



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4U4U / pdb_00004u4u
Title : Crystal structure of Lycorine bound to the yeast 80S ribosome
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Deposited on : 2014-07-24
Resolution : 3.00 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 ⓘ 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 ⓘ](#)) 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 3.00 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 411211 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	1750	Total	C	N	O	P	0	0	0
			37283	16668	6591	12274	1750			
1	6	1795	Total	C	N	O	P	0	0	0
			38238	17095	6758	12590	1795			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	C6	141	Total	C	N	O		0	0	0
			1105	708	203	194				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	c6	142	Total	C	N	O	0	0	0
			1111	711	204	196			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	D6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			
28	d6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	l2	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	M9	188	Total	C	N	O		0	0	0
			1521	935	326	260				
55	m9	188	Total	C	N	O		0	0	0
			1521	935	326	260				

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 81 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
81	sM	104	Total	C	N	O	0	0	0
			681	404	140	137			

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

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

- Molecule 83 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 84 is a protein called unknown protein chain p1.

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

- Molecule 85 is a protein called unknown protein chain p2.

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

- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	2	123	Total	Mg	0	0
			123	123		
86	S2	1	Total	Mg	0	0
			1	1		
86	S8	1	Total	Mg	0	0
			1	1		
86	D0	1	Total	Mg	0	0
			1	1		
86	D3	1	Total	Mg	0	0
			1	1		
86	D4	1	Total	Mg	0	0
			1	1		
86	SM	1	Total	Mg	0	0
			1	1		
86	1	477	Total	Mg	0	0
			477	477		
86	3	14	Total	Mg	0	0
			14	14		
86	4	21	Total	Mg	0	0
			21	21		
86	L2	1	Total	Mg	0	0
			1	1		
86	L3	2	Total	Mg	0	0
			2	2		
86	L4	2	Total	Mg	0	0
			2	2		
86	L5	2	Total	Mg	0	0
			2	2		
86	L7	2	Total	Mg	0	0
			2	2		
86	L8	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	M0	2	Total 2	Mg 2	0	0
86	M1	1	Total 1	Mg 1	0	0
86	M3	3	Total 3	Mg 3	0	0
86	M5	1	Total 1	Mg 1	0	0
86	M6	1	Total 1	Mg 1	0	0
86	M7	6	Total 6	Mg 6	0	0
86	M8	1	Total 1	Mg 1	0	0
86	M9	1	Total 1	Mg 1	0	0
86	N0	1	Total 1	Mg 1	0	0
86	N3	3	Total 3	Mg 3	0	0
86	N5	1	Total 1	Mg 1	0	0
86	N8	3	Total 3	Mg 3	0	0
86	O4	1	Total 1	Mg 1	0	0
86	O7	1	Total 1	Mg 1	0	0
86	O8	1	Total 1	Mg 1	0	0
86	Q2	1	Total 1	Mg 1	0	0
86	6	149	Total 149	Mg 149	0	0
86	s1	1	Total 1	Mg 1	0	0
86	s4	1	Total 1	Mg 1	0	0
86	s8	2	Total 2	Mg 2	0	0
86	c1	1	Total 1	Mg 1	0	0

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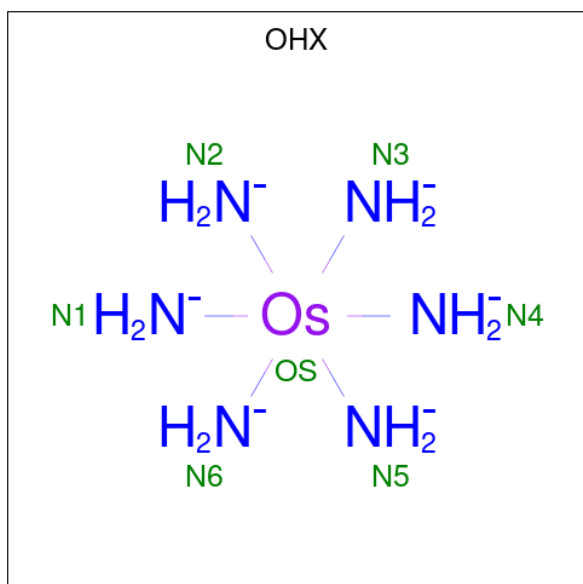
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	c7	1	Total 1	Mg 1	0	0
86	d3	2	Total 2	Mg 2	0	0
86	d4	1	Total 1	Mg 1	0	0
86	sM	2	Total 2	Mg 2	0	0
86	5	506	Total 506	Mg 506	0	0
86	7	16	Total 16	Mg 16	0	0
86	8	14	Total 14	Mg 14	0	0
86	l2	2	Total 2	Mg 2	0	0
86	l3	2	Total 2	Mg 2	0	0
86	l4	1	Total 1	Mg 1	0	0
86	l5	2	Total 2	Mg 2	0	0
86	l7	2	Total 2	Mg 2	0	0
86	l9	1	Total 1	Mg 1	0	0
86	m1	1	Total 1	Mg 1	0	0
86	m5	3	Total 3	Mg 3	0	0
86	m6	1	Total 1	Mg 1	0	0
86	m7	5	Total 5	Mg 5	0	0
86	n0	1	Total 1	Mg 1	0	0
86	n3	2	Total 2	Mg 2	0	0
86	n6	1	Total 1	Mg 1	0	0
86	n8	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	o1	2	Total	Mg	0	0
			2	2		
86	o3	2	Total	Mg	0	0
			2	2		
86	o4	1	Total	Mg	0	0
			1	1		
86	q0	1	Total	Mg	0	0
			1	1		
86	q1	1	Total	Mg	0	0
			1	1		
86	q3	1	Total	Mg	0	0
			1	1		

- Molecule 87 is osmium (III) hexammine (CCD ID: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	S8	1	Total	N	Os	0	0
			7	6	1		
87	C3	1	Total	N	Os	0	0
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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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87	M0	1	Total	N	Os	0	0
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87	M5	1	Total	N	Os	0	0
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87	M6	1	Total	N	Os	0	0
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87	M7	1	Total	N	Os	0	0
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87	M7	1	Total	N	Os	0	0
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87	N1	1	Total	N	Os	0	0
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87	N9	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	O7	1	Total	N	Os	0	0
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87	O7	1	Total	N	Os	0	0
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87	O9	1	Total	N	Os	0	0
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87	Q2	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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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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87	6	1	Total	N	Os	0	0
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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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87	s4	1	Total	N	Os	0	0
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87	s8	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	c3	1	Total	N	Os	0	0
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87	c5	1	Total	N	Os	0	0
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87	c8	1	Total	N	Os	0	0
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87	d4	1	Total	N	Os	0	0
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87	d9	1	Total	N	Os	0	0
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87	sR	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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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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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
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87	5	1	Total	N	Os	0	0
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
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87	5	1	Total	N	Os	0	0
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
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			7	6	1		
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
			7	6	1		
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87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
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			7	6	1		
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87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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87	5	1	Total	N	Os	0	0
			7	6	1		
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
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87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
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			7	6	1		
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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87	5	1	Total	N	Os	0	0
			7	6	1		
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87	5	1	Total	N	Os	0	0
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
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87	7	1	Total	N	Os	0	0
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87	8	1	Total	N	Os	0	0
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87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	8	1	Total 7	N 6	Os 1	0	0
87	8	1	Total 7	N 6	Os 1	0	0
87	8	1	Total 7	N 6	Os 1	0	0
87	8	1	Total 7	N 6	Os 1	0	0
87	8	1	Total 7	N 6	Os 1	0	0
87	8	1	Total 7	N 6	Os 1	0	0
87	8	1	Total 7	N 6	Os 1	0	0
87	8	1	Total 7	N 6	Os 1	0	0
87	8	1	Total 7	N 6	Os 1	0	0
87	8	1	Total 7	N 6	Os 1	0	0
87	8	1	Total 7	N 6	Os 1	0	0
87	13	1	Total 7	N 6	Os 1	0	0
87	13	1	Total 7	N 6	Os 1	0	0
87	14	1	Total 7	N 6	Os 1	0	0
87	14	1	Total 7	N 6	Os 1	0	0
87	15	1	Total 7	N 6	Os 1	0	0
87	15	1	Total 7	N 6	Os 1	0	0
87	15	1	Total 7	N 6	Os 1	0	0
87	19	1	Total 7	N 6	Os 1	0	0
87	m0	1	Total 7	N 6	Os 1	0	0
87	m0	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	m1	1	Total	N	Os	0	0
			7	6	1		
87	m4	1	Total	N	Os	0	0
			7	6	1		
87	m5	1	Total	N	Os	0	0
			7	6	1		
87	m6	1	Total	N	Os	0	0
			7	6	1		
87	m7	1	Total	N	Os	0	0
			7	6	1		
87	m8	1	Total	N	Os	0	0
			7	6	1		
87	m9	1	Total	N	Os	0	0
			7	6	1		
87	n3	1	Total	N	Os	0	0
			7	6	1		
87	n6	1	Total	N	Os	0	0
			7	6	1		
87	n9	1	Total	N	Os	0	0
			7	6	1		
87	o2	1	Total	N	Os	0	0
			7	6	1		
87	o3	1	Total	N	Os	0	0
			7	6	1		
87	o7	1	Total	N	Os	0	0
			7	6	1		
87	o7	1	Total	N	Os	0	0
			7	6	1		
87	q2	1	Total	N	Os	0	0
			7	6	1		

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

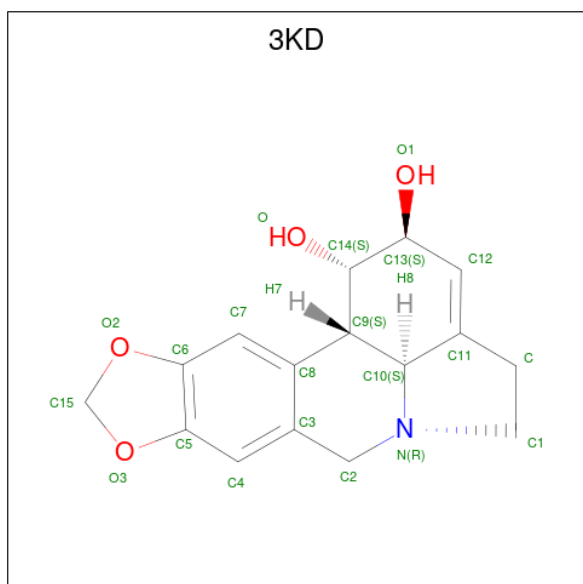
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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88	D7	1	Total	Zn	0	0
			1	1		
88	D9	1	Total	Zn	0	0
			1	1		
88	E1	1	Total	Zn	0	0
			1	1		

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

- Molecule 89 is (1S,2S,12bS,12cS)-2,4,5,7,12b,12c-hexahydro-1H-[1,3]dioxolo[4,5-j]pyrrolo[3,2,1-de]phenanthridine-1,2-diol (CCD ID: 3KD) (formula: C₁₆H₁₇NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
89	1	1	Total	C	N	O	0	0
			21	16	1	4		
89	5	1	Total	C	N	O	0	0
			21	16	1	4		

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

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	435.26Å 287.54Å 304.02Å 90.00° 98.97° 90.00°	Depositor
Resolution (Å)	73.99 – 3.00	Depositor
% Data completeness (in resolution range)	100.0 (73.99-3.00)	Depositor
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.211 , 0.259	Depositor
Wilson B-factor (Å ²)	64.9	Xtriage
Anisotropy	0.199	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411211	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 2563 ligands modelled in this entry, 1428 are monoatomic - leaving 1135 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	$\# Z > 2$
87	OHX	5	4241	-	0,6,6	-	-	-		
87	OHX	1	4201	-	0,6,6	-	-	-		
87	OHX	1	4109	-	0,6,6	-	-	-		
87	OHX	m6	202	86	0,6,6	-	-	-		
87	OHX	c8	201	-	0,6,6	-	-	-		
87	OHX	5	4102	-	0,6,6	-	-	-		
87	OHX	1	3959	-	0,6,6	-	-	-		
87	OHX	1	4100	-	0,6,6	-	-	-		
87	OHX	2	2166	-	0,6,6	-	-	-		
87	OHX	M6	202	-	0,6,6	-	-	-		
87	OHX	1	4138	-	0,6,6	-	-	-		
87	OHX	5	4195	-	0,6,6	-	-	-		
87	OHX	5	3941	86	0,6,6	-	-	-		
87	OHX	2	2157	-	0,6,6	-	-	-		
87	OHX	2	2134	-	0,6,6	-	-	-		
87	OHX	1	4073	86	0,6,6	-	-	-		
87	OHX	6	2051	-	0,6,6	-	-	-		
87	OHX	6	2199	-	0,6,6	-	-	-		
87	OHX	1	4179	-	0,6,6	-	-	-		
87	OHX	2	2132	-	0,6,6	-	-	-		
87	OHX	5	3983	-	0,6,6	-	-	-		
87	OHX	5	3979	-	0,6,6	-	-	-		
87	OHX	1	4102	-	0,6,6	-	-	-		
87	OHX	2	2083	-	0,6,6	-	-	-		
87	OHX	1	3977	-	0,6,6	-	-	-		
87	OHX	6	2173	-	0,6,6	-	-	-		
87	OHX	5	4126	-	0,6,6	-	-	-		
87	OHX	2	2087	-	0,6,6	-	-	-		
87	OHX	5	4175	-	0,6,6	-	-	-		
87	OHX	1	3982	-	0,6,6	-	-	-		
87	OHX	SR	401	-	0,6,6	-	-	-		
87	OHX	5	3971	-	0,6,6	-	-	-		
87	OHX	6	2203	-	0,6,6	-	-	-		
87	OHX	5	3999	-	0,6,6	-	-	-		
87	OHX	5	4144	-	0,6,6	-	-	-		
87	OHX	1	4171	86	0,6,6	-	-	-		
87	OHX	2	2096	-	0,6,6	-	-	-		
87	OHX	1	3945	-	0,6,6	-	-	-		
87	OHX	2	2067	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	4031	-	0,6,6	-	-	-		
87	OHX	5	3938	86	0,6,6	-	-	-		
87	OHX	7	222	-	0,6,6	-	-	-		
87	OHX	5	3973	-	0,6,6	-	-	-		
87	OHX	1	4043	-	0,6,6	-	-	-		
87	OHX	1	3875	-	0,6,6	-	-	-		
87	OHX	6	2082	-	0,6,6	-	-	-		
87	OHX	1	3924	86	0,6,6	-	-	-		
87	OHX	1	4002	-	0,6,6	-	-	-		
87	OHX	5	3970	-	0,6,6	-	-	-		
87	OHX	6	2129	-	0,6,6	-	-	-		
87	OHX	2	2116	-	0,6,6	-	-	-		
87	OHX	2	2030	-	0,6,6	-	-	-		
87	OHX	1	4208	-	0,6,6	-	-	-		
87	OHX	5	4140	-	0,6,6	-	-	-		
87	OHX	n6	202	-	0,6,6	-	-	-		
87	OHX	5	3942	-	0,6,6	-	-	-		
87	OHX	6	2108	-	0,6,6	-	-	-		
87	OHX	1	3916	-	0,6,6	-	-	-		
87	OHX	5	4158	-	0,6,6	-	-	-		
87	OHX	5	3923	-	0,6,6	-	-	-		
87	OHX	5	4089	-	0,6,6	-	-	-		
87	OHX	6	2176	-	0,6,6	-	-	-		
87	OHX	5	4182	-	0,6,6	-	-	-		
87	OHX	1	4110	-	0,6,6	-	-	-		
87	OHX	6	2138	-	0,6,6	-	-	-		
87	OHX	2	2138	-	0,6,6	-	-	-		
87	OHX	5	3993	-	0,6,6	-	-	-		
87	OHX	1	4034	-	0,6,6	-	-	-		
87	OHX	5	4082	-	0,6,6	-	-	-		
87	OHX	2	2028	-	0,6,6	-	-	-		
87	OHX	1	4160	-	0,6,6	-	-	-		
87	OHX	5	4079	-	0,6,6	-	-	-		
87	OHX	1	3988	86	0,6,6	-	-	-		
87	OHX	5	3944	-	0,6,6	-	-	-		
87	OHX	2	2088	-	0,6,6	-	-	-		
87	OHX	5	4009	86	0,6,6	-	-	-		
87	OHX	5	4035	-	0,6,6	-	-	-		
87	OHX	q2	502	86	0,6,6	-	-	-		
87	OHX	1	3957	-	0,6,6	-	-	-		
87	OHX	6	2201	-	0,6,6	-	-	-		
87	OHX	5	4239	-	0,6,6	-	-	-		
87	OHX	1	3870	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4165	-	0,6,6	-	-	-		
87	OHX	1	4085	-	0,6,6	-	-	-		
87	OHX	1	3960	-	0,6,6	-	-	-		
87	OHX	1	3980	-	0,6,6	-	-	-		
87	OHX	3	224	-	0,6,6	-	-	-		
87	OHX	M7	207	86	0,6,6	-	-	-		
87	OHX	7	224	-	0,6,6	-	-	-		
87	OHX	6	2070	-	0,6,6	-	-	-		
87	OHX	6	2114	-	0,6,6	-	-	-		
87	OHX	2	2026	86	0,6,6	-	-	-		
87	OHX	1	3946	-	0,6,6	-	-	-		
87	OHX	1	3969	-	0,6,6	-	-	-		
87	OHX	5	3945	-	0,6,6	-	-	-		
87	OHX	5	4061	-	0,6,6	-	-	-		
87	OHX	5	4240	-	0,6,6	-	-	-		
87	OHX	1	4058	86	0,6,6	-	-	-		
87	OHX	1	4112	-	0,6,6	-	-	-		
87	OHX	5	4085	-	0,6,6	-	-	-		
87	OHX	5	4205	-	0,6,6	-	-	-		
87	OHX	5	4238	-	0,6,6	-	-	-		
87	OHX	5	4218	-	0,6,6	-	-	-		
87	OHX	5	3910	-	0,6,6	-	-	-		
87	OHX	2	2079	-	0,6,6	-	-	-		
87	OHX	4	230	-	0,6,6	-	-	-		
87	OHX	2	2089	-	0,6,6	-	-	-		
87	OHX	1	3967	-	0,6,6	-	-	-		
87	OHX	1	4094	-	0,6,6	-	-	-		
87	OHX	2	2133	-	0,6,6	-	-	-		
87	OHX	6	2089	-	0,6,6	-	-	-		
87	OHX	5	4231	-	0,6,6	-	-	-		
87	OHX	6	2061	-	0,6,6	-	-	-		
87	OHX	1	3949	-	0,6,6	-	-	-		
87	OHX	3	216	86	0,6,6	-	-	-		
87	OHX	1	3926	-	0,6,6	-	-	-		
87	OHX	5	4002	-	0,6,6	-	-	-		
87	OHX	5	3982	-	0,6,6	-	-	-		
87	OHX	2	2044	-	0,6,6	-	-	-		
87	OHX	1	3962	-	0,6,6	-	-	-		
87	OHX	1	4154	-	0,6,6	-	-	-		
87	OHX	5	3914	-	0,6,6	-	-	-		
87	OHX	5	4094	-	0,6,6	-	-	-		
87	OHX	1	3981	86	0,6,6	-	-	-		
87	OHX	1	4130	86	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	2191	-	0,6,6	-	-	-		
87	OHX	5	3906	-	0,6,6	-	-	-		
87	OHX	2	2058	-	0,6,6	-	-	-		
87	OHX	1	4136	-	0,6,6	-	-	-		
87	OHX	5	4023	-	0,6,6	-	-	-		
87	OHX	5	4217	86	0,6,6	-	-	-		
87	OHX	6	2123	-	0,6,6	-	-	-		
87	OHX	2	2151	-	0,6,6	-	-	-		
87	OHX	5	4012	-	0,6,6	-	-	-		
87	OHX	1	3874	-	0,6,6	-	-	-		
87	OHX	5	3962	-	0,6,6	-	-	-		
87	OHX	5	4090	86	0,6,6	-	-	-		
87	OHX	O9	101	-	0,6,6	-	-	-		
87	OHX	7	219	-	0,6,6	-	-	-		
87	OHX	2	2109	-	0,6,6	-	-	-		
87	OHX	1	3965	-	0,6,6	-	-	-		
87	OHX	1	4149	-	0,6,6	-	-	-		
87	OHX	1	4188	-	0,6,6	-	-	-		
87	OHX	6	2086	-	0,6,6	-	-	-		
87	OHX	1	4117	86	0,6,6	-	-	-		
87	OHX	6	2158	-	0,6,6	-	-	-		
87	OHX	L3	404	-	0,6,6	-	-	-		
87	OHX	6	2171	86	0,6,6	-	-	-		
87	OHX	5	4055	-	0,6,6	-	-	-		
87	OHX	5	4196	-	0,6,6	-	-	-		
87	OHX	1	4128	86	0,6,6	-	-	-		
87	OHX	5	4138	-	0,6,6	-	-	-		
87	OHX	4	229	-	0,6,6	-	-	-		
87	OHX	6	2197	86	0,6,6	-	-	-		
87	OHX	6	2078	-	0,6,6	-	-	-		
87	OHX	5	4051	-	0,6,6	-	-	-		
87	OHX	1	3891	-	0,6,6	-	-	-		
87	OHX	5	3929	-	0,6,6	-	-	-		
87	OHX	5	4121	-	0,6,6	-	-	-		
87	OHX	5	4018	-	0,6,6	-	-	-		
87	OHX	5	4236	-	0,6,6	-	-	-		
87	OHX	1	4168	-	0,6,6	-	-	-		
87	OHX	6	2152	-	0,6,6	-	-	-		
87	OHX	1	4164	-	0,6,6	-	-	-		
87	OHX	4	226	-	0,6,6	-	-	-		
87	OHX	6	2189	-	0,6,6	-	-	-		
87	OHX	1	4063	-	0,6,6	-	-	-		
87	OHX	1	4180	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	2052	-	0,6,6	-	-	-		
87	OHX	5	4116	-	0,6,6	-	-	-		
87	OHX	2	2038	-	0,6,6	-	-	-		
87	OHX	5	3937	86	0,6,6	-	-	-		
87	OHX	1	4057	-	0,6,6	-	-	-		
87	OHX	3	225	86	0,6,6	-	-	-		
87	OHX	6	2143	-	0,6,6	-	-	-		
87	OHX	5	4168	-	0,6,6	-	-	-		
87	OHX	2	2167	-	0,6,6	-	-	-		
87	OHX	5	4137	-	0,6,6	-	-	-		
87	OHX	2	2178	-	0,6,6	-	-	-		
87	OHX	1	3968	-	0,6,6	-	-	-		
87	OHX	1	4215	86	0,6,6	-	-	-		
87	OHX	6	2092	-	0,6,6	-	-	-		
87	OHX	14	403	-	0,6,6	-	-	-		
87	OHX	5	4001	-	0,6,6	-	-	-		
87	OHX	5	4210	86	0,6,6	-	-	-		
87	OHX	4	224	-	0,6,6	-	-	-		
87	OHX	M0	303	-	0,6,6	-	-	-		
87	OHX	5	3949	-	0,6,6	-	-	-		
87	OHX	1	3898	-	0,6,6	-	-	-		
87	OHX	1	3902	-	0,6,6	-	-	-		
87	OHX	5	4222	-	0,6,6	-	-	-		
87	OHX	6	2169	-	0,6,6	-	-	-		
87	OHX	2	2037	-	0,6,6	-	-	-		
87	OHX	6	2145	-	0,6,6	-	-	-		
87	OHX	5	4215	-	0,6,6	-	-	-		
87	OHX	1	4129	-	0,6,6	-	-	-		
87	OHX	5	4087	86	0,6,6	-	-	-		
87	OHX	5	4154	-	0,6,6	-	-	-		
87	OHX	6	2193	-	0,6,6	-	-	-		
87	OHX	m5	304	-	0,6,6	-	-	-		
87	OHX	5	3955	-	0,6,6	-	-	-		
87	OHX	5	3948	-	0,6,6	-	-	-		
87	OHX	1	3984	-	0,6,6	-	-	-		
87	OHX	1	4003	-	0,6,6	-	-	-		
87	OHX	6	2206	-	0,6,6	-	-	-		
87	OHX	6	2105	-	0,6,6	-	-	-		
87	OHX	6	2155	-	0,6,6	-	-	-		
87	OHX	m0	302	-	0,6,6	-	-	-		
87	OHX	4	232	-	0,6,6	-	-	-		
87	OHX	6	2182	-	0,6,6	-	-	-		
87	OHX	1	4011	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	2186	-	0,6,6	-	-	-		
87	OHX	2	2174	-	0,6,6	-	-	-		
87	OHX	2	2124	-	0,6,6	-	-	-		
87	OHX	6	2094	86	0,6,6	-	-	-		
87	OHX	5	4076	-	0,6,6	-	-	-		
87	OHX	1	3909	-	0,6,6	-	-	-		
87	OHX	1	3934	-	0,6,6	-	-	-		
87	OHX	1	4096	-	0,6,6	-	-	-		
87	OHX	d4	202	-	0,6,6	-	-	-		
87	OHX	6	2111	-	0,6,6	-	-	-		
87	OHX	5	3939	-	0,6,6	-	-	-		
87	OHX	2	2140	-	0,6,6	-	-	-		
87	OHX	5	4033	-	0,6,6	-	-	-		
87	OHX	1	4025	-	0,6,6	-	-	-		
87	OHX	6	2096	86	0,6,6	-	-	-		
87	OHX	1	3883	-	0,6,6	-	-	-		
87	OHX	1	4088	-	0,6,6	-	-	-		
87	OHX	1	4183	-	0,6,6	-	-	-		
87	OHX	6	2120	-	0,6,6	-	-	-		
87	OHX	2	2114	-	0,6,6	-	-	-		
87	OHX	1	4045	-	0,6,6	-	-	-		
87	OHX	6	2064	-	0,6,6	-	-	-		
87	OHX	6	2194	-	0,6,6	-	-	-		
87	OHX	1	4079	-	0,6,6	-	-	-		
87	OHX	6	2181	-	0,6,6	-	-	-		
87	OHX	6	2183	-	0,6,6	-	-	-		
87	OHX	s4	302	-	0,6,6	-	-	-		
87	OHX	5	4096	-	0,6,6	-	-	-		
87	OHX	1	4098	-	0,6,6	-	-	-		
87	OHX	5	4128	-	0,6,6	-	-	-		
87	OHX	5	4186	-	0,6,6	-	-	-		
87	OHX	5	4212	-	0,6,6	-	-	-		
87	OHX	7	217	-	0,6,6	-	-	-		
87	OHX	1	4111	-	0,6,6	-	-	-		
87	OHX	1	3927	-	0,6,6	-	-	-		
87	OHX	5	4120	-	0,6,6	-	-	-		
87	OHX	1	4161	-	0,6,6	-	-	-		
87	OHX	8	227	-	0,6,6	-	-	-		
87	OHX	1	4115	86	0,6,6	-	-	-		
87	OHX	2	2022	-	0,6,6	-	-	-		
87	OHX	2	2093	-	0,6,6	-	-	-		
87	OHX	1	3944	-	0,6,6	-	-	-		
87	OHX	5	4010	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4026	86	0,6,6	-	-	-		
87	OHX	5	4242	-	0,6,6	-	-	-		
87	OHX	2	2144	-	0,6,6	-	-	-		
87	OHX	1	3877	-	0,6,6	-	-	-		
87	OHX	1	4037	-	0,6,6	-	-	-		
87	OHX	5	3919	-	0,6,6	-	-	-		
87	OHX	5	4194	86	0,6,6	-	-	-		
87	OHX	1	3918	-	0,6,6	-	-	-		
87	OHX	6	2073	86	0,6,6	-	-	-		
87	OHX	5	4105	-	0,6,6	-	-	-		
87	OHX	1	4056	-	0,6,6	-	-	-		
87	OHX	6	2100	-	0,6,6	-	-	-		
87	OHX	5	4226	86	0,6,6	-	-	-		
87	OHX	1	4018	-	0,6,6	-	-	-		
87	OHX	1	3921	86	0,6,6	-	-	-		
87	OHX	5	4054	-	0,6,6	-	-	-		
87	OHX	5	4164	-	0,6,6	-	-	-		
87	OHX	5	4208	-	0,6,6	-	-	-		
87	OHX	5	4047	-	0,6,6	-	-	-		
87	OHX	6	2154	-	0,6,6	-	-	-		
87	OHX	1	4072	-	0,6,6	-	-	-		
87	OHX	1	3951	-	0,6,6	-	-	-		
87	OHX	c5	201	-	0,6,6	-	-	-		
87	OHX	5	3922	-	0,6,6	-	-	-		
87	OHX	6	2053	-	0,6,6	-	-	-		
87	OHX	5	3998	-	0,6,6	-	-	-		
87	OHX	1	3925	-	0,6,6	-	-	-		
87	OHX	5	4024	-	0,6,6	-	-	-		
87	OHX	5	4027	86	0,6,6	-	-	-		
87	OHX	5	4117	-	0,6,6	-	-	-		
87	OHX	5	4124	86	0,6,6	-	-	-		
87	OHX	3	226	-	0,6,6	-	-	-		
87	OHX	2	2146	-	0,6,6	-	-	-		
87	OHX	6	2146	-	0,6,6	-	-	-		
87	OHX	5	4032	-	0,6,6	-	-	-		
87	OHX	5	4209	-	0,6,6	-	-	-		
87	OHX	6	2083	-	0,6,6	-	-	-		
87	OHX	1	4197	-	0,6,6	-	-	-		
87	OHX	5	3968	-	0,6,6	-	-	-		
87	OHX	1	4134	-	0,6,6	-	-	-		
87	OHX	1	4178	-	0,6,6	-	-	-		
87	OHX	1	4133	86	0,6,6	-	-	-		
87	OHX	5	3911	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4016	-	0,6,6	-	-	-		
87	OHX	5	4129	-	0,6,6	-	-	-		
87	OHX	5	3950	-	0,6,6	-	-	-		
87	OHX	2	2118	-	0,6,6	-	-	-		
87	OHX	5	3902	-	0,6,6	-	-	-		
87	OHX	8	218	-	0,6,6	-	-	-		
87	OHX	5	4153	-	0,6,6	-	-	-		
87	OHX	5	4237	-	0,6,6	-	-	-		
87	OHX	1	3879	-	0,6,6	-	-	-		
87	OHX	N9	101	-	0,6,6	-	-	-		
87	OHX	1	4204	-	0,6,6	-	-	-		
87	OHX	5	4214	-	0,6,6	-	-	-		
87	OHX	5	4034	-	0,6,6	-	-	-		
87	OHX	5	4149	86	0,6,6	-	-	-		
87	OHX	5	4013	-	0,6,6	-	-	-		
87	OHX	5	4115	-	0,6,6	-	-	-		
87	OHX	5	4147	-	0,6,6	-	-	-		
87	OHX	5	4052	-	0,6,6	-	-	-		
87	OHX	6	2161	-	0,6,6	-	-	-		
87	OHX	l3	404	-	0,6,6	-	-	-		
87	OHX	5	4045	-	0,6,6	-	-	-		
87	OHX	1	3893	-	0,6,6	-	-	-		
87	OHX	1	4198	-	0,6,6	-	-	-		
87	OHX	2	2103	-	0,6,6	-	-	-		
87	OHX	6	2103	-	0,6,6	-	-	-		
87	OHX	1	4092	-	0,6,6	-	-	-		
87	OHX	5	4077	-	0,6,6	-	-	-		
87	OHX	2	2121	-	0,6,6	-	-	-		
87	OHX	5	4073	-	0,6,6	-	-	-		
87	OHX	5	4142	86	0,6,6	-	-	-		
87	OHX	1	3873	-	0,6,6	-	-	-		
87	OHX	5	3943	-	0,6,6	-	-	-		
87	OHX	7	225	-	0,6,6	-	-	-		
87	OHX	1	4010	-	0,6,6	-	-	-		
87	OHX	l5	305	-	0,6,6	-	-	-		
87	OHX	1	4148	86	0,6,6	-	-	-		
87	OHX	6	2202	-	0,6,6	-	-	-		
87	OHX	5	4183	-	0,6,6	-	-	-		
87	OHX	C8	201	-	0,6,6	-	-	-		
87	OHX	2	2065	-	0,6,6	-	-	-		
87	OHX	2	2033	-	0,6,6	-	-	-		
87	OHX	1	4116	86	0,6,6	-	-	-		
87	OHX	1	4173	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2051	-	0,6,6	-	-	-		
87	OHX	1	3974	-	0,6,6	-	-	-		
87	OHX	5	3936	-	0,6,6	-	-	-		
87	OHX	5	3931	-	0,6,6	-	-	-		
87	OHX	5	4141	-	0,6,6	-	-	-		
87	OHX	2	2125	-	0,6,6	-	-	-		
87	OHX	5	3924	-	0,6,6	-	-	-		
87	OHX	5	4190	-	0,6,6	-	-	-		
87	OHX	1	4203	-	0,6,6	-	-	-		
87	OHX	6	2137	-	0,6,6	-	-	-		
87	OHX	5	4246	-	0,6,6	-	-	-		
87	OHX	1	4205	-	0,6,6	-	-	-		
87	OHX	1	4007	-	0,6,6	-	-	-		
87	OHX	5	4022	-	0,6,6	-	-	-		
87	OHX	1	4163	-	0,6,6	-	-	-		
87	OHX	5	3986	-	0,6,6	-	-	-		
87	OHX	5	3915	86	0,6,6	-	-	-		
87	OHX	5	4234	-	0,6,6	-	-	-		
87	OHX	1	3928	86	0,6,6	-	-	-		
87	OHX	1	4087	-	0,6,6	-	-	-		
87	OHX	5	4131	-	0,6,6	-	-	-		
87	OHX	7	226	86	0,6,6	-	-	-		
87	OHX	5	4065	-	0,6,6	-	-	-		
87	OHX	8	221	-	0,6,6	-	-	-		
87	OHX	m1	202	-	0,6,6	-	-	-		
87	OHX	6	2085	-	0,6,6	-	-	-		
87	OHX	2	2054	-	0,6,6	-	-	-		
87	OHX	6	2200	-	0,6,6	-	-	-		
87	OHX	1	4159	-	0,6,6	-	-	-		
87	OHX	1	4137	-	0,6,6	-	-	-		
87	OHX	6	2134	-	0,6,6	-	-	-		
87	OHX	5	4006	-	0,6,6	-	-	-		
87	OHX	1	4200	-	0,6,6	-	-	-		
87	OHX	6	2135	-	0,6,6	-	-	-		
87	OHX	6	2150	86	0,6,6	-	-	-		
87	OHX	5	4101	-	0,6,6	-	-	-		
87	OHX	5	4245	-	0,6,6	-	-	-		
87	OHX	1	4027	-	0,6,6	-	-	-		
87	OHX	2	2027	-	0,6,6	-	-	-		
87	OHX	5	4185	-	0,6,6	-	-	-		
87	OHX	6	2115	-	0,6,6	-	-	-		
87	OHX	5	4191	-	0,6,6	-	-	-		
87	OHX	6	2163	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	2207	-	0,6,6	-	-	-		
87	OHX	2	2076	-	0,6,6	-	-	-		
87	OHX	5	3946	-	0,6,6	-	-	-		
87	OHX	6	2132	-	0,6,6	-	-	-		
87	OHX	2	2175	-	0,6,6	-	-	-		
87	OHX	1	3976	-	0,6,6	-	-	-		
87	OHX	1	4108	-	0,6,6	-	-	-		
87	OHX	1	4192	86	0,6,6	-	-	-		
87	OHX	1	3941	-	0,6,6	-	-	-		
87	OHX	6	2160	86	0,6,6	-	-	-		
87	OHX	5	4064	-	0,6,6	-	-	-		
87	OHX	6	2177	86	0,6,6	-	-	-		
87	OHX	5	4178	86	0,6,6	-	-	-		
87	OHX	2	2036	-	0,6,6	-	-	-		
87	OHX	1	4146	-	0,6,6	-	-	-		
87	OHX	5	4114	86	0,6,6	-	-	-		
87	OHX	8	225	-	0,6,6	-	-	-		
87	OHX	1	3889	-	0,6,6	-	-	-		
87	OHX	2	2095	-	0,6,6	-	-	-		
87	OHX	1	3991	-	0,6,6	-	-	-		
87	OHX	2	2056	86	0,6,6	-	-	-		
87	OHX	5	4083	86	0,6,6	-	-	-		
87	OHX	1	4126	-	0,6,6	-	-	-		
87	OHX	1	4165	-	0,6,6	-	-	-		
87	OHX	1	3890	-	0,6,6	-	-	-		
87	OHX	O2	201	-	0,6,6	-	-	-		
87	OHX	5	4198	-	0,6,6	-	-	-		
87	OHX	5	4122	-	0,6,6	-	-	-		
87	OHX	5	3900	-	0,6,6	-	-	-		
89	3KD	5	4254	-	24,25,25	1.04	2 (8%)	30,39,39	1.06	1 (3%)
87	OHX	2	2090	-	0,6,6	-	-	-		
87	OHX	5	4107	-	0,6,6	-	-	-		
87	OHX	6	2179	-	0,6,6	-	-	-		
87	OHX	4	222	-	0,6,6	-	-	-		
87	OHX	5	4249	-	0,6,6	-	-	-		
87	OHX	1	3973	-	0,6,6	-	-	-		
87	OHX	3	218	-	0,6,6	-	-	-		
87	OHX	7	220	86	0,6,6	-	-	-		
87	OHX	6	2109	-	0,6,6	-	-	-		
87	OHX	6	2054	-	0,6,6	-	-	-		
87	OHX	n3	203	-	0,6,6	-	-	-		
87	OHX	5	3926	-	0,6,6	-	-	-		
87	OHX	1	3970	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	8	216	-	0,6,6	-	-	-		
87	OHX	2	2077	86	0,6,6	-	-	-		
87	OHX	2	2063	-	0,6,6	-	-	-		
87	OHX	1	3876	-	0,6,6	-	-	-		
87	OHX	1	3899	86	0,6,6	-	-	-		
87	OHX	1	4008	-	0,6,6	-	-	-		
87	OHX	2	2048	-	0,6,6	-	-	-		
87	OHX	6	2164	-	0,6,6	-	-	-		
87	OHX	2	2059	-	0,6,6	-	-	-		
87	OHX	5	4167	-	0,6,6	-	-	-		
87	OHX	5	4066	-	0,6,6	-	-	-		
87	OHX	6	2088	-	0,6,6	-	-	-		
87	OHX	1	4131	-	0,6,6	-	-	-		
87	OHX	5	4074	-	0,6,6	-	-	-		
87	OHX	2	2176	-	0,6,6	-	-	-		
87	OHX	1	3906	-	0,6,6	-	-	-		
87	OHX	5	4155	-	0,6,6	-	-	-		
87	OHX	sR	401	-	0,6,6	-	-	-		
87	OHX	1	4028	-	0,6,6	-	-	-		
87	OHX	1	4059	-	0,6,6	-	-	-		
87	OHX	5	4088	-	0,6,6	-	-	-		
87	OHX	7	223	-	0,6,6	-	-	-		
87	OHX	1	4124	-	0,6,6	-	-	-		
87	OHX	1	4084	-	0,6,6	-	-	-		
87	OHX	5	3976	-	0,6,6	-	-	-		
87	OHX	m9	201	-	0,6,6	-	-	-		
87	OHX	1	3929	86	0,6,6	-	-	-		
87	OHX	1	4101	-	0,6,6	-	-	-		
87	OHX	5	3956	-	0,6,6	-	-	-		
87	OHX	2	2091	-	0,6,6	-	-	-		
87	OHX	2	2073	-	0,6,6	-	-	-		
87	OHX	1	4104	-	0,6,6	-	-	-		
87	OHX	n9	101	-	0,6,6	-	-	-		
87	OHX	5	3994	86	0,6,6	-	-	-		
87	OHX	2	2021	-	0,6,6	-	-	-		
87	OHX	1	4212	-	0,6,6	-	-	-		
87	OHX	1	4181	-	0,6,6	-	-	-		
87	OHX	1	4061	-	0,6,6	-	-	-		
87	OHX	6	2107	-	0,6,6	-	-	-		
87	OHX	8	220	-	0,6,6	-	-	-		
87	OHX	1	3940	-	0,6,6	-	-	-		
87	OHX	1	3952	86	0,6,6	-	-	-		
87	OHX	1	4044	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4038	-	0,6,6	-	-	-		
87	OHX	5	3905	-	0,6,6	-	-	-		
87	OHX	5	4029	-	0,6,6	-	-	-		
87	OHX	5	4091	86	0,6,6	-	-	-		
87	OHX	6	2072	86	0,6,6	-	-	-		
87	OHX	5	4173	-	0,6,6	-	-	-		
87	OHX	2	2057	-	0,6,6	-	-	-		
87	OHX	2	2117	-	0,6,6	-	-	-		
87	OHX	5	4040	-	0,6,6	-	-	-		
87	OHX	5	4223	-	0,6,6	-	-	-		
87	OHX	8	226	-	0,6,6	-	-	-		
87	OHX	1	3983	-	0,6,6	-	-	-		
87	OHX	6	2066	-	0,6,6	-	-	-		
87	OHX	s8	303	-	0,6,6	-	-	-		
87	OHX	5	4244	-	0,6,6	-	-	-		
87	OHX	2	2170	-	0,6,6	-	-	-		
87	OHX	2	2034	-	0,6,6	-	-	-		
87	OHX	6	2151	-	0,6,6	-	-	-		
87	OHX	5	3977	-	0,6,6	-	-	-		
87	OHX	1	3871	-	0,6,6	-	-	-		
87	OHX	2	2111	-	0,6,6	-	-	-		
87	OHX	5	4170	86	0,6,6	-	-	-		
87	OHX	1	4114	-	0,6,6	-	-	-		
87	OHX	1	4053	-	0,6,6	-	-	-		
87	OHX	5	3934	-	0,6,6	-	-	-		
87	OHX	l5	303	-	0,6,6	-	-	-		
87	OHX	1	3912	-	0,6,6	-	-	-		
87	OHX	1	4106	-	0,6,6	-	-	-		
87	OHX	2	2082	-	0,6,6	-	-	-		
87	OHX	1	4118	-	0,6,6	-	-	-		
87	OHX	5	4072	-	0,6,6	-	-	-		
87	OHX	8	223	-	0,6,6	-	-	-		
87	OHX	1	4023	-	0,6,6	-	-	-		
87	OHX	6	2118	-	0,6,6	-	-	-		
87	OHX	4	225	86	0,6,6	-	-	-		
87	OHX	5	4248	86	0,6,6	-	-	-		
87	OHX	2	2123	-	0,6,6	-	-	-		
87	OHX	1	3997	-	0,6,6	-	-	-		
87	OHX	1	4093	-	0,6,6	-	-	-		
87	OHX	1	3939	-	0,6,6	-	-	-		
87	OHX	4	223	-	0,6,6	-	-	-		
87	OHX	1	4141	-	0,6,6	-	-	-		
87	OHX	1	3908	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4113	-	0,6,6	-	-	-		
87	OHX	5	4159	-	0,6,6	-	-	-		
87	OHX	5	4070	-	0,6,6	-	-	-		
87	OHX	1	4211	-	0,6,6	-	-	-		
87	OHX	5	3920	86	0,6,6	-	-	-		
87	OHX	5	4193	-	0,6,6	-	-	-		
87	OHX	2	2158	-	0,6,6	-	-	-		
87	OHX	1	3975	-	0,6,6	-	-	-		
87	OHX	2	2142	-	0,6,6	-	-	-		
87	OHX	2	2086	-	0,6,6	-	-	-		
87	OHX	1	4020	-	0,6,6	-	-	-		
87	OHX	1	4196	-	0,6,6	-	-	-		
87	OHX	6	2192	-	0,6,6	-	-	-		
87	OHX	1	3930	-	0,6,6	-	-	-		
87	OHX	1	4068	-	0,6,6	-	-	-		
87	OHX	5	4201	-	0,6,6	-	-	-		
87	OHX	o7	502	-	0,6,6	-	-	-		
87	OHX	l5	304	-	0,6,6	-	-	-		
87	OHX	s1	303	-	0,6,6	-	-	-		
87	OHX	1	4021	-	0,6,6	-	-	-		
87	OHX	5	4020	-	0,6,6	-	-	-		
87	OHX	6	2141	-	0,6,6	-	-	-		
87	OHX	5	4139	-	0,6,6	-	-	-		
87	OHX	C3	201	-	0,6,6	-	-	-		
87	OHX	6	2172	-	0,6,6	-	-	-		
87	OHX	6	2178	-	0,6,6	-	-	-		
87	OHX	2	2152	-	0,6,6	-	-	-		
87	OHX	1	3904	-	0,6,6	-	-	-		
87	OHX	5	3987	-	0,6,6	-	-	-		
87	OHX	6	2162	-	0,6,6	-	-	-		
87	OHX	1	3919	86	0,6,6	-	-	-		
87	OHX	1	4195	-	0,6,6	-	-	-		
87	OHX	5	3975	-	0,6,6	-	-	-		
87	OHX	2	2101	-	0,6,6	-	-	-		
87	OHX	2	2052	-	0,6,6	-	-	-		
87	OHX	2	2100	-	0,6,6	-	-	-		
87	OHX	1	4091	-	0,6,6	-	-	-		
87	OHX	5	4062	-	0,6,6	-	-	-		
87	OHX	6	2156	-	0,6,6	-	-	-		
87	OHX	5	3957	-	0,6,6	-	-	-		
87	OHX	3	222	-	0,6,6	-	-	-		
87	OHX	5	4037	-	0,6,6	-	-	-		
87	OHX	6	2081	86	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	8	219	-	0,6,6	-	-	-		
87	OHX	6	2055	-	0,6,6	-	-	-		
87	OHX	7	227	-	0,6,6	-	-	-		
87	OHX	5	4127	-	0,6,6	-	-	-		
87	OHX	5	4095	-	0,6,6	-	-	-		
87	OHX	1	4032	-	0,6,6	-	-	-		
87	OHX	6	2131	-	0,6,6	-	-	-		
87	OHX	1	3880	-	0,6,6	-	-	-		
87	OHX	5	3969	-	0,6,6	-	-	-		
87	OHX	1	4190	-	0,6,6	-	-	-		
87	OHX	6	2069	-	0,6,6	-	-	-		
87	OHX	2	2069	-	0,6,6	-	-	-		
87	OHX	6	2174	-	0,6,6	-	-	-		
87	OHX	1	3971	-	0,6,6	-	-	-		
87	OHX	1	3996	-	0,6,6	-	-	-		
87	OHX	1	3911	-	0,6,6	-	-	-		
87	OHX	3	221	-	0,6,6	-	-	-		
87	OHX	6	2124	-	0,6,6	-	-	-		
87	OHX	2	2043	-	0,6,6	-	-	-		
87	OHX	5	4207	-	0,6,6	-	-	-		
87	OHX	1	4144	-	0,6,6	-	-	-		
87	OHX	1	4107	-	0,6,6	-	-	-		
87	OHX	M7	208	-	0,6,6	-	-	-		
87	OHX	6	2140	-	0,6,6	-	-	-		
87	OHX	5	4080	-	0,6,6	-	-	-		
87	OHX	1	3998	-	0,6,6	-	-	-		
87	OHX	1	3992	-	0,6,6	-	-	-		
87	OHX	1	4123	-	0,6,6	-	-	-		
87	OHX	2	2155	-	0,6,6	-	-	-		
87	OHX	1	4209	-	0,6,6	-	-	-		
87	OHX	2	2106	-	0,6,6	-	-	-		
87	OHX	6	2060	-	0,6,6	-	-	-		
87	OHX	5	3907	-	0,6,6	-	-	-		
87	OHX	5	3908	-	0,6,6	-	-	-		
87	OHX	1	4151	-	0,6,6	-	-	-		
87	OHX	6	2121	-	0,6,6	-	-	-		
87	OHX	5	4211	-	0,6,6	-	-	-		
87	OHX	2	2094	-	0,6,6	-	-	-		
87	OHX	1	3900	-	0,6,6	-	-	-		
87	OHX	5	3958	-	0,6,6	-	-	-		
87	OHX	6	2112	-	0,6,6	-	-	-		
87	OHX	5	4176	-	0,6,6	-	-	-		
87	OHX	1	4217	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4204	-	0,6,6	-	-	-		
87	OHX	7	218	-	0,6,6	-	-	-		
87	OHX	1	4187	-	0,6,6	-	-	-		
87	OHX	1	3923	-	0,6,6	-	-	-		
87	OHX	5	3991	-	0,6,6	-	-	-		
87	OHX	1	4186	86	0,6,6	-	-	-		
87	OHX	5	4108	-	0,6,6	-	-	-		
87	OHX	2	2024	-	0,6,6	-	-	-		
87	OHX	1	3886	-	0,6,6	-	-	-		
87	OHX	1	3942	-	0,6,6	-	-	-		
87	OHX	1	4216	86	0,6,6	-	-	-		
87	OHX	5	4224	86	0,6,6	-	-	-		
87	OHX	m7	206	-	0,6,6	-	-	-		
87	OHX	2	2119	-	0,6,6	-	-	-		
87	OHX	5	4188	-	0,6,6	-	-	-		
87	OHX	1	4050	-	0,6,6	-	-	-		
87	OHX	1	4030	-	0,6,6	-	-	-		
87	OHX	1	4095	-	0,6,6	-	-	-		
87	OHX	1	4120	-	0,6,6	-	-	-		
87	OHX	2	2169	-	0,6,6	-	-	-		
87	OHX	2	2066	86	0,6,6	-	-	-		
87	OHX	5	4171	-	0,6,6	-	-	-		
87	OHX	1	3872	-	0,6,6	-	-	-		
87	OHX	1	4004	-	0,6,6	-	-	-		
87	OHX	5	4031	-	0,6,6	-	-	-		
87	OHX	1	4194	86	0,6,6	-	-	-		
87	OHX	2	2147	-	0,6,6	-	-	-		
87	OHX	s9	201	-	0,6,6	-	-	-		
87	OHX	1	4135	-	0,6,6	-	-	-		
87	OHX	5	3940	-	0,6,6	-	-	-		
87	OHX	2	2062	86	0,6,6	-	-	-		
87	OHX	1	4029	-	0,6,6	-	-	-		
87	OHX	1	4140	-	0,6,6	-	-	-		
87	OHX	1	4166	-	0,6,6	-	-	-		
87	OHX	5	4156	-	0,6,6	-	-	-		
87	OHX	2	2097	-	0,6,6	-	-	-		
87	OHX	2	2154	-	0,6,6	-	-	-		
87	OHX	6	2084	-	0,6,6	-	-	-		
87	OHX	5	3992	-	0,6,6	-	-	-		
87	OHX	2	2126	-	0,6,6	-	-	-		
87	OHX	6	2166	-	0,6,6	-	-	-		
87	OHX	2	2053	-	0,6,6	-	-	-		
87	OHX	1	3915	86	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4057	-	0,6,6	-	-	-		
87	OHX	8	217	-	0,6,6	-	-	-		
87	OHX	1	4005	-	0,6,6	-	-	-		
87	OHX	5	4163	-	0,6,6	-	-	-		
87	OHX	1	4042	-	0,6,6	-	-	-		
87	OHX	5	3928	-	0,6,6	-	-	-		
87	OHX	5	4059	-	0,6,6	-	-	-		
87	OHX	5	4008	-	0,6,6	-	-	-		
87	OHX	1	4143	-	0,6,6	-	-	-		
87	OHX	2	2041	86	0,6,6	-	-	-		
87	OHX	D9	102	-	0,6,6	-	-	-		
87	OHX	2	2149	-	0,6,6	-	-	-		
87	OHX	2	2060	-	0,6,6	-	-	-		
87	OHX	1	3878	-	0,6,6	-	-	-		
87	OHX	1	3978	-	0,6,6	-	-	-		
87	OHX	1	4152	-	0,6,6	-	-	-		
87	OHX	1	4145	-	0,6,6	-	-	-		
87	OHX	2	2102	-	0,6,6	-	-	-		
87	OHX	1	4038	-	0,6,6	-	-	-		
87	OHX	1	4153	-	0,6,6	-	-	-		
87	OHX	5	3953	-	0,6,6	-	-	-		
87	OHX	5	3988	-	0,6,6	-	-	-		
87	OHX	2	2135	-	0,6,6	-	-	-		
87	OHX	2	2104	-	0,6,6	-	-	-		
87	OHX	1	3903	-	0,6,6	-	-	-		
87	OHX	1	4103	-	0,6,6	-	-	-		
87	OHX	5	4187	-	0,6,6	-	-	-		
87	OHX	5	3960	86	0,6,6	-	-	-		
87	OHX	5	3980	-	0,6,6	-	-	-		
87	OHX	6	2122	-	0,6,6	-	-	-		
87	OHX	6	2067	-	0,6,6	-	-	-		
87	OHX	1	4076	86	0,6,6	-	-	-		
87	OHX	6	2204	-	0,6,6	-	-	-		
87	OHX	1	4147	-	0,6,6	-	-	-		
87	OHX	Q2	503	86	0,6,6	-	-	-		
87	OHX	1	4090	-	0,6,6	-	-	-		
87	OHX	6	2075	-	0,6,6	-	-	-		
87	OHX	1	4155	-	0,6,6	-	-	-		
87	OHX	6	2195	-	0,6,6	-	-	-		
87	OHX	6	2065	-	0,6,6	-	-	-		
87	OHX	5	4007	-	0,6,6	-	-	-		
87	OHX	5	4084	-	0,6,6	-	-	-		
87	OHX	2	2035	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3933	-	0,6,6	-	-	-		
87	OHX	2	2080	-	0,6,6	-	-	-		
87	OHX	S8	302	-	0,6,6	-	-	-		
87	OHX	1	4064	-	0,6,6	-	-	-		
87	OHX	5	4247	-	0,6,6	-	-	-		
87	OHX	1	4055	-	0,6,6	-	-	-		
87	OHX	1	4086	-	0,6,6	-	-	-		
87	OHX	2	2120	-	0,6,6	-	-	-		
87	OHX	5	4078	-	0,6,6	-	-	-		
87	OHX	5	4172	-	0,6,6	-	-	-		
87	OHX	19	202	-	0,6,6	-	-	-		
87	OHX	5	4225	-	0,6,6	-	-	-		
87	OHX	1	4184	-	0,6,6	-	-	-		
87	OHX	6	2119	-	0,6,6	-	-	-		
87	OHX	5	3974	-	0,6,6	-	-	-		
87	OHX	5	4253	86	0,6,6	-	-	-		
87	OHX	1	4017	-	0,6,6	-	-	-		
87	OHX	1	4169	-	0,6,6	-	-	-		
87	OHX	5	4203	-	0,6,6	-	-	-		
87	OHX	1	4062	-	0,6,6	-	-	-		
87	OHX	1	4121	-	0,6,6	-	-	-		
87	OHX	2	2160	-	0,6,6	-	-	-		
87	OHX	1	4206	-	0,6,6	-	-	-		
87	OHX	5	3921	-	0,6,6	-	-	-		
87	OHX	5	4123	86	0,6,6	-	-	-		
87	OHX	2	2177	-	0,6,6	-	-	-		
87	OHX	1	3990	-	0,6,6	-	-	-		
87	OHX	1	4193	-	0,6,6	-	-	-		
87	OHX	1	4132	-	0,6,6	-	-	-		
87	OHX	2	2047	-	0,6,6	-	-	-		
87	OHX	6	2130	-	0,6,6	-	-	-		
87	OHX	5	3963	86	0,6,6	-	-	-		
87	OHX	6	2128	-	0,6,6	-	-	-		
87	OHX	5	3995	86	0,6,6	-	-	-		
87	OHX	6	2062	-	0,6,6	-	-	-		
87	OHX	2	2078	-	0,6,6	-	-	-		
87	OHX	1	4172	-	0,6,6	-	-	-		
87	OHX	5	4003	-	0,6,6	-	-	-		
87	OHX	5	4017	-	0,6,6	-	-	-		
87	OHX	c1	202	-	0,6,6	-	-	-		
87	OHX	5	4130	-	0,6,6	-	-	-		
87	OHX	1	4022	-	0,6,6	-	-	-		
87	OHX	6	2059	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	2068	-	0,6,6	-	-	-		
87	OHX	5	3978	-	0,6,6	-	-	-		
87	OHX	2	2029	-	0,6,6	-	-	-		
87	OHX	5	4132	-	0,6,6	-	-	-		
87	OHX	L3	403	-	0,6,6	-	-	-		
87	OHX	o2	201	-	0,6,6	-	-	-		
87	OHX	1	4182	-	0,6,6	-	-	-		
87	OHX	3	217	86	0,6,6	-	-	-		
87	OHX	2	2129	-	0,6,6	-	-	-		
87	OHX	1	4019	-	0,6,6	-	-	-		
87	OHX	6	2136	-	0,6,6	-	-	-		
87	OHX	5	4067	86	0,6,6	-	-	-		
87	OHX	5	4150	-	0,6,6	-	-	-		
87	OHX	6	2071	-	0,6,6	-	-	-		
87	OHX	2	2071	-	0,6,6	-	-	-		
87	OHX	1	4012	-	0,6,6	-	-	-		
87	OHX	5	4106	-	0,6,6	-	-	-		
87	OHX	5	4118	-	0,6,6	-	-	-		
87	OHX	2	2110	-	0,6,6	-	-	-		
87	OHX	1	3964	-	0,6,6	-	-	-		
87	OHX	5	3997	-	0,6,6	-	-	-		
87	OHX	2	2085	-	0,6,6	-	-	-		
87	OHX	5	4021	-	0,6,6	-	-	-		
87	OHX	6	2076	86	0,6,6	-	-	-		
87	OHX	5	4143	-	0,6,6	-	-	-		
87	OHX	1	3985	-	0,6,6	-	-	-		
87	OHX	6	2175	-	0,6,6	-	-	-		
87	OHX	1	4213	86	0,6,6	-	-	-		
87	OHX	1	3950	-	0,6,6	-	-	-		
87	OHX	1	4006	-	0,6,6	-	-	-		
87	OHX	5	3964	-	0,6,6	-	-	-		
87	OHX	2	2150	-	0,6,6	-	-	-		
87	OHX	6	2104	-	0,6,6	-	-	-		
87	OHX	5	3913	-	0,6,6	-	-	-		
87	OHX	5	4086	-	0,6,6	-	-	-		
87	OHX	5	3909	-	0,6,6	-	-	-		
87	OHX	5	4233	-	0,6,6	-	-	-		
87	OHX	1	3896	86	0,6,6	-	-	-		
87	OHX	1	4049	-	0,6,6	-	-	-		
87	OHX	5	3930	86	0,6,6	-	-	-		
87	OHX	5	4100	86	0,6,6	-	-	-		
87	OHX	2	2148	-	0,6,6	-	-	-		
87	OHX	1	4167	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2050	-	0,6,6	-	-	-		
87	OHX	1	4066	-	0,6,6	-	-	-		
87	OHX	5	4036	-	0,6,6	-	-	-		
87	OHX	5	4063	-	0,6,6	-	-	-		
87	OHX	1	3956	-	0,6,6	-	-	-		
87	OHX	6	2095	-	0,6,6	-	-	-		
87	OHX	5	4152	-	0,6,6	-	-	-		
87	OHX	5	4177	86	0,6,6	-	-	-		
87	OHX	2	2032	-	0,6,6	-	-	-		
87	OHX	6	2056	-	0,6,6	-	-	-		
87	OHX	6	2180	-	0,6,6	-	-	-		
87	OHX	5	4044	-	0,6,6	-	-	-		
87	OHX	6	2153	-	0,6,6	-	-	-		
87	OHX	1	4000	-	0,6,6	-	-	-		
87	OHX	1	4075	-	0,6,6	-	-	-		
87	OHX	6	2057	-	0,6,6	-	-	-		
87	OHX	m4	201	-	0,6,6	-	-	-		
87	OHX	2	2127	-	0,6,6	-	-	-		
87	OHX	5	4119	-	0,6,6	-	-	-		
87	OHX	1	4202	-	0,6,6	-	-	-		
87	OHX	1	3961	-	0,6,6	-	-	-		
87	OHX	5	4104	-	0,6,6	-	-	-		
87	OHX	8	222	-	0,6,6	-	-	-		
87	OHX	5	4068	-	0,6,6	-	-	-		
87	OHX	1	4142	-	0,6,6	-	-	-		
87	OHX	5	3935	86	0,6,6	-	-	-		
87	OHX	6	2087	-	0,6,6	-	-	-		
87	OHX	1	4071	-	0,6,6	-	-	-		
87	OHX	2	2172	-	0,6,6	-	-	-		
87	OHX	1	4089	-	0,6,6	-	-	-		
87	OHX	2	2098	-	0,6,6	-	-	-		
87	OHX	1	4083	-	0,6,6	-	-	-		
87	OHX	m8	201	-	0,6,6	-	-	-		
87	OHX	1	4040	-	0,6,6	-	-	-		
87	OHX	5	4092	-	0,6,6	-	-	-		
87	OHX	6	2098	-	0,6,6	-	-	-		
87	OHX	O3	201	-	0,6,6	-	-	-		
87	OHX	1	4122	86	0,6,6	-	-	-		
87	OHX	6	2099	-	0,6,6	-	-	-		
87	OHX	5	3952	-	0,6,6	-	-	-		
87	OHX	5	4135	-	0,6,6	-	-	-		
87	OHX	1	4026	-	0,6,6	-	-	-		
87	OHX	5	3984	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	M9	202	-	0,6,6	-	-	-		
87	OHX	6	2077	-	0,6,6	-	-	-		
87	OHX	6	2063	-	0,6,6	-	-	-		
87	OHX	5	3989	-	0,6,6	-	-	-		
87	OHX	1	4048	-	0,6,6	-	-	-		
87	OHX	5	4184	-	0,6,6	-	-	-		
87	OHX	5	4043	-	0,6,6	-	-	-		
87	OHX	L4	403	-	0,6,6	-	-	-		
87	OHX	5	3901	-	0,6,6	-	-	-		
87	OHX	1	3897	-	0,6,6	-	-	-		
87	OHX	1	4105	-	0,6,6	-	-	-		
87	OHX	5	4011	-	0,6,6	-	-	-		
87	OHX	1	4054	-	0,6,6	-	-	-		
87	OHX	2	2055	-	0,6,6	-	-	-		
87	OHX	2	2070	-	0,6,6	-	-	-		
87	OHX	5	4206	-	0,6,6	-	-	-		
87	OHX	6	2116	-	0,6,6	-	-	-		
87	OHX	2	2168	-	0,6,6	-	-	-		
87	OHX	5	4005	-	0,6,6	-	-	-		
87	OHX	l3	403	-	0,6,6	-	-	-		
87	OHX	5	3965	-	0,6,6	-	-	-		
87	OHX	O7	103	86	0,6,6	-	-	-		
87	OHX	1	4125	-	0,6,6	-	-	-		
87	OHX	5	4042	-	0,6,6	-	-	-		
87	OHX	2	2045	-	0,6,6	-	-	-		
87	OHX	1	4113	-	0,6,6	-	-	-		
87	OHX	2	2164	-	0,6,6	-	-	-		
87	OHX	2	2075	-	0,6,6	-	-	-		
87	OHX	1	4060	-	0,6,6	-	-	-		
87	OHX	1	4067	-	0,6,6	-	-	-		
87	OHX	6	2157	-	0,6,6	-	-	-		
87	OHX	5	4200	-	0,6,6	-	-	-		
87	OHX	2	2171	-	0,6,6	-	-	-		
87	OHX	5	4098	-	0,6,6	-	-	-		
87	OHX	5	4093	-	0,6,6	-	-	-		
87	OHX	1	4074	-	0,6,6	-	-	-		
87	OHX	5	3903	-	0,6,6	-	-	-		
87	OHX	5	4041	-	0,6,6	-	-	-		
87	OHX	1	3882	-	0,6,6	-	-	-		
87	OHX	6	2091	-	0,6,6	-	-	-		
87	OHX	2	2139	-	0,6,6	-	-	-		
87	OHX	5	4219	-	0,6,6	-	-	-		
87	OHX	5	4097	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	2058	-	0,6,6	-	-	-		
87	OHX	5	4192	-	0,6,6	-	-	-		
87	OHX	1	3887	-	0,6,6	-	-	-		
87	OHX	2	2159	-	0,6,6	-	-	-		
87	OHX	1	4174	-	0,6,6	-	-	-		
87	OHX	6	2148	-	0,6,6	-	-	-		
87	OHX	6	2159	-	0,6,6	-	-	-		
87	OHX	2	2141	86	0,6,6	-	-	-		
87	OHX	5	3996	-	0,6,6	-	-	-		
87	OHX	1	4210	-	0,6,6	-	-	-		
87	OHX	2	2137	-	0,6,6	-	-	-		
87	OHX	1	3979	-	0,6,6	-	-	-		
87	OHX	1	4177	-	0,6,6	-	-	-		
87	OHX	6	2185	-	0,6,6	-	-	-		
87	OHX	5	4058	-	0,6,6	-	-	-		
87	OHX	1	3953	86	0,6,6	-	-	-		
87	OHX	1	3885	-	0,6,6	-	-	-		
87	OHX	5	4227	-	0,6,6	-	-	-		
87	OHX	2	2107	-	0,6,6	-	-	-		
87	OHX	1	4046	-	0,6,6	-	-	-		
87	OHX	2	2074	-	0,6,6	-	-	-		
87	OHX	5	4099	-	0,6,6	-	-	-		
87	OHX	1	4039	-	0,6,6	-	-	-		
87	OHX	1	3955	-	0,6,6	-	-	-		
87	OHX	5	4166	-	0,6,6	-	-	-		
87	OHX	1	3938	-	0,6,6	-	-	-		
87	OHX	6	2205	-	0,6,6	-	-	-		
87	OHX	5	3990	86	0,6,6	-	-	-		
87	OHX	1	3963	86	0,6,6	-	-	-		
87	OHX	5	4133	86	0,6,6	-	-	-		
87	OHX	5	4146	-	0,6,6	-	-	-		
87	OHX	5	4243	-	0,6,6	-	-	-		
87	OHX	6	2090	-	0,6,6	-	-	-		
87	OHX	1	3895	-	0,6,6	-	-	-		
87	OHX	5	3954	-	0,6,6	-	-	-		
87	OHX	2	2156	-	0,6,6	-	-	-		
87	OHX	6	2170	-	0,6,6	-	-	-		
87	OHX	5	4220	86	0,6,6	-	-	-		
87	OHX	2	2046	-	0,6,6	-	-	-		
87	OHX	2	2072	-	0,6,6	-	-	-		
87	OHX	1	3931	-	0,6,6	-	-	-		
87	OHX	1	3936	86	0,6,6	-	-	-		
87	OHX	1	4016	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	4162	-	0,6,6	-	-	-		
87	OHX	1	4175	-	0,6,6	-	-	-		
87	OHX	5	4103	-	0,6,6	-	-	-		
87	OHX	4	233	-	0,6,6	-	-	-		
87	OHX	5	3981	-	0,6,6	-	-	-		
87	OHX	5	4151	-	0,6,6	-	-	-		
87	OHX	2	2105	-	0,6,6	-	-	-		
87	OHX	1	3947	-	0,6,6	-	-	-		
87	OHX	5	4136	-	0,6,6	-	-	-		
87	OHX	1	4158	-	0,6,6	-	-	-		
87	OHX	m0	301	-	0,6,6	-	-	-		
87	OHX	2	2131	86	0,6,6	-	-	-		
87	OHX	2	2061	-	0,6,6	-	-	-		
87	OHX	6	2142	-	0,6,6	-	-	-		
87	OHX	5	4162	-	0,6,6	-	-	-		
87	OHX	1	3986	-	0,6,6	-	-	-		
87	OHX	3	219	-	0,6,6	-	-	-		
87	OHX	M5	302	-	0,6,6	-	-	-		
87	OHX	5	3947	-	0,6,6	-	-	-		
87	OHX	3	215	-	0,6,6	-	-	-		
87	OHX	6	2102	-	0,6,6	-	-	-		
87	OHX	1	4065	-	0,6,6	-	-	-		
87	OHX	2	2153	-	0,6,6	-	-	-		
87	OHX	1	4070	-	0,6,6	-	-	-		
87	OHX	5	3966	86	0,6,6	-	-	-		
87	OHX	1	3995	-	0,6,6	-	-	-		
87	OHX	5	4028	-	0,6,6	-	-	-		
87	OHX	1	3920	-	0,6,6	-	-	-		
87	OHX	2	2165	-	0,6,6	-	-	-		
87	OHX	6	2165	86	0,6,6	-	-	-		
87	OHX	5	4110	-	0,6,6	-	-	-		
87	OHX	5	4228	-	0,6,6	-	-	-		
87	OHX	1	4009	-	0,6,6	-	-	-		
87	OHX	5	4148	-	0,6,6	-	-	-		
87	OHX	6	2139	-	0,6,6	-	-	-		
87	OHX	5	4169	-	0,6,6	-	-	-		
87	OHX	1	3907	86	0,6,6	-	-	-		
87	OHX	5	4049	-	0,6,6	-	-	-		
87	OHX	1	4036	-	0,6,6	-	-	-		
87	OHX	N1	201	-	0,6,6	-	-	-		
87	OHX	5	4060	-	0,6,6	-	-	-		
87	OHX	6	2101	-	0,6,6	-	-	-		
87	OHX	6	2187	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3958	-	0,6,6	-	-	-		
87	OHX	1	4069	-	0,6,6	-	-	-		
87	OHX	1	4176	-	0,6,6	-	-	-		
87	OHX	5	4046	-	0,6,6	-	-	-		
87	OHX	5	4039	-	0,6,6	-	-	-		
87	OHX	1	4191	-	0,6,6	-	-	-		
87	OHX	5	4075	-	0,6,6	-	-	-		
87	OHX	1	4185	-	0,6,6	-	-	-		
87	OHX	2	2113	-	0,6,6	-	-	-		
87	OHX	8	224	-	0,6,6	-	-	-		
87	OHX	1	3922	-	0,6,6	-	-	-		
87	OHX	6	2074	-	0,6,6	-	-	-		
87	OHX	1	3987	86	0,6,6	-	-	-		
87	OHX	6	2113	-	0,6,6	-	-	-		
87	OHX	5	4180	86	0,6,6	-	-	-		
87	OHX	5	4202	-	0,6,6	-	-	-		
87	OHX	8	229	-	0,6,6	-	-	-		
87	OHX	5	3961	86	0,6,6	-	-	-		
87	OHX	5	4069	-	0,6,6	-	-	-		
87	OHX	1	4157	-	0,6,6	-	-	-		
87	OHX	5	4221	-	0,6,6	-	-	-		
87	OHX	5	4014	86	0,6,6	-	-	-		
87	OHX	5	4232	-	0,6,6	-	-	-		
87	OHX	2	2064	-	0,6,6	-	-	-		
87	OHX	5	4197	-	0,6,6	-	-	-		
87	OHX	3	220	-	0,6,6	-	-	-		
87	OHX	6	2117	86	0,6,6	-	-	-		
87	OHX	6	2079	-	0,6,6	-	-	-		
87	OHX	6	2196	-	0,6,6	-	-	-		
87	OHX	5	4250	-	0,6,6	-	-	-		
87	OHX	6	2133	-	0,6,6	-	-	-		
87	OHX	5	3959	86	0,6,6	-	-	-		
87	OHX	1	4001	-	0,6,6	-	-	-		
87	OHX	5	3985	-	0,6,6	-	-	-		
87	OHX	1	3905	-	0,6,6	-	-	-		
87	OHX	1	4099	-	0,6,6	-	-	-		
87	OHX	1	3914	-	0,6,6	-	-	-		
87	OHX	5	4199	-	0,6,6	-	-	-		
87	OHX	5	3933	-	0,6,6	-	-	-		
87	OHX	2	2092	-	0,6,6	-	-	-		
87	OHX	M8	202	-	0,6,6	-	-	-		
87	OHX	5	3912	-	0,6,6	-	-	-		
87	OHX	1	4207	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	4081	-	0,6,6	-	-	-		
87	OHX	C5	201	-	0,6,6	-	-	-		
87	OHX	1	4013	-	0,6,6	-	-	-		
87	OHX	2	2108	-	0,6,6	-	-	-		
87	OHX	1	3999	-	0,6,6	-	-	-		
87	OHX	1	4080	-	0,6,6	-	-	-		
87	OHX	6	2190	-	0,6,6	-	-	-		
87	OHX	14	402	-	0,6,6	-	-	-		
87	OHX	1	4052	-	0,6,6	-	-	-		
87	OHX	1	4170	-	0,6,6	-	-	-		
87	OHX	1	4189	-	0,6,6	-	-	-		
87	OHX	O7	104	-	0,6,6	-	-	-		
87	OHX	d9	102	-	0,6,6	-	-	-		
87	OHX	3	223	-	0,6,6	-	-	-		
87	OHX	5	4213	-	0,6,6	-	-	-		
87	OHX	2	2042	-	0,6,6	-	-	-		
87	OHX	1	4077	86	0,6,6	-	-	-		
87	OHX	1	3892	86	0,6,6	-	-	-		
87	OHX	2	2122	-	0,6,6	-	-	-		
87	OHX	2	2162	-	0,6,6	-	-	-		
87	OHX	1	3989	-	0,6,6	-	-	-		
87	OHX	5	4189	-	0,6,6	-	-	-		
87	OHX	1	4214	86	0,6,6	-	-	-		
87	OHX	2	2039	-	0,6,6	-	-	-		
87	OHX	s1	302	86	0,6,6	-	-	-		
87	OHX	1	3917	-	0,6,6	-	-	-		
87	OHX	1	3913	-	0,6,6	-	-	-		
87	OHX	1	3932	-	0,6,6	-	-	-		
87	OHX	2	2173	-	0,6,6	-	-	-		
87	OHX	8	228	-	0,6,6	-	-	-		
87	OHX	5	4111	-	0,6,6	-	-	-		
87	OHX	1	3972	-	0,6,6	-	-	-		
87	OHX	5	4161	86	0,6,6	-	-	-		
87	OHX	4	228	-	0,6,6	-	-	-		
87	OHX	1	3943	-	0,6,6	-	-	-		
87	OHX	6	2144	-	0,6,6	-	-	-		
89	3KD	1	4218	-	24,25,25	0.80	0	30,39,39	1.10	1 (3%)
87	OHX	6	2097	-	0,6,6	-	-	-		
87	OHX	5	3916	-	0,6,6	-	-	-		
87	OHX	6	2126	86	0,6,6	-	-	-		
87	OHX	1	3888	-	0,6,6	-	-	-		
87	OHX	6	2168	-	0,6,6	-	-	-		
87	OHX	5	3967	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	4051	-	0,6,6	-	-	-		
87	OHX	5	4056	-	0,6,6	-	-	-		
87	OHX	1	4035	-	0,6,6	-	-	-		
87	OHX	1	4078	-	0,6,6	-	-	-		
87	OHX	1	4041	-	0,6,6	-	-	-		
87	OHX	1	3910	86	0,6,6	-	-	-		
87	OHX	5	4019	-	0,6,6	-	-	-		
87	OHX	5	4053	86	0,6,6	-	-	-		
87	OHX	o3	203	-	0,6,6	-	-	-		
87	OHX	5	3951	-	0,6,6	-	-	-		
87	OHX	1	4156	-	0,6,6	-	-	-		
87	OHX	5	4081	-	0,6,6	-	-	-		
87	OHX	5	3925	-	0,6,6	-	-	-		
87	OHX	1	4014	-	0,6,6	-	-	-		
87	OHX	5	4157	-	0,6,6	-	-	-		
87	OHX	2	2084	-	0,6,6	-	-	-		
87	OHX	5	4160	-	0,6,6	-	-	-		
87	OHX	1	3954	-	0,6,6	-	-	-		
87	OHX	6	2149	-	0,6,6	-	-	-		
87	OHX	2	2143	-	0,6,6	-	-	-		
87	OHX	1	3948	-	0,6,6	-	-	-		
87	OHX	2	2112	-	0,6,6	-	-	-		
87	OHX	1	4127	86	0,6,6	-	-	-		
87	OHX	2	2049	-	0,6,6	-	-	-		
87	OHX	5	3917	86	0,6,6	-	-	-		
87	OHX	1	4150	-	0,6,6	-	-	-		
87	OHX	2	2145	-	0,6,6	-	-	-		
87	OHX	1	3993	-	0,6,6	-	-	-		
87	OHX	1	3994	86	0,6,6	-	-	-		
87	OHX	4	221	-	0,6,6	-	-	-		
87	OHX	6	2080	-	0,6,6	-	-	-		
87	OHX	2	2081	-	0,6,6	-	-	-		
87	OHX	2	2115	-	0,6,6	-	-	-		
87	OHX	1	4082	-	0,6,6	-	-	-		
87	OHX	6	2127	-	0,6,6	-	-	-		
87	OHX	1	3966	-	0,6,6	-	-	-		
87	OHX	6	2147	-	0,6,6	-	-	-		
87	OHX	6	2184	-	0,6,6	-	-	-		
87	OHX	5	3972	-	0,6,6	-	-	-		
87	OHX	5	4071	86	0,6,6	-	-	-		
87	OHX	5	4025	86	0,6,6	-	-	-		
87	OHX	1	4015	-	0,6,6	-	-	-		
87	OHX	1	3884	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4229	-	0,6,6	-	-	-		
87	OHX	6	2188	-	0,6,6	-	-	-		
87	OHX	5	4181	-	0,6,6	-	-	-		
87	OHX	5	3932	-	0,6,6	-	-	-		
87	OHX	1	3935	-	0,6,6	-	-	-		
87	OHX	2	2040	-	0,6,6	-	-	-		
87	OHX	5	4179	-	0,6,6	-	-	-		
87	OHX	1	4033	86	0,6,6	-	-	-		
87	OHX	1	4097	-	0,6,6	-	-	-		
87	OHX	L3	405	-	0,6,6	-	-	-		
87	OHX	c3	201	-	0,6,6	-	-	-		
87	OHX	o7	503	-	0,6,6	-	-	-		
87	OHX	D3	202	-	0,6,6	-	-	-		
87	OHX	5	3904	-	0,6,6	-	-	-		
87	OHX	1	4119	-	0,6,6	-	-	-		
87	OHX	5	4030	-	0,6,6	-	-	-		
87	OHX	5	4230	-	0,6,6	-	-	-		
87	OHX	5	4251	86	0,6,6	-	-	-		
87	OHX	7	221	86	0,6,6	-	-	-		
87	OHX	5	3927	-	0,6,6	-	-	-		
87	OHX	5	4000	-	0,6,6	-	-	-		
87	OHX	6	2167	-	0,6,6	-	-	-		
87	OHX	2	2161	-	0,6,6	-	-	-		
87	OHX	5	4004	86	0,6,6	-	-	-		
87	OHX	6	2093	-	0,6,6	-	-	-		
87	OHX	5	4048	-	0,6,6	-	-	-		
87	OHX	5	4112	-	0,6,6	-	-	-		
87	OHX	5	4252	-	0,6,6	-	-	-		
87	OHX	6	2198	-	0,6,6	-	-	-		
87	OHX	4	231	-	0,6,6	-	-	-		
87	OHX	5	3918	86	0,6,6	-	-	-		
87	OHX	2	2023	-	0,6,6	-	-	-		
87	OHX	5	4216	-	0,6,6	-	-	-		
87	OHX	1	4139	-	0,6,6	-	-	-		
87	OHX	5	4050	86	0,6,6	-	-	-		
87	OHX	2	2130	-	0,6,6	-	-	-		
87	OHX	8	230	-	0,6,6	-	-	-		
87	OHX	2	2099	-	0,6,6	-	-	-		
87	OHX	2	2128	-	0,6,6	-	-	-		
87	OHX	1	4024	-	0,6,6	-	-	-		
87	OHX	5	4235	-	0,6,6	-	-	-		
87	OHX	6	2110	-	0,6,6	-	-	-		
87	OHX	5	4125	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3901	-	0,6,6	-	-	-		
87	OHX	2	2031	-	0,6,6	-	-	-		
87	OHX	2	2068	-	0,6,6	-	-	-		
87	OHX	1	3937	-	0,6,6	-	-	-		
87	OHX	4	227	-	0,6,6	-	-	-		
87	OHX	1	4199	-	0,6,6	-	-	-		
87	OHX	1	3894	86	0,6,6	-	-	-		
87	OHX	6	2125	-	0,6,6	-	-	-		
87	OHX	2	2136	-	0,6,6	-	-	-		
87	OHX	1	4047	86	0,6,6	-	-	-		
87	OHX	1	3881	-	0,6,6	-	-	-		
87	OHX	5	4134	-	0,6,6	-	-	-		
87	OHX	2	2025	-	0,6,6	-	-	-		
87	OHX	8	215	-	0,6,6	-	-	-		
87	OHX	2	2163	-	0,6,6	-	-	-		
87	OHX	5	4015	-	0,6,6	-	-	-		
87	OHX	5	4109	86	0,6,6	-	-	-		
87	OHX	6	2106	-	0,6,6	-	-	-		
87	OHX	5	4145	86	0,6,6	-	-	-		
87	OHX	6	2050	-	0,6,6	-	-	-		
87	OHX	5	4174	86	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
89	3KD	5	4254	-	-	-	0/5/5/5
89	3KD	1	4218	-	-	-	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	5	4254	3KD	C13-C12	3.04	1.54	1.50
89	5	4254	3KD	C8-C9	-2.40	1.47	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	5	4254	3KD	O-C14-C9	-3.44	101.86	109.57
89	1	4218	3KD	O-C14-C9	-2.91	103.05	109.57

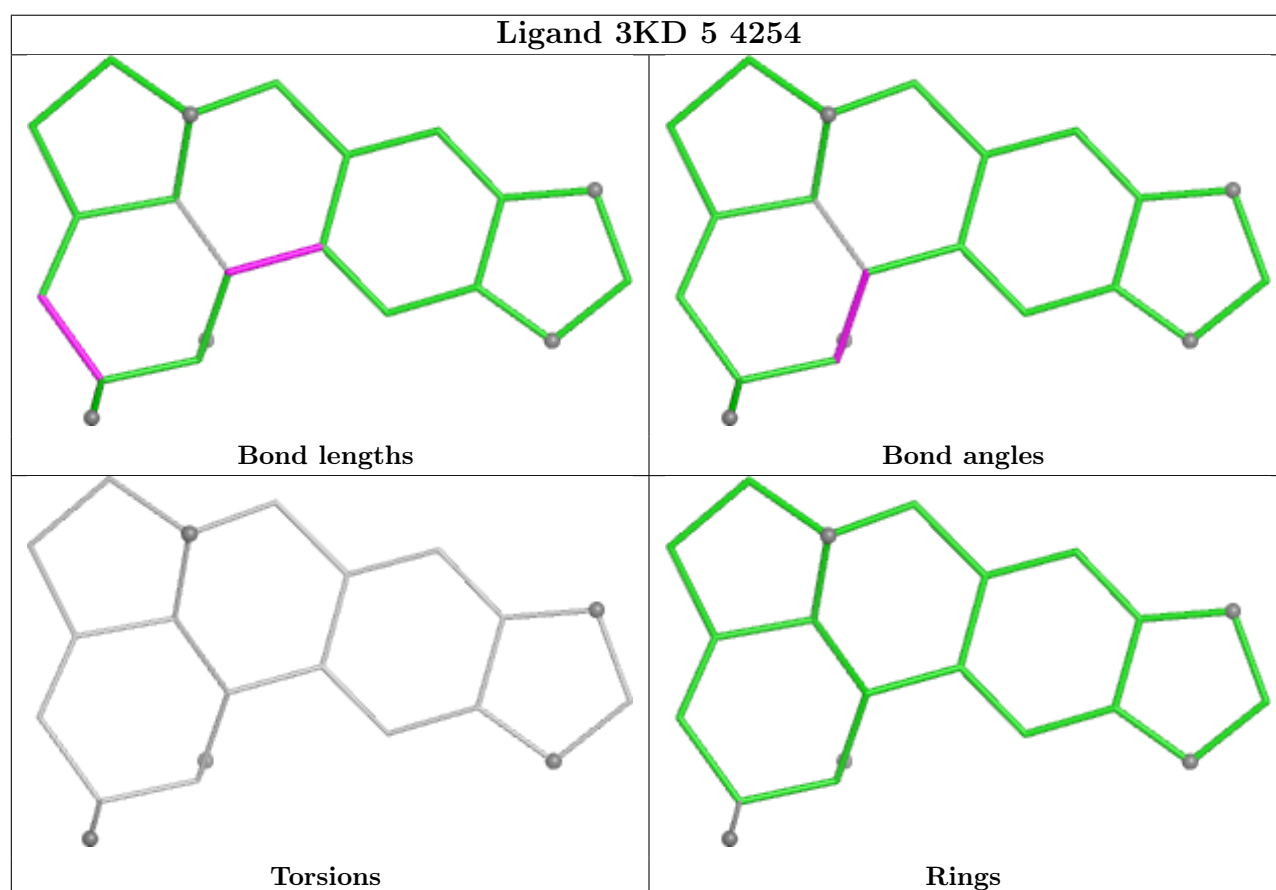
There are no chirality outliers.

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 than 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.



4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

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

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

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

5.3 Carbohydrates [i](#)

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

5.4 Ligands [i](#)

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

5.5 Other polymers [i](#)

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