wwPDB X-ray Structure Validation Summary Report (i)

Sep 15, 2026 – 11:22 pm BST

PDB ID	:	5MEI / pdb_00005mei
Title	:	Crystal structure of Agelastatin A bound to the 80S ribosome
Authors	:	McClary, B.; Zinshteyn, B.; Meyer, M.; Jouanneau, M.; Pellegrino, S.; Yusupova, G.; Schuller, A.; Reyes, J.C.P.; Lu, J.; Luo, C.; Dang, Y.; Romo, D.; Yusupov, M.; Green, R.; Liu, J.O.
Deposited on	:	2016-11-15
Resolution	:	3.50 Å(reported)

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

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

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

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

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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 Å.

There are no overall percentile quality scores available for this entry.

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

2 Entry composition (i)

There are 87 unique types of molecules in this entry. The entry contains 409590 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S ribosomal RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	l2	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
24	CX	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 46 is a protein called Suppressor protein STM1.

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

- Molecule 47 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	p0	143	Total	C	N	O	S	0	0	0
			1077	687	192	195	3			

- Molecule 48 is a protein called Suppressor protein STM1,Suppressor protein STM1,Suppressor protein Stm1 - Mol B.

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

- Molecule 49 is a protein called 40S ribosomal protein S0-A.

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

- Molecule 50 is a protein called 40S ribosomal protein S1-A.

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

- Molecule 51 is a protein called 40S ribosomal protein S2.

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

- Molecule 52 is a protein called 40S ribosomal protein S3.

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

- Molecule 53 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 54 is a protein called 40S ribosomal protein S5.

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

- Molecule 55 is a protein called 40S ribosomal protein S6-A.

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

- Molecule 56 is a protein called 40S ribosomal protein S7-A.

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

- Molecule 57 is a protein called 40S ribosomal protein S8-A.

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

- Molecule 58 is a protein called 40S ribosomal protein S9-A.

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

- Molecule 59 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	L	96	Total	C	N	O	S	0	0	0
			772	499	126	145	2			
59	c0	96	Total	C	N	O	S	0	0	0
			761	490	125	144	2			

- Molecule 60 is a protein called 40S ribosomal protein S11-A.

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

- Molecule 61 is a protein called 40S ribosomal protein S12.

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

- Molecule 62 is a protein called 40S ribosomal protein S13.

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

- Molecule 63 is a protein called 40S ribosomal protein S14-B.

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

- Molecule 64 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	Q	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	c5	135	Total	C	N	O	S	0	0	0
			1039	658	196	178	7			

- Molecule 65 is a protein called 40S ribosomal protein S16-A.

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

- Molecule 66 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	S	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			

- Molecule 67 is a protein called 40S ribosomal protein S18-A.

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

- Molecule 68 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 69 is a protein called 40S ribosomal protein S20.

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

- Molecule 70 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 71 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 72 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 73 is a protein called 40S ribosomal protein S24-A.

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

- Molecule 74 is a protein called 40S ribosomal protein S25-A.

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

- Molecule 75 is a protein called 40S ribosomal protein S26-B.

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

- Molecule 76 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 77 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 78 is a protein called 40S ribosomal protein S29-A.

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

- Molecule 79 is a protein called 40S ribosomal protein S30-A.

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

- Molecule 80 is a protein called Ubiquitin-40S ribosomal protein S31.

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

- Molecule 81 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	h	318	Total	C	N	O	S	0	0	0
			2437	1541	418	470	8			
81	sR	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

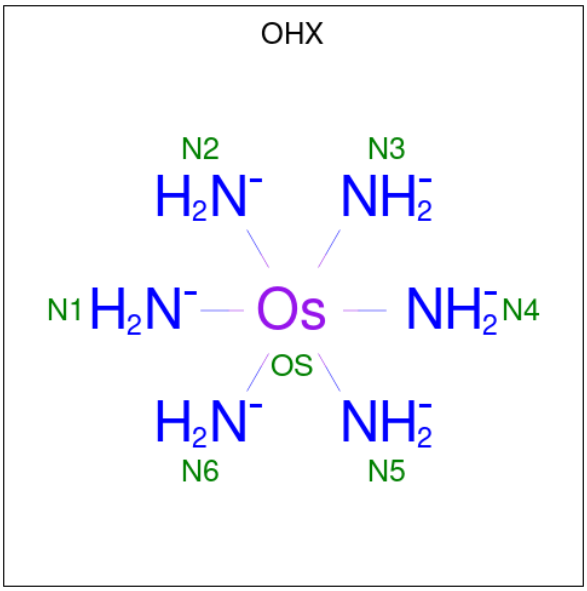
- Molecule 82 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

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

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

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



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

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

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	2	1	Total N Os 7 6 1	0	0
84	6	1	Total N Os 7 6 1	0	0
84	6	1	Total N Os 7 6 1	0	0
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84	6	1	Total N Os 7 6 1	0	0
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84	6	1	Total N Os 7 6 1	0	0
84	6	1	Total N Os 7 6 1	0	0
84	6	1	Total N Os 7 6 1	0	0
84	6	1	Total N Os 7 6 1	0	0
84	6	1	Total N Os 7 6 1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	CX	1	Total N Os 7 6 1	0	0
84	CZ	1	Total N Os 7 6 1	0	0
84	DD	1	Total N Os 7 6 1	0	0
84	DG	1	Total N Os 7 6 1	0	0
84	DH	1	Total N Os 7 6 1	0	0
84	DI	1	Total N Os 7 6 1	0	0
84	DL	1	Total N Os 7 6 1	0	0
84	DL	1	Total N Os 7 6 1	0	0
84	A	1	Total N Os 7 6 1	0	0
84	A	1	Total N Os 7 6 1	0	0
84	A	1	Total N Os 7 6 1	0	0
84	A	1	Total N Os 7 6 1	0	0
84	A	1	Total N Os 7 6 1	0	0
84	A	1	Total N Os 7 6 1	0	0
84	A	1	Total N Os 7 6 1	0	0
84	A	1	Total N Os 7 6 1	0	0
84	A	1	Total N Os 7 6 1	0	0
84	A	1	Total N Os 7 6 1	0	0
84	A	1	Total N Os 7 6 1	0	0
84	A	1	Total N Os 7 6 1	0	0

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	A	1	Total N Os 7 6 1	0	0
84	A	1	Total N Os 7 6 1	0	0
84	A	1	Total N Os 7 6 1	0	0
84	H	1	Total N Os 7 6 1	0	0
84	J	1	Total N Os 7 6 1	0	0
84	M	1	Total N Os 7 6 1	0	0
84	O	1	Total N Os 7 6 1	0	0
84	Q	1	Total N Os 7 6 1	0	0
84	T	1	Total N Os 7 6 1	0	0
84	e	1	Total N Os 7 6 1	0	0
84	h	1	Total N Os 7 6 1	0	0
84	s8	1	Total N Os 7 6 1	0	0
84	c3	1	Total N Os 7 6 1	0	0
84	c5	1	Total N Os 7 6 1	0	0
84	c8	1	Total N Os 7 6 1	0	0
84	d9	1	Total N Os 7 6 1	0	0
84	sR	1	Total N Os 7 6 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	1	490	Total Mg 490 490	0	0
85	3	12	Total Mg 12 12	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	4	21	Total Mg 21 21	0	0
85	j	2	Total Mg 2 2	0	0
85	k	2	Total Mg 2 2	0	0
85	l	2	Total Mg 2 2	0	0
85	o	3	Total Mg 3 3	0	0
85	r	1	Total Mg 1 1	0	0
85	s	1	Total Mg 1 1	0	0
85	t	2	Total Mg 2 2	0	0
85	v	1	Total Mg 1 1	0	0
85	w	1	Total Mg 1 1	0	0
85	x	5	Total Mg 5 5	0	0
85	z	2	Total Mg 2 2	0	0
85	l2	2	Total Mg 2 2	0	0
85	6	141	Total Mg 141 141	0	0
85	9	1	Total Mg 1 1	0	0
85	AB	4	Total Mg 4 4	0	0
85	AF	2	Total Mg 2 2	0	0
85	AH	1	Total Mg 1 1	0	0
85	AK	1	Total Mg 1 1	0	0
85	AP	1	Total Mg 1 1	0	0
85	i	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	AR	504	Total Mg 504 504	0	0
85	AS	20	Total Mg 20 20	0	0
85	AT	12	Total Mg 12 12	0	0
85	CD	2	Total Mg 2 2	0	0
85	CE	4	Total Mg 4 4	0	0
85	CF	1	Total Mg 1 1	0	0
85	CI	1	Total Mg 1 1	0	0
85	CK	1	Total Mg 1 1	0	0
85	CO	2	Total Mg 2 2	0	0
85	CP	2	Total Mg 2 2	0	0
85	CQ	4	Total Mg 4 4	0	0
85	CR	6	Total Mg 6 6	0	0
85	CU	2	Total Mg 2 2	0	0
85	CX	2	Total Mg 2 2	0	0
85	DA	1	Total Mg 1 1	0	0
85	DC	4	Total Mg 4 4	0	0
85	DD	1	Total Mg 1 1	0	0
85	DE	1	Total Mg 1 1	0	0
85	DF	1	Total Mg 1 1	0	0
85	DG	1	Total Mg 1 1	0	0
85	DH	2	Total Mg 2 2	0	0

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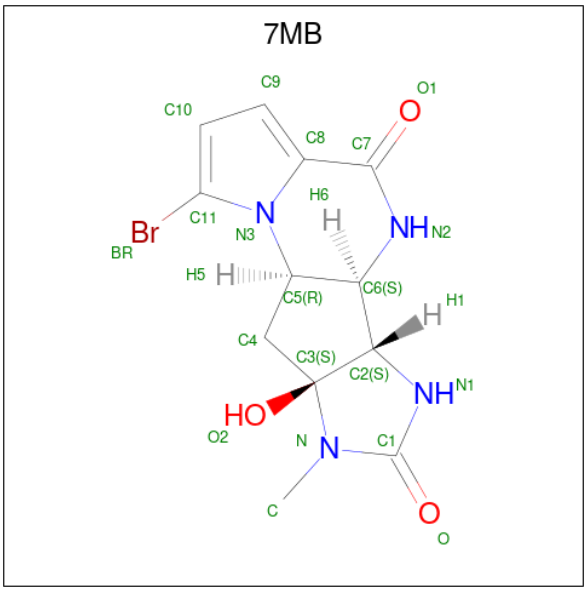
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	DI	1	Total Mg 1 1	0	0
85	DO	1	Total Mg 1 1	0	0
85	DP	1	Total Mg 1 1	0	0
85	DR	2	Total Mg 2 2	0	0
85	sM	1	Total Mg 1 1	0	0
85	A	111	Total Mg 111 111	0	0
85	D	1	Total Mg 1 1	0	0
85	F	1	Total Mg 1 1	0	0
85	Y	1	Total Mg 1 1	0	0
85	b	1	Total Mg 1 1	0	0
85	s1	1	Total Mg 1 1	0	0
85	s2	1	Total Mg 1 1	0	0
85	s6	1	Total Mg 1 1	0	0
85	s8	1	Total Mg 1 1	0	0
85	c6	1	Total Mg 1 1	0	0
85	c9	1	Total Mg 1 1	0	0
85	d3	3	Total Mg 3 3	0	0
85	d5	1	Total Mg 1 1	0	0
85	d6	1	Total Mg 1 1	0	0
85	d9	1	Total Mg 1 1	0	0

- Molecule 86 is Agelastatin A (CCD ID: 7MB) (formula: $C_{12}H_{13}BrN_4O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
86	1	1	Total	Br	C	N	O	0	0
			20	1	12	4	3		
86	AR	1	Total	Br	C	N	O	0	0
			20	1	12	4	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	AK	1	Total	Zn	0	0
			1	1		
87	AN	1	Total	Zn	0	0
			1	1		
87	AP	1	Total	Zn	0	0
			1	1		
87	AQ	1	Total	Zn	0	0
			1	1		
87	DL	1	Total	Zn	0	0
			1	1		
87	DO	1	Total	Zn	0	0
			1	1		
87	DQ	1	Total	Zn	0	0
			1	1		
87	DR	1	Total	Zn	0	0
			1	1		
87	b	1	Total	Zn	0	0
			1	1		
87	c	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	e	1	Total Zn 1 1	0	0
87	g	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

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

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	304.08Å 286.55Å 436.55Å 90.00° 99.05° 90.00°	Depositor
Resolution (Å)	98.38 – 3.50	Depositor
% Data completeness (in resolution range)	100.0 (98.38-3.50)	Depositor
R_{merge}	0.57	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 3.49Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.195 , 0.239	Depositor
Wilson B-factor (Å^2)	71.3	Xtriage
Anisotropy	0.145	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	409590	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% 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 2494 ligands modelled in this entry, 1422 are monoatomic - leaving 1072 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	1	3551	-	0,6,6	-	-	-		
84	OHX	1	3431	-	0,6,6	-	-	-		
84	OHX	AR	3629	-	0,6,6	-	-	-		
84	OHX	AR	3548	-	0,6,6	-	-	-		
84	OHX	6	1918	-	0,6,6	-	-	-		
84	OHX	1	3483	-	0,6,6	-	-	-		
84	OHX	6	1960	-	0,6,6	-	-	-		
84	OHX	AR	3518	-	0,6,6	-	-	-		
84	OHX	A	1957	85	0,6,6	-	-	-		
84	OHX	AR	3528	85	0,6,6	-	-	-		
84	OHX	AR	3561	-	0,6,6	-	-	-		
84	OHX	AR	3575	-	0,6,6	-	-	-		
84	OHX	1	3433	-	0,6,6	-	-	-		
84	OHX	1	3514	-	0,6,6	-	-	-		
84	OHX	AR	3737	-	0,6,6	-	-	-		
84	OHX	1	3730	-	0,6,6	-	-	-		
84	OHX	AR	3429	85	0,6,6	-	-	-		
84	OHX	AR	3443	-	0,6,6	-	-	-		
84	OHX	h	401	-	0,6,6	-	-	-		
84	OHX	6	2012	-	0,6,6	-	-	-		
84	OHX	1	3468	85	0,6,6	-	-	-		
84	OHX	1	3409	-	0,6,6	-	-	-		
84	OHX	1	3667	-	0,6,6	-	-	-		
84	OHX	CE	403	-	0,6,6	-	-	-		
84	OHX	1	3723	-	0,6,6	-	-	-		
84	OHX	1	3503	-	0,6,6	-	-	-		
84	OHX	1	3628	-	0,6,6	-	-	-		
84	OHX	6	2052	-	0,6,6	-	-	-		
84	OHX	1	3510	-	0,6,6	-	-	-		
84	OHX	1	3654	-	0,6,6	-	-	-		
84	OHX	AR	3442	-	0,6,6	-	-	-		
84	OHX	A	2032	-	0,6,6	-	-	-		
84	OHX	1	3476	-	0,6,6	-	-	-		
84	OHX	1	3726	-	0,6,6	-	-	-		
84	OHX	1	3511	85	0,6,6	-	-	-		
84	OHX	1	3647	-	0,6,6	-	-	-		
84	OHX	1	3725	-	0,6,6	-	-	-		
84	OHX	1	3566	85	0,6,6	-	-	-		
84	OHX	1	3641	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	A	1941	-	0,6,6	-	-	-		
84	OHX	1	3473	-	0,6,6	-	-	-		
84	OHX	1	3534	-	0,6,6	-	-	-		
84	OHX	6	1979	-	0,6,6	-	-	-		
84	OHX	AR	3476	-	0,6,6	-	-	-		
84	OHX	6	2050	-	0,6,6	-	-	-		
84	OHX	1	3553	-	0,6,6	-	-	-		
84	OHX	AR	3437	85	0,6,6	-	-	-		
84	OHX	AR	3588	-	0,6,6	-	-	-		
84	OHX	1	3715	-	0,6,6	-	-	-		
84	OHX	1	3665	-	0,6,6	-	-	-		
84	OHX	AR	3497	-	0,6,6	-	-	-		
84	OHX	AR	3532	-	0,6,6	-	-	-		
84	OHX	6	2013	-	0,6,6	-	-	-		
84	OHX	AR	3449	-	0,6,6	-	-	-		
84	OHX	A	2002	-	0,6,6	-	-	-		
84	OHX	1	3480	-	0,6,6	-	-	-		
84	OHX	A	2016	-	0,6,6	-	-	-		
84	OHX	AR	3477	-	0,6,6	-	-	-		
84	OHX	A	2009	-	0,6,6	-	-	-		
84	OHX	6	1945	-	0,6,6	-	-	-		
84	OHX	1	3563	-	0,6,6	-	-	-		
84	OHX	1	3713	-	0,6,6	-	-	-		
84	OHX	A	1950	-	0,6,6	-	-	-		
84	OHX	6	1952	-	0,6,6	-	-	-		
84	OHX	1	3402	-	0,6,6	-	-	-		
84	OHX	6	2036	-	0,6,6	-	-	-		
84	OHX	AR	3693	-	0,6,6	-	-	-		
84	OHX	6	1927	-	0,6,6	-	-	-		
84	OHX	A	2001	-	0,6,6	-	-	-		
84	OHX	A	2004	-	0,6,6	-	-	-		
84	OHX	1	3579	-	0,6,6	-	-	-		
84	OHX	6	1957	-	0,6,6	-	-	-		
84	OHX	1	3624	-	0,6,6	-	-	-		
84	OHX	1	3655	-	0,6,6	-	-	-		
84	OHX	6	1911	85	0,6,6	-	-	-		
84	OHX	6	1954	-	0,6,6	-	-	-		
84	OHX	1	3470	-	0,6,6	-	-	-		
84	OHX	1	3543	-	0,6,6	-	-	-		
84	OHX	AR	3466	-	0,6,6	-	-	-		
84	OHX	AR	3584	85	0,6,6	-	-	-		
84	OHX	A	1901	-	0,6,6	-	-	-		
84	OHX	AR	3703	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	6	1907	-	0,6,6	-	-	-		
84	OHX	A	1906	85	0,6,6	-	-	-		
84	OHX	1	3420	-	0,6,6	-	-	-		
84	OHX	6	1976	-	0,6,6	-	-	-		
84	OHX	1	3603	-	0,6,6	-	-	-		
84	OHX	1	3489	85	0,6,6	-	-	-		
84	OHX	1	3644	-	0,6,6	-	-	-		
84	OHX	1	3447	85	0,6,6	-	-	-		
84	OHX	1	3467	-	0,6,6	-	-	-		
84	OHX	1	3600	-	0,6,6	-	-	-		
84	OHX	6	1910	-	0,6,6	-	-	-		
84	OHX	1	3731	-	0,6,6	-	-	-		
84	OHX	6	1944	-	0,6,6	-	-	-		
84	OHX	AR	3493	-	0,6,6	-	-	-		
84	OHX	AR	3599	-	0,6,6	-	-	-		
84	OHX	AR	3616	-	0,6,6	-	-	-		
84	OHX	A	2018	-	0,6,6	-	-	-		
84	OHX	AR	3425	-	0,6,6	-	-	-		
84	OHX	1	3714	85	0,6,6	-	-	-		
84	OHX	AR	3521	-	0,6,6	-	-	-		
84	OHX	1	3685	-	0,6,6	-	-	-		
84	OHX	A	1969	-	0,6,6	-	-	-		
84	OHX	AR	3433	-	0,6,6	-	-	-		
84	OHX	AR	3514	-	0,6,6	-	-	-		
84	OHX	1	3601	-	0,6,6	-	-	-		
84	OHX	A	2020	-	0,6,6	-	-	-		
84	OHX	1	3517	85	0,6,6	-	-	-		
84	OHX	6	2014	-	0,6,6	-	-	-		
84	OHX	AR	3545	-	0,6,6	-	-	-		
84	OHX	1	3693	-	0,6,6	-	-	-		
84	OHX	6	2005	85	0,6,6	-	-	-		
84	OHX	6	1968	85	0,6,6	-	-	-		
84	OHX	1	3617	-	0,6,6	-	-	-		
84	OHX	6	1908	-	0,6,6	-	-	-		
84	OHX	1	3570	-	0,6,6	-	-	-		
84	OHX	AR	3560	-	0,6,6	-	-	-		
84	OHX	1	3630	-	0,6,6	-	-	-		
84	OHX	s8	301	-	0,6,6	-	-	-		
84	OHX	6	1998	-	0,6,6	-	-	-		
84	OHX	DL	102	-	0,6,6	-	-	-		
84	OHX	AR	3504	-	0,6,6	-	-	-		
84	OHX	1	3703	-	0,6,6	-	-	-		
84	OHX	6	1934	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	1	3662	85	0,6,6	-	-	-		
84	OHX	AR	3482	-	0,6,6	-	-	-		
84	OHX	1	3571	-	0,6,6	-	-	-		
84	OHX	AR	3550	-	0,6,6	-	-	-		
84	OHX	A	1942	85	0,6,6	-	-	-		
84	OHX	6	2034	-	0,6,6	-	-	-		
84	OHX	1	3616	-	0,6,6	-	-	-		
84	OHX	1	3537	-	0,6,6	-	-	-		
84	OHX	1	3689	-	0,6,6	-	-	-		
84	OHX	6	2039	-	0,6,6	-	-	-		
84	OHX	6	1909	-	0,6,6	-	-	-		
84	OHX	AR	3555	85	0,6,6	-	-	-		
84	OHX	A	1947	-	0,6,6	-	-	-		
84	OHX	6	1970	-	0,6,6	-	-	-		
84	OHX	1	3541	-	0,6,6	-	-	-		
84	OHX	AR	3462	85	0,6,6	-	-	-		
84	OHX	A	1970	-	0,6,6	-	-	-		
84	OHX	AR	3562	-	0,6,6	-	-	-		
84	OHX	1	3412	-	0,6,6	-	-	-		
84	OHX	AR	3613	85	0,6,6	-	-	-		
84	OHX	O	201	-	0,6,6	-	-	-		
84	OHX	AR	3485	-	0,6,6	-	-	-		
84	OHX	AR	3463	-	0,6,6	-	-	-		
84	OHX	1	3545	-	0,6,6	-	-	-		
84	OHX	A	1981	-	0,6,6	-	-	-		
84	OHX	A	1931	-	0,6,6	-	-	-		
84	OHX	AR	3513	-	0,6,6	-	-	-		
84	OHX	1	3649	-	0,6,6	-	-	-		
84	OHX	1	3552	-	0,6,6	-	-	-		
84	OHX	AR	3471	-	0,6,6	-	-	-		
84	OHX	6	1995	-	0,6,6	-	-	-		
84	OHX	AR	3445	-	0,6,6	-	-	-		
84	OHX	1	3676	-	0,6,6	-	-	-		
84	OHX	4	205	-	0,6,6	-	-	-		
84	OHX	1	3720	85	0,6,6	-	-	-		
84	OHX	1	3403	-	0,6,6	-	-	-		
84	OHX	1	3697	-	0,6,6	-	-	-		
84	OHX	6	2027	85	0,6,6	-	-	-		
84	OHX	6	2030	-	0,6,6	-	-	-		
84	OHX	1	3597	-	0,6,6	-	-	-		
84	OHX	A	1927	-	0,6,6	-	-	-		
84	OHX	4	207	-	0,6,6	-	-	-		
84	OHX	1	3650	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	1	3555	-	0,6,6	-	-	-		
84	OHX	AR	3411	-	0,6,6	-	-	-		
84	OHX	1	3576	85	0,6,6	-	-	-		
84	OHX	1	3705	-	0,6,6	-	-	-		
84	OHX	6	2044	-	0,6,6	-	-	-		
84	OHX	AS	201	-	0,6,6	-	-	-		
84	OHX	A	1977	-	0,6,6	-	-	-		
84	OHX	A	1946	85	0,6,6	-	-	-		
84	OHX	6	1992	-	0,6,6	-	-	-		
84	OHX	1	3687	-	0,6,6	-	-	-		
84	OHX	1	3546	-	0,6,6	-	-	-		
84	OHX	1	3502	-	0,6,6	-	-	-		
84	OHX	1	3427	-	0,6,6	-	-	-		
84	OHX	1	3682	-	0,6,6	-	-	-		
84	OHX	1	3719	-	0,6,6	-	-	-		
84	OHX	6	2016	-	0,6,6	-	-	-		
84	OHX	AC	101	-	0,6,6	-	-	-		
84	OHX	AR	3455	-	0,6,6	-	-	-		
84	OHX	6	1932	-	0,6,6	-	-	-		
84	OHX	A	2021	-	0,6,6	-	-	-		
84	OHX	AR	3547	-	0,6,6	-	-	-		
84	OHX	AR	3631	-	0,6,6	-	-	-		
84	OHX	6	1983	-	0,6,6	-	-	-		
84	OHX	AR	3571	-	0,6,6	-	-	-		
84	OHX	1	3699	-	0,6,6	-	-	-		
84	OHX	AR	3473	85	0,6,6	-	-	-		
84	OHX	A	2040	-	0,6,6	-	-	-		
84	OHX	1	3429	-	0,6,6	-	-	-		
84	OHX	6	2033	85	0,6,6	-	-	-		
84	OHX	1	3494	-	0,6,6	-	-	-		
84	OHX	6	1935	-	0,6,6	-	-	-		
84	OHX	1	3709	-	0,6,6	-	-	-		
84	OHX	AR	3544	-	0,6,6	-	-	-		
84	OHX	6	1961	-	0,6,6	-	-	-		
84	OHX	AR	3727	-	0,6,6	-	-	-		
84	OHX	1	3479	-	0,6,6	-	-	-		
84	OHX	1	3587	85	0,6,6	-	-	-		
84	OHX	4	202	-	0,6,6	-	-	-		
84	OHX	6	1928	-	0,6,6	-	-	-		
84	OHX	1	3619	-	0,6,6	-	-	-		
84	OHX	AR	3464	-	0,6,6	-	-	-		
84	OHX	6	2051	-	0,6,6	-	-	-		
84	OHX	AP	502	85	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	1	3577	-	0,6,6	-	-	-		
84	OHX	A	2012	-	0,6,6	-	-	-		
84	OHX	6	1989	-	0,6,6	-	-	-		
84	OHX	1	3456	85	0,6,6	-	-	-		
84	OHX	1	3621	-	0,6,6	-	-	-		
84	OHX	6	2032	-	0,6,6	-	-	-		
84	OHX	AK	102	85	0,6,6	-	-	-		
84	OHX	1	3707	-	0,6,6	-	-	-		
84	OHX	AR	3539	-	0,6,6	-	-	-		
84	OHX	AR	3543	-	0,6,6	-	-	-		
84	OHX	6	2028	85	0,6,6	-	-	-		
84	OHX	6	2054	-	0,6,6	-	-	-		
84	OHX	6	1987	-	0,6,6	-	-	-		
84	OHX	6	1986	-	0,6,6	-	-	-		
84	OHX	6	1959	-	0,6,6	-	-	-		
84	OHX	AR	3657	-	0,6,6	-	-	-		
84	OHX	AR	3602	-	0,6,6	-	-	-		
84	OHX	1	3469	-	0,6,6	-	-	-		
84	OHX	1	3528	-	0,6,6	-	-	-		
84	OHX	AR	3578	-	0,6,6	-	-	-		
84	OHX	1	3704	-	0,6,6	-	-	-		
84	OHX	1	3428	85	0,6,6	-	-	-		
84	OHX	6	1948	85	0,6,6	-	-	-		
84	OHX	AR	3418	-	0,6,6	-	-	-		
84	OHX	AR	3633	-	0,6,6	-	-	-		
84	OHX	1	3485	-	0,6,6	-	-	-		
84	OHX	A	1956	-	0,6,6	-	-	-		
84	OHX	AR	3641	-	0,6,6	-	-	-		
84	OHX	AR	3597	-	0,6,6	-	-	-		
84	OHX	1	3634	-	0,6,6	-	-	-		
84	OHX	6	2037	-	0,6,6	-	-	-		
84	OHX	AR	3600	85	0,6,6	-	-	-		
84	OHX	A	2006	-	0,6,6	-	-	-		
84	OHX	1	3518	-	0,6,6	-	-	-		
84	OHX	6	2029	-	0,6,6	-	-	-		
84	OHX	AR	3522	-	0,6,6	-	-	-		
84	OHX	4	208	-	0,6,6	-	-	-		
84	OHX	AR	3558	-	0,6,6	-	-	-		
84	OHX	sR	401	-	0,6,6	-	-	-		
84	OHX	6	1942	-	0,6,6	-	-	-		
84	OHX	1	3513	85	0,6,6	-	-	-		
84	OHX	3	207	-	0,6,6	-	-	-		
84	OHX	6	2023	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	AT	214	-	0,6,6	-	-	-		
84	OHX	AR	3683	-	0,6,6	-	-	-		
84	OHX	1	3443	-	0,6,6	-	-	-		
84	OHX	1	3673	-	0,6,6	-	-	-		
84	OHX	1	3729	-	0,6,6	-	-	-		
84	OHX	6	1984	-	0,6,6	-	-	-		
84	OHX	1	3506	-	0,6,6	-	-	-		
84	OHX	1	3401	-	0,6,6	-	-	-		
84	OHX	1	3620	-	0,6,6	-	-	-		
84	OHX	1	3694	-	0,6,6	-	-	-		
84	OHX	3	202	-	0,6,6	-	-	-		
84	OHX	AR	3468	-	0,6,6	-	-	-		
84	OHX	1	3561	-	0,6,6	-	-	-		
84	OHX	AR	3490	-	0,6,6	-	-	-		
84	OHX	AR	3587	-	0,6,6	-	-	-		
84	OHX	c3	201	-	0,6,6	-	-	-		
84	OHX	A	2026	-	0,6,6	-	-	-		
84	OHX	A	2000	-	0,6,6	-	-	-		
84	OHX	1	3504	-	0,6,6	-	-	-		
84	OHX	AR	3448	-	0,6,6	-	-	-		
84	OHX	1	3439	85	0,6,6	-	-	-		
84	OHX	1	3472	-	0,6,6	-	-	-		
84	OHX	6	1926	-	0,6,6	-	-	-		
84	OHX	A	1949	-	0,6,6	-	-	-		
84	OHX	AR	3673	-	0,6,6	-	-	-		
84	OHX	A	2022	-	0,6,6	-	-	-		
84	OHX	AR	3538	-	0,6,6	-	-	-		
84	OHX	6	1993	-	0,6,6	-	-	-		
84	OHX	AR	3409	-	0,6,6	-	-	-		
84	OHX	1	3670	-	0,6,6	-	-	-		
84	OHX	6	2040	-	0,6,6	-	-	-		
84	OHX	AR	3590	-	0,6,6	-	-	-		
84	OHX	AK	103	-	0,6,6	-	-	-		
84	OHX	1	3669	-	0,6,6	-	-	-		
84	OHX	AR	3496	-	0,6,6	-	-	-		
84	OHX	1	3615	-	0,6,6	-	-	-		
84	OHX	4	210	-	0,6,6	-	-	-		
84	OHX	A	2011	85	0,6,6	-	-	-		
84	OHX	A	1937	-	0,6,6	-	-	-		
84	OHX	1	3527	-	0,6,6	-	-	-		
84	OHX	1	3530	-	0,6,6	-	-	-		
84	OHX	1	3464	-	0,6,6	-	-	-		
84	OHX	1	3588	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	1	3598	-	0,6,6	-	-	-		
84	OHX	1	3661	-	0,6,6	-	-	-		
84	OHX	1	3672	-	0,6,6	-	-	-		
84	OHX	6	2026	-	0,6,6	-	-	-		
84	OHX	AR	3488	-	0,6,6	-	-	-		
84	OHX	1	3482	-	0,6,6	-	-	-		
84	OHX	1	3564	-	0,6,6	-	-	-		
84	OHX	1	3652	85	0,6,6	-	-	-		
84	OHX	6	1925	-	0,6,6	-	-	-		
84	OHX	6	1972	-	0,6,6	-	-	-		
84	OHX	AR	3697	-	0,6,6	-	-	-		
84	OHX	A	1921	85	0,6,6	-	-	-		
84	OHX	1	3512	-	0,6,6	-	-	-		
84	OHX	AR	3401	-	0,6,6	-	-	-		
84	OHX	AT	212	-	0,6,6	-	-	-		
84	OHX	4	211	-	0,6,6	-	-	-		
84	OHX	3	204	-	0,6,6	-	-	-		
84	OHX	1	3448	-	0,6,6	-	-	-		
84	OHX	1	3582	-	0,6,6	-	-	-		
84	OHX	6	1953	-	0,6,6	-	-	-		
84	OHX	1	3463	85	0,6,6	-	-	-		
84	OHX	1	3531	-	0,6,6	-	-	-		
84	OHX	1	3607	85	0,6,6	-	-	-		
84	OHX	1	3475	-	0,6,6	-	-	-		
84	OHX	1	3708	-	0,6,6	-	-	-		
84	OHX	6	1904	-	0,6,6	-	-	-		
84	OHX	AR	3404	-	0,6,6	-	-	-		
84	OHX	1	3500	-	0,6,6	-	-	-		
84	OHX	AR	3452	-	0,6,6	-	-	-		
84	OHX	1	3411	-	0,6,6	-	-	-		
84	OHX	1	3460	-	0,6,6	-	-	-		
84	OHX	A	2010	-	0,6,6	-	-	-		
84	OHX	A	1985	-	0,6,6	-	-	-		
84	OHX	6	2011	-	0,6,6	-	-	-		
84	OHX	AR	3413	-	0,6,6	-	-	-		
84	OHX	AR	3563	-	0,6,6	-	-	-		
84	OHX	1	3493	-	0,6,6	-	-	-		
84	OHX	x	201	85	0,6,6	-	-	-		
84	OHX	1	3466	-	0,6,6	-	-	-		
84	OHX	1	3627	-	0,6,6	-	-	-		
84	OHX	AR	3608	-	0,6,6	-	-	-		
84	OHX	AR	3637	-	0,6,6	-	-	-		
84	OHX	1	3536	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	1	3474	-	0,6,6	-	-	-		
84	OHX	1	3434	-	0,6,6	-	-	-		
84	OHX	AR	3554	-	0,6,6	-	-	-		
84	OHX	1	3558	-	0,6,6	-	-	-		
84	OHX	6	1930	-	0,6,6	-	-	-		
84	OHX	A	1972	-	0,6,6	-	-	-		
84	OHX	AR	3461	-	0,6,6	-	-	-		
84	OHX	AR	3556	-	0,6,6	-	-	-		
84	OHX	1	3724	-	0,6,6	-	-	-		
84	OHX	1	3418	-	0,6,6	-	-	-		
84	OHX	1	3711	-	0,6,6	-	-	-		
84	OHX	4	204	85	0,6,6	-	-	-		
84	OHX	AS	207	-	0,6,6	-	-	-		
84	OHX	1	3450	-	0,6,6	-	-	-		
84	OHX	6	2008	-	0,6,6	-	-	-		
84	OHX	AR	3439	-	0,6,6	-	-	-		
84	OHX	z	201	-	0,6,6	-	-	-		
84	OHX	1	3698	-	0,6,6	-	-	-		
84	OHX	6	1917	-	0,6,6	-	-	-		
84	OHX	6	1981	-	0,6,6	-	-	-		
84	OHX	AR	3472	-	0,6,6	-	-	-		
84	OHX	A	2028	-	0,6,6	-	-	-		
84	OHX	AR	3529	85	0,6,6	-	-	-		
84	OHX	AR	3526	-	0,6,6	-	-	-		
84	OHX	AT	218	-	0,6,6	-	-	-		
84	OHX	1	3423	-	0,6,6	-	-	-		
84	OHX	1	3575	-	0,6,6	-	-	-		
84	OHX	AR	3430	85	0,6,6	-	-	-		
84	OHX	1	3451	85	0,6,6	-	-	-		
84	OHX	AR	3441	85	0,6,6	-	-	-		
84	OHX	AR	3502	-	0,6,6	-	-	-		
84	OHX	A	2025	-	0,6,6	-	-	-		
84	OHX	AR	3481	-	0,6,6	-	-	-		
84	OHX	AE	201	-	0,6,6	-	-	-		
84	OHX	AR	3721	85	0,6,6	-	-	-		
84	OHX	1	3637	-	0,6,6	-	-	-		
84	OHX	e	101	-	0,6,6	-	-	-		
84	OHX	1	3683	-	0,6,6	-	-	-		
84	OHX	1	3562	-	0,6,6	-	-	-		
84	OHX	6	2043	-	0,6,6	-	-	-		
84	OHX	1	3425	-	0,6,6	-	-	-		
84	OHX	A	1932	-	0,6,6	-	-	-		
84	OHX	1	3404	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	AR	3604	-	0,6,6	-	-	-		
84	OHX	1	3572	-	0,6,6	-	-	-		
84	OHX	AR	3421	-	0,6,6	-	-	-		
84	OHX	AR	3607	-	0,6,6	-	-	-		
84	OHX	1	3507	-	0,6,6	-	-	-		
84	OHX	6	1978	85	0,6,6	-	-	-		
84	OHX	6	1946	85	0,6,6	-	-	-		
84	OHX	AR	3596	-	0,6,6	-	-	-		
84	OHX	AR	3701	-	0,6,6	-	-	-		
84	OHX	1	3702	-	0,6,6	-	-	-		
84	OHX	1	3645	-	0,6,6	-	-	-		
84	OHX	1	3581	85	0,6,6	-	-	-		
84	OHX	1	3728	85	0,6,6	-	-	-		
84	OHX	6	1964	-	0,6,6	-	-	-		
84	OHX	6	1997	-	0,6,6	-	-	-		
84	OHX	AR	3594	-	0,6,6	-	-	-		
84	OHX	A	1940	-	0,6,6	-	-	-		
84	OHX	6	2042	-	0,6,6	-	-	-		
84	OHX	AR	3420	-	0,6,6	-	-	-		
84	OHX	6	2048	-	0,6,6	-	-	-		
84	OHX	AR	3605	-	0,6,6	-	-	-		
84	OHX	A	2035	-	0,6,6	-	-	-		
84	OHX	1	3458	-	0,6,6	-	-	-		
84	OHX	AR	3444	-	0,6,6	-	-	-		
84	OHX	A	1998	-	0,6,6	-	-	-		
84	OHX	1	3505	-	0,6,6	-	-	-		
84	OHX	1	3441	-	0,6,6	-	-	-		
84	OHX	6	1947	-	0,6,6	-	-	-		
84	OHX	AR	3525	-	0,6,6	-	-	-		
84	OHX	AR	3564	-	0,6,6	-	-	-		
84	OHX	A	1984	-	0,6,6	-	-	-		
84	OHX	AR	3536	-	0,6,6	-	-	-		
84	OHX	1	3516	-	0,6,6	-	-	-		
84	OHX	1	3435	-	0,6,6	-	-	-		
84	OHX	1	3686	-	0,6,6	-	-	-		
84	OHX	6	2004	-	0,6,6	-	-	-		
84	OHX	AR	3506	85	0,6,6	-	-	-		
84	OHX	A	2007	-	0,6,6	-	-	-		
84	OHX	3	206	-	0,6,6	-	-	-		
84	OHX	A	1926	-	0,6,6	-	-	-		
84	OHX	6	2015	-	0,6,6	-	-	-		
84	OHX	AR	3406	-	0,6,6	-	-	-		
84	OHX	AR	3483	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	OHX	AR	3510	-	0,6,6	-	-	-		
84	OHX	AR	3533	-	0,6,6	-	-	-		
84	OHX	1	3631	-	0,6,6	-	-	-		
84	OHX	A	2017	-	0,6,6	-	-	-		
84	OHX	A	2014	-	0,6,6	-	-	-		
84	OHX	6	2045	-	0,6,6	-	-	-		
84	OHX	1	3596	-	0,6,6	-	-	-		
84	OHX	AR	3457	-	0,6,6	-	-	-		
84	OHX	AR	3520	-	0,6,6	-	-	-		
84	OHX	AR	3478	85	0,6,6	-	-	-		
84	OHX	A	2039	-	0,6,6	-	-	-		
84	OHX	1	3681	-	0,6,6	-	-	-		
84	OHX	1	3635	85	0,6,6	-	-	-		
84	OHX	1	3610	-	0,6,6	-	-	-		
84	OHX	1	3544	85	0,6,6	-	-	-		
84	OHX	6	1996	-	0,6,6	-	-	-		
84	OHX	A	1995	-	0,6,6	-	-	-		
84	OHX	1	3691	-	0,6,6	-	-	-		
84	OHX	1	3535	-	0,6,6	-	-	-		
84	OHX	1	3488	-	0,6,6	-	-	-		
84	OHX	1	3595	-	0,6,6	-	-	-		
84	OHX	1	3484	85	0,6,6	-	-	-		
84	OHX	AR	3653	-	0,6,6	-	-	-		
84	OHX	1	3688	-	0,6,6	-	-	-		
84	OHX	A	2038	-	0,6,6	-	-	-		
84	OHX	6	2020	-	0,6,6	-	-	-		
84	OHX	1	3554	-	0,6,6	-	-	-		
84	OHX	1	3660	-	0,6,6	-	-	-		
84	OHX	A	1960	-	0,6,6	-	-	-		
84	OHX	AR	3459	-	0,6,6	-	-	-		
84	OHX	AR	3495	-	0,6,6	-	-	-		
84	OHX	CK	201	-	0,6,6	-	-	-		
84	OHX	1	3605	-	0,6,6	-	-	-		
84	OHX	AR	3535	-	0,6,6	-	-	-		
84	OHX	A	1912	-	0,6,6	-	-	-		
84	OHX	1	3591	-	0,6,6	-	-	-		
84	OHX	AR	3515	-	0,6,6	-	-	-		
84	OHX	A	1974	-	0,6,6	-	-	-		
84	OHX	A	1916	-	0,6,6	-	-	-		
84	OHX	1	3407	-	0,6,6	-	-	-		
84	OHX	A	1922	-	0,6,6	-	-	-		
84	OHX	1	3486	-	0,6,6	-	-	-		
84	OHX	1	3487	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	1	3614	-	0,6,6	-	-	-		
84	OHX	k	402	-	0,6,6	-	-	-		
84	OHX	AR	3713	-	0,6,6	-	-	-		
84	OHX	6	1902	-	0,6,6	-	-	-		
84	OHX	1	3656	-	0,6,6	-	-	-		
84	OHX	1	3657	85	0,6,6	-	-	-		
84	OHX	T	201	-	0,6,6	-	-	-		
84	OHX	AR	3415	-	0,6,6	-	-	-		
84	OHX	1	3651	-	0,6,6	-	-	-		
84	OHX	1	3668	-	0,6,6	-	-	-		
84	OHX	1	3648	85	0,6,6	-	-	-		
84	OHX	AR	3592	85	0,6,6	-	-	-		
84	OHX	6	1939	-	0,6,6	-	-	-		
84	OHX	A	1986	-	0,6,6	-	-	-		
84	OHX	1	3560	-	0,6,6	-	-	-		
84	OHX	Q	201	-	0,6,6	-	-	-		
84	OHX	AR	3568	85	0,6,6	-	-	-		
84	OHX	A	1997	-	0,6,6	-	-	-		
84	OHX	AR	3565	-	0,6,6	-	-	-		
84	OHX	1	3461	85	0,6,6	-	-	-		
84	OHX	1	3633	-	0,6,6	-	-	-		
84	OHX	AT	202	-	0,6,6	-	-	-		
84	OHX	1	3663	-	0,6,6	-	-	-		
84	OHX	1	3632	-	0,6,6	-	-	-		
84	OHX	AT	208	-	0,6,6	-	-	-		
84	OHX	J	301	-	0,6,6	-	-	-		
84	OHX	A	1994	-	0,6,6	-	-	-		
84	OHX	6	1915	-	0,6,6	-	-	-		
84	OHX	6	1901	-	0,6,6	-	-	-		
84	OHX	A	2030	-	0,6,6	-	-	-		
84	OHX	AR	3417	85	0,6,6	-	-	-		
84	OHX	AR	3414	85	0,6,6	-	-	-		
84	OHX	CO	201	-	0,6,6	-	-	-		
84	OHX	AR	3436	-	0,6,6	-	-	-		
84	OHX	1	3492	85	0,6,6	-	-	-		
84	OHX	1	3442	85	0,6,6	-	-	-		
84	OHX	AR	3579	-	0,6,6	-	-	-		
84	OHX	6	1919	-	0,6,6	-	-	-		
84	OHX	AR	3512	-	0,6,6	-	-	-		
84	OHX	A	1980	-	0,6,6	-	-	-		
84	OHX	1	3638	-	0,6,6	-	-	-		
84	OHX	A	1979	-	0,6,6	-	-	-		
84	OHX	AR	3667	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	AT	204	-	0,6,6	-	-	-		
84	OHX	AR	3534	-	0,6,6	-	-	-		
84	OHX	A	1962	-	0,6,6	-	-	-		
84	OHX	6	1936	-	0,6,6	-	-	-		
84	OHX	AR	3524	-	0,6,6	-	-	-		
84	OHX	AR	3531	85	0,6,6	-	-	-		
84	OHX	1	3643	-	0,6,6	-	-	-		
84	OHX	AR	3432	-	0,6,6	-	-	-		
84	OHX	AR	3424	-	0,6,6	-	-	-		
84	OHX	1	3490	-	0,6,6	-	-	-		
84	OHX	1	3659	-	0,6,6	-	-	-		
84	OHX	6	2038	-	0,6,6	-	-	-		
84	OHX	4	203	-	0,6,6	-	-	-		
84	OHX	AR	3410	85	0,6,6	-	-	-		
84	OHX	1	3548	-	0,6,6	-	-	-		
84	OHX	AR	3549	-	0,6,6	-	-	-		
84	OHX	AR	3671	85	0,6,6	-	-	-		
84	OHX	AR	3581	-	0,6,6	-	-	-		
84	OHX	1	3520	85	0,6,6	-	-	-		
84	OHX	1	3629	-	0,6,6	-	-	-		
84	OHX	1	3664	-	0,6,6	-	-	-		
84	OHX	A	2042	-	0,6,6	-	-	-		
84	OHX	1	3408	-	0,6,6	-	-	-		
84	OHX	6	1943	-	0,6,6	-	-	-		
84	OHX	6	2009	-	0,6,6	-	-	-		
84	OHX	AR	3426	-	0,6,6	-	-	-		
84	OHX	1	3718	-	0,6,6	-	-	-		
84	OHX	AR	3567	-	0,6,6	-	-	-		
84	OHX	AR	3614	85	0,6,6	-	-	-		
84	OHX	1	3680	-	0,6,6	-	-	-		
84	OHX	A	1907	-	0,6,6	-	-	-		
84	OHX	AR	3427	-	0,6,6	-	-	-		
84	OHX	3	203	85	0,6,6	-	-	-		
84	OHX	1	3424	85	0,6,6	-	-	-		
84	OHX	AR	3403	-	0,6,6	-	-	-		
84	OHX	A	1910	-	0,6,6	-	-	-		
84	OHX	6	2010	-	0,6,6	-	-	-		
84	OHX	1	3438	-	0,6,6	-	-	-		
84	OHX	1	3666	-	0,6,6	-	-	-		
84	OHX	1	3692	-	0,6,6	-	-	-		
84	OHX	1	3549	-	0,6,6	-	-	-		
84	OHX	A	2008	-	0,6,6	-	-	-		
84	OHX	AR	3570	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	A	1990	-	0,6,6	-	-	-		
84	OHX	1	3497	-	0,6,6	-	-	-		
84	OHX	6	1906	-	0,6,6	-	-	-		
84	OHX	DH	201	-	0,6,6	-	-	-		
84	OHX	1	3515	-	0,6,6	-	-	-		
84	OHX	4	212	-	0,6,6	-	-	-		
84	OHX	1	3640	-	0,6,6	-	-	-		
84	OHX	c8	201	-	0,6,6	-	-	-		
84	OHX	1	3519	-	0,6,6	-	-	-		
84	OHX	6	2001	-	0,6,6	-	-	-		
84	OHX	6	2018	-	0,6,6	-	-	-		
84	OHX	4	206	-	0,6,6	-	-	-		
84	OHX	6	1912	-	0,6,6	-	-	-		
84	OHX	6	2031	-	0,6,6	-	-	-		
84	OHX	6	2022	-	0,6,6	-	-	-		
84	OHX	3	208	-	0,6,6	-	-	-		
84	OHX	1	3452	-	0,6,6	-	-	-		
84	OHX	1	3567	-	0,6,6	-	-	-		
84	OHX	AR	3494	85	0,6,6	-	-	-		
84	OHX	1	3444	-	0,6,6	-	-	-		
84	OHX	6	2046	-	0,6,6	-	-	-		
84	OHX	6	2057	-	0,6,6	-	-	-		
84	OHX	1	3405	-	0,6,6	-	-	-		
84	OHX	AR	3446	-	0,6,6	-	-	-		
84	OHX	1	3586	-	0,6,6	-	-	-		
84	OHX	1	3642	-	0,6,6	-	-	-		
84	OHX	AR	3621	-	0,6,6	-	-	-		
84	OHX	6	1913	-	0,6,6	-	-	-		
84	OHX	A	1982	-	0,6,6	-	-	-		
84	OHX	6	2053	-	0,6,6	-	-	-		
84	OHX	AR	3619	-	0,6,6	-	-	-		
84	OHX	1	3578	-	0,6,6	-	-	-		
84	OHX	1	3532	-	0,6,6	-	-	-		
84	OHX	1	3622	-	0,6,6	-	-	-		
84	OHX	1	3674	-	0,6,6	-	-	-		
84	OHX	1	3406	-	0,6,6	-	-	-		
84	OHX	AR	3419	85	0,6,6	-	-	-		
84	OHX	AR	3454	-	0,6,6	-	-	-		
84	OHX	AR	3589	-	0,6,6	-	-	-		
84	OHX	A	1902	-	0,6,6	-	-	-		
84	OHX	AR	3500	-	0,6,6	-	-	-		
84	OHX	AR	3412	-	0,6,6	-	-	-		
84	OHX	1	3559	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	6	1990	-	0,6,6	-	-	-		
84	OHX	AR	3546	-	0,6,6	-	-	-		
84	OHX	AR	3577	-	0,6,6	-	-	-		
84	OHX	1	3477	-	0,6,6	-	-	-		
84	OHX	6	1958	-	0,6,6	-	-	-		
84	OHX	6	2019	-	0,6,6	-	-	-		
84	OHX	1	3436	-	0,6,6	-	-	-		
84	OHX	6	2024	-	0,6,6	-	-	-		
84	OHX	6	1924	85	0,6,6	-	-	-		
84	OHX	6	1994	-	0,6,6	-	-	-		
84	OHX	AR	3456	-	0,6,6	-	-	-		
84	OHX	A	1999	-	0,6,6	-	-	-		
84	OHX	6	1985	-	0,6,6	-	-	-		
84	OHX	AR	3707	-	0,6,6	-	-	-		
84	OHX	1	3565	-	0,6,6	-	-	-		
84	OHX	A	1951	-	0,6,6	-	-	-		
84	OHX	AR	3603	-	0,6,6	-	-	-		
84	OHX	1	3495	85	0,6,6	-	-	-		
84	OHX	AR	3447	-	0,6,6	-	-	-		
84	OHX	AR	3480	85	0,6,6	-	-	-		
84	OHX	1	3524	-	0,6,6	-	-	-		
84	OHX	6	2000	-	0,6,6	-	-	-		
84	OHX	1	3618	-	0,6,6	-	-	-		
84	OHX	A	2027	-	0,6,6	-	-	-		
84	OHX	1	3525	-	0,6,6	-	-	-		
84	OHX	1	3722	85	0,6,6	-	-	-		
84	OHX	1	3462	-	0,6,6	-	-	-		
84	OHX	1	3609	-	0,6,6	-	-	-		
84	OHX	6	1931	-	0,6,6	-	-	-		
84	OHX	1	3584	-	0,6,6	-	-	-		
84	OHX	AR	3617	-	0,6,6	-	-	-		
84	OHX	6	1982	-	0,6,6	-	-	-		
84	OHX	AR	3573	-	0,6,6	-	-	-		
84	OHX	A	1992	-	0,6,6	-	-	-		
84	OHX	1	3501	-	0,6,6	-	-	-		
84	OHX	1	3594	-	0,6,6	-	-	-		
84	OHX	AR	3595	-	0,6,6	-	-	-		
84	OHX	6	1916	-	0,6,6	-	-	-		
84	OHX	A	2034	-	0,6,6	-	-	-		
84	OHX	1	3604	-	0,6,6	-	-	-		
84	OHX	1	3457	-	0,6,6	-	-	-		
84	OHX	AR	3428	-	0,6,6	-	-	-		
84	OHX	AR	3586	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	A	2041	-	0,6,6	-	-	-		
84	OHX	1	3437	-	0,6,6	-	-	-		
84	OHX	AR	3469	-	0,6,6	-	-	-		
84	OHX	AS	203	-	0,6,6	-	-	-		
84	OHX	AR	3559	-	0,6,6	-	-	-		
84	OHX	A	2019	-	0,6,6	-	-	-		
84	OHX	1	3521	-	0,6,6	-	-	-		
84	OHX	1	3417	-	0,6,6	-	-	-		
84	OHX	6	2002	-	0,6,6	-	-	-		
84	OHX	AR	3422	-	0,6,6	-	-	-		
84	OHX	AR	3405	-	0,6,6	-	-	-		
84	OHX	1	3509	-	0,6,6	-	-	-		
84	OHX	AR	3491	85	0,6,6	-	-	-		
84	OHX	1	3508	-	0,6,6	-	-	-		
84	OHX	1	3700	85	0,6,6	-	-	-		
84	OHX	1	3416	-	0,6,6	-	-	-		
84	OHX	AR	3458	85	0,6,6	-	-	-		
84	OHX	1	3410	-	0,6,6	-	-	-		
84	OHX	1	3547	-	0,6,6	-	-	-		
84	OHX	1	3550	-	0,6,6	-	-	-		
84	OHX	AR	3677	85	0,6,6	-	-	-		
84	OHX	1	3523	-	0,6,6	-	-	-		
84	OHX	AR	3408	-	0,6,6	-	-	-		
84	OHX	AR	3460	85	0,6,6	-	-	-		
84	OHX	1	3653	-	0,6,6	-	-	-		
84	OHX	AR	3517	-	0,6,6	-	-	-		
84	OHX	A	2036	-	0,6,6	-	-	-		
84	OHX	6	1950	-	0,6,6	-	-	-		
84	OHX	AR	3505	-	0,6,6	-	-	-		
84	OHX	1	3671	-	0,6,6	-	-	-		
84	OHX	6	1905	-	0,6,6	-	-	-		
84	OHX	AR	3593	-	0,6,6	-	-	-		
84	OHX	A	1987	-	0,6,6	-	-	-		
84	OHX	1	3453	85	0,6,6	-	-	-		
84	OHX	6	1974	-	0,6,6	-	-	-		
84	OHX	A	1959	-	0,6,6	-	-	-		
84	OHX	1	3710	-	0,6,6	-	-	-		
84	OHX	AR	3438	-	0,6,6	-	-	-		
84	OHX	1	3716	-	0,6,6	-	-	-		
84	OHX	1	3426	85	0,6,6	-	-	-		
84	OHX	6	2041	-	0,6,6	-	-	-		
84	OHX	AR	3527	85	0,6,6	-	-	-		
84	OHX	1	3445	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	AR	3530	-	0,6,6	-	-	-		
84	OHX	1	3422	-	0,6,6	-	-	-		
84	OHX	AR	3440	-	0,6,6	-	-	-		
84	OHX	1	3432	-	0,6,6	-	-	-		
84	OHX	AR	3582	-	0,6,6	-	-	-		
84	OHX	1	3459	-	0,6,6	-	-	-		
84	OHX	6	1923	-	0,6,6	-	-	-		
84	OHX	1	3727	-	0,6,6	-	-	-		
84	OHX	A	1917	-	0,6,6	-	-	-		
84	OHX	AR	3475	-	0,6,6	-	-	-		
84	OHX	1	3677	85	0,6,6	-	-	-		
84	OHX	6	1941	-	0,6,6	-	-	-		
84	OHX	6	2007	-	0,6,6	-	-	-		
84	OHX	AR	3622	85	0,6,6	-	-	-		
84	OHX	A	2015	-	0,6,6	-	-	-		
84	OHX	6	1966	-	0,6,6	-	-	-		
84	OHX	6	2049	-	0,6,6	-	-	-		
84	OHX	AR	3574	-	0,6,6	-	-	-		
84	OHX	r	301	-	0,6,6	-	-	-		
84	OHX	6	1937	-	0,6,6	-	-	-		
84	OHX	A	2037	-	0,6,6	-	-	-		
84	OHX	1	3465	-	0,6,6	-	-	-		
84	OHX	v	301	-	0,6,6	-	-	-		
84	OHX	AR	3540	-	0,6,6	-	-	-		
84	OHX	6	1999	-	0,6,6	-	-	-		
84	OHX	AR	3580	-	0,6,6	-	-	-		
84	OHX	A	2031	-	0,6,6	-	-	-		
84	OHX	AR	3503	-	0,6,6	-	-	-		
84	OHX	1	3455	-	0,6,6	-	-	-		
84	OHX	6	1956	-	0,6,6	-	-	-		
84	OHX	1	3569	-	0,6,6	-	-	-		
84	OHX	6	1914	-	0,6,6	-	-	-		
84	OHX	AR	3611	-	0,6,6	-	-	-		
84	OHX	1	3592	85	0,6,6	-	-	-		
84	OHX	1	3717	-	0,6,6	-	-	-		
84	OHX	6	1903	-	0,6,6	-	-	-		
84	OHX	6	2006	-	0,6,6	-	-	-		
84	OHX	1	3498	-	0,6,6	-	-	-		
84	OHX	6	1963	-	0,6,6	-	-	-		
84	OHX	AR	3591	85	0,6,6	-	-	-		
84	OHX	1	3684	85	0,6,6	-	-	-		
84	OHX	6	1975	-	0,6,6	-	-	-		
84	OHX	AR	3569	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	1	3478	-	0,6,6	-	-	-		
84	OHX	AR	3453	-	0,6,6	-	-	-		
84	OHX	6	1940	-	0,6,6	-	-	-		
84	OHX	1	3574	-	0,6,6	-	-	-		
84	OHX	AR	3627	-	0,6,6	-	-	-		
84	OHX	AR	3434	-	0,6,6	-	-	-		
84	OHX	1	3696	-	0,6,6	-	-	-		
84	OHX	A	1966	-	0,6,6	-	-	-		
84	OHX	A	2024	-	0,6,6	-	-	-		
84	OHX	1	3580	-	0,6,6	-	-	-		
84	OHX	AR	3509	85	0,6,6	-	-	-		
84	OHX	1	3414	-	0,6,6	-	-	-		
84	OHX	AR	3553	-	0,6,6	-	-	-		
84	OHX	AR	3598	-	0,6,6	-	-	-		
84	OHX	A	1911	-	0,6,6	-	-	-		
84	OHX	4	209	-	0,6,6	-	-	-		
84	OHX	AR	3479	-	0,6,6	-	-	-		
84	OHX	1	3678	-	0,6,6	-	-	-		
84	OHX	AR	3542	-	0,6,6	-	-	-		
84	OHX	AR	3691	85	0,6,6	-	-	-		
84	OHX	6	1938	-	0,6,6	-	-	-		
84	OHX	1	3611	-	0,6,6	-	-	-		
84	OHX	AR	3711	-	0,6,6	-	-	-		
84	OHX	1	3539	-	0,6,6	-	-	-		
84	OHX	1	3522	-	0,6,6	-	-	-		
84	OHX	AR	3431	-	0,6,6	-	-	-		
84	OHX	A	2005	-	0,6,6	-	-	-		
84	OHX	6	1955	-	0,6,6	-	-	-		
84	OHX	6	1965	-	0,6,6	-	-	-		
84	OHX	AR	3647	85	0,6,6	-	-	-		
84	OHX	1	3602	-	0,6,6	-	-	-		
84	OHX	1	3636	-	0,6,6	-	-	-		
84	OHX	AR	3601	-	0,6,6	-	-	-		
84	OHX	AR	3501	85	0,6,6	-	-	-		
84	OHX	AR	3508	-	0,6,6	-	-	-		
84	OHX	AR	3416	85	0,6,6	-	-	-		
84	OHX	AR	3609	-	0,6,6	-	-	-		
84	OHX	AR	3623	-	0,6,6	-	-	-		
84	OHX	1	3679	-	0,6,6	-	-	-		
84	OHX	x	202	-	0,6,6	-	-	-		
84	OHX	6	1973	-	0,6,6	-	-	-		
84	OHX	1	3706	-	0,6,6	-	-	-		
84	OHX	CV	201	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	1	3446	-	0,6,6	-	-	-		
84	OHX	1	3496	-	0,6,6	-	-	-		
84	OHX	1	3585	-	0,6,6	-	-	-		
84	OHX	AR	3572	85	0,6,6	-	-	-		
84	OHX	AR	3489	-	0,6,6	-	-	-		
84	OHX	AR	3467	-	0,6,6	-	-	-		
84	OHX	6	1921	-	0,6,6	-	-	-		
84	OHX	1	3430	-	0,6,6	-	-	-		
84	OHX	6	1929	-	0,6,6	-	-	-		
84	OHX	y	201	-	0,6,6	-	-	-		
84	OHX	4	201	-	0,6,6	-	-	-		
84	OHX	6	2056	-	0,6,6	-	-	-		
84	OHX	1	3675	85	0,6,6	-	-	-		
84	OHX	d9	101	-	0,6,6	-	-	-		
84	OHX	1	3646	-	0,6,6	-	-	-		
84	OHX	AR	3435	-	0,6,6	-	-	-		
84	OHX	6	1988	-	0,6,6	-	-	-		
84	OHX	1	3440	-	0,6,6	-	-	-		
84	OHX	1	3639	-	0,6,6	-	-	-		
84	OHX	AR	3407	-	0,6,6	-	-	-		
84	OHX	AR	3566	-	0,6,6	-	-	-		
84	OHX	AR	3687	-	0,6,6	-	-	-		
84	OHX	k	401	-	0,6,6	-	-	-		
84	OHX	AR	3511	-	0,6,6	-	-	-		
84	OHX	AR	3516	-	0,6,6	-	-	-		
84	OHX	AR	3681	-	0,6,6	-	-	-		
84	OHX	1	3573	-	0,6,6	-	-	-		
84	OHX	1	3626	-	0,6,6	-	-	-		
84	OHX	1	3612	-	0,6,6	-	-	-		
84	OHX	1	3695	-	0,6,6	-	-	-		
84	OHX	1	3613	-	0,6,6	-	-	-		
84	OHX	M	201	-	0,6,6	-	-	-		
84	OHX	A	1930	-	0,6,6	-	-	-		
84	OHX	AR	3423	-	0,6,6	-	-	-		
84	OHX	AR	3507	-	0,6,6	-	-	-		
84	OHX	A	1996	-	0,6,6	-	-	-		
84	OHX	1	3454	85	0,6,6	-	-	-		
84	OHX	AR	3519	-	0,6,6	-	-	-		
84	OHX	6	1977	-	0,6,6	-	-	-		
84	OHX	6	2021	-	0,6,6	-	-	-		
84	OHX	AR	3551	-	0,6,6	-	-	-		
84	OHX	AR	3537	-	0,6,6	-	-	-		
84	OHX	1	3538	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	AR	3541	-	0,6,6	-	-	-		
84	OHX	1	3590	-	0,6,6	-	-	-		
84	OHX	AR	3552	85	0,6,6	-	-	-		
84	OHX	6	2017	-	0,6,6	-	-	-		
86	7MB	1	4216	-	20,23,23	1.54	3 (15%)	14,38,38	1.25	2 (14%)
84	OHX	AR	3610	-	0,6,6	-	-	-		
84	OHX	AR	3451	-	0,6,6	-	-	-		
84	OHX	6	2047	-	0,6,6	-	-	-		
84	OHX	1	3415	-	0,6,6	-	-	-		
84	OHX	1	3583	-	0,6,6	-	-	-		
84	OHX	1	3589	-	0,6,6	-	-	-		
84	OHX	AR	3465	85	0,6,6	-	-	-		
84	OHX	1	3419	-	0,6,6	-	-	-		
84	OHX	6	1933	85	0,6,6	-	-	-		
84	OHX	AR	3606	-	0,6,6	-	-	-		
84	OHX	A	2029	-	0,6,6	-	-	-		
84	OHX	AR	3499	-	0,6,6	-	-	-		
84	OHX	1	3449	-	0,6,6	-	-	-		
84	OHX	A	1976	-	0,6,6	-	-	-		
84	OHX	CF	402	-	0,6,6	-	-	-		
84	OHX	6	1962	-	0,6,6	-	-	-		
84	OHX	AR	3731	-	0,6,6	-	-	-		
84	OHX	1	3557	-	0,6,6	-	-	-		
84	OHX	AR	3661	-	0,6,6	-	-	-		
84	OHX	A	1936	85	0,6,6	-	-	-		
84	OHX	A	1991	-	0,6,6	-	-	-		
84	OHX	A	1961	-	0,6,6	-	-	-		
84	OHX	1	3529	-	0,6,6	-	-	-		
84	OHX	2	201	-	0,6,6	-	-	-		
84	OHX	AR	3498	-	0,6,6	-	-	-		
84	OHX	A	1989	-	0,6,6	-	-	-		
84	OHX	1	3593	-	0,6,6	-	-	-		
84	OHX	AR	3486	85	0,6,6	-	-	-		
84	OHX	1	3499	-	0,6,6	-	-	-		
84	OHX	1	401	-	0,6,6	-	-	-		
84	OHX	6	2025	-	0,6,6	-	-	-		
84	OHX	3	201	-	0,6,6	-	-	-		
84	OHX	1	3701	-	0,6,6	-	-	-		
84	OHX	AR	3523	-	0,6,6	-	-	-		
84	OHX	6	1949	-	0,6,6	-	-	-		
84	OHX	AR	3557	-	0,6,6	-	-	-		
84	OHX	1	3623	-	0,6,6	-	-	-		
84	OHX	AR	3651	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	6	1922	-	0,6,6	-	-	-		
84	OHX	6	2055	-	0,6,6	-	-	-		
84	OHX	AG	201	-	0,6,6	-	-	-		
84	OHX	1	3540	-	0,6,6	-	-	-		
84	OHX	1	3421	-	0,6,6	-	-	-		
84	OHX	1	3413	-	0,6,6	-	-	-		
84	OHX	1	3606	85	0,6,6	-	-	-		
84	OHX	6	2003	-	0,6,6	-	-	-		
84	OHX	6	2035	-	0,6,6	-	-	-		
84	OHX	AR	3663	-	0,6,6	-	-	-		
84	OHX	AR	3450	-	0,6,6	-	-	-		
84	OHX	6	1951	-	0,6,6	-	-	-		
84	OHX	1	3608	-	0,6,6	-	-	-		
84	OHX	AR	3474	-	0,6,6	-	-	-		
84	OHX	AR	3484	-	0,6,6	-	-	-		
84	OHX	1	3471	-	0,6,6	-	-	-		
84	OHX	1	3712	-	0,6,6	-	-	-		
84	OHX	1	3625	-	0,6,6	-	-	-		
84	OHX	AR	3733	-	0,6,6	-	-	-		
84	OHX	6	1971	-	0,6,6	-	-	-		
84	OHX	6	1991	-	0,6,6	-	-	-		
84	OHX	A	1952	-	0,6,6	-	-	-		
84	OHX	6	1967	-	0,6,6	-	-	-		
84	OHX	AR	3612	-	0,6,6	-	-	-		
84	OHX	AR	3492	-	0,6,6	-	-	-		
84	OHX	AR	3723	-	0,6,6	-	-	-		
84	OHX	6	1969	85	0,6,6	-	-	-		
84	OHX	A	1971	-	0,6,6	-	-	-		
84	OHX	1	3690	-	0,6,6	-	-	-		
84	OHX	1	3568	-	0,6,6	-	-	-		
84	OHX	AR	3583	-	0,6,6	-	-	-		
84	OHX	1	3526	85	0,6,6	-	-	-		
84	OHX	6	1980	-	0,6,6	-	-	-		
84	OHX	1	3533	-	0,6,6	-	-	-		
84	OHX	AR	3402	-	0,6,6	-	-	-		
84	OHX	AR	3487	-	0,6,6	-	-	-		
84	OHX	AR	3643	85	0,6,6	-	-	-		
84	OHX	AR	3576	-	0,6,6	-	-	-		
84	OHX	A	1967	-	0,6,6	-	-	-		
84	OHX	AR	3585	-	0,6,6	-	-	-		
84	OHX	1	3481	-	0,6,6	-	-	-		
84	OHX	1	3658	85	0,6,6	-	-	-		
84	OHX	1	3721	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	OHX	DG	201	-	0,6,6	-	-	-		
84	OHX	1	3542	-	0,6,6	-	-	-		
84	OHX	1	3556	-	0,6,6	-	-	-		
84	OHX	AR	3717	85	0,6,6	-	-	-		
84	OHX	AR	3470	-	0,6,6	-	-	-		
84	OHX	3	205	-	0,6,6	-	-	-		
84	OHX	1	3491	-	0,6,6	-	-	-		
84	OHX	A	1920	-	0,6,6	-	-	-		
84	OHX	1	3599	-	0,6,6	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	7MB	1	4216	-	-	-	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	1	4216	7MB	C8-C7	-4.51	1.37	1.47
86	1	4216	7MB	C9-C8	-3.06	1.35	1.43
86	1	4216	7MB	O-C1	-2.22	1.19	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
86	1	4216	7MB	C6-C2-N1	-2.82	108.36	113.23
86	1	4216	7MB	C2-N1-C1	-2.34	108.64	113.67

There are no chirality outliers.

There are no torsion outliers.

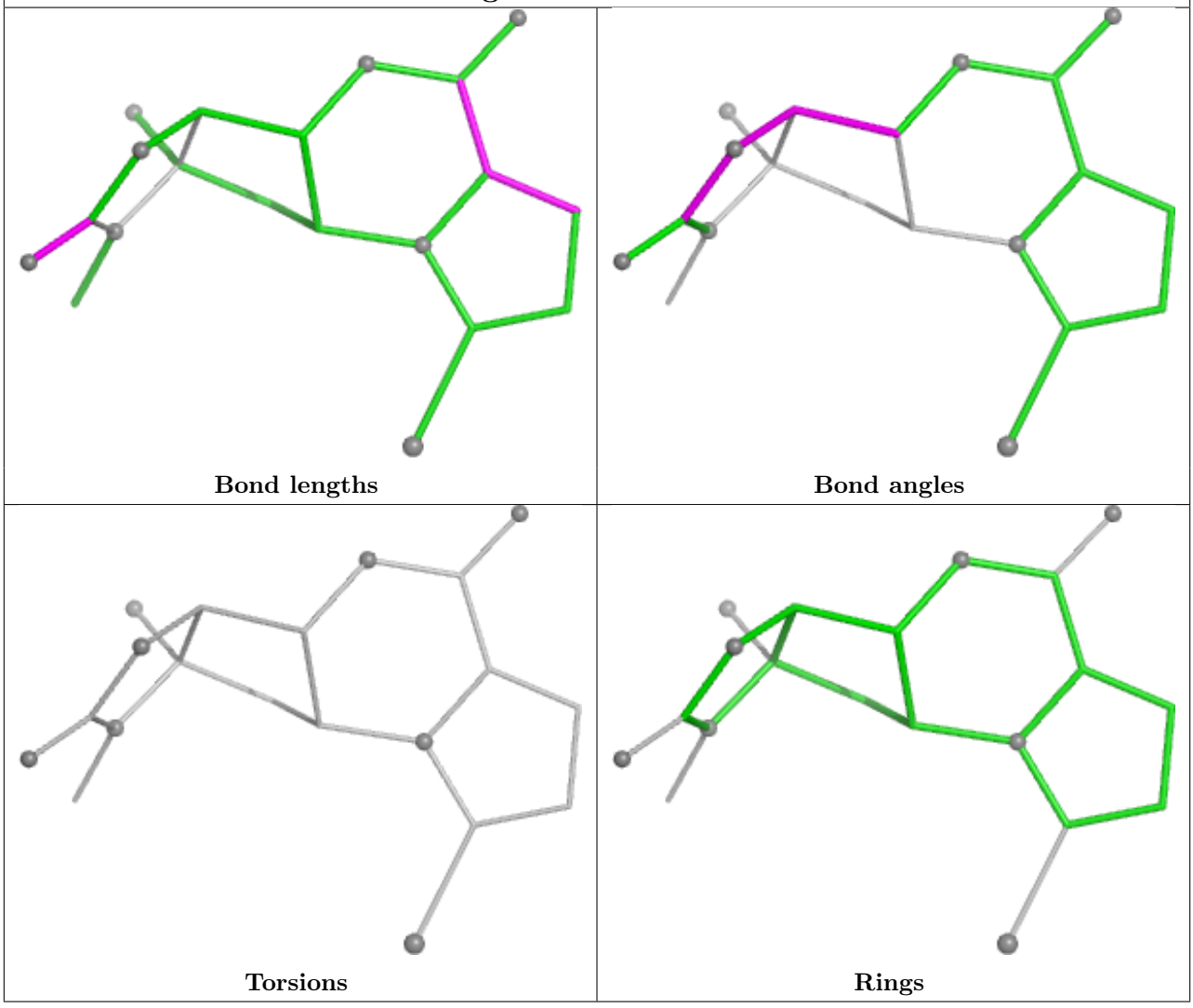
There are no ring outliers.

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 7MB 1 4216



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	sM	2
25	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	85:SER	C	119:UNK	N	44.36
1	sM	139:UNK	C	155:UNK	N	36.85
1	A	1716:C	O3'	1717:G	P	4.45

5 Fit of model and data

5.1 Protein, DNA and RNA chains

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

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

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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