Full wwPDB X-ray Structure Validation Report (i)

Sep 16, 2026 – 08:49 pm BST

PDB ID	:	4U6F / pdb_00004u6f
Title	:	Crystal structure of T-2 toxin bound to the yeast 80S ribosome
Authors	:	Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on	:	2014-07-28
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

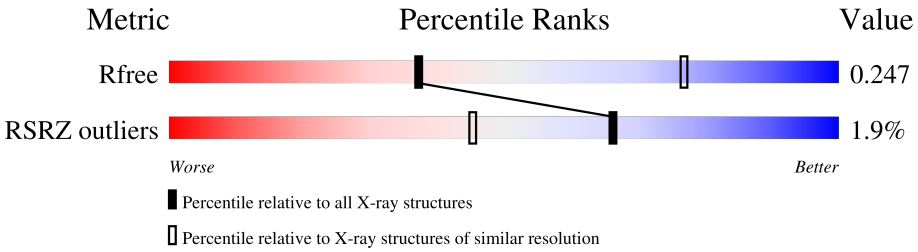
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	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.

2 Entry composition (i)

There are 88 unique types of molecules in this entry. The entry contains 411881 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	1781	Total	C	N	O	P	0	0	0
			37948	16965	6715	12487	1781			
1	6	1795	Total	C	N	O	P	0	0	0
			38238	17095	6758	12590	1795			

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S0	206	Total	C	N	O	S	0	0	0
			1577	1014	278	283	2			
2	s0	206	Total	C	N	O	S	0	0	0
			1583	1017	281	283	2			

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S1	214	Total	C	N	O	S	0	0	0
			1709	1084	310	311	4			
3	s1	216	Total	C	N	O	S	0	0	0
			1722	1091	312	315	4			

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	S2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			
4	s2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	S3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			
5	s3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			

- Molecule 6 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	S4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			
6	s4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	S5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			
7	s5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			

- Molecule 8 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	S6	226	Total	C	N	O	S	0	0	0
			1799	1129	346	321	3			
8	s6	218	Total	C	N	O	S	0	0	0
			1755	1102	337	313	3			

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	S7	184	Total	C	N	O	0	0	0
			1481	951	265	265			
9	s7	186	Total	C	N	O	0	0	0
			1491	957	267	267			

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	S8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			

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

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	S9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			
11	s9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

- Molecule 12 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	C0	96	Total	C	N	O	S	0	0	0
			773	500	126	145	2			
12	c0	96	Total	C	N	O	S	0	0	0
			762	491	125	144	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C0	89	ALA	GLY	conflict	UNP Q08745
C0	98	SER	THR	conflict	UNP Q08745
c0	89	ALA	GLY	conflict	UNP Q08745
c0	98	SER	THR	conflict	UNP Q08745

- Molecule 13 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C1	155	Total	C	N	O	S	0	0	0
			1214	775	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C1	147	ALA	GLY	conflict	UNP P0CX47
c1	147	ALA	GLY	conflict	UNP P0CX47

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	C2	124	Total	C	N	O	S	0	0	0
			892	562	156	172	2			
14	c2	124	Total	C	N	O	S	0	0	0
			892	562	156	172	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C2	104	ALA	GLY	conflict	UNP P48589
C2	110	ALA	GLY	conflict	UNP P48589
c2	104	ALA	GLY	conflict	UNP P48589
c2	110	ALA	GLY	conflict	UNP P48589

- Molecule 15 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	C3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			
15	c3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			

- Molecule 16 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	C4	127	Total	C	N	O	S	0	0	0
			891	545	182	163	1			
16	c4	128	Total	C	N	O	S	0	0	0
			949	582	188	176	3			

- Molecule 17 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	C5	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			
17	c5	135	Total	C	N	O	S	0	0	0
			1039	658	196	178	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C5	137	SER	ARG	conflict	UNP Q01855
c5	137	SER	ARG	conflict	UNP Q01855

- Molecule 18 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	C6	141	Total	C	N	O		0	0	0
			1105	708	203	194				
18	c6	142	Total	C	N	O		0	0	0
			1111	711	204	196				

- Molecule 19 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	C7	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			
19	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

- Molecule 20 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	C8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			
20	c8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			

- Molecule 21 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	C9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			
21	c9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			

- Molecule 22 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	D0	107	Total	C	N	O	S	0	0	0
			855	539	156	159	1			
22	d0	110	Total	C	N	O	S	0	0	0
			882	554	161	166	1			

- Molecule 23 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	D1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			
23	d1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			

- Molecule 24 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	D2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			
24	d2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			

- Molecule 25 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	D3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			
25	d3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			

- Molecule 26 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	D4	134	Total	C	N	O	0	0	0
			1073	676	208	189			
26	d4	134	Total	C	N	O	0	0	0
			1073	676	208	189			

- Molecule 27 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	D5	70	Total	C	N	O	0	0	0
			563	360	104	99			
27	d5	69	Total	C	N	O	0	0	0
			558	357	103	98			

- Molecule 28 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	D6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			

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

- Molecule 29 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	D7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			
29	d7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			

- Molecule 30 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	D8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			
30	d8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			
31	d9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	E0	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	E1	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			
33	e1	76	Total	C	N	O	S	0	0	0
			608	388	117	99	4			

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

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

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O	0	0	0
			1104	652	221	231			
35	sM	104	Total	C	N	O	0	0	0
			680	403	140	137			

- Molecule 36 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			
36	5	3150	Total	C	N	O	P	0	0	0
			67376	30095	12145	21987	3149			

- Molecule 37 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
37	7	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 38 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	4	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			
38	8	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	l2	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	L3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
40	l3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	L4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
41	l4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	L5	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
42	l5	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

- Molecule 43 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	L6	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
43	l6	157	Total	C	N	O	S	0	0	0
			1248	806	224	217	1			

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	L7	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
44	l7	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	l8	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	L9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
46	l9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

- Molecule 47 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	M0	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			
47	m0	213	Total	C	N	O	S	0	0	0
			1722	1094	325	297	6			

- Molecule 48 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	M1	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			
48	m1	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	M3	193	Total	C	N	O	0	0	0
			1543	962	315	266			
49	m3	194	Total	C	N	O	0	0	0
			1548	965	316	267			

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	M4	136	Total	C	N	O	S	0	0	0
			1053	675	199	177	2			
50	m4	137	Total	C	N	O	S	0	0	0
			1059	678	200	179	2			

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	M5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			
51	m5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			
52	m6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	M7	183	Total	C	N	O	0	0	0
			1420	882	281	257			
53	m7	155	Total	C	N	O	0	0	0
			1227	764	238	225			

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	M8	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			
54	m8	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	M9	188	Total	C	N	O	0	0	0
			1521	935	326	260			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	m9	188	Total 1521	C 935	N 326	O 260	0	0	0

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	N0	172	Total 1445	C 930	N 267	O 244	S 4	0	0	0
56	n0	172	Total 1445	C 930	N 267	O 244	S 4	0	0	0

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	N1	159	Total 1276	C 805	N 246	O 221	S 4	0	0	0
57	n1	159	Total 1276	C 805	N 246	O 221	S 4	0	0	0

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	N2	100	Total 796	C 516	N 131	O 149	0	0	0
58	n2	98	Total 778	C 505	N 127	O 146	0	0	0

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	N3	136	Total 1003	C 628	N 189	O 179	S 7	0	0	0
59	n3	136	Total 1003	C 628	N 189	O 179	S 7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	N4	98	Total 699	C 443	N 137	O 118	S 1	0	0	0
60	n4	135	Total 1038	C 651	N 206	O 180	S 1	0	0	0

- Molecule 61 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	N5	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			
61	n5	120	Total	C	N	O	S	0	0	0
			959	617	168	172	2			

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
62	N6	126	Total	C	N	O	0	0	0
			993	625	192	176			
62	n6	126	Total	C	N	O	0	0	0
			993	625	192	176			

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
63	N7	135	Total	C	N	O	0	0	0
			1092	710	202	180			
63	n7	135	Total	C	N	O	0	0	0
			1092	710	202	180			

- Molecule 64 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	N8	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			
64	n8	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			

- Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
65	N9	58	Total	C	N	O	0	0	0
			462	289	100	73			
65	n9	58	Total	C	N	O	0	0	0
			462	289	100	73			

- Molecule 66 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	O0	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			
66	o0	100	Total	C	N	O	S	0	0	0
			767	492	128	146	1			

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
67	O1	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			
67	o1	109	Total	C	N	O	S	0	0	0
			883	559	167	156	1			

- Molecule 68 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
68	O2	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			
68	o2	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
69	O3	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			
69	o3	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
70	O4	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			
70	o4	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O4	121	LYS	-	expression tag	UNP P87262
o4	121	LYS	-	expression tag	UNP P87262

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
71	O5	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			
71	o5	119	Total	C	N	O	S	0	0	0
			965	612	185	167	1			

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	O6	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			
72	o6	99	Total	C	N	O	S	0	0	0
			770	481	156	131	2			

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
73	O7	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			
73	o7	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			

- Molecule 74 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
74	O8	77	Total	C	N	O	0	0	0
			612	391	115	106			
74	o8	77	Total	C	N	O	0	0	0
			608	388	114	106			

- Molecule 75 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	O9	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			
75	o9	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			

- Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	Q0	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			
76	q0	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			

- Molecule 77 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	Q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			
77	q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	Q2	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			
78	q2	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	Q3	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			
79	q3	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	1			

- Molecule 81 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 82 is a protein called unknown protein chain m2.

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

- Molecule 83 is a protein called unknown protein chain p1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
83	p1	47	Total 235	C 141	N 47	O 47	0	0	0

- Molecule 84 is a protein called unknown protein chain p2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
84	p2	46	Total 230	C 138	N 46	O 46	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	2	126	Total 126	Mg 126	0	0
85	S2	1	Total 1	Mg 1	0	0
85	S8	1	Total 1	Mg 1	0	0
85	SM	1	Total 1	Mg 1	0	0
85	1	465	Total 465	Mg 465	0	0
85	3	14	Total 14	Mg 14	0	0
85	4	22	Total 22	Mg 22	0	0
85	L2	2	Total 2	Mg 2	0	0
85	L3	3	Total 3	Mg 3	0	0
85	L4	2	Total 2	Mg 2	0	0
85	L5	1	Total 1	Mg 1	0	0
85	L6	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	L7	4	Total Mg 4 4	0	0
85	L8	1	Total Mg 1 1	0	0
85	M0	2	Total Mg 2 2	0	0
85	M1	1	Total Mg 1 1	0	0
85	M3	3	Total Mg 3 3	0	0
85	M4	1	Total Mg 1 1	0	0
85	M5	2	Total Mg 2 2	0	0
85	M6	1	Total Mg 1 1	0	0
85	M7	5	Total Mg 5 5	0	0
85	M9	1	Total Mg 1 1	0	0
85	N0	2	Total Mg 2 2	0	0
85	N3	3	Total Mg 3 3	0	0
85	N5	1	Total Mg 1 1	0	0
85	N6	1	Total Mg 1 1	0	0
85	N8	6	Total Mg 6 6	0	0
85	O3	1	Total Mg 1 1	0	0
85	O4	1	Total Mg 1 1	0	0
85	O7	1	Total Mg 1 1	0	0
85	Q2	1	Total Mg 1 1	0	0
85	6	147	Total Mg 147 147	0	0
85	s1	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	s8	2	Total Mg 2 2	0	0
85	c1	2	Total Mg 2 2	0	0
85	c7	2	Total Mg 2 2	0	0
85	c8	2	Total Mg 2 2	0	0
85	d3	1	Total Mg 1 1	0	0
85	d4	1	Total Mg 1 1	0	0
85	d6	1	Total Mg 1 1	0	0
85	sM	2	Total Mg 2 2	0	0
85	5	504	Total Mg 504 504	0	0
85	7	17	Total Mg 17 17	0	0
85	8	12	Total Mg 12 12	0	0
85	l2	1	Total Mg 1 1	0	0
85	l3	3	Total Mg 3 3	0	0
85	l4	1	Total Mg 1 1	0	0
85	l5	2	Total Mg 2 2	0	0
85	l7	1	Total Mg 1 1	0	0
85	m1	2	Total Mg 2 2	0	0
85	m5	5	Total Mg 5 5	0	0
85	m6	2	Total Mg 2 2	0	0
85	m7	4	Total Mg 4 4	0	0
85	n0	1	Total Mg 1 1	0	0

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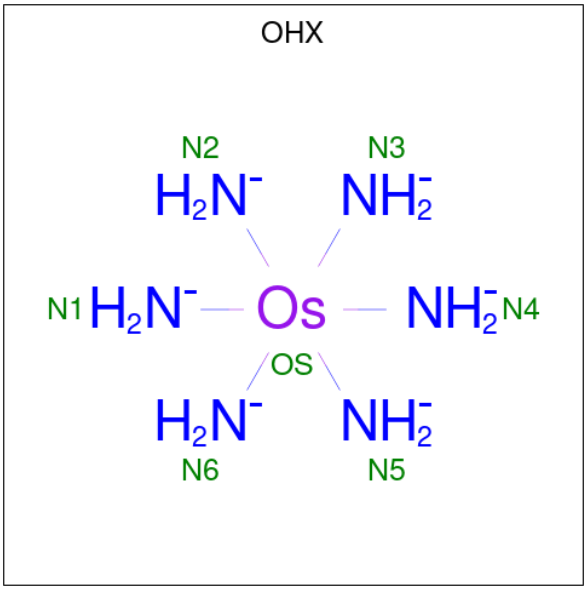
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	n3	2	Total Mg 2 2	0	0
85	n6	2	Total Mg 2 2	0	0
85	n8	3	Total Mg 3 3	0	0
85	n9	1	Total Mg 1 1	0	0
85	o0	1	Total Mg 1 1	0	0
85	o1	1	Total Mg 1 1	0	0
85	o3	1	Total Mg 1 1	0	0
85	o4	1	Total Mg 1 1	0	0
85	q0	1	Total Mg 1 1	0	0
85	q3	2	Total Mg 2 2	0	0

- Molecule 86 is osmium (III) hexammine (CCD ID: OHX) (formula: $H_{12}N_6Os$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	2	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
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86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	S8	1	Total 7	N 6	Os 1	0	0
86	S9	1	Total 7	N 6	Os 1	0	0
86	C1	1	Total 7	N 6	Os 1	0	0
86	C3	1	Total 7	N 6	Os 1	0	0
86	C5	1	Total 7	N 6	Os 1	0	0
86	C8	1	Total 7	N 6	Os 1	0	0
86	D9	1	Total 7	N 6	Os 1	0	0
86	SR	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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			7	6	1		
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	1	1	Total N Os 7 6 1	0	0
86	1	1	Total N Os 7 6 1	0	0
86	1	1	Total N Os 7 6 1	0	0
86	1	1	Total N Os 7 6 1	0	0
86	1	1	Total N Os 7 6 1	0	0
86	1	1	Total N Os 7 6 1	0	0
86	1	1	Total N Os 7 6 1	0	0
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86	1	1	Total N Os 7 6 1	0	0
86	1	1	Total N Os 7 6 1	0	0
86	1	1	Total N Os 7 6 1	0	0
86	1	1	Total N Os 7 6 1	0	0
86	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
			7	6	1		
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	L3	1	Total	N	Os	0	0
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86	L3	1	Total	N	Os	0	0
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86	L3	1	Total	N	Os	0	0
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86	L4	1	Total	N	Os	0	0
			7	6	1		
86	M0	1	Total	N	Os	0	0
			7	6	1		
86	M5	1	Total	N	Os	0	0
			7	6	1		
86	M6	1	Total	N	Os	0	0
			7	6	1		
86	M7	1	Total	N	Os	0	0
			7	6	1		
86	M7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	M8	1	Total 7	N 6	Os 1	0	0
86	M9	1	Total 7	N 6	Os 1	0	0
86	N1	1	Total 7	N 6	Os 1	0	0
86	N9	1	Total 7	N 6	Os 1	0	0
86	O1	1	Total 7	N 6	Os 1	0	0
86	O2	1	Total 7	N 6	Os 1	0	0
86	O3	1	Total 7	N 6	Os 1	0	0
86	O7	1	Total 7	N 6	Os 1	0	0
86	O7	1	Total 7	N 6	Os 1	0	0
86	Q2	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	s1	1	Total	N	Os	0	0
			7	6	1		
86	s4	1	Total	N	Os	0	0
			7	6	1		
86	s8	1	Total	N	Os	0	0
			7	6	1		
86	c3	1	Total	N	Os	0	0
			7	6	1		
86	c5	1	Total	N	Os	0	0
			7	6	1		
86	c8	1	Total	N	Os	0	0
			7	6	1		
86	d9	1	Total	N	Os	0	0
			7	6	1		
86	sR	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	7	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	l3	1	Total N Os 7 6 1	0	0
86	l3	1	Total N Os 7 6 1	0	0
86	l4	1	Total N Os 7 6 1	0	0
86	l4	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	l5	1	Total N Os 7 6 1	0	0
86	l5	1	Total N Os 7 6 1	0	0
86	l5	1	Total N Os 7 6 1	0	0
86	l9	1	Total N Os 7 6 1	0	0
86	m0	1	Total N Os 7 6 1	0	0
86	m0	1	Total N Os 7 6 1	0	0
86	m1	1	Total N Os 7 6 1	0	0
86	m4	1	Total N Os 7 6 1	0	0
86	m5	1	Total N Os 7 6 1	0	0
86	m7	1	Total N Os 7 6 1	0	0
86	n3	1	Total N Os 7 6 1	0	0
86	n5	1	Total N Os 7 6 1	0	0
86	n9	1	Total N Os 7 6 1	0	0
86	o2	1	Total N Os 7 6 1	0	0
86	o3	1	Total N Os 7 6 1	0	0
86	o7	1	Total N Os 7 6 1	0	0
86	q2	1	Total N Os 7 6 1	0	0

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	D6	1	Total Zn 1 1	0	0
87	D7	1	Total Zn 1 1	0	0

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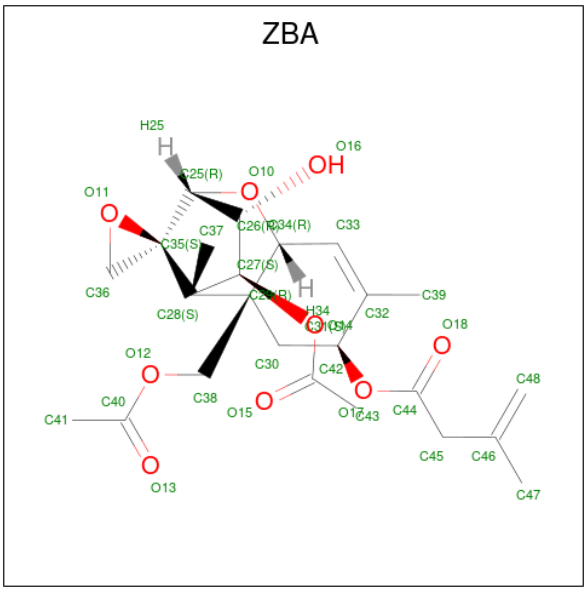
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	D9	1	Total Zn 1 1	0	0
87	E1	1	Total Zn 1 1	0	0
87	O7	1	Total Zn 1 1	0	0
87	Q0	1	Total Zn 1 1	0	0
87	Q2	1	Total Zn 1 1	0	0
87	Q3	1	Total Zn 1 1	0	0
87	d6	1	Total Zn 1 1	0	0
87	d7	1	Total Zn 1 1	0	0
87	d9	1	Total Zn 1 1	0	0
87	e1	1	Total Zn 1 1	0	0
87	o7	1	Total Zn 1 1	0	0
87	q0	1	Total Zn 1 1	0	0
87	q2	1	Total Zn 1 1	0	0
87	q3	1	Total Zn 1 1	0	0

- Molecule 88 is 12,13-Epoxytrichothec-9-ene-3,4,8,15-tetrol-4,15-diacetate-8-isovalerate (CCD ID: ZBA) (formula: $C_{24}H_{32}O_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	1	1	Total C O 33 24 9	0	0
88	5	1	Total C O 33 24 9	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	436.64Å 287.69Å 304.39Å 90.00° 98.98° 90.00°	Depositor
Resolution (Å)	300.66 – 3.10 300.66 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (300.66-3.10) 98.6 (300.66-3.10)	Depositor EDS
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.198 , 0.247 0.200 , 0.247	Depositor DCC
R_{free} test set	26422 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å^2)	71.8	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 68.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	411881	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% 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

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no oligosaccharides in this entry.

4.6 Ligand geometry

Of 2558 ligands modelled in this entry, 1425 are monoatomic - leaving 1133 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	$\#\|Z\| > 2$
86	OHX	5	4214	-	0,6,6	-	-	-		
86	OHX	2	2162	-	0,6,6	-	-	-		
86	OHX	5	4220	-	0,6,6	-	-	-		
86	OHX	1	3922	-	0,6,6	-	-	-		
86	OHX	1	4187	-	0,6,6	-	-	-		
86	OHX	2	2086	-	0,6,6	-	-	-		
86	OHX	1	4116	85	0,6,6	-	-	-		
86	OHX	5	4183	-	0,6,6	-	-	-		
86	OHX	M7	206	85	0,6,6	-	-	-		
86	OHX	1	3980	-	0,6,6	-	-	-		
86	OHX	5	3994	-	0,6,6	-	-	-		
86	OHX	L4	403	-	0,6,6	-	-	-		
86	OHX	5	4075	-	0,6,6	-	-	-		
86	OHX	2	2074	-	0,6,6	-	-	-		
86	OHX	1	4019	-	0,6,6	-	-	-		
86	OHX	6	2137	-	0,6,6	-	-	-		
86	OHX	1	3966	-	0,6,6	-	-	-		
86	OHX	5	4078	-	0,6,6	-	-	-		
86	OHX	5	4089	-	0,6,6	-	-	-		
86	OHX	5	4145	-	0,6,6	-	-	-		
86	OHX	5	3957	-	0,6,6	-	-	-		
86	OHX	5	4233	-	0,6,6	-	-	-		
86	OHX	1	3896	85	0,6,6	-	-	-		
86	OHX	1	4004	-	0,6,6	-	-	-		
86	OHX	2	2045	-	0,6,6	-	-	-		
86	OHX	1	4135	-	0,6,6	-	-	-		
86	OHX	6	2092	-	0,6,6	-	-	-		
86	OHX	1	4005	-	0,6,6	-	-	-		
86	OHX	1	4124	-	0,6,6	-	-	-		
86	OHX	2	2120	-	0,6,6	-	-	-		
86	OHX	6	2188	-	0,6,6	-	-	-		
86	OHX	5	3913	-	0,6,6	-	-	-		
86	OHX	4	224	-	0,6,6	-	-	-		
86	OHX	5	3915	-	0,6,6	-	-	-		
86	OHX	5	4065	-	0,6,6	-	-	-		
86	OHX	5	4255	85	0,6,6	-	-	-		
86	OHX	6	2196	-	0,6,6	-	-	-		
86	OHX	1	3901	-	0,6,6	-	-	-		
86	OHX	6	2181	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	4096	-	0,6,6	-	-	-		
86	OHX	5	4149	-	0,6,6	-	-	-		
86	OHX	1	4014	-	0,6,6	-	-	-		
86	OHX	5	4155	-	0,6,6	-	-	-		
86	OHX	1	3881	85	0,6,6	-	-	-		
86	OHX	2	2067	85	0,6,6	-	-	-		
86	OHX	6	2054	-	0,6,6	-	-	-		
86	OHX	1	3984	-	0,6,6	-	-	-		
86	OHX	1	4190	-	0,6,6	-	-	-		
86	OHX	6	2148	-	0,6,6	-	-	-		
86	OHX	1	4136	-	0,6,6	-	-	-		
86	OHX	5	3954	-	0,6,6	-	-	-		
86	OHX	1	3986	-	0,6,6	-	-	-		
86	OHX	1	3967	-	0,6,6	-	-	-		
86	OHX	5	3978	-	0,6,6	-	-	-		
86	OHX	7	224	-	0,6,6	-	-	-		
86	OHX	1	4130	-	0,6,6	-	-	-		
86	OHX	6	2066	-	0,6,6	-	-	-		
86	OHX	6	2205	-	0,6,6	-	-	-		
86	OHX	1	3898	85	0,6,6	-	-	-		
86	OHX	5	3920	-	0,6,6	-	-	-		
86	OHX	5	4009	-	0,6,6	-	-	-		
86	OHX	5	4187	-	0,6,6	-	-	-		
86	OHX	2	2141	-	0,6,6	-	-	-		
86	OHX	3	215	85	0,6,6	-	-	-		
86	OHX	1	4055	-	0,6,6	-	-	-		
86	OHX	Q2	503	85	0,6,6	-	-	-		
86	OHX	5	3911	-	0,6,6	-	-	-		
86	OHX	O7	104	-	0,6,6	-	-	-		
86	OHX	5	3905	-	0,6,6	-	-	-		
86	OHX	5	4047	-	0,6,6	-	-	-		
86	OHX	6	2106	-	0,6,6	-	-	-		
86	OHX	6	2185	-	0,6,6	-	-	-		
86	OHX	5	4060	-	0,6,6	-	-	-		
86	OHX	5	4070	-	0,6,6	-	-	-		
86	OHX	5	4176	-	0,6,6	-	-	-		
86	OHX	1	3874	-	0,6,6	-	-	-		
86	OHX	6	2162	-	0,6,6	-	-	-		
86	OHX	1	3926	-	0,6,6	-	-	-		
86	OHX	2	2051	-	0,6,6	-	-	-		
86	OHX	1	4159	-	0,6,6	-	-	-		
86	OHX	5	4048	-	0,6,6	-	-	-		
86	OHX	2	2114	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	3919	85	0,6,6	-	-	-		
86	OHX	C1	201	-	0,6,6	-	-	-		
86	OHX	1	3951	85	0,6,6	-	-	-		
86	OHX	l3	405	-	0,6,6	-	-	-		
86	OHX	5	3909	-	0,6,6	-	-	-		
86	OHX	2	2180	-	0,6,6	-	-	-		
86	OHX	6	2115	-	0,6,6	-	-	-		
86	OHX	6	2183	-	0,6,6	-	-	-		
86	OHX	6	2146	-	0,6,6	-	-	-		
86	OHX	6	2168	-	0,6,6	-	-	-		
86	OHX	5	4171	85	0,6,6	-	-	-		
86	OHX	5	4114	-	0,6,6	-	-	-		
86	OHX	6	2055	-	0,6,6	-	-	-		
86	OHX	6	2102	-	0,6,6	-	-	-		
86	OHX	5	4200	-	0,6,6	-	-	-		
86	OHX	1	3902	-	0,6,6	-	-	-		
86	OHX	1	4049	-	0,6,6	-	-	-		
86	OHX	6	2170	-	0,6,6	-	-	-		
86	OHX	SR	401	-	0,6,6	-	-	-		
86	OHX	1	3890	-	0,6,6	-	-	-		
86	OHX	1	4110	-	0,6,6	-	-	-		
86	OHX	1	3942	-	0,6,6	-	-	-		
86	OHX	d9	102	-	0,6,6	-	-	-		
86	OHX	5	4202	-	0,6,6	-	-	-		
86	OHX	5	4169	-	0,6,6	-	-	-		
86	OHX	1	4056	-	0,6,6	-	-	-		
86	OHX	6	2149	85	0,6,6	-	-	-		
86	OHX	6	2084	-	0,6,6	-	-	-		
86	OHX	5	3908	-	0,6,6	-	-	-		
86	OHX	6	2060	-	0,6,6	-	-	-		
86	OHX	2	2116	-	0,6,6	-	-	-		
86	OHX	2	2047	-	0,6,6	-	-	-		
86	OHX	6	2050	-	0,6,6	-	-	-		
86	OHX	1	3878	-	0,6,6	-	-	-		
86	OHX	6	2062	-	0,6,6	-	-	-		
86	OHX	6	2158	-	0,6,6	-	-	-		
86	OHX	6	2103	-	0,6,6	-	-	-		
86	OHX	2	2144	-	0,6,6	-	-	-		
86	OHX	6	2187	-	0,6,6	-	-	-		
86	OHX	5	4108	-	0,6,6	-	-	-		
86	OHX	5	3924	-	0,6,6	-	-	-		
86	OHX	6	2173	-	0,6,6	-	-	-		
86	OHX	5	4217	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	4118	-	0,6,6	-	-	-		
86	OHX	1	4119	85	0,6,6	-	-	-		
86	OHX	5	4152	-	0,6,6	-	-	-		
86	OHX	2	2101	-	0,6,6	-	-	-		
86	OHX	1	3991	-	0,6,6	-	-	-		
86	OHX	5	4134	85	0,6,6	-	-	-		
86	OHX	1	3945	-	0,6,6	-	-	-		
86	OHX	m5	306	-	0,6,6	-	-	-		
86	OHX	5	4141	-	0,6,6	-	-	-		
86	OHX	5	3955	-	0,6,6	-	-	-		
86	OHX	1	4044	-	0,6,6	-	-	-		
86	OHX	5	4064	-	0,6,6	-	-	-		
86	OHX	1	4011	-	0,6,6	-	-	-		
86	OHX	1	4095	-	0,6,6	-	-	-		
86	OHX	5	4165	-	0,6,6	-	-	-		
86	OHX	1	4143	-	0,6,6	-	-	-		
86	OHX	6	2125	-	0,6,6	-	-	-		
86	OHX	1	4057	-	0,6,6	-	-	-		
86	OHX	6	2167	-	0,6,6	-	-	-		
86	OHX	5	4082	-	0,6,6	-	-	-		
86	OHX	1	3970	-	0,6,6	-	-	-		
86	OHX	1	3998	-	0,6,6	-	-	-		
86	OHX	6	2193	-	0,6,6	-	-	-		
86	OHX	5	4098	-	0,6,6	-	-	-		
86	OHX	6	2159	85	0,6,6	-	-	-		
86	OHX	2	2046	85	0,6,6	-	-	-		
86	OHX	1	4079	-	0,6,6	-	-	-		
86	OHX	1	4167	-	0,6,6	-	-	-		
86	OHX	6	2080	-	0,6,6	-	-	-		
86	OHX	5	3902	-	0,6,6	-	-	-		
86	OHX	5	4243	-	0,6,6	-	-	-		
86	OHX	M6	202	-	0,6,6	-	-	-		
86	OHX	5	4128	-	0,6,6	-	-	-		
86	OHX	5	4191	-	0,6,6	-	-	-		
86	OHX	n9	102	-	0,6,6	-	-	-		
86	OHX	1	4101	-	0,6,6	-	-	-		
86	OHX	5	4081	-	0,6,6	-	-	-		
86	OHX	6	2199	-	0,6,6	-	-	-		
86	OHX	1	4081	-	0,6,6	-	-	-		
86	OHX	2	2121	-	0,6,6	-	-	-		
86	OHX	1	3912	85	0,6,6	-	-	-		
86	OHX	5	3943	85	0,6,6	-	-	-		
86	OHX	1	4168	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3964	-	0,6,6	-	-	-		
86	OHX	2	2070	-	0,6,6	-	-	-		
86	OHX	1	4102	-	0,6,6	-	-	-		
86	OHX	2	2163	-	0,6,6	-	-	-		
86	OHX	1	3958	-	0,6,6	-	-	-		
86	OHX	5	3983	-	0,6,6	-	-	-		
86	OHX	5	4018	-	0,6,6	-	-	-		
86	OHX	6	2117	-	0,6,6	-	-	-		
86	OHX	5	4040	-	0,6,6	-	-	-		
86	OHX	5	4041	-	0,6,6	-	-	-		
86	OHX	5	4162	85	0,6,6	-	-	-		
86	OHX	1	4001	-	0,6,6	-	-	-		
86	OHX	1	4042	-	0,6,6	-	-	-		
86	OHX	1	3929	-	0,6,6	-	-	-		
86	OHX	2	2140	-	0,6,6	-	-	-		
86	OHX	7	218	-	0,6,6	-	-	-		
86	OHX	2	2031	85	0,6,6	-	-	-		
86	OHX	2	2055	-	0,6,6	-	-	-		
86	OHX	5	3925	-	0,6,6	-	-	-		
86	OHX	1	3931	-	0,6,6	-	-	-		
86	OHX	5	4024	-	0,6,6	-	-	-		
86	OHX	6	2064	-	0,6,6	-	-	-		
86	OHX	1	3999	-	0,6,6	-	-	-		
86	OHX	7	223	-	0,6,6	-	-	-		
86	OHX	1	3916	-	0,6,6	-	-	-		
86	OHX	2	2073	-	0,6,6	-	-	-		
86	OHX	1	4173	-	0,6,6	-	-	-		
86	OHX	5	4017	85	0,6,6	-	-	-		
86	OHX	5	4107	-	0,6,6	-	-	-		
86	OHX	6	2192	-	0,6,6	-	-	-		
86	OHX	8	224	-	0,6,6	-	-	-		
86	OHX	2	2151	-	0,6,6	-	-	-		
86	OHX	2	2165	-	0,6,6	-	-	-		
86	OHX	1	4066	85	0,6,6	-	-	-		
86	OHX	1	3982	85	0,6,6	-	-	-		
86	OHX	2	2027	-	0,6,6	-	-	-		
86	OHX	6	2132	-	0,6,6	-	-	-		
88	ZBA	5	4256	85	36,36,36	1.38	2 (5%)	49,58,58	1.76	7 (14%)
86	OHX	1	4164	-	0,6,6	-	-	-		
86	OHX	6	2056	85	0,6,6	-	-	-		
86	OHX	1	4091	-	0,6,6	-	-	-		
86	OHX	2	2088	-	0,6,6	-	-	-		
86	OHX	1	3903	85	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	4138	-	0,6,6	-	-	-		
86	OHX	6	2154	-	0,6,6	-	-	-		
86	OHX	5	4013	-	0,6,6	-	-	-		
86	OHX	1	3937	-	0,6,6	-	-	-		
86	OHX	1	4166	-	0,6,6	-	-	-		
86	OHX	1	4184	-	0,6,6	-	-	-		
86	OHX	1	3917	85	0,6,6	-	-	-		
86	OHX	1	3975	-	0,6,6	-	-	-		
86	OHX	5	4025	-	0,6,6	-	-	-		
86	OHX	7	228	85	0,6,6	-	-	-		
86	OHX	6	2141	-	0,6,6	-	-	-		
86	OHX	2	2126	-	0,6,6	-	-	-		
86	OHX	2	2076	-	0,6,6	-	-	-		
86	OHX	1	3885	85	0,6,6	-	-	-		
86	OHX	1	4179	-	0,6,6	-	-	-		
86	OHX	5	3987	-	0,6,6	-	-	-		
86	OHX	5	4028	85	0,6,6	-	-	-		
86	OHX	5	4086	85	0,6,6	-	-	-		
86	OHX	1	4120	-	0,6,6	-	-	-		
86	OHX	5	4186	-	0,6,6	-	-	-		
86	OHX	C5	201	-	0,6,6	-	-	-		
86	OHX	1	3946	-	0,6,6	-	-	-		
86	OHX	1	3965	-	0,6,6	-	-	-		
86	OHX	4	231	-	0,6,6	-	-	-		
86	OHX	5	3948	-	0,6,6	-	-	-		
86	OHX	5	4029	85	0,6,6	-	-	-		
86	OHX	1	3949	-	0,6,6	-	-	-		
86	OHX	5	4175	85	0,6,6	-	-	-		
86	OHX	5	4237	-	0,6,6	-	-	-		
86	OHX	1	3886	-	0,6,6	-	-	-		
86	OHX	1	3875	-	0,6,6	-	-	-		
86	OHX	2	2172	-	0,6,6	-	-	-		
86	OHX	1	4090	-	0,6,6	-	-	-		
86	OHX	2	2060	-	0,6,6	-	-	-		
86	OHX	6	2180	-	0,6,6	-	-	-		
86	OHX	5	4076	-	0,6,6	-	-	-		
86	OHX	5	4115	85	0,6,6	-	-	-		
86	OHX	6	2099	-	0,6,6	-	-	-		
86	OHX	5	3999	-	0,6,6	-	-	-		
86	OHX	8	215	-	0,6,6	-	-	-		
86	OHX	5	4074	85	0,6,6	-	-	-		
86	OHX	7	221	85	0,6,6	-	-	-		
86	OHX	4	225	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	4031	-	0,6,6	-	-	-		
86	OHX	5	3938	85	0,6,6	-	-	-		
86	OHX	5	4236	-	0,6,6	-	-	-		
86	OHX	1	3873	-	0,6,6	-	-	-		
86	OHX	6	2048	-	0,6,6	-	-	-		
86	OHX	6	2082	-	0,6,6	-	-	-		
86	OHX	5	4205	-	0,6,6	-	-	-		
86	OHX	1	4106	85	0,6,6	-	-	-		
86	OHX	5	4054	-	0,6,6	-	-	-		
86	OHX	1	4160	-	0,6,6	-	-	-		
86	OHX	2	2081	-	0,6,6	-	-	-		
86	OHX	1	4145	-	0,6,6	-	-	-		
86	OHX	1	4170	-	0,6,6	-	-	-		
86	OHX	5	4012	85	0,6,6	-	-	-		
86	OHX	2	2062	-	0,6,6	-	-	-		
86	OHX	2	2131	-	0,6,6	-	-	-		
86	OHX	1	4096	-	0,6,6	-	-	-		
86	OHX	6	2127	-	0,6,6	-	-	-		
86	OHX	1	4030	-	0,6,6	-	-	-		
86	OHX	1	4151	-	0,6,6	-	-	-		
86	OHX	2	2030	-	0,6,6	-	-	-		
86	OHX	4	227	-	0,6,6	-	-	-		
86	OHX	6	2068	-	0,6,6	-	-	-		
86	OHX	1	3979	-	0,6,6	-	-	-		
86	OHX	2	2065	-	0,6,6	-	-	-		
86	OHX	1	3862	-	0,6,6	-	-	-		
86	OHX	1	3969	85	0,6,6	-	-	-		
86	OHX	1	3888	85	0,6,6	-	-	-		
86	OHX	1	3996	-	0,6,6	-	-	-		
86	OHX	1	4027	-	0,6,6	-	-	-		
86	OHX	1	3913	-	0,6,6	-	-	-		
86	OHX	1	4052	-	0,6,6	-	-	-		
86	OHX	6	2151	-	0,6,6	-	-	-		
86	OHX	2	2056	-	0,6,6	-	-	-		
86	OHX	5	4050	-	0,6,6	-	-	-		
86	OHX	5	4137	-	0,6,6	-	-	-		
86	OHX	1	4063	-	0,6,6	-	-	-		
86	OHX	2	2089	-	0,6,6	-	-	-		
86	OHX	5	4002	-	0,6,6	-	-	-		
86	OHX	5	3907	-	0,6,6	-	-	-		
86	OHX	1	3977	-	0,6,6	-	-	-		
86	OHX	1	4043	-	0,6,6	-	-	-		
86	OHX	1	3989	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	4071	-	0,6,6	-	-	-		
86	OHX	5	3946	-	0,6,6	-	-	-		
86	OHX	5	4240	-	0,6,6	-	-	-		
86	OHX	6	2122	-	0,6,6	-	-	-		
86	OHX	5	3949	-	0,6,6	-	-	-		
86	OHX	1	3870	-	0,6,6	-	-	-		
86	OHX	1	3935	-	0,6,6	-	-	-		
86	OHX	1	4085	-	0,6,6	-	-	-		
86	OHX	6	2186	-	0,6,6	-	-	-		
86	OHX	5	4093	-	0,6,6	-	-	-		
86	OHX	5	3940	-	0,6,6	-	-	-		
86	OHX	1	4006	-	0,6,6	-	-	-		
86	OHX	5	3974	-	0,6,6	-	-	-		
86	OHX	1	3879	-	0,6,6	-	-	-		
86	OHX	1	4192	-	0,6,6	-	-	-		
86	OHX	2	2066	-	0,6,6	-	-	-		
86	OHX	2	2145	-	0,6,6	-	-	-		
86	OHX	1	3962	-	0,6,6	-	-	-		
86	OHX	5	4010	-	0,6,6	-	-	-		
86	OHX	1	3933	-	0,6,6	-	-	-		
86	OHX	1	3959	-	0,6,6	-	-	-		
86	OHX	6	2052	-	0,6,6	-	-	-		
86	OHX	1	3944	-	0,6,6	-	-	-		
86	OHX	1	4054	-	0,6,6	-	-	-		
86	OHX	1	4104	85	0,6,6	-	-	-		
86	OHX	2	2053	-	0,6,6	-	-	-		
86	OHX	2	2113	-	0,6,6	-	-	-		
86	OHX	1	4092	-	0,6,6	-	-	-		
86	OHX	1	4163	-	0,6,6	-	-	-		
86	OHX	6	2172	-	0,6,6	-	-	-		
86	OHX	5	4087	-	0,6,6	-	-	-		
86	OHX	6	2161	-	0,6,6	-	-	-		
86	OHX	1	3871	-	0,6,6	-	-	-		
86	OHX	2	2097	-	0,6,6	-	-	-		
86	OHX	5	3993	-	0,6,6	-	-	-		
86	OHX	2	2032	-	0,6,6	-	-	-		
86	OHX	2	2094	-	0,6,6	-	-	-		
86	OHX	1	4185	-	0,6,6	-	-	-		
86	OHX	6	2150	-	0,6,6	-	-	-		
86	OHX	2	2087	-	0,6,6	-	-	-		
86	OHX	1	4062	85	0,6,6	-	-	-		
86	OHX	1	4142	-	0,6,6	-	-	-		
86	OHX	6	2171	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	6	2123	85	0,6,6	-	-	-		
86	OHX	1	4105	-	0,6,6	-	-	-		
86	OHX	6	2096	-	0,6,6	-	-	-		
86	OHX	1	3995	-	0,6,6	-	-	-		
86	OHX	5	4022	-	0,6,6	-	-	-		
86	OHX	5	4188	-	0,6,6	-	-	-		
86	OHX	5	4199	-	0,6,6	-	-	-		
86	OHX	1	3952	-	0,6,6	-	-	-		
86	OHX	6	2085	-	0,6,6	-	-	-		
86	OHX	6	2051	-	0,6,6	-	-	-		
86	OHX	2	2044	-	0,6,6	-	-	-		
86	OHX	2	2128	-	0,6,6	-	-	-		
86	OHX	1	4200	85	0,6,6	-	-	-		
86	OHX	2	2148	-	0,6,6	-	-	-		
86	OHX	5	3923	-	0,6,6	-	-	-		
86	OHX	5	4159	-	0,6,6	-	-	-		
86	OHX	5	4241	-	0,6,6	-	-	-		
86	OHX	1	3880	-	0,6,6	-	-	-		
86	OHX	2	2179	-	0,6,6	-	-	-		
86	OHX	1	4067	-	0,6,6	-	-	-		
86	OHX	5	4189	-	0,6,6	-	-	-		
86	OHX	o7	502	-	0,6,6	-	-	-		
86	OHX	1	4180	-	0,6,6	-	-	-		
86	OHX	S9	201	-	0,6,6	-	-	-		
86	OHX	5	4196	-	0,6,6	-	-	-		
86	OHX	6	2067	-	0,6,6	-	-	-		
86	OHX	s4	301	-	0,6,6	-	-	-		
86	OHX	5	3931	85	0,6,6	-	-	-		
86	OHX	5	4234	-	0,6,6	-	-	-		
86	OHX	s8	303	-	0,6,6	-	-	-		
86	OHX	1	3911	-	0,6,6	-	-	-		
86	OHX	4	235	-	0,6,6	-	-	-		
86	OHX	1	4080	-	0,6,6	-	-	-		
86	OHX	1	3908	-	0,6,6	-	-	-		
86	OHX	M7	207	-	0,6,6	-	-	-		
86	OHX	6	2095	-	0,6,6	-	-	-		
86	OHX	5	4174	-	0,6,6	-	-	-		
86	OHX	5	4181	85	0,6,6	-	-	-		
86	OHX	1	4117	85	0,6,6	-	-	-		
86	OHX	6	2107	-	0,6,6	-	-	-		
86	OHX	2	2029	-	0,6,6	-	-	-		
86	OHX	6	2116	-	0,6,6	-	-	-		
86	OHX	5	3997	85	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	4016	-	0,6,6	-	-	-		
86	OHX	5	4073	-	0,6,6	-	-	-		
86	OHX	5	4035	-	0,6,6	-	-	-		
86	OHX	1	3927	-	0,6,6	-	-	-		
86	OHX	5	3981	-	0,6,6	-	-	-		
86	OHX	1	3920	-	0,6,6	-	-	-		
86	OHX	1	4087	-	0,6,6	-	-	-		
86	OHX	2	2054	-	0,6,6	-	-	-		
86	OHX	1	3924	85	0,6,6	-	-	-		
86	OHX	1	4178	-	0,6,6	-	-	-		
86	OHX	1	4036	-	0,6,6	-	-	-		
86	OHX	2	2042	-	0,6,6	-	-	-		
86	OHX	1	4150	-	0,6,6	-	-	-		
86	OHX	5	4177	-	0,6,6	-	-	-		
86	OHX	1	4122	85	0,6,6	-	-	-		
86	OHX	5	3953	-	0,6,6	-	-	-		
86	OHX	5	4033	-	0,6,6	-	-	-		
86	OHX	1	3928	-	0,6,6	-	-	-		
86	OHX	5	4153	-	0,6,6	-	-	-		
86	OHX	2	2147	-	0,6,6	-	-	-		
86	OHX	7	222	-	0,6,6	-	-	-		
86	OHX	5	4038	-	0,6,6	-	-	-		
86	OHX	2	2104	-	0,6,6	-	-	-		
86	OHX	1	3867	-	0,6,6	-	-	-		
86	OHX	5	4062	-	0,6,6	-	-	-		
86	OHX	5	4208	-	0,6,6	-	-	-		
86	OHX	n5	201	-	0,6,6	-	-	-		
86	OHX	5	4179	85	0,6,6	-	-	-		
86	OHX	1	3910	-	0,6,6	-	-	-		
86	OHX	5	3990	-	0,6,6	-	-	-		
86	OHX	1	3941	-	0,6,6	-	-	-		
86	OHX	1	4051	-	0,6,6	-	-	-		
86	OHX	5	4231	-	0,6,6	-	-	-		
86	OHX	1	3972	-	0,6,6	-	-	-		
86	OHX	2	2149	-	0,6,6	-	-	-		
86	OHX	5	3988	-	0,6,6	-	-	-		
86	OHX	6	2118	-	0,6,6	-	-	-		
86	OHX	5	4000	-	0,6,6	-	-	-		
86	OHX	5	4140	-	0,6,6	-	-	-		
86	OHX	2	2069	-	0,6,6	-	-	-		
86	OHX	2	2077	-	0,6,6	-	-	-		
86	OHX	S8	302	-	0,6,6	-	-	-		
86	OHX	2	2048	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	2	2115	-	0,6,6	-	-	-		
86	OHX	2	2161	-	0,6,6	-	-	-		
86	OHX	5	4225	-	0,6,6	-	-	-		
86	OHX	4	233	-	0,6,6	-	-	-		
86	OHX	2	2123	-	0,6,6	-	-	-		
86	OHX	2	2153	-	0,6,6	-	-	-		
86	OHX	2	2061	85	0,6,6	-	-	-		
86	OHX	1	3894	-	0,6,6	-	-	-		
86	OHX	5	4117	-	0,6,6	-	-	-		
86	OHX	2	2103	-	0,6,6	-	-	-		
86	OHX	2	2171	-	0,6,6	-	-	-		
86	OHX	2	2095	-	0,6,6	-	-	-		
86	OHX	1	3877	-	0,6,6	-	-	-		
86	OHX	2	2064	-	0,6,6	-	-	-		
86	OHX	5	3992	85	0,6,6	-	-	-		
86	OHX	5	4213	-	0,6,6	-	-	-		
86	OHX	1	4068	-	0,6,6	-	-	-		
86	OHX	6	2071	-	0,6,6	-	-	-		
86	OHX	5	4113	-	0,6,6	-	-	-		
86	OHX	5	4207	-	0,6,6	-	-	-		
86	OHX	5	4172	-	0,6,6	-	-	-		
86	OHX	1	3985	-	0,6,6	-	-	-		
86	OHX	2	2110	-	0,6,6	-	-	-		
86	OHX	1	4109	-	0,6,6	-	-	-		
86	OHX	6	2097	-	0,6,6	-	-	-		
86	OHX	6	2165	-	0,6,6	-	-	-		
86	OHX	5	4077	-	0,6,6	-	-	-		
86	OHX	L3	404	-	0,6,6	-	-	-		
86	OHX	5	4069	-	0,6,6	-	-	-		
86	OHX	6	2143	-	0,6,6	-	-	-		
86	OHX	1	4017	-	0,6,6	-	-	-		
86	OHX	5	3928	-	0,6,6	-	-	-		
86	OHX	sR	401	-	0,6,6	-	-	-		
86	OHX	2	2102	-	0,6,6	-	-	-		
86	OHX	2	2026	-	0,6,6	-	-	-		
86	OHX	5	4246	85	0,6,6	-	-	-		
86	OHX	1	4157	-	0,6,6	-	-	-		
86	OHX	6	2160	-	0,6,6	-	-	-		
86	OHX	1	4048	-	0,6,6	-	-	-		
86	OHX	1	4138	85	0,6,6	-	-	-		
86	OHX	6	2201	-	0,6,6	-	-	-		
86	OHX	5	4127	-	0,6,6	-	-	-		
86	OHX	1	3939	85	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	4161	85	0,6,6	-	-	-		
86	OHX	6	2147	-	0,6,6	-	-	-		
86	OHX	6	2089	-	0,6,6	-	-	-		
86	OHX	2	2090	-	0,6,6	-	-	-		
86	OHX	7	219	-	0,6,6	-	-	-		
86	OHX	5	4221	-	0,6,6	-	-	-		
86	OHX	5	4116	-	0,6,6	-	-	-		
86	OHX	2	2124	-	0,6,6	-	-	-		
86	OHX	1	4025	-	0,6,6	-	-	-		
86	OHX	6	2191	-	0,6,6	-	-	-		
86	OHX	l5	305	-	0,6,6	-	-	-		
86	OHX	5	4091	85	0,6,6	-	-	-		
86	OHX	1	3976	85	0,6,6	-	-	-		
86	OHX	m0	301	-	0,6,6	-	-	-		
86	OHX	1	3863	-	0,6,6	-	-	-		
86	OHX	6	2121	-	0,6,6	-	-	-		
86	OHX	1	3938	-	0,6,6	-	-	-		
86	OHX	5	4158	-	0,6,6	-	-	-		
86	OHX	5	4226	85	0,6,6	-	-	-		
86	OHX	5	4004	-	0,6,6	-	-	-		
86	OHX	2	2050	-	0,6,6	-	-	-		
86	OHX	1	3914	-	0,6,6	-	-	-		
86	OHX	5	4059	-	0,6,6	-	-	-		
86	OHX	2	2134	-	0,6,6	-	-	-		
86	OHX	1	3932	85	0,6,6	-	-	-		
86	OHX	1	4046	-	0,6,6	-	-	-		
86	OHX	1	4100	-	0,6,6	-	-	-		
86	OHX	2	2035	-	0,6,6	-	-	-		
86	OHX	1	4156	-	0,6,6	-	-	-		
86	OHX	5	4005	-	0,6,6	-	-	-		
86	OHX	5	4254	85	0,6,6	-	-	-		
86	OHX	2	2157	-	0,6,6	-	-	-		
86	OHX	4	237	85	0,6,6	-	-	-		
86	OHX	7	217	-	0,6,6	-	-	-		
86	OHX	5	4210	-	0,6,6	-	-	-		
86	OHX	1	3906	-	0,6,6	-	-	-		
86	OHX	1	3978	-	0,6,6	-	-	-		
86	OHX	2	2033	-	0,6,6	-	-	-		
86	OHX	6	2198	-	0,6,6	-	-	-		
86	OHX	6	2073	85	0,6,6	-	-	-		
86	OHX	5	3984	-	0,6,6	-	-	-		
86	OHX	L3	406	-	0,6,6	-	-	-		
86	OHX	5	4190	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4003	-	0,6,6	-	-	-		
86	OHX	5	4015	-	0,6,6	-	-	-		
86	OHX	1	4008	-	0,6,6	-	-	-		
86	OHX	6	2058	-	0,6,6	-	-	-		
86	OHX	1	3973	-	0,6,6	-	-	-		
86	OHX	5	3986	-	0,6,6	-	-	-		
86	OHX	5	3967	85	0,6,6	-	-	-		
86	OHX	5	4130	-	0,6,6	-	-	-		
86	OHX	2	2112	-	0,6,6	-	-	-		
86	OHX	6	2049	-	0,6,6	-	-	-		
86	OHX	1	4023	-	0,6,6	-	-	-		
86	OHX	5	4097	-	0,6,6	-	-	-		
86	OHX	6	2189	-	0,6,6	-	-	-		
86	OHX	5	4123	-	0,6,6	-	-	-		
86	OHX	5	4094	-	0,6,6	-	-	-		
86	OHX	6	2152	-	0,6,6	-	-	-		
86	OHX	m1	203	-	0,6,6	-	-	-		
86	OHX	5	4055	-	0,6,6	-	-	-		
86	OHX	2	2130	-	0,6,6	-	-	-		
86	OHX	2	2071	85	0,6,6	-	-	-		
86	OHX	6	2133	-	0,6,6	-	-	-		
86	OHX	6	2076	-	0,6,6	-	-	-		
86	OHX	1	4203	85	0,6,6	-	-	-		
86	OHX	7	226	-	0,6,6	-	-	-		
86	OHX	2	2181	-	0,6,6	-	-	-		
86	OHX	2	2164	-	0,6,6	-	-	-		
86	OHX	5	3926	-	0,6,6	-	-	-		
86	OHX	1	4147	-	0,6,6	-	-	-		
86	OHX	5	4126	-	0,6,6	-	-	-		
86	OHX	6	2176	85	0,6,6	-	-	-		
86	OHX	1	4195	-	0,6,6	-	-	-		
86	OHX	6	2113	-	0,6,6	-	-	-		
86	OHX	5	3951	-	0,6,6	-	-	-		
86	OHX	2	2160	-	0,6,6	-	-	-		
86	OHX	1	3957	-	0,6,6	-	-	-		
86	OHX	O7	103	85	0,6,6	-	-	-		
86	OHX	6	2114	85	0,6,6	-	-	-		
86	OHX	2	2037	-	0,6,6	-	-	-		
86	OHX	6	2164	-	0,6,6	-	-	-		
86	OHX	5	3961	85	0,6,6	-	-	-		
86	OHX	5	4242	-	0,6,6	-	-	-		
86	OHX	6	2142	-	0,6,6	-	-	-		
86	OHX	5	4049	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	2	2082	85	0,6,6	-	-	-		
86	OHX	1	3936	-	0,6,6	-	-	-		
86	OHX	5	4218	-	0,6,6	-	-	-		
86	OHX	5	4110	85	0,6,6	-	-	-		
86	OHX	1	4053	-	0,6,6	-	-	-		
86	OHX	1	4199	-	0,6,6	-	-	-		
86	OHX	1	3930	-	0,6,6	-	-	-		
86	OHX	1	4154	-	0,6,6	-	-	-		
86	OHX	6	2094	-	0,6,6	-	-	-		
86	OHX	5	4031	-	0,6,6	-	-	-		
86	OHX	M0	303	-	0,6,6	-	-	-		
86	OHX	2	2139	-	0,6,6	-	-	-		
86	OHX	6	2104	-	0,6,6	-	-	-		
86	OHX	6	2131	-	0,6,6	-	-	-		
86	OHX	7	229	-	0,6,6	-	-	-		
86	OHX	2	2137	-	0,6,6	-	-	-		
86	OHX	5	4124	85	0,6,6	-	-	-		
86	OHX	5	4008	-	0,6,6	-	-	-		
86	OHX	5	4051	-	0,6,6	-	-	-		
86	OHX	5	4088	-	0,6,6	-	-	-		
86	OHX	5	4148	-	0,6,6	-	-	-		
86	OHX	6	2179	-	0,6,6	-	-	-		
86	OHX	5	3944	85	0,6,6	-	-	-		
86	OHX	1	3921	-	0,6,6	-	-	-		
86	OHX	2	2034	-	0,6,6	-	-	-		
86	OHX	1	3956	-	0,6,6	-	-	-		
86	OHX	2	2058	-	0,6,6	-	-	-		
86	OHX	5	4023	-	0,6,6	-	-	-		
86	OHX	5	4209	-	0,6,6	-	-	-		
86	OHX	1	4198	-	0,6,6	-	-	-		
86	OHX	5	4014	-	0,6,6	-	-	-		
86	OHX	5	4118	-	0,6,6	-	-	-		
86	OHX	1	4131	-	0,6,6	-	-	-		
86	OHX	2	2039	-	0,6,6	-	-	-		
86	OHX	2	2138	-	0,6,6	-	-	-		
86	OHX	1	4007	-	0,6,6	-	-	-		
86	OHX	1	4194	-	0,6,6	-	-	-		
86	OHX	1	4201	-	0,6,6	-	-	-		
86	OHX	2	2174	-	0,6,6	-	-	-		
86	OHX	6	2129	-	0,6,6	-	-	-		
86	OHX	5	3945	-	0,6,6	-	-	-		
86	OHX	5	3991	-	0,6,6	-	-	-		
86	OHX	7	220	85	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	8	226	-	0,6,6	-	-	-		
86	OHX	1	4098	-	0,6,6	-	-	-		
86	OHX	1	4193	-	0,6,6	-	-	-		
86	OHX	7	227	-	0,6,6	-	-	-		
86	OHX	5	4044	-	0,6,6	-	-	-		
86	OHX	5	4235	-	0,6,6	-	-	-		
86	OHX	5	4095	-	0,6,6	-	-	-		
86	OHX	1	4125	-	0,6,6	-	-	-		
86	OHX	5	3963	-	0,6,6	-	-	-		
86	OHX	1	3918	-	0,6,6	-	-	-		
86	OHX	5	3922	-	0,6,6	-	-	-		
86	OHX	5	4222	85	0,6,6	-	-	-		
86	OHX	1	4144	-	0,6,6	-	-	-		
86	OHX	5	3998	-	0,6,6	-	-	-		
86	OHX	5	4229	-	0,6,6	-	-	-		
86	OHX	2	2182	85	0,6,6	-	-	-		
86	OHX	1	3887	-	0,6,6	-	-	-		
86	OHX	5	3980	85	0,6,6	-	-	-		
86	OHX	5	4109	-	0,6,6	-	-	-		
86	OHX	5	4079	-	0,6,6	-	-	-		
86	OHX	5	4164	-	0,6,6	-	-	-		
86	OHX	l4	403	-	0,6,6	-	-	-		
86	OHX	1	4073	-	0,6,6	-	-	-		
86	OHX	5	4111	-	0,6,6	-	-	-		
86	OHX	1	4041	-	0,6,6	-	-	-		
86	OHX	1	3981	-	0,6,6	-	-	-		
86	OHX	5	4034	-	0,6,6	-	-	-		
86	OHX	2	2152	-	0,6,6	-	-	-		
86	OHX	1	4074	-	0,6,6	-	-	-		
86	OHX	5	3930	-	0,6,6	-	-	-		
86	OHX	5	3912	-	0,6,6	-	-	-		
86	OHX	5	4249	-	0,6,6	-	-	-		
86	OHX	1	3889	-	0,6,6	-	-	-		
86	OHX	1	4089	-	0,6,6	-	-	-		
86	OHX	M5	303	-	0,6,6	-	-	-		
86	OHX	4	223	-	0,6,6	-	-	-		
86	OHX	5	3958	-	0,6,6	-	-	-		
86	OHX	5	4102	-	0,6,6	-	-	-		
86	OHX	5	4247	-	0,6,6	-	-	-		
86	OHX	l3	404	-	0,6,6	-	-	-		
86	OHX	5	4248	-	0,6,6	-	-	-		
86	OHX	2	2043	-	0,6,6	-	-	-		
86	OHX	6	2163	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3891	-	0,6,6	-	-	-		
86	OHX	1	3971	-	0,6,6	-	-	-		
86	OHX	5	3956	-	0,6,6	-	-	-		
86	OHX	5	4001	-	0,6,6	-	-	-		
86	OHX	1	4129	-	0,6,6	-	-	-		
86	OHX	1	4162	-	0,6,6	-	-	-		
86	OHX	2	2109	-	0,6,6	-	-	-		
86	OHX	1	3915	-	0,6,6	-	-	-		
86	OHX	1	4065	85	0,6,6	-	-	-		
86	OHX	6	2197	85	0,6,6	-	-	-		
86	OHX	1	3872	-	0,6,6	-	-	-		
86	OHX	5	3916	85	0,6,6	-	-	-		
86	OHX	5	4173	-	0,6,6	-	-	-		
86	OHX	2	2119	-	0,6,6	-	-	-		
86	OHX	2	2170	-	0,6,6	-	-	-		
86	OHX	1	4134	-	0,6,6	-	-	-		
86	OHX	5	4216	-	0,6,6	-	-	-		
86	OHX	2	2129	-	0,6,6	-	-	-		
86	OHX	1	4137	-	0,6,6	-	-	-		
86	OHX	5	3982	85	0,6,6	-	-	-		
86	OHX	5	4215	-	0,6,6	-	-	-		
86	OHX	1	4197	85	0,6,6	-	-	-		
86	OHX	5	3903	-	0,6,6	-	-	-		
86	OHX	m4	201	-	0,6,6	-	-	-		
86	OHX	2	2117	-	0,6,6	-	-	-		
86	OHX	2	2111	-	0,6,6	-	-	-		
86	OHX	5	4166	-	0,6,6	-	-	-		
86	OHX	5	4206	-	0,6,6	-	-	-		
86	OHX	1	3860	-	0,6,6	-	-	-		
86	OHX	1	4029	-	0,6,6	-	-	-		
86	OHX	5	3975	-	0,6,6	-	-	-		
86	OHX	1	4026	-	0,6,6	-	-	-		
86	OHX	6	2126	-	0,6,6	-	-	-		
86	OHX	1	4021	85	0,6,6	-	-	-		
86	OHX	5	4011	-	0,6,6	-	-	-		
86	OHX	5	3960	85	0,6,6	-	-	-		
86	OHX	6	2166	-	0,6,6	-	-	-		
86	OHX	1	4204	85	0,6,6	-	-	-		
86	OHX	1	3974	-	0,6,6	-	-	-		
86	OHX	5	3962	85	0,6,6	-	-	-		
86	OHX	5	4103	-	0,6,6	-	-	-		
86	OHX	5	4057	-	0,6,6	-	-	-		
86	OHX	2	2175	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	4010	-	0,6,6	-	-	-		
86	OHX	1	4060	-	0,6,6	-	-	-		
86	OHX	2	2057	-	0,6,6	-	-	-		
86	OHX	1	4037	85	0,6,6	-	-	-		
86	OHX	1	4076	-	0,6,6	-	-	-		
86	OHX	6	2053	-	0,6,6	-	-	-		
86	OHX	6	2135	-	0,6,6	-	-	-		
86	OHX	C3	201	-	0,6,6	-	-	-		
86	OHX	6	2177	-	0,6,6	-	-	-		
86	OHX	1	4181	85	0,6,6	-	-	-		
86	OHX	1	4174	-	0,6,6	-	-	-		
86	OHX	5	3934	-	0,6,6	-	-	-		
86	OHX	5	4167	-	0,6,6	-	-	-		
86	OHX	2	2083	-	0,6,6	-	-	-		
86	OHX	8	220	-	0,6,6	-	-	-		
86	OHX	2	2040	-	0,6,6	-	-	-		
86	OHX	6	2100	-	0,6,6	-	-	-		
86	OHX	5	4129	-	0,6,6	-	-	-		
86	OHX	5	4133	-	0,6,6	-	-	-		
86	OHX	s1	302	-	0,6,6	-	-	-		
86	OHX	6	2155	-	0,6,6	-	-	-		
86	OHX	5	4101	-	0,6,6	-	-	-		
86	OHX	1	3994	-	0,6,6	-	-	-		
86	OHX	2	2092	-	0,6,6	-	-	-		
86	OHX	5	4252	-	0,6,6	-	-	-		
86	OHX	1	4047	85	0,6,6	-	-	-		
86	OHX	1	4075	-	0,6,6	-	-	-		
86	OHX	1	3865	-	0,6,6	-	-	-		
86	OHX	1	4078	-	0,6,6	-	-	-		
86	OHX	5	4139	-	0,6,6	-	-	-		
86	OHX	5	4168	-	0,6,6	-	-	-		
86	OHX	1	4112	-	0,6,6	-	-	-		
86	OHX	6	2194	-	0,6,6	-	-	-		
86	OHX	5	4068	-	0,6,6	-	-	-		
86	OHX	1	4188	-	0,6,6	-	-	-		
86	OHX	5	4253	-	0,6,6	-	-	-		
86	OHX	5	4160	-	0,6,6	-	-	-		
86	OHX	6	2157	-	0,6,6	-	-	-		
86	OHX	2	2098	-	0,6,6	-	-	-		
86	OHX	6	2112	-	0,6,6	-	-	-		
86	OHX	5	3966	-	0,6,6	-	-	-		
86	OHX	2	2085	-	0,6,6	-	-	-		
86	OHX	2	2178	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	4	228	85	0,6,6	-	-	-		
86	OHX	5	3969	-	0,6,6	-	-	-		
86	OHX	1	3988	-	0,6,6	-	-	-		
86	OHX	5	4026	-	0,6,6	-	-	-		
86	OHX	5	4052	-	0,6,6	-	-	-		
86	OHX	1	3869	-	0,6,6	-	-	-		
86	OHX	1	4149	-	0,6,6	-	-	-		
86	OHX	1	4155	-	0,6,6	-	-	-		
86	OHX	c8	203	-	0,6,6	-	-	-		
86	OHX	4	229	-	0,6,6	-	-	-		
86	OHX	1	3904	-	0,6,6	-	-	-		
86	OHX	5	4063	-	0,6,6	-	-	-		
86	OHX	1	4152	-	0,6,6	-	-	-		
86	OHX	D9	102	-	0,6,6	-	-	-		
86	OHX	5	4066	-	0,6,6	-	-	-		
86	OHX	6	2138	-	0,6,6	-	-	-		
88	ZBA	1	4206	85	36,36,36	1.65	3 (8%)	49,58,58	1.81	4 (8%)
86	OHX	5	3977	-	0,6,6	-	-	-		
86	OHX	5	4043	-	0,6,6	-	-	-		
86	OHX	1	3940	85	0,6,6	-	-	-		
86	OHX	1	3954	-	0,6,6	-	-	-		
86	OHX	1	3955	-	0,6,6	-	-	-		
86	OHX	1	4121	-	0,6,6	-	-	-		
86	OHX	1	4123	-	0,6,6	-	-	-		
86	OHX	6	2090	-	0,6,6	-	-	-		
86	OHX	5	4071	-	0,6,6	-	-	-		
86	OHX	5	4084	-	0,6,6	-	-	-		
86	OHX	8	227	-	0,6,6	-	-	-		
86	OHX	5	4182	-	0,6,6	-	-	-		
86	OHX	2	2105	-	0,6,6	-	-	-		
86	OHX	2	2159	-	0,6,6	-	-	-		
86	OHX	1	3868	-	0,6,6	-	-	-		
86	OHX	1	4083	-	0,6,6	-	-	-		
86	OHX	5	3917	-	0,6,6	-	-	-		
86	OHX	5	4085	-	0,6,6	-	-	-		
86	OHX	1	4082	-	0,6,6	-	-	-		
86	OHX	5	4006	-	0,6,6	-	-	-		
86	OHX	6	2105	-	0,6,6	-	-	-		
86	OHX	5	4072	-	0,6,6	-	-	-		
86	OHX	3	214	-	0,6,6	-	-	-		
86	OHX	1	3905	-	0,6,6	-	-	-		
86	OHX	5	3933	-	0,6,6	-	-	-		
86	OHX	5	3959	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	3	220	-	0,6,6	-	-	-		
86	OHX	c5	201	-	0,6,6	-	-	-		
86	OHX	1	4176	85	0,6,6	-	-	-		
86	OHX	l9	600	-	0,6,6	-	-	-		
86	OHX	1	3864	-	0,6,6	-	-	-		
86	OHX	1	4012	-	0,6,6	-	-	-		
86	OHX	6	2124	-	0,6,6	-	-	-		
86	OHX	1	3950	-	0,6,6	-	-	-		
86	OHX	6	2047	-	0,6,6	-	-	-		
86	OHX	1	4099	-	0,6,6	-	-	-		
86	OHX	5	4092	85	0,6,6	-	-	-		
86	OHX	1	3861	-	0,6,6	-	-	-		
86	OHX	8	216	-	0,6,6	-	-	-		
86	OHX	1	3919	-	0,6,6	-	-	-		
86	OHX	1	3909	-	0,6,6	-	-	-		
86	OHX	6	2077	-	0,6,6	-	-	-		
86	OHX	5	4019	-	0,6,6	-	-	-		
86	OHX	1	3968	-	0,6,6	-	-	-		
86	OHX	5	4244	-	0,6,6	-	-	-		
86	OHX	1	4032	-	0,6,6	-	-	-		
86	OHX	6	2065	-	0,6,6	-	-	-		
86	OHX	2	2122	-	0,6,6	-	-	-		
86	OHX	1	4114	-	0,6,6	-	-	-		
86	OHX	5	4142	-	0,6,6	-	-	-		
86	OHX	5	3995	-	0,6,6	-	-	-		
86	OHX	1	3876	-	0,6,6	-	-	-		
86	OHX	5	4030	85	0,6,6	-	-	-		
86	OHX	5	4151	-	0,6,6	-	-	-		
86	OHX	6	2145	-	0,6,6	-	-	-		
86	OHX	c3	201	-	0,6,6	-	-	-		
86	OHX	5	3952	-	0,6,6	-	-	-		
86	OHX	6	2134	-	0,6,6	-	-	-		
86	OHX	6	2204	-	0,6,6	-	-	-		
86	OHX	1	4024	-	0,6,6	-	-	-		
86	OHX	5	4061	-	0,6,6	-	-	-		
86	OHX	2	2150	-	0,6,6	-	-	-		
86	OHX	2	2063	-	0,6,6	-	-	-		
86	OHX	C8	201	-	0,6,6	-	-	-		
86	OHX	1	4148	-	0,6,6	-	-	-		
86	OHX	1	4202	-	0,6,6	-	-	-		
86	OHX	1	4169	-	0,6,6	-	-	-		
86	OHX	3	221	-	0,6,6	-	-	-		
86	OHX	6	2140	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	3965	-	0,6,6	-	-	-		
86	OHX	2	2156	-	0,6,6	-	-	-		
86	OHX	N1	201	-	0,6,6	-	-	-		
86	OHX	2	2052	-	0,6,6	-	-	-		
86	OHX	5	4251	-	0,6,6	-	-	-		
86	OHX	2	2038	-	0,6,6	-	-	-		
86	OHX	M9	202	-	0,6,6	-	-	-		
86	OHX	1	3997	-	0,6,6	-	-	-		
86	OHX	2	2166	-	0,6,6	-	-	-		
86	OHX	6	2093	85	0,6,6	-	-	-		
86	OHX	6	2110	-	0,6,6	-	-	-		
86	OHX	5	4180	-	0,6,6	-	-	-		
86	OHX	8	222	-	0,6,6	-	-	-		
86	OHX	5	4239	-	0,6,6	-	-	-		
86	OHX	5	4027	-	0,6,6	-	-	-		
86	OHX	1	4108	-	0,6,6	-	-	-		
86	OHX	2	2049	-	0,6,6	-	-	-		
86	OHX	2	2125	-	0,6,6	-	-	-		
86	OHX	5	4058	-	0,6,6	-	-	-		
86	OHX	2	2107	-	0,6,6	-	-	-		
86	OHX	5	4147	-	0,6,6	-	-	-		
86	OHX	5	4223	-	0,6,6	-	-	-		
86	OHX	5	4045	-	0,6,6	-	-	-		
86	OHX	o2	201	-	0,6,6	-	-	-		
86	OHX	6	2139	-	0,6,6	-	-	-		
86	OHX	1	3884	-	0,6,6	-	-	-		
86	OHX	2	2091	-	0,6,6	-	-	-		
86	OHX	5	3989	-	0,6,6	-	-	-		
86	OHX	1	4141	-	0,6,6	-	-	-		
86	OHX	6	2136	-	0,6,6	-	-	-		
86	OHX	5	3927	-	0,6,6	-	-	-		
86	OHX	5	4178	85	0,6,6	-	-	-		
86	OHX	1	4035	-	0,6,6	-	-	-		
86	OHX	1	4064	-	0,6,6	-	-	-		
86	OHX	1	4165	-	0,6,6	-	-	-		
86	OHX	6	2184	-	0,6,6	-	-	-		
86	OHX	5	4104	-	0,6,6	-	-	-		
86	OHX	1	3895	-	0,6,6	-	-	-		
86	OHX	2	2177	-	0,6,6	-	-	-		
86	OHX	6	2130	-	0,6,6	-	-	-		
86	OHX	1	3899	-	0,6,6	-	-	-		
86	OHX	5	4192	-	0,6,6	-	-	-		
86	OHX	2	2176	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	4034	-	0,6,6	-	-	-		
86	OHX	5	3968	-	0,6,6	-	-	-		
86	OHX	5	4146	-	0,6,6	-	-	-		
86	OHX	1	3963	-	0,6,6	-	-	-		
86	OHX	6	2190	-	0,6,6	-	-	-		
86	OHX	5	3910	-	0,6,6	-	-	-		
86	OHX	1	4128	-	0,6,6	-	-	-		
86	OHX	1	4191	-	0,6,6	-	-	-		
86	OHX	6	2169	-	0,6,6	-	-	-		
86	OHX	1	4022	-	0,6,6	-	-	-		
86	OHX	5	3941	-	0,6,6	-	-	-		
86	OHX	5	4039	-	0,6,6	-	-	-		
86	OHX	5	4163	-	0,6,6	-	-	-		
86	OHX	1	4158	-	0,6,6	-	-	-		
86	OHX	1	3943	-	0,6,6	-	-	-		
86	OHX	1	4175	-	0,6,6	-	-	-		
86	OHX	6	2074	-	0,6,6	-	-	-		
86	OHX	1	3983	-	0,6,6	-	-	-		
86	OHX	6	2207	-	0,6,6	-	-	-		
86	OHX	1	4018	-	0,6,6	-	-	-		
86	OHX	1	4040	-	0,6,6	-	-	-		
86	OHX	2	2108	-	0,6,6	-	-	-		
86	OHX	2	2169	-	0,6,6	-	-	-		
86	OHX	5	4219	85	0,6,6	-	-	-		
86	OHX	2	2168	-	0,6,6	-	-	-		
86	OHX	O1	201	-	0,6,6	-	-	-		
86	OHX	5	4224	-	0,6,6	-	-	-		
86	OHX	1	3925	-	0,6,6	-	-	-		
86	OHX	1	4113	-	0,6,6	-	-	-		
86	OHX	5	3964	85	0,6,6	-	-	-		
86	OHX	2	2072	-	0,6,6	-	-	-		
86	OHX	m7	205	85	0,6,6	-	-	-		
86	OHX	4	226	-	0,6,6	-	-	-		
86	OHX	4	236	-	0,6,6	-	-	-		
86	OHX	O3	202	-	0,6,6	-	-	-		
86	OHX	7	225	85	0,6,6	-	-	-		
86	OHX	2	2078	-	0,6,6	-	-	-		
86	OHX	1	4132	-	0,6,6	-	-	-		
86	OHX	2	2096	-	0,6,6	-	-	-		
86	OHX	1	4107	-	0,6,6	-	-	-		
86	OHX	6	2072	-	0,6,6	-	-	-		
86	OHX	1	4050	-	0,6,6	-	-	-		
86	OHX	5	4135	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2136	85	0,6,6	-	-	-		
86	OHX	1	4127	-	0,6,6	-	-	-		
86	OHX	6	2111	-	0,6,6	-	-	-		
86	OHX	5	3947	-	0,6,6	-	-	-		
86	OHX	6	2061	-	0,6,6	-	-	-		
86	OHX	1	4013	-	0,6,6	-	-	-		
86	OHX	1	3893	-	0,6,6	-	-	-		
86	OHX	O2	201	-	0,6,6	-	-	-		
86	OHX	2	2154	-	0,6,6	-	-	-		
86	OHX	5	4083	-	0,6,6	-	-	-		
86	OHX	5	3904	-	0,6,6	-	-	-		
86	OHX	2	2041	-	0,6,6	-	-	-		
86	OHX	6	2086	-	0,6,6	-	-	-		
86	OHX	5	3939	85	0,6,6	-	-	-		
86	OHX	1	3934	-	0,6,6	-	-	-		
86	OHX	1	3987	-	0,6,6	-	-	-		
86	OHX	1	4028	-	0,6,6	-	-	-		
86	OHX	6	2081	-	0,6,6	-	-	-		
86	OHX	1	4086	-	0,6,6	-	-	-		
86	OHX	1	4186	-	0,6,6	-	-	-		
86	OHX	3	224	85	0,6,6	-	-	-		
86	OHX	1	4020	-	0,6,6	-	-	-		
86	OHX	6	2182	-	0,6,6	-	-	-		
86	OHX	5	4122	-	0,6,6	-	-	-		
86	OHX	8	217	-	0,6,6	-	-	-		
86	OHX	5	4184	-	0,6,6	-	-	-		
86	OHX	1	3948	-	0,6,6	-	-	-		
86	OHX	2	2167	-	0,6,6	-	-	-		
86	OHX	o3	202	-	0,6,6	-	-	-		
86	OHX	1	4103	-	0,6,6	-	-	-		
86	OHX	2	2146	85	0,6,6	-	-	-		
86	OHX	5	4120	-	0,6,6	-	-	-		
86	OHX	5	4105	-	0,6,6	-	-	-		
86	OHX	1	4115	-	0,6,6	-	-	-		
86	OHX	5	3914	-	0,6,6	-	-	-		
86	OHX	2	2127	-	0,6,6	-	-	-		
86	OHX	5	3972	-	0,6,6	-	-	-		
86	OHX	5	3932	-	0,6,6	-	-	-		
86	OHX	5	4046	-	0,6,6	-	-	-		
86	OHX	1	4111	85	0,6,6	-	-	-		
86	OHX	5	4156	-	0,6,6	-	-	-		
86	OHX	6	2087	-	0,6,6	-	-	-		
86	OHX	5	4132	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	8	225	-	0,6,6	-	-	-		
86	OHX	5	4042	-	0,6,6	-	-	-		
86	OHX	1	4205	-	0,6,6	-	-	-		
86	OHX	6	2063	-	0,6,6	-	-	-		
86	OHX	1	4009	-	0,6,6	-	-	-		
86	OHX	2	2084	-	0,6,6	-	-	-		
86	OHX	1	3992	-	0,6,6	-	-	-		
86	OHX	1	4015	-	0,6,6	-	-	-		
86	OHX	2	2028	-	0,6,6	-	-	-		
86	OHX	1	4139	-	0,6,6	-	-	-		
86	OHX	5	4136	-	0,6,6	-	-	-		
86	OHX	6	2206	-	0,6,6	-	-	-		
86	OHX	5	4211	-	0,6,6	-	-	-		
86	OHX	l4	402	-	0,6,6	-	-	-		
86	OHX	6	2202	-	0,6,6	-	-	-		
86	OHX	6	2079	-	0,6,6	-	-	-		
86	OHX	5	4106	-	0,6,6	-	-	-		
86	OHX	5	4143	85	0,6,6	-	-	-		
86	OHX	1	4196	-	0,6,6	-	-	-		
86	OHX	1	4094	-	0,6,6	-	-	-		
86	OHX	1	4084	-	0,6,6	-	-	-		
86	OHX	5	3973	-	0,6,6	-	-	-		
86	OHX	8	218	-	0,6,6	-	-	-		
86	OHX	6	2119	-	0,6,6	-	-	-		
86	OHX	5	3985	-	0,6,6	-	-	-		
86	OHX	1	4016	-	0,6,6	-	-	-		
86	OHX	1	4002	-	0,6,6	-	-	-		
86	OHX	5	4036	-	0,6,6	-	-	-		
86	OHX	2	2158	-	0,6,6	-	-	-		
86	OHX	1	3907	85	0,6,6	-	-	-		
86	OHX	5	3979	-	0,6,6	-	-	-		
86	OHX	5	3996	85	0,6,6	-	-	-		
86	OHX	1	4126	-	0,6,6	-	-	-		
86	OHX	6	2083	-	0,6,6	-	-	-		
86	OHX	6	2057	-	0,6,6	-	-	-		
86	OHX	1	3960	-	0,6,6	-	-	-		
86	OHX	3	217	-	0,6,6	-	-	-		
86	OHX	1	3961	-	0,6,6	-	-	-		
86	OHX	5	4157	-	0,6,6	-	-	-		
86	OHX	1	3882	-	0,6,6	-	-	-		
86	OHX	2	2068	-	0,6,6	-	-	-		
86	OHX	5	4203	-	0,6,6	-	-	-		
86	OHX	1	4093	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	4161	-	0,6,6	-	-	-		
86	OHX	1	4153	-	0,6,6	-	-	-		
86	OHX	6	2128	-	0,6,6	-	-	-		
86	OHX	2	2143	-	0,6,6	-	-	-		
86	OHX	1	4183	85	0,6,6	-	-	-		
86	OHX	8	221	-	0,6,6	-	-	-		
86	OHX	1	4182	-	0,6,6	-	-	-		
86	OHX	6	2075	-	0,6,6	-	-	-		
86	OHX	5	3929	-	0,6,6	-	-	-		
86	OHX	8	223	-	0,6,6	-	-	-		
86	OHX	q2	502	85	0,6,6	-	-	-		
86	OHX	4	232	-	0,6,6	-	-	-		
86	OHX	l5	303	-	0,6,6	-	-	-		
86	OHX	6	2195	-	0,6,6	-	-	-		
86	OHX	5	3935	-	0,6,6	-	-	-		
86	OHX	5	3942	-	0,6,6	-	-	-		
86	OHX	2	2118	-	0,6,6	-	-	-		
86	OHX	8	228	-	0,6,6	-	-	-		
86	OHX	n3	203	-	0,6,6	-	-	-		
86	OHX	1	4072	-	0,6,6	-	-	-		
86	OHX	3	223	-	0,6,6	-	-	-		
86	OHX	5	4090	-	0,6,6	-	-	-		
86	OHX	5	3976	-	0,6,6	-	-	-		
86	OHX	5	3936	85	0,6,6	-	-	-		
86	OHX	2	2036	-	0,6,6	-	-	-		
86	OHX	1	4088	-	0,6,6	-	-	-		
86	OHX	5	4212	85	0,6,6	-	-	-		
86	OHX	1	4171	-	0,6,6	-	-	-		
86	OHX	5	4195	85	0,6,6	-	-	-		
86	OHX	1	3993	-	0,6,6	-	-	-		
86	OHX	5	4154	-	0,6,6	-	-	-		
86	OHX	1	3892	-	0,6,6	-	-	-		
86	OHX	5	4112	-	0,6,6	-	-	-		
86	OHX	5	4100	85	0,6,6	-	-	-		
86	OHX	2	2155	-	0,6,6	-	-	-		
86	OHX	l5	304	-	0,6,6	-	-	-		
86	OHX	N9	101	-	0,6,6	-	-	-		
86	OHX	6	2069	85	0,6,6	-	-	-		
86	OHX	5	4170	-	0,6,6	-	-	-		
86	OHX	5	4185	-	0,6,6	-	-	-		
86	OHX	5	3950	-	0,6,6	-	-	-		
86	OHX	5	4230	-	0,6,6	-	-	-		
86	OHX	5	4099	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	3923	-	0,6,6	-	-	-		
86	OHX	5	3906	-	0,6,6	-	-	-		
86	OHX	1	3866	-	0,6,6	-	-	-		
86	OHX	1	4140	-	0,6,6	-	-	-		
86	OHX	1	4189	-	0,6,6	-	-	-		
86	OHX	5	4056	85	0,6,6	-	-	-		
86	OHX	3	218	-	0,6,6	-	-	-		
86	OHX	6	2078	85	0,6,6	-	-	-		
86	OHX	8	219	-	0,6,6	-	-	-		
86	OHX	1	4097	-	0,6,6	-	-	-		
86	OHX	2	2142	-	0,6,6	-	-	-		
86	OHX	5	4201	-	0,6,6	-	-	-		
86	OHX	L3	405	-	0,6,6	-	-	-		
86	OHX	6	2174	-	0,6,6	-	-	-		
86	OHX	5	3970	-	0,6,6	-	-	-		
86	OHX	5	4119	-	0,6,6	-	-	-		
86	OHX	6	2091	85	0,6,6	-	-	-		
86	OHX	5	4121	-	0,6,6	-	-	-		
86	OHX	1	4070	-	0,6,6	-	-	-		
86	OHX	2	2059	-	0,6,6	-	-	-		
86	OHX	6	2088	-	0,6,6	-	-	-		
86	OHX	6	2175	-	0,6,6	-	-	-		
86	OHX	5	4125	85	0,6,6	-	-	-		
86	OHX	5	3918	-	0,6,6	-	-	-		
86	OHX	5	4232	-	0,6,6	-	-	-		
86	OHX	6	2046	-	0,6,6	-	-	-		
86	OHX	5	4144	-	0,6,6	-	-	-		
86	OHX	2	2075	-	0,6,6	-	-	-		
86	OHX	1	4058	-	0,6,6	-	-	-		
86	OHX	5	4245	-	0,6,6	-	-	-		
86	OHX	2	2135	-	0,6,6	-	-	-		
86	OHX	5	4080	-	0,6,6	-	-	-		
86	OHX	6	2178	-	0,6,6	-	-	-		
86	OHX	2	2106	-	0,6,6	-	-	-		
86	OHX	1	4177	-	0,6,6	-	-	-		
86	OHX	5	4193	-	0,6,6	-	-	-		
86	OHX	1	4146	-	0,6,6	-	-	-		
86	OHX	1	3953	-	0,6,6	-	-	-		
86	OHX	1	4033	-	0,6,6	-	-	-		
86	OHX	5	4020	-	0,6,6	-	-	-		
86	OHX	6	2153	-	0,6,6	-	-	-		
86	OHX	6	2203	-	0,6,6	-	-	-		
86	OHX	2	2099	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2080	-	0,6,6	-	-	-		
86	OHX	5	4227	-	0,6,6	-	-	-		
86	OHX	5	4238	-	0,6,6	-	-	-		
86	OHX	6	2070	85	0,6,6	-	-	-		
86	OHX	4	234	-	0,6,6	-	-	-		
86	OHX	6	2144	-	0,6,6	-	-	-		
86	OHX	3	222	-	0,6,6	-	-	-		
86	OHX	1	4039	-	0,6,6	-	-	-		
86	OHX	1	4038	-	0,6,6	-	-	-		
86	OHX	8	213	-	0,6,6	-	-	-		
86	OHX	1	3883	85	0,6,6	-	-	-		
86	OHX	2	2100	-	0,6,6	-	-	-		
86	OHX	5	4150	85	0,6,6	-	-	-		
86	OHX	5	4228	85	0,6,6	-	-	-		
86	OHX	1	3990	-	0,6,6	-	-	-		
86	OHX	3	219	-	0,6,6	-	-	-		
86	OHX	6	2098	-	0,6,6	-	-	-		
86	OHX	8	214	-	0,6,6	-	-	-		
86	OHX	5	3971	85	0,6,6	-	-	-		
86	OHX	6	2120	-	0,6,6	-	-	-		
86	OHX	6	2108	-	0,6,6	-	-	-		
86	OHX	1	4059	-	0,6,6	-	-	-		
86	OHX	5	4032	-	0,6,6	-	-	-		
86	OHX	5	4037	-	0,6,6	-	-	-		
86	OHX	2	2173	-	0,6,6	-	-	-		
86	OHX	1	4000	-	0,6,6	-	-	-		
86	OHX	5	4053	85	0,6,6	-	-	-		
86	OHX	5	4198	-	0,6,6	-	-	-		
86	OHX	6	2109	-	0,6,6	-	-	-		
86	OHX	1	4061	-	0,6,6	-	-	-		
86	OHX	1	4045	-	0,6,6	-	-	-		
86	OHX	2	2093	-	0,6,6	-	-	-		
86	OHX	5	4003	-	0,6,6	-	-	-		
86	OHX	M8	201	-	0,6,6	-	-	-		
86	OHX	6	2156	-	0,6,6	-	-	-		
86	OHX	5	3921	85	0,6,6	-	-	-		
86	OHX	5	4067	-	0,6,6	-	-	-		
86	OHX	6	2200	-	0,6,6	-	-	-		
86	OHX	5	4197	-	0,6,6	-	-	-		
86	OHX	4	230	-	0,6,6	-	-	-		
86	OHX	5	4131	-	0,6,6	-	-	-		
86	OHX	2	2132	-	0,6,6	-	-	-		
86	OHX	5	4194	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	4007	-	0,6,6	-	-	-		
86	OHX	1	4172	-	0,6,6	-	-	-		
86	OHX	6	2059	-	0,6,6	-	-	-		
86	OHX	1	3897	-	0,6,6	-	-	-		
86	OHX	1	4077	-	0,6,6	-	-	-		
86	OHX	5	4250	85	0,6,6	-	-	-		
86	OHX	2	2079	-	0,6,6	-	-	-		
86	OHX	1	4069	-	0,6,6	-	-	-		
86	OHX	3	216	85	0,6,6	-	-	-		
86	OHX	1	3900	-	0,6,6	-	-	-		
86	OHX	5	3937	-	0,6,6	-	-	-		
86	OHX	5	4021	-	0,6,6	-	-	-		
86	OHX	m0	302	-	0,6,6	-	-	-		
86	OHX	5	4204	-	0,6,6	-	-	-		
86	OHX	1	4133	-	0,6,6	-	-	-		
86	OHX	2	2133	-	0,6,6	-	-	-		
86	OHX	1	3947	-	0,6,6	-	-	-		
86	OHX	6	2101	-	0,6,6	-	-	-		
86	OHX	3	225	-	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
88	ZBA	1	4206	85	1/1/13/14	4/18/83/83	0/5/4/4
88	ZBA	5	4256	85	-	3/18/83/83	0/5/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4206	ZBA	C28-C27	-6.52	1.47	1.55
88	5	4256	ZBA	C48-C46	6.42	1.51	1.33
88	1	4206	ZBA	C48-C46	6.36	1.51	1.33
88	5	4256	ZBA	C45-C46	-4.28	1.46	1.50
88	1	4206	ZBA	C45-C46	-2.44	1.48	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
88	1	4206	ZBA	C45-C46-C48	-8.84	108.62	121.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
88	5	4256	ZBA	C45-C46-C48	-8.25	109.48	121.74
88	1	4206	ZBA	C47-C46-C48	-5.07	110.81	121.98
88	5	4256	ZBA	C47-C46-C48	-4.62	111.81	121.98
88	1	4206	ZBA	C46-C45-C44	4.54	123.94	113.26
88	5	4256	ZBA	C47-C46-C45	-3.40	110.30	116.09
88	5	4256	ZBA	O10-C34-C29	3.06	116.44	112.54
88	5	4256	ZBA	C37-C28-C27	3.02	117.03	112.12
88	1	4206	ZBA	C47-C46-C45	-2.98	111.02	116.09
88	5	4256	ZBA	C37-C28-C35	-2.17	108.32	113.12
88	5	4256	ZBA	O14-C27-C26	2.11	115.91	109.72

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
88	1	4206	ZBA	C35

All (7) torsion outliers are listed below:

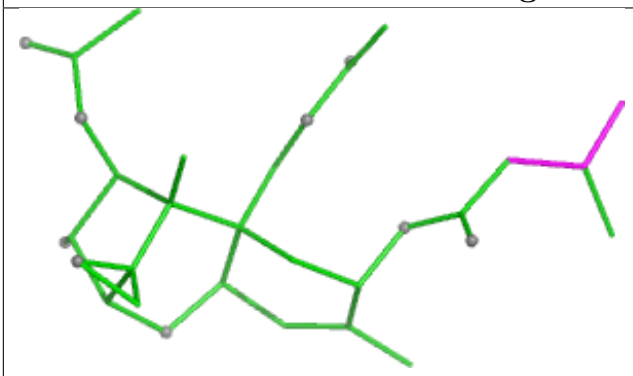
Mol	Chain	Res	Type	Atoms
88	1	4206	ZBA	C44-C45-C46-C48
88	5	4256	ZBA	C44-C45-C46-C48
88	5	4256	ZBA	C43-C42-O14-C27
88	5	4256	ZBA	O15-C42-O14-C27
88	1	4206	ZBA	O17-C44-C45-C46
88	1	4206	ZBA	C44-C45-C46-C47
88	1	4206	ZBA	O18-C44-C45-C46

There are no ring outliers.

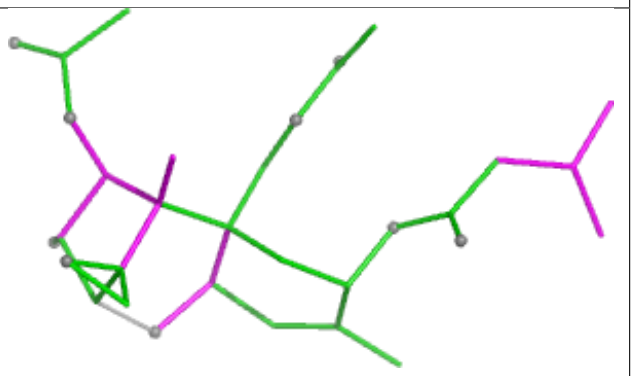
No monomer is involved in short contacts.

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.

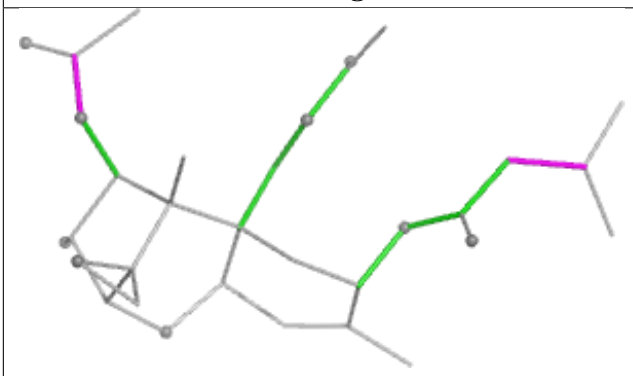
Ligand ZBA 5 4256



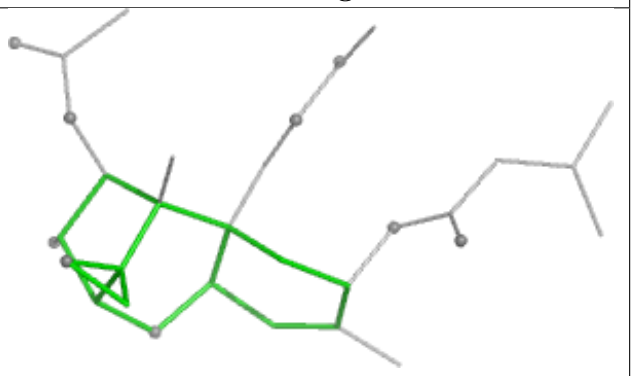
Bond lengths



Bond angles

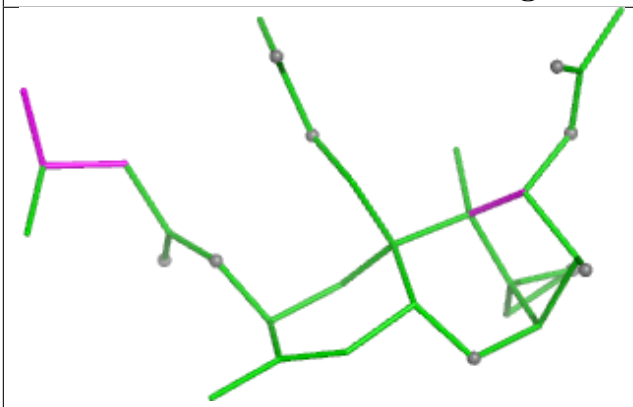


Torsions

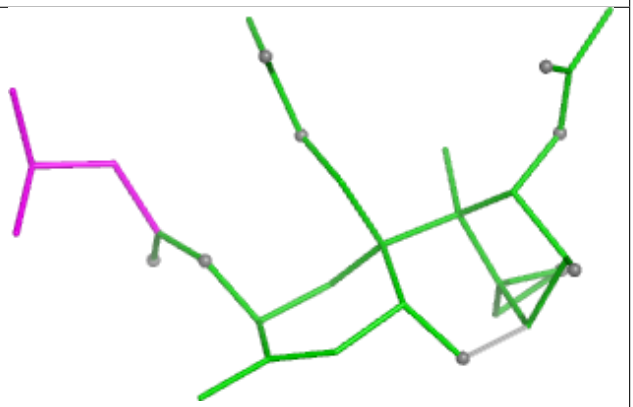


Rings

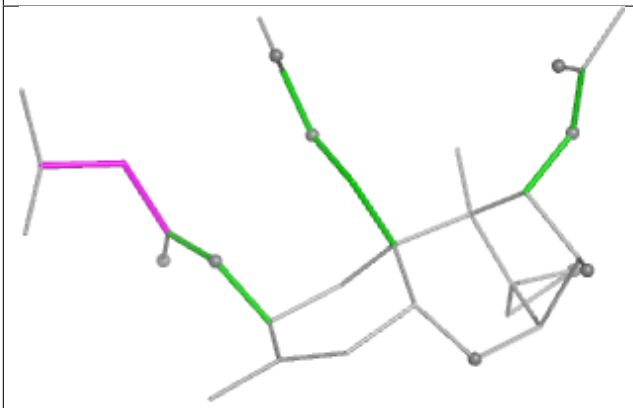
Ligand ZBA 1 4206



Bond lengths



Bond angles



Torsions



Rings

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
1	2	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1716:C	O3'	1717:G	P	4.21
1	2	1685:G	O3'	1686:C	P	2.96

5 Fit of model and data

5.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	2	1781/1800 (98%)	-0.19	27 (1%) 72 52	40, 77, 204, 284	0
1	6	1795/1800 (99%)	-0.31	22 (1%) 76 58	33, 65, 192, 277	0
2	S0	206/251 (82%)	0.47	7 (3%) 48 28	81, 100, 124, 158	0
2	s0	206/251 (82%)	0.22	6 (2%) 53 32	64, 84, 108, 128	0
3	S1	214/254 (84%)	0.72	10 (4%) 36 19	84, 125, 162, 188	0
3	s1	216/254 (85%)	0.10	1 (0%) 87 73	54, 74, 100, 137	0
4	S2	217/253 (85%)	0.53	4 (1%) 67 47	58, 77, 99, 131	0
4	s2	217/253 (85%)	0.11	6 (2%) 55 34	47, 65, 93, 105	0
5	S3	223/239 (93%)	0.53	10 (4%) 38 20	67, 79, 115, 162	0
5	s3	223/239 (93%)	0.33	3 (1%) 75 56	58, 86, 118, 136	0
6	S4	260/260 (100%)	0.21	1 (0%) 88 76	54, 78, 96, 141	0
6	s4	260/260 (100%)	-0.11	0 100 100	45, 69, 90, 145	0
7	S5	206/224 (91%)	0.29	6 (2%) 53 32	74, 99, 129, 167	0
7	s5	206/224 (91%)	0.35	8 (3%) 43 24	56, 82, 119, 151	0
8	S6	226/236 (95%)	0.51	10 (4%) 39 21	54, 91, 125, 161	0
8	s6	218/236 (92%)	0.19	3 (1%) 73 53	44, 77, 119, 146	0
9	S7	184/189 (97%)	0.48	6 (3%) 49 29	76, 108, 142, 170	0
9	s7	186/189 (98%)	0.59	11 (5%) 28 15	60, 94, 149, 171	0
10	S8	188/200 (94%)	0.22	6 (3%) 50 30	45, 61, 104, 122	0
10	s8	188/200 (94%)	0.20	4 (2%) 63 42	37, 59, 103, 120	0
11	S9	185/196 (94%)	0.37	2 (1%) 78 59	71, 86, 134, 178	0
11	s9	185/196 (94%)	-0.04	1 (0%) 87 73	53, 70, 113, 162	0
12	C0	96/105 (91%)	0.48	9 (9%) 14 8	64, 90, 132, 156	0
12	c0	96/105 (91%)	0.61	8 (8%) 17 9	70, 107, 149, 155	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	C1	155/155 (100%)	0.50	14 (9%) 15 8	45, 61, 143, 188	0
13	c1	146/155 (94%)	0.40	9 (6%) 26 14	40, 57, 114, 150	0
14	C2	124/142 (87%)	0.60	3 (2%) 59 38	110, 133, 180, 195	0
14	c2	124/142 (87%)	0.68	7 (5%) 30 16	147, 169, 211, 237	0
15	C3	150/150 (100%)	0.12	1 (0%) 84 68	52, 77, 106, 135	0
15	c3	150/150 (100%)	0.37	5 (3%) 49 29	46, 65, 87, 122	0
16	C4	127/136 (93%)	0.69	4 (3%) 51 30	56, 118, 141, 147	0
16	c4	128/136 (94%)	0.43	7 (5%) 30 16	47, 76, 91, 112	0
17	C5	124/141 (87%)	0.19	6 (4%) 35 19	57, 76, 140, 168	0
17	c5	135/141 (95%)	0.25	7 (5%) 33 17	57, 82, 122, 162	0
18	C6	141/142 (99%)	0.22	4 (2%) 55 34	68, 91, 100, 108	0
18	c6	142/142 (100%)	0.29	4 (2%) 55 34	50, 74, 89, 126	0
19	C7	120/136 (88%)	0.43	3 (2%) 58 37	71, 97, 140, 152	0
19	c7	117/136 (86%)	0.27	5 (4%) 40 22	61, 81, 123, 134	0
20	C8	145/145 (100%)	0.05	4 (2%) 55 34	60, 88, 116, 127	0
20	c8	145/145 (100%)	0.02	3 (2%) 63 42	60, 72, 117, 133	0
21	C9	143/143 (100%)	0.09	1 (0%) 84 68	70, 89, 116, 133	0
21	c9	143/143 (100%)	0.06	3 (2%) 63 42	49, 72, 94, 141	0
22	D0	107/120 (89%)	0.79	11 (10%) 12 6	60, 96, 149, 164	0
22	d0	110/120 (91%)	0.59	10 (9%) 15 8	53, 87, 154, 168	0
23	D1	87/87 (100%)	0.50	5 (5%) 29 16	83, 89, 118, 128	0
23	d1	87/87 (100%)	0.05	0 100 100	61, 72, 98, 117	0
24	D2	129/129 (100%)	0.23	1 (0%) 82 65	55, 71, 80, 90	0
24	d2	129/129 (100%)	-0.10	0 100 100	44, 54, 64, 77	0
25	D3	144/144 (100%)	0.19	2 (1%) 73 53	45, 56, 70, 117	0
25	d3	144/144 (100%)	-0.21	0 100 100	38, 45, 61, 90	0
26	D4	134/134 (100%)	0.27	2 (1%) 72 52	62, 93, 125, 139	0
26	d4	134/134 (100%)	0.05	2 (1%) 72 52	50, 79, 107, 130	0
27	D5	70/107 (65%)	0.33	2 (2%) 53 32	96, 118, 136, 148	0
27	d5	69/107 (64%)	0.25	0 100 100	67, 99, 122, 132	0
28	D6	97/97 (100%)	0.72	7 (7%) 21 11	64, 84, 153, 166	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	d6	97/97 (100%)	0.39	2 (2%) 63 42	47, 61, 105, 112	0
29	D7	81/81 (100%)	0.11	0 100 100	74, 90, 159, 176	0
29	d7	81/81 (100%)	0.31	0 100 100	55, 75, 148, 161	0
30	D8	63/66 (95%)	0.65	4 (6%) 26 14	96, 115, 142, 162	0
30	d8	63/66 (95%)	0.84	4 (6%) 26 14	75, 100, 126, 143	0
31	D9	53/55 (96%)	-0.01	0 100 100	59, 65, 90, 121	0
31	d9	53/55 (96%)	0.07	1 (1%) 66 45	56, 62, 105, 134	0
32	E0	60/60 (100%)	0.52	8 (13%) 7 4	56, 87, 157, 158	0
33	E1	71/76 (93%)	0.60	2 (2%) 55 34	91, 117, 135, 152	0
33	e1	76/76 (100%)	0.61	6 (7%) 18 10	114, 145, 167, 195	0
34	SR	318/318 (100%)	0.10	4 (1%) 75 56	71, 98, 135, 178	0
34	sR	318/318 (100%)	0.28	11 (3%) 47 27	72, 99, 132, 173	0
35	SM	159/273 (58%)	0.90	26 (16%) 4 2	55, 88, 143, 160	0
35	sM	104/273 (38%)	0.86	15 (14%) 6 3	48, 95, 166, 193	0
36	1	3149/3396 (92%)	-0.47	24 (0%) 82 65	26, 43, 141, 266	0
36	5	3150/3396 (92%)	-0.50	19 (0%) 85 70	24, 43, 133, 255	0
37	3	121/121 (100%)	-0.69	1 (0%) 82 65	33, 60, 78, 89	0
37	7	121/121 (100%)	-0.75	1 (0%) 82 65	29, 44, 59, 83	0
38	4	158/158 (100%)	-0.58	1 (0%) 85 70	30, 47, 97, 149	0
38	8	158/158 (100%)	-0.40	3 (1%) 66 45	33, 53, 106, 149	0
39	L2	252/253 (99%)	-0.08	2 (0%) 82 65	27, 41, 63, 97	0
39	l2	252/253 (99%)	-0.00	8 (3%) 50 30	28, 44, 70, 116	0
40	L3	386/386 (100%)	-0.25	2 (0%) 87 73	27, 45, 67, 135	0
40	l3	386/386 (100%)	-0.38	2 (0%) 87 73	24, 35, 53, 119	0
41	L4	361/361 (100%)	-0.28	1 (0%) 90 80	25, 38, 62, 79	0
41	l4	361/361 (100%)	-0.08	7 (1%) 66 45	28, 43, 71, 100	0
42	L5	296/296 (100%)	-0.14	1 (0%) 90 80	41, 68, 99, 137	0
42	l5	294/296 (99%)	-0.24	2 (0%) 84 68	32, 48, 88, 149	0
43	L6	156/175 (89%)	-0.32	0 100 100	32, 39, 78, 107	0
43	l6	157/175 (89%)	-0.25	0 100 100	33, 41, 78, 102	0
44	L7	222/243 (91%)	-0.34	2 (0%) 81 63	25, 33, 76, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	l7	223/243 (91%)	-0.35	1 (0%) 88 76	24, 32, 81, 160	0
45	L8	233/255 (91%)	0.28	13 (5%) 30 16	48, 63, 121, 139	0
45	l8	231/255 (90%)	0.27	5 (2%) 62 41	58, 73, 117, 141	0
46	L9	191/191 (100%)	-0.21	1 (0%) 87 73	40, 52, 73, 131	0
46	l9	191/191 (100%)	-0.37	1 (0%) 87 73	31, 40, 67, 106	0
47	M0	211/220 (95%)	-0.08	7 (3%) 49 29	34, 49, 91, 128	0
47	m0	213/220 (96%)	0.10	8 (3%) 44 25	31, 53, 88, 139	0
48	M1	169/173 (97%)	-0.13	0 100 100	50, 68, 85, 95	0
48	m1	169/173 (97%)	-0.21	1 (0%) 85 70	34, 52, 70, 93	0
49	M3	193/198 (97%)	-0.16	1 (0%) 87 73	26, 47, 103, 134	0
49	m3	194/198 (97%)	0.01	2 (1%) 79 61	32, 56, 120, 132	0
50	M4	136/137 (99%)	-0.33	0 100 100	35, 43, 64, 78	0
50	m4	137/137 (100%)	-0.35	1 (0%) 84 68	28, 37, 60, 81	0
51	M5	203/203 (100%)	-0.18	0 100 100	26, 39, 50, 58	0
51	m5	203/203 (100%)	-0.19	1 (0%) 87 73	30, 47, 59, 65	0
52	M6	197/198 (99%)	0.25	8 (4%) 41 23	23, 33, 52, 56	0
52	m6	197/198 (99%)	0.27	7 (3%) 46 26	20, 24, 49, 52	0
53	M7	183/183 (100%)	-0.05	8 (4%) 39 21	28, 36, 126, 179	0
53	m7	155/183 (84%)	-0.32	1 (0%) 85 70	21, 32, 49, 112	0
54	M8	185/185 (100%)	-0.31	1 (0%) 87 73	27, 35, 51, 79	0
54	m8	185/185 (100%)	-0.20	2 (1%) 78 59	30, 41, 53, 64	0
55	M9	188/188 (100%)	0.17	4 (2%) 63 42	40, 58, 156, 170	0
55	m9	188/188 (100%)	0.12	6 (3%) 50 30	37, 51, 132, 159	0
56	N0	172/172 (100%)	-0.29	2 (1%) 76 58	34, 41, 59, 72	0
56	n0	172/172 (100%)	-0.29	4 (2%) 61 39	26, 34, 51, 70	0
57	N1	159/159 (100%)	-0.15	0 100 100	31, 42, 94, 105	0
57	n1	159/159 (100%)	-0.19	2 (1%) 75 56	29, 35, 78, 89	0
58	N2	100/120 (83%)	0.30	2 (2%) 65 44	71, 94, 114, 143	0
58	n2	98/120 (81%)	0.37	3 (3%) 51 30	62, 85, 108, 120	0
59	N3	136/136 (100%)	-0.18	2 (1%) 72 52	30, 41, 66, 114	0
59	n3	136/136 (100%)	-0.18	3 (2%) 62 41	24, 33, 57, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
60	N4	98/155 (63%)	0.94	26 (26%) 1 1	41, 54, 188, 209	0
60	n4	135/155 (87%)	0.42	6 (4%) 39 21	33, 93, 156, 171	0
61	N5	121/141 (85%)	-0.05	1 (0%) 82 65	36, 52, 74, 138	0
61	n5	120/141 (85%)	0.11	5 (4%) 40 22	42, 60, 79, 120	0
62	N6	126/126 (100%)	-0.30	1 (0%) 82 65	34, 49, 64, 92	0
62	n6	126/126 (100%)	-0.06	2 (1%) 70 49	40, 53, 74, 106	0
63	N7	135/135 (100%)	-0.13	0 100 100	58, 77, 94, 101	0
63	n7	135/135 (100%)	0.12	1 (0%) 84 68	65, 87, 109, 119	0
64	N8	148/148 (100%)	-0.26	0 100 100	25, 37, 67, 84	0
64	n8	148/148 (100%)	-0.21	1 (0%) 84 68	27, 42, 74, 82	0
65	N9	58/58 (100%)	0.07	3 (5%) 33 17	33, 46, 102, 120	0
65	n9	58/58 (100%)	0.06	1 (1%) 69 48	29, 45, 82, 113	0
66	O0	97/104 (93%)	-0.01	2 (2%) 63 42	58, 70, 106, 124	0
66	o0	100/104 (96%)	0.29	3 (3%) 52 31	58, 73, 119, 132	0
67	O1	109/112 (97%)	-0.08	0 100 100	37, 51, 117, 140	0
67	o1	109/112 (97%)	-0.20	1 (0%) 81 63	32, 46, 108, 129	0
68	O2	127/129 (98%)	-0.36	1 (0%) 82 65	21, 35, 49, 87	0
68	o2	127/129 (98%)	-0.32	2 (1%) 70 49	24, 39, 58, 113	0
69	O3	106/106 (100%)	-0.45	0 100 100	26, 33, 53, 71	0
69	o3	106/106 (100%)	-0.37	0 100 100	22, 31, 60, 84	0
70	O4	112/120 (93%)	0.21	5 (4%) 38 20	39, 55, 113, 131	0
70	o4	112/120 (93%)	-0.00	1 (0%) 81 63	40, 57, 116, 131	0
71	O5	119/119 (100%)	-0.06	1 (0%) 82 65	38, 56, 69, 76	0
71	o5	119/119 (100%)	0.07	2 (1%) 69 48	45, 65, 79, 87	0
72	O6	99/99 (100%)	0.01	3 (3%) 52 31	44, 55, 100, 140	0
72	o6	99/99 (100%)	-0.01	0 100 100	50, 64, 98, 128	0
73	O7	87/87 (100%)	-0.08	1 (1%) 78 59	29, 35, 55, 94	0
73	o7	87/87 (100%)	-0.09	1 (1%) 78 59	31, 37, 71, 154	0
74	O8	77/77 (100%)	0.17	0 100 100	63, 83, 124, 138	0
74	o8	77/77 (100%)	0.21	0 100 100	63, 81, 111, 116	0
75	O9	50/50 (100%)	0.04	1 (2%) 65 44	37, 42, 50, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
75	o9	50/50 (100%)	0.11	1 (2%) 65 44	43, 48, 60, 71	0
76	Q0	52/52 (100%)	-0.37	0 100 100	42, 46, 66, 94	0
76	q0	52/52 (100%)	-0.55	0 100 100	28, 34, 47, 61	0
77	Q1	25/25 (100%)	0.20	1 (4%) 42 23	50, 53, 56, 64	0
77	q1	25/25 (100%)	-0.16	0 100 100	37, 44, 56, 63	0
78	Q2	105/105 (100%)	-0.19	1 (0%) 79 61	30, 45, 78, 136	0
78	q2	105/105 (100%)	-0.28	1 (0%) 79 61	33, 44, 70, 107	0
79	Q3	91/91 (100%)	-0.11	1 (1%) 78 59	32, 45, 73, 91	0
79	q3	91/91 (100%)	0.01	1 (1%) 78 59	29, 44, 63, 81	0
80	e0	62/62 (100%)	-0.02	1 (1%) 70 49	50, 75, 151, 182	0
81	p0	143/311 (45%)	0.53	6 (4%) 40 22	81, 103, 176, 185	0
82	m2	0/160	-	-	-	-
83	p1	0/47	-	-	-	-
84	p2	0/46	-	-	-	-
All	All	33094/35346 (93%)	-0.07	643 (1%) 66 45	20, 59, 133, 284	0

All (643) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	N4	86	SER	7.7
13	c1	3	THR	7.6
60	N4	88	ASP	7.4
13	C1	152	GLN	7.3
7	s5	37	GLN	7.1
7	S5	37	GLN	6.6
35	SM	85	SER	6.3
13	c1	144	ALA	6.3
47	m0	111	LEU	6.1
13	C1	2	SER	5.9
17	c5	4	ALA	5.8
13	c1	147	ALA	5.8
79	q3	2	ALA	5.6
28	D6	85	ARG	5.4
13	C1	3	THR	5.4
35	SM	84	LYS	5.3
13	c1	5	LEU	5.2
45	L8	66	SER	5.2
35	sM	82	THR	5.2

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Mol	Chain	Res	Type	RSRZ
56	N0	1	MET	5.2
22	D0	19	ILE	5.2
47	M0	112	GLN	5.2
12	c0	84	GLU	5.2
9	s7	52	ALA	5.1
13	c1	2	SER	5.1
5	S3	179	GLN	5.1
8	S6	80	ASN	5.1
81	p0	192	ASP	4.9
13	C1	150	ASN	4.8
12	C0	96	ASN	4.7
1	2	261	U	4.6
1	2	320	U	4.6
5	S3	148	LYS	4.6
60	N4	89	LEU	4.6
15	c3	15	ALA	4.6
60	N4	76	VAL	4.6
35	sM	119	ALA	4.5
60	N4	87	LEU	4.5
53	M7	184	ALA	4.5
4	s2	90	THR	4.5
1	2	676	G	4.4
22	d0	97	VAL	4.4
35	SM	83	LYS	4.3
56	n0	2	ALA	4.3
35	SM	87	THR	4.3
71	O5	120	ALA	4.3
17	c5	5	VAL	4.3
1	2	1702	A	4.2
32	E0	53	LYS	4.2
35	SM	89	ARG	4.1
12	C0	89	ALA	4.1
53	M7	161	ALA	4.1
60	N4	75	THR	4.1
7	S5	36	ALA	4.1
36	1	2522	G	4.1
73	O7	88	ALA	4.1
1	6	1491	U	4.1
28	D6	84	VAL	4.0
35	SM	88	ARG	4.0
20	C8	17	LEU	4.0
17	c5	7	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
23	D1	10	GLU	4.0
16	C4	15	GLY	4.0
60	N4	84	GLY	3.9
9	s7	12	ALA	3.9
13	C1	145	ALA	3.9
13	c1	146	ALA	3.9
1	2	913	G	3.9
65	N9	25	LYS	3.9
22	D0	108	ILE	3.9
45	L8	256	ALA	3.9
34	sR	121	MET	3.8
35	sM	83	LYS	3.8
7	s5	152	GLY	3.8
5	s3	43	PRO	3.8
36	1	2207	A	3.8
13	C1	147	ALA	3.7
71	o5	120	ALA	3.7
22	d0	98	GLN	3.7
47	m0	112	GLN	3.7
47	m0	103	LEU	3.7
39	L2	13	GLY	3.7
26	d4	18	LEU	3.6
52	m6	66	LYS	3.6
59	N3	2	SER	3.6
5	S3	142	LEU	3.6
16	c4	62	LEU	3.6
25	D3	145	SER	3.6
1	2	1699	G	3.5
52	m6	183	ALA	3.5
9	S7	41	LEU	3.5
36	1	1570	U	3.5
45	l8	124	ASP	3.5
13	C1	146	ALA	3.5
13	c1	145	ALA	3.5
55	M9	72	GLU	3.5
1	2	506	A	3.5
1	2	1700	C	3.5
36	1	1569	U	3.5
2	S0	170	ILE	3.5
15	c3	62	GLN	3.5
60	N4	72	SER	3.5
13	c1	4	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
2	S0	207	PRO	3.4
35	SM	134	ASP	3.4
55	M9	189	ALA	3.4
8	S6	163	THR	3.4
52	M6	80	PHE	3.4
63	n7	92	PHE	3.4
12	C0	95	ARG	3.4
22	D0	107	THR	3.4
36	5	1582	C	3.4
36	1	2996	U	3.4
36	1	1571	A	3.3
7	S5	152	GLY	3.3
7	s5	154	ALA	3.3
47	M0	218	ALA	3.3
8	S6	226	ILE	3.3
36	1	2401	A	3.3
35	SM	141	ALA	3.3
19	C7	110	VAL	3.3
56	n0	1	MET	3.3
36	5	1953	G	3.3
36	1	2205	U	3.3
2	s0	40	ALA	3.3
7	s5	155	ALA	3.3
37	7	73	C	3.3
39	l2	13	GLY	3.3
22	D0	120	SER	3.2
35	SM	11	ASP	3.2
60	N4	63	ILE	3.2
9	s7	4	PRO	3.2
53	M7	158	ALA	3.2
60	N4	66	GLU	3.2
22	d0	95	ALA	3.2
47	M0	221	ALA	3.2
10	s8	199	LYS	3.2
1	2	1708	U	3.2
49	m3	133	PRO	3.2
28	D6	63	ALA	3.2
35	SM	86	ASN	3.1
18	c6	142	TYR	3.1
3	S1	25	THR	3.1
18	C6	20	ALA	3.1
45	L8	250	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
9	s7	58	LEU	3.1
73	o7	88	ALA	3.1
45	L8	93	LEU	3.1
46	l9	191	LEU	3.1
16	c4	48	VAL	3.1
1	6	663	U	3.1
4	s2	92	ALA	3.1
3	S1	20	VAL	3.1
2	s0	207	PRO	3.1
60	N4	69	LYS	3.1
47	M0	219	ALA	3.1
36	5	2506	U	3.1
35	sM	155	LEU	3.0
21	c9	23	GLN	3.0
41	l4	61	SER	3.0
60	n4	68	ALA	3.0
12	C0	90	THR	3.0
17	C5	11	VAL	3.0
52	m6	184	THR	3.0
70	O4	21	LYS	3.0
9	s7	24	PHE	3.0
3	S1	140	ILE	3.0
52	M6	164	SER	3.0
55	m9	78	TYR	3.0
39	l2	248	GLY	3.0
47	M0	220	GLN	3.0
1	2	1694	A	3.0
47	m0	221	ALA	3.0
1	6	662	U	3.0
10	s8	135	LYS	3.0
12	C0	85	HIS	3.0
14	c2	123	VAL	3.0
36	5	443	G	3.0
12	c0	96	ASN	3.0
32	E0	48	THR	3.0
32	E0	47	VAL	3.0
4	S2	144	TRP	2.9
5	S3	143	ARG	2.9
33	e1	80	ARG	2.9
36	1	1349	G	2.9
48	m1	174	LYS	2.9
32	E0	50	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
20	c8	17	LEU	2.9
41	l4	63	GLU	2.9
61	n5	24	LEU	2.9
60	N4	85	ALA	2.9
55	M9	177	VAL	2.9
70	O4	23	VAL	2.9
9	s7	187	SER	2.9
40	L3	387	LEU	2.9
70	o4	33	GLN	2.9
2	s0	206	ASP	2.9
12	c0	97	PRO	2.9
60	n4	65	GLU	2.9
60	n4	66	GLU	2.9
36	1	2093	A	2.9
7	S5	24	VAL	2.9
60	n4	84	GLY	2.9
45	l8	254	ASP	2.9
9	s7	93	LEU	2.9
60	N4	90	ILE	2.9
40	l3	363	SER	2.8
1	2	1082	C	2.8
5	S3	88	ALA	2.8
4	s2	96	THR	2.8
35	sM	164	ASN	2.8
52	M6	3	VAL	2.8
1	6	678	A	2.8
39	l2	14	SER	2.8
1	6	320	U	2.8
36	1	2206	G	2.8
13	C1	151	LYS	2.8
9	s7	2	SER	2.8
15	c3	17	PRO	2.8
75	O9	46	ARG	2.8
52	m6	56	ASP	2.8
32	E0	49	LEU	2.8
35	SM	161	ASN	2.8
58	n2	11	ILE	2.8
79	Q3	92	ALA	2.8
60	N4	64	THR	2.8
2	S0	206	ASP	2.8
9	s7	8	ILE	2.8
2	S0	44	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
12	c0	81	ASN	2.8
36	1	1567	U	2.8
36	5	2971	A	2.8
36	5	3154	C	2.8
78	Q2	106	PHE	2.7
77	Q1	1	MET	2.7
56	N0	74	ASN	2.7
8	s6	169	TYR	2.7
41	l4	62	ALA	2.7
53	M7	156	ALA	2.7
60	N4	77	LYS	2.7
1	6	679	U	2.7
1	6	794	U	2.7
1	6	321	C	2.7
30	D8	21	SER	2.7
19	c7	103	ASP	2.7
21	C9	35	ASP	2.7
17	c5	8	LYS	2.7
19	C7	123	ASN	2.7
39	l2	194	ASN	2.7
16	c4	60	ALA	2.7
8	S6	41	VAL	2.7
1	2	1693	A	2.7
4	S2	90	THR	2.7
35	sM	66	ALA	2.7
55	m9	189	ALA	2.7
53	M7	165	VAL	2.7
20	c8	18	LEU	2.7
2	s0	173	ILE	2.7
60	N4	92	GLU	2.7
22	D0	67	THR	2.7
40	l3	146	ARG	2.7
44	l7	22	THR	2.7
13	C1	154	ALA	2.7
22	D0	97	VAL	2.7
35	sM	156	ASN	2.7
22	D0	110	PRO	2.7
35	sM	157	GLN	2.7
17	C5	28	MET	2.7
52	m6	100	GLU	2.7
60	N4	65	GLU	2.7
12	c0	98	SER	2.7

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Mol	Chain	Res	Type	RSRZ
33	e1	152	ALA	2.7
34	SR	180	ALA	2.7
1	2	719	U	2.7
12	C0	91	TYR	2.7
13	C1	5	LEU	2.7
28	D6	86	VAL	2.7
17	c5	6	ASN	2.7
36	5	1103	A	2.6
3	S1	63	GLY	2.6
61	n5	142	ILE	2.6
66	o0	100	ILE	2.6
13	c1	116	ARG	2.6
17	C5	9	LYS	2.6
36	5	3275	U	2.6
52	M6	100	GLU	2.6
34	sR	48	THR	2.6
11	s9	148	VAL	2.6
36	1	1581	C	2.6
59	n3	2	SER	2.6
10	S8	152	ILE	2.6
55	M9	85	ARG	2.6
59	n3	5	GLY	2.6
19	c7	87	GLU	2.6
30	d8	9	LEU	2.6
22	D0	45	ALA	2.6
33	e1	147	VAL	2.6
34	sR	279	ALA	2.6
55	m9	159	ALA	2.6
70	O4	32	ALA	2.6
1	2	793	A	2.6
1	6	1371	A	2.6
53	M7	164	LYS	2.6
42	l5	4	GLN	2.6
41	l4	54	GLU	2.6
62	N6	127	GLU	2.6
30	D8	44	VAL	2.6
45	L8	116	VAL	2.6
49	m3	195	ALA	2.6
41	l4	65	TRP	2.6
9	S7	8	ILE	2.6
18	C6	29	ILE	2.6
22	D0	20	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
13	C1	156	PHE	2.6
30	d8	24	GLY	2.6
68	o2	128	LEU	2.6
36	1	981	U	2.5
36	5	1356	U	2.5
9	S7	150	GLN	2.5
47	M0	113	GLN	2.5
58	N2	89	LEU	2.5
36	5	437	G	2.5
65	n9	22	LYS	2.5
60	N4	78	ALA	2.5
14	C2	24	ILE	2.5
27	D5	50	ILE	2.5
1	6	681	U	2.5
9	s7	16	LEU	2.5
34	SR	2	ALA	2.5
20	C8	66	LEU	2.5
28	D6	53	LEU	2.5
65	N9	59	LYS	2.5
34	sR	253	ALA	2.5
47	m0	195	ALA	2.5
1	2	132	U	2.5
56	n0	17	GLU	2.5
5	s3	115	ILE	2.5
26	D4	135	ASP	2.5
15	c3	72	MET	2.5
34	sR	12	THR	2.5
39	l2	252	THR	2.5
3	S1	61	LEU	2.5
11	S9	95	TYR	2.5
16	c4	58	TYR	2.5
23	D1	69	LEU	2.5
13	C1	149	ALA	2.5
35	sM	79	SER	2.5
4	s2	208	GLU	2.5
8	S6	78	THR	2.5
12	C0	88	PRO	2.5
9	s7	11	GLN	2.5
56	n0	138	GLN	2.5
12	C0	86	ILE	2.4
22	d0	19	ILE	2.4
60	N4	95	SER	2.4

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Mol	Chain	Res	Type	RSRZ
60	n4	72	SER	2.4
35	sM	120	GLU	2.4
38	8	80	A	2.4
2	s0	185	ARG	2.4
8	S6	168	THR	2.4
1	2	658	C	2.4
14	c2	59	LEU	2.4
58	N2	108	TYR	2.4
35	SM	9	GLY	2.4
80	e0	62	VAL	2.4
40	L3	139	GLN	2.4
42	L5	2	ALA	2.4
28	D6	79	ILE	2.4
45	L8	253	SER	2.4
35	sM	84	LYS	2.4
14	C2	88	LEU	2.4
19	c7	97	ASN	2.4
45	L8	254	ASP	2.4
22	d0	114	VAL	2.4
10	S8	167	ALA	2.4
1	2	794	U	2.4
12	C0	13	GLN	2.4
30	d8	40	ILE	2.4
3	S1	207	LEU	2.4
5	S3	37	VAL	2.4
33	e1	150	VAL	2.4
3	S1	102	GLY	2.4
4	s2	93	GLY	2.4
7	S5	209	TYR	2.4
21	c9	55	TYR	2.4
1	6	1800	A	2.4
22	D0	106	ILE	2.4
22	d0	99	ILE	2.4
68	o2	127	ALA	2.4
22	d0	18	GLN	2.4
18	c6	114	ARG	2.4
9	S7	38	LEU	2.4
14	c2	45	LEU	2.4
53	M7	162	GLU	2.4
12	c0	83	PRO	2.4
35	sM	167	PRO	2.4
2	S0	190	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
7	s5	151	GLY	2.4
23	D1	21	ASN	2.4
2	s0	204	TYR	2.4
5	S3	87	TYR	2.4
10	S8	104	ILE	2.4
41	l4	101	ALA	2.4
35	SM	165	LYS	2.4
10	S8	21	PHE	2.4
36	1	1103	A	2.4
1	6	75	U	2.4
17	c5	11	VAL	2.4
44	L7	26	VAL	2.4
1	2	1709	C	2.3
7	s5	153	GLY	2.3
3	S1	164	ILE	2.3
15	c3	16	ILE	2.3
54	m8	145	ASN	2.3
13	C1	153	PHE	2.3
62	n6	126	LEU	2.3
12	c0	94	GLU	2.3
47	m0	186	GLU	2.3
52	M6	40	GLU	2.3
35	sM	85	SER	2.3
17	C5	8	LYS	2.3
30	d8	65	ARG	2.3
61	N5	118	GLY	2.3
35	SM	138	ALA	2.3
52	m6	182	ASN	2.3
1	6	659	C	2.3
35	SM	151	LEU	2.3
36	1	1556	C	2.3
35	SM	108	GLN	2.3
62	n6	127	GLU	2.3
22	d0	118	VAL	2.3
10	S8	200	LYS	2.3
41	l4	55	LYS	2.3
8	S6	154	ARG	2.3
30	D8	6	PRO	2.3
32	E0	54	ARG	2.3
14	c2	71	ILE	2.3
60	N4	83	THR	2.3
35	SM	160	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
35	SM	153	ASP	2.3
45	L8	156	ASP	2.3
1	2	598	U	2.3
36	5	2538	U	2.3
38	8	81	U	2.3
45	l8	123	GLN	2.3
45	l8	106	LYS	2.3
72	O6	56	ARG	2.3
18	c6	3	ALA	2.3
45	L8	114	ALA	2.3
47	m0	127	ALA	2.3
53	m7	156	ALA	2.3
3	S1	46	THR	2.3
16	c4	91	THR	2.3
32	E0	61	SER	2.3
10	s8	179	CYS	2.3
54	m8	153	PHE	2.3
59	n3	4	ASN	2.3
1	2	238	U	2.3
34	sR	180	ALA	2.3
42	l5	294	ALA	2.3
13	C1	91	LEU	2.3
20	c8	3	LEU	2.3
39	l2	249	SER	2.3
39	L2	253	GLN	2.3
47	m0	220	GLN	2.3
16	c4	67	VAL	2.3
58	n2	56	VAL	2.3
52	M6	166	GLU	2.2
36	5	170	G	2.2
55	m9	183	ALA	2.2
38	8	79	A	2.2
34	sR	282	SER	2.2
18	C6	143	ARG	2.2
70	O4	22	VAL	2.2
21	c9	144	GLU	2.2
35	sM	137	GLU	2.2
66	O0	97	ASP	2.2
60	N4	68	ALA	2.2
35	SM	81	THR	2.2
1	2	600	U	2.2
12	c0	65	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	2	1701	A	2.2
1	6	506	A	2.2
18	c6	141	SER	2.2
27	D5	93	SER	2.2
52	M6	182	ASN	2.2
64	n8	120	ASN	2.2
7	s5	90	ILE	2.2
8	s6	166	GLU	2.2
23	D1	34	ILE	2.2
35	SM	13	GLU	2.2
36	1	2772	C	2.2
4	S2	163	GLY	2.2
7	S5	25	LEU	2.2
16	C4	102	LEU	2.2
51	m5	58	GLY	2.2
60	N4	81	PRO	2.2
22	d0	101	LYS	2.2
19	c7	110	VAL	2.2
45	L8	255	SER	2.2
8	S6	190	GLN	2.2
28	D6	44	ILE	2.2
1	6	1756	A	2.2
8	S6	222	GLU	2.2
35	sM	161	ASN	2.2
36	1	1954	G	2.2
44	L7	209	ASN	2.2
11	S9	181	ALA	2.2
14	C2	51	ALA	2.2
23	D1	62	ARG	2.2
57	n1	159	PHE	2.2
1	2	321	C	2.2
1	6	1399	C	2.2
14	c2	126	TRP	2.2
36	5	1581	C	2.2
8	S6	158	ILE	2.2
20	C8	35	ILE	2.2
70	O4	20	ILE	2.2
67	o1	4	LEU	2.2
16	c4	49	LYS	2.2
28	d6	98	PRO	2.2
59	N3	3	GLY	2.2
16	C4	27	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
17	C5	12	PHE	2.2
36	5	440	A	2.2
1	2	729	G	2.2
1	6	651	G	2.2
34	SR	8	VAL	2.1
53	M7	157	VAL	2.1
52	M6	112	TYR	2.1
1	6	1711	C	2.1
3	S1	188	LEU	2.1
9	S7	12	ALA	2.1
24	D2	30	SER	2.1
34	sR	284	ALA	2.1
50	m4	9	ALA	2.1
39	l2	186	PHE	2.1
78	q2	106	PHE	2.1
1	2	1370	U	2.1
36	1	1568	U	2.1
5	s3	42	THR	2.1
81	p0	4	ILE	2.1
3	s1	217	LEU	2.1
30	D8	9	LEU	2.1
33	E1	103	LEU	2.1
33	E1	143	LYS	2.1
36	1	1952	G	2.1
36	5	2095	G	2.1
18	C6	3	ALA	2.1
32	E0	2	ALA	2.1
47	M0	114	GLY	2.1
72	O6	97	SER	2.1
26	d4	26	ASP	2.1
45	L8	58	VAL	2.1
66	o0	67	VAL	2.1
1	6	718	U	2.1
5	S3	59	LEU	2.1
38	4	82	U	2.1
60	N4	70	LYS	2.1
60	N4	93	ARG	2.1
15	C3	148	ALA	2.1
22	D0	15	GLN	2.1
81	p0	107	ALA	2.1
34	sR	30	PRO	2.1
81	p0	47	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
19	C7	97	ASN	2.1
2	S0	158	VAL	2.1
35	SM	19	VAL	2.1
36	5	1192	C	2.1
31	d9	7	TRP	2.1
66	O0	104	LEU	2.1
55	m9	151	ARG	2.1
10	S8	148	ALA	2.1
45	L8	113	ALA	2.1
61	n5	23	ALA	2.1
1	6	1708	U	2.1
16	C4	99	GLN	2.1
17	C5	104	GLN	2.1
36	1	2501	U	2.1
61	n5	64	GLU	2.1
41	L4	53	SER	2.1
35	SM	105	LYS	2.1
14	c2	136	ILE	2.1
25	D3	18	HIS	2.1
33	e1	145	HIS	2.1
60	N4	80	ARG	2.1
68	O2	26	HIS	2.1
5	S3	44	THR	2.1
34	sR	72	THR	2.1
58	n2	108	TYR	2.1
1	6	720	G	2.1
17	c5	133	ALA	2.1
26	D4	126	ALA	2.1
36	1	2507	C	2.1
36	5	1032	C	2.1
71	o5	2	ALA	2.1
4	s2	87	GLN	2.1
7	s5	150	GLY	2.1
39	l2	253	GLN	2.1
45	l8	127	PRO	2.1
4	S2	80	VAL	2.0
36	5	2505	U	2.0
81	p0	105	VAL	2.0
20	C8	32	LEU	2.0
22	d0	121	ASN	2.0
34	sR	252	LEU	2.0
46	L9	191	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
55	m9	185	LEU	2.0
72	O6	98	ARG	2.0
10	s8	197	THR	2.0
14	c2	130	THR	2.0
28	d6	81	ALA	2.0
35	SM	98	GLY	2.0
45	L8	123	GLN	2.0
60	N4	79	GLN	2.0
81	p0	86	PHE	2.0
34	SR	117	LYS	2.0
54	M8	159	LYS	2.0
57	n1	104	GLU	2.0
60	n4	74	LYS	2.0
61	n5	101	GLU	2.0
1	6	1082	C	2.0
2	S0	29	VAL	2.0
36	1	2094	C	2.0
36	1	3154	C	2.0
37	3	73	C	2.0
5	S3	54	ARG	2.0
6	S4	261	LEU	2.0
75	o9	51	ILE	2.0
1	2	260	U	2.0
1	2	792	U	2.0
36	5	981	U	2.0
8	s6	168	THR	2.0
35	SM	90	ALA	2.0
33	e1	85	TYR	2.0
52	m6	67	THR	2.0
9	S7	74	GLN	2.0
19	c7	105	GLN	2.0
35	SM	21	PRO	2.0
35	SM	158	GLN	2.0
65	N9	22	LYS	2.0
49	M3	155	GLU	2.0
66	o0	104	LEU	2.0

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	2	1997	1/1	0.45	0.23	82,82,82,82	0
85	MG	o1	201	1/1	0.45	0.19	103,103,103,103	0
85	MG	1	3854	1/1	0.49	0.23	153,153,153,153	0
87	ZN	D7	101	1/1	0.51	0.13	263,263,263,263	0
85	MG	5	3776	1/1	0.57	0.24	97,97,97,97	0
85	MG	1	3623	1/1	0.63	0.20	78,78,78,78	0
85	MG	1	3754	1/1	0.63	0.22	58,58,58,58	0
85	MG	5	3797	1/1	0.68	0.16	80,80,80,80	0
85	MG	6	1909	1/1	0.68	0.29	65,65,65,65	0
85	MG	2	1992	1/1	0.68	0.28	87,87,87,87	0
85	MG	1	3855	1/1	0.69	0.33	54,54,54,54	0
86	OHX	5	4238	7/7	0.69	0.14	230,230,230,230	0
85	MG	2	1974	1/1	0.69	0.32	69,69,69,69	0
85	MG	5	3806	1/1	0.70	0.14	128,128,128,128	0
85	MG	M3	202	1/1	0.71	0.27	92,92,92,92	0
85	MG	3	213	1/1	0.71	0.21	50,50,50,50	0
85	MG	2	1955	1/1	0.72	0.31	77,77,77,77	0
85	MG	2	1954	1/1	0.73	0.25	86,86,86,86	0
85	MG	1	3648	1/1	0.73	0.38	71,71,71,71	0
85	MG	1	3667	1/1	0.73	0.22	58,58,58,58	0
85	MG	5	3774	1/1	0.74	0.21	59,59,59,59	0
86	OHX	2	2165	7/7	0.74	0.13	223,223,223,223	0
86	OHX	5	4232	7/7	0.74	0.23	193,193,193,193	0
85	MG	5	3752	1/1	0.74	0.32	67,67,67,67	0
85	MG	5	3890	1/1	0.74	0.32	51,51,51,51	0
85	MG	5	3728	1/1	0.75	0.17	81,81,81,81	0
85	MG	5	3897	1/1	0.75	0.24	47,47,47,47	0
85	MG	1	3580	1/1	0.75	0.18	41,41,41,41	0
85	MG	1	3693	1/1	0.75	0.24	55,55,55,55	0
86	OHX	6	2186	7/7	0.75	0.13	213,213,213,213	0
85	MG	2	1910	1/1	0.75	0.35	49,49,49,49	0
85	MG	1	3450	1/1	0.75	0.32	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	6	1978	1/1	0.75	0.20	80,80,80,80	0
86	OHX	1	4180	7/7	0.76	0.15	238,238,238,238	0
85	MG	2	2021	1/1	0.76	0.28	58,58,58,58	0
85	MG	5	3504	1/1	0.76	0.29	35,35,35,35	0
85	MG	5	3860	1/1	0.76	0.25	58,58,58,58	0
85	MG	5	3885	1/1	0.76	0.35	81,81,81,81	0
85	MG	5	3733	1/1	0.77	0.22	80,80,80,80	0
85	MG	m6	201	1/1	0.77	0.31	43,43,43,43	0
86	OHX	5	4199	7/7	0.77	0.14	219,219,219,219	0
86	OHX	5	4227	7/7	0.77	0.20	197,197,197,197	0
85	MG	6	1923	1/1	0.77	0.23	57,57,57,57	0
86	OHX	2	2162	7/7	0.77	0.14	218,218,218,218	0
86	OHX	5	4241	7/7	0.77	0.15	234,234,234,234	0
86	OHX	m4	201	7/7	0.77	0.11	264,264,264,264	0
85	MG	1	3468	1/1	0.77	0.20	45,45,45,45	0
85	MG	6	1907	1/1	0.78	0.31	54,54,54,54	0
85	MG	5	3808	1/1	0.78	0.21	79,79,79,79	0
86	OHX	2	2166	7/7	0.78	0.19	211,211,211,211	0
86	OHX	1	4121	7/7	0.78	0.16	193,193,193,193	0
85	MG	1	3632	1/1	0.78	0.22	52,52,52,52	0
85	MG	1	3773	1/1	0.78	0.22	70,70,70,70	0
86	OHX	6	2187	7/7	0.78	0.17	177,177,177,177	0
85	MG	1	3725	1/1	0.78	0.17	42,42,42,42	0
85	MG	5	3894	1/1	0.78	0.11	113,113,113,113	0
85	MG	5	3895	1/1	0.78	0.18	47,47,47,47	0
85	MG	6	2034	1/1	0.78	0.20	75,75,75,75	0
85	MG	c7	201	1/1	0.78	0.26	67,67,67,67	0
86	OHX	5	4243	7/7	0.78	0.15	216,216,216,216	0
86	OHX	l5	305	7/7	0.78	0.15	193,193,193,193	0
85	MG	5	3469	1/1	0.78	0.14	116,116,116,116	0
85	MG	o4	201	1/1	0.78	0.14	60,60,60,60	0
85	MG	6	2001	1/1	0.79	0.12	96,96,96,96	0
85	MG	2	1934	1/1	0.79	0.28	57,57,57,57	0
85	MG	1	3479	1/1	0.79	0.20	51,51,51,51	0
85	MG	1	3562	1/1	0.79	0.27	38,38,38,38	0
85	MG	5	3499	1/1	0.79	0.24	48,48,48,48	0
86	OHX	2	2179	7/7	0.79	0.12	232,232,232,232	0
85	MG	2	1984	1/1	0.79	0.19	62,62,62,62	0
86	OHX	1	4128	7/7	0.79	0.18	183,183,183,183	0
86	OHX	1	4170	7/7	0.79	0.15	223,223,223,223	0
85	MG	2	1947	1/1	0.79	0.24	58,58,58,58	0
86	OHX	6	2146	7/7	0.79	0.12	208,208,208,208	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	ZN	d7	101	1/1	0.79	0.14	246,246,246,246	0
85	MG	2	1973	1/1	0.80	0.27	52,52,52,52	0
85	MG	2	1926	1/1	0.80	0.28	65,65,65,65	0
86	OHX	1	4189	7/7	0.80	0.13	209,209,209,209	0
85	MG	5	3466	1/1	0.80	0.30	69,69,69,69	0
85	MG	1	3610	1/1	0.80	0.27	44,44,44,44	0
86	OHX	2	2149	7/7	0.80	0.17	173,173,173,173	0
86	OHX	6	2193	7/7	0.80	0.15	196,196,196,196	0
86	OHX	6	2194	7/7	0.80	0.15	212,212,212,212	0
86	OHX	5	4167	7/7	0.80	0.17	232,232,232,232	0
86	OHX	5	4175	7/7	0.80	0.24	139,139,139,139	0
85	MG	5	3488	1/1	0.80	0.26	46,46,46,46	0
86	OHX	2	2164	7/7	0.80	0.12	239,239,239,239	0
85	MG	6	1911	1/1	0.80	0.26	68,68,68,68	0
85	MG	2	1950	1/1	0.80	0.22	73,73,73,73	0
85	MG	1	3696	1/1	0.80	0.21	33,33,33,33	0
86	OHX	1	4105	7/7	0.80	0.17	213,213,213,213	0
86	OHX	5	4251	7/7	0.80	0.15	205,205,205,205	0
85	MG	6	1989	1/1	0.80	0.16	63,63,63,63	0
86	OHX	m0	302	7/7	0.80	0.19	171,171,171,171	0
85	MG	1	3701	1/1	0.80	0.24	56,56,56,56	0
86	OHX	n5	201	7/7	0.80	0.11	260,260,260,260	0
86	OHX	1	4136	7/7	0.80	0.20	176,176,176,176	0
86	OHX	1	4166	7/7	0.80	0.17	207,207,207,207	0
85	MG	4	210	1/1	0.81	0.20	52,52,52,52	0
85	MG	1	3750	1/1	0.81	0.13	46,46,46,46	0
86	OHX	1	4165	7/7	0.81	0.15	221,221,221,221	0
85	MG	5	3629	1/1	0.81	0.26	61,61,61,61	0
86	OHX	5	4230	7/7	0.81	0.17	174,174,174,174	0
85	MG	5	3824	1/1	0.81	0.21	80,80,80,80	0
85	MG	5	3680	1/1	0.81	0.30	71,71,71,71	0
86	OHX	1	4181	7/7	0.81	0.15	190,190,190,190	0
86	OHX	1	4183	7/7	0.81	0.19	223,223,223,223	0
86	OHX	5	4244	7/7	0.81	0.14	249,249,249,249	0
85	MG	6	2039	1/1	0.81	0.30	53,53,53,53	0
85	MG	6	1965	1/1	0.81	0.27	68,68,68,68	0
85	MG	6	1975	1/1	0.81	0.20	54,54,54,54	0
85	MG	2	2004	1/1	0.81	0.38	79,79,79,79	0
86	OHX	6	2191	7/7	0.81	0.13	232,232,232,232	0
85	MG	2	1970	1/1	0.81	0.29	76,76,76,76	0
85	MG	7	216	1/1	0.81	0.26	54,54,54,54	0
86	OHX	1	4066	7/7	0.82	0.23	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	4089	7/7	0.82	0.13	183,183,183,183	0
86	OHX	6	2198	7/7	0.82	0.13	229,229,229,229	0
86	OHX	c3	201	7/7	0.82	0.14	213,213,213,213	0
86	OHX	5	4150	7/7	0.82	0.15	180,180,180,180	0
85	MG	2	2183	1/1	0.82	0.21	70,70,70,70	0
85	MG	3	208	1/1	0.82	0.20	67,67,67,67	0
85	MG	2	1980	1/1	0.82	0.28	82,82,82,82	0
86	OHX	5	4221	7/7	0.82	0.13	202,202,202,202	0
85	MG	5	3782	1/1	0.82	0.24	64,64,64,64	0
86	OHX	1	4163	7/7	0.82	0.18	147,147,147,147	0
85	MG	1	3451	1/1	0.82	0.17	30,30,30,30	0
85	MG	1	3811	1/1	0.82	0.22	58,58,58,58	0
86	OHX	2	2127	7/7	0.82	0.17	190,190,190,190	0
85	MG	N0	202	1/1	0.82	0.17	48,48,48,48	0
86	OHX	2	2152	7/7	0.82	0.10	231,231,231,231	0
85	MG	1	3832	1/1	0.82	0.24	45,45,45,45	0
85	MG	5	3684	1/1	0.82	0.24	59,59,59,59	0
86	OHX	1	4190	7/7	0.82	0.11	225,225,225,225	0
85	MG	5	3695	1/1	0.82	0.12	63,63,63,63	0
85	MG	1	3846	1/1	0.82	0.15	102,102,102,102	0
86	OHX	2	2178	7/7	0.82	0.14	190,190,190,190	0
85	MG	2	1977	1/1	0.82	0.31	60,60,60,60	0
85	MG	5	3849	1/1	0.83	0.08	44,44,44,44	0
85	MG	5	3619	1/1	0.83	0.22	39,39,39,39	0
86	OHX	6	2188	7/7	0.83	0.11	208,208,208,208	0
85	MG	5	3869	1/1	0.83	0.14	46,46,46,46	0
86	OHX	S9	201	7/7	0.83	0.17	167,167,167,167	0
85	MG	1	3528	1/1	0.83	0.34	36,36,36,36	0
85	MG	5	3637	1/1	0.83	0.21	51,51,51,51	0
86	OHX	6	2201	7/7	0.83	0.13	215,215,215,215	0
86	OHX	6	2202	7/7	0.83	0.16	193,193,193,193	0
85	MG	1	3469	1/1	0.83	0.22	50,50,50,50	0
85	MG	6	1904	1/1	0.83	0.20	55,55,55,55	0
85	MG	6	2020	1/1	0.83	0.16	93,93,93,93	0
86	OHX	1	4132	7/7	0.83	0.13	180,180,180,180	0
86	OHX	5	4191	7/7	0.83	0.13	199,199,199,199	0
85	MG	1	3449	1/1	0.83	0.21	35,35,35,35	0
86	OHX	5	4209	7/7	0.83	0.14	203,203,203,203	0
86	OHX	5	4216	7/7	0.83	0.14	206,206,206,206	0
85	MG	3	201	1/1	0.83	0.23	51,51,51,51	0
85	MG	1	3507	1/1	0.83	0.31	26,26,26,26	0
85	MG	c7	202	1/1	0.83	0.25	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	6	1914	1/1	0.83	0.22	62,62,62,62	0
86	OHX	5	4234	7/7	0.83	0.13	217,217,217,217	0
86	OHX	2	2140	7/7	0.83	0.12	226,226,226,226	0
85	MG	1	3814	1/1	0.83	0.10	36,36,36,36	0
85	MG	6	1924	1/1	0.83	0.32	32,32,32,32	0
86	OHX	1	4186	7/7	0.83	0.13	207,207,207,207	0
86	OHX	1	4188	7/7	0.83	0.13	191,191,191,191	0
86	OHX	5	4252	7/7	0.83	0.14	174,174,174,174	0
86	OHX	l4	403	7/7	0.83	0.12	203,203,203,203	0
85	MG	4	201	1/1	0.83	0.28	50,50,50,50	0
85	MG	1	3749	1/1	0.83	0.17	75,75,75,75	0
86	OHX	M6	202	7/7	0.83	0.19	179,179,179,179	0
86	OHX	M7	206	7/7	0.83	0.23	153,153,153,153	0
85	MG	5	3556	1/1	0.83	0.30	23,23,23,23	0
86	OHX	6	2172	7/7	0.83	0.12	203,203,203,203	0
85	MG	5	3650	1/1	0.84	0.23	51,51,51,51	0
85	MG	4	217	1/1	0.84	0.08	50,50,50,50	0
85	MG	2	1953	1/1	0.84	0.29	67,67,67,67	0
85	MG	6	1951	1/1	0.84	0.23	44,44,44,44	0
85	MG	1	3801	1/1	0.84	0.16	33,33,33,33	0
86	OHX	1	4141	7/7	0.84	0.14	182,182,182,182	0
85	MG	5	3462	1/1	0.84	0.18	44,44,44,44	0
86	OHX	5	4140	7/7	0.84	0.13	185,185,185,185	0
85	MG	6	1971	1/1	0.84	0.22	54,54,54,54	0
85	MG	5	3766	1/1	0.84	0.30	39,39,39,39	0
85	MG	2	1915	1/1	0.84	0.27	46,46,46,46	0
86	OHX	5	4190	7/7	0.84	0.18	161,161,161,161	0
85	MG	2	1938	1/1	0.84	0.30	47,47,47,47	0
85	MG	5	3780	1/1	0.84	0.13	45,45,45,45	0
85	MG	5	3490	1/1	0.84	0.08	23,23,23,23	0
85	MG	2	1996	1/1	0.84	0.20	55,55,55,55	0
86	OHX	2	2159	7/7	0.84	0.12	256,256,256,256	0
86	OHX	5	4222	7/7	0.84	0.14	191,191,191,191	0
85	MG	6	1994	1/1	0.84	0.27	43,43,43,43	0
85	MG	2	1967	1/1	0.84	0.23	52,52,52,52	0
86	OHX	1	4194	7/7	0.84	0.14	223,223,223,223	0
86	OHX	1	4196	7/7	0.84	0.12	194,194,194,194	0
86	OHX	4	234	7/7	0.84	0.14	196,196,196,196	0
86	OHX	5	4239	7/7	0.84	0.12	203,203,203,203	0
86	OHX	5	4240	7/7	0.84	0.16	206,206,206,206	0
85	MG	5	3811	1/1	0.84	0.11	77,77,77,77	0
85	MG	5	3816	1/1	0.84	0.10	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	6	2137	7/7	0.84	0.14	175,175,175,175	0
85	MG	5	3616	1/1	0.84	0.20	37,37,37,37	0
86	OHX	6	2150	7/7	0.84	0.13	179,179,179,179	0
85	MG	6	2012	1/1	0.84	0.08	33,33,33,33	0
86	OHX	6	2177	7/7	0.84	0.13	219,219,219,219	0
86	OHX	6	2180	7/7	0.84	0.15	164,164,164,164	0
86	OHX	6	2184	7/7	0.84	0.16	180,180,180,180	0
85	MG	1	3853	1/1	0.84	0.14	66,66,66,66	0
85	MG	6	2021	1/1	0.84	0.24	105,105,105,105	0
85	MG	5	3870	1/1	0.84	0.14	48,48,48,48	0
85	MG	2	1912	1/1	0.85	0.22	48,48,48,48	0
85	MG	M1	201	1/1	0.85	0.19	60,60,60,60	0
85	MG	5	3540	1/1	0.85	0.39	30,30,30,30	0
85	MG	1	3839	1/1	0.85	0.22	54,54,54,54	0
85	MG	5	3588	1/1	0.85	0.24	56,56,56,56	0
85	MG	2	1928	1/1	0.85	0.37	63,63,63,63	0
85	MG	6	1902	1/1	0.85	0.20	51,51,51,51	0
86	OHX	6	2199	7/7	0.85	0.11	237,237,237,237	0
85	MG	5	3880	1/1	0.85	0.25	43,43,43,43	0
86	OHX	1	4135	7/7	0.85	0.16	198,198,198,198	0
86	OHX	6	2203	7/7	0.85	0.14	200,200,200,200	0
85	MG	1	3852	1/1	0.85	0.19	74,74,74,74	0
85	MG	1	3636	1/1	0.85	0.25	46,46,46,46	0
86	OHX	1	4155	7/7	0.85	0.12	196,196,196,196	0
85	MG	2	2022	1/1	0.85	0.29	60,60,60,60	0
85	MG	5	3655	1/1	0.85	0.17	39,39,39,39	0
85	MG	1	3455	1/1	0.85	0.30	49,49,49,49	0
85	MG	5	4258	1/1	0.85	0.11	44,44,44,44	0
86	OHX	5	4196	7/7	0.85	0.16	156,156,156,156	0
86	OHX	1	4177	7/7	0.85	0.12	205,205,205,205	0
86	OHX	5	4207	7/7	0.85	0.12	199,199,199,199	0
85	MG	6	2028	1/1	0.85	0.30	57,57,57,57	0
85	MG	1	3799	1/1	0.85	0.10	51,51,51,51	0
85	MG	n8	201	1/1	0.85	0.16	34,34,34,34	0
86	OHX	1	4184	7/7	0.85	0.14	193,193,193,193	0
86	OHX	5	4225	7/7	0.85	0.12	219,219,219,219	0
85	MG	6	1916	1/1	0.85	0.27	39,39,39,39	0
85	MG	s1	301	1/1	0.85	0.17	74,74,74,74	0
86	OHX	5	4231	7/7	0.85	0.11	217,217,217,217	0
85	MG	2	1990	1/1	0.85	0.21	64,64,64,64	0
86	OHX	5	4233	7/7	0.85	0.10	216,216,216,216	0
86	OHX	2	2139	7/7	0.85	0.14	179,179,179,179	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3806	1/1	0.85	0.23	49,49,49,49	0
85	MG	5	3423	1/1	0.85	0.21	46,46,46,46	0
85	MG	5	3433	1/1	0.85	0.23	48,48,48,48	0
86	OHX	4	237	7/7	0.85	0.14	188,188,188,188	0
85	MG	6	1934	1/1	0.85	0.17	49,49,49,49	0
86	OHX	2	2161	7/7	0.85	0.10	275,275,275,275	0
86	OHX	M7	207	7/7	0.85	0.13	186,186,186,186	0
85	MG	6	1950	1/1	0.85	0.23	51,51,51,51	0
86	OHX	5	4253	7/7	0.85	0.12	210,210,210,210	0
86	OHX	7	227	7/7	0.85	0.16	195,195,195,195	0
86	OHX	8	225	7/7	0.85	0.14	173,173,173,173	0
86	OHX	8	228	7/7	0.85	0.14	170,170,170,170	0
85	MG	1	3413	1/1	0.85	0.32	62,62,62,62	0
85	MG	1	3622	1/1	0.85	0.18	52,52,52,52	0
85	MG	6	1970	1/1	0.85	0.21	61,61,61,61	0
86	OHX	2	2171	7/7	0.85	0.14	201,201,201,201	0
86	OHX	2	2174	7/7	0.85	0.15	215,215,215,215	0
86	OHX	6	2182	7/7	0.85	0.12	199,199,199,199	0
85	MG	5	3810	1/1	0.85	0.23	35,35,35,35	0
85	MG	5	3783	1/1	0.86	0.28	84,84,84,84	0
86	OHX	2	2167	7/7	0.86	0.10	240,240,240,240	0
85	MG	6	1962	1/1	0.86	0.21	55,55,55,55	0
85	MG	5	3798	1/1	0.86	0.12	54,54,54,54	0
85	MG	4	214	1/1	0.86	0.10	42,42,42,42	0
85	MG	6	1967	1/1	0.86	0.24	47,47,47,47	0
85	MG	1	3548	1/1	0.86	0.33	44,44,44,44	0
85	MG	2	1979	1/1	0.86	0.23	62,62,62,62	0
85	MG	6	1974	1/1	0.86	0.14	51,51,51,51	0
86	OHX	6	2196	7/7	0.86	0.10	238,238,238,238	0
86	OHX	1	4098	7/7	0.86	0.15	163,163,163,163	0
85	MG	2	1907	1/1	0.86	0.30	41,41,41,41	0
86	OHX	1	4119	7/7	0.86	0.17	161,161,161,161	0
85	MG	5	3506	1/1	0.86	0.23	42,42,42,42	0
85	MG	5	3856	1/1	0.86	0.20	47,47,47,47	0
86	OHX	6	2207	7/7	0.86	0.11	219,219,219,219	0
85	MG	5	3859	1/1	0.86	0.25	60,60,60,60	0
85	MG	2	1971	1/1	0.86	0.11	65,65,65,65	0
86	OHX	5	4141	7/7	0.86	0.16	182,182,182,182	0
86	OHX	5	4144	7/7	0.86	0.12	169,169,169,169	0
85	MG	2	1904	1/1	0.86	0.22	53,53,53,53	0
86	OHX	5	4160	7/7	0.86	0.14	191,191,191,191	0
86	OHX	5	4166	7/7	0.86	0.13	192,192,192,192	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	2	1962	1/1	0.86	0.22	43,43,43,43	0
85	MG	5	3606	1/1	0.86	0.06	23,23,23,23	0
86	OHX	5	4182	7/7	0.86	0.14	185,185,185,185	0
86	OHX	5	4184	7/7	0.86	0.12	179,179,179,179	0
85	MG	6	1999	1/1	0.86	0.19	84,84,84,84	0
86	OHX	1	4164	7/7	0.86	0.11	208,208,208,208	0
85	MG	6	2000	1/1	0.86	0.17	54,54,54,54	0
86	OHX	5	4198	7/7	0.86	0.16	196,196,196,196	0
85	MG	2	1939	1/1	0.86	0.24	50,50,50,50	0
86	OHX	5	4205	7/7	0.86	0.12	186,186,186,186	0
85	MG	6	2007	1/1	0.86	0.11	55,55,55,55	0
86	OHX	1	4171	7/7	0.86	0.19	168,168,168,168	0
86	OHX	5	4210	7/7	0.86	0.17	192,192,192,192	0
86	OHX	1	4174	7/7	0.86	0.14	169,169,169,169	0
85	MG	5	3896	1/1	0.86	0.06	145,145,145,145	0
85	MG	5	3642	1/1	0.86	0.25	59,59,59,59	0
86	OHX	5	4224	7/7	0.86	0.13	209,209,209,209	0
85	MG	1	3633	1/1	0.86	0.31	53,53,53,53	0
85	MG	2	1978	1/1	0.86	0.22	41,41,41,41	0
85	MG	l2	301	1/1	0.86	0.21	43,43,43,43	0
85	MG	5	3674	1/1	0.86	0.14	35,35,35,35	0
85	MG	1	3540	1/1	0.86	0.24	59,59,59,59	0
85	MG	3	212	1/1	0.86	0.25	47,47,47,47	0
85	MG	6	2033	1/1	0.86	0.24	52,52,52,52	0
86	OHX	5	4235	7/7	0.86	0.14	206,206,206,206	0
86	OHX	5	4236	7/7	0.86	0.11	223,223,223,223	0
86	OHX	2	2122	7/7	0.86	0.15	178,178,178,178	0
85	MG	5	3714	1/1	0.86	0.17	53,53,53,53	0
86	OHX	1	4204	7/7	0.86	0.14	211,211,211,211	0
86	OHX	3	223	7/7	0.86	0.13	215,215,215,215	0
86	OHX	5	4242	7/7	0.86	0.14	168,168,168,168	0
86	OHX	4	233	7/7	0.86	0.15	154,154,154,154	0
85	MG	1	3546	1/1	0.86	0.22	46,46,46,46	0
86	OHX	4	235	7/7	0.86	0.16	180,180,180,180	0
85	MG	6	2038	1/1	0.86	0.29	50,50,50,50	0
86	OHX	2	2148	7/7	0.86	0.13	183,183,183,183	0
85	MG	1	3809	1/1	0.86	0.19	49,49,49,49	0
86	OHX	8	224	7/7	0.86	0.14	205,205,205,205	0
85	MG	6	1927	1/1	0.86	0.27	55,55,55,55	0
86	OHX	O2	201	7/7	0.86	0.13	206,206,206,206	0
85	MG	5	3773	1/1	0.86	0.15	95,95,95,95	0
85	MG	4	202	1/1	0.86	0.26	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	4	208	1/1	0.86	0.20	39,39,39,39	0
86	OHX	6	2162	7/7	0.86	0.16	170,170,170,170	0
86	OHX	6	2166	7/7	0.86	0.12	234,234,234,234	0
85	MG	1	3670	1/1	0.86	0.15	29,29,29,29	0
85	MG	6	1957	1/1	0.86	0.27	34,34,34,34	0
85	MG	6	2004	1/1	0.87	0.19	67,67,67,67	0
85	MG	2	1913	1/1	0.87	0.26	50,50,50,50	0
85	MG	5	3887	1/1	0.87	0.21	60,60,60,60	0
85	MG	5	3632	1/1	0.87	0.32	70,70,70,70	0
86	OHX	1	4157	7/7	0.87	0.12	207,207,207,207	0
86	OHX	5	4110	7/7	0.87	0.13	167,167,167,167	0
85	MG	2	1909	1/1	0.87	0.21	46,46,46,46	0
85	MG	2	1931	1/1	0.87	0.23	53,53,53,53	0
85	MG	2	1982	1/1	0.87	0.21	60,60,60,60	0
85	MG	6	1919	1/1	0.87	0.25	51,51,51,51	0
86	OHX	5	4151	7/7	0.87	0.11	172,172,172,172	0
85	MG	5	3670	1/1	0.87	0.25	53,53,53,53	0
85	MG	7	215	1/1	0.87	0.14	43,43,43,43	0
85	MG	6	2029	1/1	0.87	0.12	97,97,97,97	0
86	OHX	1	4175	7/7	0.87	0.12	191,191,191,191	0
85	MG	1	3590	1/1	0.87	0.21	42,42,42,42	0
85	MG	1	3857	1/1	0.87	0.05	37,37,37,37	0
85	MG	m7	204	1/1	0.87	0.15	34,34,34,34	0
85	MG	5	3693	1/1	0.87	0.28	52,52,52,52	0
85	MG	1	3731	1/1	0.87	0.23	59,59,59,59	0
85	MG	1	3606	1/1	0.87	0.24	39,39,39,39	0
86	OHX	2	2110	7/7	0.87	0.14	173,173,173,173	0
86	OHX	2	2118	7/7	0.87	0.12	177,177,177,177	0
85	MG	6	2044	1/1	0.87	0.35	62,62,62,62	0
86	OHX	5	4208	7/7	0.87	0.13	199,199,199,199	0
85	MG	5	3732	1/1	0.87	0.11	46,46,46,46	0
86	OHX	1	4195	7/7	0.87	0.12	196,196,196,196	0
86	OHX	5	4215	7/7	0.87	0.11	200,200,200,200	0
85	MG	2	1945	1/1	0.87	0.28	55,55,55,55	0
86	OHX	1	4198	7/7	0.87	0.15	164,164,164,164	0
86	OHX	1	4199	7/7	0.87	0.15	174,174,174,174	0
86	OHX	5	4223	7/7	0.87	0.09	228,228,228,228	0
85	MG	s8	301	1/1	0.87	0.17	43,43,43,43	0
85	MG	2	1932	1/1	0.87	0.31	37,37,37,37	0
85	MG	1	3410	1/1	0.87	0.23	39,39,39,39	0
85	MG	5	3416	1/1	0.87	0.15	41,41,41,41	0
85	MG	1	3794	1/1	0.87	0.14	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3629	1/1	0.87	0.09	41,41,41,41	0
85	MG	1	3493	1/1	0.87	0.28	70,70,70,70	0
85	MG	6	1968	1/1	0.87	0.27	43,43,43,43	0
85	MG	5	3786	1/1	0.87	0.17	23,23,23,23	0
85	MG	1	3497	1/1	0.87	0.19	34,34,34,34	0
85	MG	5	3482	1/1	0.87	0.20	32,32,32,32	0
85	MG	2	1964	1/1	0.87	0.31	59,59,59,59	0
86	OHX	2	2173	7/7	0.87	0.14	216,216,216,216	0
85	MG	L7	304	1/1	0.87	0.20	63,63,63,63	0
85	MG	5	3497	1/1	0.87	0.12	31,31,31,31	0
85	MG	1	3415	1/1	0.87	0.14	49,49,49,49	0
85	MG	1	3661	1/1	0.87	0.21	44,44,44,44	0
86	OHX	5	4250	7/7	0.87	0.13	191,191,191,191	0
85	MG	1	3827	1/1	0.87	0.22	56,56,56,56	0
86	OHX	6	2181	7/7	0.87	0.12	165,165,165,165	0
85	MG	6	1990	1/1	0.87	0.10	47,47,47,47	0
86	OHX	5	4254	7/7	0.87	0.11	191,191,191,191	0
85	MG	Q2	502	1/1	0.87	0.17	51,51,51,51	0
85	MG	5	3582	1/1	0.87	0.25	37,37,37,37	0
85	MG	1	3831	1/1	0.87	0.25	44,44,44,44	0
85	MG	5	3864	1/1	0.87	0.19	42,42,42,42	0
86	OHX	6	2190	7/7	0.87	0.10	218,218,218,218	0
86	OHX	1	4123	7/7	0.87	0.11	205,205,205,205	0
85	MG	1	3420	1/1	0.87	0.33	49,49,49,49	0
86	OHX	m1	203	7/7	0.87	0.10	213,213,213,213	0
86	OHX	1	4129	7/7	0.87	0.16	139,139,139,139	0
86	OHX	1	4131	7/7	0.87	0.14	166,166,166,166	0
85	MG	1	3669	1/1	0.87	0.23	50,50,50,50	0
86	OHX	1	4133	7/7	0.87	0.21	133,133,133,133	0
86	OHX	6	2107	7/7	0.88	0.14	161,161,161,161	0
85	MG	1	3664	1/1	0.88	0.21	49,49,49,49	0
85	MG	5	3685	1/1	0.88	0.23	69,69,69,69	0
85	MG	6	2030	1/1	0.88	0.14	62,62,62,62	0
85	MG	1	3603	1/1	0.88	0.09	48,48,48,48	0
86	OHX	6	2165	7/7	0.88	0.13	172,172,172,172	0
85	MG	5	3709	1/1	0.88	0.26	62,62,62,62	0
86	OHX	6	2171	7/7	0.88	0.11	195,195,195,195	0
86	OHX	2	2154	7/7	0.88	0.12	199,199,199,199	0
85	MG	1	3605	1/1	0.88	0.17	58,58,58,58	0
85	MG	5	3721	1/1	0.88	0.15	46,46,46,46	0
85	MG	6	2035	1/1	0.88	0.17	56,56,56,56	0
85	MG	6	2037	1/1	0.88	0.21	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3414	1/1	0.88	0.25	26,26,26,26	0
85	MG	5	3739	1/1	0.88	0.31	55,55,55,55	0
85	MG	1	3457	1/1	0.88	0.20	29,29,29,29	0
85	MG	1	3535	1/1	0.88	0.27	43,43,43,43	0
85	MG	5	3769	1/1	0.88	0.24	21,21,21,21	0
85	MG	1	3700	1/1	0.88	0.15	37,37,37,37	0
86	OHX	2	2176	7/7	0.88	0.13	199,199,199,199	0
86	OHX	2	2177	7/7	0.88	0.11	209,209,209,209	0
85	MG	1	3464	1/1	0.88	0.17	39,39,39,39	0
85	MG	c1	201	1/1	0.88	0.12	34,34,34,34	0
86	OHX	2	2181	7/7	0.88	0.11	192,192,192,192	0
86	OHX	2	2182	7/7	0.88	0.12	213,213,213,213	0
85	MG	1	3705	1/1	0.88	0.12	47,47,47,47	0
86	OHX	1	3917	7/7	0.88	0.17	129,129,129,129	0
85	MG	1	3707	1/1	0.88	0.22	48,48,48,48	0
86	OHX	s8	303	7/7	0.88	0.11	196,196,196,196	0
85	MG	1	3716	1/1	0.88	0.20	46,46,46,46	0
85	MG	6	1942	1/1	0.88	0.27	32,32,32,32	0
85	MG	5	3794	1/1	0.88	0.15	60,60,60,60	0
85	MG	1	3626	1/1	0.88	0.26	114,114,114,114	0
85	MG	5	3437	1/1	0.88	0.25	52,52,52,52	0
85	MG	5	3804	1/1	0.88	0.13	47,47,47,47	0
86	OHX	1	4124	7/7	0.88	0.13	190,190,190,190	0
86	OHX	1	4126	7/7	0.88	0.14	152,152,152,152	0
85	MG	1	3730	1/1	0.88	0.17	24,24,24,24	0
85	MG	6	1956	1/1	0.88	0.24	34,34,34,34	0
86	OHX	5	4174	7/7	0.88	0.11	204,204,204,204	0
85	MG	2	1988	1/1	0.88	0.21	88,88,88,88	0
85	MG	5	3470	1/1	0.88	0.26	53,53,53,53	0
85	MG	5	3814	1/1	0.88	0.13	62,62,62,62	0
86	OHX	5	4189	7/7	0.88	0.15	173,173,173,173	0
85	MG	5	3815	1/1	0.88	0.09	49,49,49,49	0
85	MG	5	3472	1/1	0.88	0.19	44,44,44,44	0
86	OHX	5	4195	7/7	0.88	0.16	164,164,164,164	0
86	OHX	1	4139	7/7	0.88	0.11	206,206,206,206	0
85	MG	5	3476	1/1	0.88	0.13	80,80,80,80	0
85	MG	5	3828	1/1	0.88	0.12	42,42,42,42	0
85	MG	5	3834	1/1	0.88	0.12	66,66,66,66	0
86	OHX	1	4159	7/7	0.88	0.14	160,160,160,160	0
86	OHX	1	4160	7/7	0.88	0.10	231,231,231,231	0
86	OHX	1	4161	7/7	0.88	0.20	145,145,145,145	0
85	MG	1	3744	1/1	0.88	0.29	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4214	7/7	0.88	0.17	144,144,144,144	0
85	MG	6	1964	1/1	0.88	0.14	63,63,63,63	0
85	MG	3	209	1/1	0.88	0.18	46,46,46,46	0
86	OHX	5	4217	7/7	0.88	0.16	173,173,173,173	0
85	MG	1	3745	1/1	0.88	0.25	51,51,51,51	0
85	MG	2	1921	1/1	0.88	0.28	36,36,36,36	0
85	MG	3	226	1/1	0.88	0.14	60,60,60,60	0
86	OHX	1	4172	7/7	0.88	0.12	194,194,194,194	0
85	MG	5	3505	1/1	0.88	0.23	24,24,24,24	0
85	MG	2	1963	1/1	0.88	0.24	40,40,40,40	0
86	OHX	1	4176	7/7	0.88	0.19	117,117,117,117	0
85	MG	1	3573	1/1	0.88	0.33	25,25,25,25	0
86	OHX	1	4179	7/7	0.88	0.14	189,189,189,189	0
85	MG	5	3552	1/1	0.88	0.25	40,40,40,40	0
85	MG	4	204	1/1	0.88	0.28	59,59,59,59	0
85	MG	1	3762	1/1	0.88	0.13	49,49,49,49	0
85	MG	1	3766	1/1	0.88	0.09	56,56,56,56	0
85	MG	5	3602	1/1	0.88	0.11	65,65,65,65	0
85	MG	1	3641	1/1	0.88	0.20	35,35,35,35	0
85	MG	6	1993	1/1	0.88	0.13	50,50,50,50	0
85	MG	7	207	1/1	0.88	0.26	50,50,50,50	0
86	OHX	1	4192	7/7	0.88	0.13	173,173,173,173	0
85	MG	1	3788	1/1	0.88	0.15	60,60,60,60	0
85	MG	4	218	1/1	0.88	0.15	36,36,36,36	0
86	OHX	5	4245	7/7	0.88	0.13	197,197,197,197	0
86	OHX	5	4249	7/7	0.88	0.14	211,211,211,211	0
85	MG	8	202	1/1	0.88	0.20	42,42,42,42	0
86	OHX	1	4197	7/7	0.88	0.13	181,181,181,181	0
85	MG	4	220	1/1	0.88	0.25	54,54,54,54	0
85	MG	1	3642	1/1	0.88	0.19	57,57,57,57	0
86	OHX	1	4201	7/7	0.88	0.13	202,202,202,202	0
85	MG	1	3798	1/1	0.88	0.10	43,43,43,43	0
86	OHX	7	229	7/7	0.88	0.10	208,208,208,208	0
85	MG	n6	202	1/1	0.88	0.15	37,37,37,37	0
85	MG	2	2008	1/1	0.88	0.08	46,46,46,46	0
85	MG	5	3653	1/1	0.88	0.17	57,57,57,57	0
85	MG	1	3649	1/1	0.88	0.17	56,56,56,56	0
85	MG	5	3659	1/1	0.88	0.14	44,44,44,44	0
85	MG	N8	205	1/1	0.88	0.17	42,42,42,42	0
85	MG	1	3802	1/1	0.88	0.31	102,102,102,102	0
85	MG	2	2018	1/1	0.88	0.30	56,56,56,56	0
86	OHX	M8	201	7/7	0.88	0.12	187,187,187,187	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	M9	202	7/7	0.88	0.10	209,209,209,209	0
86	OHX	2	2138	7/7	0.88	0.12	176,176,176,176	0
86	OHX	6	2163	7/7	0.89	0.12	161,161,161,161	0
85	MG	5	3796	1/1	0.89	0.09	47,47,47,47	0
86	OHX	2	2180	7/7	0.89	0.10	212,212,212,212	0
85	MG	5	3486	1/1	0.89	0.17	41,41,41,41	0
85	MG	2	2025	1/1	0.89	0.21	106,106,106,106	0
86	OHX	6	2176	7/7	0.89	0.15	178,178,178,178	0
86	OHX	S8	302	7/7	0.89	0.10	192,192,192,192	0
85	MG	2	1917	1/1	0.89	0.32	44,44,44,44	0
85	MG	5	3495	1/1	0.89	0.09	41,41,41,41	0
86	OHX	1	4021	7/7	0.89	0.16	149,149,149,149	0
86	OHX	1	4030	7/7	0.89	0.14	153,153,153,153	0
86	OHX	1	4056	7/7	0.89	0.12	161,161,161,161	0
85	MG	2	1994	1/1	0.89	0.13	84,84,84,84	0
86	OHX	1	4075	7/7	0.89	0.13	166,166,166,166	0
86	OHX	6	2189	7/7	0.89	0.10	199,199,199,199	0
85	MG	2	1935	1/1	0.89	0.25	42,42,42,42	0
85	MG	5	3501	1/1	0.89	0.24	31,31,31,31	0
86	OHX	6	2192	7/7	0.89	0.12	168,168,168,168	0
86	OHX	1	4101	7/7	0.89	0.11	188,188,188,188	0
85	MG	1	3484	1/1	0.89	0.29	44,44,44,44	0
86	OHX	1	4107	7/7	0.89	0.11	203,203,203,203	0
86	OHX	1	4112	7/7	0.89	0.13	172,172,172,172	0
85	MG	2	1936	1/1	0.89	0.27	35,35,35,35	0
85	MG	1	3607	1/1	0.89	0.07	35,35,35,35	0
85	MG	5	3517	1/1	0.89	0.23	23,23,23,23	0
85	MG	6	1903	1/1	0.89	0.28	38,38,38,38	0
85	MG	6	2010	1/1	0.89	0.11	53,53,53,53	0
86	OHX	s1	302	7/7	0.89	0.11	195,195,195,195	0
85	MG	1	3494	1/1	0.89	0.18	35,35,35,35	0
85	MG	5	3565	1/1	0.89	0.28	22,22,22,22	0
86	OHX	5	4090	7/7	0.89	0.12	163,163,163,163	0
86	OHX	5	4101	7/7	0.89	0.15	142,142,142,142	0
85	MG	6	1905	1/1	0.89	0.22	47,47,47,47	0
86	OHX	5	4120	7/7	0.89	0.13	168,168,168,168	0
85	MG	1	3834	1/1	0.89	0.18	49,49,49,49	0
85	MG	1	3615	1/1	0.89	0.21	44,44,44,44	0
85	MG	5	3604	1/1	0.89	0.10	26,26,26,26	0
85	MG	6	1910	1/1	0.89	0.21	44,44,44,44	0
86	OHX	1	4137	7/7	0.89	0.10	184,184,184,184	0
86	OHX	5	4156	7/7	0.89	0.16	161,161,161,161	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4158	7/7	0.89	0.10	184,184,184,184	0
85	MG	5	3876	1/1	0.89	0.19	32,32,32,32	0
86	OHX	5	4162	7/7	0.89	0.14	171,171,171,171	0
85	MG	1	3840	1/1	0.89	0.17	32,32,32,32	0
86	OHX	1	4144	7/7	0.89	0.10	196,196,196,196	0
86	OHX	5	4168	7/7	0.89	0.14	179,179,179,179	0
86	OHX	1	4153	7/7	0.89	0.13	154,154,154,154	0
86	OHX	1	4154	7/7	0.89	0.11	180,180,180,180	0
86	OHX	5	4180	7/7	0.89	0.14	146,146,146,146	0
85	MG	2	1959	1/1	0.89	0.28	63,63,63,63	0
85	MG	5	3621	1/1	0.89	0.12	38,38,38,38	0
85	MG	1	3502	1/1	0.89	0.28	28,28,28,28	0
85	MG	1	3504	1/1	0.89	0.29	33,33,33,33	0
85	MG	1	3628	1/1	0.89	0.09	32,32,32,32	0
85	MG	5	3641	1/1	0.89	0.13	32,32,32,32	0
85	MG	1	3741	1/1	0.89	0.13	43,43,43,43	0
85	MG	5	3649	1/1	0.89	0.15	75,75,75,75	0
85	MG	5	4259	1/1	0.89	0.24	29,29,29,29	0
85	MG	1	3743	1/1	0.89	0.16	45,45,45,45	0
86	OHX	5	4206	7/7	0.89	0.16	180,180,180,180	0
85	MG	7	213	1/1	0.89	0.11	66,66,66,66	0
85	MG	2	1983	1/1	0.89	0.28	48,48,48,48	0
85	MG	3	207	1/1	0.89	0.27	47,47,47,47	0
85	MG	1	3513	1/1	0.89	0.26	18,18,18,18	0
85	MG	5	3665	1/1	0.89	0.11	39,39,39,39	0
85	MG	1	3428	1/1	0.89	0.19	46,46,46,46	0
85	MG	2	2013	1/1	0.89	0.34	56,56,56,56	0
85	MG	1	3637	1/1	0.89	0.11	61,61,61,61	0
86	OHX	5	4219	7/7	0.89	0.12	197,197,197,197	0
85	MG	5	3407	1/1	0.89	0.11	31,31,31,31	0
85	MG	2	2014	1/1	0.89	0.29	61,61,61,61	0
85	MG	2	1960	1/1	0.89	0.26	46,46,46,46	0
85	MG	5	3425	1/1	0.89	0.10	28,28,28,28	0
85	MG	5	3431	1/1	0.89	0.15	54,54,54,54	0
86	OHX	5	4226	7/7	0.89	0.11	190,190,190,190	0
85	MG	1	3770	1/1	0.89	0.16	48,48,48,48	0
86	OHX	5	4229	7/7	0.89	0.11	210,210,210,210	0
85	MG	5	3436	1/1	0.89	0.12	27,27,27,27	0
86	OHX	1	4191	7/7	0.89	0.11	192,192,192,192	0
86	OHX	2	2131	7/7	0.89	0.10	182,182,182,182	0
85	MG	1	3647	1/1	0.89	0.20	52,52,52,52	0
85	MG	5	3730	1/1	0.89	0.28	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3731	1/1	0.89	0.14	44,44,44,44	0
86	OHX	2	2141	7/7	0.89	0.13	169,169,169,169	0
86	OHX	2	2143	7/7	0.89	0.11	202,202,202,202	0
85	MG	5	3439	1/1	0.89	0.28	55,55,55,55	0
85	MG	5	3450	1/1	0.89	0.15	43,43,43,43	0
86	OHX	1	4202	7/7	0.89	0.16	156,156,156,156	0
86	OHX	2	2151	7/7	0.89	0.17	129,129,129,129	0
85	MG	5	3455	1/1	0.89	0.17	40,40,40,40	0
86	OHX	3	224	7/7	0.89	0.14	183,183,183,183	0
85	MG	5	3750	1/1	0.89	0.24	26,26,26,26	0
86	OHX	5	4247	7/7	0.89	0.10	215,215,215,215	0
85	MG	1	3785	1/1	0.89	0.17	76,76,76,76	0
85	MG	5	3753	1/1	0.89	0.16	41,41,41,41	0
85	MG	5	3765	1/1	0.89	0.22	43,43,43,43	0
86	OHX	L3	406	7/7	0.89	0.10	218,218,218,218	0
85	MG	5	3464	1/1	0.89	0.16	37,37,37,37	0
85	MG	2	1924	1/1	0.89	0.38	59,59,59,59	0
85	MG	1	3557	1/1	0.89	0.26	40,40,40,40	0
85	MG	1	3660	1/1	0.89	0.06	41,41,41,41	0
85	MG	2	1951	1/1	0.89	0.22	40,40,40,40	0
85	MG	1	3563	1/1	0.89	0.17	30,30,30,30	0
86	OHX	8	227	7/7	0.89	0.14	151,151,151,151	0
85	MG	5	3479	1/1	0.89	0.18	58,58,58,58	0
86	OHX	2	2175	7/7	0.89	0.12	163,163,163,163	0
86	OHX	6	2141	7/7	0.89	0.12	174,174,174,174	0
85	MG	5	3480	1/1	0.89	0.27	40,40,40,40	0
86	OHX	6	2147	7/7	0.89	0.14	175,175,175,175	0
85	MG	4	221	1/1	0.89	0.31	54,54,54,54	0
86	OHX	6	2152	7/7	0.89	0.12	184,184,184,184	0
86	OHX	6	2154	7/7	0.89	0.14	192,192,192,192	0
85	MG	5	3485	1/1	0.89	0.21	46,46,46,46	0
86	OHX	6	2173	7/7	0.90	0.18	128,128,128,128	0
86	OHX	6	2175	7/7	0.90	0.11	197,197,197,197	0
86	OHX	1	4077	7/7	0.90	0.11	178,178,178,178	0
86	OHX	1	4088	7/7	0.90	0.12	159,159,159,159	0
86	OHX	6	2179	7/7	0.90	0.13	152,152,152,152	0
85	MG	1	3776	1/1	0.90	0.20	38,38,38,38	0
85	MG	6	1939	1/1	0.90	0.30	54,54,54,54	0
85	MG	6	1940	1/1	0.90	0.20	41,41,41,41	0
86	OHX	6	2183	7/7	0.90	0.13	182,182,182,182	0
86	OHX	1	4103	7/7	0.90	0.11	166,166,166,166	0
85	MG	1	3779	1/1	0.90	0.18	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3411	1/1	0.90	0.20	31,31,31,31	0
86	OHX	1	4109	7/7	0.90	0.12	157,157,157,157	0
85	MG	5	3875	1/1	0.90	0.22	40,40,40,40	0
86	OHX	1	4114	7/7	0.90	0.13	179,179,179,179	0
85	MG	6	1948	1/1	0.90	0.37	48,48,48,48	0
85	MG	5	3645	1/1	0.90	0.20	22,22,22,22	0
85	MG	5	3648	1/1	0.90	0.15	37,37,37,37	0
85	MG	5	3421	1/1	0.90	0.29	28,28,28,28	0
85	MG	5	3422	1/1	0.90	0.09	37,37,37,37	0
85	MG	5	3892	1/1	0.90	0.11	33,33,33,33	0
85	MG	1	3781	1/1	0.90	0.12	34,34,34,34	0
85	MG	1	3690	1/1	0.90	0.30	46,46,46,46	0
85	MG	2	1949	1/1	0.90	0.36	44,44,44,44	0
85	MG	2	1991	1/1	0.90	0.27	45,45,45,45	0
86	OHX	6	2206	7/7	0.90	0.10	189,189,189,189	0
85	MG	5	3900	1/1	0.90	0.21	40,40,40,40	0
85	MG	4	205	1/1	0.90	0.30	47,47,47,47	0
85	MG	1	3547	1/1	0.90	0.18	38,38,38,38	0
86	OHX	1	4138	7/7	0.90	0.15	153,153,153,153	0
86	OHX	5	3975	7/7	0.90	0.17	135,135,135,135	0
86	OHX	5	4058	7/7	0.90	0.14	169,169,169,169	0
86	OHX	5	4086	7/7	0.90	0.14	146,146,146,146	0
85	MG	1	3470	1/1	0.90	0.13	42,42,42,42	0
86	OHX	1	4140	7/7	0.90	0.11	207,207,207,207	0
86	OHX	5	4107	7/7	0.90	0.16	120,120,120,120	0
85	MG	5	3449	1/1	0.90	0.22	59,59,59,59	0
86	OHX	1	4142	7/7	0.90	0.11	195,195,195,195	0
86	OHX	5	4134	7/7	0.90	0.09	221,221,221,221	0
86	OHX	1	4143	7/7	0.90	0.11	164,164,164,164	0
85	MG	2	1946	1/1	0.90	0.12	54,54,54,54	0
86	OHX	5	4143	7/7	0.90	0.14	169,169,169,169	0
85	MG	5	3686	1/1	0.90	0.10	42,42,42,42	0
85	MG	2	2020	1/1	0.90	0.27	51,51,51,51	0
85	MG	8	206	1/1	0.90	0.13	46,46,46,46	0
86	OHX	5	4154	7/7	0.90	0.10	185,185,185,185	0
85	MG	8	210	1/1	0.90	0.10	50,50,50,50	0
86	OHX	1	4158	7/7	0.90	0.10	216,216,216,216	0
85	MG	1	3713	1/1	0.90	0.22	71,71,71,71	0
85	MG	l5	302	1/1	0.90	0.18	54,54,54,54	0
86	OHX	5	4165	7/7	0.90	0.15	155,155,155,155	0
85	MG	1	3807	1/1	0.90	0.11	48,48,48,48	0
86	OHX	1	4162	7/7	0.90	0.12	156,156,156,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	m7	202	1/1	0.90	0.20	28,28,28,28	0
85	MG	2	1981	1/1	0.90	0.23	43,43,43,43	0
85	MG	5	3719	1/1	0.90	0.28	61,61,61,61	0
86	OHX	5	4178	7/7	0.90	0.12	193,193,193,193	0
86	OHX	5	4179	7/7	0.90	0.12	189,189,189,189	0
85	MG	L2	302	1/1	0.90	0.21	37,37,37,37	0
86	OHX	5	4181	7/7	0.90	0.18	133,133,133,133	0
85	MG	L3	403	1/1	0.90	0.07	29,29,29,29	0
85	MG	6	1984	1/1	0.90	0.14	69,69,69,69	0
86	OHX	5	4186	7/7	0.90	0.11	176,176,176,176	0
86	OHX	2	2096	7/7	0.90	0.13	170,170,170,170	0
86	OHX	2	2102	7/7	0.90	0.12	165,165,165,165	0
85	MG	1	3717	1/1	0.90	0.17	24,24,24,24	0
86	OHX	5	4194	7/7	0.90	0.13	145,145,145,145	0
85	MG	M0	301	1/1	0.90	0.14	40,40,40,40	0
85	MG	2	1965	1/1	0.90	0.17	82,82,82,82	0
86	OHX	2	2124	7/7	0.90	0.10	174,174,174,174	0
85	MG	5	3735	1/1	0.90	0.27	54,54,54,54	0
86	OHX	5	4200	7/7	0.90	0.14	148,148,148,148	0
86	OHX	2	2130	7/7	0.90	0.12	180,180,180,180	0
85	MG	1	3729	1/1	0.90	0.12	39,39,39,39	0
85	MG	M9	201	1/1	0.90	0.25	56,56,56,56	0
85	MG	1	3579	1/1	0.90	0.26	32,32,32,32	0
85	MG	2	2023	1/1	0.90	0.29	61,61,61,61	0
85	MG	N8	206	1/1	0.90	0.17	32,32,32,32	0
86	OHX	5	4212	7/7	0.90	0.18	150,150,150,150	0
86	OHX	5	4213	7/7	0.90	0.12	177,177,177,177	0
85	MG	1	3732	1/1	0.90	0.20	47,47,47,47	0
86	OHX	2	2145	7/7	0.90	0.14	159,159,159,159	0
85	MG	1	3836	1/1	0.90	0.22	52,52,52,52	0
86	OHX	1	4193	7/7	0.90	0.15	158,158,158,158	0
86	OHX	5	4218	7/7	0.90	0.10	220,220,220,220	0
85	MG	1	3587	1/1	0.90	0.34	20,20,20,20	0
86	OHX	2	2150	7/7	0.90	0.10	213,213,213,213	0
85	MG	6	2019	1/1	0.90	0.10	44,44,44,44	0
85	MG	1	3589	1/1	0.90	0.29	35,35,35,35	0
85	MG	5	3779	1/1	0.90	0.16	63,63,63,63	0
86	OHX	2	2156	7/7	0.90	0.09	205,205,205,205	0
86	OHX	2	2157	7/7	0.90	0.10	182,182,182,182	0
85	MG	2	1976	1/1	0.90	0.29	60,60,60,60	0
85	MG	1	3601	1/1	0.90	0.14	32,32,32,32	0
85	MG	2	1961	1/1	0.90	0.32	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	2	2163	7/7	0.90	0.11	194,194,194,194	0
85	MG	5	3784	1/1	0.90	0.07	68,68,68,68	0
85	MG	5	3523	1/1	0.90	0.30	21,21,21,21	0
85	MG	1	3456	1/1	0.90	0.19	19,19,19,19	0
86	OHX	4	236	7/7	0.90	0.11	178,178,178,178	0
85	MG	5	3547	1/1	0.90	0.35	37,37,37,37	0
85	MG	1	3402	1/1	0.90	0.28	37,37,37,37	0
85	MG	1	3856	1/1	0.90	0.27	59,59,59,59	0
85	MG	5	3800	1/1	0.90	0.20	41,41,41,41	0
85	MG	1	3759	1/1	0.90	0.08	34,34,34,34	0
85	MG	5	3571	1/1	0.90	0.22	22,22,22,22	0
85	MG	5	3573	1/1	0.90	0.26	23,23,23,23	0
85	MG	5	3809	1/1	0.90	0.12	44,44,44,44	0
85	MG	5	3580	1/1	0.90	0.22	30,30,30,30	0
86	OHX	6	2125	7/7	0.90	0.11	165,165,165,165	0
86	OHX	5	4248	7/7	0.90	0.11	171,171,171,171	0
86	OHX	6	2127	7/7	0.90	0.21	122,122,122,122	0
85	MG	1	3524	1/1	0.90	0.15	36,36,36,36	0
85	MG	6	1922	1/1	0.90	0.19	47,47,47,47	0
85	MG	2	1930	1/1	0.90	0.15	54,54,54,54	0
85	MG	1	3467	1/1	0.90	0.17	38,38,38,38	0
86	OHX	6	2149	7/7	0.90	0.17	131,131,131,131	0
85	MG	6	2209	1/1	0.90	0.15	54,54,54,54	0
85	MG	5	3608	1/1	0.90	0.27	55,55,55,55	0
85	MG	5	3609	1/1	0.90	0.23	24,24,24,24	0
86	OHX	6	2155	7/7	0.90	0.11	179,179,179,179	0
86	OHX	6	2161	7/7	0.90	0.14	142,142,142,142	0
85	MG	5	3841	1/1	0.90	0.08	61,61,61,61	0
86	OHX	l3	405	7/7	0.90	0.11	198,198,198,198	0
85	MG	1	3673	1/1	0.90	0.20	44,44,44,44	0
86	OHX	1	4057	7/7	0.90	0.14	153,153,153,153	0
86	OHX	1	4065	7/7	0.90	0.11	190,190,190,190	0
86	OHX	6	2167	7/7	0.90	0.10	202,202,202,202	0
86	OHX	6	2169	7/7	0.90	0.09	220,220,220,220	0
86	OHX	m7	205	7/7	0.90	0.12	174,174,174,174	0
86	OHX	6	2170	7/7	0.90	0.16	154,154,154,154	0
85	MG	5	3851	1/1	0.90	0.19	52,52,52,52	0
85	MG	6	1929	1/1	0.90	0.29	48,48,48,48	0
85	MG	6	1961	1/1	0.91	0.21	38,38,38,38	0
85	MG	1	3674	1/1	0.91	0.18	53,53,53,53	0
85	MG	7	208	1/1	0.91	0.11	49,49,49,49	0
85	MG	6	1963	1/1	0.91	0.14	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	7	214	1/1	0.91	0.09	44,44,44,44	0
86	OHX	1	4134	7/7	0.91	0.10	172,172,172,172	0
85	MG	1	3686	1/1	0.91	0.12	32,32,32,32	0
85	MG	5	3442	1/1	0.91	0.24	21,21,21,21	0
86	OHX	6	2197	7/7	0.91	0.09	230,230,230,230	0
85	MG	4	212	1/1	0.91	0.09	28,28,28,28	0
85	MG	6	1966	1/1	0.91	0.17	53,53,53,53	0
85	MG	8	209	1/1	0.91	0.09	53,53,53,53	0
85	MG	5	3698	1/1	0.91	0.20	54,54,54,54	0
85	MG	5	3700	1/1	0.91	0.15	49,49,49,49	0
85	MG	l3	401	1/1	0.91	0.28	19,19,19,19	0
85	MG	5	3704	1/1	0.91	0.07	39,39,39,39	0
85	MG	m5	303	1/1	0.91	0.11	36,36,36,36	0
86	OHX	1	4146	7/7	0.91	0.14	171,171,171,171	0
86	OHX	1	4147	7/7	0.91	0.11	182,182,182,182	0
86	OHX	sR	401	7/7	0.91	0.11	191,191,191,191	0
86	OHX	1	4152	7/7	0.91	0.09	191,191,191,191	0
86	OHX	5	4020	7/7	0.91	0.13	170,170,170,170	0
85	MG	m5	305	1/1	0.91	0.15	90,90,90,90	0
85	MG	5	3707	1/1	0.91	0.15	49,49,49,49	0
85	MG	5	3453	1/1	0.91	0.14	41,41,41,41	0
86	OHX	5	4098	7/7	0.91	0.10	179,179,179,179	0
86	OHX	5	4099	7/7	0.91	0.12	157,157,157,157	0
86	OHX	5	4100	7/7	0.91	0.13	172,172,172,172	0
85	MG	5	3710	1/1	0.91	0.23	44,44,44,44	0
85	MG	1	3792	1/1	0.91	0.23	39,39,39,39	0
86	OHX	5	4108	7/7	0.91	0.13	141,141,141,141	0
85	MG	1	3527	1/1	0.91	0.27	20,20,20,20	0
86	OHX	5	4111	7/7	0.91	0.14	150,150,150,150	0
86	OHX	5	4113	7/7	0.91	0.10	171,171,171,171	0
85	MG	n9	101	1/1	0.91	0.07	22,22,22,22	0
85	MG	1	3474	1/1	0.91	0.22	58,58,58,58	0
85	MG	5	3723	1/1	0.91	0.18	47,47,47,47	0
86	OHX	2	2082	7/7	0.91	0.14	143,143,143,143	0
85	MG	5	3724	1/1	0.91	0.12	36,36,36,36	0
85	MG	1	3695	1/1	0.91	0.14	40,40,40,40	0
86	OHX	5	4149	7/7	0.91	0.15	135,135,135,135	0
86	OHX	2	2105	7/7	0.91	0.12	174,174,174,174	0
86	OHX	1	4168	7/7	0.91	0.09	195,195,195,195	0
85	MG	5	3729	1/1	0.91	0.21	22,22,22,22	0
85	MG	1	3476	1/1	0.91	0.15	43,43,43,43	0
85	MG	1	3697	1/1	0.91	0.19	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3536	1/1	0.91	0.24	39,39,39,39	0
86	OHX	5	4161	7/7	0.91	0.13	143,143,143,143	0
85	MG	1	3617	1/1	0.91	0.24	59,59,59,59	0
85	MG	1	3619	1/1	0.91	0.15	37,37,37,37	0
85	MG	1	3621	1/1	0.91	0.10	39,39,39,39	0
86	OHX	1	4178	7/7	0.91	0.11	175,175,175,175	0
86	OHX	2	2137	7/7	0.91	0.11	170,170,170,170	0
86	OHX	5	4171	7/7	0.91	0.13	166,166,166,166	0
85	MG	5	3740	1/1	0.91	0.20	35,35,35,35	0
85	MG	5	3748	1/1	0.91	0.28	24,24,24,24	0
85	MG	5	3481	1/1	0.91	0.22	43,43,43,43	0
85	MG	6	1992	1/1	0.91	0.07	52,52,52,52	0
86	OHX	1	4185	7/7	0.91	0.11	197,197,197,197	0
85	MG	2	1914	1/1	0.91	0.21	35,35,35,35	0
85	MG	1	3815	1/1	0.91	0.05	46,46,46,46	0
85	MG	6	1996	1/1	0.91	0.12	70,70,70,70	0
85	MG	1	3817	1/1	0.91	0.16	44,44,44,44	0
85	MG	N3	202	1/1	0.91	0.29	56,56,56,56	0
85	MG	N3	203	1/1	0.91	0.18	31,31,31,31	0
85	MG	1	3543	1/1	0.91	0.26	24,24,24,24	0
86	OHX	5	4193	7/7	0.91	0.11	171,171,171,171	0
85	MG	6	2005	1/1	0.91	0.35	68,68,68,68	0
85	MG	1	3544	1/1	0.91	0.16	21,21,21,21	0
85	MG	5	3781	1/1	0.91	0.08	56,56,56,56	0
86	OHX	2	2158	7/7	0.91	0.12	175,175,175,175	0
85	MG	1	3454	1/1	0.91	0.18	44,44,44,44	0
86	OHX	2	2160	7/7	0.91	0.16	143,143,143,143	0
85	MG	1	3489	1/1	0.91	0.16	23,23,23,23	0
85	MG	1	3492	1/1	0.91	0.22	60,60,60,60	0
86	OHX	1	4203	7/7	0.91	0.08	205,205,205,205	0
85	MG	1	3551	1/1	0.91	0.28	18,18,18,18	0
86	OHX	3	222	7/7	0.91	0.14	148,148,148,148	0
85	MG	5	3787	1/1	0.91	0.09	29,29,29,29	0
85	MG	5	3529	1/1	0.91	0.25	33,33,33,33	0
85	MG	2	1929	1/1	0.91	0.24	41,41,41,41	0
85	MG	6	2025	1/1	0.91	0.11	87,87,87,87	0
85	MG	5	3551	1/1	0.91	0.25	30,30,30,30	0
85	MG	1	3841	1/1	0.91	0.21	41,41,41,41	0
85	MG	1	3843	1/1	0.91	0.21	43,43,43,43	0
85	MG	2	2005	1/1	0.91	0.21	75,75,75,75	0
86	OHX	L4	403	7/7	0.91	0.10	175,175,175,175	0
85	MG	1	3849	1/1	0.91	0.29	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3572	1/1	0.91	0.30	20,20,20,20	0
85	MG	2	1986	1/1	0.91	0.11	50,50,50,50	0
85	MG	5	3575	1/1	0.91	0.39	23,23,23,23	0
85	MG	5	3812	1/1	0.91	0.21	20,20,20,20	0
85	MG	1	3500	1/1	0.91	0.30	57,57,57,57	0
86	OHX	O3	202	7/7	0.91	0.14	137,137,137,137	0
85	MG	6	1917	1/1	0.91	0.30	59,59,59,59	0
85	MG	1	3644	1/1	0.91	0.20	26,26,26,26	0
85	MG	5	3598	1/1	0.91	0.35	18,18,18,18	0
86	OHX	6	2136	7/7	0.91	0.11	154,154,154,154	0
86	OHX	C3	201	7/7	0.91	0.09	216,216,216,216	0
86	OHX	6	2139	7/7	0.91	0.11	147,147,147,147	0
85	MG	2	2011	1/1	0.91	0.31	56,56,56,56	0
86	OHX	1	4010	7/7	0.91	0.10	163,163,163,163	0
85	MG	1	3405	1/1	0.91	0.21	42,42,42,42	0
85	MG	1	3582	1/1	0.91	0.22	31,31,31,31	0
85	MG	1	3438	1/1	0.91	0.20	38,38,38,38	0
85	MG	1	3407	1/1	0.91	0.15	30,30,30,30	0
85	MG	6	1932	1/1	0.91	0.26	51,51,51,51	0
85	MG	1	3515	1/1	0.91	0.28	29,29,29,29	0
86	OHX	6	2156	7/7	0.91	0.09	175,175,175,175	0
86	OHX	6	2158	7/7	0.91	0.10	186,186,186,186	0
85	MG	1	3595	1/1	0.91	0.30	30,30,30,30	0
85	MG	5	3622	1/1	0.91	0.21	29,29,29,29	0
85	MG	5	3625	1/1	0.91	0.22	31,31,31,31	0
85	MG	d6	102	1/1	0.91	0.22	49,49,49,49	0
86	OHX	1	4094	7/7	0.91	0.09	186,186,186,186	0
85	MG	1	3668	1/1	0.91	0.08	40,40,40,40	0
85	MG	1	3775	1/1	0.91	0.10	43,43,43,43	0
85	MG	5	3415	1/1	0.91	0.16	39,39,39,39	0
86	OHX	7	226	7/7	0.91	0.13	145,145,145,145	0
85	MG	1	3516	1/1	0.91	0.31	26,26,26,26	0
86	OHX	7	228	7/7	0.91	0.16	170,170,170,170	0
85	MG	5	3419	1/1	0.91	0.18	50,50,50,50	0
85	MG	5	3420	1/1	0.91	0.19	55,55,55,55	0
85	MG	1	3777	1/1	0.91	0.24	48,48,48,48	0
85	MG	1	3518	1/1	0.91	0.31	19,19,19,19	0
86	OHX	1	4115	7/7	0.91	0.10	178,178,178,178	0
86	OHX	6	2178	7/7	0.91	0.16	128,128,128,128	0
86	OHX	1	4116	7/7	0.91	0.17	127,127,127,127	0
85	MG	6	1953	1/1	0.91	0.18	39,39,39,39	0
85	MG	1	3408	1/1	0.91	0.26	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3426	1/1	0.91	0.21	36,36,36,36	0
85	MG	1	3783	1/1	0.91	0.47	34,34,34,34	0
86	OHX	1	4125	7/7	0.91	0.11	180,180,180,180	0
86	OHX	6	2185	7/7	0.91	0.12	181,181,181,181	0
85	MG	5	3432	1/1	0.91	0.19	35,35,35,35	0
86	OHX	1	4127	7/7	0.91	0.13	198,198,198,198	0
85	MG	5	3524	1/1	0.92	0.29	30,30,30,30	0
85	MG	5	3795	1/1	0.92	0.20	43,43,43,43	0
85	MG	5	3526	1/1	0.92	0.24	24,24,24,24	0
85	MG	N5	201	1/1	0.92	0.23	57,57,57,57	0
86	OHX	1	3997	7/7	0.92	0.13	126,126,126,126	0
85	MG	5	3535	1/1	0.92	0.15	44,44,44,44	0
86	OHX	1	4014	7/7	0.92	0.13	128,128,128,128	0
85	MG	6	2006	1/1	0.92	0.23	50,50,50,50	0
86	OHX	6	2174	7/7	0.92	0.10	177,177,177,177	0
85	MG	5	3801	1/1	0.92	0.11	54,54,54,54	0
86	OHX	1	4036	7/7	0.92	0.11	147,147,147,147	0
85	MG	5	3542	1/1	0.92	0.26	21,21,21,21	0
85	MG	5	3544	1/1	0.92	0.29	20,20,20,20	0
86	OHX	1	4062	7/7	0.92	0.15	149,149,149,149	0
85	MG	5	3545	1/1	0.92	0.26	46,46,46,46	0
85	MG	N8	202	1/1	0.92	0.09	15,15,15,15	0
86	OHX	1	4070	7/7	0.92	0.11	152,152,152,152	0
86	OHX	1	4074	7/7	0.92	0.14	127,127,127,127	0
85	MG	5	3548	1/1	0.92	0.27	35,35,35,35	0
85	MG	6	2009	1/1	0.92	0.09	38,38,38,38	0
85	MG	2	1943	1/1	0.92	0.18	48,48,48,48	0
85	MG	1	3819	1/1	0.92	0.11	42,42,42,42	0
85	MG	5	3559	1/1	0.92	0.11	35,35,35,35	0
86	OHX	1	4096	7/7	0.92	0.11	185,185,185,185	0
85	MG	6	2014	1/1	0.92	0.13	84,84,84,84	0
85	MG	1	3822	1/1	0.92	0.20	45,45,45,45	0
85	MG	1	3720	1/1	0.92	0.26	58,58,58,58	0
86	OHX	1	4104	7/7	0.92	0.17	146,146,146,146	0
85	MG	1	3437	1/1	0.92	0.21	23,23,23,23	0
86	OHX	6	2195	7/7	0.92	0.10	202,202,202,202	0
85	MG	1	3727	1/1	0.92	0.12	65,65,65,65	0
85	MG	5	3846	1/1	0.92	0.21	42,42,42,42	0
85	MG	1	3639	1/1	0.92	0.14	41,41,41,41	0
85	MG	1	3406	1/1	0.92	0.22	26,26,26,26	0
86	OHX	6	2200	7/7	0.92	0.10	194,194,194,194	0
85	MG	5	3583	1/1	0.92	0.31	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3587	1/1	0.92	0.25	21,21,21,21	0
86	OHX	1	4117	7/7	0.92	0.11	177,177,177,177	0
85	MG	1	3838	1/1	0.92	0.19	47,47,47,47	0
85	MG	5	3590	1/1	0.92	0.28	25,25,25,25	0
85	MG	5	3866	1/1	0.92	0.11	44,44,44,44	0
86	OHX	s4	301	7/7	0.92	0.12	178,178,178,178	0
85	MG	1	3443	1/1	0.92	0.12	79,79,79,79	0
85	MG	1	3477	1/1	0.92	0.24	29,29,29,29	0
86	OHX	c5	201	7/7	0.92	0.10	179,179,179,179	0
85	MG	6	1913	1/1	0.92	0.29	31,31,31,31	0
85	MG	1	3478	1/1	0.92	0.21	55,55,55,55	0
85	MG	2	2001	1/1	0.92	0.10	105,105,105,105	0
86	OHX	5	4046	7/7	0.92	0.12	159,159,159,159	0
85	MG	1	3591	1/1	0.92	0.27	20,20,20,20	0
85	MG	5	3886	1/1	0.92	0.14	18,18,18,18	0
86	OHX	5	4087	7/7	0.92	0.12	137,137,137,137	0
85	MG	6	2040	1/1	0.92	0.22	50,50,50,50	0
85	MG	6	2042	1/1	0.92	0.27	40,40,40,40	0
85	MG	5	3891	1/1	0.92	0.25	34,34,34,34	0
85	MG	1	3650	1/1	0.92	0.16	50,50,50,50	0
85	MG	5	3893	1/1	0.92	0.11	19,19,19,19	0
86	OHX	5	4103	7/7	0.92	0.12	165,165,165,165	0
85	MG	1	3850	1/1	0.92	0.17	66,66,66,66	0
85	MG	1	3653	1/1	0.92	0.21	22,22,22,22	0
85	MG	1	3530	1/1	0.92	0.33	48,48,48,48	0
85	MG	1	3752	1/1	0.92	0.07	42,42,42,42	0
85	MG	5	3634	1/1	0.92	0.22	52,52,52,52	0
86	OHX	5	4116	7/7	0.92	0.13	141,141,141,141	0
85	MG	6	1928	1/1	0.92	0.24	38,38,38,38	0
86	OHX	5	4121	7/7	0.92	0.12	146,146,146,146	0
86	OHX	5	4126	7/7	0.92	0.10	178,178,178,178	0
85	MG	5	3639	1/1	0.92	0.17	31,31,31,31	0
86	OHX	5	4135	7/7	0.92	0.12	143,143,143,143	0
86	OHX	5	4136	7/7	0.92	0.10	173,173,173,173	0
86	OHX	5	4138	7/7	0.92	0.11	179,179,179,179	0
85	MG	2	1948	1/1	0.92	0.14	46,46,46,46	0
86	OHX	1	4145	7/7	0.92	0.12	130,130,130,130	0
86	OHX	5	4142	7/7	0.92	0.10	184,184,184,184	0
85	MG	d4	201	1/1	0.92	0.16	54,54,54,54	0
85	MG	7	211	1/1	0.92	0.19	31,31,31,31	0
86	OHX	1	4148	7/7	0.92	0.13	194,194,194,194	0
85	MG	6	1930	1/1	0.92	0.27	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	1	3663	1/1	0.92	0.28	56,56,56,56	0
85	MG	2	2016	1/1	0.92	0.23	53,53,53,53	0
85	MG	6	1938	1/1	0.92	0.23	38,38,38,38	0
85	MG	5	3652	1/1	0.92	0.14	19,19,19,19	0
85	MG	1	4211	1/1	0.92	0.10	50,50,50,50	0
85	MG	1	3763	1/1	0.92	0.08	84,84,84,84	0
85	MG	1	3764	1/1	0.92	0.24	17,17,17,17	0
86	OHX	5	4163	7/7	0.92	0.11	158,158,158,158	0
86	OHX	5	4164	7/7	0.92	0.13	144,144,144,144	0
85	MG	6	1945	1/1	0.92	0.34	50,50,50,50	0
85	MG	5	3668	1/1	0.92	0.12	32,32,32,32	0
85	MG	1	3665	1/1	0.92	0.11	32,32,32,32	0
85	MG	l7	301	1/1	0.92	0.26	38,38,38,38	0
86	OHX	5	4169	7/7	0.92	0.11	184,184,184,184	0
86	OHX	5	4170	7/7	0.92	0.09	181,181,181,181	0
85	MG	m5	301	1/1	0.92	0.20	25,25,25,25	0
86	OHX	5	4172	7/7	0.92	0.13	162,162,162,162	0
85	MG	1	3452	1/1	0.92	0.19	32,32,32,32	0
85	MG	5	3679	1/1	0.92	0.08	36,36,36,36	0
86	OHX	5	4177	7/7	0.92	0.12	166,166,166,166	0
86	OHX	1	4169	7/7	0.92	0.10	184,184,184,184	0
85	MG	1	3772	1/1	0.92	0.10	48,48,48,48	0
85	MG	5	3682	1/1	0.92	0.08	29,29,29,29	0
85	MG	1	3412	1/1	0.92	0.19	34,34,34,34	0
86	OHX	1	4173	7/7	0.92	0.07	251,251,251,251	0
85	MG	5	3428	1/1	0.92	0.16	22,22,22,22	0
86	OHX	5	4185	7/7	0.92	0.09	179,179,179,179	0
85	MG	2	1908	1/1	0.92	0.21	53,53,53,53	0
86	OHX	5	4187	7/7	0.92	0.12	153,153,153,153	0
86	OHX	5	4188	7/7	0.92	0.12	146,146,146,146	0
85	MG	n8	203	1/1	0.92	0.12	30,30,30,30	0
85	MG	5	3689	1/1	0.92	0.23	39,39,39,39	0
85	MG	5	3691	1/1	0.92	0.13	38,38,38,38	0
85	MG	SM	301	1/1	0.92	0.15	43,43,43,43	0
85	MG	q3	503	1/1	0.92	0.17	63,63,63,63	0
86	OHX	2	2071	7/7	0.92	0.12	170,170,170,170	0
86	OHX	1	4182	7/7	0.92	0.11	178,178,178,178	0
86	OHX	5	4197	7/7	0.92	0.10	199,199,199,199	0
85	MG	6	1958	1/1	0.92	0.31	43,43,43,43	0
86	OHX	2	2083	7/7	0.92	0.12	171,171,171,171	0
86	OHX	2	2094	7/7	0.92	0.12	160,160,160,160	0
85	MG	5	3697	1/1	0.92	0.24	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	5	3434	1/1	0.92	0.17	53,53,53,53	0
85	MG	6	1960	1/1	0.92	0.22	47,47,47,47	0
86	OHX	2	2106	7/7	0.92	0.11	205,205,205,205	0
85	MG	5	3702	1/1	0.92	0.13	71,71,71,71	0
86	OHX	2	2112	7/7	0.92	0.10	170,170,170,170	0
86	OHX	2	2114	7/7	0.92	0.08	201,201,201,201	0
85	MG	1	3614	1/1	0.92	0.12	33,33,33,33	0
85	MG	5	3705	1/1	0.92	0.07	41,41,41,41	0
85	MG	2	1927	1/1	0.92	0.39	50,50,50,50	0
85	MG	1	3677	1/1	0.92	0.19	48,48,48,48	0
86	OHX	2	2129	7/7	0.92	0.10	170,170,170,170	0
85	MG	1	3680	1/1	0.92	0.15	41,41,41,41	0
86	OHX	1	4200	7/7	0.92	0.14	148,148,148,148	0
85	MG	1	3501	1/1	0.92	0.24	15,15,15,15	0
86	OHX	2	2136	7/7	0.92	0.09	187,187,187,187	0
85	MG	1	3618	1/1	0.92	0.24	57,57,57,57	0
85	MG	1	3790	1/1	0.92	0.14	20,20,20,20	0
86	OHX	1	4205	7/7	0.92	0.11	204,204,204,204	0
85	MG	5	3460	1/1	0.92	0.23	19,19,19,19	0
85	MG	5	3461	1/1	0.92	0.09	21,21,21,21	0
86	OHX	5	4228	7/7	0.92	0.12	190,190,190,190	0
85	MG	1	3692	1/1	0.92	0.19	51,51,51,51	0
86	OHX	4	230	7/7	0.92	0.13	130,130,130,130	0
86	OHX	2	2142	7/7	0.92	0.10	189,189,189,189	0
85	MG	6	1969	1/1	0.92	0.15	47,47,47,47	0
85	MG	1	3550	1/1	0.92	0.20	34,34,34,34	0
85	MG	1	3416	1/1	0.92	0.18	34,34,34,34	0
85	MG	1	3552	1/1	0.92	0.26	21,21,21,21	0
85	MG	4	222	1/1	0.92	0.31	83,83,83,83	0
86	OHX	5	4237	7/7	0.92	0.17	128,128,128,128	0
85	MG	6	1977	1/1	0.92	0.19	33,33,33,33	0
86	OHX	M0	303	7/7	0.92	0.13	143,143,143,143	0
85	MG	1	3800	1/1	0.92	0.10	32,32,32,32	0
86	OHX	2	2153	7/7	0.92	0.09	205,205,205,205	0
85	MG	1	3554	1/1	0.92	0.22	29,29,29,29	0
85	MG	5	3744	1/1	0.92	0.11	25,25,25,25	0
85	MG	6	1986	1/1	0.92	0.09	49,49,49,49	0
85	MG	6	1987	1/1	0.92	0.13	45,45,45,45	0
85	MG	6	1988	1/1	0.92	0.09	39,39,39,39	0
85	MG	L7	301	1/1	0.92	0.09	31,31,31,31	0
85	MG	5	3757	1/1	0.92	0.13	56,56,56,56	0
85	MG	1	3699	1/1	0.92	0.26	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	6	2132	7/7	0.92	0.10	169,169,169,169	0
86	OHX	6	2135	7/7	0.92	0.11	145,145,145,145	0
85	MG	6	1991	1/1	0.92	0.20	44,44,44,44	0
85	MG	5	3768	1/1	0.92	0.09	64,64,64,64	0
85	MG	1	3555	1/1	0.92	0.32	23,23,23,23	0
85	MG	5	3496	1/1	0.92	0.20	20,20,20,20	0
86	OHX	6	2145	7/7	0.92	0.11	162,162,162,162	0
85	MG	1	3419	1/1	0.92	0.17	49,49,49,49	0
85	MG	1	3505	1/1	0.92	0.22	24,24,24,24	0
85	MG	6	1995	1/1	0.92	0.13	35,35,35,35	0
85	MG	M3	203	1/1	0.92	0.10	26,26,26,26	0
85	MG	1	3631	1/1	0.92	0.22	61,61,61,61	0
86	OHX	6	2153	7/7	0.92	0.13	146,146,146,146	0
86	OHX	l4	402	7/7	0.92	0.10	172,172,172,172	0
85	MG	1	3812	1/1	0.92	0.07	43,43,43,43	0
85	MG	5	3509	1/1	0.92	0.24	18,18,18,18	0
85	MG	5	3512	1/1	0.92	0.31	17,17,17,17	0
85	MG	5	3785	1/1	0.92	0.17	52,52,52,52	0
86	OHX	6	2159	7/7	0.92	0.12	175,175,175,175	0
85	MG	1	3404	1/1	0.92	0.32	55,55,55,55	0
85	MG	1	3570	1/1	0.92	0.26	35,35,35,35	0
85	MG	5	3790	1/1	0.92	0.19	38,38,38,38	0
86	OHX	6	2164	7/7	0.92	0.14	143,143,143,143	0
85	MG	5	3592	1/1	0.93	0.25	22,22,22,22	0
85	MG	5	3597	1/1	0.93	0.30	28,28,28,28	0
85	MG	6	1933	1/1	0.93	0.20	59,59,59,59	0
86	OHX	C5	201	7/7	0.93	0.08	198,198,198,198	0
85	MG	c1	202	1/1	0.93	0.30	51,51,51,51	0
86	OHX	1	3960	7/7	0.93	0.11	128,128,128,128	0
86	OHX	1	3984	7/7	0.93	0.12	141,141,141,141	0
86	OHX	1	3990	7/7	0.93	0.13	159,159,159,159	0
86	OHX	1	3994	7/7	0.93	0.13	127,127,127,127	0
85	MG	1	3432	1/1	0.93	0.23	32,32,32,32	0
85	MG	6	1937	1/1	0.93	0.18	35,35,35,35	0
85	MG	d3	201	1/1	0.93	0.10	43,43,43,43	0
85	MG	5	3836	1/1	0.93	0.08	38,38,38,38	0
86	OHX	1	4025	7/7	0.93	0.10	163,163,163,163	0
85	MG	5	3840	1/1	0.93	0.15	43,43,43,43	0
85	MG	1	3564	1/1	0.93	0.19	35,35,35,35	0
86	OHX	1	4043	7/7	0.93	0.12	138,138,138,138	0
86	OHX	1	4047	7/7	0.93	0.12	166,166,166,166	0
85	MG	5	3611	1/1	0.93	0.13	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3847	1/1	0.93	0.08	45,45,45,45	0
86	OHX	1	4060	7/7	0.93	0.13	131,131,131,131	0
86	OHX	1	4061	7/7	0.93	0.12	151,151,151,151	0
85	MG	5	3612	1/1	0.93	0.13	28,28,28,28	0
86	OHX	1	4063	7/7	0.93	0.13	142,142,142,142	0
86	OHX	1	4064	7/7	0.93	0.10	158,158,158,158	0
85	MG	1	3761	1/1	0.93	0.12	50,50,50,50	0
85	MG	5	3617	1/1	0.93	0.15	33,33,33,33	0
85	MG	5	3618	1/1	0.93	0.14	33,33,33,33	0
86	OHX	1	4071	7/7	0.93	0.14	136,136,136,136	0
85	MG	5	3401	1/1	0.93	0.17	52,52,52,52	0
85	MG	5	3861	1/1	0.93	0.19	54,54,54,54	0
85	MG	5	3862	1/1	0.93	0.14	40,40,40,40	0
86	OHX	1	4080	7/7	0.93	0.11	163,163,163,163	0
86	OHX	1	4081	7/7	0.93	0.12	149,149,149,149	0
86	OHX	1	4086	7/7	0.93	0.09	187,187,187,187	0
85	MG	5	3403	1/1	0.93	0.24	50,50,50,50	0
85	MG	5	3405	1/1	0.93	0.20	21,21,21,21	0
86	OHX	1	4090	7/7	0.93	0.09	177,177,177,177	0
86	OHX	1	4092	7/7	0.93	0.16	132,132,132,132	0
85	MG	5	3868	1/1	0.93	0.20	39,39,39,39	0
85	MG	5	3623	1/1	0.93	0.11	51,51,51,51	0
86	OHX	1	4097	7/7	0.93	0.11	155,155,155,155	0
85	MG	1	3651	1/1	0.93	0.09	26,26,26,26	0
85	MG	5	3873	1/1	0.93	0.33	25,25,25,25	0
86	OHX	1	4102	7/7	0.93	0.10	148,148,148,148	0
85	MG	5	3410	1/1	0.93	0.25	49,49,49,49	0
85	MG	1	3565	1/1	0.93	0.28	21,21,21,21	0
85	MG	5	3879	1/1	0.93	0.18	26,26,26,26	0
85	MG	1	3657	1/1	0.93	0.16	45,45,45,45	0
86	OHX	1	4108	7/7	0.93	0.13	160,160,160,160	0
85	MG	1	3436	1/1	0.93	0.19	32,32,32,32	0
86	OHX	1	4111	7/7	0.93	0.11	165,165,165,165	0
86	OHX	5	4031	7/7	0.93	0.14	113,113,113,113	0
85	MG	6	1949	1/1	0.93	0.21	33,33,33,33	0
85	MG	3	210	1/1	0.93	0.17	52,52,52,52	0
86	OHX	5	4067	7/7	0.93	0.12	144,144,144,144	0
86	OHX	5	4080	7/7	0.93	0.11	155,155,155,155	0
85	MG	5	3889	1/1	0.93	0.18	38,38,38,38	0
85	MG	1	3767	1/1	0.93	0.19	45,45,45,45	0
85	MG	5	3643	1/1	0.93	0.19	39,39,39,39	0
86	OHX	1	4118	7/7	0.93	0.11	180,180,180,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	2	1942	1/1	0.93	0.11	52,52,52,52	0
86	OHX	1	4120	7/7	0.93	0.10	180,180,180,180	0
85	MG	6	1955	1/1	0.93	0.33	34,34,34,34	0
86	OHX	1	4122	7/7	0.93	0.12	141,141,141,141	0
86	OHX	5	4105	7/7	0.93	0.10	175,175,175,175	0
85	MG	S8	301	1/1	0.93	0.14	48,48,48,48	0
85	MG	1	3498	1/1	0.93	0.28	23,23,23,23	0
86	OHX	5	4109	7/7	0.93	0.13	130,130,130,130	0
85	MG	1	3439	1/1	0.93	0.23	26,26,26,26	0
85	MG	5	3430	1/1	0.93	0.21	52,52,52,52	0
85	MG	5	3898	1/1	0.93	0.22	47,47,47,47	0
85	MG	4	203	1/1	0.93	0.24	28,28,28,28	0
86	OHX	5	4118	7/7	0.93	0.10	171,171,171,171	0
85	MG	5	3656	1/1	0.93	0.17	38,38,38,38	0
85	MG	1	3666	1/1	0.93	0.09	64,64,64,64	0
86	OHX	5	4122	7/7	0.93	0.11	144,144,144,144	0
86	OHX	5	4124	7/7	0.93	0.10	177,177,177,177	0
86	OHX	5	4125	7/7	0.93	0.11	157,157,157,157	0
85	MG	7	205	1/1	0.93	0.22	103,103,103,103	0
86	OHX	5	4131	7/7	0.93	0.09	181,181,181,181	0
85	MG	5	3661	1/1	0.93	0.30	46,46,46,46	0
85	MG	1	3583	1/1	0.93	0.26	36,36,36,36	0
85	MG	7	209	1/1	0.93	0.11	45,45,45,45	0
85	MG	1	3442	1/1	0.93	0.21	21,21,21,21	0
86	OHX	5	4139	7/7	0.93	0.12	172,172,172,172	0
85	MG	1	3588	1/1	0.93	0.19	29,29,29,29	0
85	MG	1	3782	1/1	0.93	0.12	41,41,41,41	0
85	MG	5	3676	1/1	0.93	0.06	69,69,69,69	0
85	MG	2	1937	1/1	0.93	0.28	34,34,34,34	0
85	MG	4	215	1/1	0.93	0.09	47,47,47,47	0
86	OHX	5	4147	7/7	0.93	0.12	179,179,179,179	0
86	OHX	5	4148	7/7	0.93	0.14	153,153,153,153	0
85	MG	8	203	1/1	0.93	0.23	32,32,32,32	0
85	MG	8	205	1/1	0.93	0.19	53,53,53,53	0
85	MG	5	3681	1/1	0.93	0.10	33,33,33,33	0
86	OHX	5	4152	7/7	0.93	0.10	193,193,193,193	0
86	OHX	5	4153	7/7	0.93	0.15	136,136,136,136	0
85	MG	1	3444	1/1	0.93	0.28	49,49,49,49	0
85	MG	2	2007	1/1	0.93	0.16	45,45,45,45	0
85	MG	8	211	1/1	0.93	0.27	58,58,58,58	0
85	MG	1	3676	1/1	0.93	0.11	39,39,39,39	0
85	MG	1	3791	1/1	0.93	0.16	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	l3	403	1/1	0.93	0.34	27,27,27,27	0
85	MG	5	3688	1/1	0.93	0.12	39,39,39,39	0
85	MG	6	1972	1/1	0.93	0.14	48,48,48,48	0
86	OHX	1	4156	7/7	0.93	0.12	173,173,173,173	0
85	MG	m1	201	1/1	0.93	0.27	51,51,51,51	0
85	MG	m1	202	1/1	0.93	0.18	41,41,41,41	0
85	MG	1	3403	1/1	0.93	0.19	29,29,29,29	0
85	MG	m5	302	1/1	0.93	0.32	33,33,33,33	0
85	MG	5	3692	1/1	0.93	0.07	43,43,43,43	0
85	MG	1	3510	1/1	0.93	0.21	18,18,18,18	0
85	MG	1	3685	1/1	0.93	0.10	42,42,42,42	0
86	OHX	5	4173	7/7	0.93	0.09	205,205,205,205	0
85	MG	m7	201	1/1	0.93	0.28	23,23,23,23	0
85	MG	5	3465	1/1	0.93	0.24	54,54,54,54	0
85	MG	L6	202	1/1	0.93	0.10	45,45,45,45	0
85	MG	n3	202	1/1	0.93	0.10	39,39,39,39	0
85	MG	n6	201	1/1	0.93	0.14	34,34,34,34	0
85	MG	6	1983	1/1	0.93	0.23	58,58,58,58	0
85	MG	2	1956	1/1	0.93	0.14	71,71,71,71	0
85	MG	5	3703	1/1	0.93	0.13	48,48,48,48	0
85	MG	5	3471	1/1	0.93	0.24	21,21,21,21	0
85	MG	L7	302	1/1	0.93	0.14	40,40,40,40	0
85	MG	5	3473	1/1	0.93	0.27	31,31,31,31	0
85	MG	5	3708	1/1	0.93	0.28	55,55,55,55	0
85	MG	5	3475	1/1	0.93	0.13	39,39,39,39	0
85	MG	L7	303	1/1	0.93	0.15	49,49,49,49	0
85	MG	2	2010	1/1	0.93	0.29	32,32,32,32	0
86	OHX	2	2084	7/7	0.93	0.10	153,153,153,153	0
86	OHX	2	2089	7/7	0.93	0.14	138,138,138,138	0
85	MG	5	3716	1/1	0.93	0.21	40,40,40,40	0
85	MG	2	1957	1/1	0.93	0.14	53,53,53,53	0
85	MG	1	3517	1/1	0.93	0.22	21,21,21,21	0
85	MG	M3	201	1/1	0.93	0.07	39,39,39,39	0
85	MG	1	3805	1/1	0.93	0.12	56,56,56,56	0
85	MG	1	3608	1/1	0.93	0.12	50,50,50,50	0
85	MG	M6	201	1/1	0.93	0.08	44,44,44,44	0
85	MG	M7	204	1/1	0.93	0.10	30,30,30,30	0
85	MG	5	3494	1/1	0.93	0.15	28,28,28,28	0
86	OHX	2	2119	7/7	0.93	0.09	163,163,163,163	0
86	OHX	2	2120	7/7	0.93	0.10	177,177,177,177	0
86	OHX	2	2121	7/7	0.93	0.09	160,160,160,160	0
85	MG	2	1968	1/1	0.93	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4211	7/7	0.93	0.09	177,177,177,177	0
86	OHX	2	2123	7/7	0.93	0.09	176,176,176,176	0
85	MG	2	1905	1/1	0.93	0.28	49,49,49,49	0
85	MG	2	1995	1/1	0.93	0.16	50,50,50,50	0
86	OHX	2	2128	7/7	0.93	0.10	168,168,168,168	0
85	MG	1	3463	1/1	0.93	0.06	30,30,30,30	0
85	MG	2	2017	1/1	0.93	0.26	43,43,43,43	0
85	MG	1	3534	1/1	0.93	0.25	12,12,12,12	0
86	OHX	2	2134	7/7	0.93	0.13	153,153,153,153	0
86	OHX	2	2135	7/7	0.93	0.10	174,174,174,174	0
85	MG	2	1920	1/1	0.93	0.35	51,51,51,51	0
86	OHX	3	221	7/7	0.93	0.10	171,171,171,171	0
85	MG	1	3711	1/1	0.93	0.10	33,33,33,33	0
85	MG	6	2008	1/1	0.93	0.18	42,42,42,42	0
85	MG	2	2019	1/1	0.93	0.15	30,30,30,30	0
86	OHX	3	225	7/7	0.93	0.10	191,191,191,191	0
85	MG	5	3755	1/1	0.93	0.16	45,45,45,45	0
86	OHX	4	231	7/7	0.93	0.10	162,162,162,162	0
85	MG	5	3516	1/1	0.93	0.15	31,31,31,31	0
85	MG	5	3759	1/1	0.93	0.08	41,41,41,41	0
85	MG	6	1901	1/1	0.93	0.23	33,33,33,33	0
85	MG	6	2011	1/1	0.93	0.26	50,50,50,50	0
86	OHX	2	2146	7/7	0.93	0.13	150,150,150,150	0
85	MG	1	3823	1/1	0.93	0.27	25,25,25,25	0
85	MG	1	3825	1/1	0.93	0.19	28,28,28,28	0
85	MG	5	3770	1/1	0.93	0.06	28,28,28,28	0
85	MG	2	1952	1/1	0.93	0.23	58,58,58,58	0
85	MG	1	3829	1/1	0.93	0.56	41,41,41,41	0
85	MG	2	1999	1/1	0.93	0.23	71,71,71,71	0
85	MG	6	2022	1/1	0.93	0.06	45,45,45,45	0
85	MG	1	3472	1/1	0.93	0.16	19,19,19,19	0
85	MG	1	3417	1/1	0.93	0.21	33,33,33,33	0
85	MG	2	2000	1/1	0.93	0.09	66,66,66,66	0
85	MG	2	1940	1/1	0.93	0.15	55,55,55,55	0
86	OHX	6	2112	7/7	0.93	0.11	138,138,138,138	0
86	OHX	6	2117	7/7	0.93	0.11	161,161,161,161	0
85	MG	6	2031	1/1	0.93	0.17	53,53,53,53	0
85	MG	6	2032	1/1	0.93	0.09	39,39,39,39	0
85	MG	5	3553	1/1	0.93	0.28	25,25,25,25	0
86	OHX	6	2133	7/7	0.93	0.13	143,143,143,143	0
86	OHX	6	2134	7/7	0.93	0.11	186,186,186,186	0
85	MG	1	3423	1/1	0.93	0.28	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4255	7/7	0.93	0.08	204,204,204,204	0
85	MG	1	3426	1/1	0.93	0.22	44,44,44,44	0
85	MG	5	3791	1/1	0.93	0.20	13,13,13,13	0
85	MG	5	3561	1/1	0.93	0.30	29,29,29,29	0
86	OHX	6	2140	7/7	0.93	0.10	163,163,163,163	0
85	MG	1	3481	1/1	0.93	0.17	24,24,24,24	0
86	OHX	6	2144	7/7	0.93	0.09	174,174,174,174	0
86	OHX	2	2169	7/7	0.93	0.09	194,194,194,194	0
85	MG	5	3569	1/1	0.93	0.24	16,16,16,16	0
85	MG	1	3735	1/1	0.93	0.13	34,34,34,34	0
85	MG	1	3483	1/1	0.93	0.07	37,37,37,37	0
85	MG	1	3847	1/1	0.93	0.13	19,19,19,19	0
86	OHX	l5	304	7/7	0.93	0.11	178,178,178,178	0
85	MG	1	3640	1/1	0.93	0.15	29,29,29,29	0
86	OHX	l9	600	7/7	0.93	0.11	151,151,151,151	0
85	MG	6	2041	1/1	0.93	0.28	50,50,50,50	0
85	MG	1	3427	1/1	0.93	0.17	22,22,22,22	0
85	MG	2	2002	1/1	0.93	0.16	53,53,53,53	0
85	MG	1	3559	1/1	0.93	0.26	34,34,34,34	0
85	MG	1	3561	1/1	0.93	0.27	14,14,14,14	0
85	MG	1	3490	1/1	0.93	0.10	46,46,46,46	0
86	OHX	6	2160	7/7	0.93	0.10	169,169,169,169	0
86	OHX	6	2168	7/7	0.94	0.09	169,169,169,169	0
85	MG	5	3644	1/1	0.94	0.10	49,49,49,49	0
86	OHX	1	4055	7/7	0.94	0.08	190,190,190,190	0
85	MG	O4	201	1/1	0.94	0.19	30,30,30,30	0
85	MG	5	3646	1/1	0.94	0.27	40,40,40,40	0
85	MG	1	3683	1/1	0.94	0.08	31,31,31,31	0
85	MG	2	1901	1/1	0.94	0.25	52,52,52,52	0
85	MG	1	3630	1/1	0.94	0.17	63,63,63,63	0
85	MG	5	3877	1/1	0.94	0.28	32,32,32,32	0
85	MG	1	3577	1/1	0.94	0.21	20,20,20,20	0
85	MG	5	3467	1/1	0.94	0.10	33,33,33,33	0
85	MG	5	3881	1/1	0.94	0.25	16,16,16,16	0
85	MG	5	3654	1/1	0.94	0.13	47,47,47,47	0
85	MG	5	3468	1/1	0.94	0.07	28,28,28,28	0
86	OHX	1	4072	7/7	0.94	0.12	152,152,152,152	0
86	OHX	1	4073	7/7	0.94	0.11	159,159,159,159	0
85	MG	1	3578	1/1	0.94	0.25	26,26,26,26	0
85	MG	5	3658	1/1	0.94	0.12	17,17,17,17	0
85	MG	6	2002	1/1	0.94	0.12	53,53,53,53	0
86	OHX	1	4078	7/7	0.94	0.10	155,155,155,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3660	1/1	0.94	0.21	24,24,24,24	0
85	MG	2	1925	1/1	0.94	0.38	52,52,52,52	0
86	OHX	1	4083	7/7	0.94	0.10	156,156,156,156	0
86	OHX	1	4085	7/7	0.94	0.12	152,152,152,152	0
85	MG	5	3664	1/1	0.94	0.19	35,35,35,35	0
85	MG	1	3635	1/1	0.94	0.17	47,47,47,47	0
85	MG	1	3499	1/1	0.94	0.28	48,48,48,48	0
85	MG	1	3539	1/1	0.94	0.29	17,17,17,17	0
86	OHX	1	4091	7/7	0.94	0.09	183,183,183,183	0
85	MG	5	3672	1/1	0.94	0.07	56,56,56,56	0
85	MG	5	3673	1/1	0.94	0.19	40,40,40,40	0
86	OHX	1	4095	7/7	0.94	0.11	161,161,161,161	0
85	MG	1	3429	1/1	0.94	0.36	30,30,30,30	0
85	MG	5	4257	1/1	0.94	0.15	26,26,26,26	0
85	MG	5	3478	1/1	0.94	0.16	21,21,21,21	0
86	OHX	1	4100	7/7	0.94	0.11	129,129,129,129	0
85	MG	3	204	1/1	0.94	0.28	30,30,30,30	0
85	MG	7	201	1/1	0.94	0.25	30,30,30,30	0
85	MG	7	204	1/1	0.94	0.20	39,39,39,39	0
85	MG	1	3542	1/1	0.94	0.26	30,30,30,30	0
85	MG	2	1972	1/1	0.94	0.11	39,39,39,39	0
86	OHX	1	4106	7/7	0.94	0.16	123,123,123,123	0
85	MG	1	3702	1/1	0.94	0.16	58,58,58,58	0
85	MG	5	3483	1/1	0.94	0.22	40,40,40,40	0
85	MG	7	210	1/1	0.94	0.20	40,40,40,40	0
86	OHX	5	3998	7/7	0.94	0.13	122,122,122,122	0
86	OHX	5	4017	7/7	0.94	0.13	115,115,115,115	0
86	OHX	1	4110	7/7	0.94	0.10	148,148,148,148	0
86	OHX	5	4027	7/7	0.94	0.11	122,122,122,122	0
86	OHX	5	4030	7/7	0.94	0.13	124,124,124,124	0
85	MG	1	3704	1/1	0.94	0.11	51,51,51,51	0
86	OHX	5	4041	7/7	0.94	0.12	140,140,140,140	0
86	OHX	5	4045	7/7	0.94	0.12	150,150,150,150	0
85	MG	6	1920	1/1	0.94	0.27	37,37,37,37	0
86	OHX	5	4055	7/7	0.94	0.11	126,126,126,126	0
86	OHX	5	4057	7/7	0.94	0.15	123,123,123,123	0
86	OHX	1	4113	7/7	0.94	0.13	122,122,122,122	0
86	OHX	5	4061	7/7	0.94	0.09	147,147,147,147	0
86	OHX	5	4066	7/7	0.94	0.11	148,148,148,148	0
85	MG	3	211	1/1	0.94	0.05	64,64,64,64	0
86	OHX	5	4073	7/7	0.94	0.09	162,162,162,162	0
86	OHX	5	4076	7/7	0.94	0.13	139,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4077	7/7	0.94	0.10	132,132,132,132	0
86	OHX	5	4078	7/7	0.94	0.10	144,144,144,144	0
85	MG	5	3489	1/1	0.94	0.21	10,10,10,10	0
85	MG	5	3690	1/1	0.94	0.20	36,36,36,36	0
85	MG	1	3789	1/1	0.94	0.21	33,33,33,33	0
86	OHX	5	4089	7/7	0.94	0.12	136,136,136,136	0
85	MG	2	1906	1/1	0.94	0.23	37,37,37,37	0
86	OHX	5	4091	7/7	0.94	0.13	127,127,127,127	0
86	OHX	5	4092	7/7	0.94	0.14	119,119,119,119	0
86	OHX	5	4094	7/7	0.94	0.11	147,147,147,147	0
85	MG	6	2023	1/1	0.94	0.15	40,40,40,40	0
85	MG	6	1926	1/1	0.94	0.15	37,37,37,37	0
85	MG	1	3706	1/1	0.94	0.21	33,33,33,33	0
85	MG	1	3545	1/1	0.94	0.13	31,31,31,31	0
86	OHX	5	4102	7/7	0.94	0.11	138,138,138,138	0
85	MG	5	3500	1/1	0.94	0.22	26,26,26,26	0
85	MG	1	3503	1/1	0.94	0.20	20,20,20,20	0
86	OHX	5	4106	7/7	0.94	0.12	163,163,163,163	0
85	MG	5	3502	1/1	0.94	0.20	18,18,18,18	0
85	MG	1	3795	1/1	0.94	0.15	75,75,75,75	0
85	MG	l5	301	1/1	0.94	0.24	49,49,49,49	0
85	MG	2	1916	1/1	0.94	0.23	31,31,31,31	0
85	MG	1	3714	1/1	0.94	0.05	26,26,26,26	0
86	OHX	5	4112	7/7	0.94	0.17	122,122,122,122	0
86	OHX	1	4130	7/7	0.94	0.14	116,116,116,116	0
86	OHX	5	4114	7/7	0.94	0.13	149,149,149,149	0
85	MG	5	3507	1/1	0.94	0.23	24,24,24,24	0
85	MG	4	206	1/1	0.94	0.18	18,18,18,18	0
85	MG	5	3510	1/1	0.94	0.18	28,28,28,28	0
85	MG	5	3712	1/1	0.94	0.14	32,32,32,32	0
85	MG	6	1936	1/1	0.94	0.21	31,31,31,31	0
85	MG	5	3515	1/1	0.94	0.25	24,24,24,24	0
85	MG	1	3418	1/1	0.94	0.23	36,36,36,36	0
85	MG	5	3720	1/1	0.94	0.22	51,51,51,51	0
86	OHX	5	4130	7/7	0.94	0.11	152,152,152,152	0
85	MG	1	3602	1/1	0.94	0.13	36,36,36,36	0
85	MG	5	3722	1/1	0.94	0.15	25,25,25,25	0
85	MG	4	211	1/1	0.94	0.14	48,48,48,48	0
85	MG	1	3719	1/1	0.94	0.10	38,38,38,38	0
86	OHX	5	4137	7/7	0.94	0.12	144,144,144,144	0
85	MG	5	3725	1/1	0.94	0.11	37,37,37,37	0
85	MG	6	1941	1/1	0.94	0.16	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	n8	202	1/1	0.94	0.17	38,38,38,38	0
85	MG	5	3528	1/1	0.94	0.28	29,29,29,29	0
85	MG	4	213	1/1	0.94	0.13	43,43,43,43	0
85	MG	5	3531	1/1	0.94	0.24	18,18,18,18	0
85	MG	5	3534	1/1	0.94	0.18	24,24,24,24	0
85	MG	6	2043	1/1	0.94	0.19	35,35,35,35	0
85	MG	5	3536	1/1	0.94	0.20	27,27,27,27	0
85	MG	5	3738	1/1	0.94	0.08	37,37,37,37	0
85	MG	5	3538	1/1	0.94	0.28	34,34,34,34	0
85	MG	5	3539	1/1	0.94	0.22	23,23,23,23	0
85	MG	1	3549	1/1	0.94	0.24	36,36,36,36	0
86	OHX	2	2091	7/7	0.94	0.11	155,155,155,155	0
85	MG	5	3745	1/1	0.94	0.11	40,40,40,40	0
86	OHX	2	2095	7/7	0.94	0.17	125,125,125,125	0
85	MG	5	3747	1/1	0.94	0.23	47,47,47,47	0
86	OHX	5	4159	7/7	0.94	0.09	152,152,152,152	0
86	OHX	2	2100	7/7	0.94	0.10	169,169,169,169	0
85	MG	6	2208	1/1	0.94	0.17	48,48,48,48	0
86	OHX	2	2103	7/7	0.94	0.08	176,176,176,176	0
85	MG	5	3543	1/1	0.94	0.24	23,23,23,23	0
85	MG	1	3723	1/1	0.94	0.15	30,30,30,30	0
86	OHX	2	2107	7/7	0.94	0.11	133,133,133,133	0
86	OHX	2	2108	7/7	0.94	0.10	157,157,157,157	0
85	MG	2	1998	1/1	0.94	0.21	27,27,27,27	0
85	MG	1	3808	1/1	0.94	0.17	34,34,34,34	0
85	MG	1	3726	1/1	0.94	0.11	48,48,48,48	0
86	OHX	2	2115	7/7	0.94	0.10	159,159,159,159	0
86	OHX	2	2116	7/7	0.94	0.10	180,180,180,180	0
85	MG	5	3550	1/1	0.94	0.23	42,42,42,42	0
85	MG	5	3760	1/1	0.94	0.22	63,63,63,63	0
85	MG	5	3764	1/1	0.94	0.13	55,55,55,55	0
85	MG	1	3654	1/1	0.94	0.12	27,27,27,27	0
86	OHX	5	4176	7/7	0.94	0.18	108,108,108,108	0
85	MG	6	1954	1/1	0.94	0.28	26,26,26,26	0
85	MG	5	3767	1/1	0.94	0.10	40,40,40,40	0
85	MG	1	3655	1/1	0.94	0.23	20,20,20,20	0
86	OHX	2	2125	7/7	0.94	0.10	168,168,168,168	0
85	MG	c8	202	1/1	0.94	0.14	52,52,52,52	0
85	MG	5	3557	1/1	0.94	0.29	44,44,44,44	0
85	MG	5	3558	1/1	0.94	0.25	20,20,20,20	0
86	OHX	1	4187	7/7	0.94	0.10	186,186,186,186	0
85	MG	1	3459	1/1	0.94	0.24	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3775	1/1	0.94	0.15	31,31,31,31	0
85	MG	1	3462	1/1	0.94	0.20	16,16,16,16	0
85	MG	5	3778	1/1	0.94	0.30	24,24,24,24	0
85	MG	L5	301	1/1	0.94	0.14	38,38,38,38	0
85	MG	sM	302	1/1	0.94	0.12	33,33,33,33	0
86	OHX	5	4192	7/7	0.94	0.11	143,143,143,143	0
85	MG	6	1959	1/1	0.94	0.23	30,30,30,30	0
85	MG	1	3816	1/1	0.94	0.12	36,36,36,36	0
85	MG	5	3404	1/1	0.94	0.09	37,37,37,37	0
85	MG	1	3553	1/1	0.94	0.21	42,42,42,42	0
85	MG	1	3486	1/1	0.94	0.24	23,23,23,23	0
85	MG	1	3737	1/1	0.94	0.12	36,36,36,36	0
85	MG	1	3740	1/1	0.94	0.12	35,35,35,35	0
85	MG	L8	301	1/1	0.94	0.22	45,45,45,45	0
86	OHX	2	2147	7/7	0.94	0.08	186,186,186,186	0
85	MG	1	3440	1/1	0.94	0.20	24,24,24,24	0
85	MG	5	3589	1/1	0.94	0.24	19,19,19,19	0
85	MG	5	3418	1/1	0.94	0.29	10,10,10,10	0
85	MG	1	3556	1/1	0.94	0.25	25,25,25,25	0
85	MG	5	3593	1/1	0.94	0.23	26,26,26,26	0
85	MG	5	3594	1/1	0.94	0.26	32,32,32,32	0
85	MG	5	3799	1/1	0.94	0.09	30,30,30,30	0
86	OHX	2	2155	7/7	0.94	0.10	161,161,161,161	0
85	MG	1	3616	1/1	0.94	0.14	36,36,36,36	0
85	MG	S2	301	1/1	0.94	0.30	57,57,57,57	0
85	MG	5	3802	1/1	0.94	0.18	46,46,46,46	0
85	MG	5	3600	1/1	0.94	0.09	36,36,36,36	0
85	MG	2	1922	1/1	0.94	0.15	45,45,45,45	0
85	MG	5	3807	1/1	0.94	0.17	40,40,40,40	0
85	MG	M5	302	1/1	0.94	0.18	48,48,48,48	0
85	MG	1	3833	1/1	0.94	0.20	25,25,25,25	0
85	MG	M7	201	1/1	0.94	0.25	50,50,50,50	0
85	MG	M7	203	1/1	0.94	0.22	27,27,27,27	0
85	MG	6	1976	1/1	0.94	0.10	35,35,35,35	0
85	MG	5	3813	1/1	0.94	0.07	38,38,38,38	0
86	OHX	2	2168	7/7	0.94	0.08	195,195,195,195	0
85	MG	1	3520	1/1	0.94	0.20	18,18,18,18	0
85	MG	2	2009	1/1	0.94	0.32	42,42,42,42	0
85	MG	N0	201	1/1	0.94	0.10	56,56,56,56	0
85	MG	5	3817	1/1	0.94	0.15	41,41,41,41	0
86	OHX	6	2064	7/7	0.94	0.14	106,106,106,106	0
86	OHX	6	2077	7/7	0.94	0.15	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	6	2095	7/7	0.94	0.12	141,141,141,141	0
86	OHX	6	2100	7/7	0.94	0.12	160,160,160,160	0
85	MG	1	3446	1/1	0.94	0.18	33,33,33,33	0
85	MG	6	1985	1/1	0.94	0.19	50,50,50,50	0
85	MG	5	3831	1/1	0.94	0.17	54,54,54,54	0
86	OHX	6	2121	7/7	0.94	0.12	123,123,123,123	0
85	MG	1	3756	1/1	0.94	0.12	43,43,43,43	0
86	OHX	6	2126	7/7	0.94	0.10	169,169,169,169	0
85	MG	1	3495	1/1	0.94	0.16	33,33,33,33	0
86	OHX	6	2128	7/7	0.94	0.10	150,150,150,150	0
85	MG	5	3837	1/1	0.94	0.28	47,47,47,47	0
85	MG	1	3624	1/1	0.94	0.17	22,22,22,22	0
85	MG	5	3445	1/1	0.94	0.10	21,21,21,21	0
85	MG	5	3844	1/1	0.94	0.25	55,55,55,55	0
85	MG	5	3626	1/1	0.94	0.16	18,18,18,18	0
85	MG	5	3628	1/1	0.94	0.08	46,46,46,46	0
85	MG	5	3848	1/1	0.94	0.07	31,31,31,31	0
86	OHX	D9	102	7/7	0.94	0.08	167,167,167,167	0
85	MG	5	3448	1/1	0.94	0.11	36,36,36,36	0
86	OHX	6	2142	7/7	0.94	0.10	178,178,178,178	0
86	OHX	1	3947	7/7	0.94	0.14	110,110,110,110	0
85	MG	5	3850	1/1	0.94	0.27	49,49,49,49	0
85	MG	N6	201	1/1	0.94	0.09	40,40,40,40	0
85	MG	5	3852	1/1	0.94	0.22	59,59,59,59	0
86	OHX	6	2148	7/7	0.94	0.10	158,158,158,158	0
86	OHX	8	221	7/7	0.94	0.14	135,135,135,135	0
86	OHX	8	223	7/7	0.94	0.11	148,148,148,148	0
86	OHX	1	3992	7/7	0.94	0.11	130,130,130,130	0
85	MG	5	3855	1/1	0.94	0.07	43,43,43,43	0
85	MG	1	3496	1/1	0.94	0.20	22,22,22,22	0
86	OHX	1	4004	7/7	0.94	0.12	143,143,143,143	0
86	OHX	1	4005	7/7	0.94	0.11	148,148,148,148	0
85	MG	5	3635	1/1	0.94	0.09	51,51,51,51	0
86	OHX	1	4011	7/7	0.94	0.10	143,143,143,143	0
86	OHX	l5	303	7/7	0.94	0.09	158,158,158,158	0
85	MG	1	3679	1/1	0.94	0.09	43,43,43,43	0
86	OHX	1	4015	7/7	0.94	0.12	130,130,130,130	0
86	OHX	1	4016	7/7	0.94	0.08	179,179,179,179	0
86	OHX	1	4020	7/7	0.94	0.10	143,143,143,143	0
85	MG	5	3454	1/1	0.94	0.27	29,29,29,29	0
85	MG	1	3531	1/1	0.94	0.20	18,18,18,18	0
85	MG	5	3863	1/1	0.94	0.09	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3456	1/1	0.94	0.07	58,58,58,58	0
86	OHX	1	4037	7/7	0.94	0.14	122,122,122,122	0
85	MG	O3	201	1/1	0.94	0.07	24,24,24,24	0
85	MG	2	1944	1/1	0.95	0.18	45,45,45,45	0
86	OHX	5	4033	7/7	0.95	0.13	103,103,103,103	0
86	OHX	5	4034	7/7	0.95	0.12	129,129,129,129	0
86	OHX	5	4040	7/7	0.95	0.09	138,138,138,138	0
85	MG	5	3554	1/1	0.95	0.19	39,39,39,39	0
85	MG	5	3699	1/1	0.95	0.08	30,30,30,30	0
85	MG	5	3438	1/1	0.95	0.13	49,49,49,49	0
86	OHX	5	4047	7/7	0.95	0.12	132,132,132,132	0
86	OHX	5	4048	7/7	0.95	0.15	111,111,111,111	0
85	MG	1	3830	1/1	0.95	0.24	27,27,27,27	0
85	MG	2	2006	1/1	0.95	0.09	80,80,80,80	0
85	MG	5	3443	1/1	0.95	0.16	38,38,38,38	0
86	OHX	5	4060	7/7	0.95	0.12	126,126,126,126	0
85	MG	5	3874	1/1	0.95	0.22	16,16,16,16	0
86	OHX	5	4064	7/7	0.95	0.09	167,167,167,167	0
86	OHX	5	4065	7/7	0.95	0.12	129,129,129,129	0
85	MG	5	3444	1/1	0.95	0.19	14,14,14,14	0
85	MG	5	3706	1/1	0.95	0.14	47,47,47,47	0
86	OHX	5	4072	7/7	0.95	0.11	123,123,123,123	0
85	MG	5	3564	1/1	0.95	0.29	15,15,15,15	0
86	OHX	5	4074	7/7	0.95	0.10	133,133,133,133	0
85	MG	5	3878	1/1	0.95	0.29	32,32,32,32	0
85	MG	L3	401	1/1	0.95	0.27	38,38,38,38	0
85	MG	5	3446	1/1	0.95	0.21	34,34,34,34	0
86	OHX	5	4079	7/7	0.95	0.12	130,130,130,130	0
85	MG	6	1931	1/1	0.95	0.13	41,41,41,41	0
86	OHX	5	4081	7/7	0.95	0.11	166,166,166,166	0
86	OHX	5	4083	7/7	0.95	0.11	150,150,150,150	0
86	OHX	5	4084	7/7	0.95	0.10	128,128,128,128	0
85	MG	5	3883	1/1	0.95	0.14	18,18,18,18	0
85	MG	1	3662	1/1	0.95	0.26	38,38,38,38	0
86	OHX	5	4088	7/7	0.95	0.09	156,156,156,156	0
85	MG	5	3713	1/1	0.95	0.07	70,70,70,70	0
85	MG	1	3471	1/1	0.95	0.25	33,33,33,33	0
85	MG	5	3888	1/1	0.95	0.19	38,38,38,38	0
86	OHX	2	2170	7/7	0.95	0.12	140,140,140,140	0
86	OHX	5	4093	7/7	0.95	0.15	122,122,122,122	0
85	MG	5	3574	1/1	0.95	0.17	22,22,22,22	0
86	OHX	5	4097	7/7	0.95	0.10	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	2	2172	7/7	0.95	0.10	155,155,155,155	0
85	MG	5	3717	1/1	0.95	0.10	64,64,64,64	0
85	MG	5	3718	1/1	0.95	0.16	38,38,38,38	0
85	MG	L6	201	1/1	0.95	0.09	39,39,39,39	0
85	MG	1	3709	1/1	0.95	0.15	61,61,61,61	0
85	MG	5	3581	1/1	0.95	0.23	28,28,28,28	0
86	OHX	5	4104	7/7	0.95	0.13	117,117,117,117	0
85	MG	6	2017	1/1	0.95	0.06	34,34,34,34	0
85	MG	6	2018	1/1	0.95	0.27	44,44,44,44	0
85	MG	2	1966	1/1	0.95	0.15	65,65,65,65	0
85	MG	1	3712	1/1	0.95	0.07	31,31,31,31	0
85	MG	5	3899	1/1	0.95	0.15	81,81,81,81	0
85	MG	1	3519	1/1	0.95	0.20	32,32,32,32	0
85	MG	2	1941	1/1	0.95	0.15	50,50,50,50	0
85	MG	5	3591	1/1	0.95	0.19	31,31,31,31	0
85	MG	1	3523	1/1	0.95	0.20	18,18,18,18	0
85	MG	6	2024	1/1	0.95	0.16	58,58,58,58	0
86	OHX	SR	401	7/7	0.95	0.09	183,183,183,183	0
86	OHX	1	3904	7/7	0.95	0.18	91,91,91,91	0
85	MG	7	203	1/1	0.95	0.19	12,12,12,12	0
86	OHX	1	3931	7/7	0.95	0.14	101,101,101,101	0
85	MG	1	3778	1/1	0.95	0.27	27,27,27,27	0
86	OHX	5	4123	7/7	0.95	0.09	165,165,165,165	0
86	OHX	1	3957	7/7	0.95	0.12	105,105,105,105	0
85	MG	5	3595	1/1	0.95	0.24	22,22,22,22	0
86	OHX	1	3974	7/7	0.95	0.12	129,129,129,129	0
86	OHX	5	4127	7/7	0.95	0.08	175,175,175,175	0
86	OHX	1	3978	7/7	0.95	0.15	112,112,112,112	0
85	MG	7	206	1/1	0.95	0.25	25,25,25,25	0
86	OHX	1	3989	7/7	0.95	0.14	115,115,115,115	0
85	MG	6	2027	1/1	0.95	0.25	49,49,49,49	0
85	MG	M0	302	1/1	0.95	0.09	43,43,43,43	0
85	MG	1	3594	1/1	0.95	0.23	17,17,17,17	0
86	OHX	1	3995	7/7	0.95	0.13	107,107,107,107	0
85	MG	5	3741	1/1	0.95	0.10	33,33,33,33	0
86	OHX	1	4002	7/7	0.95	0.12	138,138,138,138	0
85	MG	5	3742	1/1	0.95	0.08	52,52,52,52	0
85	MG	5	3743	1/1	0.95	0.21	19,19,19,19	0
85	MG	5	3601	1/1	0.95	0.06	40,40,40,40	0
86	OHX	4	229	7/7	0.95	0.09	127,127,127,127	0
86	OHX	5	4146	7/7	0.95	0.11	135,135,135,135	0
85	MG	1	3421	1/1	0.95	0.22	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	4012	7/7	0.95	0.10	149,149,149,149	0
85	MG	5	3603	1/1	0.95	0.21	35,35,35,35	0
85	MG	8	201	1/1	0.95	0.23	23,23,23,23	0
85	MG	1	3634	1/1	0.95	0.10	37,37,37,37	0
86	OHX	1	4019	7/7	0.95	0.09	139,139,139,139	0
85	MG	5	3749	1/1	0.95	0.09	47,47,47,47	0
86	OHX	L3	405	7/7	0.95	0.11	121,121,121,121	0
86	OHX	5	4155	7/7	0.95	0.12	122,122,122,122	0
85	MG	5	3605	1/1	0.95	0.14	40,40,40,40	0
86	OHX	1	4022	7/7	0.95	0.09	161,161,161,161	0
86	OHX	1	4024	7/7	0.95	0.11	130,130,130,130	0
85	MG	5	3751	1/1	0.95	0.09	46,46,46,46	0
86	OHX	1	4027	7/7	0.95	0.12	122,122,122,122	0
85	MG	1	3721	1/1	0.95	0.14	36,36,36,36	0
86	OHX	1	4031	7/7	0.95	0.10	162,162,162,162	0
85	MG	5	3607	1/1	0.95	0.11	28,28,28,28	0
85	MG	M5	301	1/1	0.95	0.14	31,31,31,31	0
85	MG	5	3756	1/1	0.95	0.07	37,37,37,37	0
85	MG	1	3851	1/1	0.95	0.23	41,41,41,41	0
86	OHX	1	4049	7/7	0.95	0.08	191,191,191,191	0
86	OHX	1	4050	7/7	0.95	0.13	113,113,113,113	0
86	OHX	1	4051	7/7	0.95	0.11	129,129,129,129	0
86	OHX	6	2105	7/7	0.95	0.12	132,132,132,132	0
86	OHX	1	4053	7/7	0.95	0.10	148,148,148,148	0
85	MG	1	3422	1/1	0.95	0.12	33,33,33,33	0
86	OHX	6	2113	7/7	0.95	0.12	132,132,132,132	0
86	OHX	6	2114	7/7	0.95	0.12	138,138,138,138	0
85	MG	1	3786	1/1	0.95	0.09	45,45,45,45	0
86	OHX	6	2119	7/7	0.95	0.10	145,145,145,145	0
85	MG	5	3614	1/1	0.95	0.11	22,22,22,22	0
86	OHX	6	2122	7/7	0.95	0.09	158,158,158,158	0
86	OHX	6	2123	7/7	0.95	0.10	161,161,161,161	0
86	OHX	6	2124	7/7	0.95	0.11	118,118,118,118	0
85	MG	5	3615	1/1	0.95	0.08	32,32,32,32	0
86	OHX	5	4183	7/7	0.95	0.07	186,186,186,186	0
85	MG	1	3724	1/1	0.95	0.20	12,12,12,12	0
85	MG	2	1993	1/1	0.95	0.10	42,42,42,42	0
85	MG	M7	205	1/1	0.95	0.14	27,27,27,27	0
86	OHX	6	2130	7/7	0.95	0.09	159,159,159,159	0
85	MG	2	1985	1/1	0.95	0.07	54,54,54,54	0
85	MG	1	3480	1/1	0.95	0.25	27,27,27,27	0
85	MG	1	3678	1/1	0.95	0.18	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	4068	7/7	0.95	0.10	143,143,143,143	0
86	OHX	1	4069	7/7	0.95	0.10	139,139,139,139	0
85	MG	1	3793	1/1	0.95	0.08	41,41,41,41	0
85	MG	5	3624	1/1	0.95	0.21	26,26,26,26	0
85	MG	3	203	1/1	0.95	0.08	94,94,94,94	0
85	MG	m7	203	1/1	0.95	0.14	47,47,47,47	0
85	MG	1	3533	1/1	0.95	0.07	28,28,28,28	0
85	MG	n3	201	1/1	0.95	0.24	13,13,13,13	0
86	OHX	1	4076	7/7	0.95	0.12	145,145,145,145	0
85	MG	5	3627	1/1	0.95	0.13	43,43,43,43	0
86	OHX	5	4202	7/7	0.95	0.10	132,132,132,132	0
86	OHX	5	4203	7/7	0.95	0.09	139,139,139,139	0
85	MG	5	3493	1/1	0.95	0.28	47,47,47,47	0
85	MG	3	206	1/1	0.95	0.23	19,19,19,19	0
85	MG	5	3631	1/1	0.95	0.13	40,40,40,40	0
86	OHX	1	4082	7/7	0.95	0.18	116,116,116,116	0
85	MG	N8	201	1/1	0.95	0.07	41,41,41,41	0
85	MG	5	3633	1/1	0.95	0.08	24,24,24,24	0
85	MG	2	1933	1/1	0.95	0.23	46,46,46,46	0
85	MG	N8	204	1/1	0.95	0.10	48,48,48,48	0
85	MG	1	3482	1/1	0.95	0.22	41,41,41,41	0
86	OHX	6	2157	7/7	0.95	0.12	136,136,136,136	0
85	MG	5	3638	1/1	0.95	0.16	40,40,40,40	0
86	OHX	2	2043	7/7	0.95	0.13	98,98,98,98	0
86	OHX	2	2066	7/7	0.95	0.09	146,146,146,146	0
86	OHX	1	4093	7/7	0.95	0.09	137,137,137,137	0
85	MG	1	3734	1/1	0.95	0.24	55,55,55,55	0
86	OHX	5	4220	7/7	0.95	0.10	119,119,119,119	0
86	OHX	2	2078	7/7	0.95	0.09	164,164,164,164	0
85	MG	5	3793	1/1	0.95	0.13	43,43,43,43	0
85	MG	c8	201	1/1	0.95	0.29	56,56,56,56	0
85	MG	1	3684	1/1	0.95	0.10	64,64,64,64	0
86	OHX	1	4099	7/7	0.95	0.08	165,165,165,165	0
86	OHX	2	2087	7/7	0.95	0.11	134,134,134,134	0
85	MG	5	3503	1/1	0.95	0.10	38,38,38,38	0
85	MG	2	2012	1/1	0.95	0.36	63,63,63,63	0
85	MG	1	3738	1/1	0.95	0.08	35,35,35,35	0
85	MG	1	3804	1/1	0.95	0.17	26,26,26,26	0
85	MG	5	3647	1/1	0.95	0.10	31,31,31,31	0
85	MG	1	3645	1/1	0.95	0.07	40,40,40,40	0
85	MG	1	3646	1/1	0.95	0.09	34,34,34,34	0
85	MG	6	1979	1/1	0.95	0.12	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3651	1/1	0.95	0.11	29,29,29,29	0
85	MG	5	3511	1/1	0.95	0.24	16,16,16,16	0
85	MG	6	1980	1/1	0.95	0.11	43,43,43,43	0
85	MG	5	3513	1/1	0.95	0.13	20,20,20,20	0
85	MG	1	3613	1/1	0.95	0.17	40,40,40,40	0
86	OHX	2	2111	7/7	0.95	0.08	157,157,157,157	0
85	MG	5	3406	1/1	0.95	0.13	29,29,29,29	0
85	MG	1	3538	1/1	0.95	0.19	33,33,33,33	0
85	MG	5	3518	1/1	0.95	0.20	30,30,30,30	0
85	MG	6	1906	1/1	0.95	0.20	35,35,35,35	0
85	MG	1	3694	1/1	0.95	0.09	52,52,52,52	0
85	MG	5	3662	1/1	0.95	0.42	38,38,38,38	0
85	MG	5	3414	1/1	0.95	0.21	21,21,21,21	0
85	MG	5	3820	1/1	0.95	0.08	85,85,85,85	0
85	MG	5	3527	1/1	0.95	0.14	45,45,45,45	0
85	MG	1	3746	1/1	0.95	0.15	58,58,58,58	0
85	MG	5	3829	1/1	0.95	0.11	31,31,31,31	0
85	MG	1	3465	1/1	0.95	0.14	39,39,39,39	0
86	OHX	2	2126	7/7	0.95	0.10	155,155,155,155	0
85	MG	5	3417	1/1	0.95	0.10	25,25,25,25	0
86	OHX	7	224	7/7	0.95	0.09	146,146,146,146	0
86	OHX	7	225	7/7	0.95	0.10	137,137,137,137	0
85	MG	1	3813	1/1	0.95	0.10	51,51,51,51	0
85	MG	6	1912	1/1	0.95	0.26	35,35,35,35	0
85	MG	5	3839	1/1	0.95	0.13	23,23,23,23	0
85	MG	2	1923	1/1	0.95	0.24	44,44,44,44	0
86	OHX	8	219	7/7	0.95	0.12	131,131,131,131	0
85	MG	5	3678	1/1	0.95	0.13	42,42,42,42	0
86	OHX	8	222	7/7	0.95	0.09	169,169,169,169	0
85	MG	1	3751	1/1	0.95	0.11	35,35,35,35	0
85	MG	6	1915	1/1	0.95	0.22	43,43,43,43	0
85	MG	1	3541	1/1	0.95	0.20	18,18,18,18	0
86	OHX	8	226	7/7	0.95	0.08	171,171,171,171	0
85	MG	5	3541	1/1	0.95	0.19	17,17,17,17	0
85	MG	1	3487	1/1	0.95	0.18	26,26,26,26	0
85	MG	1	3508	1/1	0.95	0.23	13,13,13,13	0
85	MG	6	1998	1/1	0.95	0.36	45,45,45,45	0
85	MG	1	3757	1/1	0.95	0.17	42,42,42,42	0
85	MG	5	3546	1/1	0.95	0.21	21,21,21,21	0
86	OHX	c8	203	7/7	0.95	0.09	160,160,160,160	0
86	OHX	2	2144	7/7	0.95	0.08	190,190,190,190	0
85	MG	4	216	1/1	0.95	0.10	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3488	1/1	0.95	0.13	41,41,41,41	0
86	OHX	5	4002	7/7	0.95	0.11	118,118,118,118	0
86	OHX	5	4006	7/7	0.95	0.11	117,117,117,117	0
85	MG	1	3430	1/1	0.95	0.20	41,41,41,41	0
85	MG	6	2003	1/1	0.95	0.09	63,63,63,63	0
85	MG	1	3703	1/1	0.95	0.08	33,33,33,33	0
86	OHX	1	4149	7/7	0.95	0.11	159,159,159,159	0
88	ZBA	1	4206	33/33	0.95	0.11	26,26,26,26	0
86	OHX	5	4042	7/7	0.96	0.08	134,134,134,134	0
86	OHX	5	4044	7/7	0.96	0.09	143,143,143,143	0
85	MG	5	3562	1/1	0.96	0.25	18,18,18,18	0
86	OHX	1	3922	7/7	0.96	0.12	100,100,100,100	0
86	OHX	1	4167	7/7	0.96	0.09	126,126,126,126	0
85	MG	l4	401	1/1	0.96	0.09	44,44,44,44	0
86	OHX	5	4050	7/7	0.96	0.13	111,111,111,111	0
86	OHX	5	4053	7/7	0.96	0.13	114,114,114,114	0
86	OHX	1	3939	7/7	0.96	0.11	111,111,111,111	0
86	OHX	1	3940	7/7	0.96	0.10	94,94,94,94	0
86	OHX	1	3946	7/7	0.96	0.11	115,115,115,115	0
85	MG	1	3845	1/1	0.96	0.25	65,65,65,65	0
85	MG	5	3675	1/1	0.96	0.09	33,33,33,33	0
85	MG	6	2045	1/1	0.96	0.22	46,46,46,46	0
86	OHX	1	3963	7/7	0.96	0.11	113,113,113,113	0
86	OHX	1	3967	7/7	0.96	0.10	111,111,111,111	0
86	OHX	1	3973	7/7	0.96	0.11	117,117,117,117	0
86	OHX	5	4069	7/7	0.96	0.09	126,126,126,126	0
86	OHX	5	4070	7/7	0.96	0.09	138,138,138,138	0
86	OHX	5	4071	7/7	0.96	0.10	136,136,136,136	0
85	MG	5	3568	1/1	0.96	0.29	21,21,21,21	0
85	MG	1	3797	1/1	0.96	0.09	61,61,61,61	0
86	OHX	1	3979	7/7	0.96	0.11	110,110,110,110	0
86	OHX	5	4075	7/7	0.96	0.12	149,149,149,149	0
86	OHX	1	3983	7/7	0.96	0.10	110,110,110,110	0
85	MG	5	3570	1/1	0.96	0.25	21,21,21,21	0
86	OHX	1	3986	7/7	0.96	0.10	143,143,143,143	0
86	OHX	1	3987	7/7	0.96	0.10	137,137,137,137	0
85	MG	1	3753	1/1	0.96	0.16	40,40,40,40	0
85	MG	5	3803	1/1	0.96	0.12	33,33,33,33	0
85	MG	1	3848	1/1	0.96	0.10	69,69,69,69	0
85	MG	5	3683	1/1	0.96	0.20	38,38,38,38	0
86	OHX	5	4085	7/7	0.96	0.10	121,121,121,121	0
85	MG	6	1981	1/1	0.96	0.19	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	3996	7/7	0.96	0.08	139,139,139,139	0
85	MG	s8	302	1/1	0.96	0.07	38,38,38,38	0
86	OHX	1	3998	7/7	0.96	0.09	137,137,137,137	0
86	OHX	1	3999	7/7	0.96	0.09	128,128,128,128	0
86	OHX	1	4000	7/7	0.96	0.12	121,121,121,121	0
86	OHX	1	4001	7/7	0.96	0.09	122,122,122,122	0
85	MG	6	1982	1/1	0.96	0.13	42,42,42,42	0
86	OHX	1	4003	7/7	0.96	0.09	143,143,143,143	0
85	MG	5	3577	1/1	0.96	0.22	37,37,37,37	0
85	MG	5	3579	1/1	0.96	0.20	22,22,22,22	0
86	OHX	1	4006	7/7	0.96	0.09	155,155,155,155	0
85	MG	L4	401	1/1	0.96	0.13	48,48,48,48	0
85	MG	5	3477	1/1	0.96	0.30	23,23,23,23	0
85	MG	L4	402	1/1	0.96	0.07	36,36,36,36	0
85	MG	6	1918	1/1	0.96	0.21	29,29,29,29	0
85	MG	1	3600	1/1	0.96	0.15	23,23,23,23	0
86	OHX	3	215	7/7	0.96	0.10	127,127,127,127	0
86	OHX	3	220	7/7	0.96	0.08	151,151,151,151	0
85	MG	1	3687	1/1	0.96	0.25	42,42,42,42	0
86	OHX	1	4018	7/7	0.96	0.09	140,140,140,140	0
85	MG	5	3818	1/1	0.96	0.15	44,44,44,44	0
85	MG	5	3819	1/1	0.96	0.07	34,34,34,34	0
85	MG	1	3688	1/1	0.96	0.06	30,30,30,30	0
86	OHX	4	227	7/7	0.96	0.09	142,142,142,142	0
86	OHX	4	228	7/7	0.96	0.11	114,114,114,114	0
85	MG	q0	202	1/1	0.96	0.05	45,45,45,45	0
86	OHX	1	4023	7/7	0.96	0.08	153,153,153,153	0
86	OHX	5	4117	7/7	0.96	0.11	134,134,134,134	0
85	MG	5	3823	1/1	0.96	0.10	34,34,34,34	0
86	OHX	5	4119	7/7	0.96	0.12	118,118,118,118	0
85	MG	1	3722	1/1	0.96	0.10	80,80,80,80	0
86	OHX	2	2046	7/7	0.96	0.13	114,114,114,114	0
86	OHX	2	2058	7/7	0.96	0.12	124,124,124,124	0
86	OHX	2	2059	7/7	0.96	0.10	135,135,135,135	0
86	OHX	1	4032	7/7	0.96	0.10	132,132,132,132	0
86	OHX	L3	404	7/7	0.96	0.10	130,130,130,130	0
86	OHX	2	2060	7/7	0.96	0.10	143,143,143,143	0
85	MG	5	3825	1/1	0.96	0.15	51,51,51,51	0
86	OHX	5	4129	7/7	0.96	0.07	150,150,150,150	0
86	OHX	1	4040	7/7	0.96	0.10	131,131,131,131	0
86	OHX	2	2068	7/7	0.96	0.11	120,120,120,120	0
86	OHX	5	4132	7/7	0.96	0.09	152,152,152,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4133	7/7	0.96	0.10	127,127,127,127	0
86	OHX	M5	303	7/7	0.96	0.10	119,119,119,119	0
86	OHX	1	4044	7/7	0.96	0.10	139,139,139,139	0
86	OHX	1	4045	7/7	0.96	0.09	157,157,157,157	0
86	OHX	1	4046	7/7	0.96	0.08	165,165,165,165	0
86	OHX	2	2069	7/7	0.96	0.10	147,147,147,147	0
86	OHX	1	4048	7/7	0.96	0.13	129,129,129,129	0
85	MG	5	3826	1/1	0.96	0.19	43,43,43,43	0
86	OHX	2	2076	7/7	0.96	0.08	153,153,153,153	0
86	OHX	2	2077	7/7	0.96	0.10	137,137,137,137	0
86	OHX	1	4052	7/7	0.96	0.07	195,195,195,195	0
86	OHX	6	2085	7/7	0.96	0.10	132,132,132,132	0
86	OHX	6	2086	7/7	0.96	0.11	113,113,113,113	0
86	OHX	6	2091	7/7	0.96	0.10	131,131,131,131	0
85	MG	5	3827	1/1	0.96	0.06	34,34,34,34	0
86	OHX	6	2098	7/7	0.96	0.09	135,135,135,135	0
86	OHX	6	2099	7/7	0.96	0.10	151,151,151,151	0
86	OHX	1	4054	7/7	0.96	0.07	167,167,167,167	0
86	OHX	6	2101	7/7	0.96	0.10	156,156,156,156	0
86	OHX	6	2103	7/7	0.96	0.10	122,122,122,122	0
86	OHX	2	2079	7/7	0.96	0.10	131,131,131,131	0
86	OHX	2	2080	7/7	0.96	0.11	126,126,126,126	0
86	OHX	6	2108	7/7	0.96	0.10	125,125,125,125	0
86	OHX	5	4157	7/7	0.96	0.10	133,133,133,133	0
86	OHX	6	2111	7/7	0.96	0.09	143,143,143,143	0
86	OHX	2	2081	7/7	0.96	0.08	149,149,149,149	0
86	OHX	1	4059	7/7	0.96	0.08	166,166,166,166	0
85	MG	1	3491	1/1	0.96	0.16	23,23,23,23	0
86	OHX	6	2116	7/7	0.96	0.09	132,132,132,132	0
85	MG	sM	301	1/1	0.96	0.05	36,36,36,36	0
85	MG	5	3830	1/1	0.96	0.20	21,21,21,21	0
86	OHX	6	2120	7/7	0.96	0.09	131,131,131,131	0
86	OHX	2	2085	7/7	0.96	0.09	161,161,161,161	0
85	MG	1	3571	1/1	0.96	0.24	16,16,16,16	0
86	OHX	2	2088	7/7	0.96	0.08	156,156,156,156	0
85	MG	1	3522	1/1	0.96	0.25	20,20,20,20	0
86	OHX	1	4067	7/7	0.96	0.08	128,128,128,128	0
86	OHX	2	2090	7/7	0.96	0.09	137,137,137,137	0
85	MG	1	3574	1/1	0.96	0.24	12,12,12,12	0
85	MG	1	3434	1/1	0.96	0.12	38,38,38,38	0
85	MG	1	3858	1/1	0.96	0.21	30,30,30,30	0
85	MG	1	4207	1/1	0.96	0.17	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	2	2099	7/7	0.96	0.09	164,164,164,164	0
85	MG	6	1997	1/1	0.96	0.05	45,45,45,45	0
85	MG	5	3409	1/1	0.96	0.23	26,26,26,26	0
85	MG	5	3498	1/1	0.96	0.24	27,27,27,27	0
86	OHX	2	2104	7/7	0.96	0.07	153,153,153,153	0
86	OHX	6	2138	7/7	0.96	0.10	136,136,136,136	0
85	MG	1	4208	1/1	0.96	0.08	18,18,18,18	0
85	MG	1	4210	1/1	0.96	0.11	40,40,40,40	0
85	MG	1	3728	1/1	0.96	0.20	30,30,30,30	0
85	MG	6	1935	1/1	0.96	0.28	47,47,47,47	0
86	OHX	6	2143	7/7	0.96	0.08	139,139,139,139	0
85	MG	M4	201	1/1	0.96	0.08	44,44,44,44	0
86	OHX	1	4084	7/7	0.96	0.07	189,189,189,189	0
85	MG	1	3810	1/1	0.96	0.22	56,56,56,56	0
85	MG	5	3610	1/1	0.96	0.22	26,26,26,26	0
86	OHX	1	4087	7/7	0.96	0.08	163,163,163,163	0
85	MG	3	202	1/1	0.96	0.17	46,46,46,46	0
85	MG	5	3857	1/1	0.96	0.13	96,96,96,96	0
86	OHX	6	2151	7/7	0.96	0.09	129,129,129,129	0
85	MG	5	3858	1/1	0.96	0.07	29,29,29,29	0
85	MG	1	3769	1/1	0.96	0.08	43,43,43,43	0
85	MG	5	3613	1/1	0.96	0.25	44,44,44,44	0
85	MG	1	3511	1/1	0.96	0.28	35,35,35,35	0
85	MG	3	205	1/1	0.96	0.17	23,23,23,23	0
85	MG	1	3526	1/1	0.96	0.23	19,19,19,19	0
85	MG	1	3512	1/1	0.96	0.26	19,19,19,19	0
85	MG	5	3424	1/1	0.96	0.18	42,42,42,42	0
86	OHX	5	4204	7/7	0.96	0.10	133,133,133,133	0
85	MG	5	3867	1/1	0.96	0.12	42,42,42,42	0
85	MG	6	1946	1/1	0.96	0.20	39,39,39,39	0
85	MG	1	3774	1/1	0.96	0.12	41,41,41,41	0
85	MG	5	3427	1/1	0.96	0.22	29,29,29,29	0
85	MG	5	3872	1/1	0.96	0.22	15,15,15,15	0
85	MG	1	3612	1/1	0.96	0.10	31,31,31,31	0
85	MG	5	3736	1/1	0.96	0.12	43,43,43,43	0
86	OHX	2	2132	7/7	0.96	0.07	205,205,205,205	0
85	MG	1	3733	1/1	0.96	0.14	27,27,27,27	0
85	MG	5	3519	1/1	0.96	0.33	17,17,17,17	0
85	MG	5	3520	1/1	0.96	0.22	17,17,17,17	0
85	MG	5	3522	1/1	0.96	0.26	33,33,33,33	0
85	MG	6	2015	1/1	0.96	0.07	34,34,34,34	0
85	MG	N3	201	1/1	0.96	0.24	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3525	1/1	0.96	0.25	23,23,23,23	0
85	MG	1	3818	1/1	0.96	0.07	34,34,34,34	0
85	MG	5	3746	1/1	0.96	0.22	32,32,32,32	0
85	MG	2	2024	1/1	0.96	0.09	75,75,75,75	0
85	MG	1	3821	1/1	0.96	0.07	20,20,20,20	0
85	MG	1	3558	1/1	0.96	0.18	13,13,13,13	0
85	MG	5	3636	1/1	0.96	0.18	36,36,36,36	0
85	MG	5	3530	1/1	0.96	0.14	18,18,18,18	0
85	MG	1	3514	1/1	0.96	0.29	18,18,18,18	0
85	MG	1	3824	1/1	0.96	0.18	16,16,16,16	0
85	MG	5	3640	1/1	0.96	0.17	51,51,51,51	0
85	MG	5	3440	1/1	0.96	0.11	25,25,25,25	0
85	MG	N8	203	1/1	0.96	0.18	24,24,24,24	0
85	MG	5	3758	1/1	0.96	0.14	55,55,55,55	0
85	MG	1	3780	1/1	0.96	0.13	43,43,43,43	0
85	MG	2	1975	1/1	0.96	0.33	59,59,59,59	0
85	MG	5	3761	1/1	0.96	0.07	34,34,34,34	0
85	MG	2	1903	1/1	0.96	0.11	31,31,31,31	0
85	MG	5	3901	1/1	0.96	0.13	25,25,25,25	0
85	MG	1	3675	1/1	0.96	0.11	37,37,37,37	0
85	MG	1	3742	1/1	0.96	0.07	45,45,45,45	0
85	MG	1	3431	1/1	0.96	0.23	30,30,30,30	0
85	MG	2	1987	1/1	0.96	0.11	47,47,47,47	0
85	MG	7	202	1/1	0.96	0.12	33,33,33,33	0
85	MG	5	3451	1/1	0.96	0.16	19,19,19,19	0
85	MG	1	3593	1/1	0.96	0.38	18,18,18,18	0
85	MG	5	3771	1/1	0.96	0.10	40,40,40,40	0
85	MG	1	3835	1/1	0.96	0.15	37,37,37,37	0
85	MG	1	3475	1/1	0.96	0.16	25,25,25,25	0
85	MG	5	3549	1/1	0.96	0.34	45,45,45,45	0
86	OHX	6	2204	7/7	0.96	0.08	179,179,179,179	0
86	OHX	6	2205	7/7	0.96	0.07	221,221,221,221	0
85	MG	1	3747	1/1	0.96	0.07	37,37,37,37	0
85	MG	5	3777	1/1	0.96	0.07	34,34,34,34	0
85	MG	5	3457	1/1	0.96	0.25	16,16,16,16	0
85	MG	5	3657	1/1	0.96	0.15	41,41,41,41	0
85	MG	5	3458	1/1	0.96	0.18	23,23,23,23	0
85	MG	5	3459	1/1	0.96	0.12	76,76,76,76	0
85	MG	1	3569	1/1	0.96	0.15	16,16,16,16	0
85	MG	5	3555	1/1	0.96	0.23	27,27,27,27	0
86	OHX	d9	102	7/7	0.96	0.07	165,165,165,165	0
86	OHX	1	4151	7/7	0.96	0.09	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	8	218	7/7	0.96	0.09	130,130,130,130	0
86	OHX	5	3965	7/7	0.96	0.13	101,101,101,101	0
85	MG	1	3597	1/1	0.96	0.16	30,30,30,30	0
86	OHX	5	3977	7/7	0.96	0.12	97,97,97,97	0
86	OHX	5	3979	7/7	0.96	0.12	102,102,102,102	0
86	OHX	5	3997	7/7	0.96	0.09	133,133,133,133	0
85	MG	5	3663	1/1	0.96	0.07	44,44,44,44	0
85	MG	8	204	1/1	0.96	0.18	34,34,34,34	0
85	MG	6	1973	1/1	0.96	0.16	38,38,38,38	0
86	OHX	5	4009	7/7	0.96	0.10	128,128,128,128	0
86	OHX	5	4015	7/7	0.96	0.09	112,112,112,112	0
86	OHX	5	4016	7/7	0.96	0.10	161,161,161,161	0
85	MG	1	3598	1/1	0.96	0.17	17,17,17,17	0
86	OHX	5	4019	7/7	0.96	0.11	118,118,118,118	0
85	MG	8	207	1/1	0.96	0.06	52,52,52,52	0
86	OHX	5	4023	7/7	0.96	0.10	129,129,129,129	0
85	MG	8	208	1/1	0.96	0.08	31,31,31,31	0
86	OHX	m0	301	7/7	0.96	0.10	136,136,136,136	0
85	MG	5	3667	1/1	0.96	0.06	16,16,16,16	0
85	MG	1	3599	1/1	0.96	0.21	20,20,20,20	0
85	MG	5	3792	1/1	0.96	0.06	47,47,47,47	0
85	MG	5	3560	1/1	0.96	0.26	20,20,20,20	0
86	OHX	5	4035	7/7	0.96	0.10	139,139,139,139	0
86	OHX	5	4039	7/7	0.96	0.09	147,147,147,147	0
87	ZN	Q2	501	1/1	0.96	0.12	89,89,89,89	0
85	MG	1	3844	1/1	0.96	0.14	34,34,34,34	0
87	ZN	q2	501	1/1	0.96	0.10	85,85,85,85	0
86	OHX	1	3914	7/7	0.96	0.11	116,116,116,116	0
85	MG	6	1921	1/1	0.97	0.33	45,45,45,45	0
85	MG	1	3586	1/1	0.97	0.28	19,19,19,19	0
86	OHX	5	4062	7/7	0.97	0.08	153,153,153,153	0
86	OHX	5	4063	7/7	0.97	0.08	131,131,131,131	0
85	MG	1	3671	1/1	0.97	0.18	15,15,15,15	0
86	OHX	1	4058	7/7	0.97	0.11	114,114,114,114	0
85	MG	1	3401	1/1	0.97	0.14	28,28,28,28	0
85	MG	5	3737	1/1	0.97	0.12	40,40,40,40	0
86	OHX	5	4068	7/7	0.97	0.07	161,161,161,161	0
85	MG	8	212	1/1	0.97	0.20	21,21,21,21	0
85	MG	6	2036	1/1	0.97	0.19	42,42,42,42	0
85	MG	1	3828	1/1	0.97	0.20	23,23,23,23	0
85	MG	5	3833	1/1	0.97	0.10	47,47,47,47	0
85	MG	1	3560	1/1	0.97	0.25	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3578	1/1	0.97	0.19	32,32,32,32	0
85	MG	1	3708	1/1	0.97	0.06	50,50,50,50	0
85	MG	5	3838	1/1	0.97	0.06	62,62,62,62	0
85	MG	1	3787	1/1	0.97	0.12	27,27,27,27	0
86	OHX	O1	201	7/7	0.97	0.10	121,121,121,121	0
85	MG	5	3441	1/1	0.97	0.22	32,32,32,32	0
85	MG	5	3508	1/1	0.97	0.30	21,21,21,21	0
85	MG	5	3843	1/1	0.97	0.14	30,30,30,30	0
86	OHX	5	4082	7/7	0.97	0.10	109,109,109,109	0
86	OHX	6	2071	7/7	0.97	0.08	115,115,115,115	0
85	MG	M7	202	1/1	0.97	0.12	24,24,24,24	0
86	OHX	6	2078	7/7	0.97	0.09	109,109,109,109	0
86	OHX	6	2082	7/7	0.97	0.09	110,110,110,110	0
86	OHX	6	2084	7/7	0.97	0.08	123,123,123,123	0
85	MG	m5	304	1/1	0.97	0.08	33,33,33,33	0
85	MG	5	3586	1/1	0.97	0.29	15,15,15,15	0
86	OHX	6	2089	7/7	0.97	0.10	128,128,128,128	0
86	OHX	6	2090	7/7	0.97	0.08	119,119,119,119	0
85	MG	1	3643	1/1	0.97	0.09	23,23,23,23	0
86	OHX	6	2092	7/7	0.97	0.09	123,123,123,123	0
86	OHX	6	2094	7/7	0.97	0.10	131,131,131,131	0
86	OHX	5	4095	7/7	0.97	0.09	128,128,128,128	0
86	OHX	5	4096	7/7	0.97	0.07	156,156,156,156	0
85	MG	1	3710	1/1	0.97	0.07	29,29,29,29	0
86	OHX	6	2097	7/7	0.97	0.07	139,139,139,139	0
85	MG	1	3441	1/1	0.97	0.20	30,30,30,30	0
86	OHX	1	4079	7/7	0.97	0.07	188,188,188,188	0
85	MG	2	1958	1/1	0.97	0.31	45,45,45,45	0
85	MG	5	3514	1/1	0.97	0.16	39,39,39,39	0
86	OHX	6	2102	7/7	0.97	0.07	121,121,121,121	0
85	MG	n0	201	1/1	0.97	0.10	33,33,33,33	0
85	MG	5	3666	1/1	0.97	0.10	20,20,20,20	0
86	OHX	6	2106	7/7	0.97	0.10	117,117,117,117	0
85	MG	5	3854	1/1	0.97	0.09	58,58,58,58	0
85	MG	5	3754	1/1	0.97	0.22	35,35,35,35	0
86	OHX	6	2109	7/7	0.97	0.08	134,134,134,134	0
85	MG	1	3458	1/1	0.97	0.17	45,45,45,45	0
85	MG	2	2015	1/1	0.97	0.21	43,43,43,43	0
85	MG	1	3715	1/1	0.97	0.23	41,41,41,41	0
85	MG	1	3620	1/1	0.97	0.06	29,29,29,29	0
86	OHX	6	2115	7/7	0.97	0.08	133,133,133,133	0
86	OHX	5	4115	7/7	0.97	0.13	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	5	3596	1/1	0.97	0.25	15,15,15,15	0
85	MG	o0	201	1/1	0.97	0.12	51,51,51,51	0
86	OHX	6	2118	7/7	0.97	0.10	130,130,130,130	0
85	MG	5	3452	1/1	0.97	0.22	30,30,30,30	0
85	MG	1	3796	1/1	0.97	0.07	52,52,52,52	0
85	MG	5	3763	1/1	0.97	0.05	50,50,50,50	0
85	MG	q3	502	1/1	0.97	0.13	45,45,45,45	0
85	MG	5	3599	1/1	0.97	0.18	37,37,37,37	0
86	OHX	2	2034	7/7	0.97	0.12	102,102,102,102	0
86	OHX	2	2040	7/7	0.97	0.10	116,116,116,116	0
85	MG	5	3677	1/1	0.97	0.09	32,32,32,32	0
85	MG	5	3521	1/1	0.97	0.29	23,23,23,23	0
86	OHX	5	4128	7/7	0.97	0.06	183,183,183,183	0
86	OHX	2	2052	7/7	0.97	0.09	115,115,115,115	0
86	OHX	6	2129	7/7	0.97	0.07	146,146,146,146	0
86	OHX	2	2053	7/7	0.97	0.09	126,126,126,126	0
86	OHX	6	2131	7/7	0.97	0.08	122,122,122,122	0
86	OHX	2	2055	7/7	0.97	0.10	122,122,122,122	0
86	OHX	C1	201	7/7	0.97	0.07	148,148,148,148	0
86	OHX	2	2056	7/7	0.97	0.08	131,131,131,131	0
86	OHX	2	2057	7/7	0.97	0.09	132,132,132,132	0
86	OHX	C8	201	7/7	0.97	0.10	103,103,103,103	0
85	MG	1	3842	1/1	0.97	0.07	33,33,33,33	0
85	MG	1	3682	1/1	0.97	0.23	51,51,51,51	0
86	OHX	1	3889	7/7	0.97	0.13	91,91,91,91	0
85	MG	1	3461	1/1	0.97	0.13	19,19,19,19	0
86	OHX	2	2065	7/7	0.97	0.08	133,133,133,133	0
85	MG	5	3871	1/1	0.97	0.13	14,14,14,14	0
86	OHX	1	3918	7/7	0.97	0.11	93,93,93,93	0
86	OHX	2	2067	7/7	0.97	0.09	123,123,123,123	0
86	OHX	1	3926	7/7	0.97	0.11	101,101,101,101	0
86	OHX	1	3929	7/7	0.97	0.10	100,100,100,100	0
85	MG	6	1943	1/1	0.97	0.28	42,42,42,42	0
86	OHX	1	3932	7/7	0.97	0.12	98,98,98,98	0
86	OHX	1	3933	7/7	0.97	0.10	104,104,104,104	0
86	OHX	1	3934	7/7	0.97	0.09	104,104,104,104	0
85	MG	6	1944	1/1	0.97	0.23	31,31,31,31	0
86	OHX	2	2070	7/7	0.97	0.07	154,154,154,154	0
86	OHX	1	3941	7/7	0.97	0.09	115,115,115,115	0
86	OHX	1	3944	7/7	0.97	0.10	115,115,115,115	0
85	MG	1	3568	1/1	0.97	0.21	20,20,20,20	0
86	OHX	2	2072	7/7	0.97	0.10	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	3954	7/7	0.97	0.08	131,131,131,131	0
86	OHX	1	3955	7/7	0.97	0.09	106,106,106,106	0
86	OHX	1	3956	7/7	0.97	0.08	126,126,126,126	0
86	OHX	2	2074	7/7	0.97	0.08	133,133,133,133	0
86	OHX	1	3959	7/7	0.97	0.10	107,107,107,107	0
85	MG	1	3758	1/1	0.97	0.23	49,49,49,49	0
86	OHX	1	3962	7/7	0.97	0.08	129,129,129,129	0
85	MG	1	3529	1/1	0.97	0.24	17,17,17,17	0
86	OHX	1	3965	7/7	0.97	0.11	123,123,123,123	0
86	OHX	1	3966	7/7	0.97	0.09	114,114,114,114	0
85	MG	5	3687	1/1	0.97	0.12	35,35,35,35	0
86	OHX	1	3968	7/7	0.97	0.08	133,133,133,133	0
86	OHX	1	3969	7/7	0.97	0.09	111,111,111,111	0
86	OHX	1	3970	7/7	0.97	0.09	116,116,116,116	0
86	OHX	1	3971	7/7	0.97	0.13	95,95,95,95	0
86	OHX	1	3972	7/7	0.97	0.25	99,99,99,99	0
85	MG	1	3760	1/1	0.97	0.12	61,61,61,61	0
85	MG	5	3463	1/1	0.97	0.20	17,17,17,17	0
85	MG	1	3409	1/1	0.97	0.15	24,24,24,24	0
85	MG	1	3625	1/1	0.97	0.10	26,26,26,26	0
86	OHX	1	3980	7/7	0.97	0.09	127,127,127,127	0
86	OHX	1	3981	7/7	0.97	0.10	124,124,124,124	0
86	OHX	1	4150	7/7	0.97	0.10	119,119,119,119	0
86	OHX	1	3982	7/7	0.97	0.09	131,131,131,131	0
85	MG	5	3882	1/1	0.97	0.16	23,23,23,23	0
85	MG	6	1952	1/1	0.97	0.25	36,36,36,36	0
86	OHX	1	3985	7/7	0.97	0.09	118,118,118,118	0
85	MG	5	3884	1/1	0.97	0.16	38,38,38,38	0
86	OHX	2	2086	7/7	0.97	0.08	148,148,148,148	0
86	OHX	1	3988	7/7	0.97	0.09	142,142,142,142	0
85	MG	5	3402	1/1	0.97	0.14	20,20,20,20	0
85	MG	5	3694	1/1	0.97	0.06	40,40,40,40	0
86	OHX	1	3991	7/7	0.97	0.07	152,152,152,152	0
85	MG	1	3424	1/1	0.97	0.14	38,38,38,38	0
86	OHX	1	3993	7/7	0.97	0.11	102,102,102,102	0
85	MG	5	3696	1/1	0.97	0.19	33,33,33,33	0
85	MG	O7	102	1/1	0.97	0.20	42,42,42,42	0
86	OHX	2	2092	7/7	0.97	0.09	123,123,123,123	0
85	MG	1	3572	1/1	0.97	0.21	15,15,15,15	0
85	MG	5	3788	1/1	0.97	0.26	78,78,78,78	0
85	MG	1	3765	1/1	0.97	0.11	62,62,62,62	0
86	OHX	2	2097	7/7	0.97	0.07	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	2	2098	7/7	0.97	0.08	155,155,155,155	0
85	MG	1	3658	1/1	0.97	0.07	25,25,25,25	0
85	MG	5	3701	1/1	0.97	0.13	33,33,33,33	0
86	OHX	2	2101	7/7	0.97	0.09	131,131,131,131	0
85	MG	1	3448	1/1	0.97	0.24	32,32,32,32	0
85	MG	L3	402	1/1	0.97	0.17	26,26,26,26	0
86	OHX	1	4007	7/7	0.97	0.10	139,139,139,139	0
86	OHX	1	4008	7/7	0.97	0.08	130,130,130,130	0
86	OHX	1	4009	7/7	0.97	0.09	120,120,120,120	0
85	MG	1	3435	1/1	0.97	0.12	33,33,33,33	0
85	MG	1	3575	1/1	0.97	0.18	16,16,16,16	0
85	MG	6	2016	1/1	0.97	0.09	58,58,58,58	0
86	OHX	1	4013	7/7	0.97	0.09	130,130,130,130	0
85	MG	1	3771	1/1	0.97	0.13	48,48,48,48	0
85	MG	6	1908	1/1	0.97	0.24	44,44,44,44	0
86	OHX	2	2109	7/7	0.97	0.10	129,129,129,129	0
86	OHX	1	4017	7/7	0.97	0.06	155,155,155,155	0
86	OHX	5	3929	7/7	0.97	0.12	72,72,72,72	0
86	OHX	5	3932	7/7	0.97	0.13	94,94,94,94	0
86	OHX	5	3943	7/7	0.97	0.13	94,94,94,94	0
86	OHX	5	3944	7/7	0.97	0.10	90,90,90,90	0
86	OHX	5	3949	7/7	0.97	0.12	83,83,83,83	0
86	OHX	5	3957	7/7	0.97	0.11	98,98,98,98	0
86	OHX	5	3958	7/7	0.97	0.11	94,94,94,94	0
86	OHX	5	3962	7/7	0.97	0.09	82,82,82,82	0
85	MG	1	3859	1/1	0.97	0.32	27,27,27,27	0
85	MG	1	3425	1/1	0.97	0.11	20,20,20,20	0
86	OHX	5	3976	7/7	0.97	0.11	107,107,107,107	0
85	MG	5	3711	1/1	0.97	0.11	66,66,66,66	0
85	MG	5	3630	1/1	0.97	0.16	34,34,34,34	0
86	OHX	5	3981	7/7	0.97	0.12	97,97,97,97	0
86	OHX	5	3982	7/7	0.97	0.14	97,97,97,97	0
86	OHX	5	3986	7/7	0.97	0.09	102,102,102,102	0
86	OHX	5	3987	7/7	0.97	0.10	102,102,102,102	0
86	OHX	5	3993	7/7	0.97	0.09	110,110,110,110	0
86	OHX	5	3995	7/7	0.97	0.10	104,104,104,104	0
86	OHX	5	3996	7/7	0.97	0.19	95,95,95,95	0
85	MG	2	2003	1/1	0.97	0.11	64,64,64,64	0
85	MG	5	3805	1/1	0.97	0.10	58,58,58,58	0
86	OHX	5	3999	7/7	0.97	0.15	102,102,102,102	0
86	OHX	2	2117	7/7	0.97	0.09	134,134,134,134	0
86	OHX	5	4003	7/7	0.97	0.10	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3484	1/1	0.97	0.22	13,13,13,13	0
86	OHX	5	4007	7/7	0.97	0.10	102,102,102,102	0
85	MG	5	3715	1/1	0.97	0.15	53,53,53,53	0
86	OHX	5	4013	7/7	0.97	0.08	127,127,127,127	0
86	OHX	5	4014	7/7	0.97	0.08	113,113,113,113	0
86	OHX	1	4028	7/7	0.97	0.08	154,154,154,154	0
86	OHX	1	4029	7/7	0.97	0.12	105,105,105,105	0
85	MG	1	4209	1/1	0.97	0.05	69,69,69,69	0
86	OHX	5	4018	7/7	0.97	0.08	110,110,110,110	0
85	MG	1	3698	1/1	0.97	0.16	41,41,41,41	0
85	MG	5	3487	1/1	0.97	0.20	35,35,35,35	0
86	OHX	7	219	7/7	0.97	0.10	103,103,103,103	0
86	OHX	5	4022	7/7	0.97	0.09	119,119,119,119	0
86	OHX	1	4033	7/7	0.97	0.09	133,133,133,133	0
86	OHX	5	4024	7/7	0.97	0.09	112,112,112,112	0
86	OHX	5	4025	7/7	0.97	0.09	124,124,124,124	0
86	OHX	5	4026	7/7	0.97	0.10	119,119,119,119	0
85	MG	1	3411	1/1	0.97	0.16	27,27,27,27	0
86	OHX	8	216	7/7	0.97	0.09	112,112,112,112	0
86	OHX	8	217	7/7	0.97	0.08	140,140,140,140	0
86	OHX	5	4029	7/7	0.97	0.09	118,118,118,118	0
85	MG	1	4212	1/1	0.97	0.08	26,26,26,26	0
86	OHX	8	220	7/7	0.97	0.08	133,133,133,133	0
86	OHX	1	4039	7/7	0.97	0.08	117,117,117,117	0
86	OHX	5	4032	7/7	0.97	0.13	103,103,103,103	0
85	MG	1	3453	1/1	0.97	0.21	30,30,30,30	0
86	OHX	1	4041	7/7	0.97	0.08	135,135,135,135	0
86	OHX	3	216	7/7	0.97	0.09	119,119,119,119	0
86	OHX	5	4037	7/7	0.97	0.10	115,115,115,115	0
86	OHX	3	217	7/7	0.97	0.09	116,116,116,116	0
86	OHX	3	219	7/7	0.97	0.07	145,145,145,145	0
86	OHX	l3	404	7/7	0.97	0.08	108,108,108,108	0
85	MG	7	212	1/1	0.97	0.15	63,63,63,63	0
85	MG	5	3492	1/1	0.97	0.10	40,40,40,40	0
86	OHX	5	4043	7/7	0.97	0.23	99,99,99,99	0
85	MG	1	3609	1/1	0.97	0.06	32,32,32,32	0
85	MG	1	3736	1/1	0.97	0.06	35,35,35,35	0
85	MG	2	1989	1/1	0.97	0.19	54,54,54,54	0
85	MG	5	3727	1/1	0.97	0.07	29,29,29,29	0
85	MG	5	3566	1/1	0.97	0.20	17,17,17,17	0
86	OHX	5	4049	7/7	0.97	0.08	138,138,138,138	0
86	OHX	2	2133	7/7	0.97	0.09	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4051	7/7	0.97	0.09	131,131,131,131	0
86	OHX	m5	306	7/7	0.97	0.09	131,131,131,131	0
86	OHX	5	4052	7/7	0.97	0.08	134,134,134,134	0
85	MG	5	3567	1/1	0.97	0.40	42,42,42,42	0
86	OHX	o3	202	7/7	0.97	0.10	119,119,119,119	0
86	OHX	5	4054	7/7	0.97	0.08	139,139,139,139	0
85	MG	5	3821	1/1	0.97	0.09	50,50,50,50	0
86	OHX	5	4056	7/7	0.97	0.10	109,109,109,109	0
85	MG	5	3429	1/1	0.97	0.12	26,26,26,26	0
85	MG	1	3521	1/1	0.97	0.18	40,40,40,40	0
88	ZBA	5	4256	33/33	0.97	0.09	24,24,24,24	0
86	OHX	1	3937	7/7	0.98	0.07	108,108,108,108	0
86	OHX	1	3938	7/7	0.98	0.10	98,98,98,98	0
86	OHX	2	2113	7/7	0.98	0.07	120,120,120,120	0
85	MG	6	2026	1/1	0.98	0.14	56,56,56,56	0
85	MG	1	3460	1/1	0.98	0.21	15,15,15,15	0
86	OHX	1	3942	7/7	0.98	0.08	110,110,110,110	0
86	OHX	3	214	7/7	0.98	0.09	98,98,98,98	0
86	OHX	1	3943	7/7	0.98	0.08	129,129,129,129	0
85	MG	L2	301	1/1	0.98	0.05	31,31,31,31	0
85	MG	1	3506	1/1	0.98	0.28	28,28,28,28	0
86	OHX	3	218	7/7	0.98	0.06	128,128,128,128	0
85	MG	5	3576	1/1	0.98	0.18	20,20,20,20	0
86	OHX	1	3949	7/7	0.98	0.09	103,103,103,103	0
86	OHX	1	3950	7/7	0.98	0.08	103,103,103,103	0
86	OHX	1	3951	7/7	0.98	0.10	106,106,106,106	0
86	OHX	1	3952	7/7	0.98	0.16	82,82,82,82	0
86	OHX	1	3953	7/7	0.98	0.07	116,116,116,116	0
85	MG	1	3537	1/1	0.98	0.32	20,20,20,20	0
86	OHX	4	225	7/7	0.98	0.09	102,102,102,102	0
86	OHX	4	226	7/7	0.98	0.06	125,125,125,125	0
85	MG	1	3681	1/1	0.98	0.10	41,41,41,41	0
85	MG	1	3748	1/1	0.98	0.10	19,19,19,19	0
85	MG	1	3652	1/1	0.98	0.23	38,38,38,38	0
85	MG	2	1918	1/1	0.98	0.30	40,40,40,40	0
85	MG	o3	201	1/1	0.98	0.10	34,34,34,34	0
86	OHX	4	232	7/7	0.98	0.06	147,147,147,147	0
86	OHX	1	3961	7/7	0.98	0.08	104,104,104,104	0
85	MG	1	3445	1/1	0.98	0.06	36,36,36,36	0
85	MG	5	3474	1/1	0.98	0.19	48,48,48,48	0
86	OHX	1	3964	7/7	0.98	0.06	113,113,113,113	0
85	MG	5	3762	1/1	0.98	0.10	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3585	1/1	0.98	0.27	13,13,13,13	0
86	OHX	2	2028	7/7	0.98	0.13	80,80,80,80	0
86	OHX	2	2031	7/7	0.98	0.10	90,90,90,90	0
86	OHX	2	2033	7/7	0.98	0.09	97,97,97,97	0
85	MG	1	3576	1/1	0.98	0.13	19,19,19,19	0
86	OHX	2	2036	7/7	0.98	0.10	102,102,102,102	0
86	OHX	2	2038	7/7	0.98	0.09	106,106,106,106	0
85	MG	6	1947	1/1	0.98	0.19	27,27,27,27	0
86	OHX	2	2041	7/7	0.98	0.08	97,97,97,97	0
86	OHX	5	4145	7/7	0.98	0.07	144,144,144,144	0
86	OHX	1	3975	7/7	0.98	0.15	99,99,99,99	0
86	OHX	1	3976	7/7	0.98	0.07	124,124,124,124	0
86	OHX	5	3931	7/7	0.98	0.09	96,96,96,96	0
86	OHX	1	3977	7/7	0.98	0.06	117,117,117,117	0
86	OHX	2	2042	7/7	0.98	0.11	97,97,97,97	0
85	MG	1	3718	1/1	0.98	0.07	61,61,61,61	0
86	OHX	5	3946	7/7	0.98	0.09	88,88,88,88	0
86	OHX	5	3947	7/7	0.98	0.10	85,85,85,85	0
86	OHX	O7	103	7/7	0.98	0.09	99,99,99,99	0
86	OHX	5	3950	7/7	0.98	0.08	89,89,89,89	0
86	OHX	5	3952	7/7	0.98	0.09	98,98,98,98	0
86	OHX	5	3953	7/7	0.98	0.10	89,89,89,89	0
86	OHX	5	3954	7/7	0.98	0.10	106,106,106,106	0
86	OHX	5	3955	7/7	0.98	0.09	100,100,100,100	0
86	OHX	O7	104	7/7	0.98	0.12	100,100,100,100	0
86	OHX	Q2	503	7/7	0.98	0.12	90,90,90,90	0
86	OHX	5	3960	7/7	0.98	0.09	92,92,92,92	0
86	OHX	5	3961	7/7	0.98	0.08	77,77,77,77	0
86	OHX	6	2050	7/7	0.98	0.10	69,69,69,69	0
86	OHX	5	3963	7/7	0.98	0.08	94,94,94,94	0
86	OHX	6	2054	7/7	0.98	0.10	83,83,83,83	0
86	OHX	5	3966	7/7	0.98	0.12	86,86,86,86	0
86	OHX	5	3968	7/7	0.98	0.09	99,99,99,99	0
86	OHX	5	3971	7/7	0.98	0.08	98,98,98,98	0
86	OHX	5	3974	7/7	0.98	0.10	88,88,88,88	0
86	OHX	6	2063	7/7	0.98	0.09	92,92,92,92	0
85	MG	5	3832	1/1	0.98	0.10	65,65,65,65	0
86	OHX	6	2065	7/7	0.98	0.08	105,105,105,105	0
86	OHX	5	3978	7/7	0.98	0.08	110,110,110,110	0
86	OHX	6	2066	7/7	0.98	0.11	107,107,107,107	0
86	OHX	6	2069	7/7	0.98	0.08	99,99,99,99	0
86	OHX	6	2070	7/7	0.98	0.13	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	3983	7/7	0.98	0.09	103,103,103,103	0
86	OHX	5	3984	7/7	0.98	0.12	81,81,81,81	0
86	OHX	2	2048	7/7	0.98	0.07	108,108,108,108	0
86	OHX	6	2072	7/7	0.98	0.12	88,88,88,88	0
86	OHX	5	3988	7/7	0.98	0.09	98,98,98,98	0
86	OHX	5	3990	7/7	0.98	0.07	101,101,101,101	0
86	OHX	5	3991	7/7	0.98	0.08	124,124,124,124	0
86	OHX	6	2074	7/7	0.98	0.09	125,125,125,125	0
86	OHX	5	3994	7/7	0.98	0.12	96,96,96,96	0
86	OHX	6	2076	7/7	0.98	0.07	111,111,111,111	0
86	OHX	2	2049	7/7	0.98	0.07	121,121,121,121	0
86	OHX	2	2051	7/7	0.98	0.07	121,121,121,121	0
86	OHX	6	2079	7/7	0.98	0.07	119,119,119,119	0
86	OHX	6	2080	7/7	0.98	0.08	107,107,107,107	0
86	OHX	5	4000	7/7	0.98	0.07	125,125,125,125	0
86	OHX	5	4001	7/7	0.98	0.07	113,113,113,113	0
86	OHX	6	2081	7/7	0.98	0.08	113,113,113,113	0
85	MG	1	3656	1/1	0.98	0.13	31,31,31,31	0
86	OHX	5	4004	7/7	0.98	0.08	108,108,108,108	0
86	OHX	5	4005	7/7	0.98	0.16	82,82,82,82	0
86	OHX	6	2083	7/7	0.98	0.07	117,117,117,117	0
85	MG	1	3755	1/1	0.98	0.10	42,42,42,42	0
86	OHX	5	4008	7/7	0.98	0.10	112,112,112,112	0
86	OHX	5	4201	7/7	0.98	0.15	91,91,91,91	0
86	OHX	2	2054	7/7	0.98	0.08	112,112,112,112	0
86	OHX	5	4010	7/7	0.98	0.06	135,135,135,135	0
86	OHX	5	4012	7/7	0.98	0.09	101,101,101,101	0
85	MG	5	3835	1/1	0.98	0.11	28,28,28,28	0
86	OHX	6	2088	7/7	0.98	0.07	121,121,121,121	0
85	MG	5	3533	1/1	0.98	0.17	33,33,33,33	0
85	MG	1	3509	1/1	0.98	0.14	25,25,25,25	0
85	MG	1	3473	1/1	0.98	0.20	12,12,12,12	0
85	MG	5	3772	1/1	0.98	0.08	50,50,50,50	0
85	MG	1	3689	1/1	0.98	0.17	35,35,35,35	0
86	OHX	2	2061	7/7	0.98	0.07	116,116,116,116	0
86	OHX	5	4021	7/7	0.98	0.09	124,124,124,124	0
86	OHX	6	2096	7/7	0.98	0.09	128,128,128,128	0
86	OHX	2	2062	7/7	0.98	0.07	120,120,120,120	0
86	OHX	2	2063	7/7	0.98	0.09	121,121,121,121	0
86	OHX	2	2064	7/7	0.98	0.08	133,133,133,133	0
85	MG	5	3537	1/1	0.98	0.27	17,17,17,17	0
85	MG	5	3842	1/1	0.98	0.08	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4028	7/7	0.98	0.07	125,125,125,125	0
85	MG	1	3837	1/1	0.98	0.24	28,28,28,28	0
85	MG	1	3659	1/1	0.98	0.16	35,35,35,35	0
86	OHX	6	2104	7/7	0.98	0.08	135,135,135,135	0
85	MG	1	3691	1/1	0.98	0.08	27,27,27,27	0
85	MG	5	3435	1/1	0.98	0.14	23,23,23,23	0
85	MG	1	3525	1/1	0.98	0.16	16,16,16,16	0
85	MG	1	3485	1/1	0.98	0.24	35,35,35,35	0
86	OHX	5	4036	7/7	0.98	0.09	103,103,103,103	0
85	MG	1	3581	1/1	0.98	0.21	23,23,23,23	0
86	OHX	5	4038	7/7	0.98	0.09	118,118,118,118	0
86	OHX	6	2110	7/7	0.98	0.07	132,132,132,132	0
86	OHX	2	2075	7/7	0.98	0.06	132,132,132,132	0
85	MG	1	3433	1/1	0.98	0.11	29,29,29,29	0
85	MG	7	230	1/1	0.98	0.22	30,30,30,30	0
85	MG	5	3491	1/1	0.98	0.16	40,40,40,40	0
85	MG	5	3853	1/1	0.98	0.10	39,39,39,39	0
85	MG	1	3447	1/1	0.98	0.05	33,33,33,33	0
85	MG	1	3584	1/1	0.98	0.28	18,18,18,18	0
85	MG	1	3611	1/1	0.98	0.17	25,25,25,25	0
85	MG	1	3768	1/1	0.98	0.08	56,56,56,56	0
85	MG	4	207	1/1	0.98	0.18	26,26,26,26	0
85	MG	5	3789	1/1	0.98	0.09	36,36,36,36	0
85	MG	5	3726	1/1	0.98	0.04	46,46,46,46	0
85	MG	1	3585	1/1	0.98	0.23	17,17,17,17	0
85	MG	4	209	1/1	0.98	0.05	45,45,45,45	0
86	OHX	5	4246	7/7	0.98	0.09	93,93,93,93	0
85	MG	5	3669	1/1	0.98	0.06	27,27,27,27	0
85	MG	5	3447	1/1	0.98	0.10	29,29,29,29	0
85	MG	5	3671	1/1	0.98	0.09	25,25,25,25	0
85	MG	l3	402	1/1	0.98	0.05	44,44,44,44	0
86	OHX	2	2093	7/7	0.98	0.07	138,138,138,138	0
86	OHX	5	4059	7/7	0.98	0.07	121,121,121,121	0
85	MG	2	1919	1/1	0.98	0.24	46,46,46,46	0
86	OHX	1	4026	7/7	0.98	0.08	116,116,116,116	0
85	MG	6	2013	1/1	0.98	0.11	59,59,59,59	0
86	OHX	7	217	7/7	0.98	0.10	94,94,94,94	0
86	OHX	7	218	7/7	0.98	0.08	93,93,93,93	0
85	MG	5	3734	1/1	0.98	0.09	28,28,28,28	0
86	OHX	7	221	7/7	0.98	0.13	100,100,100,100	0
86	OHX	7	222	7/7	0.98	0.08	103,103,103,103	0
86	OHX	7	223	7/7	0.98	0.07	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	6	1925	1/1	0.98	0.20	42,42,42,42	0
85	MG	1	3466	1/1	0.98	0.10	35,35,35,35	0
85	MG	2	1902	1/1	0.98	0.20	24,24,24,24	0
85	MG	1	3566	1/1	0.98	0.21	13,13,13,13	0
86	OHX	1	3876	7/7	0.98	0.11	71,71,71,71	0
86	OHX	1	4034	7/7	0.98	0.07	121,121,121,121	0
86	OHX	8	215	7/7	0.98	0.06	124,124,124,124	0
86	OHX	1	4035	7/7	0.98	0.06	149,149,149,149	0
86	OHX	1	3877	7/7	0.98	0.13	67,67,67,67	0
85	MG	1	3672	1/1	0.98	0.10	70,70,70,70	0
86	OHX	1	4038	7/7	0.98	0.08	119,119,119,119	0
86	OHX	1	3890	7/7	0.98	0.11	75,75,75,75	0
86	OHX	1	3893	7/7	0.98	0.10	77,77,77,77	0
86	OHX	1	3894	7/7	0.98	0.08	88,88,88,88	0
86	OHX	1	4042	7/7	0.98	0.06	139,139,139,139	0
86	OHX	1	3898	7/7	0.98	0.08	82,82,82,82	0
86	OHX	1	3902	7/7	0.98	0.10	87,87,87,87	0
85	MG	5	3620	1/1	0.98	0.09	37,37,37,37	0
86	OHX	1	3905	7/7	0.98	0.09	97,97,97,97	0
86	OHX	1	3907	7/7	0.98	0.08	89,89,89,89	0
86	OHX	1	3908	7/7	0.98	0.08	89,89,89,89	0
86	OHX	1	3909	7/7	0.98	0.08	98,98,98,98	0
86	OHX	1	3910	7/7	0.98	0.12	92,92,92,92	0
86	OHX	1	3911	7/7	0.98	0.09	94,94,94,94	0
85	MG	1	3567	1/1	0.98	0.16	21,21,21,21	0
86	OHX	1	3915	7/7	0.98	0.10	92,92,92,92	0
86	OHX	1	3916	7/7	0.98	0.08	86,86,86,86	0
85	MG	1	3739	1/1	0.98	0.12	20,20,20,20	0
85	MG	1	3532	1/1	0.98	0.26	34,34,34,34	0
86	OHX	1	3919	7/7	0.98	0.13	77,77,77,77	0
86	OHX	1	3920	7/7	0.98	0.10	102,102,102,102	0
86	OHX	1	3921	7/7	0.98	0.10	92,92,92,92	0
85	MG	1	3592	1/1	0.98	0.21	9,9,9,9	0
86	OHX	1	3924	7/7	0.98	0.10	82,82,82,82	0
85	MG	m6	202	1/1	0.98	0.09	30,30,30,30	0
86	OHX	o2	201	7/7	0.98	0.10	107,107,107,107	0
86	OHX	1	3927	7/7	0.98	0.09	102,102,102,102	0
86	OHX	o7	502	7/7	0.98	0.08	101,101,101,101	0
85	MG	4	219	1/1	0.98	0.08	37,37,37,37	0
87	ZN	E1	501	1/1	0.98	0.04	106,106,106,106	0
86	OHX	1	3930	7/7	0.98	0.08	102,102,102,102	0
85	MG	2	1969	1/1	0.98	0.25	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	ZN	e1	501	1/1	0.98	0.04	147,147,147,147	0
85	MG	2	1911	1/1	0.98	0.26	39,39,39,39	0
85	MG	5	3412	1/1	0.98	0.14	31,31,31,31	0
85	MG	5	3413	1/1	0.98	0.14	31,31,31,31	0
85	MG	1	3803	1/1	0.99	0.12	56,56,56,56	0
86	OHX	N9	101	7/7	0.99	0.10	65,65,65,65	0
85	MG	5	3845	1/1	0.99	0.13	32,32,32,32	0
86	OHX	5	3902	7/7	0.99	0.10	47,47,47,47	0
86	OHX	5	3904	7/7	0.99	0.10	68,68,68,68	0
86	OHX	5	3906	7/7	0.99	0.10	51,51,51,51	0
86	OHX	5	3907	7/7	0.99	0.09	55,55,55,55	0
86	OHX	5	3908	7/7	0.99	0.12	65,65,65,65	0
86	OHX	5	3909	7/7	0.99	0.09	64,64,64,64	0
86	OHX	5	3910	7/7	0.99	0.10	58,58,58,58	0
86	OHX	5	3911	7/7	0.99	0.07	64,64,64,64	0
86	OHX	5	3912	7/7	0.99	0.13	64,64,64,64	0
86	OHX	5	3914	7/7	0.99	0.07	61,61,61,61	0
86	OHX	5	3915	7/7	0.99	0.11	65,65,65,65	0
86	OHX	5	3917	7/7	0.99	0.10	66,66,66,66	0
86	OHX	5	3918	7/7	0.99	0.09	71,71,71,71	0
86	OHX	5	3919	7/7	0.99	0.08	64,64,64,64	0
86	OHX	5	3922	7/7	0.99	0.08	69,69,69,69	0
86	OHX	5	3923	7/7	0.99	0.06	65,65,65,65	0
86	OHX	5	3924	7/7	0.99	0.09	63,63,63,63	0
86	OHX	5	3925	7/7	0.99	0.07	67,67,67,67	0
86	OHX	5	3926	7/7	0.99	0.10	71,71,71,71	0
86	OHX	5	3927	7/7	0.99	0.07	71,71,71,71	0
86	OHX	5	3928	7/7	0.99	0.06	65,65,65,65	0
85	MG	1	3604	1/1	0.99	0.25	41,41,41,41	0
86	OHX	5	3930	7/7	0.99	0.07	79,79,79,79	0
86	OHX	2	2044	7/7	0.99	0.06	96,96,96,96	0
86	OHX	2	2045	7/7	0.99	0.06	96,96,96,96	0
86	OHX	5	3933	7/7	0.99	0.07	70,70,70,70	0
86	OHX	5	3934	7/7	0.99	0.08	72,72,72,72	0
86	OHX	5	3935	7/7	0.99	0.10	86,86,86,86	0
86	OHX	5	3936	7/7	0.99	0.07	76,76,76,76	0
86	OHX	5	3937	7/7	0.99	0.06	81,81,81,81	0
86	OHX	5	3938	7/7	0.99	0.06	77,77,77,77	0
86	OHX	5	3940	7/7	0.99	0.08	74,74,74,74	0
86	OHX	5	3941	7/7	0.99	0.07	84,84,84,84	0
86	OHX	5	3942	7/7	0.99	0.08	93,93,93,93	0
86	OHX	2	2073	7/7	0.99	0.05	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3784	1/1	0.99	0.05	58,58,58,58	0
86	OHX	5	3945	7/7	0.99	0.08	93,93,93,93	0
86	OHX	6	2047	7/7	0.99	0.11	70,70,70,70	0
86	OHX	6	2048	7/7	0.99	0.10	64,64,64,64	0
86	OHX	5	3948	7/7	0.99	0.08	80,80,80,80	0
86	OHX	6	2049	7/7	0.99	0.07	71,71,71,71	0
86	OHX	1	3923	7/7	0.99	0.07	102,102,102,102	0
86	OHX	5	3951	7/7	0.99	0.09	100,100,100,100	0
86	OHX	6	2051	7/7	0.99	0.09	75,75,75,75	0
86	OHX	6	2052	7/7	0.99	0.09	74,74,74,74	0
86	OHX	6	2053	7/7	0.99	0.10	78,78,78,78	0
86	OHX	2	2047	7/7	0.99	0.06	103,103,103,103	0
86	OHX	5	3956	7/7	0.99	0.06	89,89,89,89	0
86	OHX	6	2055	7/7	0.99	0.10	73,73,73,73	0
86	OHX	6	2056	7/7	0.99	0.10	80,80,80,80	0
86	OHX	5	3959	7/7	0.99	0.07	86,86,86,86	0
86	OHX	6	2057	7/7	0.99	0.07	79,79,79,79	0
86	OHX	6	2058	7/7	0.99	0.08	78,78,78,78	0
86	OHX	6	2059	7/7	0.99	0.07	92,92,92,92	0
86	OHX	6	2060	7/7	0.99	0.06	85,85,85,85	0
86	OHX	5	3964	7/7	0.99	0.05	88,88,88,88	0
86	OHX	6	2061	7/7	0.99	0.08	85,85,85,85	0
86	OHX	6	2062	7/7	0.99	0.05	92,92,92,92	0
86	OHX	5	3967	7/7	0.99	0.07	91,91,91,91	0
86	OHX	1	3925	7/7	0.99	0.07	84,84,84,84	0
86	OHX	5	3969	7/7	0.99	0.08	96,96,96,96	0
86	OHX	5	3970	7/7	0.99	0.07	88,88,88,88	0
85	MG	1	3627	1/1	0.99	0.17	77,77,77,77	0
86	OHX	5	3972	7/7	0.99	0.07	94,94,94,94	0
86	OHX	5	3973	7/7	0.99	0.08	91,91,91,91	0
85	MG	5	3822	1/1	0.99	0.06	48,48,48,48	0
86	OHX	1	3928	7/7	0.99	0.06	78,78,78,78	0
86	OHX	6	2067	7/7	0.99	0.11	99,99,99,99	0
86	OHX	6	2068	7/7	0.99	0.10	96,96,96,96	0
86	OHX	2	2050	7/7	0.99	0.04	122,122,122,122	0
86	OHX	1	3862	7/7	0.99	0.10	67,67,67,67	0
86	OHX	5	3980	7/7	0.99	0.10	83,83,83,83	0
86	OHX	1	3864	7/7	0.99	0.12	56,56,56,56	0
86	OHX	1	3866	7/7	0.99	0.11	62,62,62,62	0
86	OHX	6	2073	7/7	0.99	0.06	113,113,113,113	0
86	OHX	1	3867	7/7	0.99	0.07	65,65,65,65	0
86	OHX	5	3985	7/7	0.99	0.08	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	6	2075	7/7	0.99	0.09	96,96,96,96	0
86	OHX	1	3868	7/7	0.99	0.10	63,63,63,63	0
86	OHX	1	3935	7/7	0.99	0.10	94,94,94,94	0
86	OHX	5	3989	7/7	0.99	0.08	82,82,82,82	0
86	OHX	1	3936	7/7	0.99	0.07	101,101,101,101	0
86	OHX	7	220	7/7	0.99	0.05	108,108,108,108	0
86	OHX	1	3869	7/7	0.99	0.09	64,64,64,64	0
86	OHX	5	3992	7/7	0.99	0.06	84,84,84,84	0
86	OHX	1	3870	7/7	0.99	0.08	69,69,69,69	0
86	OHX	1	3871	7/7	0.99	0.09	63,63,63,63	0
86	OHX	1	3874	7/7	0.99	0.10	66,66,66,66	0
86	OHX	1	3875	7/7	0.99	0.06	69,69,69,69	0
85	MG	1	3826	1/1	0.99	0.22	10,10,10,10	0
85	MG	5	3865	1/1	0.99	0.06	69,69,69,69	0
86	OHX	1	3878	7/7	0.99	0.07	67,67,67,67	0
86	OHX	8	214	7/7	0.99	0.10	60,60,60,60	0
86	OHX	6	2087	7/7	0.99	0.06	114,114,114,114	0
86	OHX	1	3945	7/7	0.99	0.06	106,106,106,106	0
86	OHX	1	3879	7/7	0.99	0.09	70,70,70,70	0
86	OHX	1	3880	7/7	0.99	0.08	69,69,69,69	0
86	OHX	1	3948	7/7	0.99	0.12	89,89,89,89	0
86	OHX	1	3881	7/7	0.99	0.09	70,70,70,70	0
86	OHX	6	2093	7/7	0.99	0.06	114,114,114,114	0
86	OHX	1	3882	7/7	0.99	0.07	78,78,78,78	0
86	OHX	1	3884	7/7	0.99	0.09	76,76,76,76	0
86	OHX	1	3885	7/7	0.99	0.06	69,69,69,69	0
86	OHX	1	3888	7/7	0.99	0.10	76,76,76,76	0
86	OHX	5	4011	7/7	0.99	0.07	71,71,71,71	0
86	OHX	2	2026	7/7	0.99	0.10	75,75,75,75	0
86	OHX	2	2027	7/7	0.99	0.10	79,79,79,79	0
86	OHX	1	3891	7/7	0.99	0.09	75,75,75,75	0
86	OHX	1	3892	7/7	0.99	0.07	76,76,76,76	0
86	OHX	4	223	7/7	0.99	0.10	63,63,63,63	0
86	OHX	1	3958	7/7	0.99	0.08	70,70,70,70	0
85	MG	1	3596	1/1	0.99	0.27	11,11,11,11	0
86	OHX	2	2029	7/7	0.99	0.07	80,80,80,80	0
86	OHX	1	3895	7/7	0.99	0.07	67,67,67,67	0
86	OHX	1	3896	7/7	0.99	0.07	83,83,83,83	0
86	OHX	1	3897	7/7	0.99	0.08	74,74,74,74	0
86	OHX	2	2030	7/7	0.99	0.08	79,79,79,79	0
86	OHX	1	3899	7/7	0.99	0.08	78,78,78,78	0
86	OHX	1	3900	7/7	0.99	0.07	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	3901	7/7	0.99	0.06	79,79,79,79	0
85	MG	5	3584	1/1	0.99	0.27	16,16,16,16	0
86	OHX	n3	203	7/7	0.99	0.10	89,89,89,89	0
86	OHX	2	2032	7/7	0.99	0.07	88,88,88,88	0
86	OHX	n9	102	7/7	0.99	0.09	67,67,67,67	0
85	MG	5	3532	1/1	0.99	0.24	16,16,16,16	0
86	OHX	1	3906	7/7	0.99	0.07	85,85,85,85	0
85	MG	5	3563	1/1	0.99	0.23	13,13,13,13	0
86	OHX	q2	502	7/7	0.99	0.10	93,93,93,93	0
86	OHX	2	2035	7/7	0.99	0.08	94,94,94,94	0
87	ZN	D9	101	1/1	0.99	0.03	67,67,67,67	0
85	MG	1	3820	1/1	0.99	0.05	51,51,51,51	0
86	OHX	2	2037	7/7	0.99	0.09	95,95,95,95	0
85	MG	1	3638	1/1	0.99	0.11	34,34,34,34	0
87	ZN	d9	101	1/1	0.99	0.02	60,60,60,60	0
86	OHX	1	3912	7/7	0.99	0.07	90,90,90,90	0
86	OHX	1	3913	7/7	0.99	0.08	93,93,93,93	0
86	OHX	2	2039	7/7	0.99	0.06	91,91,91,91	0
85	MG	5	3408	1/1	0.99	0.02	22,22,22,22	0
86	OHX	1	3886	7/7	1.00	0.05	69,69,69,69	0
86	OHX	1	3887	7/7	1.00	0.06	71,71,71,71	0
86	OHX	5	3916	7/7	1.00	0.07	68,68,68,68	0
86	OHX	1	3873	7/7	1.00	0.07	65,65,65,65	0
86	OHX	6	2046	7/7	1.00	0.09	60,60,60,60	0
86	OHX	1	3861	7/7	1.00	0.07	47,47,47,47	0
86	OHX	5	3939	7/7	1.00	0.05	72,72,72,72	0
86	OHX	5	3920	7/7	1.00	0.06	64,64,64,64	0
86	OHX	5	3921	7/7	1.00	0.06	71,71,71,71	0
86	OHX	5	3903	7/7	1.00	0.10	46,46,46,46	0
86	OHX	4	224	7/7	1.00	0.07	64,64,64,64	0
87	ZN	D6	500	1/1	1.00	0.02	73,73,73,73	0
86	OHX	5	3905	7/7	1.00	0.07	55,55,55,55	0
86	OHX	1	3865	7/7	1.00	0.08	55,55,55,55	0
86	OHX	1	3860	7/7	1.00	0.09	43,43,43,43	0
87	ZN	O7	101	1/1	1.00	0.01	32,32,32,32	0
87	ZN	Q0	500	1/1	1.00	0.02	42,42,42,42	0
86	OHX	N1	201	7/7	1.00	0.06	66,66,66,66	0
87	ZN	Q3	501	1/1	1.00	0.01	50,50,50,50	0
87	ZN	d6	101	1/1	1.00	0.02	54,54,54,54	0
86	OHX	1	3883	7/7	1.00	0.07	72,72,72,72	0
86	OHX	8	213	7/7	1.00	0.08	62,62,62,62	0
86	OHX	1	3863	7/7	1.00	0.09	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	ZN	o7	501	1/1	1.00	0.01	35,35,35,35	0
87	ZN	q0	201	1/1	1.00	0.02	32,32,32,32	0
86	OHX	1	3903	7/7	1.00	0.05	75,75,75,75	0
87	ZN	q3	501	1/1	1.00	0.02	61,61,61,61	0
86	OHX	1	3872	7/7	1.00	0.08	62,62,62,62	0
86	OHX	5	3913	7/7	1.00	0.07	58,58,58,58	0

5.5 Other polymers

There are no such residues in this entry.