1	0.93	0.15	66,66,66,66	0
84	OHX	1	3525	7/7	0.93	0.19	114,114,114,115	0
85	MG	1	3811	1/1	0.93	0.14	44,44,44,44	0
85	MG	AR	3850	1/1	0.93	0.23	24,24,24,24	0
84	OHX	A	1941	7/7	0.93	0.15	136,137,137,137	0
85	MG	AR	4106	1/1	0.93	0.08	46,46,46,46	0
85	MG	1	3972	1/1	0.93	0.28	45,45,45,45	0
85	MG	1	4160	1/1	0.93	0.09	34,34,34,34	0
84	OHX	AR	3653	7/7	0.93	0.18	120,120,121,121	0
85	MG	AR	4110	1/1	0.93	0.14	46,46,46,46	0
85	MG	1	4163	1/1	0.93	0.14	44,44,44,44	0
84	OHX	1	3637	7/7	0.93	0.14	140,140,140,141	0
85	MG	1	3977	1/1	0.93	0.09	48,48,48,48	0
85	MG	AR	3860	1/1	0.93	0.26	23,23,23,23	0
85	MG	AR	4118	1/1	0.93	0.12	31,31,31,31	0
85	MG	1	4168	1/1	0.93	0.28	20,20,20,20	0
84	OHX	A	1952	7/7	0.93	0.20	128,129,129,129	0
85	MG	A	2076	1/1	0.93	0.28	51,51,51,51	0
84	OHX	AR	3595	7/7	0.93	0.17	131,131,131,132	0
85	MG	AR	4124	1/1	0.93	0.11	39,39,39,39	0
84	OHX	1	3608	7/7	0.93	0.17	118,119,119,119	0
85	MG	AR	3874	1/1	0.93	0.32	27,27,27,27	0
84	OHX	1	3722	1/7	0.93	0.20	136,136,136,136	0
85	MG	1	4173	1/1	0.93	0.32	36,36,36,36	0
84	OHX	6	1988	7/7	0.93	0.16	133,133,133,134	0
85	MG	1	3822	1/1	0.93	0.28	18,18,18,18	0
84	OHX	A	1963	7/7	0.93	0.14	150,151,152,152	0
84	OHX	AR	3494	7/7	0.93	0.17	124,125,125,125	0
84	OHX	1	3553	7/7	0.93	0.20	121,122,122,122	0
85	MG	1	3831	1/1	0.93	0.29	26,26,26,26	0
84	OHX	6	1990	7/7	0.93	0.19	129,130,130,130	0
85	MG	1	3995	1/1	0.93	0.15	34,34,34,34	0
85	MG	AR	3895	1/1	0.93	0.27	43,43,43,43	0
85	MG	1	3996	1/1	0.93	0.16	64,64,64,64	0
85	MG	1	4198	1/1	0.93	0.34	43,43,43,43	0
85	MG	1	3997	1/1	0.93	0.15	54,54,54,54	0
85	MG	1	3998	1/1	0.93	0.10	36,36,36,36	0
85	MG	1	4203	1/1	0.93	0.18	31,31,31,31	0
85	MG	AR	4147	1/1	0.93	0.06	31,31,31,31	0
85	MG	1	4205	1/1	0.93	0.24	31,31,31,31	0
84	OHX	AR	3520	7/7	0.93	0.20	112,112,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	3905	1/1	0.93	0.25	29,29,29,29	0
84	OHX	c1	201	7/7	0.93	0.18	147,148,148,149	0
85	MG	1	3837	1/1	0.93	0.24	26,26,26,26	0
85	MG	6	2149	1/1	0.93	0.23	46,46,46,46	0
84	OHX	AR	3521	7/7	0.93	0.16	117,118,118,118	0
85	MG	AR	4159	1/1	0.93	0.13	36,36,36,36	0
84	OHX	6	2025	7/7	0.93	0.21	120,120,121,121	0
85	MG	1	4010	1/1	0.93	0.16	30,30,30,30	0
84	OHX	AR	3526	7/7	0.93	0.18	117,117,117,118	0
84	OHX	6	1991	7/7	0.93	0.16	133,134,134,135	0
84	OHX	6	1940	7/7	0.93	0.13	149,150,151,151	0
84	OHX	6	1946	7/7	0.93	0.20	127,128,128,129	0
85	MG	AR	3926	1/1	0.93	0.29	33,33,33,33	0
84	OHX	A	1982	7/7	0.93	0.19	121,122,122,122	0
85	MG	AR	3932	1/1	0.93	0.14	63,63,63,63	0
85	MG	A	2116	1/1	0.93	0.24	67,67,67,67	0
85	MG	AR	3933	1/1	0.93	0.25	24,24,24,24	0
85	MG	AR	4173	1/1	0.93	0.12	53,53,53,53	0
85	MG	3	215	1/1	0.93	0.35	31,31,31,31	0
84	OHX	AR	3536	7/7	0.93	0.17	123,124,124,124	0
84	OHX	1	3595	7/7	0.93	0.14	140,140,140,140	0
85	MG	1	3860	1/1	0.93	0.29	36,36,36,36	0
85	MG	AR	3939	1/1	0.93	0.27	31,31,31,31	0
84	OHX	6	1955	7/7	0.93	0.12	179,179,179,179	0
84	OHX	AR	3541	7/7	0.93	0.22	125,125,125,125	0
85	MG	1	3864	1/1	0.93	0.17	38,38,38,38	0
85	MG	AR	4187	1/1	0.93	0.18	36,36,36,36	0
84	OHX	1	3611	7/7	0.93	0.24	119,119,119,120	0
85	MG	4	218	1/1	0.93	0.31	49,49,49,49	0
85	MG	AR	4193	1/1	0.93	0.18	38,38,38,38	0
85	MG	A	2133	1/1	0.93	0.28	72,72,72,72	0
85	MG	1	3736	1/1	0.93	0.27	31,31,31,31	0
84	OHX	1	3526	7/7	0.93	0.19	114,115,115,115	0
85	MG	1	4034	1/1	0.93	0.23	42,42,42,42	0
85	MG	AR	4199	1/1	0.93	0.21	45,45,45,45	0
85	MG	AR	4200	1/1	0.93	0.18	48,48,48,48	0
85	MG	1	4035	1/1	0.93	0.20	47,47,47,47	0
85	MG	1	3872	1/1	0.93	0.32	32,32,32,32	0
85	MG	1	4037	1/1	0.93	0.07	30,30,30,30	0
84	OHX	AR	3548	7/7	0.93	0.18	121,121,122,122	0
85	MG	AR	4206	1/1	0.93	0.16	33,33,33,33	0
85	MG	4	230	1/1	0.93	0.07	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	3964	1/1	0.93	0.16	35,35,35,35	0
85	MG	6	2182	1/1	0.93	0.20	83,83,83,83	0
84	OHX	AR	3549	7/7	0.93	0.17	116,117,117,117	0
85	MG	1	3875	1/1	0.93	0.25	23,23,23,23	0
84	OHX	3	207	7/7	0.93	0.14	137,138,138,138	0
85	MG	AR	4216	1/1	0.93	0.16	44,44,44,44	0
84	OHX	A	1998	7/7	0.93	0.15	158,159,160,160	0
84	OHX	AR	3553	7/7	0.93	0.19	113,113,113,113	0
85	MG	1	3748	1/1	0.93	0.24	44,44,44,44	0
84	OHX	AR	3558	7/7	0.93	0.15	137,137,137,137	0
84	OHX	6	2000	7/7	0.93	0.18	130,130,131,131	0
84	OHX	AR	3560	7/7	0.93	0.14	135,135,136,136	0
85	MG	1	4055	1/1	0.93	0.11	33,33,33,33	0
85	MG	1	3896	1/1	0.93	0.25	36,36,36,36	0
84	OHX	6	1964	7/7	0.93	0.18	123,123,124,124	0
85	MG	1	3898	1/1	0.93	0.26	33,33,33,33	0
84	OHX	6	1966	7/7	0.93	0.16	133,133,134,134	0
85	MG	T	202	1/1	0.93	0.11	97,97,97,97	0
85	MG	1	3758	1/1	0.93	0.18	32,32,32,32	0
85	MG	AR	3993	1/1	0.93	0.21	28,28,28,28	0
85	MG	1	3759	1/1	0.93	0.11	41,41,41,41	0
85	MG	1	4071	1/1	0.93	0.11	40,40,40,40	0
85	MG	1	4072	1/1	0.93	0.30	46,46,46,46	0
85	MG	1	4073	1/1	0.93	0.18	40,40,40,40	0
85	MG	1	3904	1/1	0.93	0.29	25,25,25,25	0
85	MG	1	4077	1/1	0.93	0.11	33,33,33,33	0
85	MG	x	207	1/1	0.93	0.15	33,33,33,33	0
84	OHX	6	1968	7/7	0.93	0.21	122,122,123,123	0
85	MG	6	2053	1/1	0.93	0.27	41,41,41,41	0
84	OHX	AR	3743	7/7	0.93	0.28	109,109,109,109	0
85	MG	d6	102	1/1	0.93	0.20	38,38,38,38	0
85	MG	AR	3754	1/1	0.93	0.28	40,40,40,40	0
84	OHX	AR	3744	7/7	0.93	0.26	109,110,110,110	0
84	OHX	6	1969	7/7	0.93	0.18	127,127,128,128	0
85	MG	AR	4012	1/1	0.93	0.17	30,30,30,30	0
85	MG	AS	213	1/1	0.93	0.18	26,26,26,26	0
84	OHX	AS	208	7/7	0.93	0.14	138,139,139,139	0
85	MG	1	3765	1/1	0.93	0.27	21,21,21,21	0
85	MG	1	3725	1/1	0.94	0.29	34,34,34,34	0
85	MG	6	2084	1/1	0.94	0.19	48,48,48,48	0
84	OHX	1	3670	7/7	0.94	0.22	111,111,111,111	0
84	OHX	1	3531	7/7	0.94	0.20	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	4035	1/1	0.94	0.11	43,43,43,43	0
84	OHX	1	3534	7/7	0.94	0.18	113,113,113,113	0
84	OHX	6	1919	7/7	0.94	0.16	121,121,122,122	0
84	OHX	6	1932	7/7	0.94	0.17	132,132,133,133	0
84	OHX	AR	3679	7/7	0.94	0.12	153,153,153,154	0
85	MG	1	3990	1/1	0.94	0.15	24,24,24,24	0
84	OHX	AR	3567	7/7	0.94	0.15	121,121,121,121	0
85	MG	AR	4045	1/1	0.94	0.23	55,55,55,55	0
85	MG	1	4155	1/1	0.94	0.09	53,53,53,53	0
85	MG	1	3994	1/1	0.94	0.14	47,47,47,47	0
84	OHX	1	3481	7/7	0.94	0.17	116,117,117,117	0
84	OHX	A	1990	7/7	0.94	0.16	135,135,136,136	0
85	MG	1	3738	1/1	0.94	0.23	28,28,28,28	0
85	MG	1	3855	1/1	0.94	0.16	44,44,44,44	0
85	MG	AT	225	1/1	0.94	0.22	53,53,53,53	0
85	MG	1	4162	1/1	0.94	0.15	40,40,40,40	0
85	MG	1	3739	1/1	0.94	0.11	51,51,51,51	0
85	MG	1	4001	1/1	0.94	0.24	47,47,47,47	0
85	MG	AR	3832	1/1	0.94	0.25	30,30,30,30	0
85	MG	1	4166	1/1	0.94	0.19	47,47,47,47	0
85	MG	AR	3834	1/1	0.94	0.16	33,33,33,33	0
85	MG	1	4002	1/1	0.94	0.07	37,37,37,37	0
84	OHX	6	1941	7/7	0.94	0.15	120,120,121,121	0
85	MG	AR	3837	1/1	0.94	0.28	19,19,19,19	0
85	MG	AR	4067	1/1	0.94	0.10	34,34,34,34	0
85	MG	1	3741	1/1	0.94	0.18	37,37,37,37	0
85	MG	1	4005	1/1	0.94	0.13	36,36,36,36	0
84	OHX	AR	3570	7/7	0.94	0.19	120,121,121,121	0
84	OHX	AK	102	7/7	0.94	0.18	105,105,105,105	0
85	MG	AR	4073	1/1	0.94	0.13	40,40,40,40	0
84	OHX	1	3565	7/7	0.94	0.15	131,131,131,131	0
84	OHX	AR	3472	7/7	0.94	0.18	111,111,111,112	0
85	MG	1	3869	1/1	0.94	0.33	34,34,34,34	0
85	MG	1	4176	1/1	0.94	0.29	34,34,34,34	0
84	OHX	AR	3474	7/7	0.94	0.19	114,114,114,115	0
85	MG	1	4182	1/1	0.94	0.15	25,25,25,25	0
85	MG	CQ	202	1/1	0.94	0.19	32,32,32,32	0
85	MG	AR	3852	1/1	0.94	0.10	37,37,37,37	0
85	MG	AR	4082	1/1	0.94	0.18	24,24,24,24	0
85	MG	AR	4083	1/1	0.94	0.30	31,31,31,31	0
85	MG	AR	4084	1/1	0.94	0.08	34,34,34,34	0
84	OHX	AR	3493	7/7	0.94	0.16	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	1	3566	7/7	0.94	0.17	113,113,114,114	0
84	OHX	AR	3495	7/7	0.94	0.18	113,113,114,114	0
85	MG	1	4187	1/1	0.94	0.15	43,43,43,43	0
85	MG	AR	3857	1/1	0.94	0.27	20,20,20,20	0
85	MG	6	2122	1/1	0.94	0.24	61,61,61,61	0
84	OHX	AR	3581	7/7	0.94	0.21	109,109,109,109	0
85	MG	1	3754	1/1	0.94	0.21	37,37,37,37	0
85	MG	1	4193	1/1	0.94	0.23	23,23,23,23	0
85	MG	AR	4097	1/1	0.94	0.19	40,40,40,40	0
85	MG	AR	3863	1/1	0.94	0.30	21,21,21,21	0
85	MG	6	2127	1/1	0.94	0.19	54,54,54,54	0
85	MG	1	3878	1/1	0.94	0.26	24,24,24,24	0
85	MG	1	4195	1/1	0.94	0.28	29,29,29,29	0
85	MG	AR	3869	1/1	0.94	0.32	31,31,31,31	0
85	MG	AR	4103	1/1	0.94	0.17	47,47,47,47	0
84	OHX	AR	3582	7/7	0.94	0.19	114,114,114,114	0
84	OHX	AR	3501	7/7	0.94	0.18	113,113,114,114	0
84	OHX	1	3503	7/7	0.94	0.14	127,128,128,129	0
85	MG	AR	3880	1/1	0.94	0.27	42,42,42,42	0
85	MG	AR	3881	1/1	0.94	0.21	30,30,30,30	0
84	OHX	AT	209	7/7	0.94	0.17	121,121,122,122	0
85	MG	AR	4111	1/1	0.94	0.08	37,37,37,37	0
84	OHX	AR	3512	7/7	0.94	0.16	118,118,119,119	0
85	MG	1	4032	1/1	0.94	0.18	42,42,42,42	0
85	MG	1	4033	1/1	0.94	0.22	58,58,58,58	0
85	MG	1	4209	1/1	0.94	0.32	48,48,48,48	0
85	MG	A	2058	1/1	0.94	0.34	46,46,46,46	0
85	MG	1	3892	1/1	0.94	0.20	23,23,23,23	0
85	MG	A	2060	1/1	0.94	0.39	55,55,55,55	0
85	MG	A	2061	1/1	0.94	0.34	59,59,59,59	0
84	OHX	AT	211	7/7	0.94	0.13	137,138,138,138	0
85	MG	A	2063	1/1	0.94	0.33	51,51,51,51	0
84	OHX	A	2009	7/7	0.94	0.19	126,126,127,127	0
85	MG	AR	3894	1/1	0.94	0.31	45,45,45,45	0
84	OHX	6	1995	7/7	0.94	0.16	133,134,134,135	0
84	OHX	1	3520	7/7	0.94	0.16	123,123,124,124	0
85	MG	1	4218	1/1	0.94	0.14	32,32,32,32	0
84	OHX	AR	3645	7/7	0.94	0.20	118,118,118,118	0
85	MG	AR	3899	1/1	0.94	0.24	45,45,45,45	0
84	OHX	3	202	7/7	0.94	0.21	115,116,116,116	0
85	MG	1	4041	1/1	0.94	0.20	45,45,45,45	0
84	OHX	1	3571	7/7	0.94	0.18	111,111,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3771	1/1	0.94	0.14	33,33,33,33	0
85	MG	AR	3904	1/1	0.94	0.25	21,21,21,21	0
84	OHX	1	3483	7/7	0.94	0.17	113,113,113,113	0
85	MG	3	217	1/1	0.94	0.11	40,40,40,40	0
85	MG	AR	4138	1/1	0.94	0.22	28,28,28,28	0
85	MG	1	3907	1/1	0.94	0.34	40,40,40,40	0
84	OHX	1	3514	7/7	0.94	0.17	112,112,112,112	0
84	OHX	1	3554	7/7	0.94	0.16	129,129,130,130	0
85	MG	1	3775	1/1	0.94	0.19	32,32,32,32	0
84	OHX	AR	3594	7/7	0.94	0.18	114,114,115,115	0
85	MG	1	3917	1/1	0.94	0.23	30,30,30,30	0
85	MG	AR	3919	1/1	0.94	0.40	34,34,34,34	0
85	MG	1	3777	1/1	0.94	0.07	30,30,30,30	0
85	MG	6	2164	1/1	0.94	0.17	53,53,53,53	0
84	OHX	1	3543	7/7	0.94	0.15	119,119,120,120	0
85	MG	1	4059	1/1	0.94	0.21	51,51,51,51	0
85	MG	1	4060	1/1	0.94	0.19	44,44,44,44	0
85	MG	AR	3931	1/1	0.94	0.21	17,17,17,17	0
85	MG	AR	4154	1/1	0.94	0.09	39,39,39,39	0
85	MG	4	224	1/1	0.94	0.27	33,33,33,33	0
85	MG	1	3779	1/1	0.94	0.46	55,55,55,55	0
85	MG	AR	4157	1/1	0.94	0.30	75,75,75,75	0
85	MG	AR	4158	1/1	0.94	0.14	29,29,29,29	0
84	OHX	4	203	7/7	0.94	0.20	106,107,107,107	0
85	MG	1	4065	1/1	0.94	0.24	48,48,48,48	0
85	MG	1	4069	1/1	0.94	0.10	46,46,46,46	0
85	MG	1	3784	1/1	0.94	0.20	26,26,26,26	0
84	OHX	1	3600	7/7	0.94	0.11	150,150,150,150	0
84	OHX	1	3581	7/7	0.94	0.20	112,113,113,113	0
84	OHX	AR	3539	7/7	0.94	0.12	127,128,128,128	0
84	OHX	4	211	7/7	0.94	0.14	138,139,139,140	0
85	MG	AR	3944	1/1	0.94	0.16	38,38,38,38	0
84	OHX	4	212	7/7	0.94	0.17	128,128,128,128	0
84	OHX	DH	201	7/7	0.94	0.19	113,113,113,113	0
84	OHX	A	1915	7/7	0.94	0.15	142,143,143,144	0
85	MG	AR	3950	1/1	0.94	0.17	47,47,47,47	0
85	MG	4	238	1/1	0.94	0.08	35,35,35,35	0
85	MG	4	239	1/1	0.94	0.28	43,43,43,43	0
85	MG	4	240	1/1	0.94	0.22	32,32,32,32	0
84	OHX	A	1918	7/7	0.94	0.18	128,129,129,129	0
84	OHX	A	1927	7/7	0.94	0.14	138,138,139,139	0
85	MG	AR	4183	1/1	0.94	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	l	402	1/1	0.94	0.13	57,57,57,57	0
85	MG	1	4083	1/1	0.94	0.06	41,41,41,41	0
85	MG	AR	3963	1/1	0.94	0.17	49,49,49,49	0
85	MG	l	404	1/1	0.94	0.19	35,35,35,35	0
85	MG	AR	3965	1/1	0.94	0.15	50,50,50,50	0
84	OHX	A	1932	7/7	0.94	0.15	141,142,142,143	0
84	OHX	AR	3544	7/7	0.94	0.20	109,109,110,110	0
85	MG	AR	3970	1/1	0.94	0.11	50,50,50,50	0
84	OHX	AR	3715	7/7	0.94	0.14	118,118,119,119	0
84	OHX	A	1945	7/7	0.94	0.14	143,144,144,145	0
84	OHX	AR	3545	7/7	0.94	0.24	108,108,108,108	0
85	MG	AR	4201	1/1	0.94	0.08	35,35,35,35	0
85	MG	AR	3975	1/1	0.94	0.08	31,31,31,31	0
85	MG	v	302	1/1	0.94	0.16	36,36,36,36	0
84	OHX	1	3582	7/7	0.94	0.17	121,121,121,121	0
85	MG	1	3946	1/1	0.94	0.13	34,34,34,34	0
85	MG	w	202	1/1	0.94	0.13	31,31,31,31	0
85	MG	AG	202	1/1	0.94	0.08	43,43,43,43	0
85	MG	AR	4208	1/1	0.94	0.13	57,57,57,57	0
84	OHX	6	1976	7/7	0.94	0.13	146,147,147,148	0
85	MG	AR	3746	1/1	0.94	0.15	58,58,58,58	0
84	OHX	1	3603	7/7	0.94	0.20	123,123,124,124	0
85	MG	AR	3988	1/1	0.94	0.32	50,50,50,50	0
85	MG	1	3950	1/1	0.94	0.12	38,38,38,38	0
84	OHX	A	1956	7/7	0.94	0.15	133,133,134,134	0
84	OHX	1	3583	7/7	0.94	0.16	131,132,132,132	0
85	MG	AR	3752	1/1	0.94	0.17	37,37,37,37	0
85	MG	A	2147	1/1	0.94	0.08	79,79,79,79	0
84	OHX	1	3625	7/7	0.94	0.14	135,135,135,135	0
85	MG	lR	201	1/1	0.94	0.22	26,26,26,26	0
85	MG	AR	4221	1/1	0.94	0.10	35,35,35,35	0
85	MG	1	3810	1/1	0.94	0.13	32,32,32,32	0
84	OHX	AR	3555	7/7	0.94	0.17	115,115,115,115	0
84	OHX	A	1962	7/7	0.94	0.17	132,133,133,134	0
84	OHX	AR	3556	7/7	0.94	0.22	109,109,109,109	0
84	OHX	AR	3557	7/7	0.94	0.16	123,123,124,124	0
84	OHX	A	1965	7/7	0.94	0.18	134,135,135,136	0
84	OHX	1	3646	7/7	0.94	0.17	117,118,118,118	0
85	MG	AR	4231	1/1	0.94	0.18	32,32,32,32	0
85	MG	AR	4233	1/1	0.94	0.18	31,31,31,31	0
84	OHX	h	401	7/7	0.94	0.12	175,176,177,177	0
85	MG	AR	4235	1/1	0.94	0.24	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	A	1967	7/7	0.94	0.17	119,119,120,120	0
85	MG	AR	4238	1/1	0.94	0.07	36,36,36,36	0
85	MG	1	3969	1/1	0.94	0.24	41,41,41,41	0
85	MG	AR	4009	1/1	0.94	0.14	37,37,37,37	0
84	OHX	1	3647	7/7	0.94	0.19	118,118,118,118	0
85	MG	AR	4245	1/1	0.94	0.22	26,26,26,26	0
84	OHX	AR	3616	7/7	0.94	0.22	109,110,110,110	0
84	OHX	AR	3672	7/7	0.94	0.23	109,110,110,110	0
84	OHX	A	1974	7/7	0.94	0.13	167,167,168,168	0
85	MG	1	4123	1/1	0.94	0.13	51,51,51,51	0
84	OHX	A	1975	7/7	0.94	0.12	156,158,158,158	0
85	MG	1	4127	1/1	0.94	0.20	45,45,45,45	0
85	MG	d3	202	1/1	0.94	0.30	47,47,47,47	0
85	MG	1	4128	1/1	0.94	0.13	51,51,51,51	0
85	MG	1	4129	1/1	0.94	0.27	33,33,33,33	0
84	OHX	1	3544	7/7	0.94	0.21	116,117,117,117	0
86	HN8	1	4223	22/22	0.94	0.12	32,32,32,32	0
85	MG	1	3832	1/1	0.94	0.19	26,26,26,26	0
85	MG	AR	3793	1/1	0.94	0.17	29,29,29,29	0
85	MG	1	4132	1/1	0.94	0.11	86,86,86,86	0
85	MG	1	4134	1/1	0.94	0.11	63,63,63,63	0
85	MG	1	4136	1/1	0.94	0.10	40,40,40,40	0
84	OHX	sR	401	7/7	0.94	0.13	161,161,162,162	0
85	MG	1	3981	1/1	0.94	0.17	50,50,50,50	0
84	OHX	4	208	7/7	0.95	0.23	106,106,106,106	0
84	OHX	1	3570	7/7	0.95	0.12	144,144,145,145	0
85	MG	AR	3781	1/1	0.95	0.15	23,23,23,23	0
85	MG	AR	4256	1/1	0.95	0.32	49,49,49,49	0
84	OHX	1	3549	7/7	0.95	0.17	120,120,120,120	0
85	MG	AR	4258	1/1	0.95	0.23	34,34,34,34	0
84	OHX	AR	3614	7/7	0.95	0.21	114,114,114,114	0
85	MG	AR	4260	1/1	0.95	0.34	6,6,6,6	0
85	MG	1	3794	1/1	0.95	0.20	34,34,34,34	0
84	OHX	1	3527	7/7	0.95	0.13	135,135,136,136	0
85	MG	1	3796	1/1	0.95	0.26	18,18,18,18	0
85	MG	AR	3789	1/1	0.95	0.10	36,36,36,36	0
85	MG	1	4118	1/1	0.95	0.09	43,43,43,43	0
85	MG	AR	3791	1/1	0.95	0.15	34,34,34,34	0
84	OHX	A	2024	7/7	0.95	0.13	151,152,153,153	0
85	MG	1	4120	1/1	0.95	0.42	27,27,27,27	0
85	MG	AR	3794	1/1	0.95	0.13	34,34,34,34	0
84	OHX	1	3528	7/7	0.95	0.18	119,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3799	1/1	0.95	0.09	37,37,37,37	0
84	OHX	1	3462	7/7	0.95	0.18	119,120,120,120	0
84	OHX	1	3576	7/7	0.95	0.14	131,131,132,132	0
85	MG	1	4125	1/1	0.95	0.12	23,23,23,23	0
85	MG	AR	4036	1/1	0.95	0.09	41,41,41,41	0
85	MG	1	4126	1/1	0.95	0.41	33,33,33,33	0
84	OHX	1	3630	7/7	0.95	0.22	113,113,114,114	0
85	MG	AR	3805	1/1	0.95	0.19	36,36,36,36	0
84	OHX	6	1981	7/7	0.95	0.15	139,140,140,140	0
85	MG	AR	3808	1/1	0.95	0.09	28,28,28,28	0
85	MG	1	3961	1/1	0.95	0.10	40,40,40,40	0
84	OHX	1	3473	7/7	0.95	0.13	114,115,115,115	0
84	OHX	6	1983	7/7	0.95	0.15	128,129,129,129	0
84	OHX	AR	3697	7/7	0.95	0.18	114,115,115,115	0
85	MG	1	4133	1/1	0.95	0.07	51,51,51,51	0
85	MG	AR	4049	1/1	0.95	0.14	50,50,50,50	0
84	OHX	AR	3551	7/7	0.95	0.14	129,129,130,130	0
85	MG	1	4135	1/1	0.95	0.21	51,51,51,51	0
84	OHX	k	401	7/7	0.95	0.16	118,118,118,118	0
85	MG	AR	4055	1/1	0.95	0.12	40,40,40,40	0
85	MG	1	3809	1/1	0.95	0.29	39,39,39,39	0
84	OHX	1	3578	7/7	0.95	0.20	107,107,107,107	0
85	MG	AR	3823	1/1	0.95	0.18	39,39,39,39	0
85	MG	1	4139	1/1	0.95	0.10	31,31,31,31	0
85	MG	AR	3825	1/1	0.95	0.28	33,33,33,33	0
84	OHX	AR	3554	7/7	0.95	0.18	112,112,112,112	0
85	MG	CG	303	1/1	0.95	0.06	62,62,62,62	0
84	OHX	1	3579	7/7	0.95	0.17	119,120,120,120	0
85	MG	1	4144	1/1	0.95	0.07	53,53,53,53	0
85	MG	1	3974	1/1	0.95	0.18	28,28,28,28	0
85	MG	AR	4065	1/1	0.95	0.09	31,31,31,31	0
85	MG	1	4146	1/1	0.95	0.10	48,48,48,48	0
85	MG	1	4147	1/1	0.95	0.14	48,48,48,48	0
84	OHX	A	1933	7/7	0.95	0.14	122,122,122,123	0
84	OHX	AR	3630	7/7	0.95	0.15	124,125,125,125	0
84	OHX	v	301	7/7	0.95	0.19	113,113,114,114	0
84	OHX	A	1943	7/7	0.95	0.16	133,133,134,134	0
85	MG	6	2100	1/1	0.95	0.25	36,36,36,36	0
84	OHX	1	3607	7/7	0.95	0.14	122,122,122,122	0
85	MG	AR	3839	1/1	0.95	0.21	33,33,33,33	0
84	OHX	1	3715	7/7	0.95	0.10	166,166,167,167	0
84	OHX	1	3580	7/7	0.95	0.16	115,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3821	1/1	0.95	0.32	66,66,66,66	0
85	MG	1	4157	1/1	0.95	0.28	60,60,60,60	0
84	OHX	A	1951	7/7	0.95	0.11	145,145,146,146	0
84	OHX	M	201	7/7	0.95	0.17	137,137,138,138	0
85	MG	1	3824	1/1	0.95	0.22	25,25,25,25	0
85	MG	1	3825	1/1	0.95	0.36	31,31,31,31	0
85	MG	1	3827	1/1	0.95	0.29	32,32,32,32	0
85	MG	DH	203	1/1	0.95	0.11	31,31,31,31	0
84	OHX	1	3508	7/7	0.95	0.16	113,114,114,114	0
85	MG	1	3991	1/1	0.95	0.06	66,66,66,66	0
84	OHX	6	1902	7/7	0.95	0.37	136,136,137,137	0
84	OHX	T	201	7/7	0.95	0.16	145,146,146,147	0
84	OHX	A	1954	7/7	0.95	0.14	135,136,136,136	0
85	MG	AR	4093	1/1	0.95	0.12	46,46,46,46	0
84	OHX	6	1905	7/7	0.95	0.29	132,133,133,134	0
84	OHX	A	1957	7/7	0.95	0.18	133,134,134,134	0
84	OHX	6	1907	7/7	0.95	0.30	135,136,136,137	0
84	OHX	1	3555	7/7	0.95	0.17	111,111,112,112	0
85	MG	AR	3861	1/1	0.95	0.14	30,30,30,30	0
85	MG	1	3838	1/1	0.95	0.25	33,33,33,33	0
84	OHX	6	1921	7/7	0.95	0.14	141,141,142,143	0
84	OHX	AR	3566	7/7	0.95	0.16	115,115,115,116	0
85	MG	1	3843	1/1	0.95	0.15	24,24,24,24	0
85	MG	AR	3866	1/1	0.95	0.19	34,34,34,34	0
85	MG	AR	4105	1/1	0.95	0.08	42,42,42,42	0
85	MG	1	4179	1/1	0.95	0.21	38,38,38,38	0
85	MG	1	3844	1/1	0.95	0.19	28,28,28,28	0
85	MG	AR	3870	1/1	0.95	0.28	33,33,33,33	0
85	MG	AR	3873	1/1	0.95	0.25	31,31,31,31	0
85	MG	1	3845	1/1	0.95	0.24	18,18,18,18	0
85	MG	6	2128	1/1	0.95	0.25	47,47,47,47	0
85	MG	AR	4112	1/1	0.95	0.10	54,54,54,54	0
85	MG	AR	3876	1/1	0.95	0.22	27,27,27,27	0
84	OHX	AR	3642	7/7	0.95	0.16	122,122,122,122	0
84	OHX	6	1929	7/7	0.95	0.11	157,158,159,159	0
84	OHX	1	3510	7/7	0.95	0.19	111,111,111,111	0
84	OHX	1	3557	7/7	0.95	0.18	117,118,118,118	0
85	MG	A	2067	1/1	0.95	0.44	64,64,64,64	0
84	OHX	1	3487	7/7	0.95	0.16	115,115,116,116	0
85	MG	AR	4120	1/1	0.95	0.09	31,31,31,31	0
85	MG	AR	4121	1/1	0.95	0.09	27,27,27,27	0
84	OHX	A	1968	7/7	0.95	0.16	125,125,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	6	1943	7/7	0.95	0.13	124,124,125,125	0
85	MG	1	3856	1/1	0.95	0.28	24,24,24,24	0
85	MG	1	4019	1/1	0.95	0.14	42,42,42,42	0
84	OHX	AR	3572	7/7	0.95	0.19	118,119,119,119	0
85	MG	AR	3892	1/1	0.95	0.17	31,31,31,31	0
85	MG	1	3859	1/1	0.95	0.24	28,28,28,28	0
85	MG	1	3730	1/1	0.95	0.22	36,36,36,36	0
85	MG	1	4025	1/1	0.95	0.19	32,32,32,32	0
84	OHX	6	1944	7/7	0.95	0.12	143,143,144,144	0
84	OHX	A	1973	7/7	0.95	0.12	167,168,169,169	0
84	OHX	AR	3574	7/7	0.95	0.19	112,113,113,113	0
85	MG	1	4208	1/1	0.95	0.22	37,37,37,37	0
85	MG	AR	4136	1/1	0.95	0.13	36,36,36,36	0
84	OHX	6	2003	7/7	0.95	0.16	126,126,127,127	0
84	OHX	A	1976	7/7	0.95	0.17	123,124,124,124	0
84	OHX	1	3480	7/7	0.95	0.14	119,119,119,120	0
85	MG	1	3870	1/1	0.95	0.30	47,47,47,47	0
84	OHX	6	1947	7/7	0.95	0.14	121,122,122,122	0
84	OHX	6	1949	7/7	0.95	0.12	135,136,136,136	0
85	MG	AR	4143	1/1	0.95	0.10	34,34,34,34	0
84	OHX	AR	3430	7/7	0.95	0.16	107,107,107,107	0
85	MG	AR	3908	1/1	0.95	0.32	25,25,25,25	0
84	OHX	AR	3460	7/7	0.95	0.15	112,112,112,112	0
85	MG	1	4220	1/1	0.95	0.32	35,35,35,35	0
85	MG	1	4221	1/1	0.95	0.41	35,35,35,35	0
84	OHX	AR	3467	7/7	0.95	0.15	108,109,109,109	0
85	MG	A	2098	1/1	0.95	0.29	65,65,65,65	0
85	MG	AR	4150	1/1	0.95	0.10	44,44,44,44	0
84	OHX	1	3497	7/7	0.95	0.11	125,125,126,126	0
85	MG	AR	3916	1/1	0.95	0.29	19,19,19,19	0
85	MG	1	3877	1/1	0.95	0.36	36,36,36,36	0
85	MG	6	2163	1/1	0.95	0.09	48,48,48,48	0
85	MG	AR	3921	1/1	0.95	0.21	38,38,38,38	0
85	MG	3	214	1/1	0.95	0.16	34,34,34,34	0
84	OHX	A	1984	7/7	0.95	0.14	130,130,131,131	0
85	MG	6	2166	1/1	0.95	0.33	53,53,53,53	0
84	OHX	6	1953	7/7	0.95	0.14	132,133,133,134	0
85	MG	AR	3928	1/1	0.95	0.26	39,39,39,39	0
85	MG	1	3749	1/1	0.95	0.18	24,24,24,24	0
84	OHX	A	1986	7/7	0.95	0.13	168,169,170,170	0
84	OHX	A	1987	7/7	0.95	0.14	128,128,129,129	0
84	OHX	A	1988	7/7	0.95	0.13	139,140,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	6	2172	1/1	0.95	0.08	38,38,38,38	0
85	MG	1	3890	1/1	0.95	0.35	34,34,34,34	0
84	OHX	6	1954	7/7	0.95	0.10	178,178,178,178	0
84	OHX	1	3562	7/7	0.95	0.14	121,121,121,121	0
84	OHX	6	1956	7/7	0.95	0.12	174,174,175,175	0
84	OHX	A	1992	7/7	0.95	0.15	140,141,142,142	0
84	OHX	AR	3499	7/7	0.95	0.12	125,126,126,126	0
84	OHX	1	3697	7/7	0.95	0.13	119,119,120,120	0
84	OHX	AR	3502	7/7	0.95	0.18	113,114,114,114	0
85	MG	1	3901	1/1	0.95	0.32	39,39,39,39	0
85	MG	AR	3947	1/1	0.95	0.23	44,44,44,44	0
85	MG	A	2125	1/1	0.95	0.31	56,56,56,56	0
84	OHX	AR	3503	7/7	0.95	0.15	120,120,121,121	0
84	OHX	3	204	7/7	0.95	0.12	124,125,125,125	0
85	MG	1	4066	1/1	0.95	0.18	20,20,20,20	0
84	OHX	AR	3511	7/7	0.95	0.17	108,108,108,108	0
84	OHX	1	3498	7/7	0.95	0.16	115,116,116,116	0
84	OHX	AR	3515	7/7	0.95	0.18	113,113,114,114	0
85	MG	AR	3956	1/1	0.95	0.11	29,29,29,29	0
85	MG	6	2190	1/1	0.95	0.28	66,66,66,66	0
84	OHX	6	1963	7/7	0.95	0.17	125,125,126,126	0
85	MG	AR	3959	1/1	0.95	0.10	32,32,32,32	0
85	MG	AR	4197	1/1	0.95	0.10	35,35,35,35	0
85	MG	1	3912	1/1	0.95	0.30	22,22,22,22	0
85	MG	AR	3961	1/1	0.95	0.24	43,43,43,43	0
85	MG	1	3769	1/1	0.95	0.06	45,45,45,45	0
85	MG	1	4075	1/1	0.95	0.14	41,41,41,41	0
85	MG	1	4076	1/1	0.95	0.15	64,64,64,64	0
84	OHX	AS	206	7/7	0.95	0.14	124,124,125,125	0
84	OHX	AR	3519	7/7	0.95	0.20	108,109,109,109	0
85	MG	AR	3967	1/1	0.95	0.25	42,42,42,42	0
84	OHX	1	3564	7/7	0.95	0.14	126,126,127,127	0
84	OHX	1	3521	7/7	0.95	0.19	116,117,117,117	0
85	MG	j	301	1/1	0.95	0.13	29,29,29,29	0
85	MG	AB	203	1/1	0.95	0.29	32,32,32,32	0
84	OHX	AR	3523	7/7	0.95	0.20	107,108,108,108	0
85	MG	AR	4211	1/1	0.95	0.13	73,73,73,73	0
85	MG	AB	205	1/1	0.95	0.15	40,40,40,40	0
85	MG	1	3922	1/1	0.95	0.30	45,45,45,45	0
84	OHX	AT	205	7/7	0.95	0.19	108,108,108,108	0
84	OHX	AT	206	7/7	0.95	0.15	123,124,124,124	0
85	MG	AP	503	1/1	0.95	0.13	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	A	2010	7/7	0.95	0.13	157,158,158,159	0
85	MG	o	301	1/1	0.95	0.09	34,34,34,34	0
84	OHX	1	3524	7/7	0.95	0.18	116,117,117,117	0
84	OHX	1	3500	7/7	0.95	0.17	119,120,120,120	0
85	MG	1	3780	1/1	0.95	0.15	17,17,17,17	0
84	OHX	1	3455	7/7	0.95	0.14	127,127,127,128	0
85	MG	t	203	1/1	0.95	0.14	29,29,29,29	0
85	MG	1	3782	1/1	0.95	0.27	58,58,58,58	0
85	MG	1	4095	1/1	0.95	0.06	61,61,61,61	0
85	MG	AR	4228	1/1	0.95	0.21	27,27,27,27	0
85	MG	AR	3758	1/1	0.95	0.19	37,37,37,37	0
84	OHX	4	206	7/7	0.95	0.14	116,116,116,116	0
84	OHX	AR	3530	7/7	0.95	0.18	112,113,113,113	0
85	MG	s8	302	1/1	0.95	0.20	51,51,51,51	0
85	MG	AR	4232	1/1	0.95	0.18	28,28,28,28	0
85	MG	1	3934	1/1	0.95	0.32	54,54,54,54	0
84	OHX	4	207	7/7	0.95	0.17	118,119,119,119	0
85	MG	AR	3763	1/1	0.95	0.27	17,17,17,17	0
85	MG	d3	201	1/1	0.95	0.27	49,49,49,49	0
85	MG	1	4102	1/1	0.95	0.15	57,57,57,57	0
84	OHX	AR	3532	7/7	0.95	0.12	135,136,136,137	0
85	MG	1	3938	1/1	0.95	0.07	34,34,34,34	0
85	MG	AR	4004	1/1	0.95	0.08	32,32,32,32	0
85	MG	AR	4243	1/1	0.95	0.21	30,30,30,30	0
86	HN8	AR	4263	22/22	0.95	0.13	27,27,27,27	22
84	OHX	AR	3533	7/7	0.95	0.18	111,111,111,111	0
85	MG	1	3940	1/1	0.95	0.22	43,43,43,43	0
85	MG	1	3789	1/1	0.95	0.19	42,42,42,42	0
85	MG	AR	3773	1/1	0.95	0.26	41,41,41,41	0
85	MG	1	4108	1/1	0.95	0.07	42,42,42,42	0
85	MG	AR	3777	1/1	0.95	0.07	37,37,37,37	0
85	MG	AR	3778	1/1	0.95	0.24	42,42,42,42	0
85	MG	1	3817	1/1	0.96	0.16	23,23,23,23	0
84	OHX	A	1950	7/7	0.96	0.14	127,128,128,128	0
84	OHX	1	3533	7/7	0.96	0.11	149,149,150,150	0
84	OHX	AR	3547	7/7	0.96	0.18	116,116,116,117	0
84	OHX	6	1945	7/7	0.96	0.14	126,127,127,128	0
85	MG	AR	4081	1/1	0.96	0.15	55,55,55,55	0
84	OHX	AR	3629	7/7	0.96	0.11	141,141,141,142	0
84	OHX	A	1955	7/7	0.96	0.10	145,146,147,147	0
85	MG	1	4100	1/1	0.96	0.09	53,53,53,53	0
84	OHX	1	3451	7/7	0.96	0.16	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3957	1/1	0.96	0.16	37,37,37,37	0
84	OHX	AR	3550	7/7	0.96	0.19	107,107,107,107	0
84	OHX	1	3505	7/7	0.96	0.18	116,116,117,117	0
85	MG	CE	403	1/1	0.96	0.28	22,22,22,22	0
84	OHX	1	3506	7/7	0.96	0.15	109,109,110,110	0
84	OHX	1	3538	7/7	0.96	0.13	125,125,125,126	0
84	OHX	6	1952	7/7	0.96	0.10	148,148,148,148	0
84	OHX	4	204	7/7	0.96	0.18	108,108,108,108	0
85	MG	1	3833	1/1	0.96	0.32	24,24,24,24	0
84	OHX	4	205	7/7	0.96	0.17	106,106,106,106	0
85	MG	AR	4096	1/1	0.96	0.21	54,54,54,54	0
85	MG	CJ	301	1/1	0.96	0.27	78,78,78,78	0
85	MG	CK	202	1/1	0.96	0.06	44,44,44,44	0
85	MG	j	302	1/1	0.96	0.07	35,35,35,35	0
84	OHX	1	3431	7/7	0.96	0.25	114,114,114,114	0
85	MG	k	403	1/1	0.96	0.12	30,30,30,30	0
85	MG	k	404	1/1	0.96	0.34	32,32,32,32	0
85	MG	1	3970	1/1	0.96	0.18	31,31,31,31	0
85	MG	CP	503	1/1	0.96	0.15	38,38,38,38	0
84	OHX	1	3458	7/7	0.96	0.14	116,116,116,117	0
84	OHX	6	1957	7/7	0.96	0.11	129,130,130,131	0
84	OHX	AR	3401	7/7	0.96	0.41	121,121,121,122	0
85	MG	AR	3907	1/1	0.96	0.29	25,25,25,25	0
85	MG	1	4117	1/1	0.96	0.09	41,41,41,41	0
85	MG	1	3840	1/1	0.96	0.13	78,78,78,78	0
85	MG	AR	3910	1/1	0.96	0.15	23,23,23,23	0
85	MG	CR	204	1/1	0.96	0.08	46,46,46,46	0
85	MG	CR	205	1/1	0.96	0.13	31,31,31,31	0
85	MG	AR	3911	1/1	0.96	0.24	40,40,40,40	0
85	MG	CX	203	1/1	0.96	0.23	19,19,19,19	0
84	OHX	AR	3405	7/7	0.96	0.35	119,119,120,120	0
84	OHX	AR	3427	7/7	0.96	0.24	110,110,111,111	0
84	OHX	6	1958	7/7	0.96	0.14	126,127,127,127	0
84	OHX	A	1972	7/7	0.96	0.10	148,148,148,148	0
84	OHX	AR	3441	7/7	0.96	0.13	116,117,117,117	0
84	OHX	AR	3456	7/7	0.96	0.15	117,117,117,117	0
85	MG	AR	3918	1/1	0.96	0.25	27,27,27,27	0
85	MG	DH	202	1/1	0.96	0.20	40,40,40,40	0
84	OHX	1	3460	7/7	0.96	0.13	118,118,118,119	0
85	MG	AR	3920	1/1	0.96	0.26	27,27,27,27	0
84	OHX	AR	3463	7/7	0.96	0.14	110,110,111,111	0
85	MG	1	3850	1/1	0.96	0.21	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	DQ	203	1/1	0.96	0.13	45,45,45,45	0
84	OHX	1	3542	7/7	0.96	0.16	119,119,120,120	0
84	OHX	AR	3471	7/7	0.96	0.16	109,109,109,109	0
85	MG	AR	3925	1/1	0.96	0.23	34,34,34,34	0
85	MG	AB	207	1/1	0.96	0.09	34,34,34,34	0
85	MG	AF	201	1/1	0.96	0.27	41,41,41,41	0
84	OHX	AR	3731	7/7	0.96	0.17	117,117,117,117	0
85	MG	1	3854	1/1	0.96	0.35	34,34,34,34	0
84	OHX	1	3511	7/7	0.96	0.15	109,109,109,109	0
85	MG	AK	103	1/1	0.96	0.20	36,36,36,36	0
84	OHX	AR	3473	7/7	0.96	0.11	111,111,112,112	0
85	MG	1	3992	1/1	0.96	0.07	40,40,40,40	0
84	OHX	1	3573	7/7	0.96	0.14	131,131,132,132	0
85	MG	1	3858	1/1	0.96	0.19	25,25,25,25	0
85	MG	6	2057	1/1	0.96	0.31	51,51,51,51	0
84	OHX	AR	3476	7/7	0.96	0.15	109,109,109,109	0
85	MG	AR	3751	1/1	0.96	0.16	36,36,36,36	0
84	OHX	AR	3477	7/7	0.96	0.14	112,112,113,113	0
84	OHX	AR	3479	7/7	0.96	0.15	110,110,110,110	0
85	MG	1	3862	1/1	0.96	0.24	52,52,52,52	0
85	MG	AR	3755	1/1	0.96	0.21	56,56,56,56	0
84	OHX	AR	3480	7/7	0.96	0.15	113,114,114,114	0
85	MG	1	4142	1/1	0.96	0.17	38,38,38,38	0
84	OHX	AR	3483	7/7	0.96	0.15	111,111,111,111	0
84	OHX	AR	3484	7/7	0.96	0.14	114,114,114,114	0
85	MG	AR	3952	1/1	0.96	0.23	28,28,28,28	0
85	MG	1	3866	1/1	0.96	0.09	34,34,34,34	0
84	OHX	AR	3490	7/7	0.96	0.16	112,112,112,113	0
84	OHX	AR	3492	7/7	0.96	0.13	116,116,117,117	0
85	MG	AR	3764	1/1	0.96	0.12	33,33,33,33	0
84	OHX	1	3513	7/7	0.96	0.17	113,113,114,114	0
85	MG	1	4007	1/1	0.96	0.16	29,29,29,29	0
85	MG	1	4008	1/1	0.96	0.10	37,37,37,37	0
84	OHX	6	1965	7/7	0.96	0.16	116,117,117,117	0
85	MG	1	4153	1/1	0.96	0.07	39,39,39,39	0
84	OHX	1	3438	7/7	0.96	0.21	117,117,117,117	0
85	MG	1	4011	1/1	0.96	0.14	44,44,44,44	0
84	OHX	AR	3496	7/7	0.96	0.17	112,113,113,113	0
84	OHX	AS	207	7/7	0.96	0.13	122,122,122,123	0
85	MG	6	2078	1/1	0.96	0.27	42,42,42,42	0
84	OHX	6	1967	7/7	0.96	0.15	126,127,127,127	0
84	OHX	1	3515	7/7	0.96	0.18	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	4164	1/1	0.96	0.09	41,41,41,41	0
84	OHX	1	3466	7/7	0.96	0.14	114,115,115,115	0
85	MG	AR	3972	1/1	0.96	0.20	39,39,39,39	0
84	OHX	1	3548	7/7	0.96	0.13	134,134,134,134	0
85	MG	1	4018	1/1	0.96	0.15	38,38,38,38	0
85	MG	1	3768	1/1	0.96	0.18	36,36,36,36	0
84	OHX	AT	203	7/7	0.96	0.14	117,117,117,117	0
85	MG	AR	3787	1/1	0.96	0.31	31,31,31,31	0
85	MG	1	3881	1/1	0.96	0.23	31,31,31,31	0
85	MG	AR	4176	1/1	0.96	0.05	33,33,33,33	0
85	MG	AR	4177	1/1	0.96	0.22	32,32,32,32	0
85	MG	1	3882	1/1	0.96	0.29	32,32,32,32	0
85	MG	6	2089	1/1	0.96	0.28	44,44,44,44	0
85	MG	1	4024	1/1	0.96	0.08	61,61,61,61	0
85	MG	AR	3982	1/1	0.96	0.15	53,53,53,53	0
85	MG	AR	3983	1/1	0.96	0.05	33,33,33,33	0
85	MG	1	3883	1/1	0.96	0.24	22,22,22,22	0
85	MG	AR	3985	1/1	0.96	0.25	35,35,35,35	0
84	OHX	AT	204	7/7	0.96	0.16	105,105,105,106	0
85	MG	AR	3987	1/1	0.96	0.20	31,31,31,31	0
85	MG	1	3885	1/1	0.96	0.24	20,20,20,20	0
85	MG	AR	3989	1/1	0.96	0.20	44,44,44,44	0
84	OHX	1	3518	7/7	0.96	0.19	109,110,110,110	0
84	OHX	1	3490	7/7	0.96	0.14	113,113,113,113	0
84	OHX	1	3492	7/7	0.96	0.14	117,118,118,118	0
85	MG	AR	3800	1/1	0.96	0.28	33,33,33,33	0
84	OHX	AR	3513	7/7	0.96	0.09	150,151,151,151	0
84	OHX	AR	3514	7/7	0.96	0.15	112,112,112,113	0
85	MG	1	4177	1/1	0.96	0.22	27,27,27,27	0
84	OHX	1	3493	7/7	0.96	0.15	115,116,116,116	0
84	OHX	AR	3516	7/7	0.96	0.15	112,112,112,112	0
84	OHX	1	3522	7/7	0.96	0.16	120,121,121,121	0
84	OHX	AR	3518	7/7	0.96	0.12	118,119,119,119	0
84	OHX	1	3469	7/7	0.96	0.14	117,117,118,118	0
85	MG	1	4185	1/1	0.96	0.24	27,27,27,27	0
84	OHX	1	3585	7/7	0.96	0.16	115,115,116,116	0
84	OHX	1	3618	7/7	0.96	0.08	190,190,190,190	0
85	MG	1	4188	1/1	0.96	0.20	28,28,28,28	0
85	MG	AR	4007	1/1	0.96	0.11	29,29,29,29	0
85	MG	1	4189	1/1	0.96	0.24	27,27,27,27	0
85	MG	AR	4212	1/1	0.96	0.07	31,31,31,31	0
85	MG	1	3783	1/1	0.96	0.21	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	AR	4010	1/1	0.96	0.11	30,30,30,30	0
85	MG	1	4191	1/1	0.96	0.23	29,29,29,29	0
85	MG	AR	3818	1/1	0.96	0.25	37,37,37,37	0
85	MG	AR	3819	1/1	0.96	0.24	37,37,37,37	0
85	MG	AR	3820	1/1	0.96	0.21	43,43,43,43	0
85	MG	A	2129	1/1	0.96	0.16	57,57,57,57	0
85	MG	1	3905	1/1	0.96	0.43	38,38,38,38	0
84	OHX	AR	3522	7/7	0.96	0.15	114,114,115,115	0
84	OHX	1	3471	7/7	0.96	0.16	112,112,113,113	0
84	OHX	1	3587	7/7	0.96	0.13	133,133,133,134	0
85	MG	1	4047	1/1	0.96	0.11	57,57,57,57	0
85	MG	AR	3826	1/1	0.96	0.17	23,23,23,23	0
85	MG	1	4199	1/1	0.96	0.30	24,24,24,24	0
85	MG	1	4048	1/1	0.96	0.32	33,33,33,33	0
84	OHX	1	3499	7/7	0.96	0.17	111,111,111,111	0
85	MG	1	3911	1/1	0.96	0.30	21,21,21,21	0
85	MG	1	4204	1/1	0.96	0.26	34,34,34,34	0
84	OHX	6	1909	7/7	0.96	0.21	137,138,138,139	0
84	OHX	6	1914	7/7	0.96	0.20	133,133,134,134	0
84	OHX	AR	3609	7/7	0.96	0.21	107,107,107,107	0
85	MG	6	2126	1/1	0.96	0.15	53,53,53,53	0
85	MG	1	3916	1/1	0.96	0.12	26,26,26,26	0
85	MG	AR	4033	1/1	0.96	0.07	40,40,40,40	0
84	OHX	1	3446	7/7	0.96	0.14	116,116,116,116	0
84	OHX	1	3590	7/7	0.96	0.13	137,138,138,138	0
84	OHX	6	1925	7/7	0.96	0.15	122,122,122,123	0
85	MG	AR	4242	1/1	0.96	0.34	35,35,35,35	0
85	MG	6	2131	1/1	0.96	0.16	44,44,44,44	0
85	MG	AR	4038	1/1	0.96	0.18	35,35,35,35	0
84	OHX	6	1927	7/7	0.96	0.14	124,124,125,125	0
85	MG	1	4214	1/1	0.96	0.29	43,43,43,43	0
85	MG	AR	4247	1/1	0.96	0.24	22,22,22,22	0
84	OHX	AR	3534	7/7	0.96	0.17	109,109,109,109	0
85	MG	AR	4249	1/1	0.96	0.27	24,24,24,24	0
84	OHX	A	1903	7/7	0.96	0.32	149,149,150,150	0
84	OHX	A	1909	7/7	0.96	0.12	151,151,152,153	0
85	MG	AR	3847	1/1	0.96	0.09	38,38,38,38	0
85	MG	AR	3848	1/1	0.96	0.19	31,31,31,31	0
85	MG	1	4068	1/1	0.96	0.19	42,42,42,42	0
84	OHX	A	1913	7/7	0.96	0.19	126,126,127,127	0
84	OHX	1	3476	7/7	0.96	0.17	111,111,111,112	0
84	OHX	6	1931	7/7	0.96	0.14	115,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	A	1926	7/7	0.96	0.12	127,127,127,128	0
84	OHX	1	3530	7/7	0.96	0.13	138,138,139,139	0
85	MG	3	213	1/1	0.96	0.40	48,48,48,48	0
84	OHX	A	1928	7/7	0.96	0.14	125,126,126,126	0
84	OHX	A	1930	7/7	0.96	0.15	122,122,123,123	0
84	OHX	6	1934	7/7	0.96	0.11	139,139,140,140	0
84	OHX	AR	3540	7/7	0.96	0.19	108,108,108,108	0
84	OHX	A	1934	7/7	0.96	0.11	132,132,133,133	0
85	MG	6	2151	1/1	0.96	0.09	60,60,60,60	0
84	OHX	6	1938	7/7	0.96	0.11	130,131,131,131	0
84	OHX	A	1936	7/7	0.96	0.14	126,127,127,128	0
85	MG	d4	201	1/1	0.96	0.14	53,53,53,53	0
84	OHX	AR	3542	7/7	0.96	0.10	152,152,152,153	0
84	OHX	A	1942	7/7	0.96	0.12	133,133,134,134	0
84	OHX	3	203	7/7	0.96	0.14	118,118,118,119	0
84	OHX	1	3560	7/7	0.96	0.15	111,112,112,112	0
85	MG	4	219	1/1	0.96	0.35	42,42,42,42	0
85	MG	AR	4070	1/1	0.96	0.08	50,50,50,50	0
85	MG	AS	227	1/1	0.96	0.07	45,45,45,45	0
84	OHX	1	3502	7/7	0.96	0.18	114,114,114,114	0
85	MG	AR	3871	1/1	0.96	0.25	28,28,28,28	0
84	OHX	AR	3625	7/7	0.96	0.12	134,134,134,134	0
84	OHX	A	1949	7/7	0.96	0.11	148,149,149,149	0
85	MG	4	223	1/1	0.96	0.28	27,27,27,27	0
84	OHX	AR	3415	7/7	0.97	0.31	109,109,110,110	0
84	OHX	AR	3416	7/7	0.97	0.22	114,114,115,115	0
84	OHX	AR	3423	7/7	0.97	0.24	110,111,111,111	0
85	MG	1	3967	1/1	0.97	0.08	38,38,38,38	0
85	MG	1	3968	1/1	0.97	0.14	29,29,29,29	0
84	OHX	1	3486	7/7	0.97	0.12	116,117,117,117	0
85	MG	x	209	1/1	0.97	0.29	39,39,39,39	0
85	MG	AR	3927	1/1	0.97	0.23	35,35,35,35	0
85	MG	z	202	1/1	0.97	0.07	59,59,59,59	0
85	MG	AR	3929	1/1	0.97	0.24	25,25,25,25	0
85	MG	AR	4115	1/1	0.97	0.11	46,46,46,46	0
84	OHX	6	1939	7/7	0.97	0.11	131,132,132,133	0
84	OHX	AR	3432	7/7	0.97	0.20	117,117,117,118	0
84	OHX	AR	3433	7/7	0.97	0.17	110,110,110,111	0
84	OHX	CE	401	7/7	0.97	0.12	114,114,115,115	0
84	OHX	AR	3435	7/7	0.97	0.17	112,113,113,113	0
85	MG	1	3826	1/1	0.97	0.21	33,33,33,33	0
84	OHX	AR	3436	7/7	0.97	0.18	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	CQ	203	1/1	0.97	0.07	34,34,34,34	0
85	MG	AR	3937	1/1	0.97	0.29	27,27,27,27	0
84	OHX	AR	3439	7/7	0.97	0.20	119,120,120,120	0
84	OHX	1	3443	7/7	0.97	0.17	119,120,120,120	0
84	OHX	AR	3442	7/7	0.97	0.16	112,112,112,112	0
84	OHX	AR	3444	7/7	0.97	0.13	112,112,112,112	0
84	OHX	AR	3445	7/7	0.97	0.14	107,107,107,107	0
84	OHX	AR	3447	7/7	0.97	0.17	112,112,112,112	0
84	OHX	AR	3450	7/7	0.97	0.13	127,127,127,128	0
84	OHX	AR	3453	7/7	0.97	0.10	106,106,107,107	0
84	OHX	AR	3455	7/7	0.97	0.13	111,112,112,112	0
84	OHX	A	1901	7/7	0.97	0.32	127,127,127,128	0
85	MG	AR	3768	1/1	0.97	0.09	39,39,39,39	0
85	MG	1	4143	1/1	0.97	0.13	29,29,29,29	0
84	OHX	1	3445	7/7	0.97	0.16	111,112,112,112	0
84	OHX	A	1904	7/7	0.97	0.21	133,134,134,134	0
84	OHX	A	1908	7/7	0.97	0.19	141,142,143,143	0
85	MG	AR	3775	1/1	0.97	0.13	22,22,22,22	0
84	OHX	AR	3459	7/7	0.97	0.19	114,114,115,115	0
84	OHX	A	1910	7/7	0.97	0.17	138,139,139,140	0
85	MG	DO	202	1/1	0.97	0.14	42,42,42,42	0
84	OHX	A	1911	7/7	0.97	0.18	139,140,141,141	0
84	OHX	A	1912	7/7	0.97	0.17	137,137,138,138	0
84	OHX	1	3489	7/7	0.97	0.12	113,113,114,114	0
85	MG	6	2079	1/1	0.97	0.16	45,45,45,45	0
84	OHX	1	3568	7/7	0.97	0.13	115,116,116,116	0
84	OHX	A	1916	7/7	0.97	0.14	136,137,137,138	0
85	MG	1	3999	1/1	0.97	0.12	41,41,41,41	0
84	OHX	AR	3464	7/7	0.97	0.13	106,106,106,106	0
85	MG	AR	3786	1/1	0.97	0.21	25,25,25,25	0
84	OHX	A	1921	7/7	0.97	0.14	142,143,144,144	0
85	MG	AR	3969	1/1	0.97	0.14	60,60,60,60	0
84	OHX	A	1924	7/7	0.97	0.11	132,132,133,133	0
84	OHX	AR	3466	7/7	0.97	0.12	120,120,121,121	0
84	OHX	1	3403	7/7	0.97	0.28	113,113,113,114	0
84	OHX	AR	3578	7/7	0.97	0.15	109,109,110,110	0
84	OHX	A	1929	7/7	0.97	0.12	123,123,124,124	0
84	OHX	AR	3469	7/7	0.97	0.10	121,122,122,122	0
84	OHX	A	1931	7/7	0.97	0.10	139,140,140,140	0
85	MG	1	4164	1/1	0.97	0.12	58,58,58,58	0
84	OHX	1	3529	7/7	0.97	0.13	115,115,115,116	0
84	OHX	4	201	7/7	0.97	0.29	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	6	1948	7/7	0.97	0.11	127,128,128,128	0
84	OHX	1	3491	7/7	0.97	0.12	120,120,121,121	0
85	MG	6	2097	1/1	0.97	0.38	46,46,46,46	0
84	OHX	1	3404	7/7	0.97	0.32	120,120,121,121	0
85	MG	AR	4168	1/1	0.97	0.09	65,65,65,65	0
84	OHX	A	1937	7/7	0.97	0.11	153,154,155,155	0
84	OHX	A	1940	7/7	0.97	0.11	137,138,138,139	0
85	MG	AR	3806	1/1	0.97	0.09	57,57,57,57	0
84	OHX	6	1951	7/7	0.97	0.10	134,134,135,135	0
85	MG	1	3868	1/1	0.97	0.32	29,29,29,29	0
84	OHX	AR	3478	7/7	0.97	0.12	110,110,110,111	0
85	MG	AR	3810	1/1	0.97	0.21	27,27,27,27	0
84	OHX	1	3532	7/7	0.97	0.08	159,159,159,159	0
85	MG	1	4020	1/1	0.97	0.07	34,34,34,34	0
84	OHX	A	1944	7/7	0.97	0.10	138,139,139,140	0
84	OHX	1	3452	7/7	0.97	0.12	109,109,109,109	0
84	OHX	AR	3589	7/7	0.97	0.15	109,110,110,110	0
84	OHX	AR	3481	7/7	0.97	0.14	106,106,107,107	0
84	OHX	A	1948	7/7	0.97	0.09	139,140,140,140	0
84	OHX	1	3495	7/7	0.97	0.12	114,115,115,115	0
84	OHX	1	3496	7/7	0.97	0.11	115,115,115,115	0
84	OHX	AR	3696	7/7	0.97	0.12	112,113,113,113	0
85	MG	1	3745	1/1	0.97	0.25	31,31,31,31	0
85	MG	AR	4190	1/1	0.97	0.05	30,30,30,30	0
84	OHX	AR	3486	7/7	0.97	0.14	111,111,111,111	0
84	OHX	AR	3487	7/7	0.97	0.13	107,107,107,107	0
85	MG	AR	4195	1/1	0.97	0.09	63,63,63,63	0
84	OHX	AR	3488	7/7	0.97	0.11	118,118,119,119	0
84	OHX	1	3453	7/7	0.97	0.11	120,120,120,120	0
84	OHX	1	3405	7/7	0.97	0.38	124,125,125,125	0
84	OHX	1	3456	7/7	0.97	0.14	111,111,111,111	0
85	MG	1	3886	1/1	0.97	0.23	21,21,21,21	0
84	OHX	6	1959	7/7	0.97	0.11	137,138,138,139	0
85	MG	1	4196	1/1	0.97	0.24	30,30,30,30	0
84	OHX	1	3409	7/7	0.97	0.27	116,116,117,117	0
84	OHX	1	3459	7/7	0.97	0.12	108,108,108,108	0
85	MG	1	3756	1/1	0.97	0.11	32,32,32,32	0
84	OHX	AR	3497	7/7	0.97	0.10	124,125,125,126	0
85	MG	1	4043	1/1	0.97	0.17	27,27,27,27	0
84	OHX	AR	3498	7/7	0.97	0.09	123,123,123,124	0
84	OHX	1	3414	7/7	0.97	0.24	109,109,109,109	0
84	OHX	AR	3500	7/7	0.97	0.11	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	1	3415	7/7	0.97	0.31	123,124,124,124	0
84	OHX	1	3504	7/7	0.97	0.10	127,127,127,128	0
85	MG	1	4049	1/1	0.97	0.08	32,32,32,32	0
85	MG	1	4050	1/1	0.97	0.07	31,31,31,31	0
84	OHX	1	3420	7/7	0.97	0.25	118,118,118,118	0
85	MG	1	4052	1/1	0.97	0.18	21,21,21,21	0
84	OHX	AR	3504	7/7	0.97	0.13	110,110,110,110	0
84	OHX	AR	3505	7/7	0.97	0.16	114,114,115,115	0
84	OHX	1	3428	7/7	0.97	0.24	126,126,127,127	0
84	OHX	AR	3509	7/7	0.97	0.15	106,106,106,106	0
85	MG	AR	4031	1/1	0.97	0.19	39,39,39,39	0
84	OHX	AR	3510	7/7	0.97	0.12	117,118,118,118	0
84	OHX	1	3470	7/7	0.97	0.14	115,115,115,115	0
84	OHX	1	3430	7/7	0.97	0.13	110,110,110,110	0
85	MG	1	4222	1/1	0.97	0.31	13,13,13,13	0
85	MG	AR	4226	1/1	0.97	0.21	24,24,24,24	0
85	MG	1	3910	1/1	0.97	0.24	19,19,19,19	0
84	OHX	1	3509	7/7	0.97	0.12	119,120,120,120	0
84	OHX	1	3472	7/7	0.97	0.12	110,111,111,111	0
84	OHX	1	3401	7/7	0.97	0.40	114,114,115,115	0
84	OHX	1	3512	7/7	0.97	0.19	110,110,110,110	0
85	MG	1	4067	1/1	0.97	0.08	40,40,40,40	0
84	OHX	6	1901	7/7	0.97	0.36	119,120,120,120	0
85	MG	AR	4043	1/1	0.97	0.06	37,37,37,37	0
84	OHX	1	3474	7/7	0.97	0.14	122,122,123,123	0
85	MG	AR	4236	1/1	0.97	0.27	23,23,23,23	0
85	MG	1	3918	1/1	0.97	0.07	31,31,31,31	0
84	OHX	6	1904	7/7	0.97	0.24	124,124,124,125	0
84	OHX	1	3475	7/7	0.97	0.12	117,117,118,118	0
84	OHX	1	3434	7/7	0.97	0.22	126,127,127,127	0
84	OHX	6	1908	7/7	0.97	0.24	120,120,121,121	0
85	MG	AR	3867	1/1	0.97	0.26	18,18,18,18	0
84	OHX	1	3516	7/7	0.97	0.12	116,117,117,117	0
84	OHX	6	1911	7/7	0.97	0.20	134,135,135,135	0
85	MG	AR	4054	1/1	0.97	0.09	55,55,55,55	0
84	OHX	AR	3525	7/7	0.97	0.12	119,119,120,120	0
85	MG	1	4078	1/1	0.97	0.14	24,24,24,24	0
85	MG	AR	3872	1/1	0.97	0.28	43,43,43,43	0
84	OHX	1	3477	7/7	0.97	0.15	109,109,109,109	0
84	OHX	6	1917	7/7	0.97	0.15	131,131,132,132	0
84	OHX	6	1918	7/7	0.97	0.12	116,117,117,117	0
84	OHX	AR	3529	7/7	0.97	0.17	108,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	1	3435	7/7	0.97	0.18	114,114,114,114	0
84	OHX	6	1920	7/7	0.97	0.10	133,133,134,134	0
84	OHX	1	3436	7/7	0.97	0.22	115,115,115,115	0
85	MG	1	4086	1/1	0.97	0.09	32,32,32,32	0
85	MG	AR	4066	1/1	0.97	0.11	56,56,56,56	0
84	OHX	6	1924	7/7	0.97	0.09	134,135,135,135	0
85	MG	AR	3884	1/1	0.97	0.27	22,22,22,22	0
85	MG	1	3935	1/1	0.97	0.22	47,47,47,47	0
85	MG	1	4090	1/1	0.97	0.15	42,42,42,42	0
85	MG	AR	3887	1/1	0.97	0.21	21,21,21,21	0
85	MG	AR	3888	1/1	0.97	0.23	24,24,24,24	0
84	OHX	1	3482	7/7	0.97	0.13	117,117,117,117	0
84	OHX	AR	3535	7/7	0.97	0.12	114,115,115,115	0
84	OHX	1	3402	7/7	0.97	0.37	114,115,115,115	0
85	MG	6	2179	1/1	0.97	0.28	43,43,43,43	0
84	OHX	6	1928	7/7	0.97	0.11	126,126,127,127	0
84	OHX	1	3682	7/7	0.97	0.15	110,110,111,111	0
85	MG	AS	222	1/1	0.97	0.20	44,44,44,44	0
84	OHX	AS	202	7/7	0.97	0.10	124,124,125,125	0
85	MG	1	4097	1/1	0.97	0.11	70,70,70,70	0
84	OHX	AS	203	7/7	0.97	0.11	116,116,116,116	0
84	OHX	AS	204	7/7	0.97	0.12	113,113,113,113	0
84	OHX	AS	205	7/7	0.97	0.14	113,113,114,114	0
84	OHX	1	3440	7/7	0.97	0.17	110,110,111,111	0
85	MG	1	3947	1/1	0.97	0.10	26,26,26,26	0
84	OHX	3	201	7/7	0.97	0.13	121,121,121,122	0
84	OHX	A	2008	7/7	0.97	0.13	132,132,133,133	0
84	OHX	6	1933	7/7	0.97	0.12	116,116,117,117	0
84	OHX	1	3523	7/7	0.97	0.10	119,119,120,120	0
84	OHX	6	1935	7/7	0.97	0.13	121,121,121,122	0
84	OHX	AP	502	7/7	0.97	0.15	112,113,113,113	0
84	OHX	6	1936	7/7	0.97	0.13	116,116,117,117	0
84	OHX	AR	3402	7/7	0.97	0.40	113,113,113,113	0
85	MG	r	302	1/1	0.97	0.14	37,37,37,37	0
85	MG	1	3956	1/1	0.97	0.10	34,34,34,34	0
84	OHX	AR	3403	7/7	0.97	0.22	110,110,110,110	0
84	OHX	AR	3404	7/7	0.97	0.32	112,112,112,112	0
84	OHX	6	1937	7/7	0.97	0.11	119,120,120,120	0
85	MG	AT	230	1/1	0.97	0.19	39,39,39,39	0
85	MG	1	3960	1/1	0.97	0.07	33,33,33,33	0
85	MG	AB	206	1/1	0.97	0.21	26,26,26,26	0
84	OHX	AR	3406	7/7	0.97	0.34	112,112,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	AR	3411	7/7	0.97	0.28	106,106,106,106	0
84	OHX	AR	3413	7/7	0.97	0.24	107,107,107,107	0
88	ZN	g	501	1/1	0.97	0.07	119,119,119,119	0
85	MG	CE	405	1/1	0.97	0.34	26,26,26,26	0
88	ZN	e1	501	1/1	0.97	0.05	153,153,153,153	0
84	OHX	1	3429	7/7	0.98	0.16	110,110,110,110	0
85	MG	1	3889	1/1	0.98	0.28	23,23,23,23	0
84	OHX	AT	201	7/7	0.98	0.30	109,109,110,110	0
85	MG	1	3891	1/1	0.98	0.25	17,17,17,17	0
84	OHX	AT	202	7/7	0.98	0.25	106,106,106,106	0
85	MG	1	3893	1/1	0.98	0.16	26,26,26,26	0
85	MG	6	2055	1/1	0.98	0.32	49,49,49,49	0
84	OHX	1	3411	7/7	0.98	0.23	111,112,112,112	0
84	OHX	1	3461	7/7	0.98	0.11	110,110,111,111	0
85	MG	AR	3878	1/1	0.98	0.17	31,31,31,31	0
85	MG	AR	3879	1/1	0.98	0.26	22,22,22,22	0
85	MG	AR	4186	1/1	0.98	0.05	33,33,33,33	0
84	OHX	AR	3475	7/7	0.98	0.11	116,116,116,116	0
84	OHX	1	3412	7/7	0.98	0.26	114,114,115,115	0
84	OHX	1	3463	7/7	0.98	0.10	121,121,122,122	0
84	OHX	1	3464	7/7	0.98	0.11	109,109,109,109	0
85	MG	AR	4192	1/1	0.98	0.16	29,29,29,29	0
84	OHX	1	3465	7/7	0.98	0.12	117,117,117,117	0
84	OHX	1	3432	7/7	0.98	0.22	117,117,117,117	0
84	OHX	6	1942	7/7	0.98	0.10	135,135,136,136	0
84	OHX	AR	3482	7/7	0.98	0.10	111,112,112,112	0
84	OHX	1	3467	7/7	0.98	0.13	123,123,124,124	0
84	OHX	1	3468	7/7	0.98	0.11	116,117,117,117	0
84	OHX	AR	3485	7/7	0.98	0.09	114,114,115,115	0
84	OHX	1	3433	7/7	0.98	0.19	118,119,119,119	0
84	OHX	1	3413	7/7	0.98	0.22	112,113,113,113	0
84	OHX	AC	101	7/7	0.98	0.26	114,115,115,115	0
84	OHX	1	3407	7/7	0.98	0.27	106,106,107,107	0
84	OHX	AR	3491	7/7	0.98	0.13	108,108,109,109	0
84	OHX	1	3408	7/7	0.98	0.28	112,112,112,113	0
84	OHX	1	3437	7/7	0.98	0.19	116,117,117,117	0
84	OHX	1	3416	7/7	0.98	0.18	109,109,109,109	0
84	OHX	1	3439	7/7	0.98	0.13	109,109,109,109	0
85	MG	1	4178	1/1	0.98	0.15	28,28,28,28	0
84	OHX	1	3417	7/7	0.98	0.23	116,117,117,117	0
85	MG	AR	4053	1/1	0.98	0.22	30,30,30,30	0
84	OHX	1	3441	7/7	0.98	0.15	116,116,116,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	2	201	7/7	0.98	0.25	119,119,120,120	0
84	OHX	CV	201	7/7	0.98	0.28	117,117,117,117	0
85	MG	AR	3757	1/1	0.98	0.18	31,31,31,31	0
84	OHX	CX	201	7/7	0.98	0.10	116,116,116,116	0
84	OHX	1	3478	7/7	0.98	0.10	125,125,125,126	0
84	OHX	DD	101	7/7	0.98	0.23	113,114,114,114	0
84	OHX	1	3479	7/7	0.98	0.09	108,109,109,109	0
84	OHX	DQ	201	7/7	0.98	0.13	111,111,111,111	0
84	OHX	6	1903	7/7	0.98	0.28	117,118,118,118	0
85	MG	1	3929	1/1	0.98	0.17	34,34,34,34	0
84	OHX	A	1902	7/7	0.98	0.23	122,122,123,123	0
84	OHX	AR	3407	7/7	0.98	0.28	113,113,113,113	0
84	OHX	AR	3408	7/7	0.98	0.26	107,107,107,107	0
84	OHX	A	1905	7/7	0.98	0.23	128,129,129,129	0
85	MG	1	4062	1/1	0.98	0.14	45,45,45,45	0
84	OHX	A	1906	7/7	0.98	0.18	142,143,143,143	0
85	MG	1	4197	1/1	0.98	0.19	32,32,32,32	0
84	OHX	A	1907	7/7	0.98	0.14	133,134,134,134	0
84	OHX	AR	3409	7/7	0.98	0.33	120,120,120,121	0
84	OHX	AR	3410	7/7	0.98	0.26	109,109,109,110	0
84	OHX	1	3442	7/7	0.98	0.17	120,121,121,121	0
85	MG	1	4202	1/1	0.98	0.21	19,19,19,19	0
84	OHX	AR	3507	7/7	0.98	0.09	123,123,123,123	0
84	OHX	AR	3508	7/7	0.98	0.15	109,109,109,109	0
84	OHX	AR	3412	7/7	0.98	0.22	109,109,109,109	0
84	OHX	A	1914	7/7	0.98	0.13	126,127,127,127	0
85	MG	1	3943	1/1	0.98	0.17	37,37,37,37	0
84	OHX	1	3418	7/7	0.98	0.22	114,115,115,115	0
85	MG	AR	4241	1/1	0.98	0.22	17,17,17,17	0
84	OHX	AR	3414	7/7	0.98	0.24	113,113,114,114	0
84	OHX	A	1917	7/7	0.98	0.11	130,131,131,131	0
84	OHX	6	1906	7/7	0.98	0.24	122,123,123,124	0
85	MG	1	4212	1/1	0.98	0.21	39,39,39,39	0
84	OHX	A	1919	7/7	0.98	0.11	121,122,122,122	0
84	OHX	A	1920	7/7	0.98	0.09	128,128,129,129	0
84	OHX	1	3444	7/7	0.98	0.16	116,116,117,117	0
85	MG	1	4216	1/1	0.98	0.21	23,23,23,23	0
84	OHX	A	1922	7/7	0.98	0.09	123,124,124,124	0
85	MG	AR	4092	1/1	0.98	0.26	47,47,47,47	0
85	MG	AR	3940	1/1	0.98	0.24	21,21,21,21	0
84	OHX	A	1923	7/7	0.98	0.10	124,125,125,125	0
84	OHX	AR	3417	7/7	0.98	0.17	111,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	A	1925	7/7	0.98	0.07	136,137,137,137	0
84	OHX	AR	3418	7/7	0.98	0.23	116,116,117,117	0
85	MG	AR	3945	1/1	0.98	0.06	40,40,40,40	0
85	MG	AR	3798	1/1	0.98	0.24	33,33,33,33	0
85	MG	AR	3799	1/1	0.98	0.09	22,22,22,22	0
84	OHX	AR	3419	7/7	0.98	0.23	122,122,123,123	0
84	OHX	AR	3420	7/7	0.98	0.25	113,114,114,114	0
84	OHX	AR	3421	7/7	0.98	0.20	113,113,113,113	0
85	MG	1	4089	1/1	0.98	0.19	42,42,42,42	0
84	OHX	AR	3422	7/7	0.98	0.23	112,112,112,112	0
84	OHX	1	3406	7/7	0.98	0.30	108,108,108,108	0
84	OHX	AR	3424	7/7	0.98	0.22	112,112,113,113	0
84	OHX	AR	3425	7/7	0.98	0.14	105,106,106,106	0
84	OHX	AR	3426	7/7	0.98	0.20	111,112,112,112	0
84	OHX	1	3484	7/7	0.98	0.09	125,126,126,126	0
84	OHX	AR	3428	7/7	0.98	0.14	115,115,115,116	0
84	OHX	6	1910	7/7	0.98	0.23	119,120,120,120	0
84	OHX	A	1938	7/7	0.98	0.12	126,127,127,127	0
84	OHX	A	1939	7/7	0.98	0.10	140,141,141,142	0
85	MG	6	2135	1/1	0.98	0.12	49,49,49,49	0
85	MG	6	2136	1/1	0.98	0.08	52,52,52,52	0
84	OHX	AR	3431	7/7	0.98	0.18	109,109,110,110	0
84	OHX	1	3421	7/7	0.98	0.27	115,115,116,116	0
84	OHX	6	1912	7/7	0.98	0.14	122,122,123,123	0
84	OHX	6	1913	7/7	0.98	0.17	133,134,135,135	0
84	OHX	1	3448	7/7	0.98	0.13	117,117,117,117	0
84	OHX	AR	3437	7/7	0.98	0.14	108,108,108,108	0
85	MG	1	3975	1/1	0.98	0.17	42,42,42,42	0
85	MG	1	3847	1/1	0.98	0.31	28,28,28,28	0
85	MG	4	225	1/1	0.98	0.17	25,25,25,25	0
84	OHX	AR	3438	7/7	0.98	0.15	108,108,108,108	0
84	OHX	6	1916	7/7	0.98	0.15	119,120,120,120	0
84	OHX	AR	3440	7/7	0.98	0.14	125,125,125,126	0
84	OHX	1	3449	7/7	0.98	0.16	117,117,118,118	0
84	OHX	1	3450	7/7	0.98	0.09	121,122,122,123	0
85	MG	1	3982	1/1	0.98	0.21	32,32,32,32	0
84	OHX	AR	3443	7/7	0.98	0.10	116,116,117,117	0
84	OHX	1	3422	7/7	0.98	0.21	116,116,117,117	0
85	MG	1	3733	1/1	0.98	0.23	26,26,26,26	0
84	OHX	1	3423	7/7	0.98	0.23	120,120,121,121	0
85	MG	1	3735	1/1	0.98	0.13	24,24,24,24	0
84	OHX	AR	3446	7/7	0.98	0.12	112,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	OHX	1	3424	7/7	0.98	0.18	115,115,115,115	0
84	OHX	AR	3448	7/7	0.98	0.13	115,115,115,115	0
84	OHX	AR	3449	7/7	0.98	0.12	116,117,117,117	0
84	OHX	6	1922	7/7	0.98	0.09	121,122,122,122	0
84	OHX	AR	3451	7/7	0.98	0.13	114,114,114,114	0
84	OHX	AR	3452	7/7	0.98	0.12	121,121,122,122	0
84	OHX	A	1961	7/7	0.98	0.09	149,150,151,151	0
84	OHX	6	1923	7/7	0.98	0.10	121,121,122,122	0
84	OHX	AR	3454	7/7	0.98	0.10	112,112,113,113	0
85	MG	AR	3846	1/1	0.98	0.28	33,33,33,33	0
84	OHX	1	3454	7/7	0.98	0.10	111,111,111,111	0
85	MG	1	3747	1/1	0.98	0.26	37,37,37,37	0
84	OHX	1	3425	7/7	0.98	0.20	108,109,109,109	0
85	MG	AR	3999	1/1	0.98	0.15	44,44,44,44	0
84	OHX	AR	3457	7/7	0.98	0.10	108,108,108,109	0
84	OHX	AR	3458	7/7	0.98	0.11	114,114,114,115	0
84	OHX	6	1926	7/7	0.98	0.09	120,121,121,121	0
84	OHX	1	3494	7/7	0.98	0.10	119,119,120,120	0
84	OHX	AR	3461	7/7	0.98	0.11	110,111,111,111	0
84	OHX	AR	3462	7/7	0.98	0.09	116,116,116,116	0
84	OHX	AS	201	7/7	0.98	0.18	119,119,119,120	0
85	MG	CQ	204	1/1	0.98	0.20	30,30,30,30	0
84	OHX	1	3426	7/7	0.98	0.21	120,120,120,120	0
85	MG	1	3757	1/1	0.98	0.14	38,38,38,38	0
84	OHX	4	202	7/7	0.98	0.29	112,112,112,113	0
85	MG	v	304	1/1	0.98	0.33	52,52,52,52	0
85	MG	6	2181	1/1	0.98	0.04	95,95,95,95	0
84	OHX	AR	3465	7/7	0.98	0.14	118,118,118,118	0
84	OHX	6	1930	7/7	0.98	0.10	121,121,122,122	0
84	OHX	1	3535	7/7	0.98	0.12	111,111,111,112	0
84	OHX	AR	3468	7/7	0.98	0.10	124,124,125,125	0
84	OHX	1	3457	7/7	0.98	0.12	126,127,127,128	0
84	OHX	AR	3470	7/7	0.98	0.09	115,116,116,116	0
85	MG	AR	4018	1/1	0.98	0.13	36,36,36,36	0
85	MG	AR	4172	1/1	0.98	0.08	65,65,65,65	0
85	MG	DC	204	1/1	0.98	0.07	35,35,35,35	0
84	OHX	1	3410	7/7	0.98	0.30	112,112,112,112	0
85	MG	AR	4175	1/1	0.99	0.10	35,35,35,35	0
85	MG	1	4063	1/1	0.99	0.04	38,38,38,38	0
85	MG	1	4181	1/1	0.99	0.16	23,23,23,23	0
85	MG	1	3839	1/1	0.99	0.10	27,27,27,27	0
84	OHX	1	3427	7/7	0.99	0.19	112,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3895	1/1	0.99	0.30	28,28,28,28	0
84	OHX	AR	3434	7/7	0.99	0.14	111,111,111,111	0
85	MG	AR	3770	1/1	0.99	0.21	32,32,32,32	0
84	OHX	AR	3489	7/7	0.99	0.07	114,114,114,114	0
84	OHX	AR	3429	7/7	0.99	0.10	112,112,112,112	0
85	MG	1	4112	1/1	0.99	0.21	32,32,32,32	0
85	MG	AR	3954	1/1	0.99	0.15	44,44,44,44	0
85	MG	AR	3774	1/1	0.99	0.04	30,30,30,30	0
84	OHX	6	1915	7/7	0.99	0.09	119,119,120,120	0
85	MG	1	4031	1/1	0.99	0.25	21,21,21,21	0
84	OHX	1	3419	7/7	0.99	0.16	107,107,107,107	0
85	MG	AS	230	1/1	0.99	0.29	36,36,36,36	0
85	MG	AR	4191	1/1	0.99	0.07	58,58,58,58	0
85	MG	1	3829	1/1	0.99	0.27	16,16,16,16	0
88	ZN	DQ	202	1/1	0.99	0.04	63,63,63,63	0
85	MG	AR	4131	1/1	0.99	0.07	39,39,39,39	0
88	ZN	e	102	1/1	0.99	0.04	79,79,79,79	0
84	OHX	1	3447	7/7	0.99	0.10	113,113,113,113	0
85	MG	1	3914	1/1	0.99	0.25	19,19,19,19	0
88	ZN	d9	102	1/1	0.99	0.05	83,83,83,83	0
85	MG	1	3903	1/1	0.99	0.26	21,21,21,21	0
88	ZN	DR	501	1/1	1.00	0.04	59,59,59,59	0
88	ZN	b	102	1/1	1.00	0.06	71,71,71,71	0
88	ZN	AN	500	1/1	1.00	0.01	38,38,38,38	0
88	ZN	AP	501	1/1	1.00	0.04	61,61,61,61	0
88	ZN	AQ	501	1/1	1.00	0.03	56,56,56,56	0
88	ZN	d6	103	1/1	1.00	0.02	53,53,53,53	0
88	ZN	DL	101	1/1	1.00	0.02	41,41,41,41	0
88	ZN	DO	201	1/1	1.00	0.02	32,32,32,32	0
88	ZN	AK	101	1/1	1.00	0.02	34,34,34,34	0

5.5 Other polymers (i)

There are no such residues in this entry.