



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 16, 2017 – 10:34 am GMT

PDB ID : 4U4R
Title : Crystal structure of Lactimidomycin bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 2.80 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	FAILED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28986

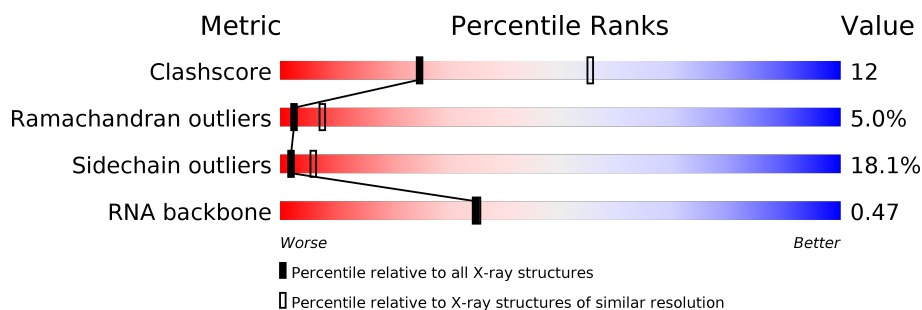
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RNA backbone	2435	1007 (3.10-2.50)





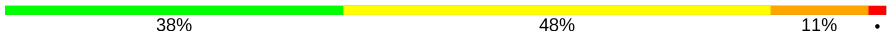

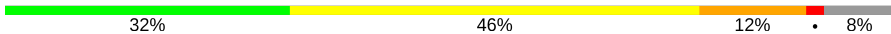

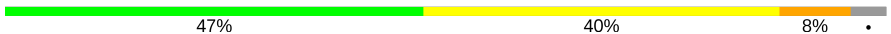

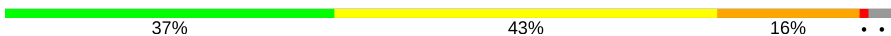

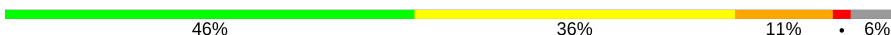







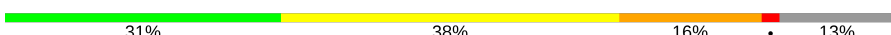




The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	2	1800	
1	6	1800	
2	S0	251	
2	s0	251	
3	S1	254	
3	s1	254	


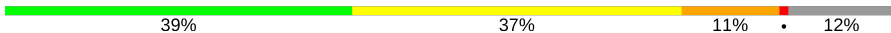



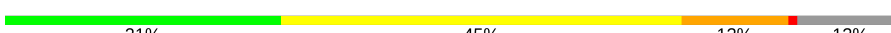





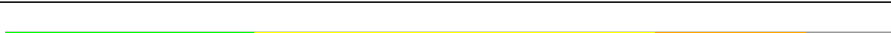


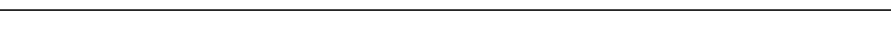




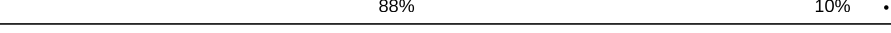





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Mol	Chain	Length	Quality of chain
4	S2	253	
4	s2	253	
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	
15	c3	150	
16	C4	136	





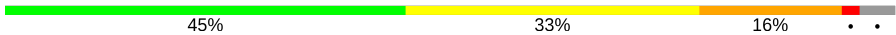


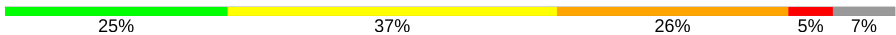

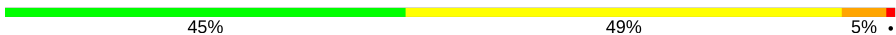

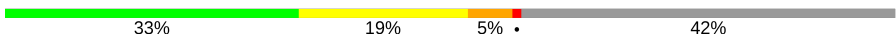













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Mol	Chain	Length	Quality of chain
16	c4	136	
17	C5	141	
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107	
27	d5	107	
28	D6	97	
28	d6	97	







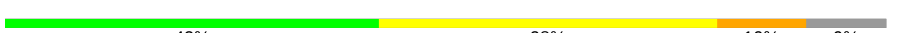







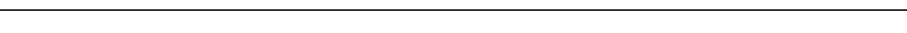




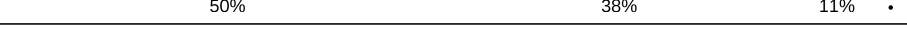





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Mol	Chain	Length	Quality of chain
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	












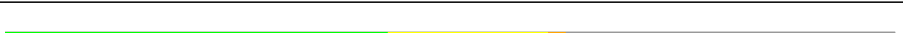


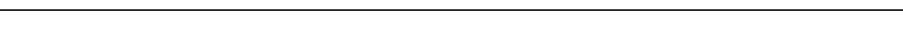




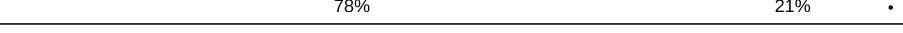





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Mol	Chain	Length	Quality of chain
42	L5	296	
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	
53	m7	183	
54	M8	185	















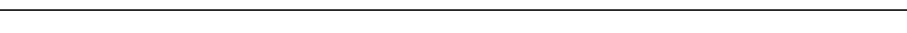




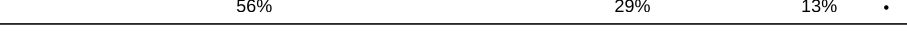

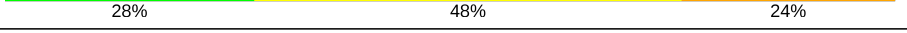



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Mol	Chain	Length	Quality of chain
54	m8	185	
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	104	
66	o0	104	






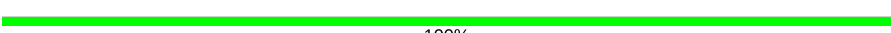
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Mol	Chain	Length	Quality of chain
67	O1	112	
67	o1	112	
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	119	
70	o4	119	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	

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Mol	Chain	Length	Quality of chain
79	q3	91	
80	e0	62	
81	m2	160	
82	p0	311	
83	p1	47	
84	p2	46	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	1	3943	-	-	X	-
86	OHX	1	3962	-	-	X	-
86	OHX	1	3964	-	-	X	-
86	OHX	1	3976	-	-	X	-
86	OHX	1	3980	-	-	X	-
86	OHX	1	4007	-	-	X	-
86	OHX	1	4023	-	-	X	-
86	OHX	1	4032	-	-	X	-
86	OHX	1	4036	-	-	X	-
86	OHX	1	4047	-	-	X	-
86	OHX	1	4048	-	-	X	-
86	OHX	1	4056	-	-	X	-
86	OHX	1	4059	-	-	X	-
86	OHX	1	4060	-	-	X	-
86	OHX	1	4061	-	-	X	-
86	OHX	1	4065	-	-	X	-
86	OHX	1	4071	-	-	X	-
86	OHX	1	4084	-	-	X	-
86	OHX	1	4088	-	-	X	-
86	OHX	1	4089	-	-	X	-
86	OHX	1	4118	-	-	X	-
86	OHX	1	4143	-	-	X	-
86	OHX	1	4149	-	-	X	-
86	OHX	1	4153	-	-	X	-
86	OHX	1	4157	-	-	X	-
86	OHX	1	4158	-	-	X	-
86	OHX	1	4159	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	1	4163	-	-	X	-
86	OHX	1	4166	-	-	X	-
86	OHX	1	4175	-	-	X	-
86	OHX	1	4177	-	-	X	-
86	OHX	1	4200	-	-	X	-
86	OHX	2	2032	-	-	X	-
86	OHX	2	2045	-	-	X	-
86	OHX	2	2076	-	-	X	-
86	OHX	2	2084	-	-	X	-
86	OHX	2	2086	-	-	X	-
86	OHX	2	2090	-	-	X	-
86	OHX	2	2091	-	-	X	-
86	OHX	2	2096	-	-	X	-
86	OHX	2	2099	-	-	X	-
86	OHX	2	2109	-	-	X	-
86	OHX	2	2116	-	-	X	-
86	OHX	2	2132	-	-	X	-
86	OHX	2	2147	-	-	X	-
86	OHX	2	2155	-	-	X	-
86	OHX	2	2163	-	-	X	-
86	OHX	5	3962	-	-	X	-
86	OHX	5	3973	-	-	X	-
86	OHX	5	3978	-	-	X	-
86	OHX	5	4000	-	-	X	-
86	OHX	5	4001	-	-	X	-
86	OHX	5	4011	-	-	X	-
86	OHX	5	4020	-	-	X	-
86	OHX	5	4033	-	-	X	-
86	OHX	5	4034	-	-	X	-
86	OHX	5	4055	-	-	X	-
86	OHX	5	4065	-	-	X	-
86	OHX	5	4066	-	-	X	-
86	OHX	5	4074	-	-	X	-
86	OHX	5	4081	-	-	X	-
86	OHX	5	4090	-	-	X	-
86	OHX	5	4093	-	-	X	-
86	OHX	5	4094	-	-	X	-
86	OHX	5	4141	-	-	X	-
86	OHX	5	4187	-	-	X	-
86	OHX	5	4189	-	-	X	-
86	OHX	5	4190	-	-	X	-
86	OHX	5	4196	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	5	4197	-	-	X	-
86	OHX	5	4198	-	-	X	-
86	OHX	5	4201	-	-	X	-
86	OHX	5	4212	-	-	X	-
86	OHX	5	4215	-	-	X	-
86	OHX	5	4222	-	-	X	-
86	OHX	5	4234	-	-	X	-
86	OHX	5	4241	-	-	X	-
86	OHX	6	2060	-	-	X	-
86	OHX	6	2121	-	-	X	-
86	OHX	6	2147	-	-	X	-
86	OHX	6	2171	-	-	X	-
86	OHX	7	218	-	-	X	-
86	OHX	7	219	-	-	X	-
86	OHX	7	224	-	-	X	-
86	OHX	7	226	-	-	X	-
86	OHX	8	215	-	-	X	-
86	OHX	8	223	-	-	X	-
86	OHX	8	224	-	-	X	-
86	OHX	C1	201	-	-	X	-
86	OHX	C5	201	-	-	X	-
86	OHX	O7	103	-	-	X	-
86	OHX	O9	101	-	-	X	-
87	ZN	Q2	501	-	-	X	-

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411226 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		0	0	0
			1481	951	265	265				
9	s7	186	Total	C	N	O		0	0	0
			1491	957	267	267				

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

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

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

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

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

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

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

There are 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
			890	560	156	172	2			
14	c2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

- 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			
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			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	19	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			
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	S	0	0	0
			993	625	192	176				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 Unknown protein m2.

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

- Molecule 82 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 83 is a protein called Unknown protein p1.

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

- Molecule 84 is a protein called Unknown protein p2.

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

- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L7	2	Total 2	Mg 2	0	0
85	m7	5	Total 5	Mg 5	0	0
85	n8	4	Total 4	Mg 4	0	0
85	o1	1	Total 1	Mg 1	0	0
85	N5	1	Total 1	Mg 1	0	0
85	6	147	Total 147	Mg 147	0	0
85	sM	2	Total 2	Mg 2	0	0
85	O4	1	Total 1	Mg 1	0	0
85	m5	1	Total 1	Mg 1	0	0
85	l3	1	Total 1	Mg 1	0	0
85	M1	1	Total 1	Mg 1	0	0
85	n0	2	Total 2	Mg 2	0	0
85	d6	1	Total 1	Mg 1	0	0
85	2	126	Total 126	Mg 126	0	0
85	O3	1	Total 1	Mg 1	0	0
85	L4	3	Total 3	Mg 3	0	0
85	l7	1	Total 1	Mg 1	0	0
85	M5	2	Total 2	Mg 2	0	0
85	l4	1	Total 1	Mg 1	0	0
85	L8	1	Total 1	Mg 1	0	0
85	o4	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	M9	1	Total 1	Mg 1	0	0
85	q0	1	Total 1	Mg 1	0	0
85	SM	1	Total 1	Mg 1	0	0
85	c8	2	Total 2	Mg 2	0	0
85	M0	2	Total 2	Mg 2	0	0
85	c1	1	Total 1	Mg 1	0	0
85	5	504	Total 504	Mg 504	0	0
85	L5	1	Total 1	Mg 1	0	0
85	O7	1	Total 1	Mg 1	0	0
85	s6	1	Total 1	Mg 1	0	0
85	Q2	1	Total 1	Mg 1	0	0
85	n9	2	Total 2	Mg 2	0	0
85	1	475	Total 475	Mg 475	0	0
85	d2	1	Total 1	Mg 1	0	0
85	n6	2	Total 2	Mg 2	0	0
85	S8	1	Total 1	Mg 1	0	0
85	m1	2	Total 2	Mg 2	0	0
85	d3	1	Total 1	Mg 1	0	0
85	q3	1	Total 1	Mg 1	0	0
85	o3	2	Total 2	Mg 2	0	0
85	M3	4	Total 4	Mg 4	0	0

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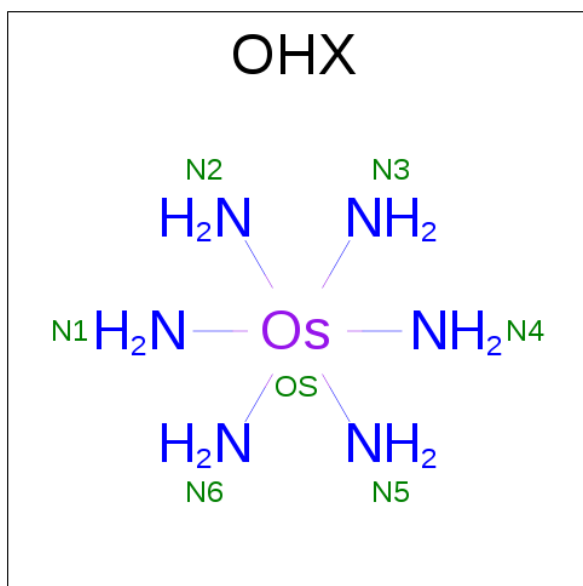
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	N3	3	Total 3	Mg 3	0	0
85	N8	2	Total 2	Mg 2	0	0
85	4	21	Total 21	Mg 21	0	0
85	L2	1	Total 1	Mg 1	0	0
85	l5	3	Total 3	Mg 3	0	0
85	C3	1	Total 1	Mg 1	0	0
85	M7	6	Total 6	Mg 6	0	0
85	m4	1	Total 1	Mg 1	0	0
85	L6	1	Total 1	Mg 1	0	0
85	s1	1	Total 1	Mg 1	0	0
85	m6	1	Total 1	Mg 1	0	0
85	s8	2	Total 2	Mg 2	0	0
85	c7	1	Total 1	Mg 1	0	0
85	7	15	Total 15	Mg 15	0	0
85	n3	2	Total 2	Mg 2	0	0
85	q1	1	Total 1	Mg 1	0	0
85	L3	2	Total 2	Mg 2	0	0
85	l2	2	Total 2	Mg 2	0	0
85	8	13	Total 13	Mg 13	0	0
85	M6	1	Total 1	Mg 1	0	0
85	N0	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	3	14	Total	Mg	0	0
			14	14		

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	L3	1	Total 7	N 6	Os 1	0	0
86	L3	1	Total 7	N 6	Os 1	0	0
86	L4	1	Total 7	N 6	Os 1	0	0
86	L6	1	Total 7	N 6	Os 1	0	0
86	M0	1	Total 7	N 6	Os 1	0	0
86	M5	1	Total 7	N 6	Os 1	0	0
86	M5	1	Total 7	N 6	Os 1	0	0
86	M6	1	Total 7	N 6	Os 1	0	0
86	M7	1	Total 7	N 6	Os 1	0	0
86	M7	1	Total 7	N 6	Os 1	0	0
86	M9	1	Total 7	N 6	Os 1	0	0
86	N9	1	Total 7	N 6	Os 1	0	0
86	O2	1	Total 7	N 6	Os 1	0	0
86	O3	1	Total 7	N 6	Os 1	0	0
86	O7	1	Total 7	N 6	Os 1	0	0
86	O7	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	O9	1	Total	N	Os	0	0
			7	6	1		
86	Q2	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	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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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
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86	s1	1	Total 7	N 6	Os 1	0	0
86	s4	1	Total 7	N 6	Os 1	0	0
86	s8	1	Total 7	N 6	Os 1	0	0
86	s9	1	Total 7	N 6	Os 1	0	0
86	c1	1	Total 7	N 6	Os 1	0	0
86	c3	1	Total 7	N 6	Os 1	0	0
86	c5	1	Total 7	N 6	Os 1	0	0

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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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			7	6	1		

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	13	1	Total 7	N 6	Os 1	0	0
86	13	1	Total 7	N 6	Os 1	0	0
86	13	1	Total 7	N 6	Os 1	0	0
86	14	1	Total 7	N 6	Os 1	0	0
86	14	1	Total 7	N 6	Os 1	0	0
86	15	1	Total 7	N 6	Os 1	0	0
86	15	1	Total 7	N 6	Os 1	0	0
86	15	1	Total 7	N 6	Os 1	0	0
86	19	1	Total 7	N 6	Os 1	0	0
86	m0	1	Total 7	N 6	Os 1	0	0
86	m0	1	Total 7	N 6	Os 1	0	0
86	m1	1	Total 7	N 6	Os 1	0	0
86	m4	1	Total 7	N 6	Os 1	0	0
86	m5	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	m6	1	Total	N	Os	0	0
			7	6	1		
86	m7	1	Total	N	Os	0	0
			7	6	1		
86	m8	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o2	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	o4	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

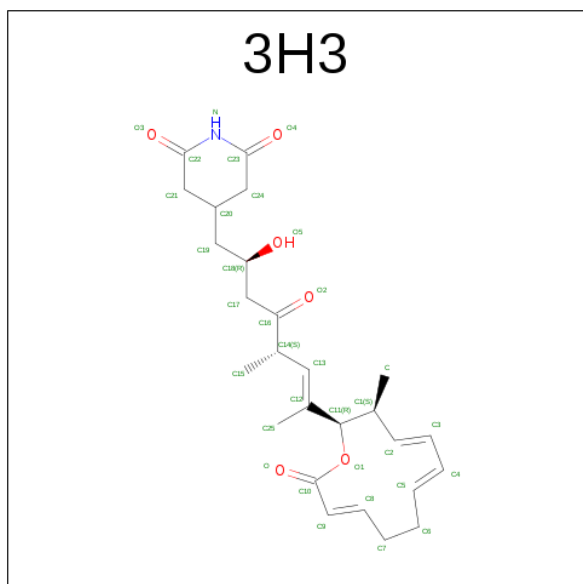
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	q0	1	Total	Zn	0	0
			1	1		
87	D6	1	Total	Zn	0	0
			1	1		
87	Q2	1	Total	Zn	0	0
			1	1		
87	e1	1	Total	Zn	0	0
			1	1		
87	Q3	1	Total	Zn	0	0
			1	1		
87	D9	1	Total	Zn	0	0
			1	1		
87	E1	1	Total	Zn	0	0
			1	1		
87	Q0	1	Total	Zn	0	0
			1	1		
87	d7	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	q3	1	Total	Zn	0	0
			1	1		
87	d9	1	Total	Zn	0	0
			1	1		
87	D7	1	Total	Zn	0	0
			1	1		
87	d6	1	Total	Zn	0	0
			1	1		
87	o7	1	Total	Zn	0	0
			1	1		
87	O7	1	Total	Zn	0	0
			1	1		
87	q2	1	Total	Zn	0	0
			1	1		

- Molecule 88 is 4-{(2R,5S,6E)-2-hydroxy-5-methyl-7-[(2R,3S,4E,6Z,10E)-3-methyl-12-oxooxacyclododeca-4,6,10-trien-2-yl]-4-oxooct-6-en-1-yl}piperidine-2,6-dione (three-letter code: 3H3) (formula: C₂₆H₃₅NO₆).



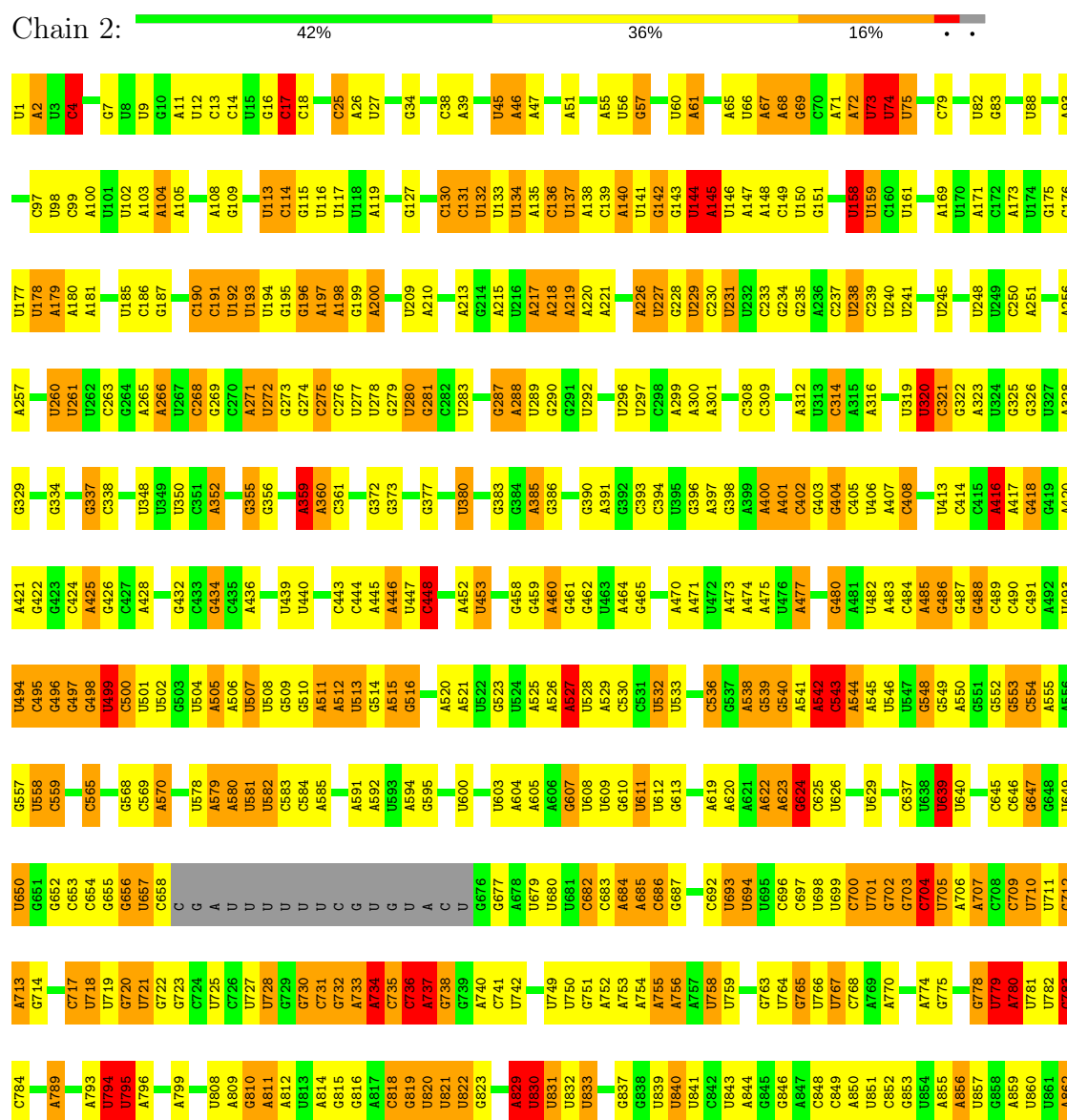
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
88	1	1	Total	C	N	O	0	0
			33	26	1	6		
88	5	1	Total	C	N	O	0	0
			33	26	1	6		

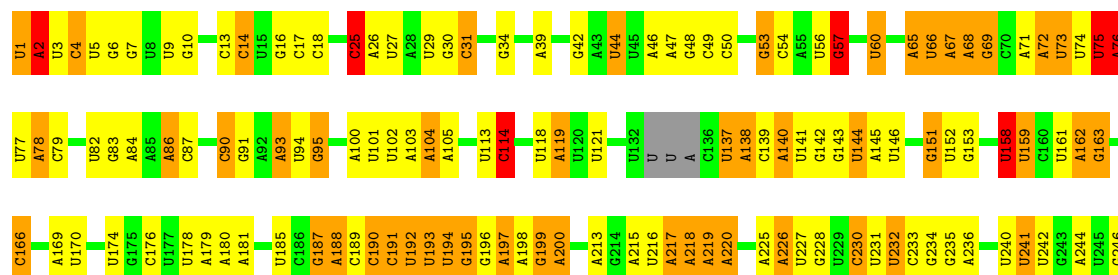
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

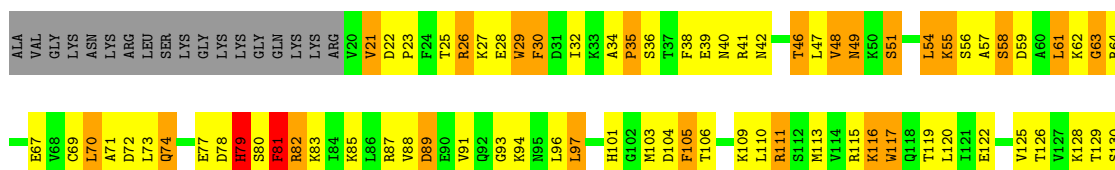
Note EDS failed to run properly.

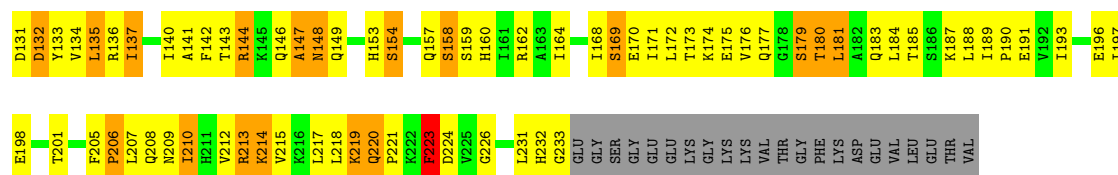
• Molecule 1: 18S ribosomal RNA





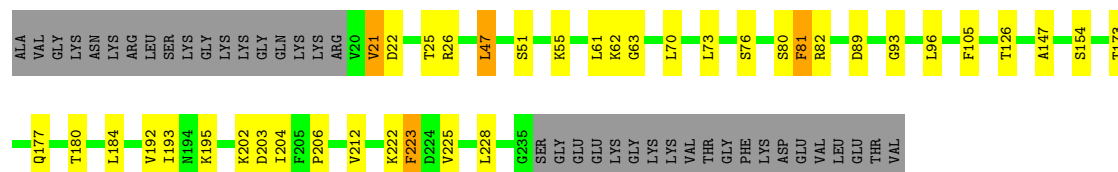
G1428	A1344	C1248	U1175	A1091	G1016	C934	U843	G785	C886	G616	G549	G486	C402	U327	A247
G1429	A1345	U1249	C1177	A1092	U1017	U935	U846	U766	G688	U617	A550	G487	G403	A328	U248
C1431	A1346	U1251	G1176	U1095	U1018	G942	G846	U767	G689	A618	C554	G488	G404	G329	U249
U1432	U1350	U1252	G1178	C1096	C1022	C943	A847	G1179	G690	A620	A555	C489	C405	C250	C250
U1434	G1351	U1254	C1180	U1098	A1026	U945	C848	A770	C591	A621	A556	C491	U406	A331	A251
G1435	G1354	U1255	A1183	U1099	A1027	U946	A856	A774	U694	A622	G557	U492	C408	U332	U252
U1437	A1357	G1256	U1184	G1100	C1028	U947	U857	G775	U695	A623	U558	U494	C409	G344	U260
U1442	G1358	U1257	A1185	G1101	A1030	A951	U857	G778	C896	G624	C559	C495	A416	U335	U261
C1443	C1359	U1259	C1192	U1103	U1031	A859	A859	G779	U698	A629	U563	G496	A417	G336	C263
U1445	A1360	G1263	A1193	G1107	C1033	G957	A862	A780	U699	A630	C565	G497	A418	C338	C264
A1446	U1361	G1264	A1194	G1108	C1034	U958	A863	U781	C700	U633	C566	U499	A421	A344	A271
C1447	U1363	U1268	C1196	G1109	G1035	U959	U864	G783	G702	A635	C569	U502	G424	U348	G272
G1448	G1364	U1269	A1197	G1121	A1036	U960	G868	A788	C704	A636	A570	G503	C424	U349	G273
U1449	C1365	G1274	C1198	A1125	A1039	U965	G871	A789	U705	C637	G571	U504	A425	U350	G274
U1450	U1366	C1279	G1199	G1126	G1047	A970	G876	A793	A706	U638	C572	A505	G426	C351	C275
G1455	A1370	C1280	G1200	C1122	G1041	U966	G872	U794	G711	U640	C574	A506	G429	A352	C276
C1457	A1371	U1281	G1201	A1123	C1045	A967	U873	U795	G712	G646	C577	U507	G430	C354	U277
G1458	C1379	U1283	C1207	G1129	G1048	A971	G879	U800	G713	G647	C578	U508	G431	G355	G279
C1459	A1382	U1284	A1208	G1130	U1049	A972	G891	G801	A715	G648	C579	A511	C432	G357	U280
A1460	G1385	U1285	C1209	G1133	G1050	A973	U894	A804	C716	G652	C581	U513	C433	U358	G281
G1462	U1287	U1286	C1210	A1133	G1051	A978	G895	U805	C717	C653	C582	A514	A437	A359	U282
C1463	A1388	G1288	G1212	C1134	G1052	A979	G895	A806	C718	C654	C583	A515	A438	A360	U283
G1464	C1389	U1293	G1213	A1138	G1053	G980	A898	A807	U719	G655	C584	U517	U439	C361	G287
C1465	U1390	C1216	C1217	A1144	U1057	G981	A906	A811	G720	G656	A585	A518	C443	G362	G291
A1471	A1391	G1218	A1217	U1145	U1058	G986	G901	A812	G721	U657	C586	A519	C444	A369	U292
C1472	C1393	G1219	G1218	U1146	U1059	A987	G902	U813	G722	C658	C587	A520	A445	A370	U297
U1473	G1394	A1219	A1219	G1147	U1060	A988	U903	G815	G723	C660	C589	A521	C448	U374	C298
G1477	G1395	C1220	C1220	A1147	G1064	C990	A905	G816	U727	A661	C590	U522	C449	C376	A299
G1478	U1396	A1312	A1226	C1148	A1065	G991	A906	A817	U728	U665	C592	A527	U453	A377	A301
A1479	U1397	A1313	A1227	G1149	A1068	A992	G910	C818	G729	U666	U693	U528	U454	A378	U306
G1480	C1399	U1314	G1228	A1151	A1069	A993	U911	G819	G730	A667	C594	A529	C455	U379	G307
C1481	A1400	G1316	G1229	A1152	C1070	G994	U912	U821	U733	C668	C595	U530	C308	U380	C308
C1482	A1401	C1317	A1230	G1153	U1071	U996	U913	U822	A734	G669	C597	U532	C309	C381	C310
A1487	G1402	G1318	U1231	G1154	C1072	G997	G914	G823	A737	U670	U600	U533	C310	G362	G311
G1488	G1408	A1321	A1234	G1155	G1073	C1000	A915	G824	G738	G	A601	A534	A312	G383	U311
U1489	G1409	C1235	C1235	C1156	G1074	A1001	U916	U825	A737	U	A602	A535	A312	A377	A312
U1491	U1431	G1330	A1236	C1157	C1075	G1002	U917	U826	U742	A673	U603	C536	A471	A387	U313
A1492	U1413	C1332	G1237	C1158	U1078	A1003	U918	U827	U742	C674	A604	A538	C314	G388	G314
A1493	U1414	C1333	A1238	C1159	U1079	U1004	A919	U828	C747	U675	A605	C539	A315	G389	A315
C1494	U1415	U1239	U1238	A1160	U1080	A1005	U921	A829	G751	A678	A606	G540	C394	G390	U319
C1495	G1416	G1334	C1240	C1161	A1081	C1006	G922	U831	U752	U679	U608	A541	A477	C394	U320
U1496	A1417	U1335	G1241	A1163	C1082	C1007	A923	U832	A753	U680	U609	A543	A481	A397	G321
U1497	G1418	A1336	A1242	A1166	G1083	C1010	A926	U833	A754	U681	G610	A544	U482	A397	G322
G1498	C1338	C1387	G1243	G1167	A1084	G1085	A931	U834	A755	C682	C613	A545	U482	C398	A323
	A1425	C1339	A1244	G1187	A1085	G1085	C931	U835	A756	C683	C614	U546	A483	A399	U324
	C1426	U1340	G1245	A1171	A1088	G1088	U932	U836	A757	A694	C615	U547	C484	A400	G325
A1503	A1427	A1341	U1247	G1172	A1088	U1015	A933	G838	U758	A695	A615	G548	A485	A401	G326





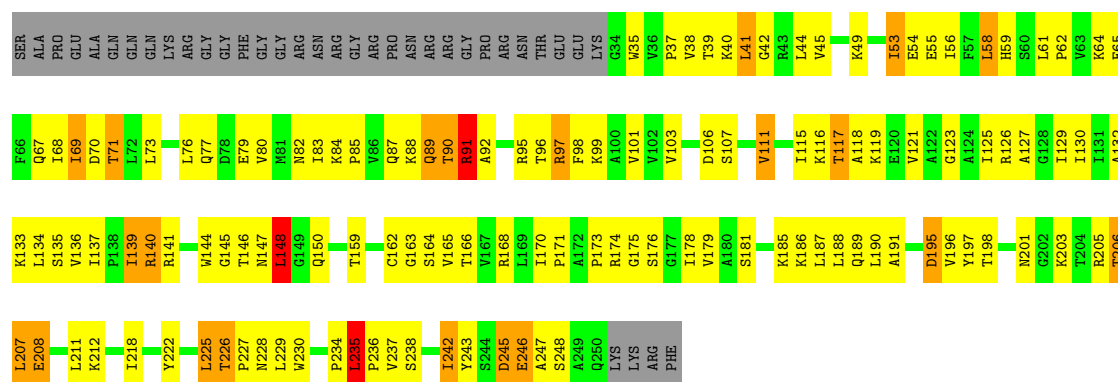
• Molecule 3: 40S ribosomal protein S1-A

Chain s1: 70% 14% 15%



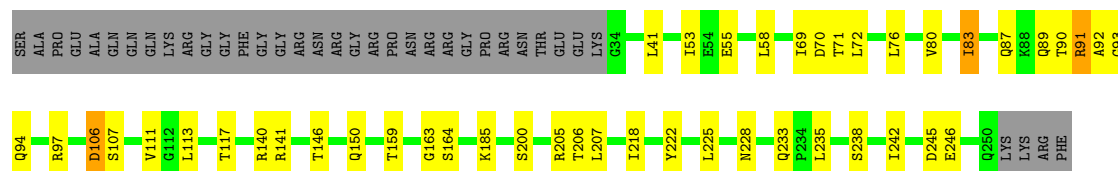
• Molecule 4: 40S ribosomal protein S2

Chain S2: 34% 42% 8% 14%



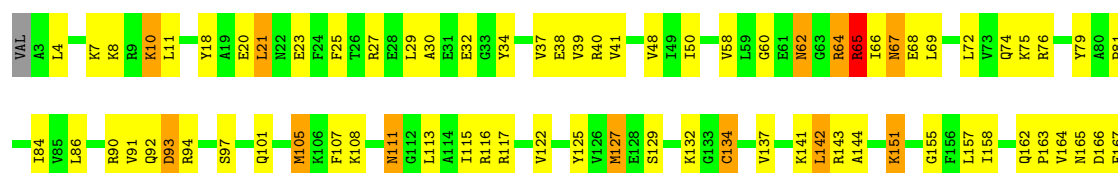
• Molecule 4: 40S ribosomal protein S2

Chain s2: 68% 17% 14%

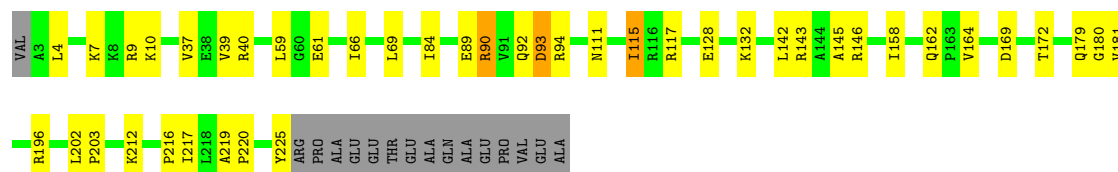
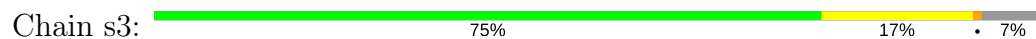


• Molecule 5: 40S ribosomal protein S3

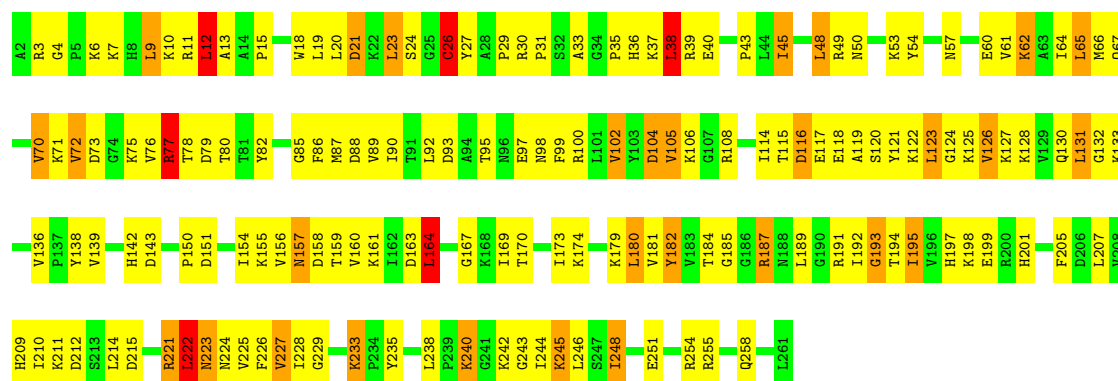
Chain S3: 46% 38% 9% 7%



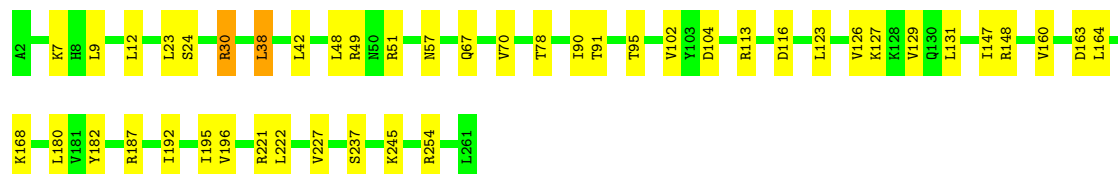
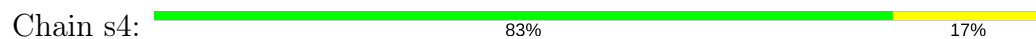
- Molecule 5: 40S ribosomal protein S3



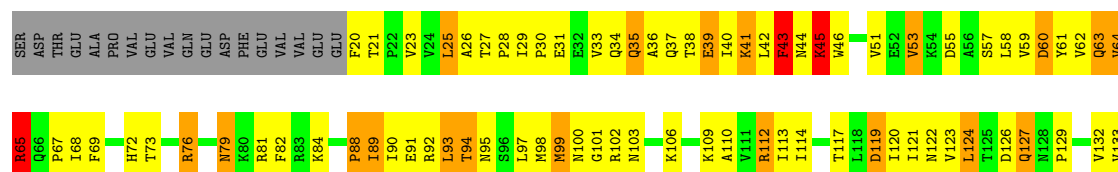
- Molecule 6: 40S ribosomal protein S4-A

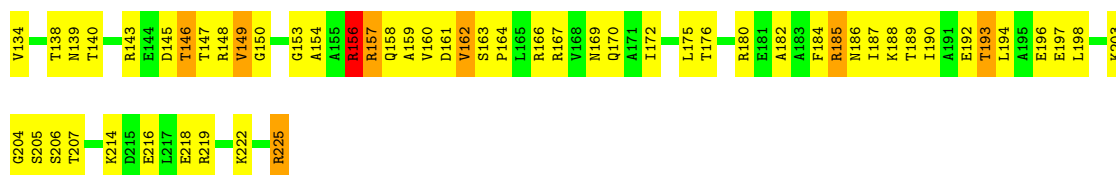


- Molecule 6: 40S ribosomal protein S4-A



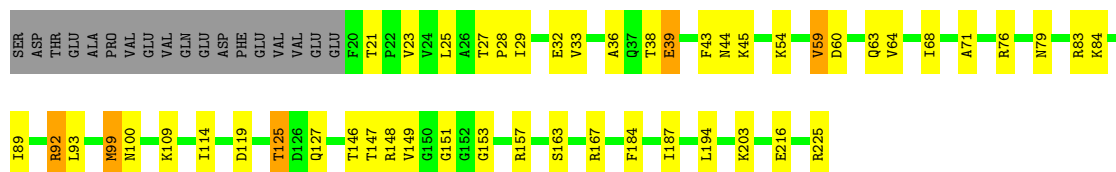
- Molecule 7: 40S ribosomal protein S5





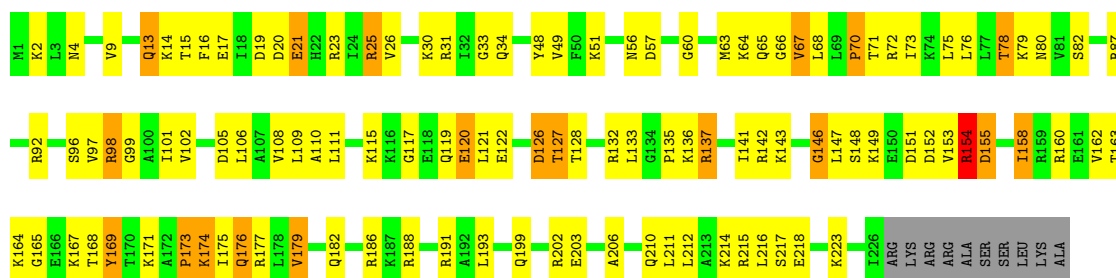
• Molecule 7: 40S ribosomal protein S5

Chain s5: 70% 20% 8%



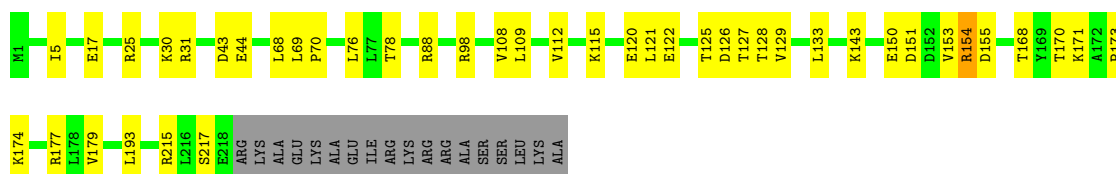
• Molecule 8: 40S ribosomal protein S6-A

Chain S6: 47% 40% 8%



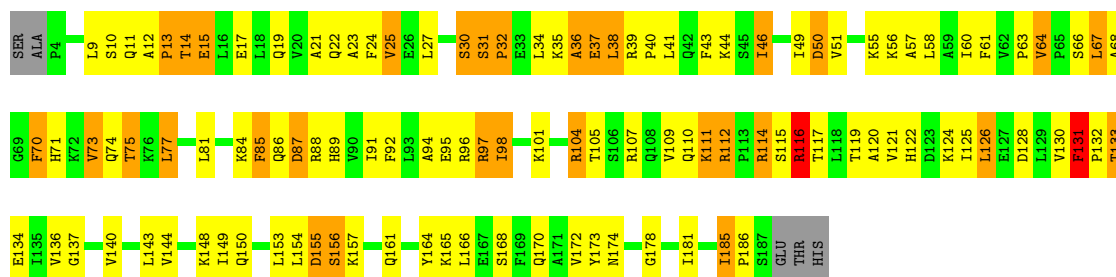
• Molecule 8: 40S ribosomal protein S6-A

Chain s6: 74% 18% 8%

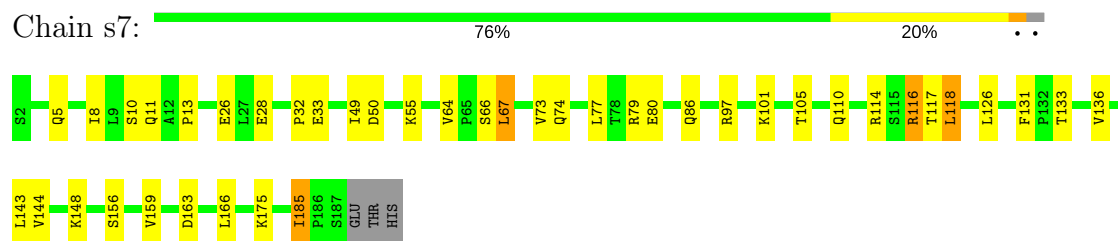


• Molecule 9: 40S ribosomal protein S7-A

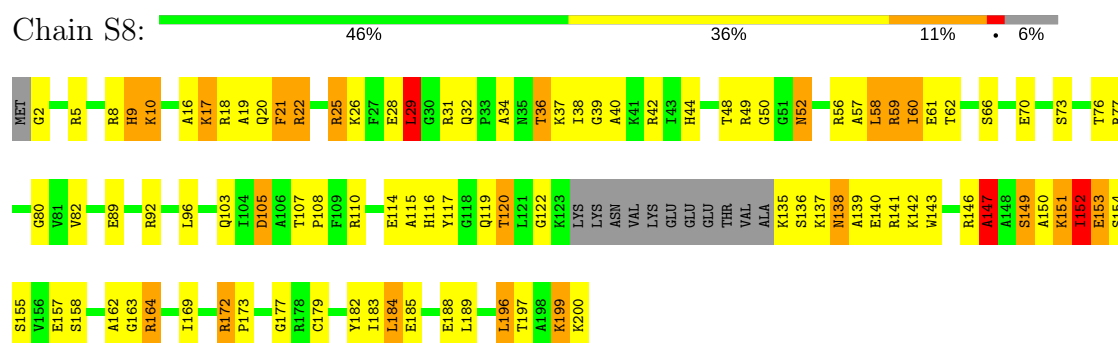
Chain S7: 37% 43% 16%



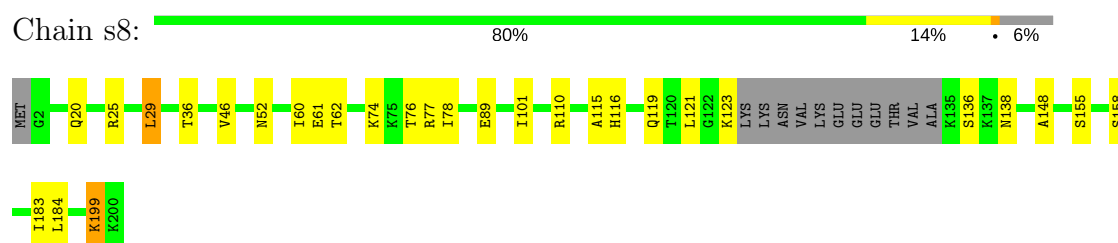
- Molecule 9: 40S ribosomal protein S7-A



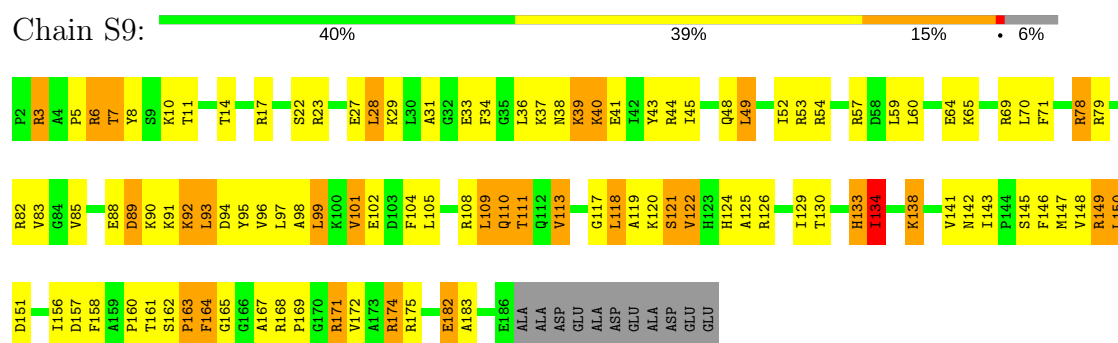
- Molecule 10: 40S ribosomal protein S8-A



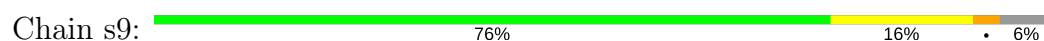
- Molecule 10: 40S ribosomal protein S8-A

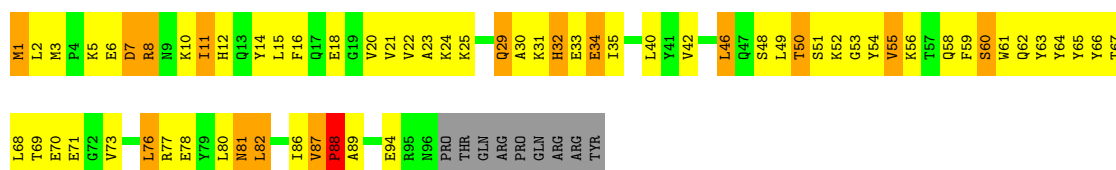
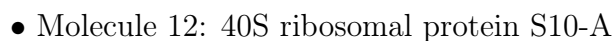


- Molecule 11: 40S ribosomal protein S9-A



- Molecule 11: 40S ribosomal protein S9-A



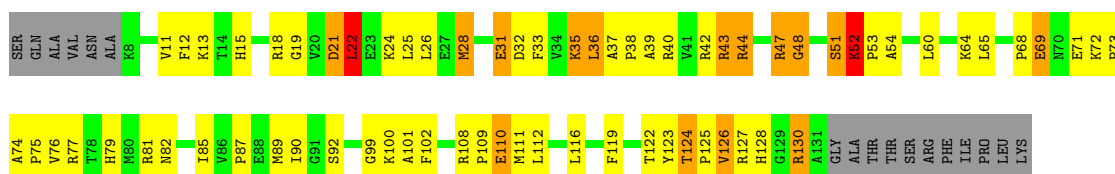


M1	L2	M3	P4	K5	L15	V20	V21	V22	A23	K24	P27	A30	K31	H32	E33	F34	I35	D36	V85	K86	T87	T67	E71	L82	P83	F84	HIS	ILE	V87	P88	I92	P95	N96	P97	T98	GLN	ARG	PRO	GLN	ARG	ARG	PRO
----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

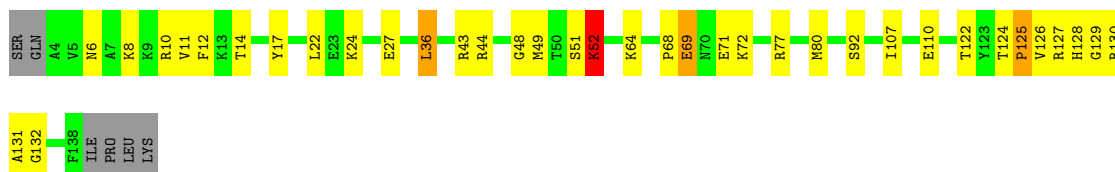
R82	R83	R84	R85	R86	R87	R88	R89	R90	R91	R92	R93	R94	R95	R96	R97	R98	R99	R100	E101	P108	P109	H110	P113	Q118	V123	T124	V125	P130	I131	S132	K133	T134	V135	R136	F137	N138	V139	L140	K141	V142	S143	A144	A145	F145	A154	K155	F156
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

GLN	S2
PHE	L5
ALA	T6
LYS	V7
PHE	E10
	N21
	K26
	T27
	R30
	T31
	K32
	R33
	L40
	T44
	T47
	D55
	K56
	F60
	T61
	R67
	T74
	M80
	T83
	V109
	A114
	V123
	R129
	S132
	K133
	V140
	S143
	A144
	A145
	A146
	A147
	LYS
	ALA
	ASP
	LYS

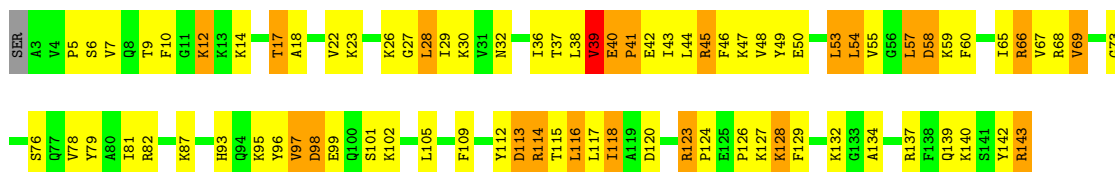
SER	ASP	V66	T67	E68	A69	V70	I71	I72	K73	L74	V75	E76	G77	L78	D81	P82	E83	K84	R85	V86	P87	L88	I89	K90	V91	A92	D93	A94	K95	Q96	L97	A101	G102	L103	I106	D107	R108	A112	V115	V116	G117	A118	S119	V120	V121	V122	V123	K124	N125	V126	G127	A128	E129	N130	T131	P132				
	VAL					VAL	VAL	GLU	VAL	GLN	GLU	GLU	THR	VAL	VAL	GLN	THR	A20	E21	V22	T23	T24	E25	D26	A27	L28	K29	V30	V31	L32	R33			L36	V37	H38	D39	G40	L41	A42	R43	G44	L45	R46	E47	S48	T49	K50	A51	L52	T53	R54	G55	E56	A57	L58	S59	V60	V61	L62



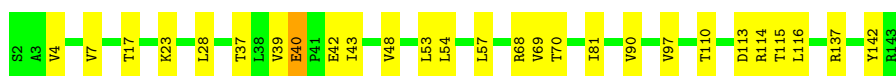
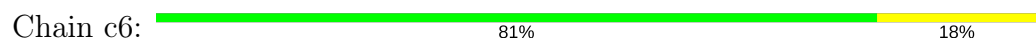
• Molecule 17: 40S ribosomal protein S15



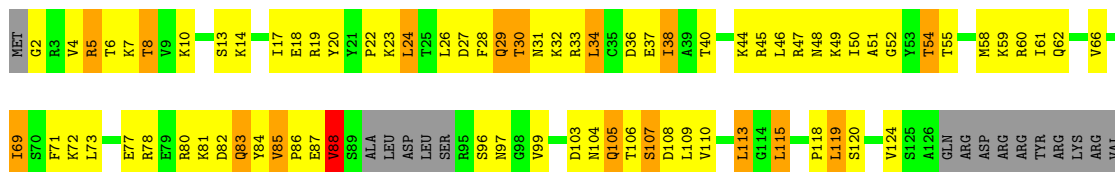
• Molecule 18: 40S ribosomal protein S16-A



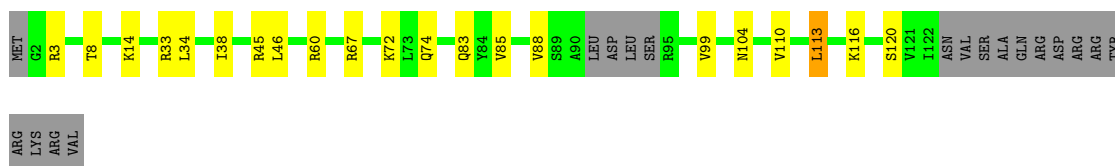
• Molecule 18: 40S ribosomal protein S16-A



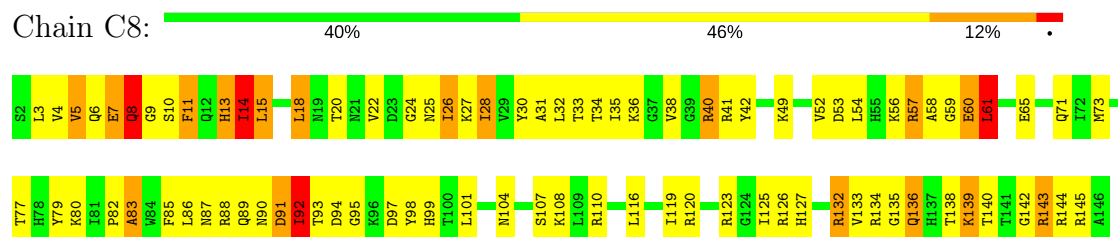
• Molecule 19: 40S ribosomal protein S17-A



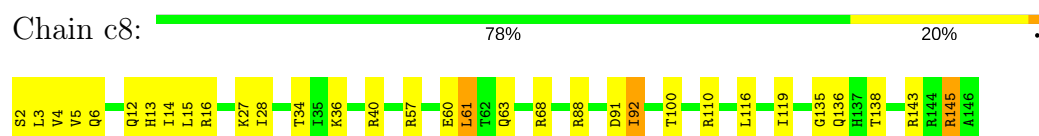
• Molecule 19: 40S ribosomal protein S17-A



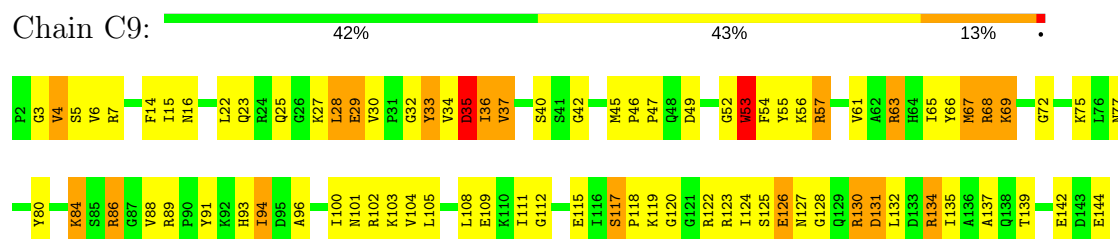
- Molecule 20: 40S ribosomal protein S18-A



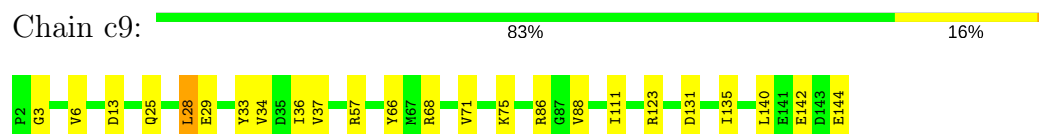
- Molecule 20: 40S ribosomal protein S18-A



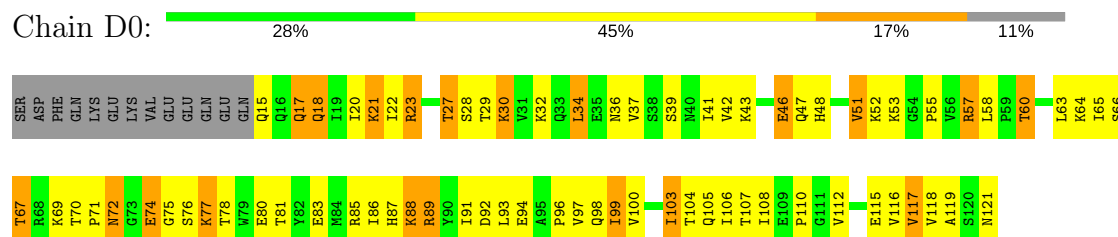
- Molecule 21: 40S ribosomal protein S19-A



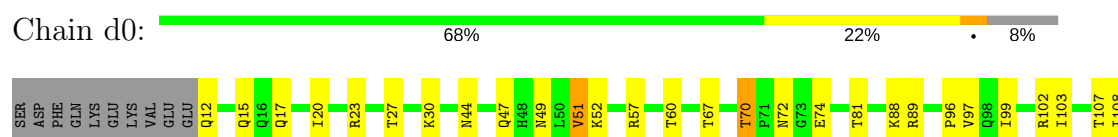
- Molecule 21: 40S ribosomal protein S19-A



- Molecule 22: 40S ribosomal protein S20



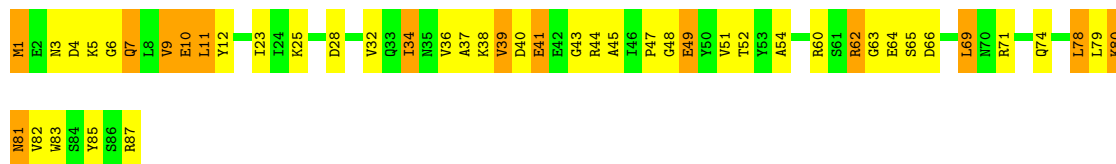
- Molecule 22: 40S ribosomal protein S20





- Molecule 23: 40S ribosomal protein S21-A

Chain D1: 46% 38% 16%



- Molecule 23: 40S ribosomal protein S21-A

Chain d1: 75% 25%



- Molecule 24: 40S ribosomal protein S22-A

Chain D2: 47% 45% 7%



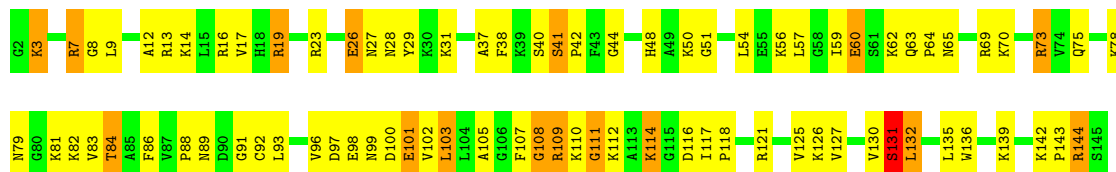
- Molecule 24: 40S ribosomal protein S22-A

Chain d2: 88% 12%



- Molecule 25: 40S ribosomal protein S23-A

Chain D3: 43% 45% 11%

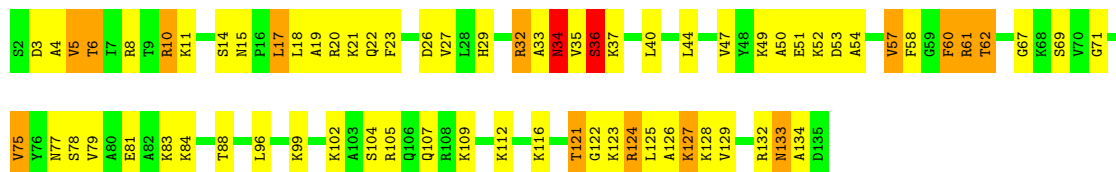


- Molecule 25: 40S ribosomal protein S23-A


Chain d3: 88% 10%

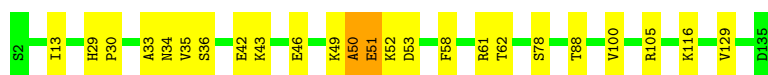
- Molecule 26: 40S ribosomal protein S24-A

Chain D4:  47% 41% 10%



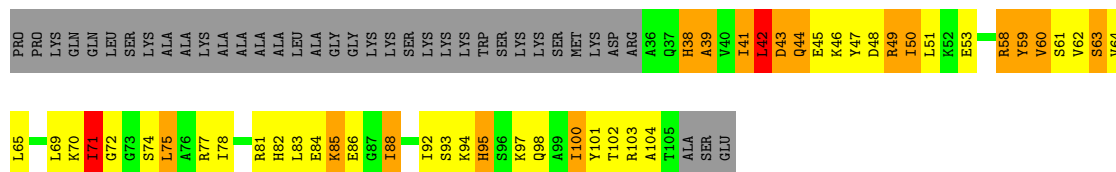
- Molecule 26: 40S ribosomal protein S24-A

Chain d4:  82% 16%



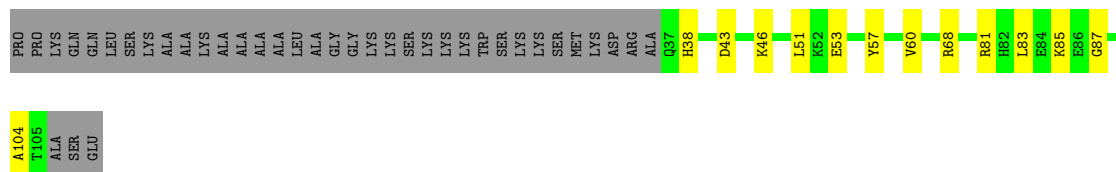
- Molecule 27: 40S ribosomal protein S25-A

Chain D5:  21% 28% 15% 3% 33%



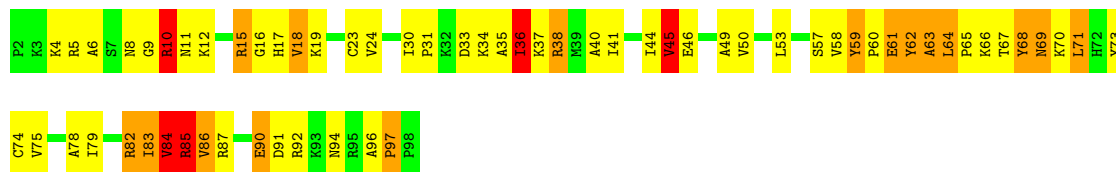
- Molecule 27: 40S ribosomal protein S25-A

Chain d5:  52% 12% 36%




- Molecule 28: 40S ribosomal protein S26-B

Chain D6:



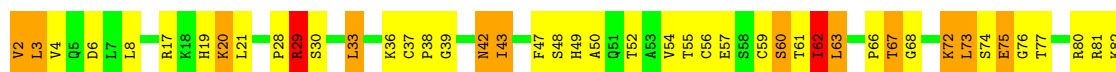
- Molecule 28: 40S ribosomal protein S26-B

Chain d6:  78% 21% .




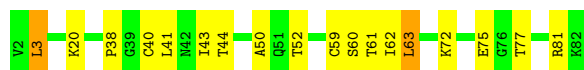
- Molecule 29: 40S ribosomal protein S27-A

Chain D7:  44% 38% 15% .



- Molecule 29: 40S ribosomal protein S27-A

Chain d7:  78% 20% .




- Molecule 30: 40S ribosomal protein S28-A

Chain D8:  35% 52% 8% 5% .



- Molecule 30: 40S ribosomal protein S28-A

Chain d8:  79% 14% 5% .



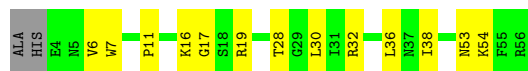
- Molecule 31: 40S ribosomal protein S29-A

Chain D9:  45% 33% 16% .



- Molecule 31: 40S ribosomal protein S29-A

Chain d9:  73% 24% .



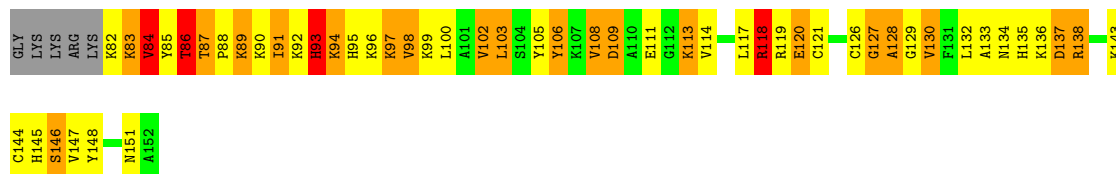
- Molecule 32: 40S ribosomal protein S30-A

Chain E0:  53% 37% 8% .



- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1: 25% 37% 26% 5% 7%



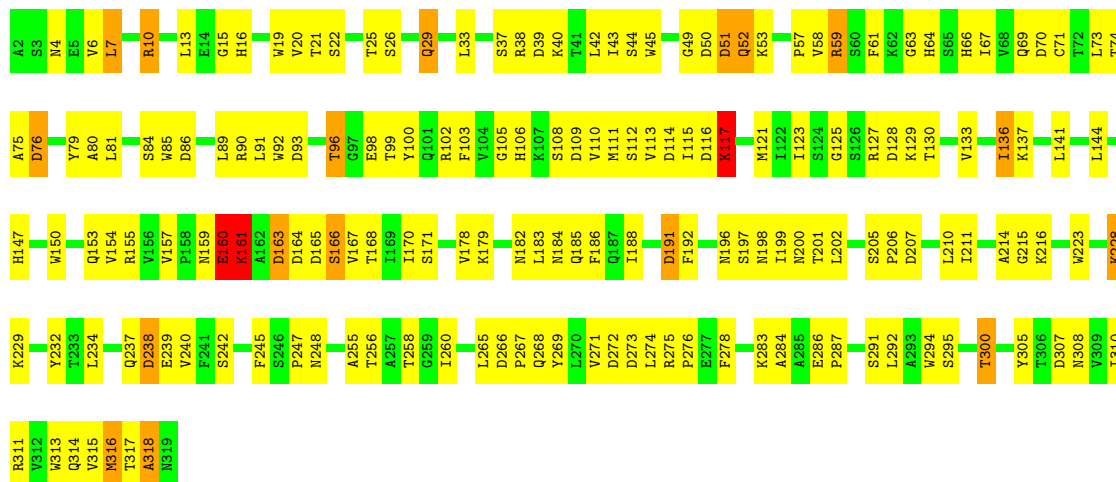
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1: 57% 37% 5%



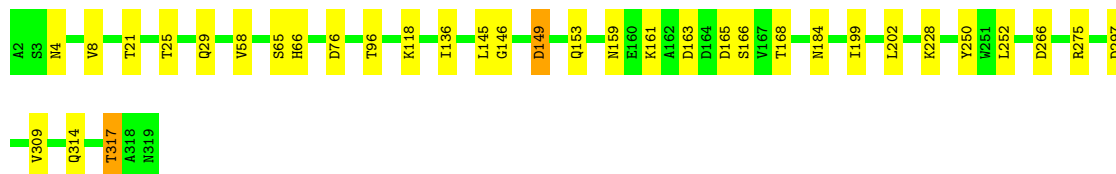
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR: 45% 49% 5%



- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

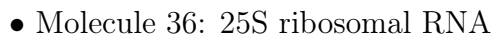
Chain sR: 89% 10%



- Molecule 35: Suppressor protein STM1

G1513	G1444	A1381	G1310	U1241	U1167	C1107	G1020	C948	A882	G805	U719	A653	G590	G510	U
G1514	U1445	G1382	G1313	G1242	U1168	U1108	G1024	C949	A883	A806	A720	C654	G591	G511	U
G1517	A1446	G1383	G1314	A1244	A1169	U1109	A1025	U954	A884	A807	G721	C655	A592	C515	U
G1520	U1448	A1386	U1315	A1245	G1171	U1111	U1028	U956	G887	G810	G728	G658	G596	A516	U
G1521	G1450	G1387	G1316	G1246	U1175	G1113	G1029	U957	G887	A810	C729	G659	G597	G517	G
U1522	C1451	G1389	G1319	U1247	C1176	G1114	A1030	C958	A888	U811	C730	A660	A598	G518	G
U1523	G1390	U1389	C1320	G1248	U1177	U1115	G1036	C959	C990	U814	A735	G661	C599	U520	C
A1524	C1391	G1392	U1322	G1255	G1178	G1116	A1036	U960	G894	G815	A736	U662	G600	A521	C
U1525	A1393	G1323	G1323	G1256	U1179	G1117	A1036	C961	A895	A816	A737	U663	G601	A522	U
C1527	A1394	U1324	U1324	G1257	U1181	C1118	G1043	G963	A896	C818	G737	U664	A603	U528	C
G1528	G1395	U1325	U1325	U1258	A1182	A1120	G1043	G964	U897	U819	G742	A665	G604	A529	G
G1536	C1396	A1326	A1326	A1259	C1183	U1121	A1047	A965	U898	C670	C743	C670	U605	A530	U
U1540	C1397	C1327	C1327	A1260	U1184	U1122	A1048	U966	U899	U671	U748	U671	C606	G530	C
G1541	U1398	U1328	U1328	G1261	A1189	U1123	C1049	A967	G900	A672	U748	A672	A507	U534	C
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G1547	G1400	A1330	A1330	A1263	U1191	U1125	U1051	C969	G908	G674	G750	G674	G609	U536	U
G1548	A1401	U1331	U1331	G1264	U1191	G1126	U1052	A970	U903	G675	G760	G675	G610	A537	U
U1549	C1402	U1334	U1334	U1265	C1192	G1127	A1053	G971	A904	U829	G760	G676	A611	G538	G
A1549	G1403	G1335	G1335	G1266	A1193	U1128	A1054	A972	U905	A850	G763	A677	U612	U541	U
U1550	U1405	U1336	U1336	U1267	G1194	A1129	U1054	A973	G907	G832	G763	G678	G613	U541	U
G1551	U1337	U1337	U1337	G1268	A1195	A1130	U1060	C975	G909	U834	G764	U679	G614	C544	G
G1552	C1338	C1338	C1338	A1270	U1200	C1132	A1062	U976	G910	G835	G765	U681	C618	U545	U
U1553	U1409	G1339	G1339	A1271	A1200	A1133	G1063	C977	G912	A836	U767	U682	A619	C546	A
G1554	U1410	G1340	G1340	C1272	C1201	G1134	U1064	G978	C911	U837	G768	U683	U620	G547	G
U1555	C1411	U1341	U1341	A1273	A1202	A1135	A1065	U979	G913	G838	G769	G684	A622	G548	G
G1556	G1412	C1342	C1342	A1274	A1136	A1136	G1066	A980	A914	G839	G770	G685	A622	G548	G
A1557	G1413	U1343	U1343	C1275	G1207	C1137	U1069	U981	G915	C840	A771	G686	U623	A551	G
G1558	C1414	G1345	G1345	U1276	U1208	U1138	C1089	C982	A917	A841	U772	U687	G624	G552	A
U1559	U1415	U1346	U1346	C1277	G1209	G1139	U1070	A983	A917	G688	G773	G688	G625	U553	A
G1560	G1416	G1347	G1347	U1278	U1210	G1140	U1071	U988	A920	U846	U776	U689	U626	A554	U
U1561	U1418	U1350	U1350	C1279	U1211	C1141	U1072	U988	A921	A847	U777	U690	U627	U555	C
C1562	A1419	A1351	A1351	G1281	A1212	G1142	U1073	G993	U922	A848	U777	A691	A628	U556	U
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G1582	C1508	G1374	G1374	G1237	G1237	A1163	A1103	C1016	C944	G878	C802	A716	C850	U587	U507
A1583	U1509	U1442	U1442	C1238	C1238	G1164	A1105	C1017	C945	U879	C803	C717	G651	G588	U508
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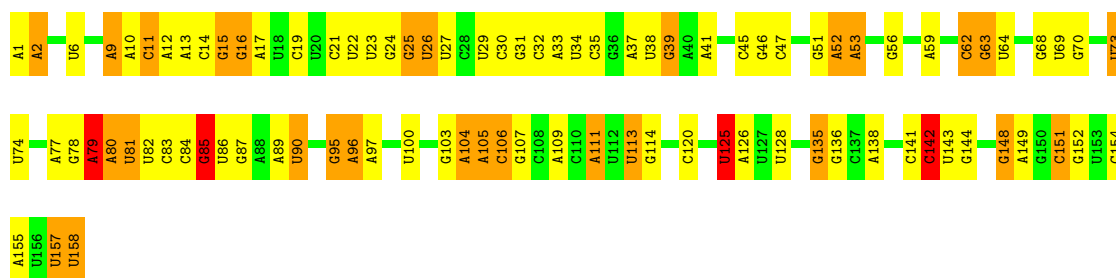


Frequency	Percentage
Daily	36%
Often	38%
Sometimes	16%
Rarely	7%
Never	1%



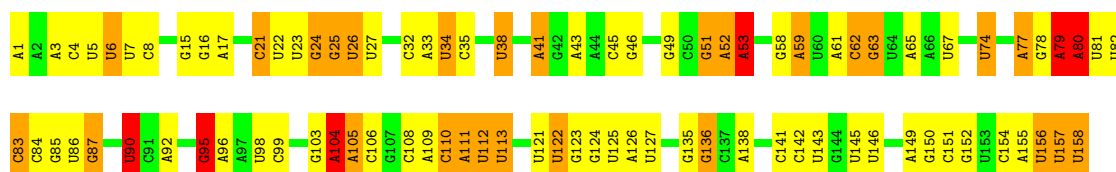
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		A1435	G1370	A1303	A1221	G1152	U1078	A1003	A936	U874	U798	U719	C641	G567	C
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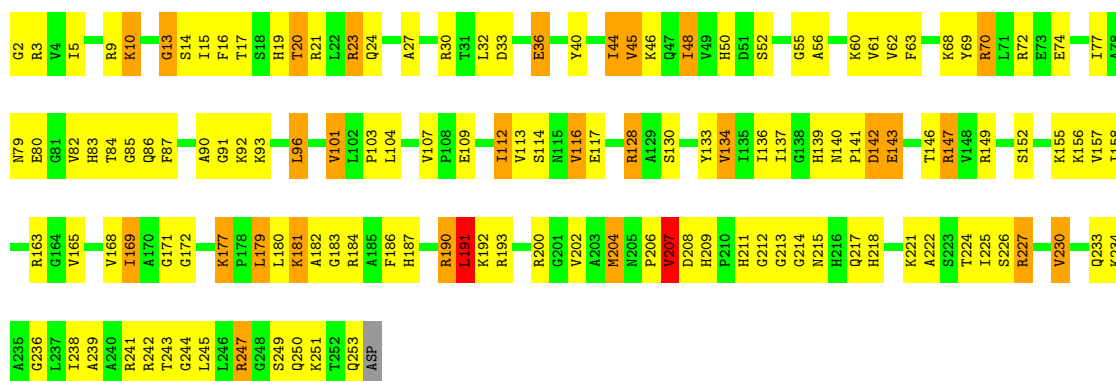
• Molecule 38: 5.8S ribosomal RNA

Chain 8: 44% 35% 17%



• Molecule 39: 60S ribosomal protein L2-A

Chain L2: 46% 42% 11%



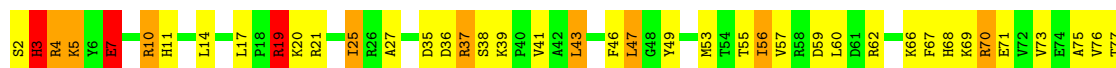
• Molecule 39: 60S ribosomal protein L2-A

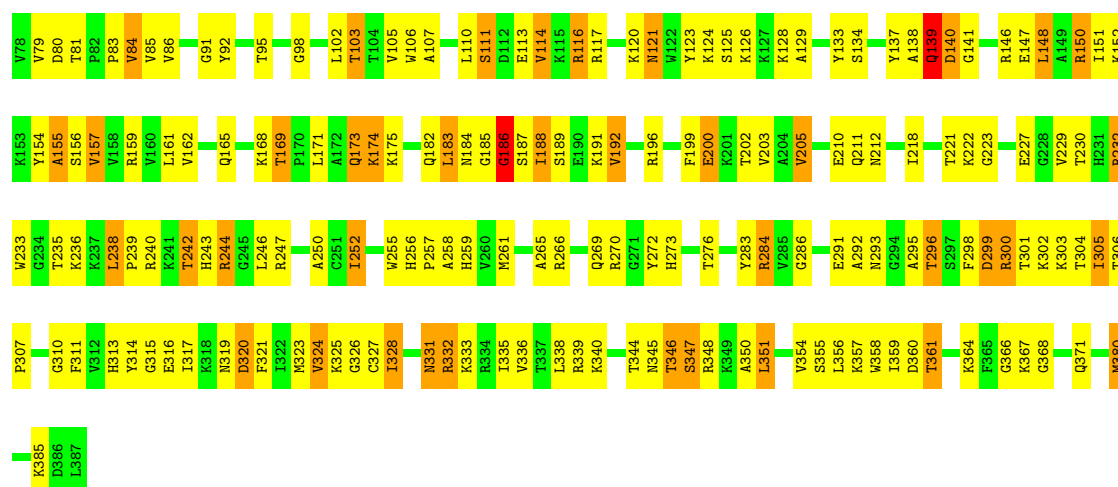
Chain l2: 81% 16%



• Molecule 40: 60S ribosomal protein L3

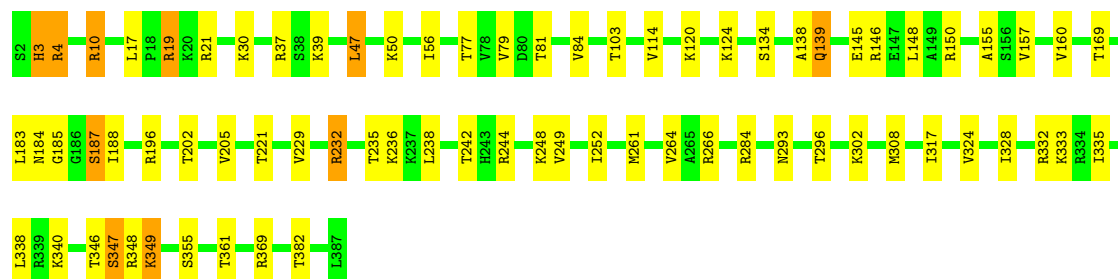
Chain L3: 44% 42% 12%





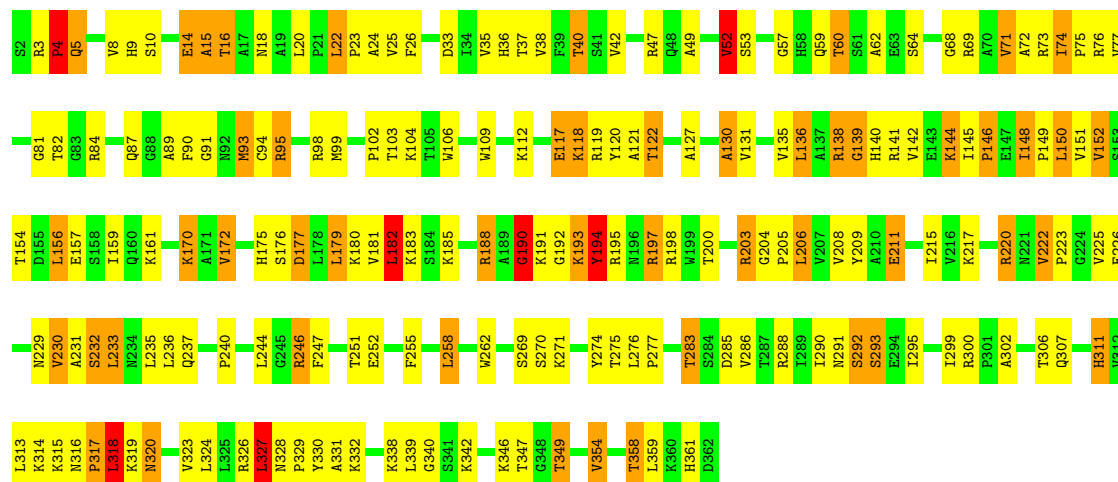
• Molecule 40: 60S ribosomal protein L3

Chain 13: 81% 17% .



• Molecule 41: 60S ribosomal protein L4-A

Chain L4: 47% 37% 14% .



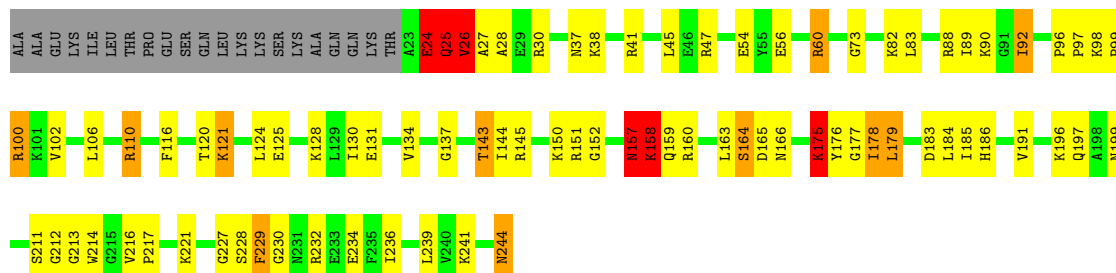
• Molecule 41: 60S ribosomal protein L4-A

Chain l4: 81% 18% .



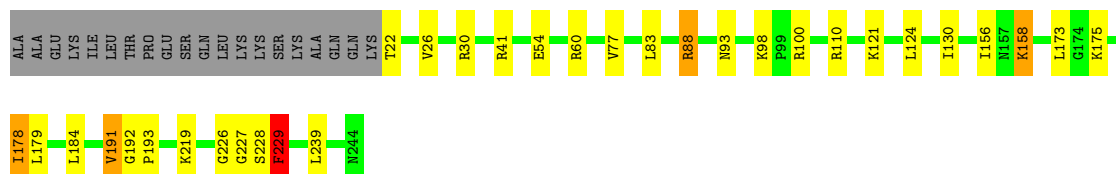
• Molecule 44: 60S ribosomal protein L7-A

Chain L7: 57% 27% 5% 9%



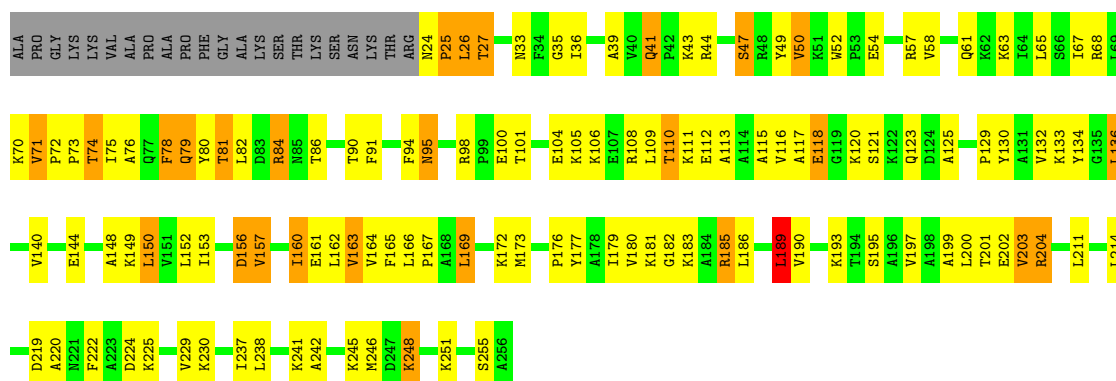
• Molecule 44: 60S ribosomal protein L7-A

Chain L7: 79% 11% 8%



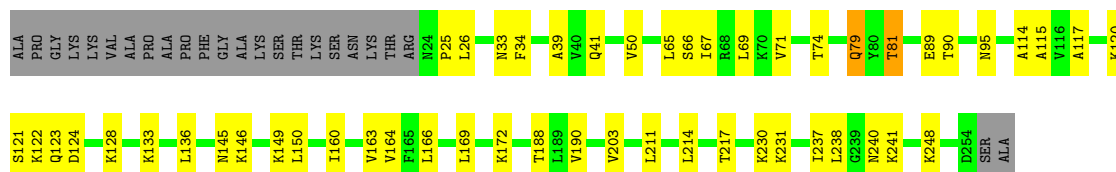
• Molecule 45: 60S ribosomal protein L8-A

Chain L8: 42% 38% 10% 9%

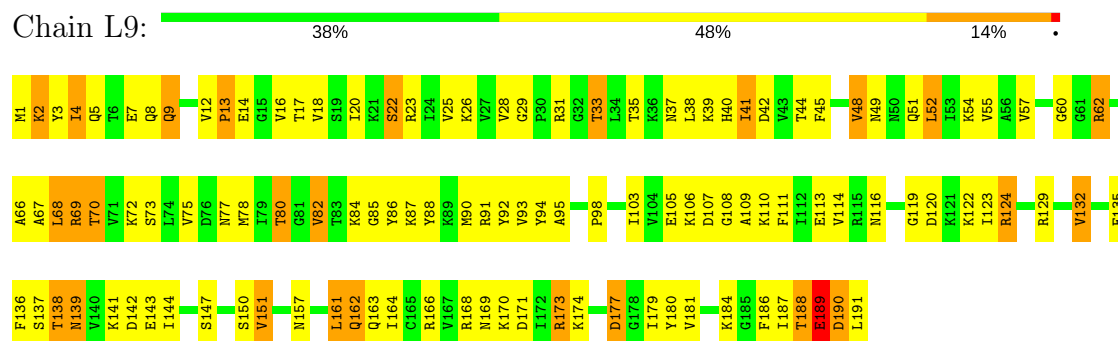


• Molecule 45: 60S ribosomal protein L8-A

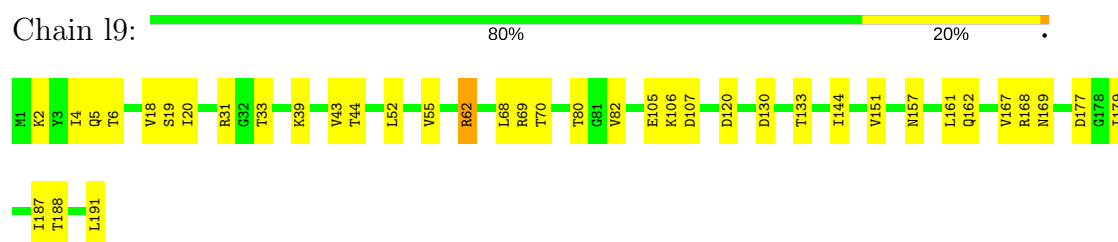
Chain L8: 70% 20% 9%



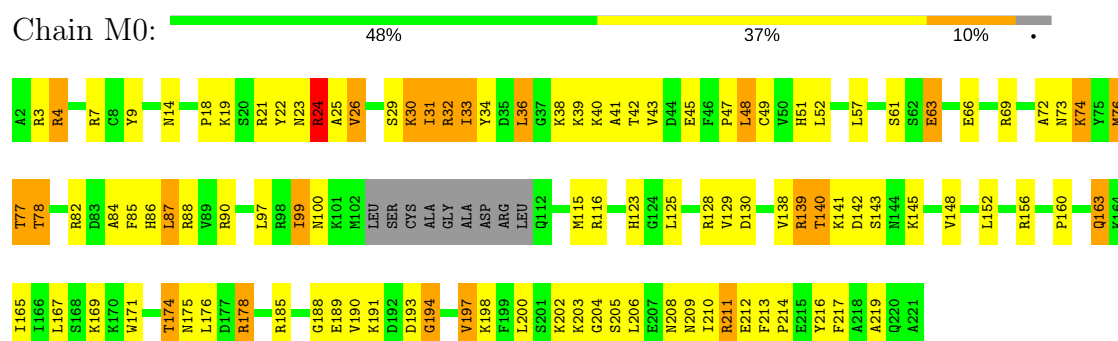
- Molecule 46: 60S ribosomal protein L9-A



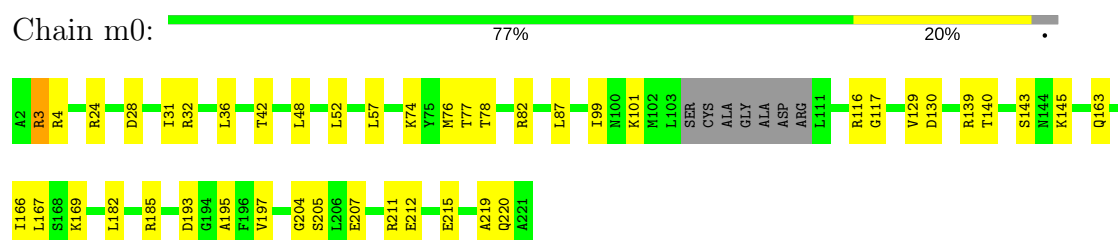
- Molecule 46: 60S ribosomal protein L9-A



- Molecule 47: 60S ribosomal protein L10

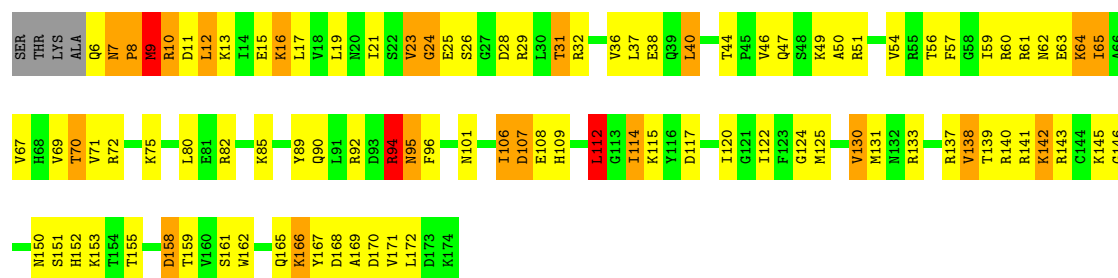


- Molecule 47: 60S ribosomal protein L10



- Molecule 48: 60S ribosomal protein L11-B





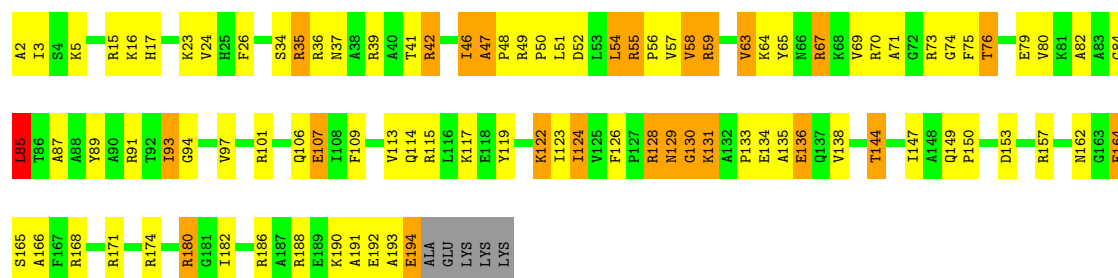
- Molecule 48: 60S ribosomal protein L11-B

Chain m1: 79% 17% ..



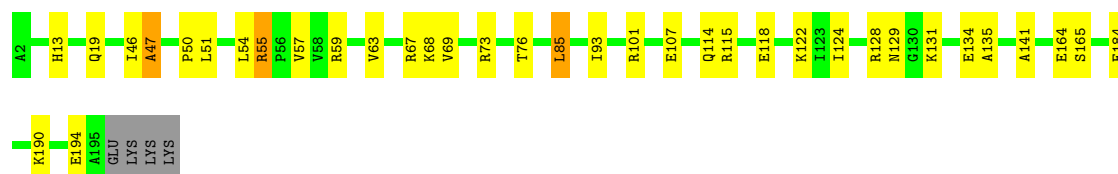
- Molecule 49: 60S ribosomal protein L13-A

Chain M3: 49% 35% 12% ..



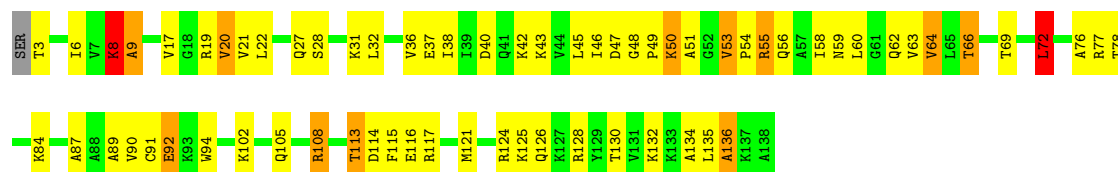
- Molecule 49: 60S ribosomal protein L13-A

Chain m3: 80% 17% ..

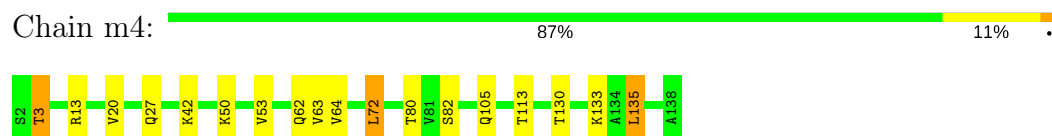


- Molecule 50: 60S ribosomal protein L14-A

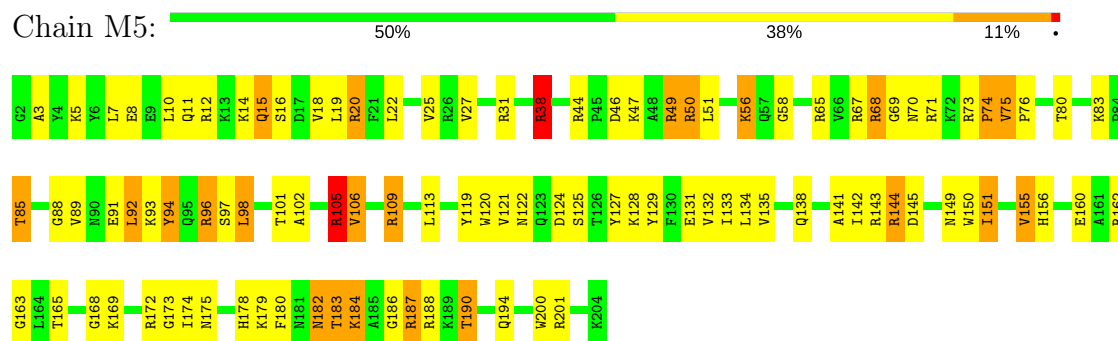
Chain M4: 50% 39% 8% ..



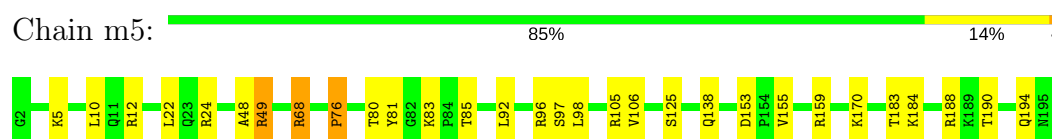
- Molecule 50: 60S ribosomal protein L14-A



- Molecule 51: 60S ribosomal protein L15-A



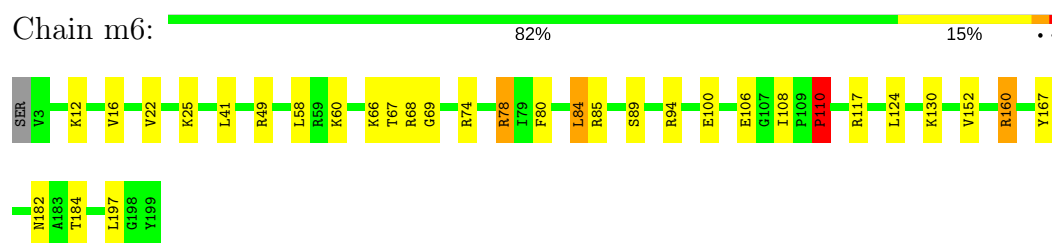
- Molecule 51: 60S ribosomal protein L15-A



- Molecule 52: 60S ribosomal protein L16-A

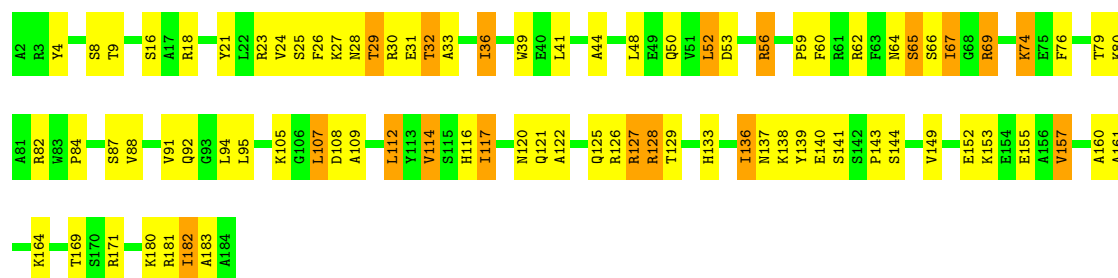


- Molecule 52: 60S ribosomal protein L16-A



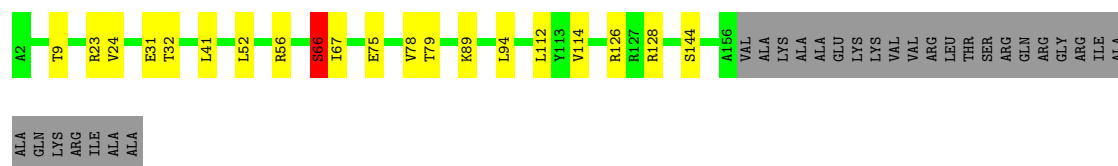
- Molecule 53: 60S ribosomal protein L17-A





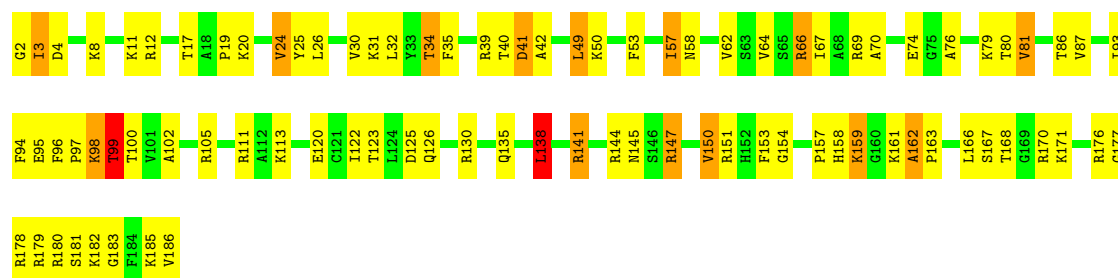
• Molecule 53: 60S ribosomal protein L17-A

Chain m7: 74% 10% 15%



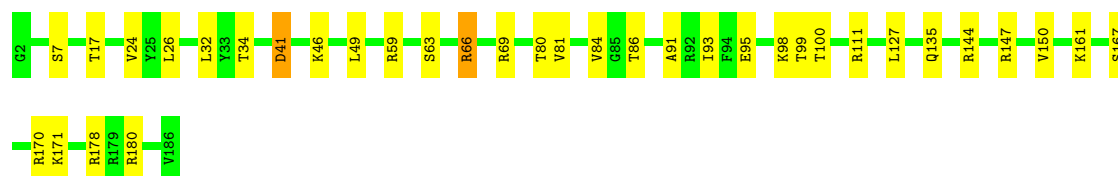
• Molecule 54: 60S ribosomal protein L18-A

Chain M8: 52% 39% 8%



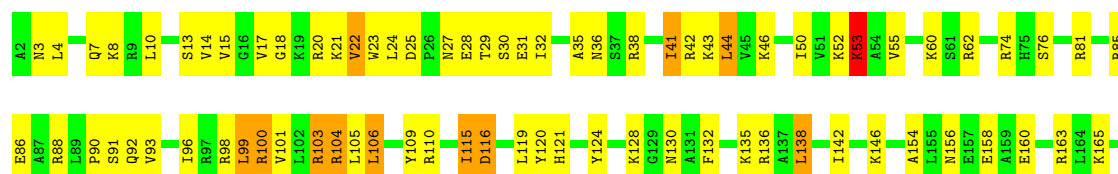
• Molecule 54: 60S ribosomal protein L18-A

Chain m8: 81% 18%



• Molecule 55: 60S ribosomal protein L19-A

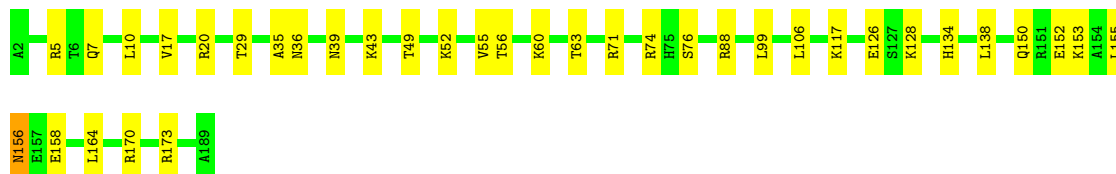
Chain M9: 55% 39% 6%





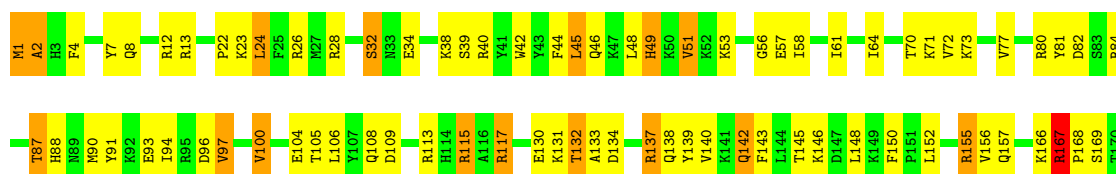
• Molecule 55: 60S ribosomal protein L19-A

Chain m9: 81% 19%



• Molecule 56: 60S ribosomal protein L20-A

Chain N0: 53% 36% 10%



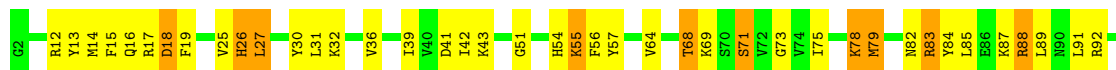
• Molecule 56: 60S ribosomal protein L20-A

Chain n0: 84% 15%



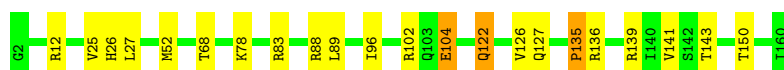
• Molecule 57: 60S ribosomal protein L21-A

Chain N1: 51% 35% 13%



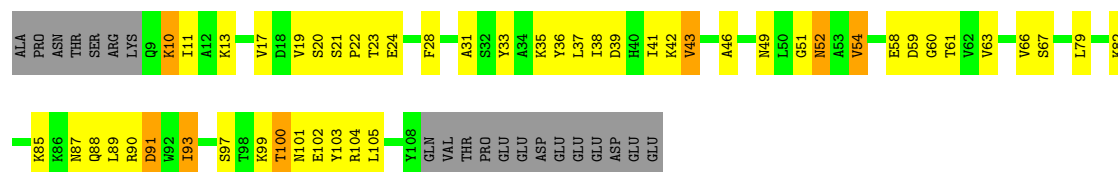
• Molecule 57: 60S ribosomal protein L21-A

Chain n1: 86% 12%



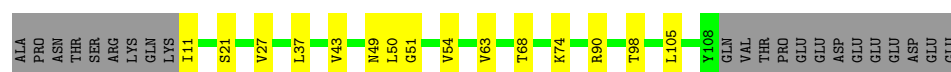
• Molecule 58: 60S ribosomal protein L22-A

Chain N2: 



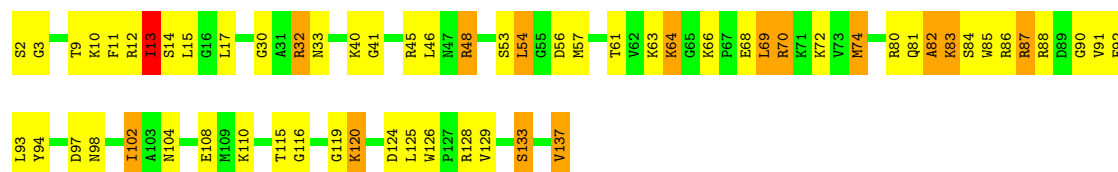
- Molecule 58: 60S ribosomal protein L22-A

Chain n2: 



- Molecule 59: 60S ribosomal protein L23-A

Chain N3: 



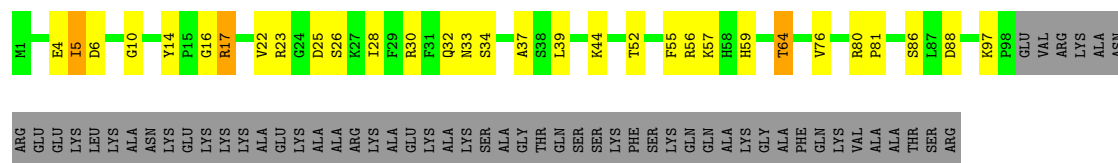
- Molecule 59: 60S ribosomal protein L23-A

Chain n3: 




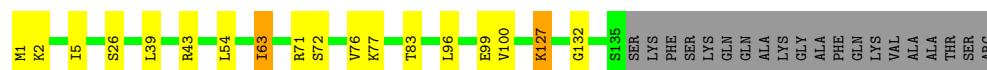
- Molecule 60: 60S ribosomal protein L24-A

Chain N4: 

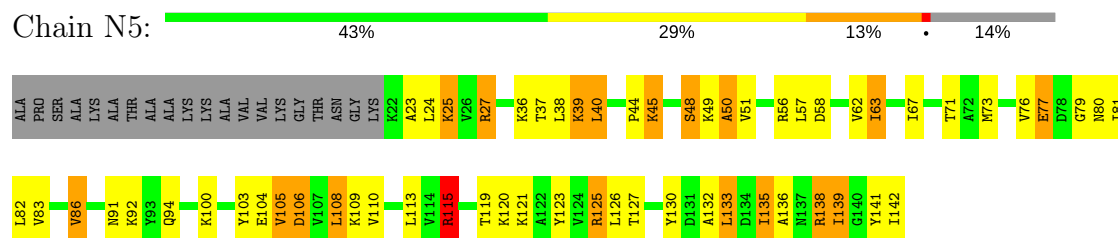


- Molecule 60: 60S ribosomal protein L24-A

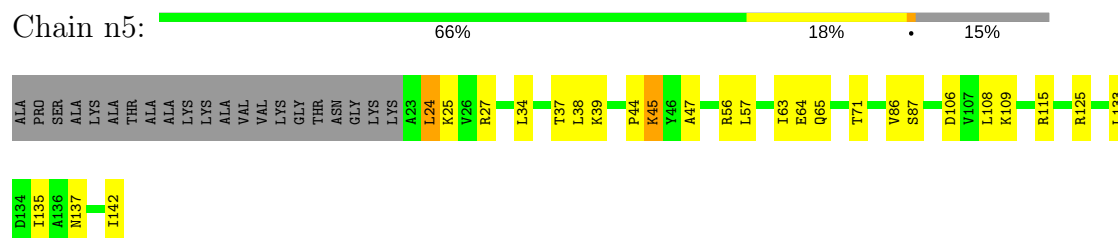
Chain n4: 



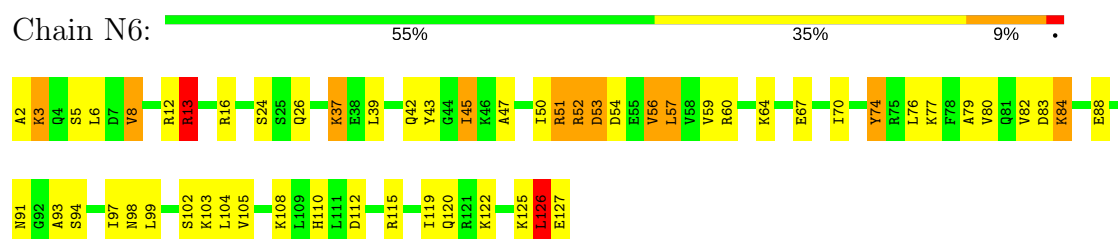
- Molecule 61: 60S ribosomal protein L25



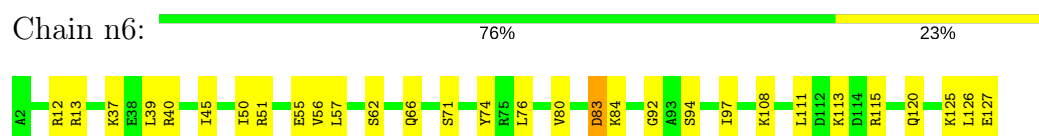
• Molecule 61: 60S ribosomal protein L25



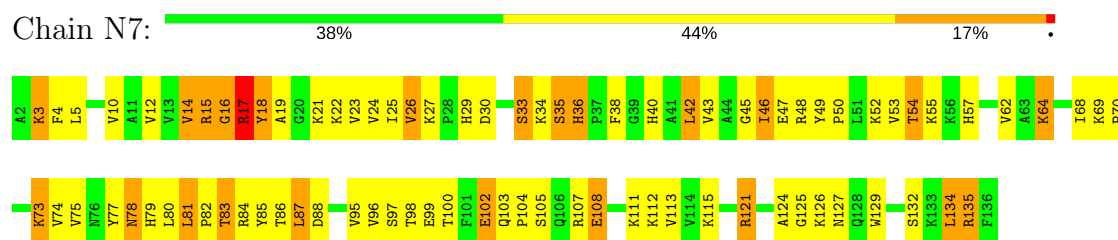
• Molecule 62: 60S ribosomal protein L26-A



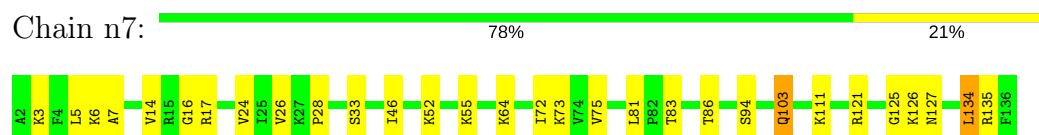
• Molecule 62: 60S ribosomal protein L26-A



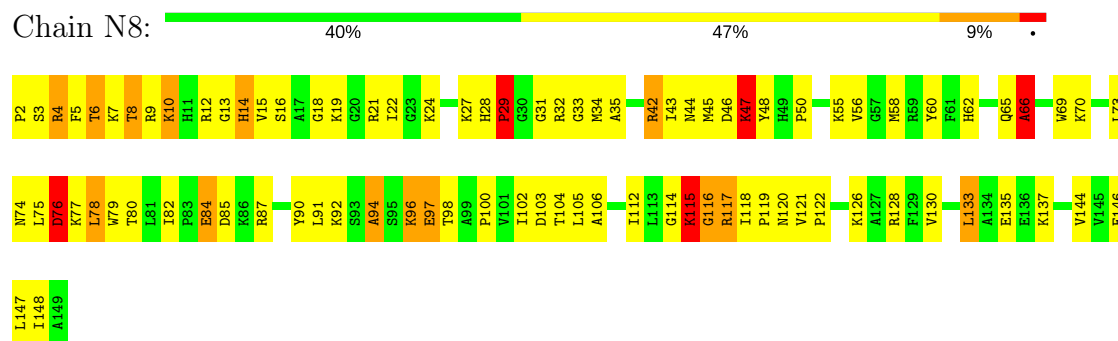
• Molecule 63: 60S ribosomal protein L27-A



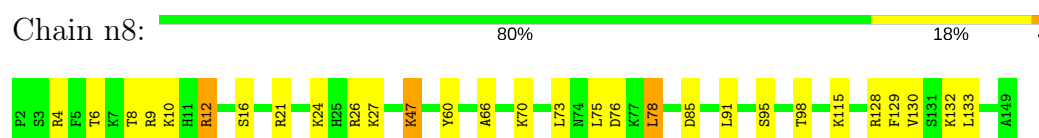
• Molecule 63: 60S ribosomal protein L27-A



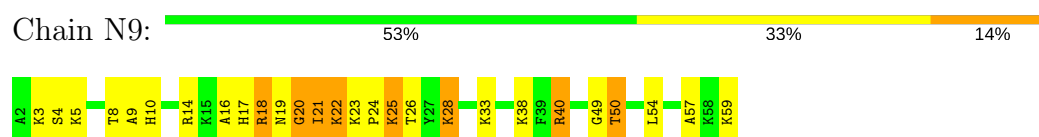
- Molecule 64: 60S ribosomal protein L28



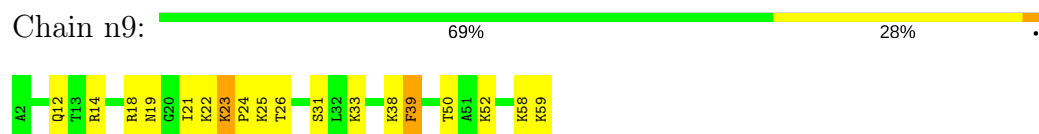
- Molecule 64: 60S ribosomal protein L28



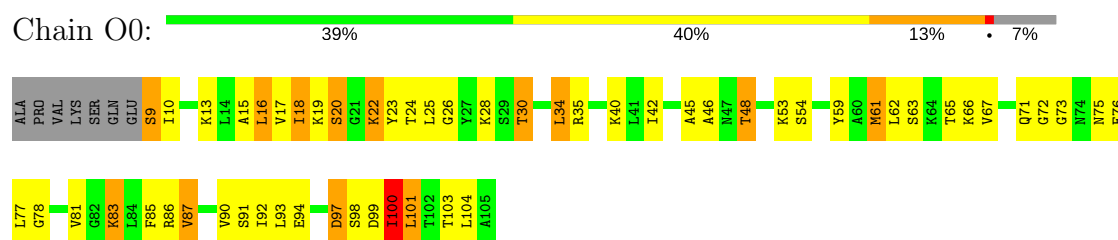
- Molecule 65: 60S ribosomal protein L29



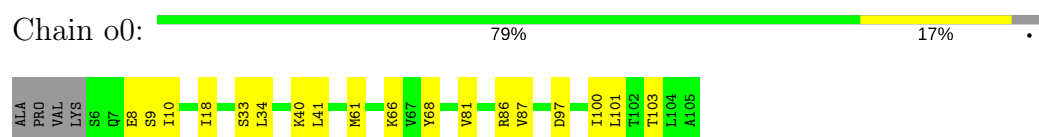
- Molecule 65: 60S ribosomal protein L29



- Molecule 66: 60S ribosomal protein L30

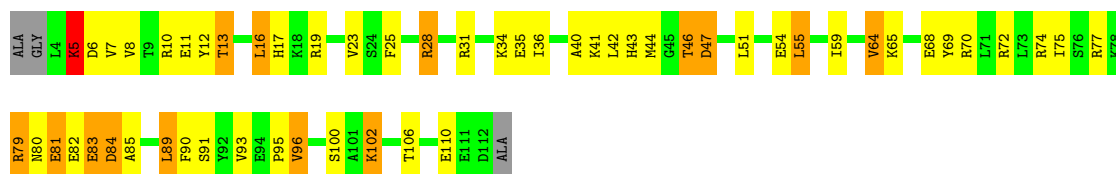


- Molecule 66: 60S ribosomal protein L30




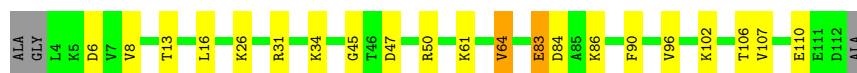
- Molecule 67: 60S ribosomal protein L31-A

Chain O1: 



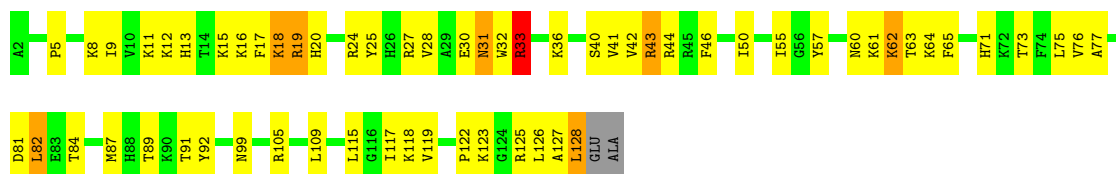
- Molecule 67: 60S ribosomal protein L31-A

Chain o1: 




- Molecule 68: 60S ribosomal protein L32

Chain O2: 



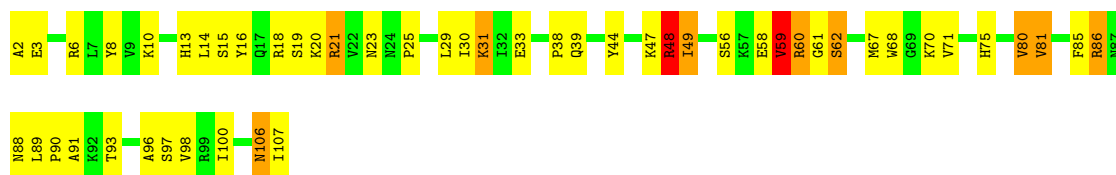
- Molecule 68: 60S ribosomal protein L32

Chain o2: 




- Molecule 69: 60S ribosomal protein L33-A

Chain O3: 

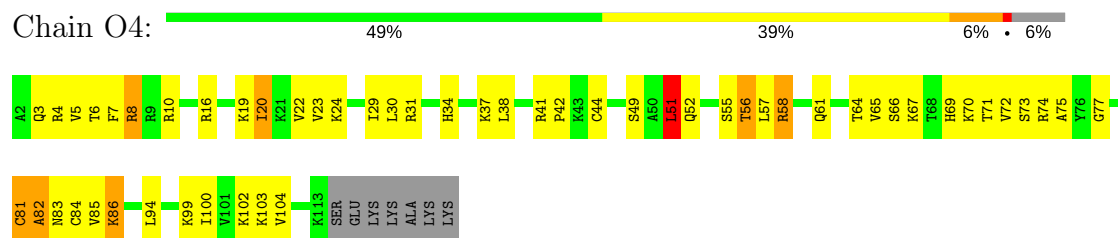


- Molecule 69: 60S ribosomal protein L33-A

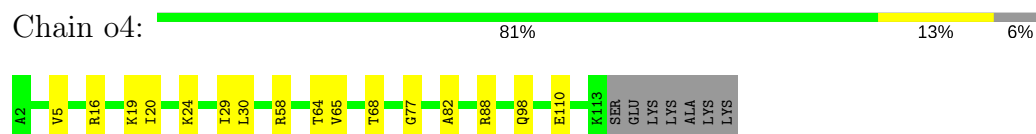
Chain o3: 



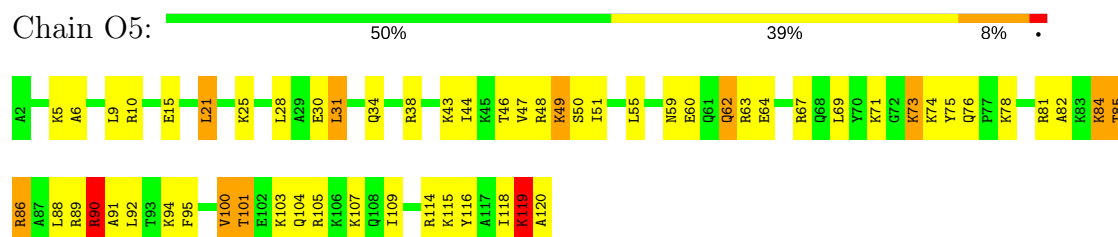
- Molecule 70: 60S ribosomal protein L34-A



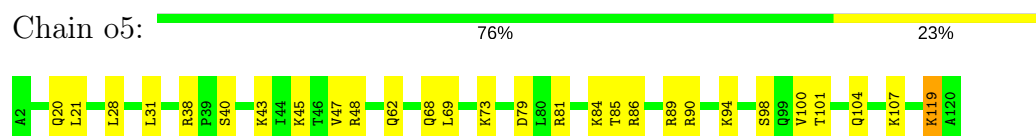
- Molecule 70: 60S ribosomal protein L34-A



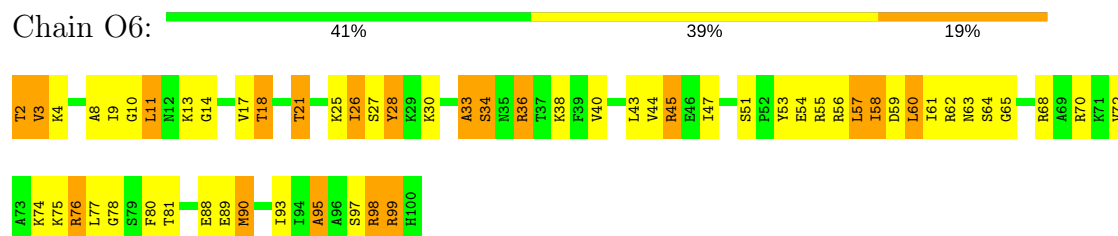
- Molecule 71: 60S ribosomal protein L35-A



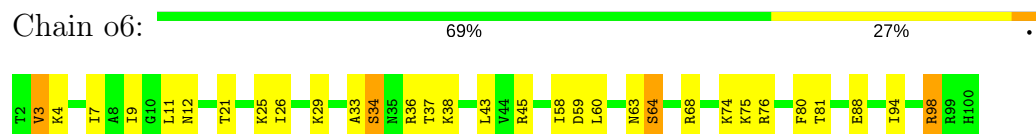
- Molecule 71: 60S ribosomal protein L35-A



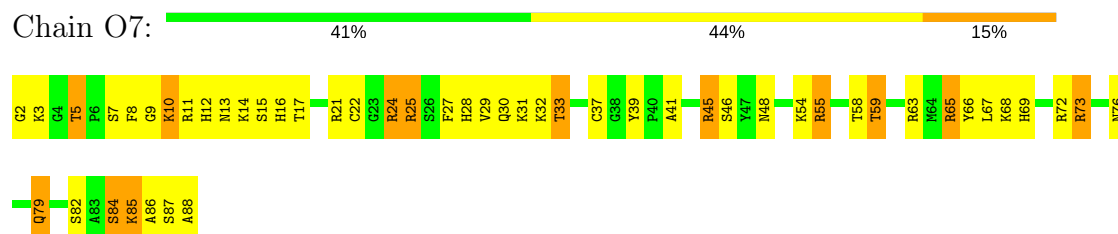
- Molecule 72: 60S ribosomal protein L36-A



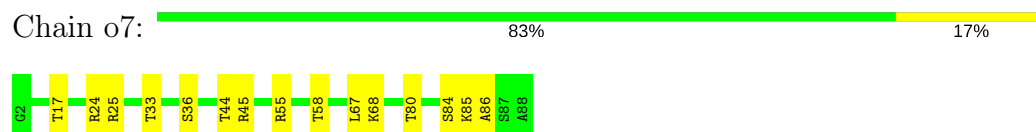
- Molecule 72: 60S ribosomal protein L36-A



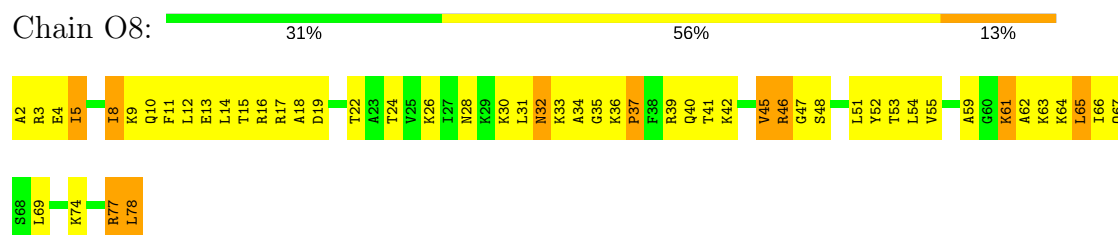
- Molecule 73: 60S ribosomal protein L37-A



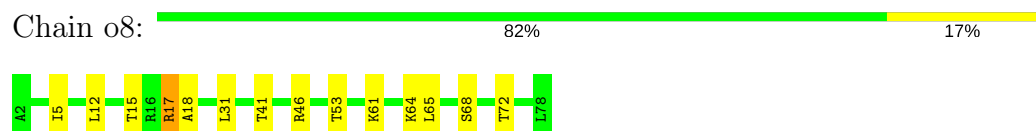
- Molecule 73: 60S ribosomal protein L37-A



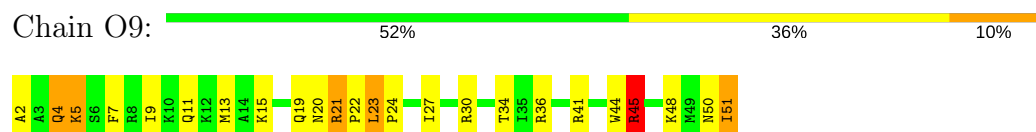
- Molecule 74: 60S ribosomal protein L38



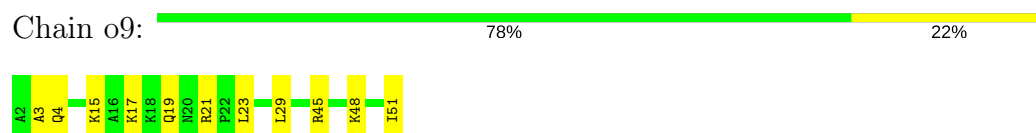
- Molecule 74: 60S ribosomal protein L38



- Molecule 75: 60S ribosomal protein L39

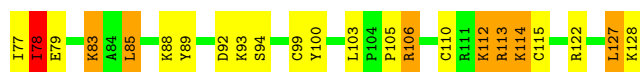


- Molecule 75: 60S ribosomal protein L39



- Molecule 76: Ubiquitin-60S ribosomal protein L40





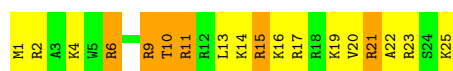
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0: 85% 13%



- Molecule 77: 60S ribosomal protein L41-A

Chain Q1: 28% 48% 24%



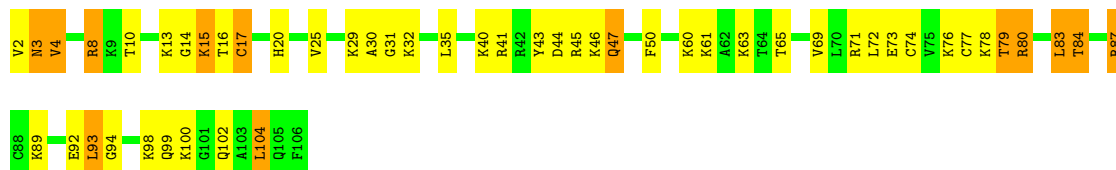
- Molecule 77: 60S ribosomal protein L41-A

Chain q1: 64% 32%



- Molecule 78: 60S ribosomal protein L42-A

Chain Q2: 51% 36% 12%



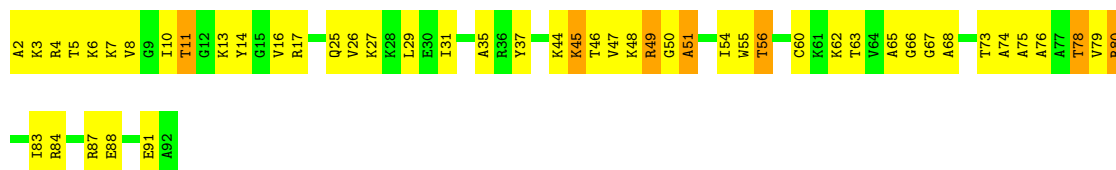
- Molecule 78: 60S ribosomal protein L42-A

Chain q2: 79% 21%




- Molecule 79: 60S ribosomal protein L43-A

Chain Q3: 45% 47% 8%



- Molecule 79: 60S ribosomal protein L43-A

Chain q3:  85% 15%



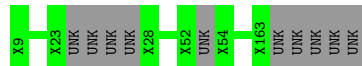
- Molecule 80: 40S ribosomal protein S30-A

Chain e0:  76% 23% .




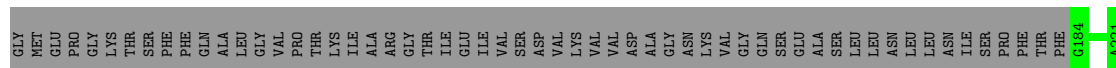
- Molecule 81: Unknown protein m2

Chain m2:  94% 6%



- Molecule 82: 60S acidic ribosomal protein P0

Chain p0:  39% 7% 54%



- Molecule 83: Unknown protein p1

Chain p1:  100%

There are no outlier residues recorded for this chain.

- Molecule 84: Unknown protein p2

Chain p2:  100%

There are no outlier residues recorded for this chain.

4 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	436.64Å 287.69Å 304.39Å 90.00° 98.98° 90.00°	Depositor
Resolution (Å)	300.66 – 2.80	Depositor
% Data completeness (in resolution range)	99.6 (300.66-2.80)	Depositor
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.208 , 0.246	Depositor
Wilson B-factor (Å ²)	60.5	Xtriage
Anisotropy	0.227	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411226	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% 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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 3H3, OHX, MG

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 $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2	0.75	5/41698 (0.0%)	1.30	337/64972 (0.5%)
1	6	0.87	23/42765 (0.1%)	1.40	490/66634 (0.7%)
2	S0	0.47	0/1617	0.67	0/2215
2	s0	0.53	0/1623	0.76	2/2222 (0.1%)
3	S1	0.37	0/1735	0.62	0/2335
3	s1	0.52	0/1748	0.71	1/2352 (0.0%)
4	S2	0.51	0/1665	0.67	0/2263
4	s2	0.61	0/1665	0.79	0/2263
5	S3	0.50	0/1759	0.65	0/2368
5	s3	0.48	0/1759	0.62	0/2368
6	S4	0.51	0/2109	0.74	2/2839 (0.1%)
6	s4	0.57	0/2109	0.79	1/2839 (0.0%)
7	S5	0.43	0/1629	0.60	0/2202
7	s5	0.46	0/1629	0.66	1/2202 (0.0%)
8	S6	0.48	0/1823	0.65	0/2439
8	s6	0.58	0/1779	0.72	1/2379 (0.0%)
9	S7	0.46	0/1506	0.65	0/2028
9	s7	0.54	0/1516	0.70	1/2043 (0.0%)
10	S8	0.58	0/1514	0.79	3/2021 (0.1%)
10	s8	0.64	0/1514	0.77	1/2021 (0.0%)
11	S9	0.50	0/1519	0.69	0/2035
11	s9	0.59	0/1519	0.74	0/2035
12	C0	0.45	0/790	0.69	1/1069 (0.1%)
12	c0	0.40	0/777	0.63	3/1049 (0.3%)
13	C1	0.59	0/1240	0.71	0/1675
13	c1	0.66	0/1194	0.86	0/1610
14	C2	0.37	0/898	0.62	0/1220
14	c2	0.31	0/898	0.58	1/1220 (0.1%)
15	C3	0.50	0/1215	0.71	2/1638 (0.1%)
15	c3	0.61	0/1215	0.77	0/1638
16	C4	0.38	0/901	0.65	0/1217
16	c4	0.54	0/960	0.77	1/1290 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.50	0/998	0.67	0/1341
17	c5	0.51	0/1060	0.68	1/1426 (0.1%)
18	C6	0.47	0/1125	0.74	3/1510 (0.2%)
18	c6	0.50	0/1131	0.69	0/1518
19	C7	0.46	0/935	0.65	0/1254
19	c7	0.50	0/914	0.70	0/1224
20	C8	0.49	0/1211	0.67	0/1628
20	c8	0.51	0/1211	0.73	1/1628 (0.1%)
21	C9	0.48	0/1130	0.68	0/1517
21	c9	0.51	0/1130	0.71	0/1517
22	D0	0.48	0/865	0.66	0/1169
22	d0	0.49	0/892	0.68	0/1205
23	D1	0.47	0/693	0.66	0/935
23	d1	0.57	0/693	0.80	0/935
24	D2	0.55	0/1038	0.75	1/1395 (0.1%)
24	d2	0.68	0/1038	0.75	0/1395
25	D3	0.63	0/1139	0.79	1/1518 (0.1%)
25	d3	0.73	0/1139	0.83	3/1518 (0.2%)
26	D4	0.48	0/1087	0.63	0/1449
26	d4	0.53	0/1087	0.72	0/1449
27	D5	0.42	0/571	0.71	0/768
27	d5	0.45	0/566	0.63	0/761
28	D6	0.47	0/782	0.67	0/1047
28	d6	0.59	0/782	0.75	0/1047
29	D7	0.46	0/620	0.68	1/838 (0.1%)
29	d7	0.52	0/620	0.73	0/838
30	D8	0.36	0/499	0.56	0/670
30	d8	0.44	0/499	0.67	0/670
31	D9	0.56	0/452	0.82	1/600 (0.2%)
31	d9	0.58	0/452	0.72	0/600
32	E0	0.49	0/483	0.65	0/643
33	E1	0.49	0/577	0.83	0/770
33	e1	0.43	0/619	0.75	1/822 (0.1%)
34	SR	1.06	2/2494 (0.1%)	1.50	6/3393 (0.2%)
34	sR	0.41	0/2495	0.58	0/3395
35	SM	0.55	0/1113	0.71	2/1502 (0.1%)
35	sM	0.51	0/683	0.68	1/923 (0.1%)
36	1	1.16	152/75394 (0.2%)	1.67	1955/117545 (1.7%)
36	5	1.20	176/75414 (0.2%)	1.69	1938/117575 (1.6%)
37	3	0.96	4/2883 (0.1%)	1.42	33/4491 (0.7%)
37	7	1.13	7/2883 (0.2%)	1.63	50/4491 (1.1%)
38	4	1.11	2/3746 (0.1%)	1.60	70/5832 (1.2%)
38	8	1.00	5/3746 (0.1%)	1.51	46/5832 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.75	0/1948	0.87	2/2617 (0.1%)
39	l2	0.82	1/1946 (0.1%)	0.95	5/2614 (0.2%)
40	L3	0.77	2/3146 (0.1%)	0.88	2/4228 (0.0%)
40	l3	0.85	1/3146 (0.0%)	0.96	11/4228 (0.3%)
41	L4	0.86	3/2800 (0.1%)	1.02	10/3790 (0.3%)
41	l4	0.79	0/2800	0.94	6/3790 (0.2%)
42	L5	0.59	0/2425	0.72	0/3271
42	l5	0.78	0/2408	0.83	3/3248 (0.1%)
43	L6	0.77	0/1260	0.85	3/1694 (0.2%)
43	l6	0.78	0/1269	0.85	0/1705
44	L7	0.85	1/1821 (0.1%)	0.90	0/2451
44	l7	0.86	1/1828 (0.1%)	0.91	5/2461 (0.2%)
45	L8	0.59	0/1836	0.69	1/2481 (0.0%)
45	l8	0.57	0/1795	0.69	0/2429
46	L9	0.70	0/1539	0.79	0/2073
46	l9	0.80	0/1539	0.85	0/2073
47	M0	0.76	0/1741	0.88	3/2335 (0.1%)
47	m0	0.82	0/1758	0.89	0/2358
48	M1	0.55	0/1374	0.74	1/1842 (0.1%)
48	m1	0.67	0/1374	0.83	2/1842 (0.1%)
49	M3	0.77	0/1568	0.91	3/2106 (0.1%)
49	m3	0.75	0/1573	0.89	4/2113 (0.2%)
50	M4	0.79	0/1068	0.87	2/1438 (0.1%)
50	m4	0.81	0/1074	0.84	1/1446 (0.1%)
51	M5	0.78	0/1757	0.97	3/2354 (0.1%)
51	m5	0.72	0/1757	0.83	0/2354
52	M6	0.93	3/1585 (0.2%)	1.00	7/2128 (0.3%)
52	m6	1.06	2/1585 (0.1%)	1.04	9/2128 (0.4%)
53	M7	0.84	0/1443	0.87	0/1944
53	m7	0.93	1/1250 (0.1%)	0.89	0/1683
54	M8	0.84	0/1465	0.95	4/1965 (0.2%)
54	m8	0.76	0/1465	0.94	2/1965 (0.1%)
55	M9	0.58	0/1538	0.68	0/2050
55	m9	0.65	0/1538	0.72	0/2050
56	N0	0.81	0/1481	0.87	3/1990 (0.2%)
56	n0	0.84	0/1481	0.92	1/1990 (0.1%)
57	N1	0.81	0/1300	0.86	0/1743
57	n1	0.86	1/1300 (0.1%)	0.86	0/1743
58	N2	0.46	0/812	0.61	0/1099
58	n2	0.53	0/794	0.66	0/1076
59	N3	0.78	0/1018	0.94	5/1369 (0.4%)
59	n3	0.85	0/1018	0.93	4/1369 (0.3%)
60	N4	0.61	0/712	0.69	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.68	0/1052	0.72	0/1398
61	N5	0.65	0/979	0.82	1/1321 (0.1%)
61	n5	0.68	0/974	0.84	0/1314
62	N6	0.76	0/1004	0.94	4/1341 (0.3%)
62	n6	0.68	0/1004	0.82	0/1341
63	N7	0.54	0/1118	0.72	0/1497
63	n7	0.52	0/1118	0.66	0/1497
64	N8	0.86	0/1204	0.97	4/1612 (0.2%)
64	n8	0.84	0/1204	0.97	4/1612 (0.2%)
65	N9	0.85	0/473	0.81	1/629 (0.2%)
65	n9	0.90	0/473	0.93	2/629 (0.3%)
66	O0	0.53	0/751	0.68	0/1008
66	o0	0.55	0/775	0.67	0/1040
67	O1	0.68	0/890	0.75	0/1196
67	o1	0.85	1/897 (0.1%)	0.86	0/1205
68	O2	0.87	0/1041	0.95	4/1394 (0.3%)
68	o2	0.89	0/1041	1.02	5/1394 (0.4%)
69	O3	0.92	0/868	0.90	3/1168 (0.3%)
69	o3	0.98	1/868 (0.1%)	0.92	2/1168 (0.2%)
70	O4	0.62	0/890	0.80	1/1189 (0.1%)
70	o4	0.67	0/890	0.74	0/1189
71	O5	0.71	1/978 (0.1%)	0.84	2/1301 (0.2%)
71	o5	0.62	0/974	0.71	0/1297
72	O6	0.68	0/778	0.84	0/1034
72	o6	0.60	0/777	0.74	0/1033
73	O7	0.89	1/696 (0.1%)	1.00	2/923 (0.2%)
73	o7	0.75	0/696	0.88	1/923 (0.1%)
74	O8	0.52	0/618	0.64	0/826
74	o8	0.49	0/614	0.67	0/822
75	O9	0.89	1/443 (0.2%)	0.96	1/588 (0.2%)
75	o9	0.81	0/443	0.95	0/588
76	Q0	0.73	0/423	0.90	1/562 (0.2%)
76	q0	0.89	0/423	0.92	1/562 (0.2%)
77	Q1	0.70	0/234	0.93	0/300
77	q1	0.94	0/234	1.05	1/300 (0.3%)
78	Q2	1.00	1/860 (0.1%)	0.99	2/1136 (0.2%)
78	q2	0.83	2/860 (0.2%)	0.87	0/1136
79	Q3	0.73	0/701	0.84	0/934
79	q3	0.78	0/701	0.88	0/934
80	e0	0.58	0/499	0.77	0/665
82	p0	0.46	0/1092	0.62	0/1474
All	All	0.92	400/430070 (0.1%)	1.33	5106/631356 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	S0	0	1
7	s5	0	2
9	S7	0	1
10	S8	0	1
16	C4	0	2
17	c5	0	1
19	C7	0	1
22	d0	0	1
25	D3	0	1
25	d3	0	1
26	d4	0	2
27	D5	0	1
28	D6	0	3
31	d9	0	1
33	E1	0	1
34	SR	0	2
39	L2	0	1
39	l2	0	2
40	l3	0	2
41	L4	0	2
41	l4	0	1
42	L5	0	1
42	l5	0	2
43	l6	0	1
44	L7	0	1
44	l7	0	2
51	M5	0	1
52	M6	0	2
52	m6	0	1
53	M7	0	1
53	m7	0	1
57	N1	0	1
59	n3	0	1
62	n6	0	1
63	N7	0	1
63	n7	0	1
64	n8	0	2
65	N9	0	1
65	n9	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
67	O1	0	1
67	o1	0	1
72	O6	0	1
All	All	0	57

The worst 5 of 400 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	SR	160	GLU	C-N	-38.52	0.45	1.34
34	SR	161	LYS	C-N	-29.42	0.66	1.34
78	Q2	17	CYS	CB-SG	16.03	2.09	1.82
36	5	1152	G	N9-C4	-13.26	1.27	1.38
39	l2	213	GLY	C-O	9.71	1.39	1.23

The worst 5 of 5106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	SR	161	LYS	O-C-N	-48.73	44.74	122.70
34	SR	160	GLU	C-N-CA	-43.07	14.02	121.70
34	SR	160	GLU	CA-C-N	-38.98	31.43	117.20
36	5	1152	G	N3-C4-C5	26.73	141.96	128.60
36	5	1152	G	N3-C4-N9	-24.27	111.44	126.00

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
16	C4	124	ASP	Peptide
2	S0	188	LEU	Peptide
9	S7	131	PHE	Peptide
10	S8	147	ALA	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37283	0	18757	748	0
1	6	38238	0	19241	711	0
2	S0	1577	0	1567	139	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	145	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	111	0
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	93	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	146	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	130	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	106	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	106	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	98	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	116	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	58	0
12	c0	762	0	699	0	0
13	C1	1214	0	1259	59	0
13	c1	1168	0	1231	0	0
14	C2	890	0	887	64	0
14	c2	890	0	887	0	0
15	C3	1192	0	1255	76	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	91	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	74	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	90	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	68	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	89	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	84	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	d0	882	0	939	0	0
23	D1	684	0	672	54	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	65	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	72	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	70	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	52	0
27	d5	558	0	598	0	0
28	D6	769	0	814	84	0
28	d6	769	0	814	0	0
29	D7	610	0	631	49	0
29	d7	610	0	631	0	0
30	D8	497	0	535	34	0
30	d8	497	0	535	0	0
31	D9	442	0	428	33	0
31	d9	442	0	428	0	0
32	E0	475	0	525	25	0
33	E1	566	0	602	63	0
33	e1	608	0	657	0	0
34	SR	2441	0	2395	133	0
34	sR	2442	0	2392	0	0
35	SM	1104	0	996	67	0
35	sM	680	0	607	0	0
36	1	67355	0	33840	1037	0
36	5	67376	0	33857	1042	0
37	3	2579	0	1304	39	0
37	7	2579	0	1304	39	0
38	4	3353	0	1695	51	0
38	8	3353	0	1695	58	0
39	L2	1914	0	1981	137	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	218	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	173	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	169	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	61	0
43	l6	1248	0	1339	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	L7	1784	0	1862	74	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	114	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	106	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1736	107	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	84	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	94	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	54	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	118	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	83	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	81	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	87	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	77	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	71	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	72	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	29	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	62	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	18	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	65	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	51	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	80	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	94	0
64	n8	1173	0	1215	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	N9	462	0	491	28	0
65	n9	462	0	491	0	0
66	O0	743	0	797	52	0
66	o0	767	0	816	0	0
67	O1	876	0	912	40	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	48	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	45	0
69	o3	850	0	880	0	0
70	O4	880	0	945	53	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	61	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	55	0
72	o6	770	0	846	0	0
73	O7	681	0	683	55	0
73	o7	681	0	683	0	0
74	O8	612	0	682	46	0
74	o8	608	0	671	0	0
75	O9	436	0	475	31	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	26	0
76	q0	417	0	455	0	0
77	Q1	233	0	284	25	0
77	q1	233	0	284	0	0
78	Q2	847	0	916	51	0
78	q2	847	0	914	0	0
79	Q3	694	0	734	44	0
79	q3	694	0	734	0	0
80	e0	491	0	542	0	0
81	m2	750	0	175	0	0
82	p0	1077	0	1041	0	0
83	p1	235	0	51	0	0
84	p2	230	0	50	0	0
85	1	475	0	0	0	0
85	2	126	0	0	0	0
85	3	14	0	0	0	0
85	4	21	0	0	0	0
85	5	504	0	0	0	0
85	6	147	0	0	0	0
85	7	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	8	13	0	0	0	0
85	C3	1	0	0	0	0
85	L2	1	0	0	0	0
85	L3	2	0	0	0	0
85	L4	3	0	0	0	0
85	L5	1	0	0	0	0
85	L6	1	0	0	0	0
85	L7	2	0	0	0	0
85	L8	1	0	0	0	0
85	M0	2	0	0	0	0
85	M1	1	0	0	0	0
85	M3	4	0	0	0	0
85	M5	2	0	0	0	0
85	M6	1	0	0	0	0
85	M7	6	0	0	0	0
85	M9	1	0	0	0	0
85	N0	1	0	0	0	0
85	N3	3	0	0	0	0
85	N5	1	0	0	0	0
85	N8	2	0	0	0	0
85	O3	1	0	0	0	0
85	O4	1	0	0	0	0
85	O7	1	0	0	0	0
85	Q2	1	0	0	0	0
85	S8	1	0	0	0	0
85	SM	1	0	0	0	0
85	c1	1	0	0	0	0
85	c7	1	0	0	0	0
85	c8	2	0	0	0	0
85	d2	1	0	0	0	0
85	d3	1	0	0	0	0
85	d6	1	0	0	0	0
85	l2	2	0	0	0	0
85	l3	1	0	0	0	0
85	l4	1	0	0	0	0
85	l5	3	0	0	0	0
85	l7	1	0	0	0	0
85	m1	2	0	0	0	0
85	m4	1	0	0	0	0
85	m5	1	0	0	0	0
85	m6	1	0	0	0	0
85	m7	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	n0	2	0	0	0	0
85	n3	2	0	0	0	0
85	n6	2	0	0	0	0
85	n8	4	0	0	0	0
85	n9	2	0	0	0	0
85	o1	1	0	0	0	0
85	o3	2	0	0	0	0
85	o4	2	0	0	0	0
85	q0	1	0	0	0	0
85	q1	1	0	0	0	0
85	q3	1	0	0	0	0
85	s1	1	0	0	0	0
85	s6	1	0	0	0	0
85	s8	2	0	0	0	0
85	sM	2	0	0	0	0
86	1	2436	0	0	247	0
86	2	1106	0	0	132	0
86	3	84	0	0	5	0
86	4	105	0	0	5	0
86	5	2471	0	0	233	0
86	6	1106	0	0	97	0
86	7	84	0	0	12	0
86	8	112	0	0	21	0
86	C1	7	0	0	7	0
86	C3	7	0	0	1	0
86	C5	7	0	0	4	0
86	C8	7	0	0	1	0
86	D9	7	0	0	1	0
86	L3	14	0	0	1	0
86	L4	7	0	0	2	0
86	L6	7	0	0	0	0
86	M0	7	0	0	0	0
86	M5	14	0	0	2	0
86	M6	7	0	0	1	0
86	M7	14	0	0	1	0
86	M9	7	0	0	1	0
86	N9	7	0	0	1	0
86	O2	7	0	0	0	0
86	O3	7	0	0	0	0
86	O7	14	0	0	6	0
86	O9	7	0	0	4	0
86	Q2	7	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	S8	7	0	0	1	0
86	SR	7	0	0	0	0
86	c1	7	0	0	0	0
86	c3	7	0	0	0	0
86	c5	7	0	0	0	0
86	c8	7	0	0	0	0
86	d4	7	0	0	0	0
86	d9	7	0	0	0	0
86	l3	21	0	0	0	0
86	l4	14	0	0	0	0
86	l5	21	0	0	0	0
86	l9	7	0	0	0	0
86	m0	14	0	0	0	0
86	m1	7	0	0	0	0
86	m4	7	0	0	0	0
86	m5	7	0	0	0	0
86	m6	7	0	0	0	0
86	m7	7	0	0	0	0
86	m8	7	0	0	0	0
86	n3	7	0	0	0	0
86	n9	7	0	0	0	0
86	o2	7	0	0	0	0
86	o3	7	0	0	0	0
86	o4	7	0	0	0	0
86	o7	7	0	0	0	0
86	q2	7	0	0	0	0
86	s1	14	0	0	0	0
86	s4	7	0	0	0	0
86	s8	7	0	0	0	0
86	s9	7	0	0	0	0
86	sR	7	0	0	0	0
87	D6	1	0	0	0	0
87	D7	1	0	0	0	0
87	D9	1	0	0	0	0
87	E1	1	0	0	0	0
87	O7	1	0	0	0	0
87	Q0	1	0	0	0	0
87	Q2	1	0	0	3	0
87	Q3	1	0	0	0	0
87	d6	1	0	0	0	0
87	d7	1	0	0	0	0
87	d9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	e1	1	0	0	0	0
87	o7	1	0	0	0	0
87	q0	1	0	0	0	0
87	q2	1	0	0	0	0
87	q3	1	0	0	0	0
88	1	33	0	35	1	0
88	5	33	0	35	1	0
All	All	411226	0	297341	8413	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 8413 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:M6:66:LYS:NZ	52:M6:66:LYS:CE	1.48	1.54
78:Q2:17:CYS:CB	78:Q2:17:CYS:SG	2.09	1.40
78:Q2:17:CYS:CB	87:Q2:501:ZN:ZN	1.31	1.09
40:L3:296:THR:HG22	40:L3:298:PHE:H	1.82	1.07
36:5:2403:G:N2	36:5:2404:A:N7	2.03	1.03

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	154 (76%)	27 (13%)	23 (11%)	0	1
2	s0	204/251 (81%)	161 (79%)	27 (13%)	16 (8%)	1	2
3	S1	212/254 (84%)	152 (72%)	31 (15%)	29 (14%)	0	1
3	s1	214/254 (84%)	179 (84%)	23 (11%)	12 (6%)	2	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	S2	215/253 (85%)	181 (84%)	25 (12%)	9 (4%)	3	10
4	s2	215/253 (85%)	187 (87%)	16 (7%)	12 (6%)	2	6
5	S3	221/239 (92%)	198 (90%)	14 (6%)	9 (4%)	3	11
5	s3	221/239 (92%)	193 (87%)	15 (7%)	13 (6%)	2	5
6	S4	258/260 (99%)	219 (85%)	27 (10%)	12 (5%)	3	8
6	s4	258/260 (99%)	223 (86%)	23 (9%)	12 (5%)	3	8
7	S5	204/224 (91%)	162 (79%)	21 (10%)	21 (10%)	0	1
7	s5	204/224 (91%)	164 (80%)	23 (11%)	17 (8%)	1	2
8	S6	224/236 (95%)	195 (87%)	21 (9%)	8 (4%)	4	13
8	s6	216/236 (92%)	194 (90%)	14 (6%)	8 (4%)	4	13
9	S7	182/189 (96%)	143 (79%)	21 (12%)	18 (10%)	1	1
9	s7	184/189 (97%)	148 (80%)	22 (12%)	14 (8%)	1	2
10	S8	184/200 (92%)	159 (86%)	12 (6%)	13 (7%)	1	3
10	s8	184/200 (92%)	164 (89%)	11 (6%)	9 (5%)	2	8
11	S9	183/196 (93%)	159 (87%)	15 (8%)	9 (5%)	2	8
11	s9	183/196 (93%)	148 (81%)	23 (13%)	12 (7%)	1	4
12	C0	94/105 (90%)	74 (79%)	14 (15%)	6 (6%)	1	4
12	c0	92/105 (88%)	63 (68%)	16 (17%)	13 (14%)	0	1
13	C1	153/155 (99%)	125 (82%)	18 (12%)	10 (6%)	1	4
13	c1	144/155 (93%)	117 (81%)	18 (12%)	9 (6%)	1	4
14	C2	122/142 (86%)	70 (57%)	26 (21%)	26 (21%)	0	0
14	c2	122/142 (86%)	71 (58%)	29 (24%)	22 (18%)	0	0
15	C3	148/150 (99%)	132 (89%)	13 (9%)	3 (2%)	9	28
15	c3	148/150 (99%)	123 (83%)	16 (11%)	9 (6%)	2	4
16	C4	125/136 (92%)	97 (78%)	16 (13%)	12 (10%)	1	1
16	c4	126/136 (93%)	101 (80%)	15 (12%)	10 (8%)	1	2
17	C5	122/141 (86%)	95 (78%)	16 (13%)	11 (9%)	1	1
17	c5	133/141 (94%)	97 (73%)	16 (12%)	20 (15%)	0	0
18	C6	139/142 (98%)	121 (87%)	13 (9%)	5 (4%)	4	13
18	c6	140/142 (99%)	121 (86%)	11 (8%)	8 (6%)	2	5
19	C7	116/136 (85%)	87 (75%)	22 (19%)	7 (6%)	2	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	c7	113/136 (83%)	96 (85%)	11 (10%)	6 (5%)	2	7
20	C8	143/145 (99%)	121 (85%)	11 (8%)	11 (8%)	1	2
20	c8	143/145 (99%)	115 (80%)	21 (15%)	7 (5%)	2	8
21	C9	141/143 (99%)	122 (86%)	14 (10%)	5 (4%)	4	14
21	c9	141/143 (99%)	122 (86%)	14 (10%)	5 (4%)	4	14
22	D0	105/120 (88%)	88 (84%)	15 (14%)	2 (2%)	9	30
22	d0	108/120 (90%)	85 (79%)	15 (14%)	8 (7%)	1	3
23	D1	85/87 (98%)	69 (81%)	10 (12%)	6 (7%)	1	3
23	d1	85/87 (98%)	75 (88%)	5 (6%)	5 (6%)	2	5
24	D2	127/129 (98%)	113 (89%)	13 (10%)	1 (1%)	22	55
24	d2	127/129 (98%)	116 (91%)	10 (8%)	1 (1%)	22	55
25	D3	142/144 (99%)	117 (82%)	14 (10%)	11 (8%)	1	2
25	d3	142/144 (99%)	131 (92%)	10 (7%)	1 (1%)	25	59
26	D4	132/134 (98%)	110 (83%)	14 (11%)	8 (6%)	2	4
26	d4	132/134 (98%)	106 (80%)	15 (11%)	11 (8%)	1	2
27	D5	68/107 (64%)	51 (75%)	9 (13%)	8 (12%)	0	1
27	d5	67/107 (63%)	48 (72%)	13 (19%)	6 (9%)	1	1
28	D6	95/97 (98%)	69 (73%)	12 (13%)	14 (15%)	0	0
28	d6	95/97 (98%)	73 (77%)	14 (15%)	8 (8%)	1	2
29	D7	79/81 (98%)	62 (78%)	12 (15%)	5 (6%)	1	4
29	d7	79/81 (98%)	60 (76%)	10 (13%)	9 (11%)	0	1
30	D8	61/66 (92%)	51 (84%)	7 (12%)	3 (5%)	2	8
30	d8	61/66 (92%)	46 (75%)	10 (16%)	5 (8%)	1	2
31	D9	51/55 (93%)	41 (80%)	7 (14%)	3 (6%)	2	5
31	d9	51/55 (93%)	42 (82%)	5 (10%)	4 (8%)	1	2
32	E0	58/60 (97%)	45 (78%)	12 (21%)	1 (2%)	11	34
33	E1	69/76 (91%)	36 (52%)	14 (20%)	19 (28%)	0	0
33	e1	74/76 (97%)	38 (51%)	16 (22%)	20 (27%)	0	0
34	SR	316/318 (99%)	274 (87%)	29 (9%)	13 (4%)	3	11
34	sR	316/318 (99%)	268 (85%)	40 (13%)	8 (2%)	6	22
35	SM	155/273 (57%)	109 (70%)	26 (17%)	20 (13%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	sM	98/273 (36%)	61 (62%)	24 (24%)	13 (13%)	0	1
39	L2	250/253 (99%)	226 (90%)	20 (8%)	4 (2%)	11	36
39	l2	250/253 (99%)	214 (86%)	27 (11%)	9 (4%)	4	13
40	L3	384/386 (100%)	340 (88%)	31 (8%)	13 (3%)	4	15
40	l3	384/386 (100%)	350 (91%)	25 (6%)	9 (2%)	7	25
41	L4	359/361 (99%)	315 (88%)	23 (6%)	21 (6%)	2	5
41	l4	359/361 (99%)	308 (86%)	38 (11%)	13 (4%)	4	13
42	L5	294/296 (99%)	253 (86%)	23 (8%)	18 (6%)	2	4
42	l5	292/296 (99%)	262 (90%)	21 (7%)	9 (3%)	5	16
43	L6	152/175 (87%)	141 (93%)	8 (5%)	3 (2%)	9	28
43	l6	153/175 (87%)	132 (86%)	17 (11%)	4 (3%)	6	21
44	L7	220/243 (90%)	205 (93%)	6 (3%)	9 (4%)	3	11
44	l7	221/243 (91%)	203 (92%)	15 (7%)	3 (1%)	13	39
45	L8	231/255 (91%)	193 (84%)	30 (13%)	8 (4%)	4	14
45	l8	229/255 (90%)	184 (80%)	25 (11%)	20 (9%)	1	2
46	L9	189/191 (99%)	170 (90%)	14 (7%)	5 (3%)	6	21
46	l9	189/191 (99%)	173 (92%)	10 (5%)	6 (3%)	5	16
47	M0	207/220 (94%)	185 (89%)	17 (8%)	5 (2%)	7	23
47	m0	209/220 (95%)	181 (87%)	20 (10%)	8 (4%)	4	12
48	M1	167/173 (96%)	133 (80%)	20 (12%)	14 (8%)	1	2
48	m1	167/173 (96%)	146 (87%)	11 (7%)	10 (6%)	2	5
49	M3	191/198 (96%)	164 (86%)	19 (10%)	8 (4%)	3	10
49	m3	192/198 (97%)	164 (85%)	17 (9%)	11 (6%)	2	5
50	M4	134/137 (98%)	118 (88%)	11 (8%)	5 (4%)	4	13
50	m4	135/137 (98%)	127 (94%)	6 (4%)	2 (2%)	12	37
51	M5	201/203 (99%)	188 (94%)	7 (4%)	6 (3%)	5	17
51	m5	201/203 (99%)	180 (90%)	14 (7%)	7 (4%)	4	14
52	M6	195/198 (98%)	185 (95%)	6 (3%)	4 (2%)	8	27
52	m6	195/198 (98%)	185 (95%)	8 (4%)	2 (1%)	18	50
53	M7	181/183 (99%)	159 (88%)	16 (9%)	6 (3%)	4	15
53	m7	153/183 (84%)	140 (92%)	10 (6%)	3 (2%)	9	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	M8	183/185 (99%)	169 (92%)	10 (6%)	4 (2%)	8	26
54	m8	183/185 (99%)	165 (90%)	11 (6%)	7 (4%)	4	12
55	M9	186/188 (99%)	173 (93%)	12 (6%)	1 (0%)	32	67
55	m9	186/188 (99%)	175 (94%)	8 (4%)	3 (2%)	11	36
56	N0	170/172 (99%)	157 (92%)	11 (6%)	2 (1%)	15	44
56	n0	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	10	32
57	N1	157/159 (99%)	138 (88%)	14 (9%)	5 (3%)	5	16
57	n1	157/159 (99%)	143 (91%)	10 (6%)	4 (2%)	6	22
58	N2	98/120 (82%)	79 (81%)	15 (15%)	4 (4%)	3	11
58	n2	96/120 (80%)	84 (88%)	9 (9%)	3 (3%)	5	16
59	N3	134/136 (98%)	126 (94%)	7 (5%)	1 (1%)	25	59
59	n3	134/136 (98%)	125 (93%)	8 (6%)	1 (1%)	25	59
60	N4	96/155 (62%)	77 (80%)	14 (15%)	5 (5%)	2	7
60	n4	133/155 (86%)	113 (85%)	12 (9%)	8 (6%)	2	5
61	N5	119/141 (84%)	110 (92%)	8 (7%)	1 (1%)	22	55
61	n5	118/141 (84%)	100 (85%)	13 (11%)	5 (4%)	3	10
62	N6	124/126 (98%)	114 (92%)	6 (5%)	4 (3%)	5	16
62	n6	124/126 (98%)	113 (91%)	6 (5%)	5 (4%)	3	11
63	N7	133/135 (98%)	111 (84%)	12 (9%)	10 (8%)	1	2
63	n7	133/135 (98%)	111 (84%)	14 (10%)	8 (6%)	2	5
64	N8	146/148 (99%)	122 (84%)	16 (11%)	8 (6%)	2	6
64	n8	146/148 (99%)	126 (86%)	16 (11%)	4 (3%)	6	20
65	N9	56/58 (97%)	49 (88%)	5 (9%)	2 (4%)	4	13
65	n9	56/58 (97%)	43 (77%)	9 (16%)	4 (7%)	1	3
66	O0	95/104 (91%)	87 (92%)	6 (6%)	2 (2%)	8	27
66	o0	98/104 (94%)	89 (91%)	7 (7%)	2 (2%)	9	28
67	O1	107/112 (96%)	95 (89%)	7 (6%)	5 (5%)	3	8
67	o1	107/112 (96%)	98 (92%)	5 (5%)	4 (4%)	4	13
68	O2	125/129 (97%)	116 (93%)	8 (6%)	1 (1%)	22	55
68	o2	125/129 (97%)	111 (89%)	11 (9%)	3 (2%)	7	23
69	O3	104/106 (98%)	101 (97%)	2 (2%)	1 (1%)	18	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	o3	104/106 (98%)	92 (88%)	7 (7%)	5 (5%)	2	8
70	O4	110/119 (92%)	103 (94%)	4 (4%)	3 (3%)	6	20
70	o4	110/119 (92%)	100 (91%)	8 (7%)	2 (2%)	10	32
71	O5	117/119 (98%)	108 (92%)	5 (4%)	4 (3%)	4	15
71	o5	117/119 (98%)	106 (91%)	9 (8%)	2 (2%)	11	34
72	O6	97/99 (98%)	78 (80%)	11 (11%)	8 (8%)	1	2
72	o6	97/99 (98%)	81 (84%)	9 (9%)	7 (7%)	1	3
73	O7	85/87 (98%)	76 (89%)	6 (7%)	3 (4%)	4	14
73	o7	85/87 (98%)	72 (85%)	10 (12%)	3 (4%)	4	14
74	O8	75/77 (97%)	62 (83%)	10 (13%)	3 (4%)	3	11
74	o8	75/77 (97%)	66 (88%)	6 (8%)	3 (4%)	3	11
75	O9	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
75	o9	48/50 (96%)	44 (92%)	3 (6%)	1 (2%)	8	27
76	Q0	50/52 (96%)	48 (96%)	0	2 (4%)	3	11
76	q0	50/52 (96%)	49 (98%)	0	1 (2%)	9	28
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	23 (100%)	0	0	100	100
78	Q2	103/105 (98%)	90 (87%)	10 (10%)	3 (3%)	5	18
78	q2	103/105 (98%)	92 (89%)	8 (8%)	3 (3%)	5	18
79	Q3	89/91 (98%)	80 (90%)	7 (8%)	2 (2%)	8	26
79	q3	89/91 (98%)	80 (90%)	8 (9%)	1 (1%)	17	47
80	e0	60/62 (97%)	47 (78%)	9 (15%)	4 (7%)	1	4
82	p0	139/311 (45%)	117 (84%)	19 (14%)	3 (2%)	8	26
All	All	22333/24141 (92%)	19119 (86%)	2092 (9%)	1122 (5%)	2	7

5 of 1122 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	39	ASN
2	S0	66	ALA
2	S0	103	THR
2	S0	158	VAL
2	S0	163	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/209 (78%)	134 (82%)	30 (18%)	2	6
2	s0	165/209 (79%)	131 (79%)	34 (21%)	1	4
3	S1	191/223 (86%)	162 (85%)	29 (15%)	3	10
3	s1	192/223 (86%)	162 (84%)	30 (16%)	3	9
4	S2	176/204 (86%)	137 (78%)	39 (22%)	1	3
4	s2	176/204 (86%)	139 (79%)	37 (21%)	1	4
5	S3	182/194 (94%)	149 (82%)	33 (18%)	2	6
5	s3	182/194 (94%)	149 (82%)	33 (18%)	2	6
6	S4	221/221 (100%)	182 (82%)	39 (18%)	2	6
6	s4	221/221 (100%)	187 (85%)	34 (15%)	3	9
7	S5	173/190 (91%)	140 (81%)	33 (19%)	2	5
7	s5	173/190 (91%)	138 (80%)	35 (20%)	1	4
8	S6	188/201 (94%)	155 (82%)	33 (18%)	2	6
8	s6	187/201 (93%)	152 (81%)	35 (19%)	2	5
9	S7	165/169 (98%)	140 (85%)	25 (15%)	3	10
9	s7	165/169 (98%)	134 (81%)	31 (19%)	2	5
10	S8	150/161 (93%)	128 (85%)	22 (15%)	3	10
10	s8	150/161 (93%)	129 (86%)	21 (14%)	4	12
11	S9	158/165 (96%)	123 (78%)	35 (22%)	1	3
11	s9	158/165 (96%)	128 (81%)	30 (19%)	2	5
12	C0	77/98 (79%)	58 (75%)	19 (25%)	1	2
12	c0	73/98 (74%)	61 (84%)	12 (16%)	2	8
13	C1	129/136 (95%)	104 (81%)	25 (19%)	1	5
13	c1	129/136 (95%)	107 (83%)	22 (17%)	2	7
14	C2	88/118 (75%)	68 (77%)	20 (23%)	1	3
14	c2	88/118 (75%)	65 (74%)	23 (26%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	C3	127/127 (100%)	101 (80%)	26 (20%)	1	4
15	c3	127/127 (100%)	105 (83%)	22 (17%)	2	7
16	C4	81/104 (78%)	61 (75%)	20 (25%)	1	2
16	c4	97/104 (93%)	75 (77%)	22 (23%)	1	3
17	C5	101/117 (86%)	86 (85%)	15 (15%)	3	10
17	c5	103/117 (88%)	83 (81%)	20 (19%)	1	5
18	C6	117/118 (99%)	94 (80%)	23 (20%)	1	4
18	c6	118/118 (100%)	98 (83%)	20 (17%)	2	7
19	C7	94/124 (76%)	70 (74%)	24 (26%)	0	2
19	c7	92/124 (74%)	76 (83%)	16 (17%)	2	7
20	C8	128/128 (100%)	102 (80%)	26 (20%)	1	4
20	c8	128/128 (100%)	101 (79%)	27 (21%)	1	3
21	C9	115/115 (100%)	93 (81%)	22 (19%)	2	5
21	c9	115/115 (100%)	95 (83%)	20 (17%)	2	7
22	D0	100/113 (88%)	74 (74%)	26 (26%)	0	1
22	d0	103/113 (91%)	80 (78%)	23 (22%)	1	3
23	D1	74/74 (100%)	60 (81%)	14 (19%)	2	5
23	d1	74/74 (100%)	57 (77%)	17 (23%)	1	2
24	D2	110/110 (100%)	94 (86%)	16 (14%)	4	11
24	d2	110/110 (100%)	96 (87%)	14 (13%)	5	15
25	D3	119/119 (100%)	97 (82%)	22 (18%)	2	5
25	d3	119/119 (100%)	104 (87%)	15 (13%)	5	16
26	D4	112/112 (100%)	93 (83%)	19 (17%)	2	7
26	d4	112/112 (100%)	99 (88%)	13 (12%)	6	19
27	D5	61/88 (69%)	43 (70%)	18 (30%)	0	1
27	d5	61/88 (69%)	54 (88%)	7 (12%)	6	20
28	D6	83/83 (100%)	66 (80%)	17 (20%)	1	4
28	d6	83/83 (100%)	69 (83%)	14 (17%)	2	7
29	D7	70/70 (100%)	57 (81%)	13 (19%)	2	5
29	d7	70/70 (100%)	59 (84%)	11 (16%)	3	9
30	D8	56/59 (95%)	44 (79%)	12 (21%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	d8	56/59 (95%)	48 (86%)	8 (14%)	4	11
31	D9	47/48 (98%)	38 (81%)	9 (19%)	2	5
31	d9	47/48 (98%)	39 (83%)	8 (17%)	2	7
32	E0	51/51 (100%)	41 (80%)	10 (20%)	1	4
33	E1	62/66 (94%)	47 (76%)	15 (24%)	1	2
33	e1	66/66 (100%)	48 (73%)	18 (27%)	0	1
34	SR	260/261 (100%)	237 (91%)	23 (9%)	12	33
34	sR	260/261 (100%)	232 (89%)	28 (11%)	7	22
35	SM	97/228 (42%)	79 (81%)	18 (19%)	2	5
35	sM	54/228 (24%)	47 (87%)	7 (13%)	5	14
39	L2	193/195 (99%)	157 (81%)	36 (19%)	2	5
39	l2	192/195 (98%)	155 (81%)	37 (19%)	1	5
40	L3	321/322 (100%)	258 (80%)	63 (20%)	1	4
40	l3	320/322 (99%)	255 (80%)	65 (20%)	1	4
41	L4	288/288 (100%)	239 (83%)	49 (17%)	2	7
41	l4	288/288 (100%)	235 (82%)	53 (18%)	2	5
42	L5	244/244 (100%)	194 (80%)	50 (20%)	1	4
42	l5	243/244 (100%)	192 (79%)	51 (21%)	1	4
43	L6	134/152 (88%)	115 (86%)	19 (14%)	4	12
43	l6	135/152 (89%)	111 (82%)	24 (18%)	2	6
44	L7	186/204 (91%)	162 (87%)	24 (13%)	5	15
44	l7	187/204 (92%)	159 (85%)	28 (15%)	3	10
45	L8	187/207 (90%)	154 (82%)	33 (18%)	2	6
45	l8	177/207 (86%)	143 (81%)	34 (19%)	1	5
46	L9	171/171 (100%)	139 (81%)	32 (19%)	2	5
46	l9	171/171 (100%)	137 (80%)	34 (20%)	1	4
47	M0	177/186 (95%)	144 (81%)	33 (19%)	2	5
47	m0	179/186 (96%)	142 (79%)	37 (21%)	1	4
48	M1	147/150 (98%)	119 (81%)	28 (19%)	2	5
48	m1	147/150 (98%)	125 (85%)	22 (15%)	3	10
49	M3	154/158 (98%)	126 (82%)	28 (18%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	m3	154/158 (98%)	130 (84%)	24 (16%)	3	9
50	M4	107/108 (99%)	86 (80%)	21 (20%)	1	4
50	m4	108/108 (100%)	90 (83%)	18 (17%)	2	7
51	M5	175/175 (100%)	146 (83%)	29 (17%)	2	8
51	m5	175/175 (100%)	148 (85%)	27 (15%)	3	9
52	M6	160/161 (99%)	137 (86%)	23 (14%)	4	11
52	m6	160/161 (99%)	132 (82%)	28 (18%)	2	6
53	M7	140/145 (97%)	113 (81%)	27 (19%)	1	5
53	m7	125/145 (86%)	108 (86%)	17 (14%)	4	13
54	M8	150/150 (100%)	125 (83%)	25 (17%)	2	7
54	m8	150/150 (100%)	122 (81%)	28 (19%)	2	5
55	M9	153/153 (100%)	133 (87%)	20 (13%)	5	14
55	m9	153/153 (100%)	119 (78%)	34 (22%)	1	3
56	N0	156/156 (100%)	128 (82%)	28 (18%)	2	6
56	n0	156/156 (100%)	132 (85%)	24 (15%)	3	9
57	N1	136/136 (100%)	108 (79%)	28 (21%)	1	4
57	n1	136/136 (100%)	116 (85%)	20 (15%)	3	10
58	N2	87/106 (82%)	76 (87%)	11 (13%)	5	16
58	n2	85/106 (80%)	73 (86%)	12 (14%)	4	12
59	N3	104/104 (100%)	90 (86%)	14 (14%)	4	13
59	n3	104/104 (100%)	95 (91%)	9 (9%)	12	33
60	N4	57/129 (44%)	52 (91%)	5 (9%)	12	33
60	n4	100/129 (78%)	88 (88%)	12 (12%)	6	18
61	N5	104/117 (89%)	79 (76%)	25 (24%)	1	2
61	n5	104/117 (89%)	80 (77%)	24 (23%)	1	2
62	N6	109/109 (100%)	88 (81%)	21 (19%)	1	5
62	n6	109/109 (100%)	84 (77%)	25 (23%)	1	3
63	N7	115/115 (100%)	91 (79%)	24 (21%)	1	4
63	n7	115/115 (100%)	92 (80%)	23 (20%)	1	4
64	N8	118/118 (100%)	97 (82%)	21 (18%)	2	6
64	n8	118/118 (100%)	95 (80%)	23 (20%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
65	N9	46/46 (100%)	38 (83%)	8 (17%)	2	7
65	n9	46/46 (100%)	35 (76%)	11 (24%)	1	2
66	O0	81/87 (93%)	66 (82%)	15 (18%)	2	5
66	o0	84/87 (97%)	68 (81%)	16 (19%)	2	5
67	O1	92/96 (96%)	72 (78%)	20 (22%)	1	3
67	o1	94/96 (98%)	77 (82%)	17 (18%)	2	6
68	O2	109/110 (99%)	94 (86%)	15 (14%)	4	12
68	o2	109/110 (99%)	92 (84%)	17 (16%)	3	9
69	O3	90/90 (100%)	76 (84%)	14 (16%)	3	9
69	o3	90/90 (100%)	82 (91%)	8 (9%)	11	32
70	O4	95/101 (94%)	78 (82%)	17 (18%)	2	6
70	o4	95/101 (94%)	81 (85%)	14 (15%)	3	10
71	O5	104/104 (100%)	83 (80%)	21 (20%)	1	4
71	o5	103/104 (99%)	76 (74%)	27 (26%)	0	1
72	O6	81/81 (100%)	60 (74%)	21 (26%)	0	1
72	o6	80/81 (99%)	52 (65%)	28 (35%)	0	0
73	O7	70/70 (100%)	58 (83%)	12 (17%)	2	7
73	o7	70/70 (100%)	59 (84%)	11 (16%)	3	9
74	O8	68/68 (100%)	55 (81%)	13 (19%)	2	5
74	o8	67/68 (98%)	55 (82%)	12 (18%)	2	6
75	O9	45/45 (100%)	36 (80%)	9 (20%)	1	4
75	o9	45/45 (100%)	35 (78%)	10 (22%)	1	3
76	Q0	47/47 (100%)	40 (85%)	7 (15%)	3	10
76	q0	47/47 (100%)	40 (85%)	7 (15%)	3	10
77	Q1	23/23 (100%)	15 (65%)	8 (35%)	0	0
77	q1	23/23 (100%)	14 (61%)	9 (39%)	0	0
78	Q2	90/90 (100%)	76 (84%)	14 (16%)	3	9
78	q2	90/90 (100%)	73 (81%)	17 (19%)	2	5
79	Q3	71/71 (100%)	61 (86%)	10 (14%)	4	12
79	q3	71/71 (100%)	58 (82%)	13 (18%)	2	6
80	e0	53/53 (100%)	41 (77%)	12 (23%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
82	p0	105/253 (42%)	84 (80%)	21 (20%)	1	4
All	All	18729/20239 (92%)	15348 (82%)	3381 (18%)	2	6

5 of 3381 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
67	O1	110	GLU
7	s5	216	GLU
64	n8	10	LYS
70	O4	86	LYS
2	s0	172	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
48	M1	95	ASN
61	N5	80	ASN
61	n5	111	ASN
53	M7	125	GLN
59	N3	81	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	449 (25%)	0
1	6	1792/1800 (99%)	430 (23%)	0
36	1	3145/3396 (92%)	609 (19%)	0
36	5	3145/3396 (92%)	613 (19%)	0
37	3	120/121 (99%)	17 (14%)	0
37	7	120/121 (99%)	15 (12%)	0
38	4	157/158 (99%)	35 (22%)	0
38	8	157/158 (99%)	37 (23%)	0
All	All	10383/10950 (94%)	2205 (21%)	0

5 of 2205 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C

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Mol	Chain	Res	Type
1	2	17	C
1	2	25	C
1	2	26	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2559 ligands modelled in this entry, 1424 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	$\# Z > 2$
86	OHX	1	3868	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3869	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3870	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3871	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3872	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3880	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3888	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3889	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3890	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3891	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3923	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3966	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4009	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4052	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4095	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4138	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	1	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4181	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
88	3H3	1	4216	-	33,34,34	1.01	4 (12%)	32,45,45	1.47	6 (18%)
86	OHX	2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	2	2032	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2074	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2117	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2147	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2160	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	231	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	4	232	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	233	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	234	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	235	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	236	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3935	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3942	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3978	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4021	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4064	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4107	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4150	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4193	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4232	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4233	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4234	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4235	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4236	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4237	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4238	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4239	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4240	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4241	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4242	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4243	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4244	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4245	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4246	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4247	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4248	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4249	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4250	-	0,6,6	0.00	-	0,15,15	0.00	-
88	3H3	5	4251	-	33,34,34	1.13	2 (6%)	32,45,45	1.31	4 (12%)
86	OHX	6	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2074	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2117	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2160	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2189	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2203	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	D9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L4	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	207	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	M7	208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	N9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	Q2	503	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	S8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c1	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c8	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	d4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	d9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	305	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	306	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l9	600	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m1	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m5	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n9	3803	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o4	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o7	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s1	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s1	303	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	s4	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s8	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	sR	401	-	0,6,6	0.00	-	0,15,15	0.00	-

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	OHX	1	3868	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3869	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3870	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3871	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3872	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3873	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3874	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3875	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3876	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3877	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3878	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3879	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3880	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3881	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3882	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3883	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3884	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3885	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3886	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3887	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3888	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3889	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3890	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3891	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3892	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3893	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3894	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3895	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3896	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3897	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3898	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3899	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3900	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3901	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3902	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3903	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3904	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3905	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3906	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3907	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3908	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3909	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3910	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3911	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3912	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3913	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3914	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3915	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3916	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3917	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3918	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3919	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3920	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3921	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3922	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3923	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3924	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3925	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3926	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3927	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3928	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3929	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3930	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3931	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3932	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3933	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3934	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3935	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3936	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3937	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3938	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3939	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3940	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3941	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3942	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3943	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3944	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3945	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3946	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3947	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3948	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3949	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3950	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3951	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3952	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3953	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3954	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3955	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3956	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3957	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3958	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3959	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3960	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3961	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3962	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3963	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3964	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3965	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3966	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3967	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3968	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3969	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3970	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3971	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3972	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3973	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3974	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3975	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3976	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3977	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3978	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3979	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3980	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3981	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3982	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3983	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3984	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3985	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3986	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3987	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3988	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3989	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3990	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3991	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3992	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3993	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3994	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3995	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3996	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3997	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3998	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3999	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4000	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4001	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4002	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4003	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4004	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4005	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4006	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4007	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4008	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4009	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4010	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4011	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4012	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4013	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4014	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4015	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4016	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4017	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4018	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4019	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4020	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4021	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4022	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4023	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4024	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4025	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4026	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4027	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4028	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4029	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4030	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4031	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4032	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4033	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4034	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4035	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4036	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4037	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4038	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4039	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4040	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4041	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4042	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4043	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4044	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4045	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4046	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4047	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4048	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4049	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4050	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4051	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4052	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4053	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4054	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4055	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4056	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4057	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4058	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4059	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4060	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4061	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4062	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4063	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4064	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4065	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4066	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4067	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4068	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4069	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4070	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4071	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4072	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4073	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4074	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4075	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4076	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4077	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4078	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4079	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4080	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4081	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4082	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4083	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4084	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4085	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4086	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4087	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4088	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4089	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4090	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4091	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4092	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4093	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4094	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4095	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4096	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4097	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4098	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4099	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4100	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4101	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4102	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4103	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4104	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4105	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4106	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4107	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4108	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4109	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4110	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4111	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4112	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4113	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4114	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4115	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4116	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4117	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4118	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4119	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4120	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4121	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4122	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4123	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4124	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4125	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4126	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4127	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4128	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4129	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4130	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4131	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4132	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4133	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4134	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4135	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4136	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4137	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4138	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4139	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4140	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4141	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4142	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4143	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4144	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4145	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4146	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4147	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4148	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4149	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4150	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4151	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4152	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4153	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4154	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4155	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4156	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4157	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4158	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4159	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4160	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4161	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4162	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4163	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4164	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4165	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4166	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4167	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4168	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4169	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4170	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4171	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4172	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4173	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4174	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4175	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4176	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4177	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4178	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4179	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4180	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4181	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4182	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4183	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4184	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4185	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4186	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4187	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4188	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4189	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4190	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4191	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4192	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4193	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4194	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4195	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4196	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4197	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4198	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4199	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4200	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4201	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4202	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4203	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4204	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4205	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4206	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4207	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4208	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4209	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4210	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4211	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4212	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4213	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4214	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4215	-	-	0/0/0/0	0/0/0/0
88	3H3	1	4216	-	-	0/39/51/51	0/1/2/2
86	OHX	2	2024	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2025	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2029	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2030	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2031	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2032	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2033	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2034	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2035	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2036	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2037	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2038	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2039	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2040	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2041	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2042	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2043	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2044	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2045	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2046	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2047	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2048	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2049	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2050	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2051	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2052	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2053	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2054	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2055	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2056	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2057	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2058	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2059	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2060	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2061	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2062	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2063	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2064	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2065	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2066	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2067	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2068	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2069	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2070	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2071	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2072	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2073	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2074	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2075	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2076	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2077	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2078	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2079	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2080	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2081	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2082	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2083	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2084	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2085	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2086	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2087	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2088	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2089	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2090	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2091	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2092	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2093	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2094	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2095	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2096	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2097	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2098	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2099	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2100	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2101	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2102	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2103	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2104	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2105	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2106	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2107	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2108	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2109	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2110	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2111	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2112	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2113	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2114	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2115	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2116	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2117	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2118	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2119	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2120	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2121	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2122	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2123	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2124	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2125	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2126	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2127	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2128	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2129	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2130	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2131	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2132	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2133	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2134	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2135	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2136	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2137	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2138	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2139	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2140	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2141	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2142	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2143	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2144	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2145	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2146	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2147	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2148	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2149	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2150	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2151	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2152	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2153	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2154	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2155	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2156	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2157	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2158	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2159	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2160	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2161	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2162	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2163	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2164	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2165	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2166	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2167	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2168	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2169	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2170	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2171	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2172	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2173	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2174	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2175	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2176	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2177	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2178	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2179	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2180	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2181	-	-	0/0/0/0	0/0/0/0
86	OHX	3	215	-	-	0/0/0/0	0/0/0/0
86	OHX	3	216	-	-	0/0/0/0	0/0/0/0
86	OHX	3	217	-	-	0/0/0/0	0/0/0/0
86	OHX	3	218	-	-	0/0/0/0	0/0/0/0
86	OHX	3	219	-	-	0/0/0/0	0/0/0/0
86	OHX	3	220	-	-	0/0/0/0	0/0/0/0
86	OHX	3	221	-	-	0/0/0/0	0/0/0/0
86	OHX	3	222	-	-	0/0/0/0	0/0/0/0
86	OHX	3	223	-	-	0/0/0/0	0/0/0/0
86	OHX	3	224	-	-	0/0/0/0	0/0/0/0
86	OHX	3	225	-	-	0/0/0/0	0/0/0/0
86	OHX	3	226	-	-	0/0/0/0	0/0/0/0
86	OHX	4	222	-	-	0/0/0/0	0/0/0/0
86	OHX	4	223	-	-	0/0/0/0	0/0/0/0
86	OHX	4	224	-	-	0/0/0/0	0/0/0/0
86	OHX	4	225	-	-	0/0/0/0	0/0/0/0
86	OHX	4	226	-	-	0/0/0/0	0/0/0/0
86	OHX	4	227	-	-	0/0/0/0	0/0/0/0
86	OHX	4	228	-	-	0/0/0/0	0/0/0/0
86	OHX	4	229	-	-	0/0/0/0	0/0/0/0
86	OHX	4	230	-	-	0/0/0/0	0/0/0/0
86	OHX	4	231	-	-	0/0/0/0	0/0/0/0
86	OHX	4	232	-	-	0/0/0/0	0/0/0/0
86	OHX	4	233	-	-	0/0/0/0	0/0/0/0
86	OHX	4	234	-	-	0/0/0/0	0/0/0/0
86	OHX	4	235	-	-	0/0/0/0	0/0/0/0
86	OHX	4	236	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3898	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3899	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3900	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3901	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3902	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3903	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3904	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3905	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3906	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3907	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3908	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3909	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3910	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3911	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3912	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3913	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3914	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3915	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3916	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3917	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3918	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3919	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3920	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3921	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3922	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3923	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3924	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3925	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3926	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3927	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3928	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3929	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3930	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3931	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3932	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3933	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3934	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3935	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3936	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3937	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3938	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3939	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3940	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3941	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3942	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3943	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3944	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3945	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3946	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3947	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3948	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3949	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3950	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3951	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3952	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3953	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3954	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3955	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3956	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3957	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3958	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3959	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3960	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3961	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3962	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3963	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3964	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3965	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3966	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3967	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3968	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3969	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3970	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3971	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3972	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3973	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3974	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3975	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3976	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3977	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3978	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3979	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3980	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3981	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3982	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3983	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3984	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3985	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3986	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3987	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3988	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3989	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3990	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3991	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3992	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3993	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3994	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3995	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3996	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3997	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3998	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3999	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4000	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4001	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4002	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4003	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4004	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4005	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4006	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4007	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4008	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4009	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4010	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4011	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4012	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4013	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4014	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4015	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4016	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4017	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4018	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4019	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4020	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4021	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4022	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4023	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4024	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4025	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4026	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4027	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4028	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4029	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4030	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4031	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4032	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4033	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4034	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4035	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4036	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4037	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4038	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4039	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4040	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4041	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4042	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4043	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4044	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4045	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4046	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4047	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4048	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4049	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4050	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4051	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4052	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4053	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4054	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4055	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4056	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4057	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4058	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4059	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4060	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4061	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4062	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4063	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4064	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4065	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4066	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4067	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4068	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4069	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4070	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4071	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4072	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4073	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4074	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4075	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4076	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4077	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4078	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4079	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4080	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4081	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4082	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4083	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4084	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4085	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4086	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4087	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4088	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4089	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4090	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4091	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4092	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4093	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4094	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4095	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4096	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4097	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4098	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4099	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4100	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4101	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4102	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4103	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4104	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4105	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4106	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4107	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4108	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4109	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4110	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4111	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4112	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4113	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4114	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4115	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4116	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4117	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4118	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4119	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4120	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4121	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4122	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4123	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4124	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4125	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4126	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4127	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4128	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4129	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4130	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4131	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4132	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4133	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4134	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4135	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4136	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4137	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4138	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4139	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4140	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4141	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4142	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4143	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4144	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4145	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4146	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4147	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4148	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4149	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4150	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4151	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4152	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4153	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4154	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4155	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4156	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4157	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4158	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4159	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4160	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4161	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4162	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4163	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4164	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4165	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4166	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4167	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4168	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4169	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4170	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4171	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4172	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4173	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4174	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4175	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4176	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4177	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4178	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4179	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4180	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4181	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4182	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4183	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4184	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4185	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4186	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4187	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4188	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4189	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4190	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4191	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4192	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4193	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4194	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4195	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4196	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4197	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4198	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4199	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4200	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4201	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4202	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4203	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4204	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4205	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4206	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4207	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4208	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4209	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4210	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4211	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4212	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4213	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4214	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4215	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4216	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4217	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4218	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4219	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4220	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4221	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4222	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4223	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4224	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4225	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4226	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4227	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4228	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4229	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4230	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4231	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4232	86	-	0/0/0/0	0/0/0/0
86	OHX	5	4233	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4234	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4235	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4236	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4237	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4238	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4239	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4240	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4241	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4242	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4243	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4244	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4245	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4246	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4247	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4248	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4249	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4250	-	-	0/0/0/0	0/0/0/0
88	3H3	5	4251	-	-	0/39/51/51	0/1/2/2
86	OHX	6	2047	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2049	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2050	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2051	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2052	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2053	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2054	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2055	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2056	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2057	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2058	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2059	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2060	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2061	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2062	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2063	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2064	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2065	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2066	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2067	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2068	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2069	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2070	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2071	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2072	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2073	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2074	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2075	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2076	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2077	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2078	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2079	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2080	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2081	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2082	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2083	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2084	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2085	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2086	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2087	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2088	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2089	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2090	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2091	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2092	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2093	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2094	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2095	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2096	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2097	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2098	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2099	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2100	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2101	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2102	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2103	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2104	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2105	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2106	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2107	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2108	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2109	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2110	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2111	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2112	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2113	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2114	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2115	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2116	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2117	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2118	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2119	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2120	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2121	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2122	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2123	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2124	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2125	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2126	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2127	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2128	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2129	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2130	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2131	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2132	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2133	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2134	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2135	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2136	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2137	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2138	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2139	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2140	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2141	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2142	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2143	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2144	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2145	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2146	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2147	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2148	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2149	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2150	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2151	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2152	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2153	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2154	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2155	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2156	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2157	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2158	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2159	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2160	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2161	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2162	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2163	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2164	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2165	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2166	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2167	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2168	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2169	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2170	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2171	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2172	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2173	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2174	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2175	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2176	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2177	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2178	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2179	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2180	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2181	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2182	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2183	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2184	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2185	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2186	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2187	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2188	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2189	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2190	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2191	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2192	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2193	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2194	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2195	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2196	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2197	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2198	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2199	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2200	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2201	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2202	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2203	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2204	-	-	0/0/0/0	0/0/0/0
86	OHX	7	216	-	-	0/0/0/0	0/0/0/0
86	OHX	7	217	-	-	0/0/0/0	0/0/0/0
86	OHX	7	218	-	-	0/0/0/0	0/0/0/0
86	OHX	7	219	-	-	0/0/0/0	0/0/0/0
86	OHX	7	220	-	-	0/0/0/0	0/0/0/0
86	OHX	7	221	-	-	0/0/0/0	0/0/0/0
86	OHX	7	222	-	-	0/0/0/0	0/0/0/0
86	OHX	7	223	-	-	0/0/0/0	0/0/0/0
86	OHX	7	224	-	-	0/0/0/0	0/0/0/0
86	OHX	7	225	-	-	0/0/0/0	0/0/0/0
86	OHX	7	226	-	-	0/0/0/0	0/0/0/0
86	OHX	7	227	-	-	0/0/0/0	0/0/0/0
86	OHX	8	214	-	-	0/0/0/0	0/0/0/0
86	OHX	8	215	-	-	0/0/0/0	0/0/0/0
86	OHX	8	216	-	-	0/0/0/0	0/0/0/0
86	OHX	8	217	-	-	0/0/0/0	0/0/0/0
86	OHX	8	218	-	-	0/0/0/0	0/0/0/0
86	OHX	8	219	-	-	0/0/0/0	0/0/0/0
86	OHX	8	220	-	-	0/0/0/0	0/0/0/0
86	OHX	8	221	-	-	0/0/0/0	0/0/0/0
86	OHX	8	222	-	-	0/0/0/0	0/0/0/0
86	OHX	8	223	-	-	0/0/0/0	0/0/0/0
86	OHX	8	224	-	-	0/0/0/0	0/0/0/0
86	OHX	8	225	-	-	0/0/0/0	0/0/0/0
86	OHX	8	226	-	-	0/0/0/0	0/0/0/0
86	OHX	8	227	-	-	0/0/0/0	0/0/0/0
86	OHX	8	228	-	-	0/0/0/0	0/0/0/0
86	OHX	8	229	-	-	0/0/0/0	0/0/0/0
86	OHX	C1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	D9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	403	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	404	-	-	0/0/0/0	0/0/0/0
86	OHX	L4	404	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	L6	202	-	-	0/0/0/0	0/0/0/0
86	OHX	M0	303	-	-	0/0/0/0	0/0/0/0
86	OHX	M5	303	-	-	0/0/0/0	0/0/0/0
86	OHX	M5	304	-	-	0/0/0/0	0/0/0/0
86	OHX	M6	202	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	207	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	208	-	-	0/0/0/0	0/0/0/0
86	OHX	M9	202	-	-	0/0/0/0	0/0/0/0
86	OHX	N9	101	-	-	0/0/0/0	0/0/0/0
86	OHX	O2	201	-	-	0/0/0/0	0/0/0/0
86	OHX	O3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	103	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	104	-	-	0/0/0/0	0/0/0/0
86	OHX	O9	101	-	-	0/0/0/0	0/0/0/0
86	OHX	Q2	503	-	-	0/0/0/0	0/0/0/0
86	OHX	S8	302	-	-	0/0/0/0	0/0/0/0
86	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
86	OHX	c1	202	-	-	0/0/0/0	0/0/0/0
86	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c8	203	-	-	0/0/0/0	0/0/0/0
86	OHX	d4	201	-	-	0/0/0/0	0/0/0/0
86	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	402	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	403	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	404	-	-	0/0/0/0	0/0/0/0
86	OHX	l4	402	-	-	0/0/0/0	0/0/0/0
86	OHX	l4	403	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	304	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	305	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	306	-	-	0/0/0/0	0/0/0/0
86	OHX	l9	600	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	301	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
86	OHX	m1	203	-	-	0/0/0/0	0/0/0/0
86	OHX	m4	202	-	-	0/0/0/0	0/0/0/0
86	OHX	m5	302	-	-	0/0/0/0	0/0/0/0
86	OHX	m6	202	-	-	0/0/0/0	0/0/0/0
86	OHX	m7	206	-	-	0/0/0/0	0/0/0/0
86	OHX	m8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	n3	203	-	-	0/0/0/0	0/0/0/0
86	OHX	n9	3803	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	o2	201	-	-	0/0/0/0	0/0/0/0
86	OHX	o3	203	-	-	0/0/0/0	0/0/0/0
86	OHX	o4	203	-	-	0/0/0/0	0/0/0/0
86	OHX	o7	502	-	-	0/0/0/0	0/0/0/0
86	OHX	q2	502	-	-	0/0/0/0	0/0/0/0
86	OHX	s1	302	-	-	0/0/0/0	0/0/0/0
86	OHX	s1	303	-	-	0/0/0/0	0/0/0/0
86	OHX	s4	301	-	-	0/0/0/0	0/0/0/0
86	OHX	s8	303	-	-	0/0/0/0	0/0/0/0
86	OHX	s9	201	-	-	0/0/0/0	0/0/0/0
86	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	5	4251	3H3	C15-C14	-2.59	1.50	1.53
88	1	4216	3H3	C15-C14	-2.59	1.50	1.53
88	1	4216	3H3	C14-C13	2.04	1.54	1.51
88	1	4216	3H3	C14-C16	2.40	1.54	1.52
88	1	4216	3H3	C3-C2	3.37	1.47	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4216	3H3	C-C1-C2	-3.18	102.02	110.07
88	1	4216	3H3	O1-C11-C12	-2.64	103.55	109.40
88	1	4216	3H3	C6-C7-C8	-2.24	106.97	112.93
88	5	4251	3H3	C6-C7-C8	-2.11	107.32	112.93
88	1	4216	3H3	C8-C9-C10	-2.08	117.49	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

465 monomers are involved in 778 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3873	OHX	1	0
86	1	3875	OHX	1	0
86	1	3876	OHX	1	0
86	1	3883	OHX	1	0
86	1	3886	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3887	OHX	1	0
86	1	3888	OHX	1	0
86	1	3896	OHX	1	0
86	1	3897	OHX	1	0
86	1	3898	OHX	1	0
86	1	3903	OHX	1	0
86	1	3911	OHX	1	0
86	1	3915	OHX	1	0
86	1	3924	OHX	1	0
86	1	3931	OHX	1	0
86	1	3935	OHX	2	0
86	1	3937	OHX	1	0
86	1	3938	OHX	1	0
86	1	3943	OHX	6	0
86	1	3945	OHX	1	0
86	1	3948	OHX	1	0
86	1	3952	OHX	1	0
86	1	3955	OHX	3	0
86	1	3958	OHX	1	0
86	1	3961	OHX	1	0
86	1	3962	OHX	5	0
86	1	3964	OHX	7	0
86	1	3967	OHX	1	0
86	1	3968	OHX	3	0
86	1	3970	OHX	1	0
86	1	3971	OHX	1	0
86	1	3973	OHX	1	0
86	1	3976	OHX	7	0
86	1	3979	OHX	1	0
86	1	3980	OHX	5	0
86	1	3983	OHX	1	0
86	1	3985	OHX	1	0
86	1	3986	OHX	2	0
86	1	3987	OHX	2	0
86	1	3990	OHX	1	0
86	1	3993	OHX	1	0
86	1	3995	OHX	1	0
86	1	4002	OHX	2	0
86	1	4005	OHX	1	0
86	1	4006	OHX	1	0
86	1	4007	OHX	8	0
86	1	4010	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	4011	OHX	1	0
86	1	4012	OHX	1	0
86	1	4014	OHX	1	0
86	1	4016	OHX	1	0
86	1	4017	OHX	1	0
86	1	4021	OHX	1	0
86	1	4023	OHX	7	0
86	1	4031	OHX	2	0
86	1	4032	OHX	6	0
86	1	4034	OHX	2	0
86	1	4036	OHX	6	0
86	1	4037	OHX	1	0
86	1	4038	OHX	1	0
86	1	4041	OHX	3	0
86	1	4042	OHX	1	0
86	1	4043	OHX	2	0
86	1	4044	OHX	2	0
86	1	4046	OHX	2	0
86	1	4047	OHX	4	0
86	1	4048	OHX	7	0
86	1	4049	OHX	1	0
86	1	4051	OHX	2	0
86	1	4054	OHX	1	0
86	1	4056	OHX	6	0
86	1	4059	OHX	7	0
86	1	4060	OHX	4	0
86	1	4061	OHX	5	0
86	1	4064	OHX	1	0
86	1	4065	OHX	8	0
86	1	4066	OHX	1	0
86	1	4068	OHX	1	0
86	1	4070	OHX	1	0
86	1	4071	OHX	6	0
86	1	4076	OHX	3	0
86	1	4077	OHX	1	0
86	1	4079	OHX	1	0
86	1	4083	OHX	1	0
86	1	4084	OHX	8	0
86	1	4088	OHX	7	0
86	1	4089	OHX	4	0
86	1	4092	OHX	1	0
86	1	4094	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	4095	OHX	1	0
86	1	4098	OHX	1	0
86	1	4099	OHX	1	0
86	1	4100	OHX	1	0
86	1	4102	OHX	1	0
86	1	4103	OHX	1	0
86	1	4111	OHX	1	0
86	1	4113	OHX	1	0
86	1	4118	OHX	6	0
86	1	4122	OHX	2	0
86	1	4123	OHX	1	0
86	1	4125	OHX	1	0
86	1	4128	OHX	1	0
86	1	4134	OHX	1	0
86	1	4135	OHX	3	0
86	1	4136	OHX	3	0
86	1	4138	OHX	3	0
86	1	4142	OHX	3	0
86	1	4143	OHX	6	0
86	1	4144	OHX	1	0
86	1	4146	OHX	2	0
86	1	4147	OHX	1	0
86	1	4149	OHX	6	0
86	1	4151	OHX	1	0
86	1	4153	OHX	7	0
86	1	4157	OHX	5	0
86	1	4158	OHX	4	0
86	1	4159	OHX	6	0
86	1	4163	OHX	5	0
86	1	4166	OHX	6	0
86	1	4167	OHX	2	0
86	1	4168	OHX	1	0
86	1	4170	OHX	2	0
86	1	4171	OHX	1	0
86	1	4172	OHX	1	0
86	1	4175	OHX	8	0
86	1	4177	OHX	6	0
86	1	4178	OHX	1	0
86	1	4179	OHX	1	0
86	1	4182	OHX	1	0
86	1	4183	OHX	1	0
86	1	4184	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	4186	OHX	1	0
86	1	4187	OHX	1	0
86	1	4194	OHX	1	0
86	1	4196	OHX	1	0
86	1	4198	OHX	1	0
86	1	4200	OHX	6	0
86	1	4201	OHX	1	0
86	1	4203	OHX	1	0
86	1	4205	OHX	2	0
86	1	4208	OHX	1	0
86	1	4209	OHX	1	0
86	1	4210	OHX	1	0
88	1	4216	3H3	1	0
86	2	2027	OHX	2	0
86	2	2032	OHX	7	0
86	2	2037	OHX	3	0
86	2	2039	OHX	1	0
86	2	2040	OHX	2	0
86	2	2043	OHX	1	0
86	2	2045	OHX	6	0
86	2	2046	OHX	1	0
86	2	2048	OHX	1	0
86	2	2049	OHX	1	0
86	2	2052	OHX	1	0
86	2	2054	OHX	1	0
86	2	2058	OHX	1	0
86	2	2059	OHX	1	0
86	2	2063	OHX	1	0
86	2	2065	OHX	1	0
86	2	2071	OHX	1	0
86	2	2072	OHX	1	0
86	2	2073	OHX	1	0
86	2	2074	OHX	1	0
86	2	2075	OHX	1	0
86	2	2076	OHX	6	0
86	2	2077	OHX	1	0
86	2	2079	OHX	1	0
86	2	2083	OHX	1	0
86	2	2084	OHX	4	0
86	2	2085	OHX	1	0
86	2	2086	OHX	4	0
86	2	2087	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	2	2090	OHX	6	0
86	2	2091	OHX	6	0
86	2	2093	OHX	2	0
86	2	2094	OHX	1	0
86	2	2095	OHX	1	0
86	2	2096	OHX	6	0
86	2	2097	OHX	1	0
86	2	2099	OHX	7	0
86	2	2105	OHX	1	0
86	2	2109	OHX	7	0
86	2	2110	OHX	1	0
86	2	2111	OHX	2	0
86	2	2115	OHX	2	0
86	2	2116	OHX	7	0
86	2	2117	OHX	1	0
86	2	2119	OHX	1	0
86	2	2121	OHX	2	0
86	2	2127	OHX	1	0
86	2	2128	OHX	1	0
86	2	2130	OHX	2	0
86	2	2131	OHX	1	0
86	2	2132	OHX	8	0
86	2	2133	OHX	1	0
86	2	2137	OHX	1	0
86	2	2139	OHX	1	0
86	2	2142	OHX	1	0
86	2	2144	OHX	1	0
86	2	2145	OHX	1	0
86	2	2146	OHX	2	0
86	2	2147	OHX	7	0
86	2	2150	OHX	1	0
86	2	2155	OHX	4	0
86	2	2156	OHX	1	0
86	2	2157	OHX	1	0
86	2	2158	OHX	3	0
86	2	2160	OHX	2	0
86	2	2161	OHX	2	0
86	2	2162	OHX	1	0
86	2	2163	OHX	6	0
86	2	2166	OHX	1	0
86	2	2167	OHX	2	0
86	2	2168	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	2	2169	OHX	1	0
86	2	2170	OHX	1	0
86	2	2172	OHX	2	0
86	2	2173	OHX	2	0
86	2	2174	OHX	1	0
86	3	216	OHX	1	0
86	3	218	OHX	3	0
86	3	223	OHX	2	0
86	3	226	OHX	1	0
86	4	223	OHX	1	0
86	4	224	OHX	1	0
86	4	227	OHX	1	0
86	4	232	OHX	2	0
86	5	3904	OHX	1	0
86	5	3906	OHX	2	0
86	5	3912	OHX	1	0
86	5	3921	OHX	1	0
86	5	3924	OHX	3	0
86	5	3941	OHX	1	0
86	5	3942	OHX	3	0
86	5	3948	OHX	1	0
86	5	3949	OHX	1	0
86	5	3953	OHX	1	0
86	5	3955	OHX	2	0
86	5	3957	OHX	1	0
86	5	3959	OHX	1	0
86	5	3962	OHX	4	0
86	5	3966	OHX	1	0
86	5	3969	OHX	1	0
86	5	3972	OHX	1	0
86	5	3973	OHX	6	0
86	5	3978	OHX	8	0
86	5	3987	OHX	1	0
86	5	3991	OHX	2	0
86	5	3999	OHX	1	0
86	5	4000	OHX	5	0
86	5	4001	OHX	7	0
86	5	4002	OHX	2	0
86	5	4003	OHX	1	0
86	5	4007	OHX	1	0
86	5	4011	OHX	6	0
86	5	4013	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	4017	OHX	1	0
86	5	4020	OHX	6	0
86	5	4023	OHX	3	0
86	5	4024	OHX	2	0
86	5	4026	OHX	1	0
86	5	4030	OHX	1	0
86	5	4033	OHX	4	0
86	5	4034	OHX	4	0
86	5	4039	OHX	1	0
86	5	4046	OHX	1	0
86	5	4049	OHX	1	0
86	5	4051	OHX	1	0
86	5	4052	OHX	1	0
86	5	4054	OHX	3	0
86	5	4055	OHX	6	0
86	5	4059	OHX	1	0
86	5	4061	OHX	1	0
86	5	4065	OHX	5	0
86	5	4066	OHX	7	0
86	5	4068	OHX	1	0
86	5	4072	OHX	1	0
86	5	4074	OHX	5	0
86	5	4076	OHX	1	0
86	5	4079	OHX	1	0
86	5	4081	OHX	4	0
86	5	4088	OHX	1	0
86	5	4089	OHX	1	0
86	5	4090	OHX	7	0
86	5	4091	OHX	1	0
86	5	4092	OHX	1	0
86	5	4093	OHX	4	0
86	5	4094	OHX	6	0
86	5	4096	OHX	1	0
86	5	4097	OHX	1	0
86	5	4099	OHX	1	0
86	5	4102	OHX	2	0
86	5	4106	OHX	1	0
86	5	4108	OHX	3	0
86	5	4109	OHX	1	0
86	5	4110	OHX	1	0
86	5	4117	OHX	3	0
86	5	4118	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	4119	OHX	1	0
86	5	4125	OHX	1	0
86	5	4127	OHX	1	0
86	5	4128	OHX	1	0
86	5	4129	OHX	1	0
86	5	4130	OHX	1	0
86	5	4131	OHX	1	0
86	5	4132	OHX	1	0
86	5	4136	OHX	2	0
86	5	4138	OHX	1	0
86	5	4140	OHX	2	0
86	5	4141	OHX	6	0
86	5	4144	OHX	1	0
86	5	4145	OHX	1	0
86	5	4146	OHX	1	0
86	5	4151	OHX	1	0
86	5	4152	OHX	1	0
86	5	4157	OHX	2	0
86	5	4160	OHX	2	0
86	5	4161	OHX	1	0
86	5	4166	OHX	1	0
86	5	4170	OHX	1	0
86	5	4176	OHX	1	0
86	5	4177	OHX	2	0
86	5	4178	OHX	2	0
86	5	4179	OHX	1	0
86	5	4181	OHX	1	0
86	5	4182	OHX	1	0
86	5	4183	OHX	1	0
86	5	4185	OHX	1	0
86	5	4187	OHX	7	0
86	5	4189	OHX	7	0
86	5	4190	OHX	6	0
86	5	4191	OHX	1	0
86	5	4193	OHX	1	0
86	5	4196	OHX	9	0
86	5	4197	OHX	7	0
86	5	4198	OHX	7	0
86	5	4199	OHX	3	0
86	5	4200	OHX	1	0
86	5	4201	OHX	5	0
86	5	4203	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	4204	OHX	1	0
86	5	4205	OHX	1	0
86	5	4206	OHX	1	0
86	5	4207	OHX	2	0
86	5	4212	OHX	6	0
86	5	4214	OHX	1	0
86	5	4215	OHX	8	0
86	5	4219	OHX	1	0
86	5	4221	OHX	1	0
86	5	4222	OHX	6	0
86	5	4224	OHX	2	0
86	5	4225	OHX	1	0
86	5	4226	OHX	1	0
86	5	4227	OHX	1	0
86	5	4230	OHX	2	0
86	5	4232	OHX	2	0
86	5	4234	OHX	6	0
86	5	4235	OHX	1	0
86	5	4238	OHX	2	0
86	5	4241	OHX	7	0
86	5	4242	OHX	1	0
86	5	4247	OHX	2	0
86	5	4249	OHX	1	0
88	5	4251	3H3	1	0
86	6	2055	OHX	1	0
86	6	2060	OHX	6	0
86	6	2061	OHX	1	0
86	6	2062	OHX	1	0
86	6	2066	OHX	1	0
86	6	2067	OHX	1	0
86	6	2071	OHX	1	0
86	6	2073	OHX	1	0
86	6	2074	OHX	2	0
86	6	2075	OHX	2	0
86	6	2089	OHX	1	0
86	6	2093	OHX	1	0
86	6	2094	OHX	1	0
86	6	2096	OHX	1	0
86	6	2097	OHX	1	0
86	6	2101	OHX	3	0
86	6	2102	OHX	1	0
86	6	2103	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	6	2107	OHX	1	0
86	6	2108	OHX	1	0
86	6	2112	OHX	1	0
86	6	2113	OHX	1	0
86	6	2115	OHX	2	0
86	6	2118	OHX	1	0
86	6	2120	OHX	2	0
86	6	2121	OHX	8	0
86	6	2122	OHX	1	0
86	6	2123	OHX	1	0
86	6	2124	OHX	1	0
86	6	2125	OHX	1	0
86	6	2126	OHX	3	0
86	6	2128	OHX	2	0
86	6	2130	OHX	1	0
86	6	2135	OHX	1	0
86	6	2136	OHX	1	0
86	6	2138	OHX	1	0
86	6	2142	OHX	1	0
86	6	2143	OHX	1	0
86	6	2144	OHX	1	0
86	6	2146	OHX	1	0
86	6	2147	OHX	7	0
86	6	2149	OHX	1	0
86	6	2150	OHX	1	0
86	6	2151	OHX	1	0
86	6	2154	OHX	2	0
86	6	2155	OHX	1	0
86	6	2156	OHX	2	0
86	6	2157	OHX	1	0
86	6	2159	OHX	3	0
86	6	2160	OHX	1	0
86	6	2162	OHX	1	0
86	6	2163	OHX	1	0
86	6	2165	OHX	1	0
86	6	2168	OHX	1	0
86	6	2170	OHX	1	0
86	6	2171	OHX	8	0
86	6	2175	OHX	1	0
86	6	2178	OHX	1	0
86	6	2180	OHX	1	0
86	6	2182	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	6	2183	OHX	1	0
86	6	2188	OHX	1	0
86	6	2189	OHX	2	0
86	6	2190	OHX	2	0
86	6	2192	OHX	1	0
86	6	2195	OHX	1	0
86	6	2196	OHX	1	0
86	6	2202	OHX	2	0
86	7	217	OHX	1	0
86	7	218	OHX	6	0
86	7	219	OHX	4	0
86	7	221	OHX	1	0
86	7	224	OHX	4	0
86	7	226	OHX	6	0
86	8	214	OHX	2	0
86	8	215	OHX	6	0
86	8	216	OHX	1	0
86	8	218	OHX	1	0
86	8	219	OHX	2	0
86	8	222	OHX	2	0
86	8	223	OHX	6	0
86	8	224	OHX	6	0
86	8	225	OHX	1	0
86	C1	201	OHX	7	0
86	C3	202	OHX	1	0
86	C5	201	OHX	4	0
86	C8	201	OHX	1	0
86	D9	102	OHX	1	0
86	L3	403	OHX	1	0
86	L4	404	OHX	2	0
86	M5	303	OHX	1	0
86	M5	304	OHX	1	0
86	M6	202	OHX	1	0
86	M7	207	OHX	1	0
86	M9	202	OHX	1	0
86	N9	101	OHX	1	0
86	O7	103	OHX	6	0
86	O9	101	OHX	4	0
86	Q2	503	OHX	2	0
86	S8	302	OHX	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	SR	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SR	161:LYS	C	162:ALA	N	0.66
1	SR	160:GLU	C	161:LYS	N	0.45

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

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

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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