wwPDB X-ray Structure Validation Summary Report (i)

Sep 15, 2026 – 11:41 pm BST

PDB ID	:	8P4V / pdb_00008p4v
Title	:	80S yeast ribosome in complex with HaterumaimideQ
Authors	:	Terrosu, S.; Yusupov, M.
Deposited on	:	2023-05-23
Resolution	:	3.16 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 (i)

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

The reported resolution of this entry is 3.16 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 89 unique types of molecules in this entry. The entry contains 409267 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	3147	Total	C	N	O	P	0	0	0
			67313	30067	12134	21965	3147			

- 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 Large ribosomal subunit protein uL5B.

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	6	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 protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	7	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			
25	CY	124	Total	C	N	O	S	0	0	0
			836	525	166	144	1			

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	8	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			

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

- Molecule 27 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	9	126	Total	C	N	O	0	0	0
			993	625	192	176			
27	DA	124	Total	C	N	O	0	0	0
			976	614	190	172			

- Molecule 28 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	AA	135	Total	C	N	O	0	0	0
			1092	710	202	180			
28	DB	135	Total	C	N	O	0	0	0
			1087	706	201	180			

- Molecule 29 is a protein called 60S ribosomal protein L28.

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

- Molecule 30 is a protein called 60S ribosomal protein L29.

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

- Molecule 31 is a protein called 60S ribosomal protein L30.

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

- Molecule 32 is a protein called 60S ribosomal protein L31-A.

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

- Molecule 33 is a protein called 60S ribosomal protein L32.

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

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 35 is a protein called 60S ribosomal protein L34-A.

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

- Molecule 36 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 37 is a protein called 60S ribosomal protein L36-A.

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

- Molecule 38 is a protein called 60S ribosomal protein L37-A.

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

- Molecule 39 is a protein called 60S ribosomal protein L38.

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

- Molecule 40 is a protein called 60S ribosomal protein L39.

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

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 42 is a protein called 60S ribosomal protein L41-A.

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

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

- Molecule 43 is a protein called 60S ribosomal protein L42-A.

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

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 45 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	i	159	Total	C	N	O	0	0	0
			1104	652	221	231			
45	sM	63	Total	C	N	O	0	0	0
			475	280	99	96			

- Molecule 46 is a protein called 60S acidic protein P0.

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

- Molecule 47 is a RNA chain called 18S ribosomal RNA.

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

- Molecule 48 is a protein called 40S ribosomal protein S0-A.

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

- Molecule 49 is a protein called 40S ribosomal protein S1-A.

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

- Molecule 50 is a protein called 40S ribosomal protein S2.

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

- Molecule 51 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 52 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 53 is a protein called 40S ribosomal protein S5.

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

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

- Molecule 54 is a protein called 40S ribosomal protein S6-A.

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

- Molecule 55 is a protein called 40S ribosomal protein S7-A.

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

- Molecule 56 is a protein called 40S ribosomal protein S8-A.

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

- Molecule 57 is a protein called 40S ribosomal protein S9-A.

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

- Molecule 58 is a protein called 40S ribosomal protein S10-A.

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

- Molecule 59 is a protein called 40S ribosomal protein S11-A.

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

- Molecule 60 is a protein called 40S ribosomal protein S12.

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

- Molecule 61 is a protein called 40S ribosomal protein S13.

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

- Molecule 62 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
62	P	127	Total	C	N	O	S	0	0	0
			886	541	182	162	1			
62	c4	128	Total	C	N	O	S	0	0	0
			949	582	188	176	3			

- Molecule 63 is a protein called 40S ribosomal protein S15.

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

- Molecule 64 is a protein called 40S ribosomal protein S16-A.

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

- Molecule 65 is a protein called 40S ribosomal protein S17-B.

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

- Molecule 66 is a protein called 40S ribosomal protein S18-A.

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

- Molecule 67 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 68 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 69 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 70 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 71 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 72 is a protein called 40S ribosomal protein S24-A.

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

- Molecule 73 is a protein called 40S ribosomal protein S25-A.

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

- Molecule 74 is a protein called Small ribosomal subunit protein eS26B.

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

- Molecule 75 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 76 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 77 is a protein called Small ribosomal subunit protein uS14A.

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

- Molecule 78 is a protein called 40S ribosomal protein S30-A.

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

- Molecule 79 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	g	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			
79	e1	51	Total	C	N	O	S	0	0	0
			397	249	73	71	4			

- Molecule 80 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	h	318	Total	C	N	O	S	0	0	0
			2437	1541	418	470	8			

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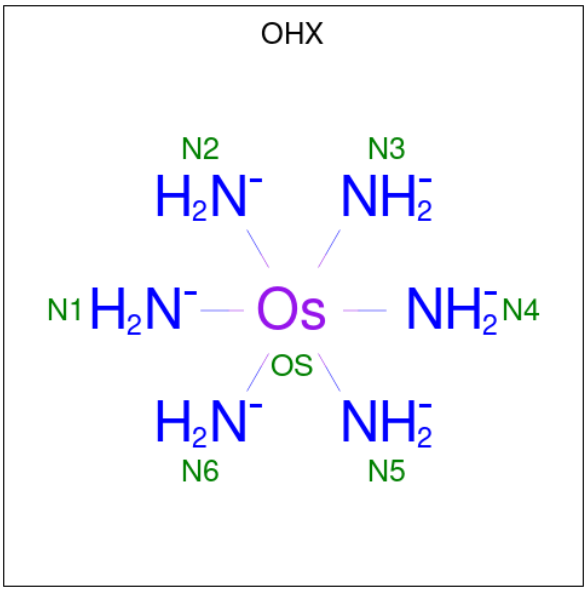
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	Rb	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 81 is a protein called 40S ribosomal protein S17-A.

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

- Molecule 82 is osmium (III) hexammine (CCD ID: OHX) (formula: $H_{12}N_6Os$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
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82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
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82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
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82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
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82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
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82	1	1	Total N Os 7 6 1	0	0
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82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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82	1	1	Total N Os 7 6 1	0	0
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82	1	1	Total N Os 7 6 1	0	0
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82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 14 12 2	0	1
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
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82	1	1	Total N Os 7 6 1	0	0
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82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
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82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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82	1	1	Total N Os 7 6 1	0	0
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82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	1	Total N Os 7 6 1	0	0
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82	1	1	Total N Os 7 6 1	0	0
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82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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82	1	1	Total N Os 7 6 1	0	0
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82	1	1	Total N Os 7 6 1	0	0
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82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 6 5 1	0	0
82	1	1	Total N Os 7 6 1	0	0
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82	1	1	Total N Os 7 6 1	0	0
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82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
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82	1	1	Total N Os 7 6 1	0	0
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82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 7 6 1	0	0
82	1	1	Total N Os 6 5 1	0	0
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82	3	1	Total N Os 7 6 1	0	0
82	3	1	Total N Os 7 6 1	0	0
82	3	1	Total N Os 7 6 1	0	0
82	3	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	3	1	Total N Os 7 6 1	0	0
82	3	1	Total N Os 7 6 1	0	0
82	3	1	Total N Os 7 6 1	0	0
82	3	1	Total N Os 7 6 1	0	0
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82	4	1	Total N Os 7 6 1	0	0
82	4	1	Total N Os 7 6 1	0	0
82	4	1	Total N Os 7 6 1	0	0
82	k	1	Total N Os 7 6 1	0	0
82	k	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	l	1	Total N Os 7 6 1	0	0
82	r	1	Total N Os 7 6 1	0	0
82	v	1	Total N Os 7 6 1	0	0
82	z	1	Total N Os 7 6 1	0	0
82	2	1	Total N Os 7 6 1	0	0
82	AC	1	Total N Os 7 6 1	0	0
82	AG	1	Total N Os 7 6 1	0	0
82	AK	1	Total N Os 7 6 1	0	0
82	AK	1	Total N Os 7 6 1	0	0
82	AP	1	Total N Os 7 6 1	0	0
82	AR	1	Total N Os 7 6 1	0	0
82	AR	1	Total N Os 7 6 1	0	0
82	AR	1	Total N Os 7 6 1	0	0
82	AR	1	Total N Os 7 6 1	0	0
82	AR	1	Total N Os 7 6 1	0	0
82	AR	1	Total N Os 7 6 1	0	0
82	AR	1	Total N Os 7 6 1	0	0
82	AR	1	Total N Os 7 6 1	0	0
82	AR	1	Total N Os 7 6 1	0	0
82	AR	1	Total N Os 7 6 1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	AT	1	Total N Os 7 6 1	0	0
82	CE	1	Total N Os 7 6 1	0	0
82	CE	1	Total N Os 7 6 1	0	0
82	CG	1	Total N Os 7 6 1	0	0
82	CG	1	Total N Os 7 6 1	0	0
82	CG	1	Total N Os 7 6 1	0	0
82	CH	1	Total N Os 7 6 1	0	0
82	CK	1	Total N Os 7 6 1	0	0
82	CL	1	Total N Os 7 6 1	0	0
82	CL	1	Total N Os 7 6 1	0	0
82	CP	1	Total N Os 7 6 1	0	0
82	CS	1	Total N Os 7 6 1	0	0
82	CV	1	Total N Os 7 6 1	0	0
82	CX	1	Total N Os 7 6 1	0	0
82	DD	1	Total N Os 7 6 1	0	0
82	DH	1	Total N Os 7 6 1	0	0
82	DL	1	Total N Os 7 6 1	0	0
82	DQ	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
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82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 14 12 2	0	1
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 14 12 2	0	1
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	A	1	Total N Os 7 6 1	0	0
82	J	1	Total N Os 7 6 1	0	0
82	O	1	Total N Os 7 6 1	0	0
82	Q	1	Total N Os 7 6 1	0	0
82	T	1	Total N Os 7 6 1	0	0
82	U	1	Total N Os 7 6 1	0	0
82	h	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	1
			14	12	2		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	sR	1	Total N Os 7 6 1	0	0
82	sR	1	Total N Os 7 6 1	0	0
82	sR	1	Total N Os 7 6 1	0	0
82	sR	1	Total N Os 7 6 1	0	0
82	sR	1	Total N Os 7 6 1	0	0
82	sR	1	Total N Os 7 6 1	0	0
82	sR	1	Total N Os 7 6 1	0	0
82	sR	1	Total N Os 7 6 1	0	0
82	sR	1	Total N Os 7 6 1	0	0
82	sR	1	Total N Os 7 6 1	0	0
82	sR	1	Total N Os 7 6 1	0	0
82	sR	1	Total N Os 7 6 1	0	0
82	sR	1	Total N Os 7 6 1	0	0
82	Rb	1	Total N Os 7 6 1	0	0
82	s1	1	Total N Os 7 6 1	0	0
82	s4	1	Total N Os 7 6 1	0	0
82	s8	1	Total N Os 7 6 1	0	0
82	c3	1	Total N Os 7 6 1	0	0
82	c5	1	Total N Os 7 6 1	0	0
82	c7	1	Total N Os 7 6 1	0	0
82	c8	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	d4	1	Total N Os 7 6 1	0	0

- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	1	486	Total Mg 486 486	0	0
83	3	12	Total Mg 12 12	0	0
83	4	18	Total Mg 18 18	0	0
83	j	2	Total Mg 2 2	0	0
83	k	2	Total Mg 2 2	0	0
83	l	4	Total Mg 4 4	0	0
83	m	1	Total Mg 1 1	0	0
83	o	3	Total Mg 3 3	0	0
83	r	2	Total Mg 2 2	0	0
83	s	1	Total Mg 1 1	0	0
83	t	2	Total Mg 2 2	0	0
83	u	1	Total Mg 1 1	0	0
83	v	4	Total Mg 4 4	0	0
83	w	1	Total Mg 1 1	0	0
83	x	8	Total Mg 8 8	0	0
83	y	1	Total Mg 1 1	0	0
83	z	1	Total Mg 1 1	0	0
83	6	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	9	1	Total Mg 1 1	0	0
83	AB	5	Total Mg 5 5	0	0
83	AC	1	Total Mg 1 1	0	0
83	AF	2	Total Mg 2 2	0	0
83	AG	1	Total Mg 1 1	0	0
83	AH	2	Total Mg 2 2	0	0
83	AI	1	Total Mg 1 1	0	0
83	AP	1	Total Mg 1 1	0	0
83	i	1	Total Mg 1 1	0	0
83	AR	498	Total Mg 498 498	0	0
83	AS	19	Total Mg 19 19	0	0
83	AT	19	Total Mg 19 19	0	0
83	CD	1	Total Mg 1 1	0	0
83	CE	3	Total Mg 3 3	0	0
83	CF	5	Total Mg 5 5	0	0
83	CG	1	Total Mg 1 1	0	0
83	CI	2	Total Mg 2 2	0	0
83	CJ	1	Total Mg 1 1	0	0
83	CK	1	Total Mg 1 1	0	0
83	CL	2	Total Mg 2 2	0	0
83	CM	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	CO	1	Total Mg 1 1	0	0
83	CP	5	Total Mg 5 5	0	0
83	CQ	3	Total Mg 3 3	0	0
83	CR	8	Total Mg 8 8	0	0
83	CU	1	Total Mg 1 1	0	0
83	CX	1	Total Mg 1 1	0	0
83	DA	2	Total Mg 2 2	0	0
83	DC	2	Total Mg 2 2	0	0
83	DD	1	Total Mg 1 1	0	0
83	DH	2	Total Mg 2 2	0	0
83	DI	3	Total Mg 3 3	0	0
83	DL	2	Total Mg 2 2	0	0
83	DO	2	Total Mg 2 2	0	0
83	DP	1	Total Mg 1 1	0	0
83	DQ	2	Total Mg 2 2	0	0
83	sM	2	Total Mg 2 2	0	0
83	A	135	Total Mg 135 135	0	0
83	D	2	Total Mg 2 2	0	0
83	F	1	Total Mg 1 1	0	0
83	O	1	Total Mg 1 1	0	0
83	P	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	S	1	Total Mg 1 1	0	0
83	X	1	Total Mg 1 1	0	0
83	Y	1	Total Mg 1 1	0	0
83	b	1	Total Mg 1 1	0	0
83	sR	149	Total Mg 149 149	0	0
83	s1	1	Total Mg 1 1	0	0
83	s2	1	Total Mg 1 1	0	0
83	s4	1	Total Mg 1 1	0	0
83	s6	1	Total Mg 1 1	0	0
83	s8	2	Total Mg 2 2	0	0
83	s9	1	Total Mg 1 1	0	0
83	c1	1	Total Mg 1 1	0	0
83	c3	1	Total Mg 1 1	0	0
83	c4	2	Total Mg 2 2	0	0
83	c6	1	Total Mg 1 1	0	0
83	c8	1	Total Mg 1 1	0	0
83	c9	2	Total Mg 2 2	0	0
83	d3	3	Total Mg 3 3	0	0
83	d4	3	Total Mg 3 3	0	0
83	d5	1	Total Mg 1 1	0	0
83	d6	2	Total Mg 2 2	0	0

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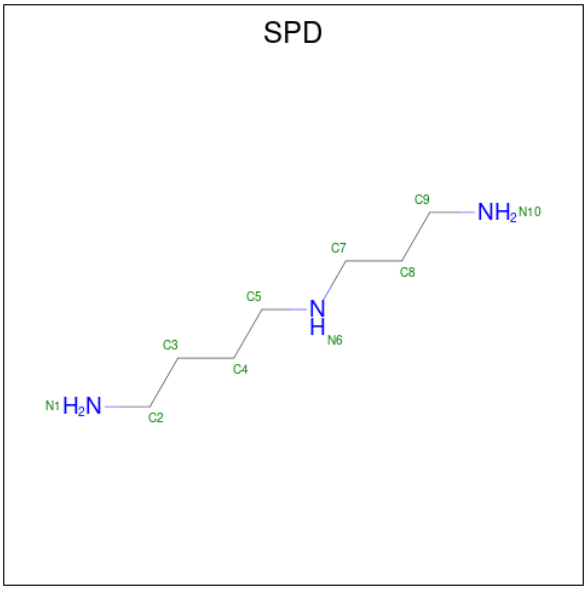
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	d9	1	Total Mg 1 1	0	0

- Molecule 84 is POTASSIUM ION (CCD ID: K) (formula: K).

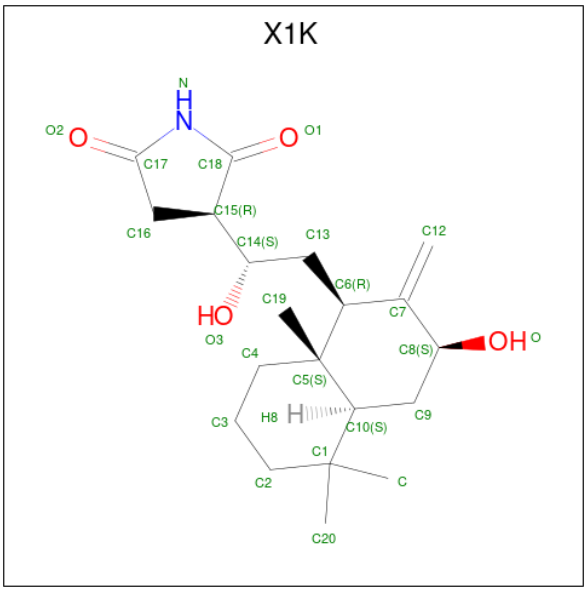
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	1	1	Total K 1 1	0	0
84	j	1	Total K 1 1	0	0
84	AR	4	Total K 4 4	0	0
84	sR	1	Total K 1 1	0	0

- Molecule 85 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	1	1	Total C N 10 7 3	0	0
85	AR	1	Total C N 10 7 3	0	0

- Molecule 86 is (3 {R})-3-[(1 {S})-2-[(1 {R},3 {S},4 {a} {S},8 {a} {S})-5,5,8 {a}-trimethyl-2-methylidene-3-oxidanyl-3,4,4 {a},6,7,8-hexahydro-1 {H}-naphthalen-1-yl]-1-oxidanyl-ethyl]pyrrolidine-2,5-dione (CCD ID: X1K) (formula: $C_{20}H_{31}NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	1	1	Total C N O 25 20 1 4	0	0
86	AR	1	Total C N O 25 20 1 4	0	0

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

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

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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

- Molecule 88 is OSMIUM ION (CCD ID: OS) (formula: Os).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	A	1	Total Os 1 1	0	0

- Molecule 89 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
89	1	148	Total O 148 148	0	0
89	4	14	Total O 14 14	0	0
89	j	1	Total O 1 1	0	0
89	x	4	Total O 4 4	0	0
89	AE	2	Total O 2 2	0	0
89	AO	1	Total O 1 1	0	0
89	AR	210	Total O 210 210	0	0
89	CD	1	Total O 1 1	0	0
89	CF	7	Total O 7 7	0	0
89	CI	1	Total O 1 1	0	0
89	CP	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
89	CR	1	Total O 1 1	0	0
89	CT	1	Total O 1 1	0	0
89	DG	1	Total O 1 1	0	0
89	A	57	Total O 57 57	0	0
89	R	1	Total O 1 1	0	0
89	S	6	Total O 6 6	0	0
89	Y	1	Total O 1 1	0	0
89	sR	41	Total O 41 41	0	0
89	s8	1	Total O 1 1	0	0
89	c1	1	Total O 1 1	0	0
89	c7	2	Total O 2 2	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	302.58Å 285.05Å 433.72Å 90.00° 98.89° 90.00°	Depositor
Resolution (Å)	206.30 – 3.16	Depositor
% Data completeness (in resolution range)	98.1 (206.30-3.16)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.52 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.223 , 0.251	Depositor
Wilson B-factor (Å^2)	72.9	Xtriage
Anisotropy	0.178	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	409267	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% 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 2462 ligands modelled in this entry, 1 is modelled with single atom and 1500 are monoatomic - leaving 961 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	$\#\|Z\| > 2$
82	OHX	A	1923	-	0,6,6	-	-	-		
82	OHX	A	1969	-	0,6,6	-	-	-		
82	OHX	CV	201	-	0,6,6	-	-	-		
82	OHX	AR	3650	-	0,6,6	-	-	-		
82	OHX	1	3481	-	0,6,6	-	-	-		
82	OHX	AR	3618	-	0,6,6	-	-	-		
82	OHX	AR	3671	-	0,6,6	-	-	-		
82	OHX	AR	3480	-	0,6,6	-	-	-		
82	OHX	AR	3623	-	0,6,6	-	-	-		
82	OHX	1	4106	-	0,6,6	-	-	-		
82	OHX	AS	205	-	0,6,6	-	-	-		
82	OHX	4	206	-	0,6,6	-	-	-		
82	OHX	AR	4148	-	0,6,6	-	-	-		
82	OHX	AR	3525	-	0,6,6	-	-	-		
82	OHX	3	202	-	0,6,6	-	-	-		
82	OHX	AR	4150	83	0,6,6	-	-	-		
82	OHX	AT	215	-	0,6,6	-	-	-		
82	OHX	A	1919	-	0,6,6	-	-	-		
82	OHX	1	3486	-	0,6,6	-	-	-		
82	OHX	1	3443	-	0,6,6	-	-	-		
82	OHX	1	3495	-	0,6,6	-	-	-		
82	OHX	sR	2176	-	0,6,6	-	-	-		
82	OHX	1	3410	-	0,6,6	-	-	-		
82	OHX	sR	1965	-	0,6,6	-	-	-		
82	OHX	c7	201	-	0,6,6	-	-	-		
82	OHX	A	1917	-	0,6,6	-	-	-		
82	OHX	sR	2172	-	0,6,6	-	-	-		
82	OHX	1	3448	83	0,6,6	-	-	-		
82	OHX	sR	1959	-	0,6,6	-	-	-		
82	OHX	1	3463	-	0,6,6	-	-	-		
82	OHX	1	4075	-	0,6,6	-	-	-		
82	OHX	AR	3572	-	0,6,6	-	-	-		
82	OHX	1	4058	-	0,6,6	-	-	-		
82	OHX	sR	1922	-	0,6,6	-	-	-		
82	OHX	1	3538	-	0,6,6	-	-	-		
82	OHX	sR	1949	-	0,6,6	-	-	-		
82	OHX	AR	4139	-	0,6,6	-	-	-		
82	OHX	A	1922	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	A	2109	-	0,6,6	-	-	-		
82	OHX	r	303	-	0,6,6	-	-	-		
82	OHX	1	4107	83	0,6,6	-	-	-		
82	OHX	CE	401	-	0,6,6	-	-	-		
82	OHX	sR	1992	-	0,6,6	-	-	-		
82	OHX	AR	3485	-	0,6,6	-	-	-		
82	OHX	sR	1996	-	0,6,6	-	-	-		
82	OHX	1	4131	-	0,6,6	-	-	-		
82	OHX	A	1908	-	0,6,6	-	-	-		
82	OHX	1	3548	-	0,6,6	-	-	-		
82	OHX	1	3471	-	0,6,6	-	-	-		
82	OHX	AS	204	-	0,6,6	-	-	-		
82	OHX	1	3602	83	0,6,6	-	-	-		
82	OHX	AR	4161	-	0,6,6	-	-	-		
82	OHX	1	3502	-	0,6,6	-	-	-		
82	OHX	AR	3558	-	0,6,6	-	-	-		
82	OHX	AR	3595	-	0,6,6	-	-	-		
82	OHX	A	2141	-	0,6,6	-	-	-		
82	OHX	sR	1933	-	0,6,6	-	-	-		
82	OHX	1	3439	-	0,6,6	-	-	-		
82	OHX	AR	4136	-	0,6,6	-	-	-		
82	OHX	AR	3477	-	0,6,6	-	-	-		
82	OHX	1	3550	-	0,6,6	-	-	-		
82	OHX	1	4051	-	0,6,6	-	-	-		
82	OHX	A	1968	-	0,6,6	-	-	-		
82	OHX	AT	210	-	0,6,6	-	-	-		
82	OHX	A	1927	-	0,6,6	-	-	-		
82	OHX	1	3506	-	0,6,6	-	-	-		
82	OHX	4	209	-	0,6,6	-	-	-		
82	OHX	A	2129	-	0,6,6	-	-	-		
82	OHX	1	4135	-	0,6,6	-	-	-		
82	OHX	sR	1991	-	0,6,6	-	-	-		
82	OHX	1	4093	83	0,6,6	-	-	-		
82	OHX	A	2139	-	0,6,6	-	-	-		
82	OHX	1	3547	-	0,6,6	-	-	-		
82	OHX	1	3401	-	0,6,6	-	-	-		
82	OHX	1	3474	-	0,6,6	-	-	-		
82	OHX	1	4073	-	0,6,6	-	-	-		
82	OHX	AR	3413	-	0,6,6	-	-	-		
82	OHX	1	3426	-	0,6,6	-	-	-		
82	OHX	1	3581	-	0,6,6	-	-	-		
82	OHX	1	3442	83	0,6,6	-	-	-		
82	OHX	A	1903	83	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	1	3533	-	0,6,6	-	-	-		
82	OHX	sR	2001	-	0,6,6	-	-	-		
82	OHX	1	4138	-	0,6,6	-	-	-		
82	OHX	1	4142	-	0,6,6	-	-	-		
82	OHX	1	4056	83	0,6,6	-	-	-		
82	OHX	AR	3636	-	0,6,6	-	-	-		
82	OHX	AR	3628	-	0,6,6	-	-	-		
82	OHX	J	301	-	0,6,6	-	-	-		
82	OHX	4	202	-	0,6,6	-	-	-		
82	OHX	sR	2022	-	0,6,6	-	-	-		
86	X1K	AR	4205	-	27,27,27	0.68	2 (7%)	35,43,43	1.92	9 (25%)
82	OHX	1	3470	83	0,6,6	-	-	-		
82	OHX	AR	3537	-	0,6,6	-	-	-		
82	OHX	AS	203	-	0,6,6	-	-	-		
82	OHX	AR	3455	-	0,6,6	-	-	-		
82	OHX	AR	3585	-	0,6,6	-	-	-		
82	OHX	1	4083	-	0,6,6	-	-	-		
82	OHX	3	220	83	0,6,6	-	-	-		
82	OHX	AR	3407	83	0,6,6	-	-	-		
82	OHX	AR	3633	-	0,6,6	-	-	-		
82	OHX	1	3532	-	0,6,6	-	-	-		
82	OHX	1	3560	-	0,6,6	-	-	-		
82	OHX	sR	1953	-	0,6,6	-	-	-		
82	OHX	1	3487	-	0,6,6	-	-	-		
82	OHX	sR	1982	-	0,6,6	-	-	-		
82	OHX	sR	1943	-	0,6,6	-	-	-		
82	OHX	A	1934	-	0,6,6	-	-	-		
82	OHX	A	1940[A]	-	0,6,6	-	-	-		
82	OHX	AR	4116	-	0,6,6	-	-	-		
82	OHX	A	1967	-	0,6,6	-	-	-		
82	OHX	sR	2178	83	0,6,6	-	-	-		
82	OHX	1	3600	-	0,6,6	-	-	-		
82	OHX	1	4120	-	0,6,6	-	-	-		
82	OHX	O	201	-	0,6,6	-	-	-		
82	OHX	1	3491	-	0,6,6	-	-	-		
82	OHX	CL	302	-	0,6,6	-	-	-		
82	OHX	1	3475	-	0,6,6	-	-	-		
82	OHX	AR	3637	83	0,6,6	-	-	-		
82	OHX	A	2123	-	0,6,6	-	-	-		
82	OHX	AR	3607	-	0,6,6	-	-	-		
86	X1K	1	4181	-	27,27,27	0.49	1 (3%)	35,43,43	2.30	8 (22%)
82	OHX	AR	4143	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	AR	3483	-	0,6,6	-	-	-		
82	OHX	1	3578	-	0,6,6	-	-	-		
82	OHX	A	1946	-	0,6,6	-	-	-		
82	OHX	1	3557	-	0,6,6	-	-	-		
82	OHX	1	4102	-	0,6,6	-	-	-		
82	OHX	4	205	-	0,6,6	-	-	-		
82	OHX	1	3562	-	0,6,6	-	-	-		
82	OHX	AR	3617	-	0,6,6	-	-	-		
82	OHX	1	3492	-	0,6,6	-	-	-		
82	OHX	1	3456	-	0,6,6	-	-	-		
82	OHX	AR	3561	-	0,6,6	-	-	-		
82	OHX	1	4074	-	0,6,6	-	-	-		
82	OHX	A	2130	-	0,6,6	-	-	-		
82	OHX	sR	1917	-	0,6,6	-	-	-		
82	OHX	CH	201	-	0,6,6	-	-	-		
82	OHX	1	3497	-	0,6,6	-	-	-		
82	OHX	AR	3430	-	0,6,6	-	-	-		
82	OHX	sR	1932	-	0,6,6	-	-	-		
82	OHX	3	206	-	0,6,6	-	-	-		
82	OHX	1	4091	-	0,6,6	-	-	-		
82	OHX	sR	1985	-	0,6,6	-	-	-		
82	OHX	AR	3503	-	0,6,6	-	-	-		
82	OHX	1	3586	-	0,6,6	-	-	-		
82	OHX	sR	1919	-	0,6,6	-	-	-		
82	OHX	1	3504	-	0,6,6	-	-	-		
82	OHX	1	3546	-	0,6,6	-	-	-		
82	OHX	1	4101	-	0,6,6	-	-	-		
82	OHX	AR	3435	-	0,6,6	-	-	-		
82	OHX	AR	3606	-	0,6,6	-	-	-		
82	OHX	A	1912	-	0,6,6	-	-	-		
82	OHX	AT	216	-	0,6,6	-	-	-		
82	OHX	AR	4147	-	0,6,6	-	-	-		
82	OHX	1	3599	-	0,6,6	-	-	-		
82	OHX	1	3468	-	0,6,6	-	-	-		
82	OHX	AR	4138	-	0,6,6	-	-	-		
82	OHX	sR	1910	-	0,6,6	-	-	-		
82	OHX	AS	209	-	0,6,6	-	-	-		
82	OHX	A	1902	-	0,6,6	-	-	-		
82	OHX	A	2136	-	0,6,6	-	-	-		
82	OHX	AR	3415	-	0,6,6	-	-	-		
82	OHX	1	3433	-	0,6,6	-	-	-		
82	OHX	sR	1958	-	0,6,6	-	-	-		
82	OHX	AR	3605	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	1	3416	-	0,6,6	-	-	-		
82	OHX	1	4079	-	0,6,6	-	-	-		
82	OHX	AR	3669	-	0,5,6	-	-	-		
82	OHX	1	4123	-	0,6,6	-	-	-		
82	OHX	1	4098	-	0,6,6	-	-	-		
82	OHX	1	3449	-	0,6,6	-	-	-		
82	OHX	AR	3450	-	0,6,6	-	-	-		
82	OHX	AR	3440	83	0,6,6	-	-	-		
82	OHX	AT	208	-	0,6,6	-	-	-		
82	OHX	A	1948	-	0,6,6	-	-	-		
82	OHX	1	4060	-	0,6,6	-	-	-		
82	OHX	AT	233	-	0,6,6	-	-	-		
82	OHX	sR	1981	-	0,6,6	-	-	-		
82	OHX	1	4155	-	0,6,6	-	-	-		
82	OHX	AR	3469	-	0,6,6	-	-	-		
82	OHX	sR	2004	-	0,6,6	-	-	-		
82	OHX	1	4092	83	0,6,6	-	-	-		
82	OHX	AR	3463	83	0,6,6	-	-	-		
82	OHX	sR	1934	83	0,6,6	-	-	-		
82	OHX	A	2105	-	0,6,6	-	-	-		
82	OHX	1	3514	-	0,6,6	-	-	-		
82	OHX	1	3466	-	0,6,6	-	-	-		
82	OHX	1	3568	-	0,6,6	-	-	-		
82	OHX	1	3593	-	0,6,6	-	-	-		
82	OHX	AR	3420	-	0,6,6	-	-	-		
82	OHX	AR	3551	-	0,6,6	-	-	-		
82	OHX	A	1906	-	0,6,6	-	-	-		
82	OHX	A	1955	-	0,6,6	-	-	-		
82	OHX	sR	1963	-	0,6,6	-	-	-		
82	OHX	A	1944	83	0,6,6	-	-	-		
82	OHX	1	3518	-	0,6,6	-	-	-		
82	OHX	AR	3641	-	0,6,6	-	-	-		
82	OHX	AR	3549	83	0,6,6	-	-	-		
82	OHX	sR	1964	-	0,6,6	-	-	-		
82	OHX	1	3431	-	0,6,6	-	-	-		
82	OHX	sR	1911	-	0,6,6	-	-	-		
82	OHX	A	2131	-	0,6,6	-	-	-		
82	OHX	sR	1968	-	0,6,6	-	-	-		
82	OHX	4	211	-	0,6,6	-	-	-		
82	OHX	1	3422	-	0,6,6	-	-	-		
82	OHX	AR	4163	-	0,6,6	-	-	-		
82	OHX	A	2120	-	0,6,6	-	-	-		
82	OHX	1	3483	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	1	4118	-	0,6,6	-	-	-		
82	OHX	sR	1993	-	0,6,6	-	-	-		
82	OHX	AR	3465	-	0,6,6	-	-	-		
82	OHX	sR	1914	-	0,6,6	-	-	-		
82	OHX	1	3500	-	0,6,6	-	-	-		
82	OHX	1	4122	-	0,6,6	-	-	-		
82	OHX	1	3530	-	0,6,6	-	-	-		
82	OHX	sR	1970	83	0,6,6	-	-	-		
82	OHX	1	4097	-	0,6,6	-	-	-		
82	OHX	AR	3646	-	0,6,6	-	-	-		
82	OHX	A	1954	-	0,5,6	-	-	-		
82	OHX	AR	3408	-	0,6,6	-	-	-		
82	OHX	1	4141	-	0,6,6	-	-	-		
82	OHX	1	3523	-	0,6,6	-	-	-		
82	OHX	sR	1903	-	0,6,6	-	-	-		
82	OHX	1	3445	-	0,6,6	-	-	-		
82	OHX	AR	3409	-	0,6,6	-	-	-		
82	OHX	A	2143	-	0,6,6	-	-	-		
82	OHX	AR	3452	-	0,6,6	-	-	-		
82	OHX	sR	1947	-	0,6,6	-	-	-		
82	OHX	sR	1952	-	0,6,6	-	-	-		
82	OHX	AR	3441	-	0,6,6	-	-	-		
82	OHX	1	3554	83	0,6,6	-	-	-		
82	OHX	sR	2016	-	0,6,6	-	-	-		
82	OHX	1	4100	-	0,6,6	-	-	-		
82	OHX	A	2102	-	0,6,6	-	-	-		
82	OHX	1	3406	-	0,6,6	-	-	-		
82	OHX	CX	201	-	0,6,6	-	-	-		
82	OHX	1	4104	-	0,6,6	-	-	-		
82	OHX	AR	3427	-	0,6,6	-	-	-		
82	OHX	1	4111	-	0,6,6	-	-	-		
82	OHX	AR	3627	-	0,6,6	-	-	-		
82	OHX	A	1972	-	0,6,6	-	-	-		
82	OHX	1	3591	-	0,6,6	-	-	-		
82	OHX	1	3505	-	0,6,6	-	-	-		
82	OHX	AR	3436	-	0,6,6	-	-	-		
82	OHX	AR	3645	-	0,6,6	-	-	-		
82	OHX	A	1939	-	0,6,6	-	-	-		
82	OHX	AR	3470	-	0,6,6	-	-	-		
82	OHX	AR	3660	-	0,6,6	-	-	-		
82	OHX	1	4146	-	0,6,6	-	-	-		
82	OHX	1	4143	-	0,6,6	-	-	-		
82	OHX	1	3598	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	A	1943	-	0,6,6	-	-	-		
82	OHX	AR	3424	-	0,6,6	-	-	-		
82	OHX	sR	1966	-	0,6,6	-	-	-		
82	OHX	sR	1974	-	0,6,6	-	-	-		
82	OHX	AR	3461	-	0,6,6	-	-	-		
82	OHX	AR	4142	-	0,6,6	-	-	-		
82	OHX	A	1957	-	0,6,6	-	-	-		
82	OHX	1	3446	83	0,6,6	-	-	-		
82	OHX	A	2134	-	0,6,6	-	-	-		
82	OHX	1	3535[A]	-	0,6,6	-	-	-		
82	OHX	A	1916	-	0,6,6	-	-	-		
82	OHX	1	4147	-	0,6,6	-	-	-		
82	OHX	AR	3616	-	0,6,6	-	-	-		
82	OHX	sR	1920	-	0,6,6	-	-	-		
82	OHX	sR	1997	-	0,6,6	-	-	-		
82	OHX	1	4084	-	0,6,6	-	-	-		
82	OHX	1	4114[B]	-	0,6,6	-	-	-		
82	OHX	1	4140	-	0,6,6	-	-	-		
82	OHX	A	1904	-	0,6,6	-	-	-		
82	OHX	1	3566	-	0,6,6	-	-	-		
82	OHX	sR	1937	-	0,6,6	-	-	-		
82	OHX	A	1973	-	0,6,6	-	-	-		
82	OHX	AR	3491	-	0,6,6	-	-	-		
82	OHX	AR	3475	-	0,6,6	-	-	-		
82	OHX	AS	208	-	0,6,6	-	-	-		
82	OHX	A	1936	-	0,6,6	-	-	-		
82	OHX	A	1945	-	0,6,6	-	-	-		
82	OHX	DH	202	-	0,6,6	-	-	-		
82	OHX	3	219	-	0,6,6	-	-	-		
82	OHX	A	1907	-	0,6,6	-	-	-		
82	OHX	A	2122	-	0,6,6	-	-	-		
82	OHX	4	229	-	0,6,6	-	-	-		
82	OHX	AR	3515	-	0,6,6	-	-	-		
82	OHX	AR	3530	-	0,6,6	-	-	-		
82	OHX	1	3575	-	0,6,6	-	-	-		
82	OHX	AR	3666	-	0,6,6	-	-	-		
82	OHX	1	4130	-	0,6,6	-	-	-		
82	OHX	sR	1923	-	0,6,6	-	-	-		
82	OHX	sR	1977	-	0,6,6	-	-	-		
82	OHX	CP	302	-	0,6,6	-	-	-		
82	OHX	sR	1961	-	0,6,6	-	-	-		
82	OHX	sR	1998	-	0,6,6	-	-	-		
82	OHX	AR	3640	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	1	3404	-	0,6,6	-	-	-		
82	OHX	1	3525	-	0,6,6	-	-	-		
82	OHX	AR	4152	-	0,6,6	-	-	-		
82	OHX	CG	302	-	0,6,6	-	-	-		
82	OHX	A	2124	-	0,6,6	-	-	-		
82	OHX	AR	3533	-	0,6,6	-	-	-		
82	OHX	1	3447	83	0,6,6	-	-	-		
82	OHX	1	3545	-	0,6,6	-	-	-		
82	OHX	1	4088	-	0,6,6	-	-	-		
82	OHX	1	4050	-	0,6,6	-	-	-		
82	OHX	AR	3661	-	0,6,6	-	-	-		
82	OHX	A	1915	-	0,6,6	-	-	-		
82	OHX	A	1942	-	0,6,6	-	-	-		
82	OHX	A	1935	-	0,6,6	-	-	-		
82	OHX	1	3493	-	0,6,6	-	-	-		
82	OHX	AR	3629	-	0,6,6	-	-	-		
82	OHX	AR	3496	-	0,6,6	-	-	-		
82	OHX	4	213	-	0,6,6	-	-	-		
82	OHX	AR	3412	-	0,6,6	-	-	-		
82	OHX	AR	3546	-	0,6,6	-	-	-		
82	OHX	1	4103	-	0,6,6	-	-	-		
82	OHX	A	2126[A]	83	0,6,6	-	-	-		
82	OHX	sR	1980	-	0,6,6	-	-	-		
82	OHX	sR	1916[B]	-	0,6,6	-	-	-		
82	OHX	AR	3425	-	0,6,6	-	-	-		
82	OHX	1	3583	-	0,6,6	-	-	-		
82	OHX	A	1956	-	0,6,6	-	-	-		
82	OHX	1	4077	-	0,6,6	-	-	-		
82	OHX	AR	4154	-	0,6,6	-	-	-		
82	OHX	A	2140	-	0,6,6	-	-	-		
82	OHX	sR	1918	-	0,6,6	-	-	-		
82	OHX	1	3579	83	0,6,6	-	-	-		
82	OHX	1	3534	-	0,6,6	-	-	-		
82	OHX	AR	3562	83	0,6,6	-	-	-		
82	OHX	AR	4140	-	0,6,6	-	-	-		
82	OHX	A	1960	-	0,6,6	-	-	-		
82	OHX	A	2107	-	0,6,6	-	-	-		
82	OHX	AR	3490	-	0,6,6	-	-	-		
82	OHX	1	3451	-	0,6,6	-	-	-		
82	OHX	1	3522	-	0,6,6	-	-	-		
82	OHX	1	4076	-	0,6,6	-	-	-		
82	OHX	sR	2003	83	0,6,6	-	-	-		
82	OHX	1	3480	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	c3	202	-	0,6,6	-	-	-		
82	OHX	1	3520	-	0,6,6	-	-	-		
82	OHX	1	3452	-	0,6,6	-	-	-		
82	OHX	AT	213	-	0,6,6	-	-	-		
82	OHX	A	1951	-	0,6,6	-	-	-		
82	OHX	sR	1925	-	0,6,6	-	-	-		
82	OHX	1	4152	-	0,6,6	-	-	-		
82	OHX	AR	3492	83	0,6,6	-	-	-		
82	OHX	AR	3625	-	0,6,6	-	-	-		
82	OHX	1	3536	-	0,6,6	-	-	-		
82	OHX	AR	3498	-	0,6,6	-	-	-		
82	OHX	AR	3500	-	0,6,6	-	-	-		
82	OHX	sR	1935	-	0,6,6	-	-	-		
82	OHX	1	3424	-	0,6,6	-	-	-		
82	OHX	1	3462	-	0,6,6	-	-	-		
82	OHX	1	3571	-	0,6,6	-	-	-		
82	OHX	A	1966	-	0,6,6	-	-	-		
82	OHX	A	2103	-	0,6,6	-	-	-		
82	OHX	sR	2006	-	0,6,6	-	-	-		
82	OHX	AR	3471	-	0,6,6	-	-	-		
82	OHX	AR	3411	-	0,6,6	-	-	-		
82	OHX	A	2132	-	0,6,6	-	-	-		
82	OHX	Q	201	-	0,6,6	-	-	-		
82	OHX	AR	3488	-	0,6,6	-	-	-		
82	OHX	AG	202	-	0,6,6	-	-	-		
82	OHX	AR	4159	-	0,6,6	-	-	-		
82	OHX	3	201	-	0,6,6	-	-	-		
82	OHX	1	3423	-	0,6,6	-	-	-		
82	OHX	1	3428	83	0,6,6	-	-	-		
82	OHX	AR	3621	-	0,6,6	-	-	-		
82	OHX	AR	4144	-	0,6,6	-	-	-		
82	OHX	sR	1941	-	0,6,6	-	-	-		
82	OHX	AR	3418	-	0,6,6	-	-	-		
82	OHX	AR	3468	-	0,6,6	-	-	-		
82	OHX	AR	3479	-	0,6,6	-	-	-		
82	OHX	sR	1913	-	0,6,6	-	-	-		
82	OHX	1	3467	83	0,6,6	-	-	-		
82	OHX	AT	235	-	0,6,6	-	-	-		
82	OHX	1	3414	-	0,6,6	-	-	-		
82	OHX	1	4153	-	0,6,6	-	-	-		
82	OHX	AR	3473	83	0,6,6	-	-	-		
82	OHX	1	3595	-	0,6,6	-	-	-		
82	OHX	AR	3482	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	AR	3527	-	0,6,6	-	-	-		
82	OHX	AR	4156	-	0,6,6	-	-	-		
82	OHX	A	1965	-	0,6,6	-	-	-		
82	OHX	sR	1916[A]	-	0,6,6	-	-	-		
82	OHX	AR	4153	-	0,6,6	-	-	-		
82	OHX	AC	102	-	0,6,6	-	-	-		
82	OHX	AR	3639	-	0,6,6	-	-	-		
82	OHX	4	208	83	0,6,6	-	-	-		
82	OHX	sR	1931	-	0,6,6	-	-	-		
82	OHX	1	3461	-	0,6,6	-	-	-		
82	OHX	1	3515	-	0,6,6	-	-	-		
82	OHX	h	401	-	0,6,6	-	-	-		
82	OHX	sR	1928	-	0,6,6	-	-	-		
82	OHX	1	3553	-	0,6,6	-	-	-		
82	OHX	A	1924	-	0,6,6	-	-	-		
82	OHX	1	3476	-	0,6,6	-	-	-		
82	OHX	AR	3429	-	0,6,6	-	-	-		
82	OHX	1	4072	-	0,6,6	-	-	-		
82	OHX	AR	3406	-	0,6,6	-	-	-		
82	OHX	A	2110	-	0,6,6	-	-	-		
82	OHX	AR	3643	83	0,6,6	-	-	-		
82	OHX	AR	3663	-	0,6,6	-	-	-		
82	OHX	1	3552	-	0,6,6	-	-	-		
82	OHX	AR	3478	-	0,6,6	-	-	-		
82	OHX	1	3408	-	0,6,6	-	-	-		
82	OHX	A	2104	-	0,6,6	-	-	-		
82	OHX	sR	1901	-	0,6,6	-	-	-		
82	OHX	sR	1945	-	0,6,6	-	-	-		
82	OHX	1	3563	-	0,6,6	-	-	-		
82	OHX	A	1926	-	0,6,6	-	-	-		
82	OHX	1	3569	-	0,6,6	-	-	-		
82	OHX	AR	4146	-	0,6,6	-	-	-		
82	OHX	A	1918	-	0,6,6	-	-	-		
82	OHX	1	3572	-	0,6,6	-	-	-		
82	OHX	AR	4157	-	0,6,6	-	-	-		
82	OHX	sR	1988	-	0,6,6	-	-	-		
82	OHX	A	2142	-	0,6,6	-	-	-		
82	OHX	CG	304	-	0,6,6	-	-	-		
82	OHX	3	222	-	0,6,6	-	-	-		
82	OHX	1	3437	83	0,6,6	-	-	-		
82	OHX	1	3402	-	0,6,6	-	-	-		
82	OHX	AP	502	83	0,6,6	-	-	-		
82	OHX	AR	3487	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	1	3512	-	0,6,6	-	-	-		
82	OHX	sR	1957	-	0,6,6	-	-	-		
82	OHX	1	3558	-	0,6,6	-	-	-		
82	OHX	AR	3499	-	0,6,6	-	-	-		
82	OHX	AR	3489	-	0,6,6	-	-	-		
82	OHX	sR	1972	-	0,6,6	-	-	-		
82	OHX	1	3432	-	0,6,6	-	-	-		
82	OHX	1	4109	-	0,6,6	-	-	-		
82	OHX	AR	3434	-	0,6,6	-	-	-		
82	OHX	AR	4160	-	0,6,6	-	-	-		
82	OHX	sR	2025	-	0,6,6	-	-	-		
82	OHX	AR	3648	83	0,6,6	-	-	-		
82	OHX	A	1938	-	0,6,6	-	-	-		
82	OHX	1	3594	-	0,6,6	-	-	-		
82	OHX	sR	2021	-	0,6,6	-	-	-		
82	OHX	1	3601	-	0,6,6	-	-	-		
82	OHX	AR	3403	-	0,6,6	-	-	-		
82	OHX	AR	3651	-	0,6,6	-	-	-		
82	OHX	sR	1995	-	0,6,6	-	-	-		
82	OHX	sR	1915	-	0,6,6	-	-	-		
82	OHX	A	2128	83	0,6,6	-	-	-		
82	OHX	AR	3647	-	0,6,6	-	-	-		
82	OHX	1	4151	-	0,6,6	-	-	-		
82	OHX	sR	2005	-	0,6,6	-	-	-		
82	OHX	AR	3486	-	0,6,6	-	-	-		
82	OHX	1	3577	-	0,6,6	-	-	-		
82	OHX	A	1914	-	0,6,6	-	-	-		
82	OHX	1	3510	-	0,6,6	-	-	-		
82	OHX	sR	1986	-	0,6,6	-	-	-		
82	OHX	1	3589	-	0,6,6	-	-	-		
82	OHX	AR	4137	-	0,6,6	-	-	-		
82	OHX	1	3421	83	0,6,6	-	-	-		
82	OHX	A	2119	-	0,6,6	-	-	-		
82	OHX	1	3573	-	0,6,6	-	-	-		
82	OHX	1	4085	-	0,6,6	-	-	-		
82	OHX	AR	3446	-	0,6,6	-	-	-		
82	OHX	A	2111	-	0,6,6	-	-	-		
82	OHX	sR	1994	-	0,6,6	-	-	-		
82	OHX	A	1949	-	0,6,6	-	-	-		
82	OHX	1	3430	83	0,6,6	-	-	-		
82	OHX	1	3537	83	0,6,6	-	-	-		
82	OHX	1	3604	-	0,6,6	-	-	-		
82	OHX	1	3407	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	AR	3423	-	0,6,6	-	-	-		
82	OHX	1	3427	-	0,6,6	-	-	-		
82	OHX	1	3561	-	0,6,6	-	-	-		
82	OHX	sR	1904	-	0,6,6	-	-	-		
82	OHX	AR	3548	-	0,6,6	-	-	-		
82	OHX	1	3584	-	0,6,6	-	-	-		
82	OHX	1	3539	-	0,6,6	-	-	-		
82	OHX	AR	3458	83	0,6,6	-	-	-		
82	OHX	sR	1936	-	0,6,6	-	-	-		
82	OHX	sR	1960	-	0,6,6	-	-	-		
82	OHX	1	4116	83	0,6,6	-	-	-		
82	OHX	1	3457	-	0,6,6	-	-	-		
82	OHX	1	3542	83	0,6,6	-	-	-		
82	OHX	A	2113	-	0,6,6	-	-	-		
82	OHX	1	3444	-	0,6,6	-	-	-		
82	OHX	AS	207	-	0,6,6	-	-	-		
82	OHX	A	2121	-	0,6,6	-	-	-		
82	OHX	3	204	83	0,6,6	-	-	-		
82	OHX	k	404	-	0,6,6	-	-	-		
82	OHX	1	3438	-	0,6,6	-	-	-		
82	OHX	1	3485	83	0,6,6	-	-	-		
82	OHX	1	3605	-	0,6,6	-	-	-		
82	OHX	sR	1969	-	0,6,6	-	-	-		
82	OHX	s8	301	-	0,6,6	-	-	-		
82	OHX	A	1950	-	0,6,6	-	-	-		
82	OHX	AR	3540	-	0,6,6	-	-	-		
82	OHX	1	4108	-	0,6,6	-	-	-		
82	OHX	1	3603	-	0,6,6	-	-	-		
82	OHX	A	1932	-	0,6,6	-	-	-		
82	OHX	1	3489	-	0,6,6	-	-	-		
82	OHX	4	212	-	0,6,6	-	-	-		
82	OHX	AR	3404	-	0,6,6	-	-	-		
82	OHX	AT	207	-	0,6,6	-	-	-		
82	OHX	sR	1930	-	0,6,6	-	-	-		
82	OHX	AR	3401	-	0,6,6	-	-	-		
82	OHX	CG	303	-	0,6,6	-	-	-		
82	OHX	sR	2009	-	0,6,6	-	-	-		
82	OHX	AR	3426	-	0,6,6	-	-	-		
82	OHX	AR	3632	-	0,6,6	-	-	-		
82	OHX	A	2117	-	0,6,6	-	-	-		
82	OHX	1	4128	-	0,6,6	-	-	-		
82	OHX	AR	3536	-	0,6,6	-	-	-		
82	OHX	AR	3442	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	sR	1927	-	0,6,6	-	-	-		
82	OHX	4	210	-	0,6,6	-	-	-		
82	OHX	A	1928	83	0,6,6	-	-	-		
82	OHX	AR	3462	-	0,6,6	-	-	-		
82	OHX	AR	3419	83	0,6,6	-	-	-		
82	OHX	AR	3421	-	0,6,6	-	-	-		
82	OHX	3	203	-	0,6,6	-	-	-		
82	OHX	sR	1921	-	0,6,6	-	-	-		
82	OHX	sR	1975	-	0,6,6	-	-	-		
82	OHX	U	201	-	0,6,6	-	-	-		
82	OHX	AR	4149	83	0,6,6	-	-	-		
82	OHX	AR	3649	-	0,6,6	-	-	-		
82	OHX	1	3450	-	0,6,6	-	-	-		
82	OHX	AR	3668	-	0,6,6	-	-	-		
82	OHX	3	221	-	0,6,6	-	-	-		
82	OHX	A	1958	-	0,6,6	-	-	-		
82	OHX	AR	3428	-	0,6,6	-	-	-		
82	OHX	2	201	-	0,6,6	-	-	-		
82	OHX	1	3472	-	0,6,6	-	-	-		
82	OHX	1	3540	-	0,6,6	-	-	-		
82	OHX	1	3464	-	0,6,6	-	-	-		
82	OHX	1	3459	-	0,6,6	-	-	-		
82	OHX	AR	3439	-	0,6,6	-	-	-		
82	OHX	sR	2007	-	0,6,6	-	-	-		
82	OHX	1	3580	-	0,6,6	-	-	-		
82	OHX	AR	4141	-	0,6,6	-	-	-		
82	OHX	AR	3417	-	0,6,6	-	-	-		
82	OHX	AR	3597	83	0,6,6	-	-	-		
82	OHX	AT	212	-	0,6,6	-	-	-		
82	OHX	A	2115	83	0,6,6	-	-	-		
82	OHX	A	2125	-	0,6,6	-	-	-		
82	OHX	1	3499	-	0,6,6	-	-	-		
82	OHX	AR	3631	-	0,6,6	-	-	-		
82	OHX	1	3484	-	0,6,6	-	-	-		
82	OHX	T	201	-	0,6,6	-	-	-		
82	OHX	1	3590	83	0,6,6	-	-	-		
82	OHX	AR	3662	-	0,6,6	-	-	-		
82	OHX	DD	102	-	0,6,6	-	-	-		
82	OHX	A	1901	-	0,6,6	-	-	-		
82	OHX	1	3434	-	0,6,6	-	-	-		
82	OHX	1	3455	-	0,6,6	-	-	-		
82	OHX	AR	3559	-	0,6,6	-	-	-		
82	OHX	3	205	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	AR	3653	-	0,6,6	-	-	-		
82	OHX	AR	3657	-	0,6,6	-	-	-		
82	OHX	AR	3659	-	0,6,6	-	-	-		
82	OHX	AR	4120	-	0,6,6	-	-	-		
82	OHX	1	3511	-	0,6,6	-	-	-		
82	OHX	A	2145	-	0,6,6	-	-	-		
82	OHX	k	403	-	0,6,6	-	-	-		
82	OHX	AR	3467	-	0,6,6	-	-	-		
82	OHX	sR	2017	-	0,6,6	-	-	-		
82	OHX	1	3494	83	0,6,6	-	-	-		
82	OHX	A	2144	-	0,6,6	-	-	-		
82	OHX	1	4086	-	0,6,6	-	-	-		
82	OHX	1	3477	-	0,6,6	-	-	-		
82	OHX	A	2106	-	0,6,6	-	-	-		
82	OHX	l	405	-	0,6,6	-	-	-		
82	OHX	AR	3630	-	0,6,6	-	-	-		
82	OHX	A	1976	-	0,6,6	-	-	-		
82	OHX	AR	3456	-	0,6,6	-	-	-		
82	OHX	1	3521	-	0,6,6	-	-	-		
82	OHX	AR	3626	-	0,6,6	-	-	-		
82	OHX	AR	3655	-	0,6,6	-	-	-		
82	OHX	A	1963	-	0,6,6	-	-	-		
82	OHX	1	3420	-	0,6,6	-	-	-		
82	OHX	sR	2175	-	0,6,6	-	-	-		
82	OHX	1	3596	-	0,6,6	-	-	-		
82	OHX	AR	4162	-	0,6,6	-	-	-		
82	OHX	1	4126	-	0,6,6	-	-	-		
82	OHX	AR	3652	-	0,6,6	-	-	-		
82	OHX	sR	2015	-	0,6,6	-	-	-		
82	OHX	1	3549	-	0,6,6	-	-	-		
82	OHX	sR	2010	-	0,6,6	-	-	-		
85	SPD	AR	4204	-	9,9,9	0.33	0	8,8,8	0.88	0
82	OHX	sR	1946	-	0,6,6	-	-	-		
82	OHX	1	3436	-	0,6,6	-	-	-		
82	OHX	1	3418	-	0,6,6	-	-	-		
82	OHX	1	4129	-	0,6,6	-	-	-		
82	OHX	sR	1912	-	0,6,6	-	-	-		
82	OHX	1	3564	-	0,6,6	-	-	-		
82	OHX	1	3519	-	0,6,6	-	-	-		
82	OHX	AR	3443	-	0,6,6	-	-	-		
82	OHX	sR	1939	-	0,6,6	-	-	-		
82	OHX	sR	1990	-	0,6,6	-	-	-		
82	OHX	sR	2000	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
85	SPD	1	4180	-	9,9,9	0.33	0	8,8,8	0.92	0
82	OHX	sR	1938	-	0,6,6	-	-	-		
82	OHX	A	2135	-	0,6,6	-	-	-		
82	OHX	1	3524	-	0,6,6	-	-	-		
82	OHX	sR	2024	-	0,6,6	-	-	-		
82	OHX	AR	3438	-	0,6,6	-	-	-		
82	OHX	1	3465	83	0,6,6	-	-	-		
82	OHX	AR	3448	-	0,6,6	-	-	-		
82	OHX	CK	201	-	0,6,6	-	-	-		
82	OHX	A	1947	-	0,6,6	-	-	-		
82	OHX	1	4114[A]	-	0,6,6	-	-	-		
82	OHX	1	3567	-	0,6,6	-	-	-		
82	OHX	AR	3665	-	0,6,6	-	-	-		
82	OHX	sR	1940	-	0,6,6	-	-	-		
82	OHX	1	3409	-	0,6,6	-	-	-		
82	OHX	AR	4151	-	0,6,6	-	-	-		
82	OHX	1	3498	-	0,6,6	-	-	-		
82	OHX	AR	3460	-	0,6,6	-	-	-		
82	OHX	A	1911	83	0,6,6	-	-	-		
82	OHX	sR	1909	-	0,6,6	-	-	-		
82	OHX	A	1909	-	0,6,6	-	-	-		
82	OHX	1	4150	83	0,6,6	-	-	-		
82	OHX	AR	3656	-	0,6,6	-	-	-		
82	OHX	1	3574	-	0,6,6	-	-	-		
82	OHX	AK	103	-	0,6,6	-	-	-		
82	OHX	1	3597	-	0,6,6	-	-	-		
82	OHX	sR	1948	-	0,6,6	-	-	-		
82	OHX	A	1930	-	0,6,6	-	-	-		
82	OHX	AR	3635	-	0,6,6	-	-	-		
82	OHX	AR	3658	-	0,6,6	-	-	-		
82	OHX	1	3411	-	0,6,6	-	-	-		
82	OHX	1	3453	83	0,6,6	-	-	-		
82	OHX	AR	3476	-	0,6,6	-	-	-		
82	OHX	sR	1956	-	0,6,6	-	-	-		
82	OHX	4	201	-	0,6,6	-	-	-		
82	OHX	A	1962	-	0,6,6	-	-	-		
82	OHX	AR	3497	-	0,6,6	-	-	-		
82	OHX	1	4121	-	0,6,6	-	-	-		
82	OHX	1	4081	-	0,6,6	-	-	-		
82	OHX	sR	1984	-	0,6,6	-	-	-		
82	OHX	1	3559	-	0,6,6	-	-	-		
82	OHX	AR	3402	-	0,6,6	-	-	-		
82	OHX	1	4096	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	A	1953	-	0,6,6	-	-	-		
82	OHX	AR	3466	83	0,6,6	-	-	-		
82	OHX	1	4087	-	0,6,6	-	-	-		
82	OHX	A	1937	-	0,6,6	-	-	-		
82	OHX	sR	1907	-	0,6,6	-	-	-		
82	OHX	1	3528	-	0,6,6	-	-	-		
82	OHX	v	301	-	0,6,6	-	-	-		
82	OHX	sR	1987	-	0,6,6	-	-	-		
82	OHX	A	1941	-	0,6,6	-	-	-		
82	OHX	sR	1983	-	0,6,6	-	-	-		
82	OHX	1	3435	-	0,6,6	-	-	-		
82	OHX	1	3509	-	0,6,6	-	-	-		
82	OHX	1	4078	-	0,6,6	-	-	-		
82	OHX	1	4136	-	0,6,6	-	-	-		
82	OHX	z	202	-	0,6,6	-	-	-		
82	OHX	AR	3416	83	0,6,6	-	-	-		
82	OHX	A	2112	-	0,6,6	-	-	-		
82	OHX	A	1905	-	0,6,6	-	-	-		
82	OHX	A	1977	-	0,6,6	-	-	-		
82	OHX	AR	3422	-	0,6,6	-	-	-		
82	OHX	1	4124	-	0,6,6	-	-	-		
82	OHX	1	3517	-	0,6,6	-	-	-		
82	OHX	1	4149	-	0,6,6	-	-	-		
82	OHX	1	4080	-	0,6,6	-	-	-		
82	OHX	sR	1906	-	0,6,6	-	-	-		
82	OHX	A	2146	-	0,6,6	-	-	-		
82	OHX	1	3585	-	0,6,6	-	-	-		
82	OHX	AR	3432	-	0,6,6	-	-	-		
82	OHX	A	1970	-	0,6,6	-	-	-		
82	OHX	sR	1944	-	0,6,6	-	-	-		
82	OHX	1	4082	-	0,6,6	-	-	-		
82	OHX	1	3415	-	0,6,6	-	-	-		
82	OHX	1	3582	-	0,6,6	-	-	-		
82	OHX	sR	1908	-	0,6,6	-	-	-		
82	OHX	AR	3502	-	0,6,6	-	-	-		
82	OHX	AR	3600	-	0,6,6	-	-	-		
82	OHX	A	1913	-	0,6,6	-	-	-		
82	OHX	1	3526	-	0,6,6	-	-	-		
82	OHX	1	3570	-	0,6,6	-	-	-		
82	OHX	AT	214	-	0,6,6	-	-	-		
82	OHX	1	3440	-	0,6,6	-	-	-		
82	OHX	1	4089	-	0,6,6	-	-	-		
82	OHX	AS	201	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	1	3516	-	0,6,6	-	-	-		
82	OHX	AR	3543	-	0,6,6	-	-	-		
82	OHX	AR	3445	-	0,6,6	-	-	-		
82	OHX	1	3405	-	0,6,6	-	-	-		
82	OHX	1	3541	-	0,6,6	-	-	-		
82	OHX	sR	2012	-	0,6,6	-	-	-		
82	OHX	A	1920	-	0,6,6	-	-	-		
82	OHX	1	3490	-	0,6,6	-	-	-		
82	OHX	1	3587	83	0,6,6	-	-	-		
82	OHX	A	1921	-	0,6,6	-	-	-		
82	OHX	1	3478	-	0,6,6	-	-	-		
82	OHX	sR	1976	83	0,6,6	-	-	-		
82	OHX	1	4148	-	0,6,6	-	-	-		
82	OHX	sR	1924	-	0,6,6	-	-	-		
82	OHX	CE	402	-	0,6,6	-	-	-		
82	OHX	sR	1954	-	0,6,6	-	-	-		
82	OHX	1	3460	-	0,6,6	-	-	-		
82	OHX	A	1959	-	0,6,6	-	-	-		
82	OHX	1	4145	-	0,6,6	-	-	-		
82	OHX	1	4132	-	0,6,6	-	-	-		
82	OHX	1	3458	-	0,6,6	-	-	-		
82	OHX	1	3531	-	0,6,6	-	-	-		
82	OHX	AR	3472	-	0,6,6	-	-	-		
82	OHX	A	1910	-	0,6,6	-	-	-		
82	OHX	1	3555	83	0,6,6	-	-	-		
82	OHX	AR	3431	-	0,6,6	-	-	-		
82	OHX	AR	3642	-	0,6,6	-	-	-		
82	OHX	sR	2014	-	0,6,6	-	-	-		
82	OHX	1	4139	-	0,6,6	-	-	-		
82	OHX	sR	1929	83	0,6,6	-	-	-		
82	OHX	sR	1926	83	0,6,6	-	-	-		
82	OHX	1	3496	-	0,6,6	-	-	-		
82	OHX	A	2138	-	0,6,6	-	-	-		
82	OHX	sR	1971	-	0,6,6	-	-	-		
82	OHX	sR	1979	-	0,6,6	-	-	-		
82	OHX	AK	102	83	0,6,6	-	-	-		
82	OHX	AT	211	83	0,6,6	-	-	-		
82	OHX	1	4127	-	0,6,6	-	-	-		
82	OHX	sR	2011	-	0,6,6	-	-	-		
82	OHX	1	3507	-	0,6,6	-	-	-		
82	OHX	AR	3414	83	0,6,6	-	-	-		
82	OHX	1	4137	83	0,6,6	-	-	-		
82	OHX	AR	3437	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	AR	3613	-	0,6,6	-	-	-		
82	OHX	1	4144	1	0,5,6	-	-	-		
82	OHX	1	4154	-	0,6,6	-	-	-		
82	OHX	sR	1978	-	0,6,6	-	-	-		
82	OHX	1	3479	-	0,6,6	-	-	-		
82	OHX	1	4125	-	0,6,6	-	-	-		
82	OHX	A	1925	-	0,6,6	-	-	-		
82	OHX	1	3413	-	0,6,6	-	-	-		
82	OHX	1	3417	83	0,6,6	-	-	-		
82	OHX	AR	3405	-	0,6,6	-	-	-		
82	OHX	AR	3457	-	0,6,6	-	-	-		
82	OHX	AR	4158	-	0,6,6	-	-	-		
82	OHX	AR	3638	-	0,6,6	-	-	-		
82	OHX	1	3527	-	0,6,6	-	-	-		
82	OHX	AR	3410	-	0,6,6	-	-	-		
82	OHX	1	4099	-	0,5,6	-	-	-		
82	OHX	1	3429	-	0,6,6	-	-	-		
82	OHX	sR	1973	-	0,6,6	-	-	-		
82	OHX	sR	1950	-	0,6,6	-	-	-		
82	OHX	A	2133	-	0,6,6	-	-	-		
82	OHX	CL	303	-	0,6,6	-	-	-		
82	OHX	AR	3610	-	0,6,6	-	-	-		
82	OHX	1	4090	-	0,6,6	-	-	-		
82	OHX	1	4110	-	0,6,6	-	-	-		
82	OHX	AR	3449	-	0,6,6	-	-	-		
82	OHX	sR	2167	-	0,6,6	-	-	-		
82	OHX	1	3565	-	0,6,6	-	-	-		
82	OHX	AR	3447	-	0,6,6	-	-	-		
82	OHX	1	4117	-	0,6,6	-	-	-		
82	OHX	1	4112	-	0,6,6	-	-	-		
82	OHX	4	204	-	0,6,6	-	-	-		
82	OHX	sR	1942	-	0,6,6	-	-	-		
82	OHX	1	3488	-	0,6,6	-	-	-		
82	OHX	AR	3620	-	0,6,6	-	-	-		
82	OHX	1	3419	-	0,6,6	-	-	-		
82	OHX	sR	1955	-	0,6,6	-	-	-		
82	OHX	1	3588	-	0,6,6	-	-	-		
82	OHX	1	3503	-	0,6,6	-	-	-		
82	OHX	AR	3493	-	0,6,6	-	-	-		
82	OHX	A	1931	-	0,6,6	-	-	-		
82	OHX	sR	1967	-	0,6,6	-	-	-		
82	OHX	AR	3619	-	0,6,6	-	-	-		
82	OHX	DL	103	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	1	3556	-	0,6,6	-	-	-		
82	OHX	1	3535[B]	-	0,6,6	-	-	-		
82	OHX	AR	3459	-	0,6,6	-	-	-		
82	OHX	A	1933	-	0,6,6	-	-	-		
82	OHX	AT	201	-	0,6,6	-	-	-		
82	OHX	1	3592	83	0,6,6	-	-	-		
82	OHX	1	4115	83	0,6,6	-	-	-		
82	OHX	1	3473	-	0,6,6	-	-	-		
82	OHX	1	4113	-	0,6,6	-	-	-		
82	OHX	1	3544	-	0,6,6	-	-	-		
82	OHX	1	4134	-	0,6,6	-	-	-		
82	OHX	1	3529	-	0,6,6	-	-	-		
82	OHX	1	3482	-	0,6,6	-	-	-		
82	OHX	1	4062	-	0,6,6	-	-	-		
82	OHX	1	3469	-	0,6,6	-	-	-		
82	OHX	4	228	-	0,6,6	-	-	-		
82	OHX	1	3441	-	0,6,6	-	-	-		
82	OHX	1	4119	-	0,6,6	-	-	-		
82	OHX	sR	1989	-	0,6,6	-	-	-		
82	OHX	1	3543	-	0,6,6	-	-	-		
82	OHX	AS	206	-	0,6,6	-	-	-		
82	OHX	1	3501	-	0,6,6	-	-	-		
82	OHX	AR	3453	-	0,6,6	-	-	-		
82	OHX	AR	3444	-	0,6,6	-	-	-		
82	OHX	AR	3481	-	0,6,6	-	-	-		
82	OHX	1	3425	-	0,6,6	-	-	-		
82	OHX	sR	1999	-	0,6,6	-	-	-		
82	OHX	1	3513	-	0,6,6	-	-	-		
82	OHX	1	4105	-	0,6,6	-	-	-		
82	OHX	AR	3501	-	0,6,6	-	-	-		
82	OHX	1	3403	-	0,6,6	-	-	-		
82	OHX	1	3508	-	0,6,6	-	-	-		
82	OHX	1	3576	-	0,6,6	-	-	-		
82	OHX	4	207	-	0,6,6	-	-	-		
82	OHX	AR	3451	-	0,6,6	-	-	-		
82	OHX	1	4094	-	0,6,6	-	-	-		
82	OHX	sR	1962	-	0,6,6	-	-	-		
82	OHX	1	3551	-	0,6,6	-	-	-		
82	OHX	AT	234	-	0,6,6	-	-	-		
82	OHX	sR	2002	-	0,6,6	-	-	-		
82	OHX	1	4133	-	0,6,6	-	-	-		
82	OHX	A	1971	-	0,6,6	-	-	-		
82	OHX	AR	3670	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	OHX	1	4095	-	0,6,6	-	-	-		
82	OHX	A	2114	-	0,6,6	-	-	-		
82	OHX	A	2116	-	0,6,6	-	-	-		
82	OHX	AR	3433	-	0,6,6	-	-	-		
82	OHX	CS	201	-	0,6,6	-	-	-		
82	OHX	AR	3667	-	0,6,6	-	-	-		
82	OHX	AT	202	-	0,6,6	-	-	-		
82	OHX	sR	1951	-	0,6,6	-	-	-		
82	OHX	AR	3615	83	0,6,6	-	-	-		
82	OHX	AT	209	-	0,6,6	-	-	-		
82	OHX	A	2126[B]	-	0,6,6	-	-	-		
82	OHX	DQ	502	83	0,6,6	-	-	-		
82	OHX	AS	202	-	0,6,6	-	-	-		
82	OHX	AT	206	-	0,6,6	-	-	-		
82	OHX	1	3412	-	0,6,6	-	-	-		
82	OHX	1	3454	-	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	X1K	AR	4205	-	-	0/8/58/58	0/3/3/3
86	X1K	1	4181	-	-	2/8/58/58	0/3/3/3
85	SPD	AR	4204	-	-	2/7/7/7	-
85	SPD	1	4180	-	-	2/7/7/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	AR	4205	X1K	C1-C10	-2.44	1.52	1.56
86	AR	4205	X1K	C5-C10	2.09	1.59	1.56
86	1	4181	X1K	C5-C10	2.03	1.59	1.56

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
86	1	4181	X1K	C1-C10-C5	-7.82	107.86	116.78
86	1	4181	X1K	C20-C1-C2	-5.82	97.05	109.03
86	AR	4205	X1K	C1-C10-C5	-5.21	110.83	116.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
86	1	4181	X1K	C20-C1-C	-4.51	101.24	107.89
86	AR	4205	X1K	C20-C1-C	-4.22	101.68	107.89

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	1	4181	X1K	C13-C14-C15-C16
85	AR	4204	SPD	C3-C4-C5-N6
85	1	4180	SPD	C3-C4-C5-N6
86	1	4181	X1K	C6-C13-C14-C15
85	AR	4204	SPD	N1-C2-C3-C4

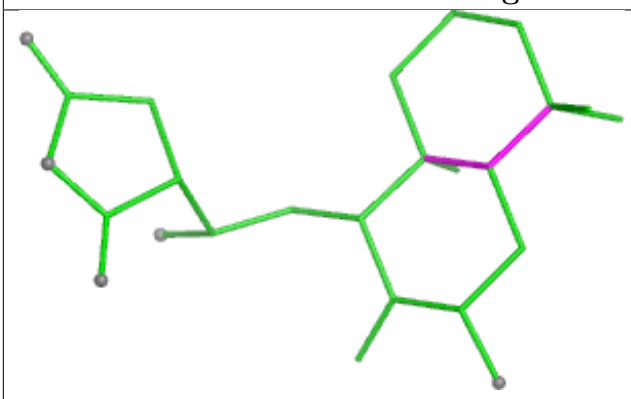
There are no ring outliers.

2 monomers are involved in 2 short contacts:

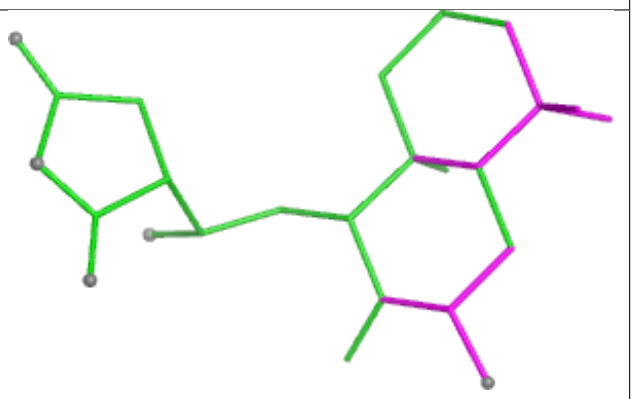
Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	AR	3440	OHX	0	1
82	CG	304	OHX	0	1

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.

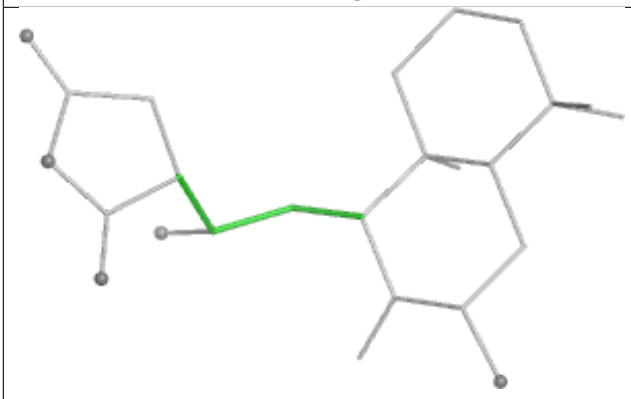
Ligand X1K AR 4205



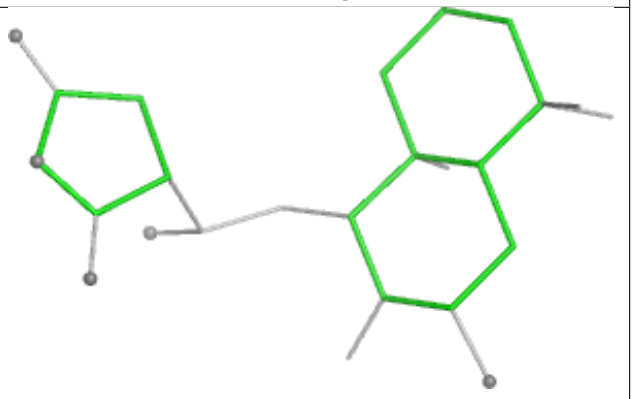
Bond lengths



Bond angles

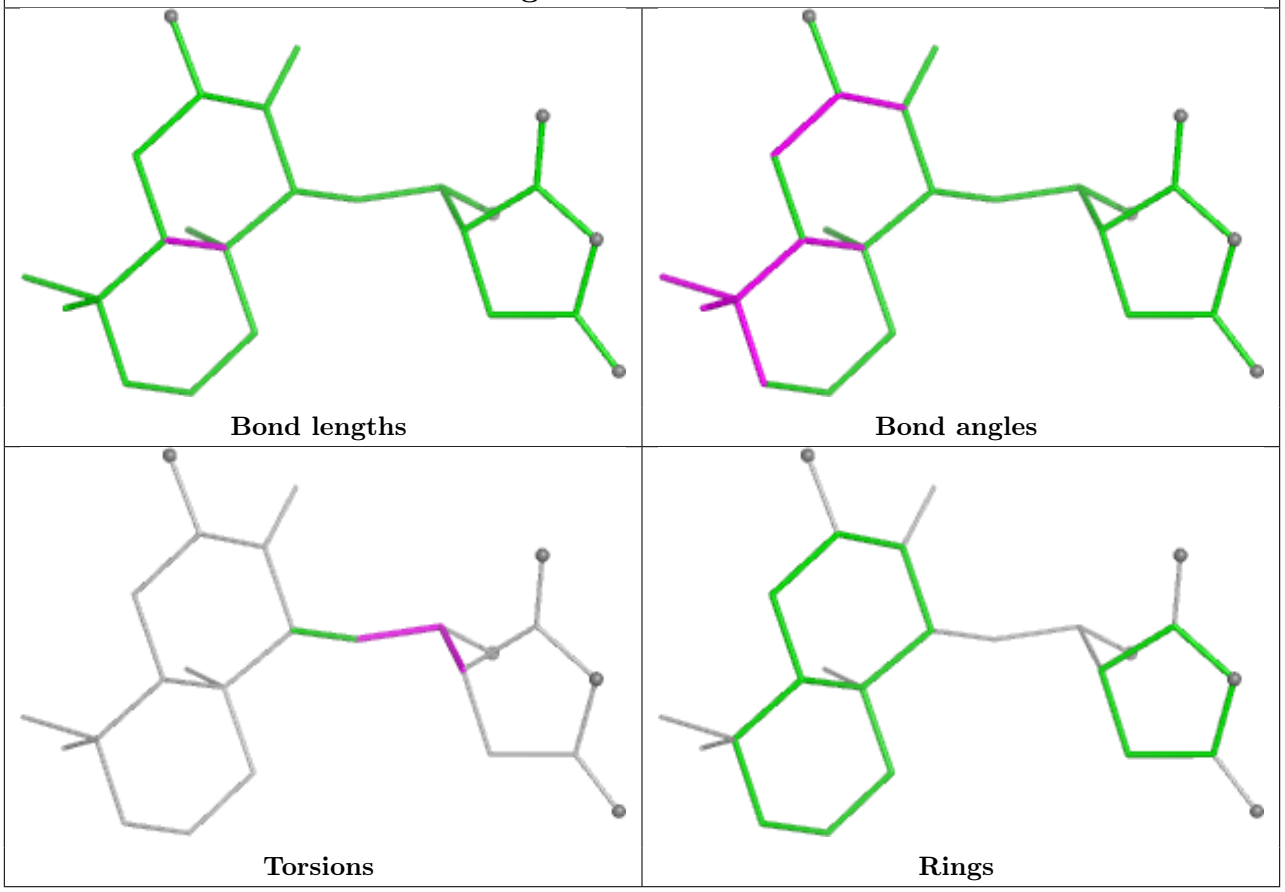


Torsions



Rings

Ligand X1K 1 4181



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
58	c0	1
47	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	c0	84:GLU	C	87:HIS	N	9.31
1	A	1716:C	O3'	1717:G	P	4.49

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.