



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 16, 2017 – 10:04 am GMT

PDB ID : 4U3N  
Title : Crystal structure of CCA trinucleotide bound to the yeast 80S ribosome  
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.  
Deposited on : 2014-07-22  
Resolution : 3.20 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](mailto: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.

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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	:	<b>FAILED</b>
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

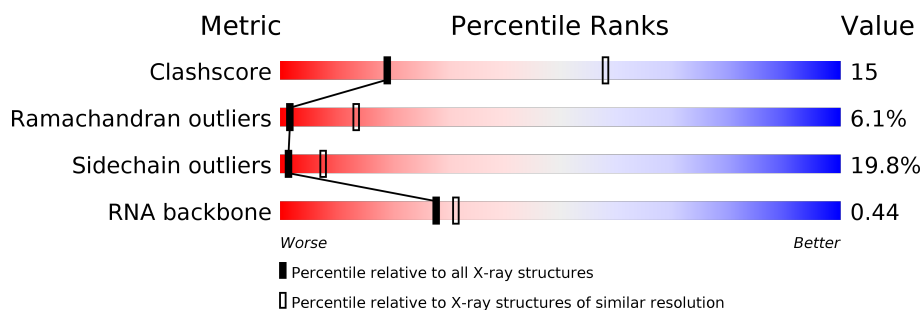
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RNA backbone	2435	1045 (3.60-2.80)

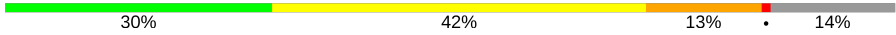



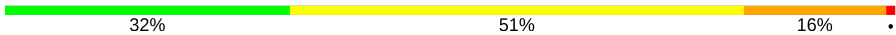

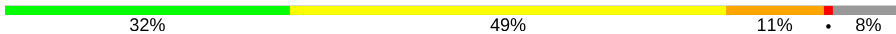

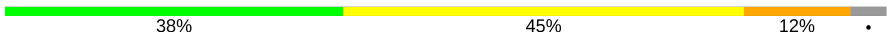

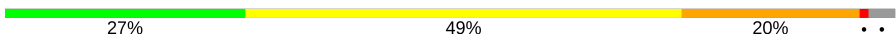

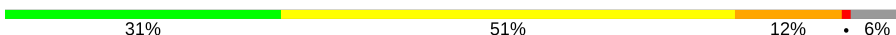

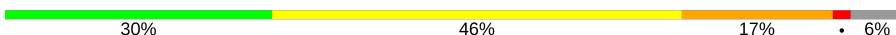

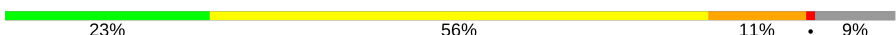


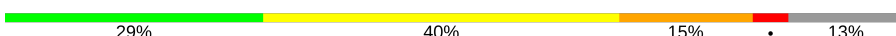





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	

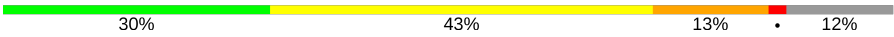

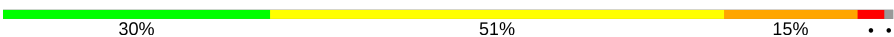

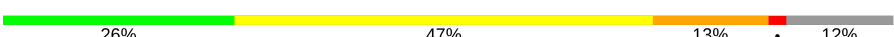

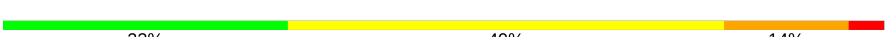

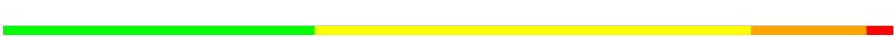

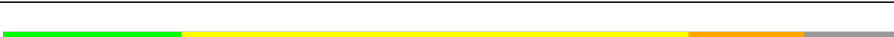


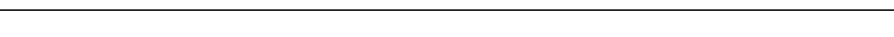








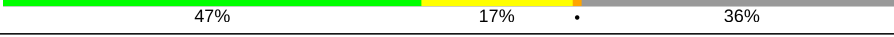
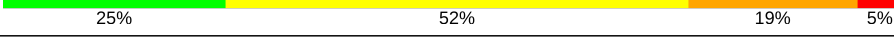

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Mol	Chain	Length	Quality of chain
4	S2	253	
4	s2	253	
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	
15	c3	150	
16	C4	136	
16	c4	136	


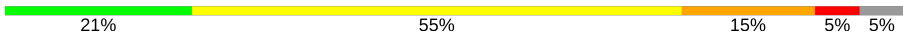



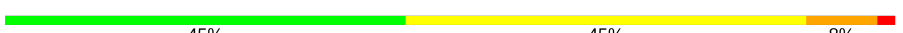
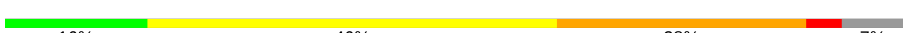




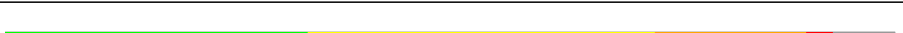


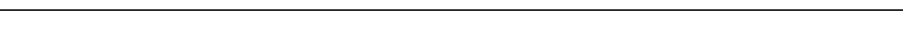




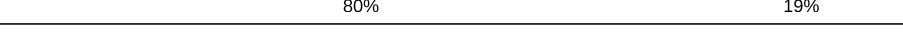





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Mol	Chain	Length	Quality of chain
17	C5	141	
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107	
27	d5	107	
28	D6	97	
28	d6	97	
29	D7	81	

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Mol	Chain	Length	Quality of chain
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
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	
42	L5	296	
42	l5	296	


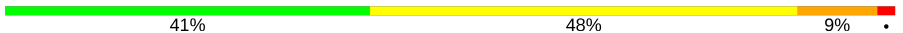



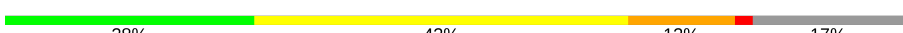





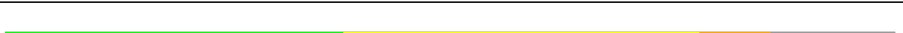


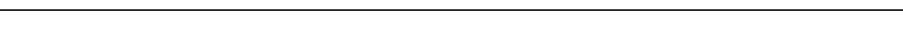

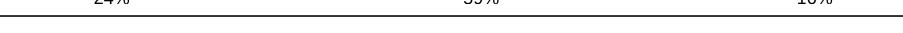


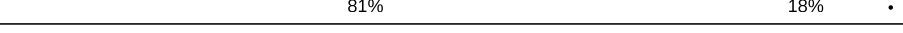


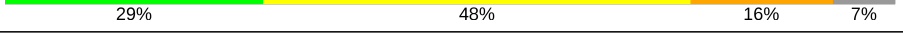


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Mol	Chain	Length	Quality of chain
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	
53	m7	183	
54	M8	185	
54	m8	185	
55	M9	188	



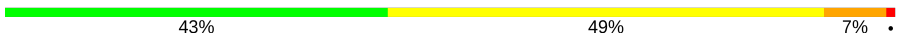



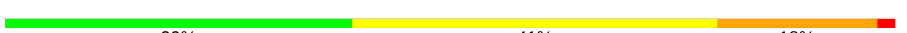







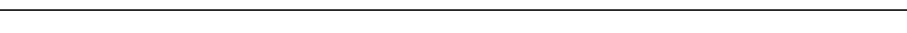




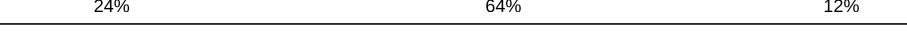

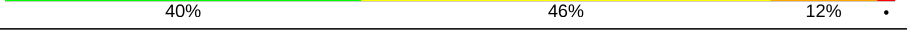



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Mol	Chain	Length	Quality of chain
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	104	
66	o0	104	
67	O1	112	
67	o1	112	

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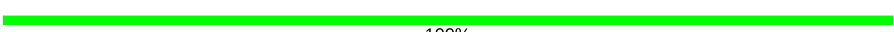
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Mol	Chain	Length	Quality of chain
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	119	
70	o4	119	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	
79	q3	91	
80	c0	105	

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Mol	Chain	Length	Quality of chain
81	e0	62	 69% 29% 2%
82	e1	76	 55% 36% 8%
83	m2	160	 94% 6%
84	p0	311	 37% 8% 54%
85	p1	47	 100%
86	p2	46	 100%

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
88	OHX	1	3982	-	-	X	-
88	OHX	1	4015	-	-	X	-
88	OHX	1	4170	-	-	X	-
88	OHX	1	4186	-	-	X	-
88	OHX	2	2044	-	-	X	-
88	OHX	2	2099	-	-	X	-
88	OHX	5	3981	-	-	X	-
88	OHX	5	4014	-	-	X	-
88	OHX	5	4023	-	-	X	-
88	OHX	5	4203	-	-	X	-
88	OHX	5	4205	-	-	X	-
88	OHX	5	4222	-	-	X	-
88	OHX	5	4248	-	-	X	-
88	OHX	6	2105	-	-	X	-
88	OHX	6	2143	-	-	X	-
88	OHX	8	218	-	-	X	-
88	OHX	8	225	-	-	X	-
88	OHX	C5	201	-	-	X	-

## 2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 411288 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			

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

- 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			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

- Molecule 80 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	c0	96	Total	C	N	O	S	0	0	0
			762	491	125	144	2			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 81 is a protein called 40S ribosomal protein S30-A.

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

- Molecule 82 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	e1	76	Total	C	N	O	S	0	0	0
			608	388	117	99	4			

- Molecule 83 is a protein called UNKNOWN PROTEIN m2.

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

- Molecule 84 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 85 is a protein called UNKNOWN PROTEIN p1.

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

- Molecule 86 is a protein called UNKNOWN PROTEIN p2.

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

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	L7	4	Total	Mg	0	0
			4	4		
87	n8	3	Total	Mg	0	0
			3	3		
87	o1	1	Total	Mg	0	0
			1	1		
87	N5	1	Total	Mg	0	0
			1	1		
87	6	144	Total	Mg	0	0
			144	144		
87	sM	1	Total	Mg	0	0
			1	1		
87	O4	1	Total	Mg	0	0
			1	1		
87	m5	5	Total	Mg	0	0
			5	5		
87	l3	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	M1	1	Total 1	Mg 1	0	0
87	d6	1	Total 1	Mg 1	0	0
87	2	124	Total 124	Mg 124	0	0
87	n0	3	Total 3	Mg 3	0	0
87	L4	1	Total 1	Mg 1	0	0
87	l7	1	Total 1	Mg 1	0	0
87	M5	2	Total 2	Mg 2	0	0
87	c9	1	Total 1	Mg 1	0	0
87	L8	1	Total 1	Mg 1	0	0
87	D3	1	Total 1	Mg 1	0	0
87	o4	1	Total 1	Mg 1	0	0
87	M9	1	Total 1	Mg 1	0	0
87	q0	1	Total 1	Mg 1	0	0
87	SM	1	Total 1	Mg 1	0	0
87	c8	1	Total 1	Mg 1	0	0
87	M0	2	Total 2	Mg 2	0	0
87	c1	1	Total 1	Mg 1	0	0
87	5	502	Total 502	Mg 502	0	0
87	L5	1	Total 1	Mg 1	0	0
87	O7	1	Total 1	Mg 1	0	0
87	s6	1	Total 1	Mg 1	0	0

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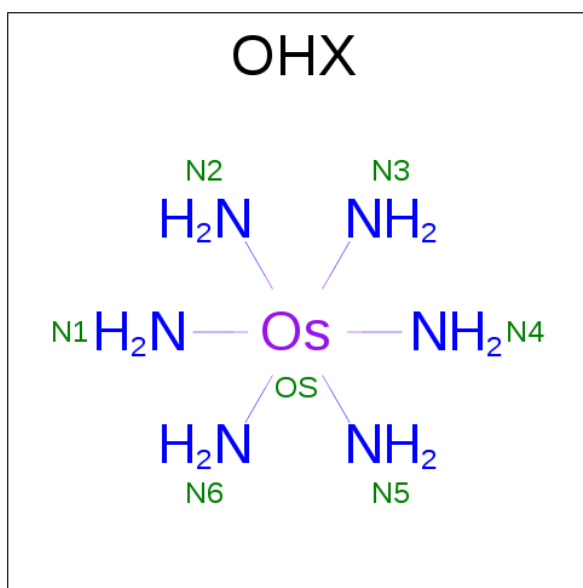
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	l4	2	Total 2	Mg 2	0	0
87	d4	1	Total 1	Mg 1	0	0
87	1	477	Total 477	Mg 477	0	0
87	d3	1	Total 1	Mg 1	0	0
87	S8	1	Total 1	Mg 1	0	0
87	m1	2	Total 2	Mg 2	0	0
87	O2	1	Total 1	Mg 1	0	0
87	q3	2	Total 2	Mg 2	0	0
87	o3	1	Total 1	Mg 1	0	0
87	M3	2	Total 2	Mg 2	0	0
87	N3	3	Total 3	Mg 3	0	0
87	4	19	Total 19	Mg 19	0	0
87	n6	2	Total 2	Mg 2	0	0
87	S4	2	Total 2	Mg 2	0	0
87	L2	1	Total 1	Mg 1	0	0
87	l5	2	Total 2	Mg 2	0	0
87	m7	5	Total 5	Mg 5	0	0
87	M7	4	Total 4	Mg 4	0	0
87	N8	5	Total 5	Mg 5	0	0
87	s1	1	Total 1	Mg 1	0	0
87	m6	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	s8	3	Total 3	Mg 3	0	0
87	c7	2	Total 2	Mg 2	0	0
87	7	15	Total 15	Mg 15	0	0
87	n3	2	Total 2	Mg 2	0	0
87	q1	1	Total 1	Mg 1	0	0
87	L3	3	Total 3	Mg 3	0	0
87	O5	1	Total 1	Mg 1	0	0
87	l2	1	Total 1	Mg 1	0	0
87	8	16	Total 16	Mg 16	0	0
87	M6	1	Total 1	Mg 1	0	0
87	N0	1	Total 1	Mg 1	0	0
87	3	14	Total 14	Mg 14	0	0

- Molecule 88 is osmium (III) hexammine (three-letter code: OHX) (formula:  $\text{H}_{12}\text{N}_6\text{Os}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	S8	1	Total 7	N 6	Os 1	0	0
88	C3	1	Total 7	N 6	Os 1	0	0
88	C5	1	Total 7	N 6	Os 1	0	0
88	C8	1	Total 7	N 6	Os 1	0	0
88	D3	1	Total 7	N 6	Os 1	0	0
88	D9	1	Total 7	N 6	Os 1	0	0
88	SR	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
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88	3	1	Total	N	Os	0	0
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88	3	1	Total	N	Os	0	0
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			7	6	1		
88	3	1	Total	N	Os	0	0
			7	6	1		
88	3	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	3	1	Total	N	Os	0	0
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88	3	1	Total	N	Os	0	0
			7	6	1		
88	3	1	Total	N	Os	0	0
			7	6	1		
88	4	1	Total	N	Os	0	0
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88	4	1	Total	N	Os	0	0
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88	4	1	Total	N	Os	0	0
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88	4	1	Total	N	Os	0	0
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88	4	1	Total	N	Os	0	0
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88	4	1	Total	N	Os	0	0
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88	4	1	Total	N	Os	0	0
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88	4	1	Total	N	Os	0	0
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88	4	1	Total	N	Os	0	0
			7	6	1		
88	4	1	Total	N	Os	0	0
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88	L3	1	Total	N	Os	0	0
			7	6	1		
88	L3	1	Total	N	Os	0	0
			7	6	1		
88	L3	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	L4	1	Total	N	Os	0	0
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88	M0	1	Total	N	Os	0	0
			7	6	1		
88	M5	1	Total	N	Os	0	0
			7	6	1		
88	M7	1	Total	N	Os	0	0
			7	6	1		
88	M7	1	Total	N	Os	0	0
			7	6	1		
88	M8	1	Total	N	Os	0	0
			7	6	1		
88	M9	1	Total	N	Os	0	0
			7	6	1		
88	N9	1	Total	N	Os	0	0
			7	6	1		
88	O3	1	Total	N	Os	0	0
			7	6	1		
88	O7	1	Total	N	Os	0	0
			7	6	1		
88	O7	1	Total	N	Os	0	0
			7	6	1		
88	6	1	Total	N	Os	0	0
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			7	6	1		
88	6	1	Total	N	Os	0	0
			7	6	1		
88	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
			7	6	1		
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
			7	6	1		
88	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	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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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	6	1	Total 7	N 6	Os 1	0	0
88	s1	1	Total 7	N 6	Os 1	0	0
88	s1	1	Total 7	N 6	Os 1	0	0
88	s8	1	Total 7	N 6	Os 1	0	0
88	c1	1	Total 7	N 6	Os 1	0	0
88	c3	1	Total 7	N 6	Os 1	0	0
88	c5	1	Total 7	N 6	Os 1	0	0
88	c8	1	Total 7	N 6	Os 1	0	0
88	d4	1	Total 7	N 6	Os 1	0	0
88	d9	1	Total 7	N 6	Os 1	0	0
88	sR	1	Total 7	N 6	Os 1	0	0
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88	5	1	Total 7	N 6	Os 1	0	0
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88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	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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88	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
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			7	6	1		
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88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	13	1	Total	N	Os	0	0
			7	6	1		
88	13	1	Total	N	Os	0	0
			7	6	1		
88	13	1	Total	N	Os	0	0
			7	6	1		

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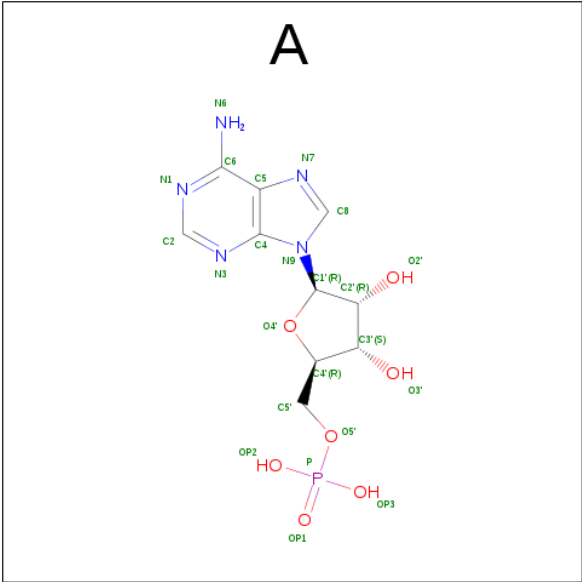
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	l4	1	Total	N	Os	0	0
			7	6	1		
88	l4	1	Total	N	Os	0	0
			7	6	1		
88	l5	1	Total	N	Os	0	0
			7	6	1		
88	l5	1	Total	N	Os	0	0
			7	6	1		
88	l5	1	Total	N	Os	0	0
			7	6	1		
88	l5	1	Total	N	Os	0	0
			7	6	1		
88	l9	1	Total	N	Os	0	0
			7	6	1		
88	m0	1	Total	N	Os	0	0
			7	6	1		
88	m0	1	Total	N	Os	0	0
			7	6	1		
88	m1	1	Total	N	Os	0	0
			7	6	1		
88	m4	1	Total	N	Os	0	0
			7	6	1		
88	m5	1	Total	N	Os	0	0
			7	6	1		
88	m6	1	Total	N	Os	0	0
			7	6	1		
88	n3	1	Total	N	Os	0	0
			7	6	1		
88	n3	1	Total	N	Os	0	0
			7	6	1		
88	n9	1	Total	N	Os	0	0
			7	6	1		
88	o3	1	Total	N	Os	0	0
			7	6	1		
88	o7	1	Total	N	Os	0	0
			7	6	1		
88	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

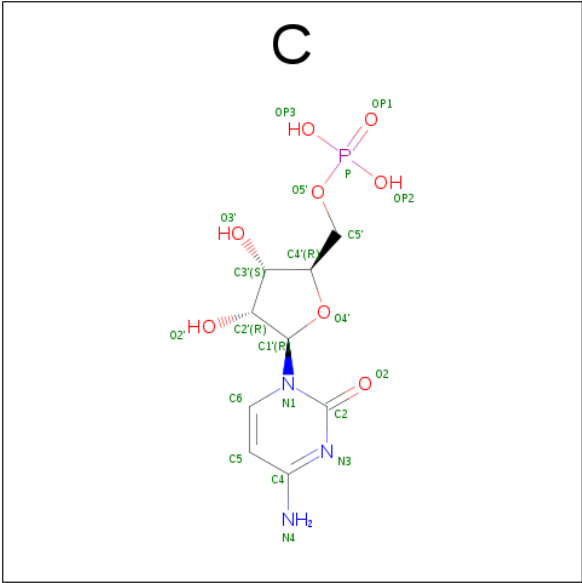
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
89	q0	1	Total Zn 1 1	0	0
89	D6	1	Total Zn 1 1	0	0
89	Q2	1	Total Zn 1 1	0	0
89	e1	1	Total Zn 1 1	0	0
89	Q3	1	Total Zn 1 1	0	0
89	D9	1	Total Zn 1 1	0	0
89	E1	1	Total Zn 1 1	0	0
89	Q0	1	Total Zn 1 1	0	0
89	d7	1	Total Zn 1 1	0	0
89	q3	1	Total Zn 1 1	0	0
89	d9	1	Total Zn 1 1	0	0
89	D7	1	Total Zn 1 1	0	0
89	d6	1	Total Zn 1 1	0	0
89	o7	1	Total Zn 1 1	0	0
89	O7	1	Total Zn 1 1	0	0
89	q2	1	Total Zn 1 1	0	0

- Molecule 90 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula:  $C_{10}H_{14}N_5O_7P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
90	1	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
90	5	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 91 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>3</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
91	Q2	1	Total	C	N	O	P	0	0
			20	9	3	7	1		

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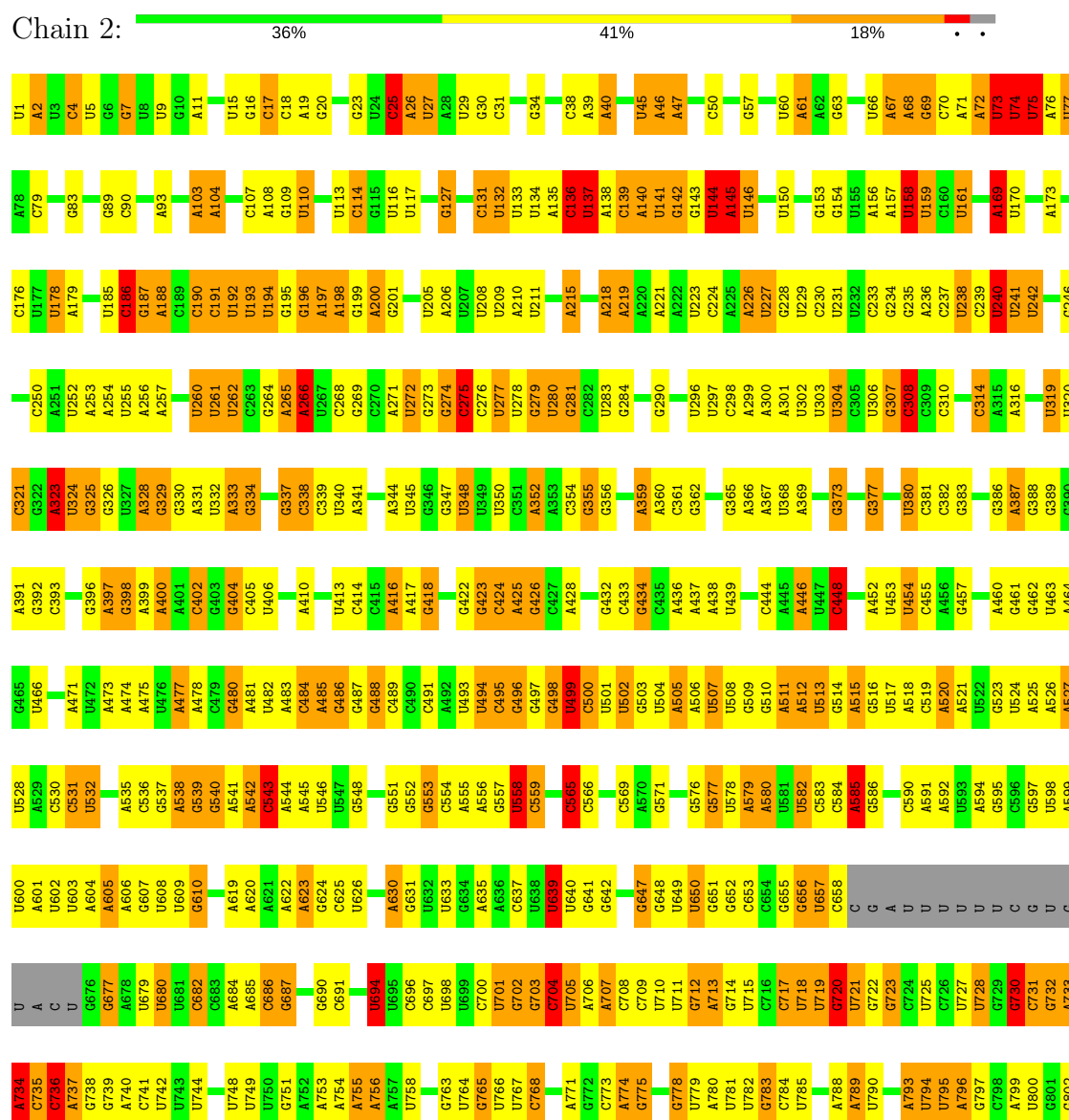
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
91	Q2	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
91	q2	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
91	q2	1	Total	C	N	O	P	0	0
			20	9	3	7	1		

### 3 Residue-property plots

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





Response	Percentage
Yes, the U.S. is responsible	37%
No, the U.S. is not responsible	42%
Don't know	18%
Refuse to answer	3%

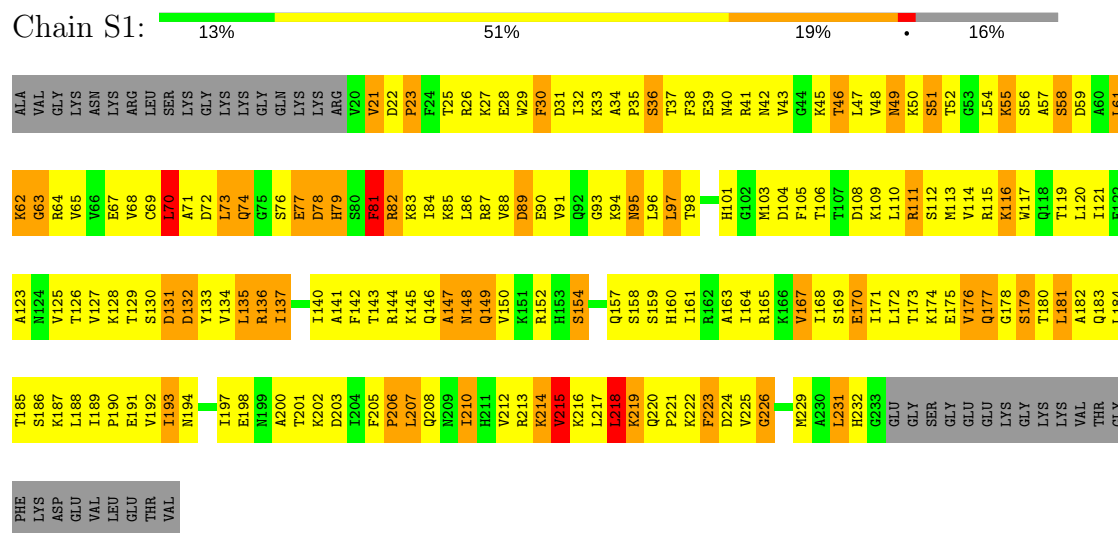




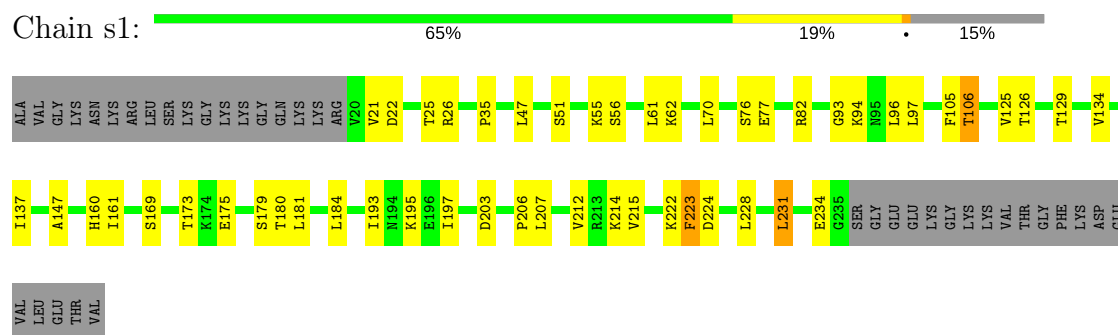
A1242	G1164	U1079	C1007	G858	A793	U715	G648	C569	U502	G432	G357	G279	A206	C136	A72
G1243	G1165	U1080	C1010	U861	U795	C716	U649	A570	G503	C433	U358	U280	A209	U137	U73
A1244	A1166	A1081	G934	A862	U795	C717	U650	G571	A504	G434	A359	G281	U210	C139	U74
G1245	G1167	C1082	G1011	A861	A796	U718	G651	G574	A505	A437	A360	C282	A207	A140	A76
G1246	A1171	A1087	U935	A863	G797	U719	G652	G574	A506	A438	G362	U283	A213	U141	U77
U1249	G1172	A1088	G936	U864	U800	C720	C653	G577	U507	U439	G363	G287	G214	G142	A78
U1250	C1173	G937	G938	A865	G801	G722	C654	U578	U508	C444	A366	G290	A215	G143	C79
U1251	C1174	G867	G939	G866	A804	G723	C655	U579	G509	A445	A367	G291	U216	U144	U82
U1252	U1175	A1092	A940	C868	A805	U727	C658	A581	A511	A446	A367	G292	A217	A145	G83
U1253	G1176	A869	A941	C869	A806	U728	A661	U582	A512	U447	A367	U292	A218	U146	A84
U1254	C1177	C870	C1022	C870	A807	U729	U662	C583	U513	U448	G372	U293	A219	U150	A85
G1255	G1178	G871	C943	U662	A807	G730	U662	C584	A514	C449	G373	C294	A220	G151	A86
A1256	G1179	C872	A944	U665	U808	G730	U665	C584	A515	U450	G373	A295	A221	U152	C87
U1257	C1180	U873	A944	U666	A809	A733	U666	C587	G516	U451	C376	A299	C224	U153	U88
U1258	U1099	C874	C950	U667	G810	A734	U667	U588	A518	A452	G377	A301	A225	G154	G89
U1259	G875	C875	A951	C668	A811	A734	C668	U588	C519	U453	G377	A301	A225	U155	C90
U1260	U1185	C876	A952	U670	A812	A737	U670	A591	A520	U454	U380	C308	U227	A156	A93
G1261	U1191	G879	A955	U670	A813	G738	U670	A592	A521	C455	C381	C308	U228	A157	U94
U1262	G1192	C880	C956	G	G814	G738	G	U593	A522	U455	C382	C309	U229	U158	U94
G1263	A1193	C881	C957	U	G815	A752	U	U594	G523	A460	C383	C310	U230	U159	U95
G1264	A1194	A881	G958	A881	G816	A753	A881	A594	U524	A461	C384	U311	U231	C160	G96
C1195	C1195	U887	U958	U887	G816	A754	A887	A595	U524	G461	C384	U311	U231	C160	G96
G1267	A1196	U888	C1034	A888	G819	A755	U888	A596	A525	U462	C385	U312	U232	U161	C99
G1268	G1197	U889	G1035	A889	U820	A756	U889	A597	A526	U463	C386	U313	U233	A162	C99
U1269	G1198	U890	C1036	U889	U821	G751	G876	U600	A527	A464	C387	C314	U234	G163	A100
G1270	G1199	U891	A1037	U890	U822	A752	G877	A604	U528	G467	C390	A315	U235	A164	U101
G1271	G1200	U892	U1038	U891	G823	A753	A878	A605	A529	A468	C391	A316	U236	G165	U102
G1272	G1201	U893	C1039	U892	G824	A754	A879	A606	C530	A469	C392	A317	U237	A166	A103
C1274	A1202	U894	A1040	U893	U825	A755	U880	A606	C530	C469	C393	U318	U240	A168	A104
G1279	U1206	U895	G1041	U894	U826	A756	U881	A606	A534	A470	C394	U319	U241	U170	U106
C1280	U1206	U896	G1042	U895	U827	A756	U882	U609	A535	A471	C395	U320	U242	A171	C107
G1281	G1212	U897	C1045	U896	U828	A760	C882	G610	C536	U472	C396	U321	U243	C176	A108
U1282	G1213	U900	U1052	U897	U829	C768	C883	U611	G537	A473	C397	G322	U244	U177	G109
U1283	U1214	U901	G1053	U902	A830	U764	A884	U612	A538	A474	C398	G323	U245	U178	U110
C1284	C1215	A905	U1054	A906	U831	C765	A885	U613	G539	A475	C399	G324	U246	U179	U111
G1285	C1216	U906	U1055	A907	U832	U766	C886	U614	G540	U476	A400	G325	U247	A180	U112
U1286	A1217	U907	U1056	U908	U833	U767	C887	U615	A541	U477	A401	G326	U248	A181	C114
A1287	G1218	U908	U1057	U909	U834	U768	C888	U616	C542	A478	C402	G327	U249	A182	C114
G1288	U1219	U909	U1058	U910	U835	A769	U890	U617	A543	A479	C403	G328	U250	A183	G115
U1289	A1220	U910	U1059	U911	U836	A770	U891	U618	A544	A480	C404	G329	A251	U184	U116
U1290	U1231	U911	U1060	U912	U837	C772	C892	A620	U545	A481	C405	U332	C258	U185	U117
G1294	U1225	U912	U1061	U913	U838	C773	C893	A621	U546	A482	C406	G336	U259	U186	U118
U1295	A1226	U913	U1062	U914	U839	C774	C894	A622	G548	U483	C407	G337	U260	G186	A119
G1297	A1227	U914	U1063	U915	U840	C775	C895	A623	G549	U484	C408	G338	U261	G187	U120
U1298	G1228	U915	U1064	U916	U841	C776	C896	A624	A550	U485	A416	C339	U262	G188	C126
G1299	G1229	U916	U1065	U917	U842	C777	C897	A625	A551	U486	A417	C340	U263	A189	U121
U1305	U1230	U917	U1066	U918	U843	C778	C898	A626	A552	U487	A418	U341	A265	C190	G123
U1306	U1231	U918	U1067	U919	U844	C779	C899	U626	A553	U488	G418	C342	A266	C191	U124
G1308	U1232	U919	U1068	U920	U845	C780	C900	U627	A554	U489	G419	C343	U267	U192	U125
U1309	G1233	U920	U1069	U921	U846	C781	C901	U628	A555	U490	G420	C344	C270	U193	A126
C1309	A1234	U921	U1070	U922	U847	C782	C902	U629	A556	U491	G421	C345	C271	U194	G127
C1235	C1235	U922	U1071	U923	U848	C783	C903	U630	A557	U492	G422	C346	C272	U195	C130
A1312	A1312	U923	U1072	U924	U849	C784	C904	U631	A558	U493	G423	C347	C273	G196	C130
A1313	A1313	U924	U1073	U925	U850	C785	C905	U632	A559	U494	G424	C348	C274	G197	C131
U1314	U1239	U925	U1074	U926	U851	C786	C906	U633	A560	U495	G425	C349	C275	A198	U132
U1315	U1240	U926	U1075	U927	U852	C787	C907	U634	A561	U496	G426	C350	C276	G199	U
G1316	G1241	U927	U1076	U928	U853	C788	C908	U635	A562	U497	G427	C351	C277	A200	U
			U1077	U929	U854	C789	C909	U636	A563	U498	G428	C352	C278	G200	A
			U1078	U930	U855	C790	C910	U637	A564	U499	G429	C353	C279	G201	
			U1079	U931	U856	C791	C911	U638	A565	U500	G430	C354	C280	G202	
			U1080	U932	U857	C792	C912	U639	A566	U501	G431	C355	C281	G203	
			U1081	U933	U858	C793	C913	U640	A567			C356	C282	G204	
			U1082	U934	U859	C794	C914	U641	A568			C357	C283	G205	
			U1083	U935	U860	C795	C915	U642	A569			C358	C284	G206	
			U1084	U936	U861	C796	C916	U643	A570			C359	C285	G207	
			U1085	U937	U862	C797	C917	U644	A571			C360	C286	G208	
			U1086	U938	U863	C798	C918	U645	A572			C361	C287	G209	
			U1087	U939	U864	C799	C919	U646	A573			C362	C288	G210	
			U1088	U940	U865	C800	C920	U647	A574			C363	C289	G211	
			U1089	U941	U866	C801	C921	U648	A575			C364	C290	G212	
			U1090	U942	U867	C802	C922	U649	A576			C365	C291	G213	
			U1091	U943	U868	C803	C923	U650	A577			C366	C292	G214	
			U1092	U944	U869	C804	C924	U651	A578			C367	C293	G215	
			U1093	U945	U870	C805	C925	U652	A579			C368	C294	G216	
			U1094	U946	U871	C806	C926	U653	A580			C369	C295	G217	
			U1095	U947	U872	C807	C927	U654	A581			C370	C296	G218	
			U1096	U948	U873	C808	C928	U655	A582			C371	C297	G219	
			U1097	U949	U874	C809	C929	U656	A583			C372	C298	G220	
			U1098	U950	U875	C810	C930	U657	A584			C373	C299	G221	
			U1099	U951	U876	C811	C931	U658	A585			C374	C300	G222	
			U1100	U952	U877	C812	C932	U659	A586			C375	C301	G223	
			U1101	U953	U878	C813	C933	U660	A587			C376	C302	G224	
			U1102	U954	U879	C814	C934	U661	A588			C377	C303	G225	
			U1103	U955	U880	C815	C935	U662	A589			C378	C304	G226	
			U1104	U956	U881	C816	C936	U663	A590			C379	C305	G227	
			U1105	U957	U882	C817	C937	U664	A591			C380	C306	G228	
			U1106	U958	U883	C818	C938	U665	A592			C381	C307	G229	
			U1107	U959	U884	C819	C939	U666	A593			C382	C308	G230	
			U1108	U960	U885	C820	C940	U667	A594			C383	C309	G231	
			U1109	U961	U886	C821	C941	U668	A595			C384	C310	G232	
			U1110	U962	U887	C822	C942	U669	A596			C385	C311	G233	
			U1111	U963	U888	C823	C943	U670	A597			C386	C312	G234	
			U1112	U964	U889	C824	C944	U671							



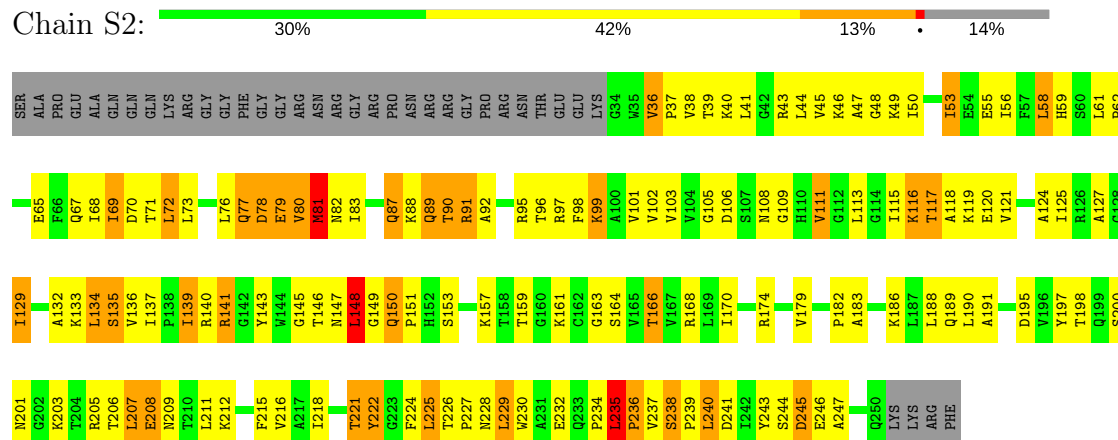
- Molecule 3: 40S ribosomal protein S1-A



- Molecule 3: 40S ribosomal protein S1-A

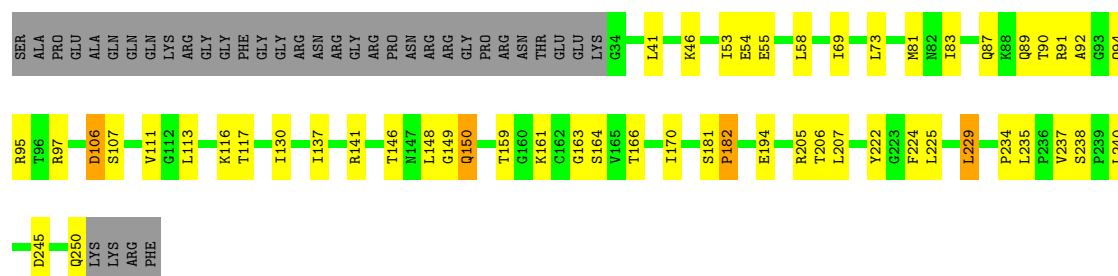


- Molecule 4: 40S ribosomal protein S2



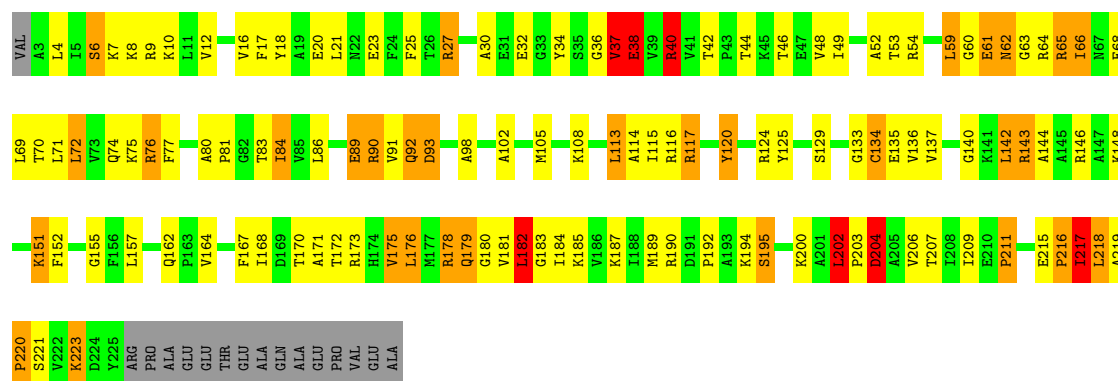
- Molecule 4: 40S ribosomal protein S2





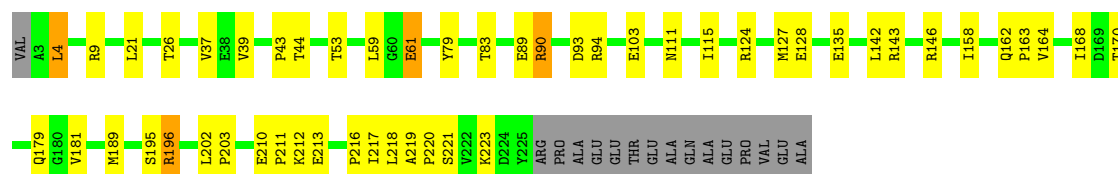
• Molecule 5: 40S ribosomal protein S3

Chain S3: 41% 36% 13% 7%



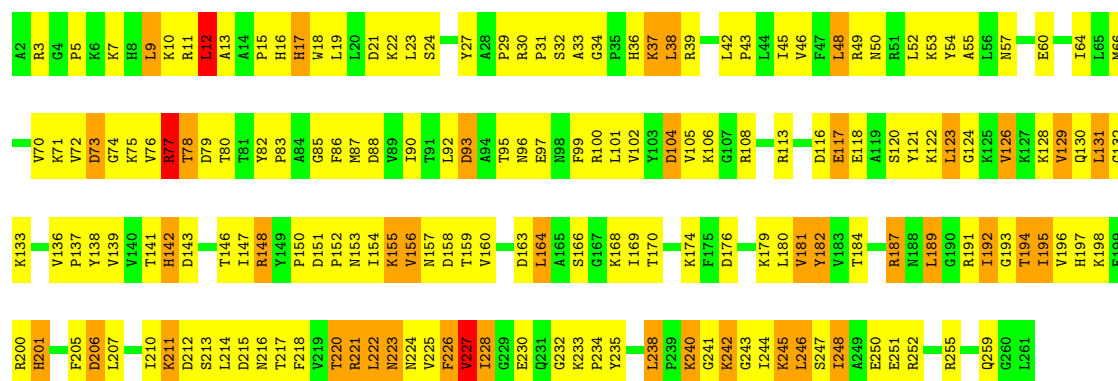
• Molecule 5: 40S ribosomal protein S3

Chain s3: 72% 20% 7%

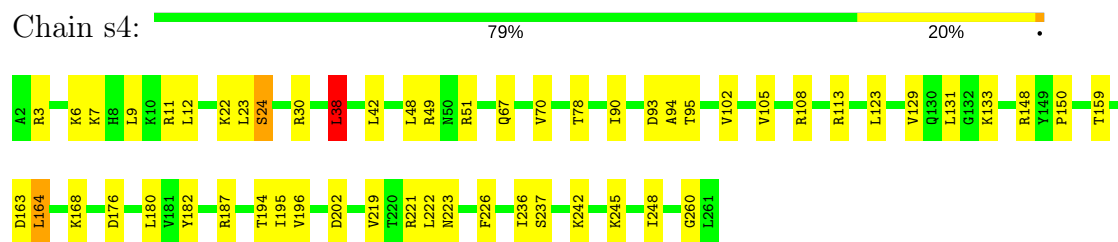


• Molecule 6: 40S ribosomal protein S4-A

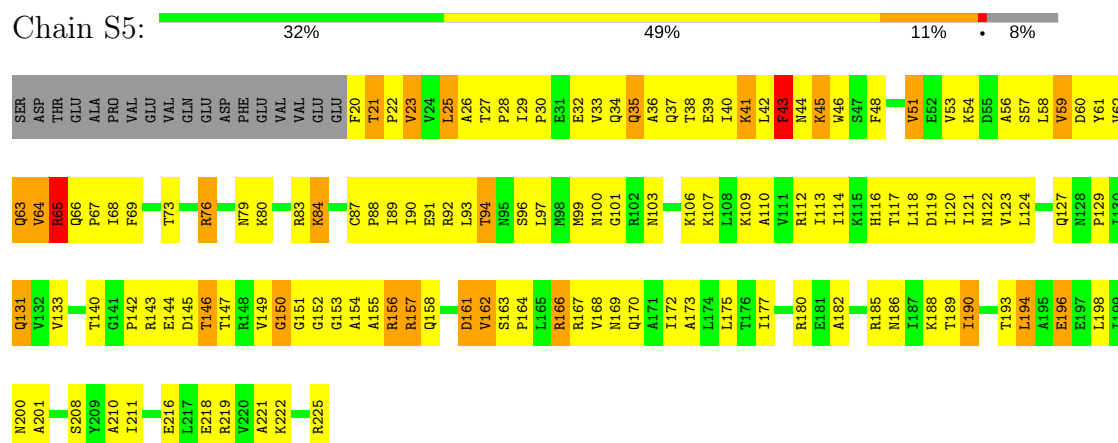
Chain S4: 32% 51% 16%



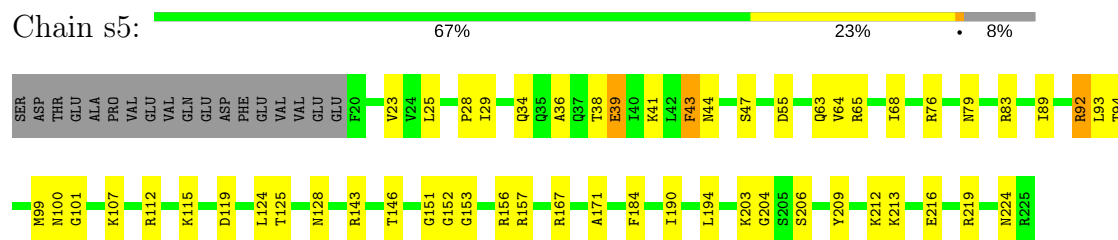
• Molecule 6: 40S ribosomal protein S4-A



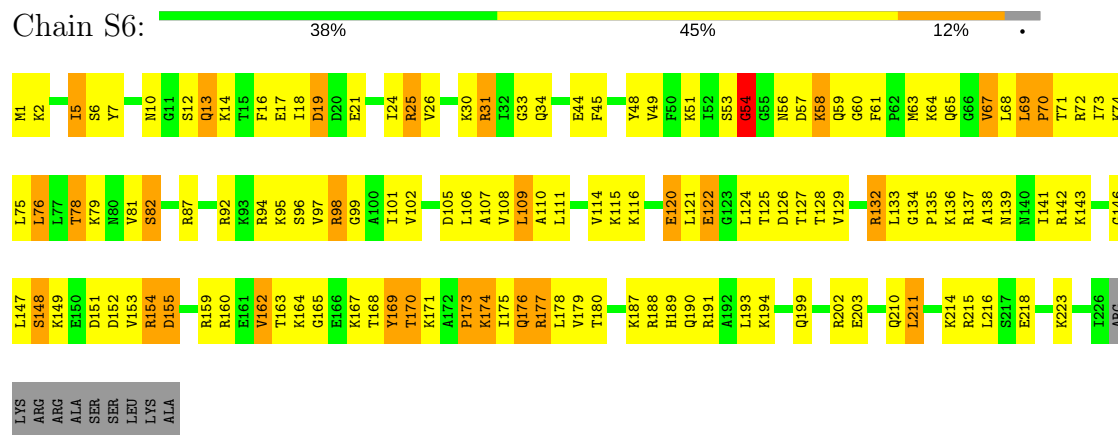
• Molecule 7: 40S ribosomal protein S5



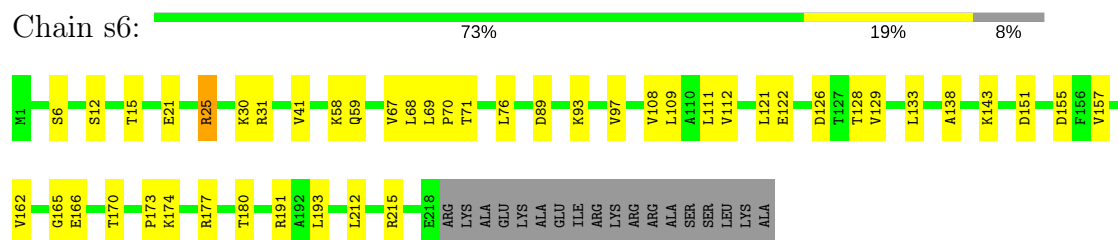
• Molecule 7: 40S ribosomal protein S5



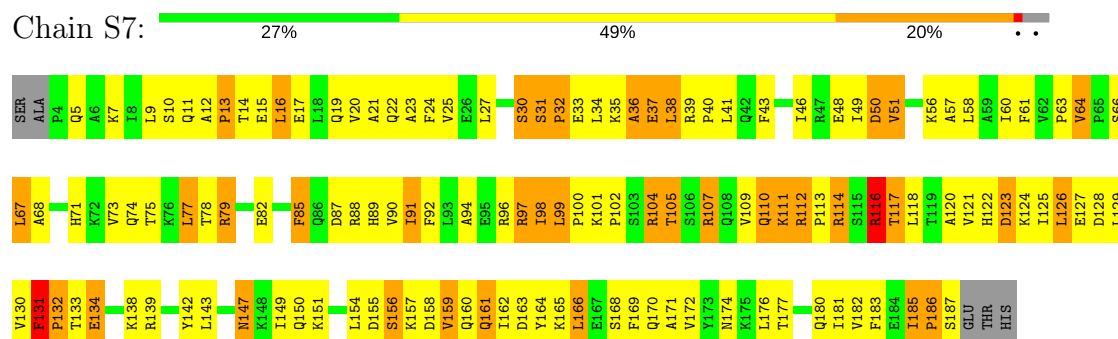
• Molecule 8: 40S ribosomal protein S6-A



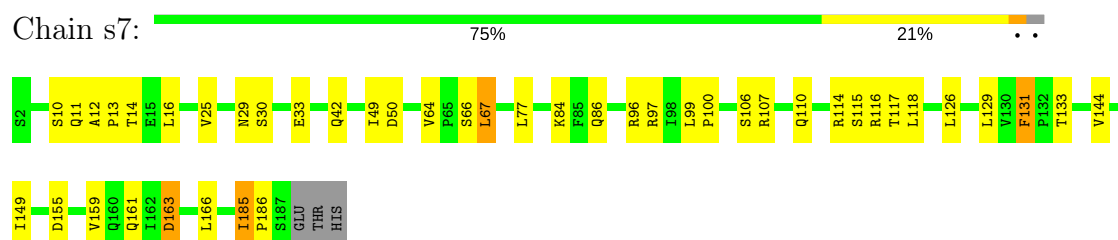
• Molecule 8: 40S ribosomal protein S6-A



• Molecule 9: 40S ribosomal protein S7-A



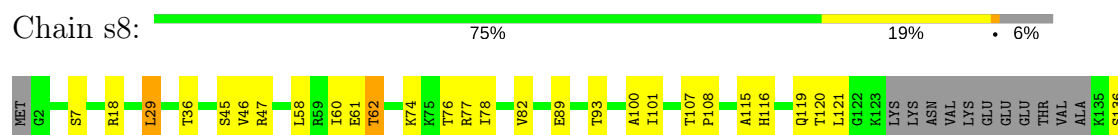
• Molecule 9: 40S ribosomal protein S7-A



• Molecule 10: 40S ribosomal protein S8-A



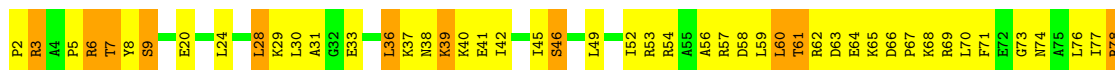
• Molecule 10: 40S ribosomal protein S8-A





• Molecule 11: 40S ribosomal protein S9-A

Chain S9: 30% 46% 17% 6%



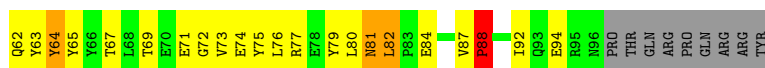
• Molecule 11: 40S ribosomal protein S9-A

Chain s9: 76% 17% 6%



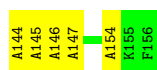
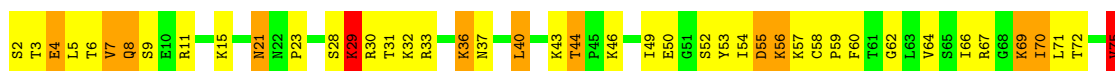
• Molecule 12: 40S ribosomal protein S10-A

Chain C0: 23% 56% 11% 9%



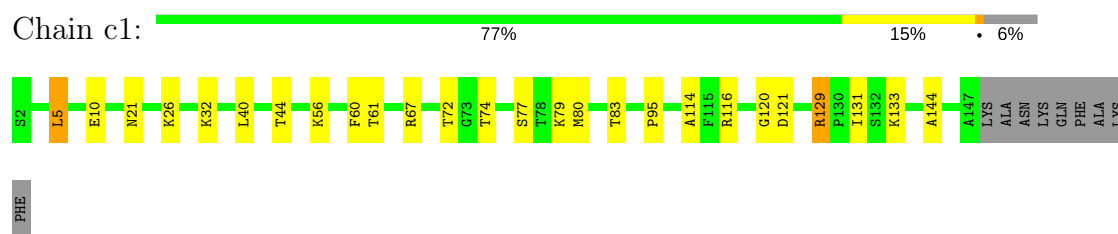
• Molecule 13: 40S ribosomal protein S11-A

Chain C1: 39% 46% 13%



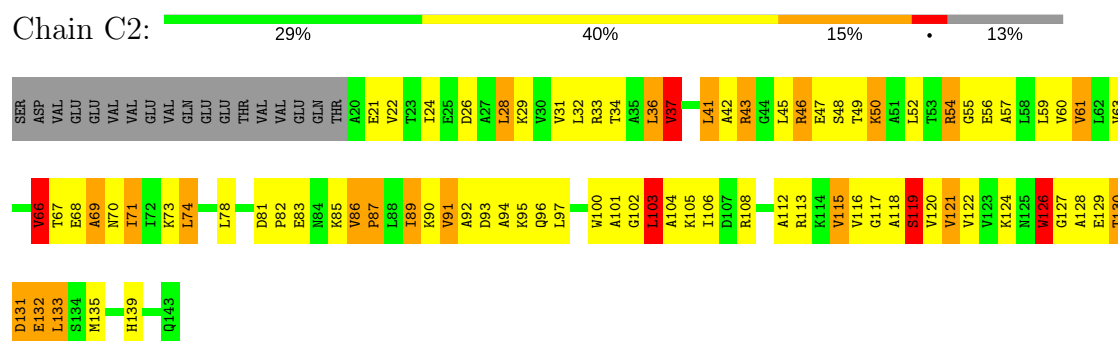
• Molecule 13: 40S ribosomal protein S11-A

Chain c1:



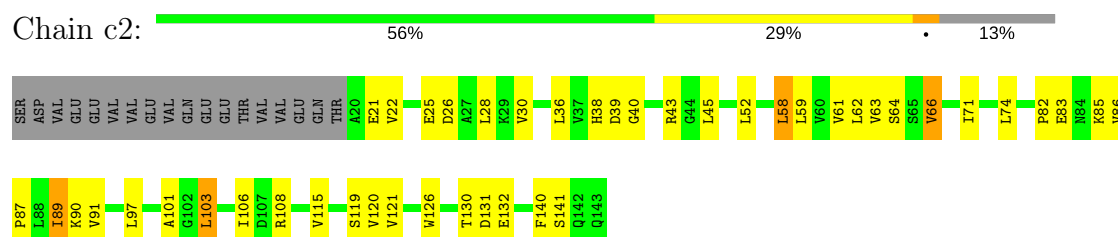
- Molecule 14: 40S ribosomal protein S12

Chain C2:



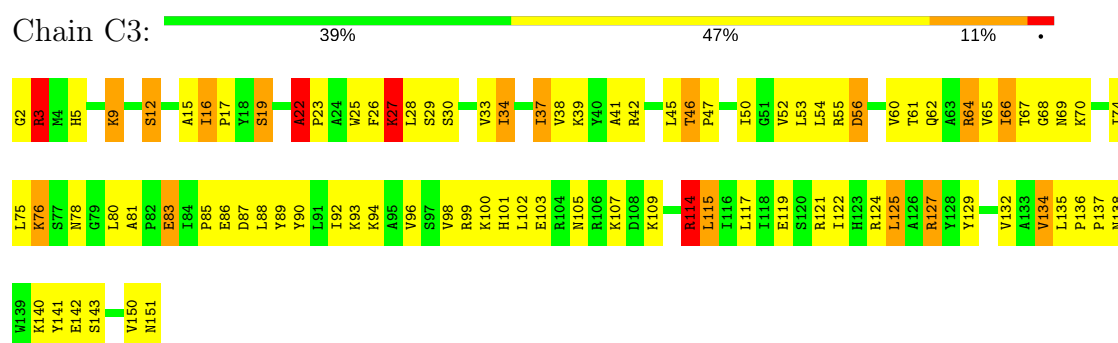
- Molecule 14: 40S ribosomal protein S12

Chain c2:



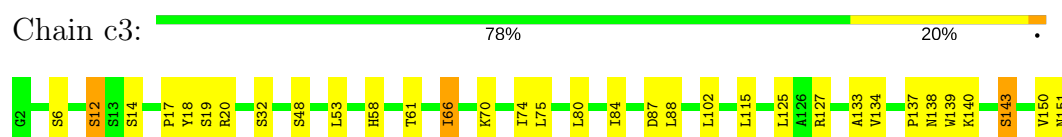
- Molecule 15: 40S ribosomal protein S13

Chain C3:



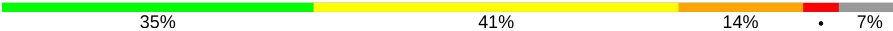
- Molecule 15: 40S ribosomal protein S13

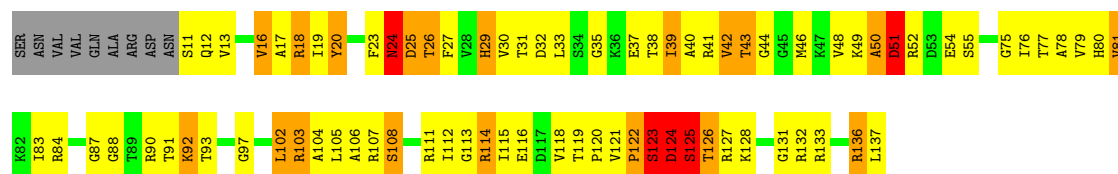
Chain c3:



- Molecule 16: 40S ribosomal protein S14-A

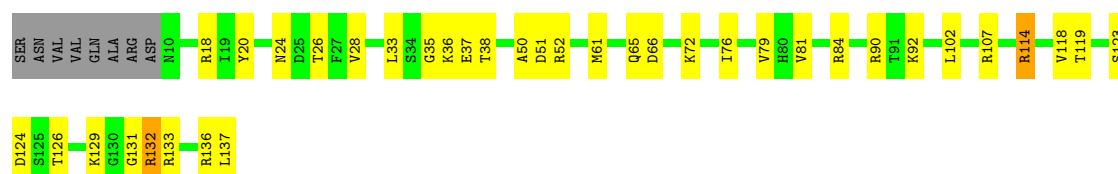


Chain C4: 



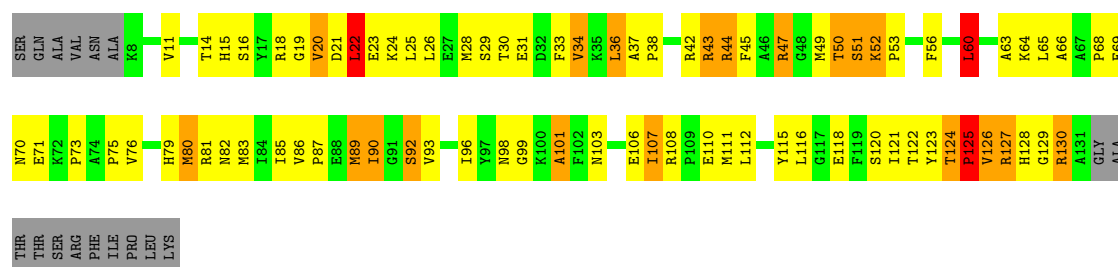
• Molecule 16: 40S ribosomal protein S14-A

Chain c4: 



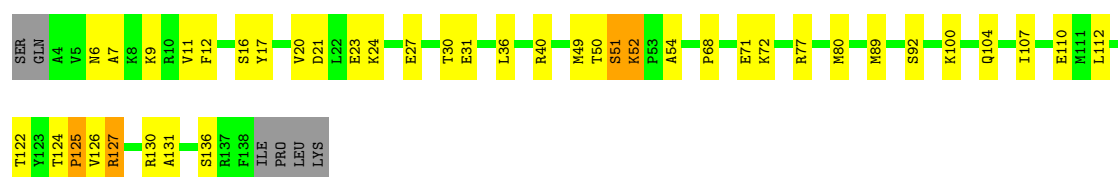
• Molecule 17: 40S ribosomal protein S15

Chain C5: 

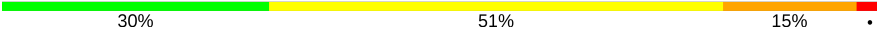


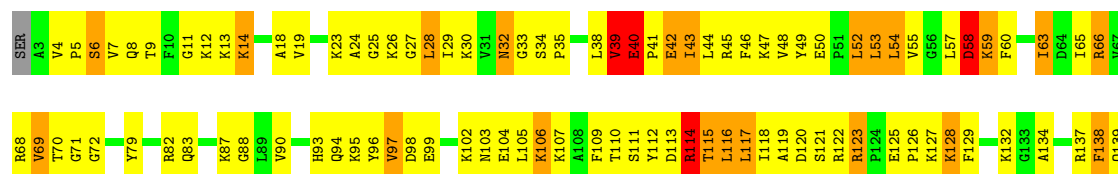
• Molecule 17: 40S ribosomal protein S15

Chain c5: 



• Molecule 18: 40S ribosomal protein S16-A

Chain C6: 





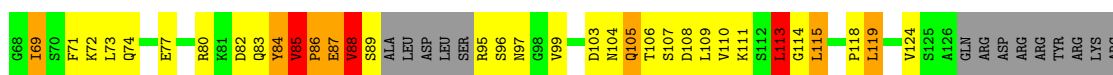
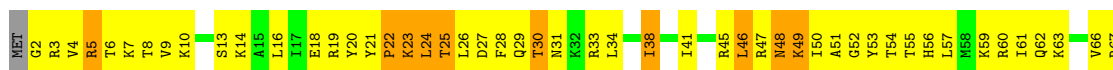
• Molecule 18: 40S ribosomal protein S16-A

Chain c6: 78% 20%



• Molecule 19: 40S ribosomal protein S17-A

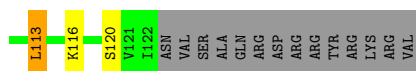
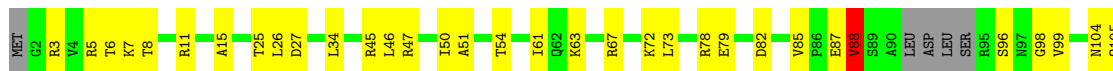
Chain C7: 26% 47% 13% 12%



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• Molecule 19: 40S ribosomal protein S17-A

Chain c7: 60% 25% 14%



• Molecule 20: 40S ribosomal protein S18-A

Chain C8: 32% 49% 14%



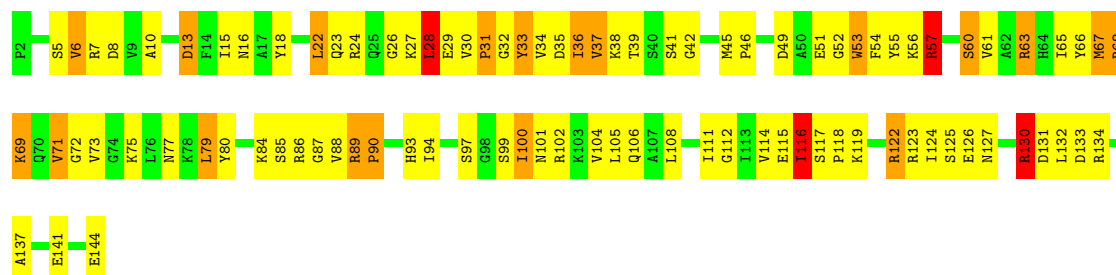
• Molecule 20: 40S ribosomal protein S18-A

Chain c8: 76% 21%



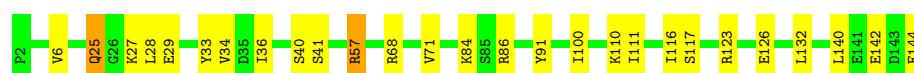
- Molecule 21: 40S ribosomal protein S19-A

Chain C9: 35% 49% 13%



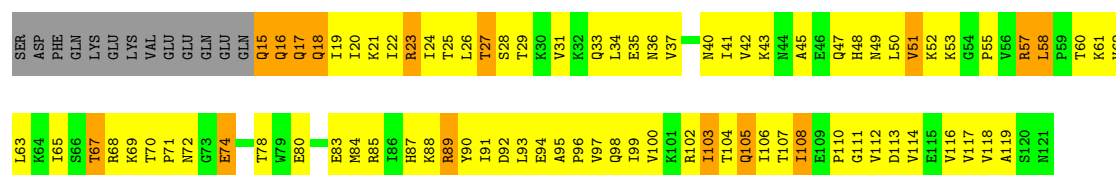
- Molecule 21: 40S ribosomal protein S19-A

Chain c9: 81% 17%



- Molecule 22: 40S ribosomal protein S20

Chain D0: 20% 57% 13% 11%



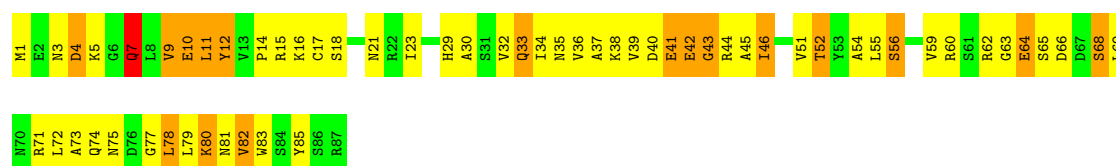
- Molecule 22: 40S ribosomal protein S20

Chain d0: 57% 33% 8%

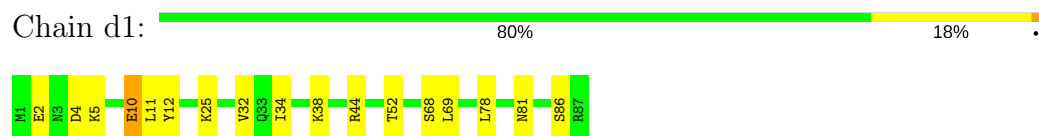


- Molecule 23: 40S ribosomal protein S21-A

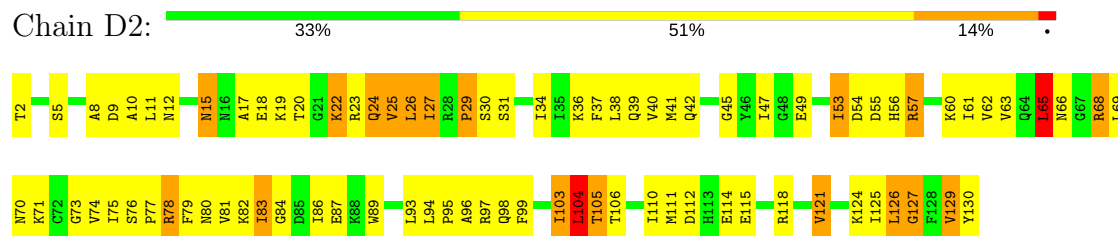
Chain D1: 31% 48% 20%



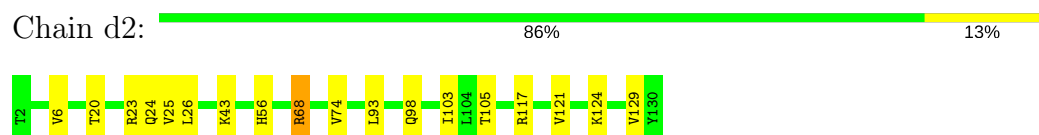
- Molecule 23: 40S ribosomal protein S21-A



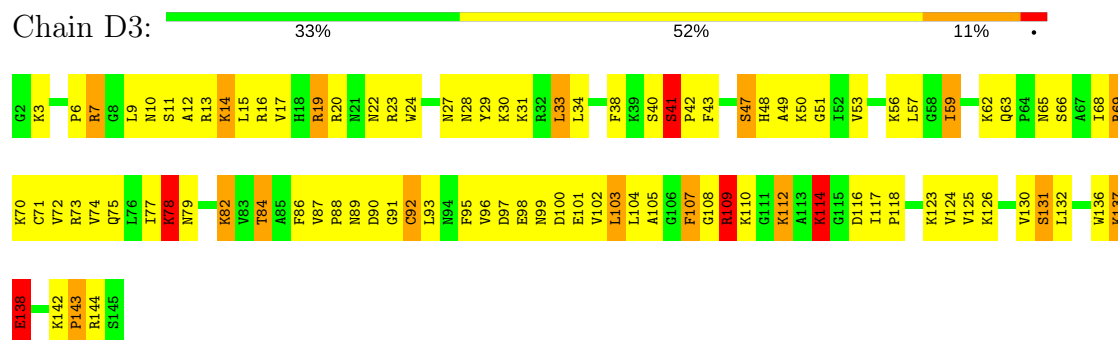
- Molecule 24: 40S ribosomal protein S22-A



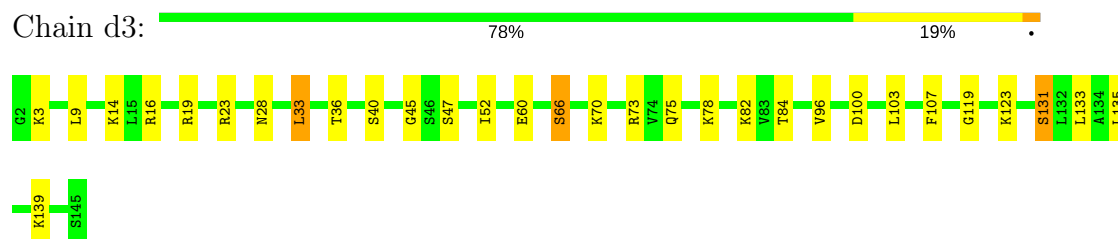
- Molecule 24: 40S ribosomal protein S22-A



- Molecule 25: 40S ribosomal protein S23-A

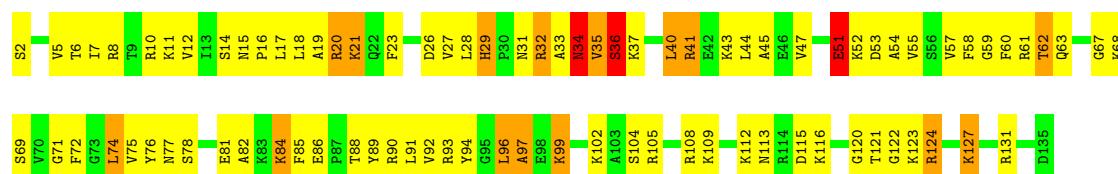


- Molecule 25: 40S ribosomal protein S23-A



- Molecule 26: 40S ribosomal protein S24-A





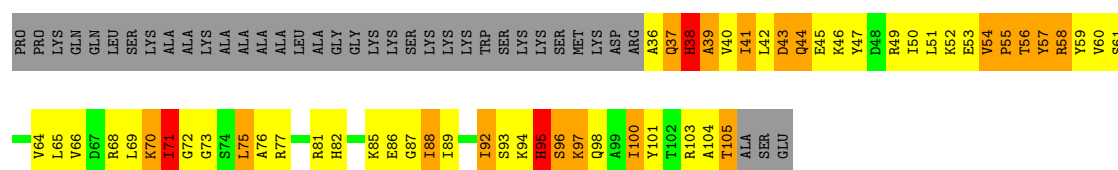
- Molecule 26: 40S ribosomal protein S24-A

Chain d4: 78% 21% ..



- Molecule 27: 40S ribosomal protein S25-A

Chain D5: 13% 33% 17% 35%



- Molecule 27: 40S ribosomal protein S25-A

Chain d5: 47% 17% 36%



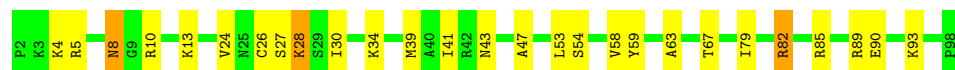
- Molecule 28: 40S ribosomal protein S26-B

Chain D6: 25% 52% 19% 5%

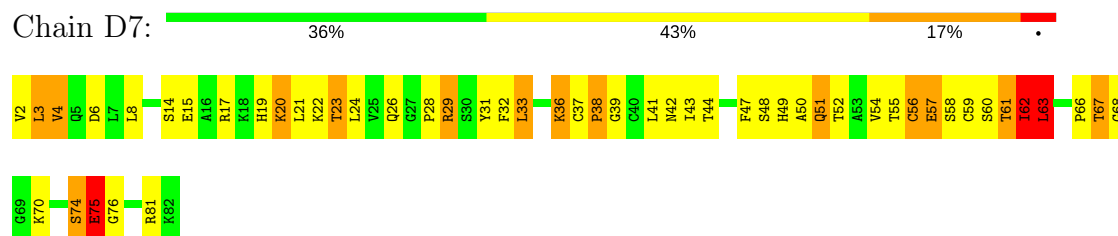


- Molecule 28: 40S ribosomal protein S26-B

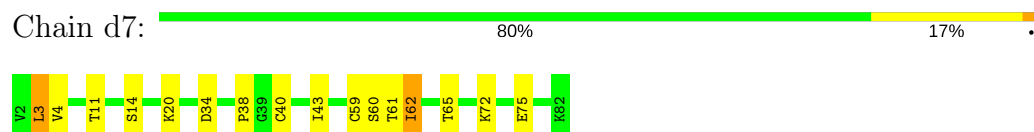
Chain d6: 72% 25%



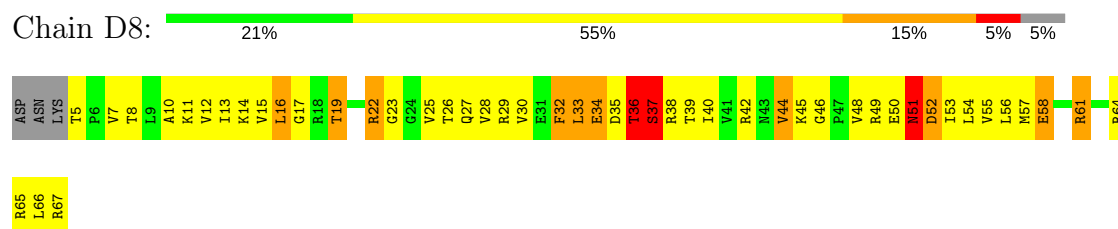
- Molecule 29: 40S ribosomal protein S27-A



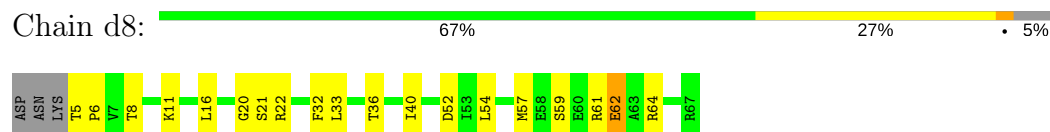
- Molecule 29: 40S ribosomal protein S27-A



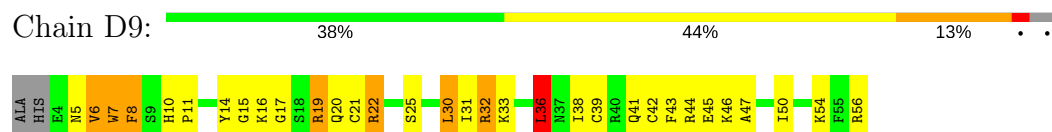
- Molecule 30: 40S ribosomal protein S28-A



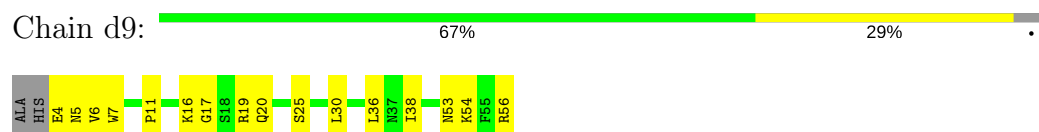
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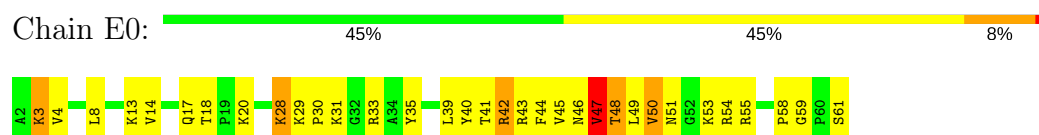
- Molecule 31: 40S ribosomal protein S29-A



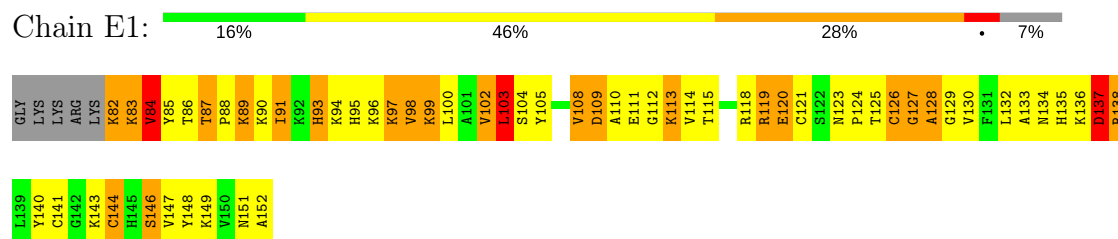
- Molecule 31: 40S ribosomal protein S29-A



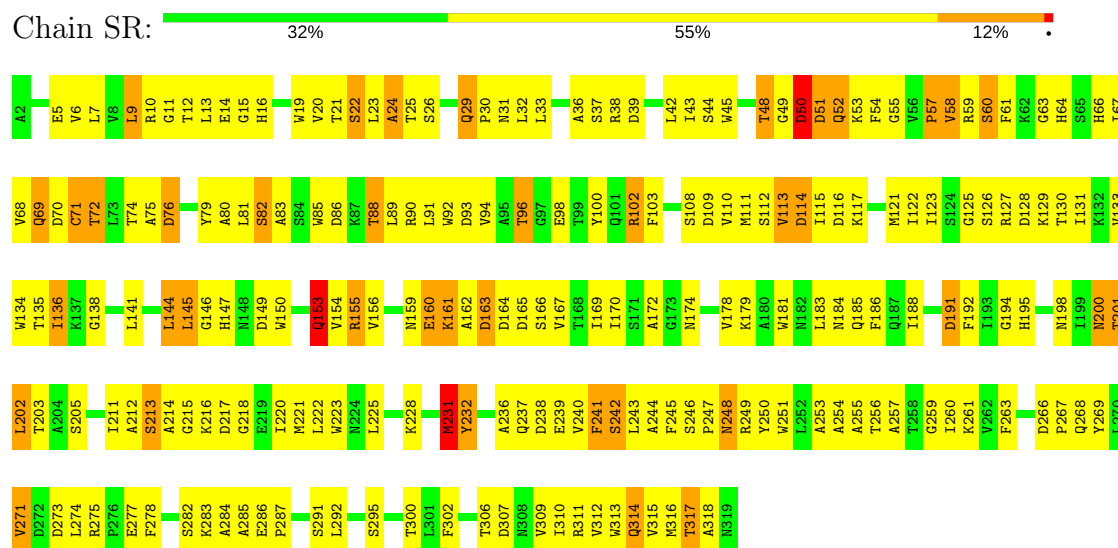
- Molecule 32: 40S ribosomal protein S30-A



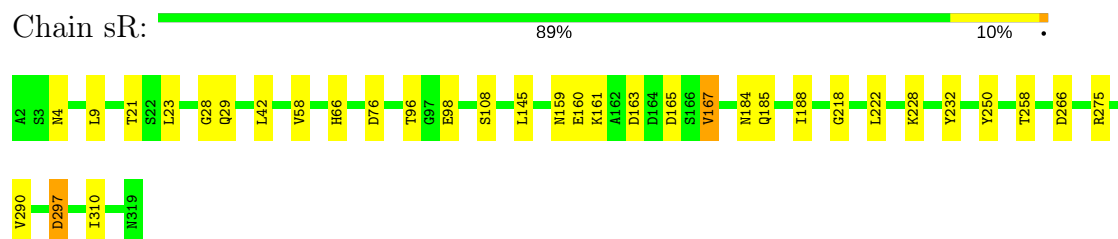
- Molecule 33: Ubiquitin-40S ribosomal protein S31



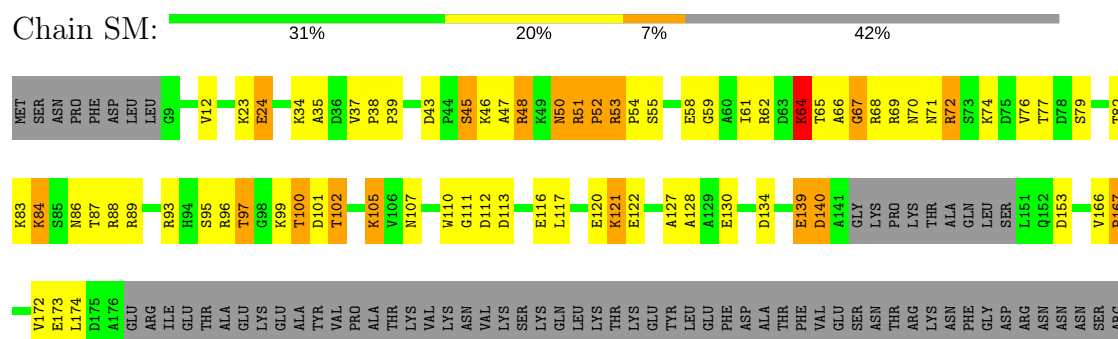
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



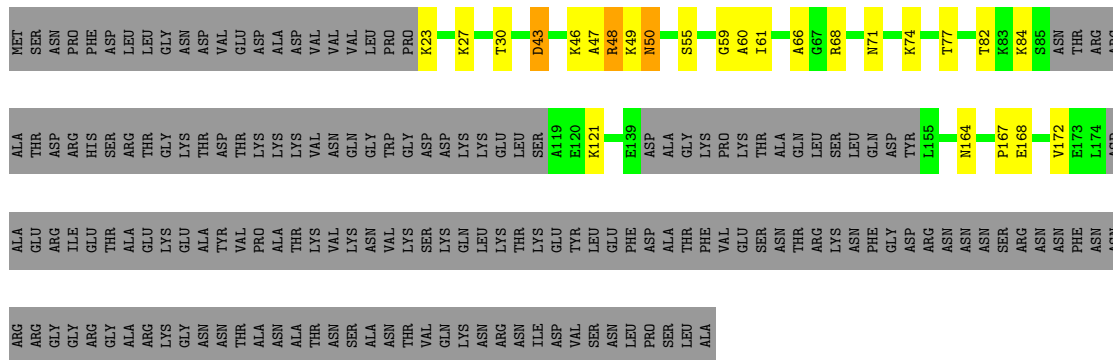
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



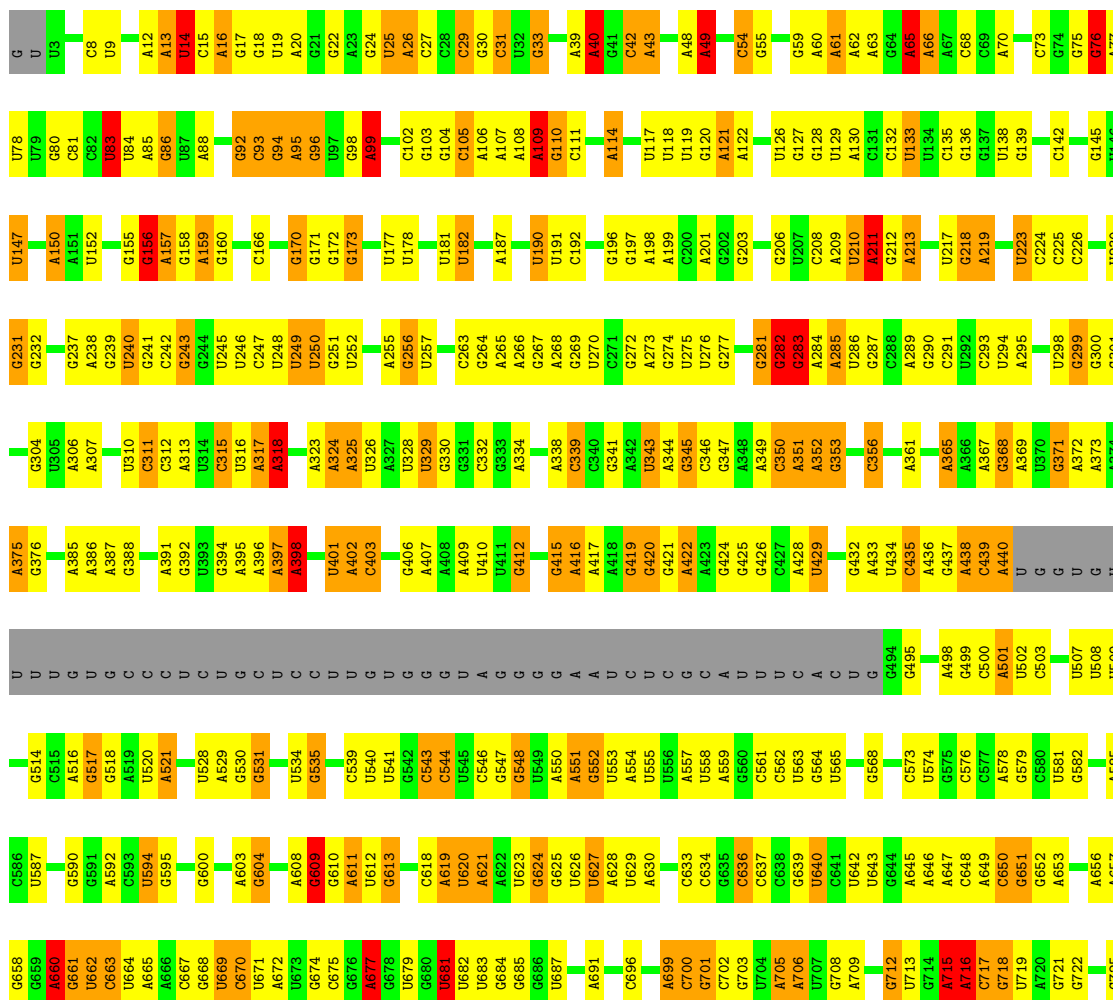
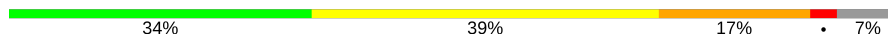
- Molecule 35: Suppressor protein STM1



## Chain sM:



Chain 1:





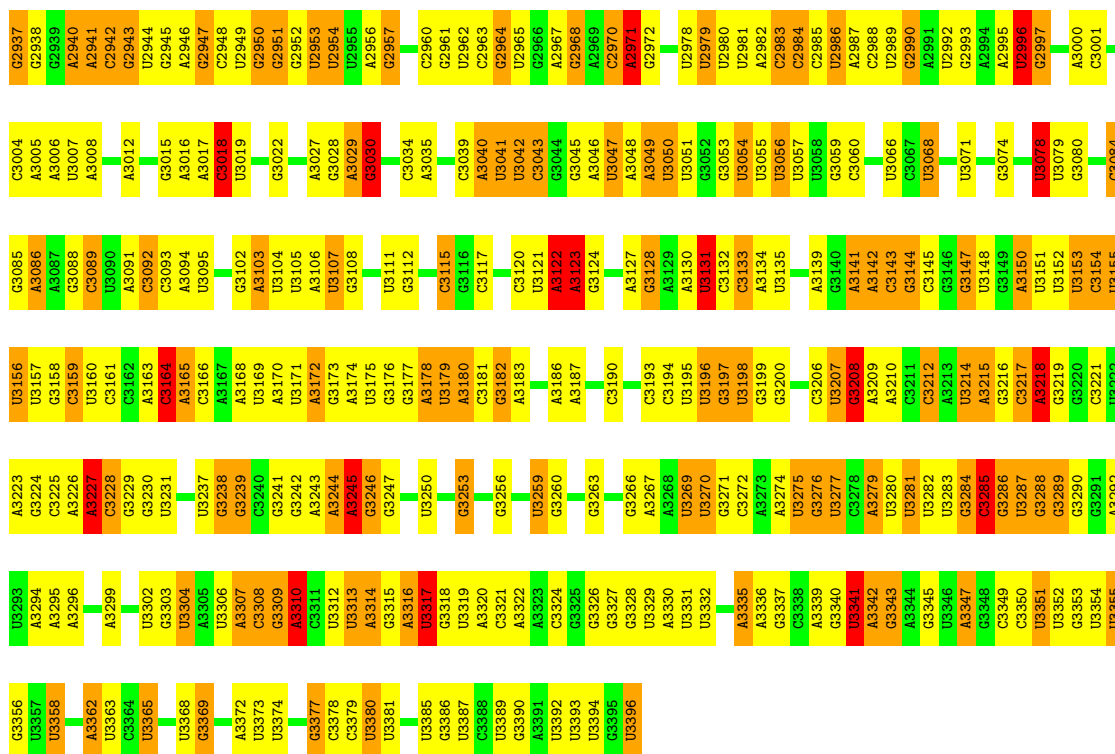
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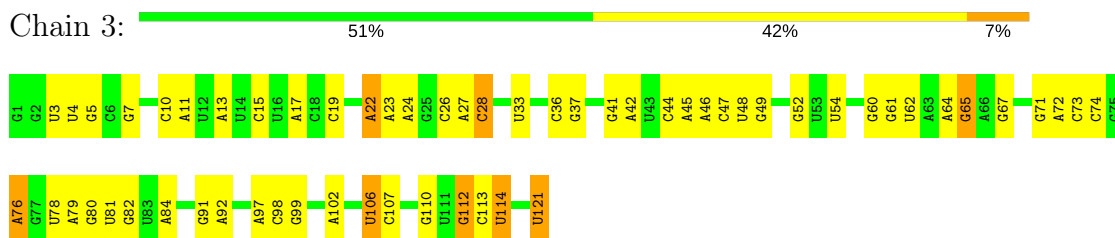


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U1765	U1647	U1648	U1765	U1649	U1650	U1651	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	G1273	G1200	G1131	U1060	A986	A915	U844	A765	C682	
G1766	U1648	U1649	G1766	U1650	U1651	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	G1274	G1201	G1132	U1061	A987	A916	U845	A766	C683	
G1769	U1649	U1650	G1769	U1651	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	G1275	G1202	G1133	U1062	A988	A917	U846	A767	C684	
G1770	U1650	U1651	G1770	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	G1276	G1203	G1134	U1063	A989	A918	U847	A768	C685	
G1771	U1651	U1652	G1771	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	G1277	G1204	G1135	U1064	A990	A919	U848	A769	C686	
G1772	U1652	U1653	G1772	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	G1278	G1205	G1136	U1065	A991	A920	U849	A770	C687	
G1773	U1653	U1654	G1773	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	G1279	G1206	G1137	U1066	A992	A921	U850	A771	C688	
C1774	U1654	U1655	C1774	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	G1280	G1207	G1138	U1067	A993	A922	U851	A772	C689	
U1687	U1655	U1656	U1687	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	G1281	G1208	G1139	U1068	A994	A923	U852	A773	C690	
G1778	U1656	U1657	G1778	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	G1282	G1209	G1140	U1069	A995	A924	U853	A774	C691	
C1779	U1657	U1658	C1779	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	G1283	G1210	G1141	U1070	A996	A925	U854	A775	C692	
G1843	U1658	U1659	G1843	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	G1284	G1211	G1142	U1071	A997	A926	U855	A776	C693	
G1844	U1659	U1660	G1844	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	G1285	G1212	G1143	U1072	A998	A927	U856	A777	C694	
G1845	U1660																										

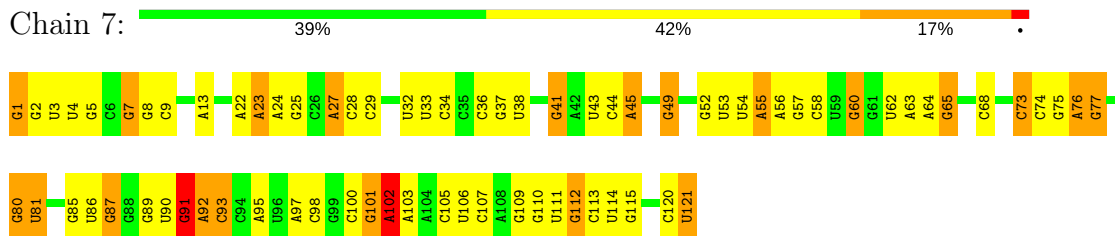




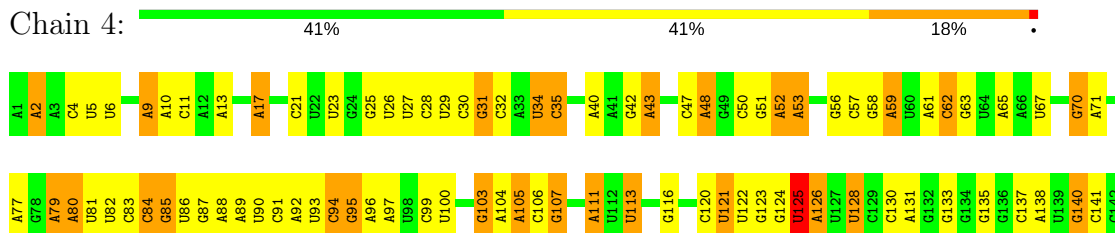
- Molecule 37: 5S ribosomal RNA



- Molecule 37: 5S ribosomal RNA

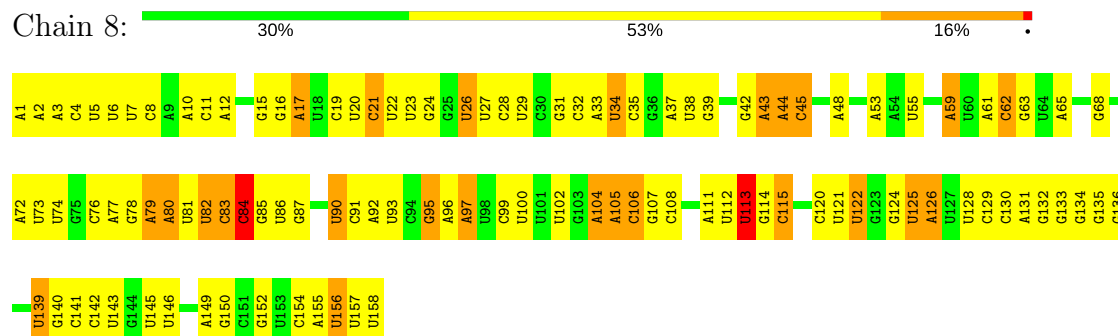


- Molecule 38: 5.8S ribosomal RNA

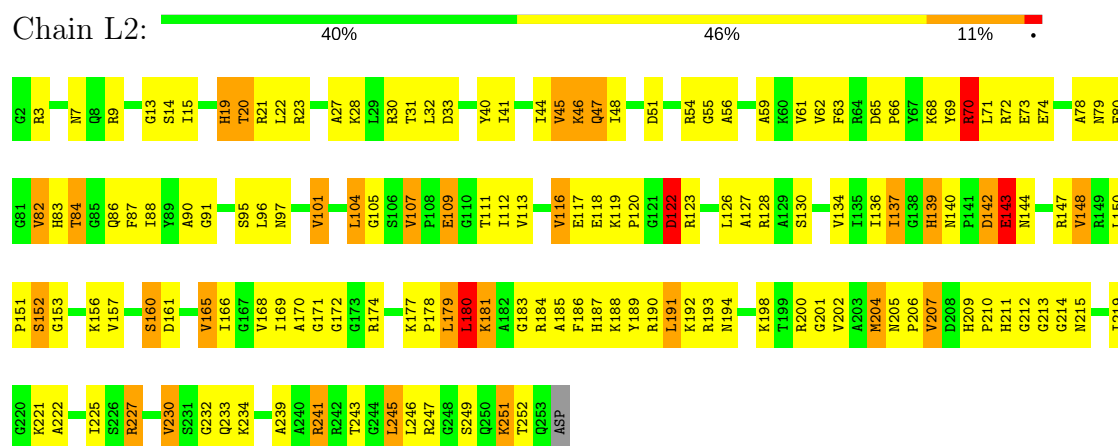




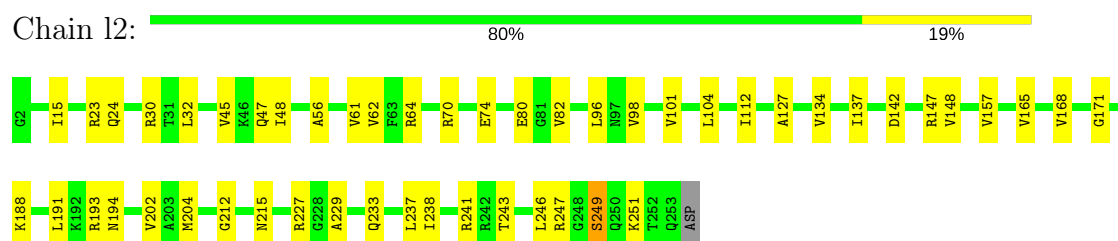
• Molecule 38: 5.8S ribosomal RNA



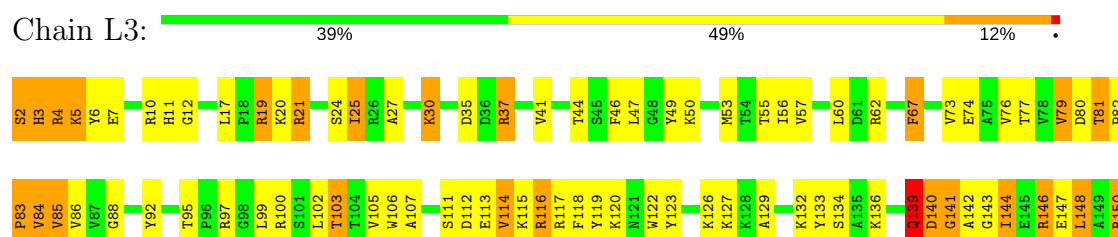
• Molecule 39: 60S ribosomal protein L2-A

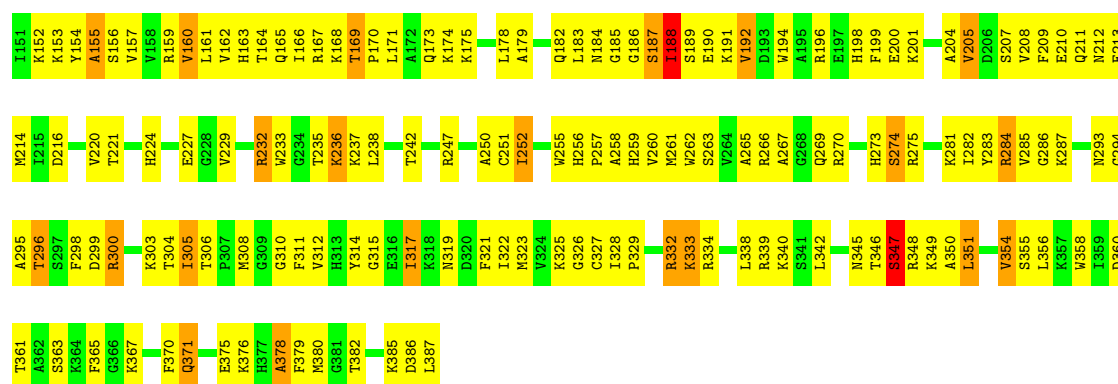


• Molecule 39: 60S ribosomal protein L2-A

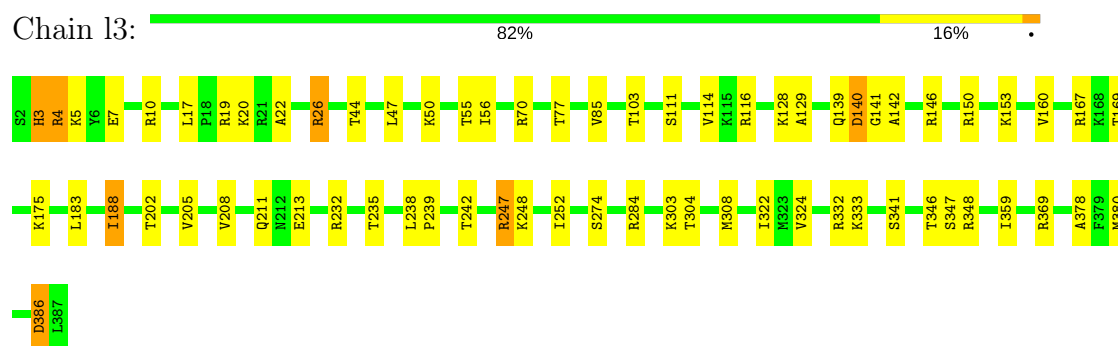


• Molecule 40: 60S ribosomal protein L3

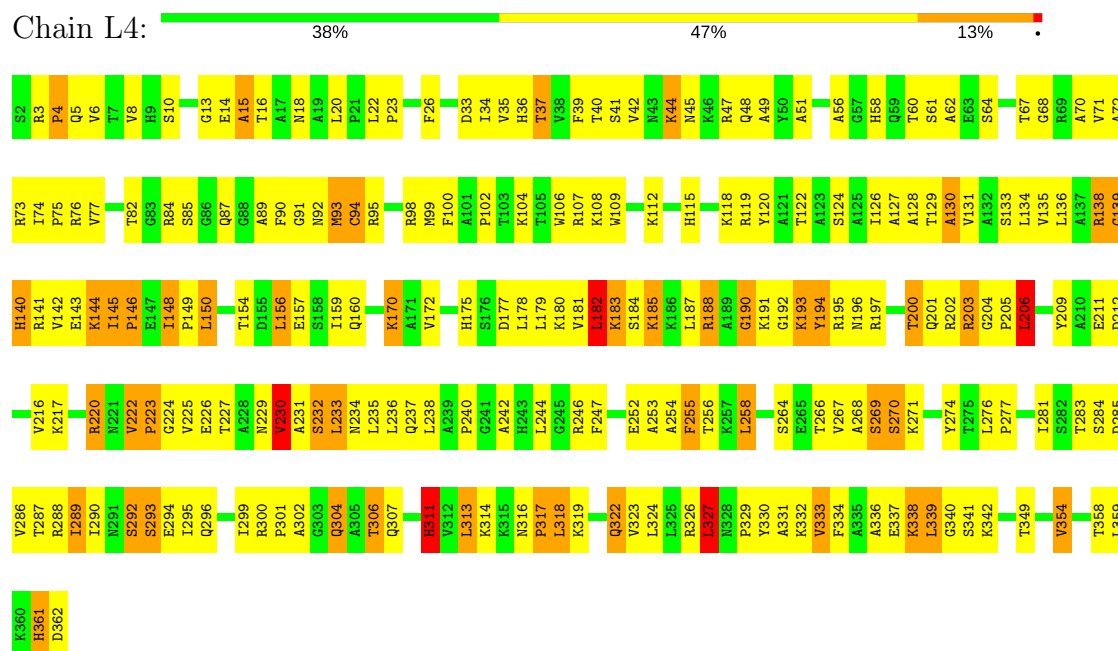




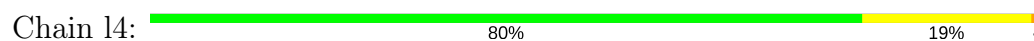
• Molecule 40: 60S ribosomal protein L3



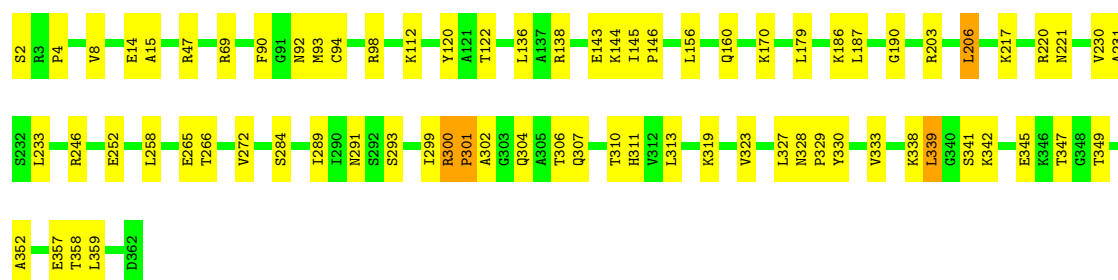
• Molecule 41: 60S ribosomal protein L4-A



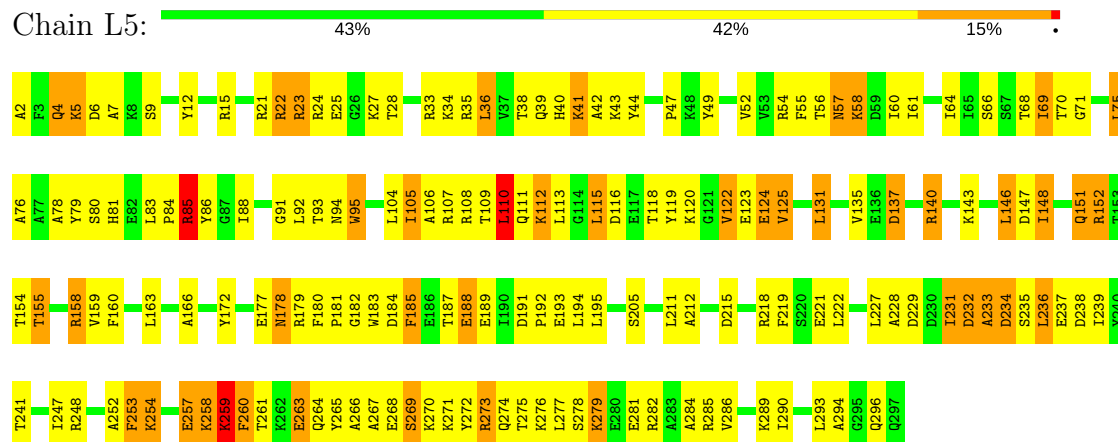
• Molecule 41: 60S ribosomal protein L4-A



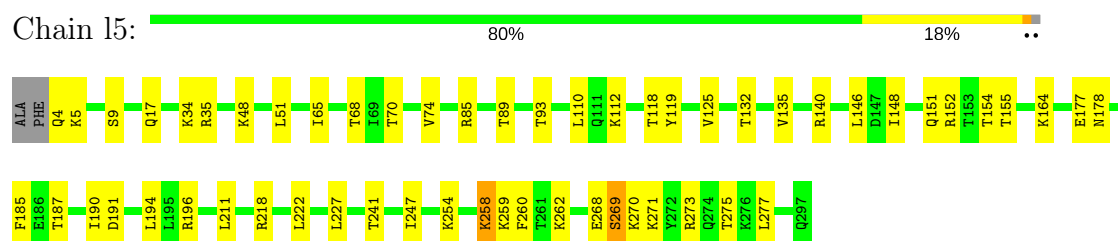




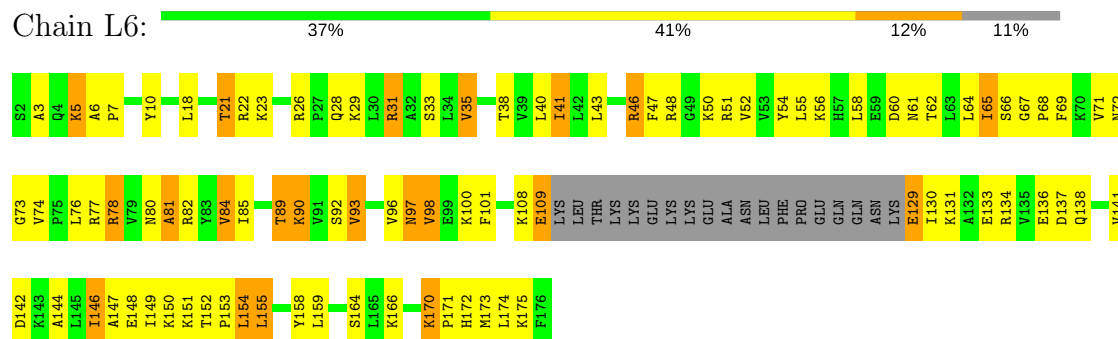
- Molecule 42: 60S ribosomal protein L5

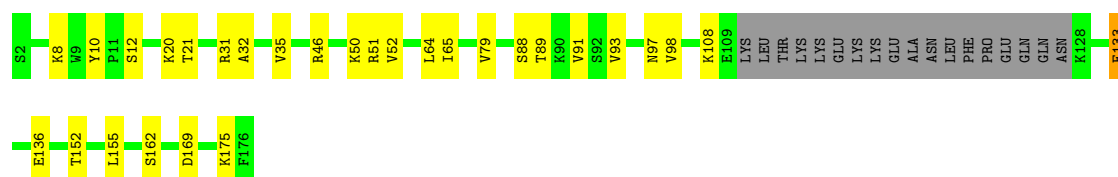


- Molecule 42: 60S ribosomal protein L5



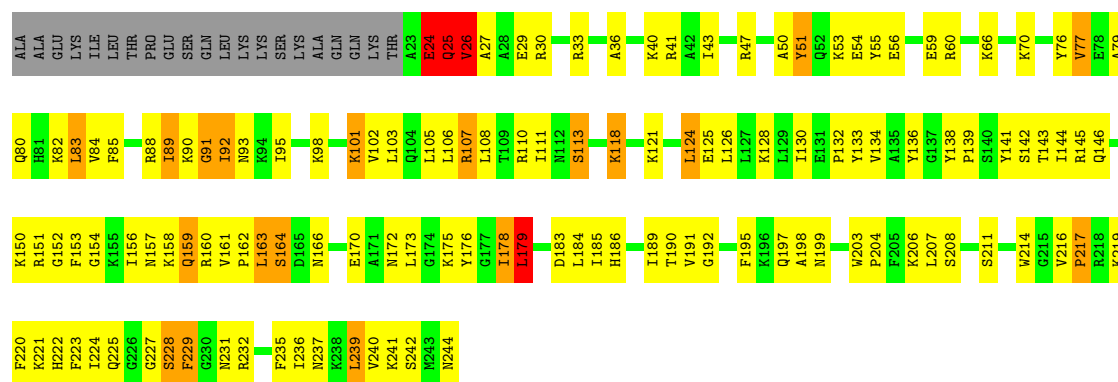
- Molecule 43: 60S ribosomal protein L6-A





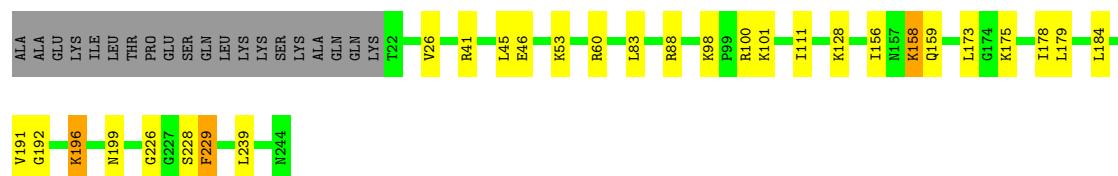
• Molecule 44: 60S ribosomal protein L7-A

Chain L7: 38% 44% 8% 9%



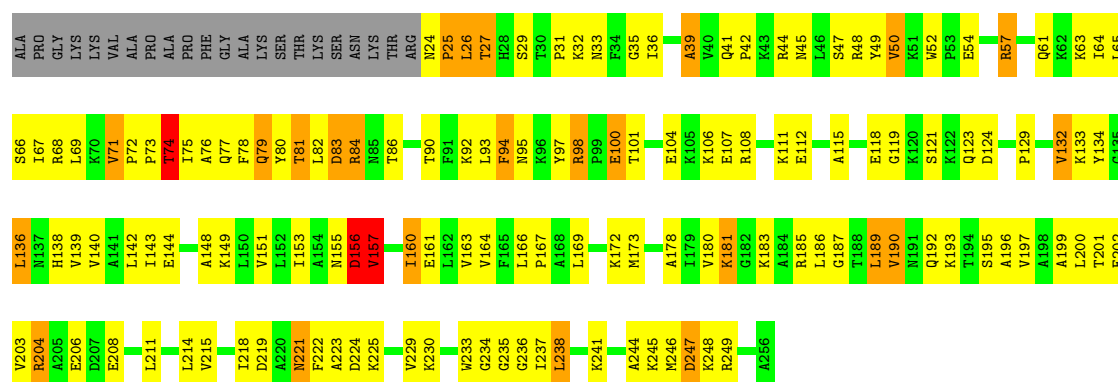
• Molecule 44: 60S ribosomal protein L7-A

Chain L7: 80% 11% 8%



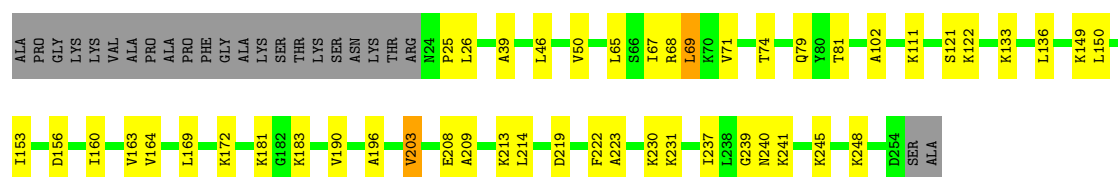
• Molecule 45: 60S ribosomal protein L8-A

Chain L8: 36% 44% 9% 9%



• Molecule 45: 60S ribosomal protein L8-A

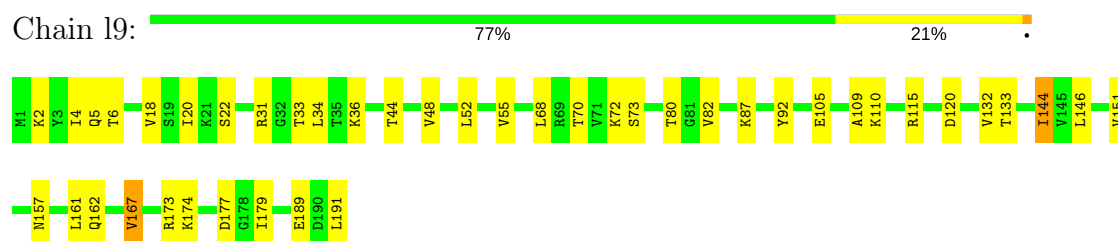
Chain L8: 72% 18% 9%



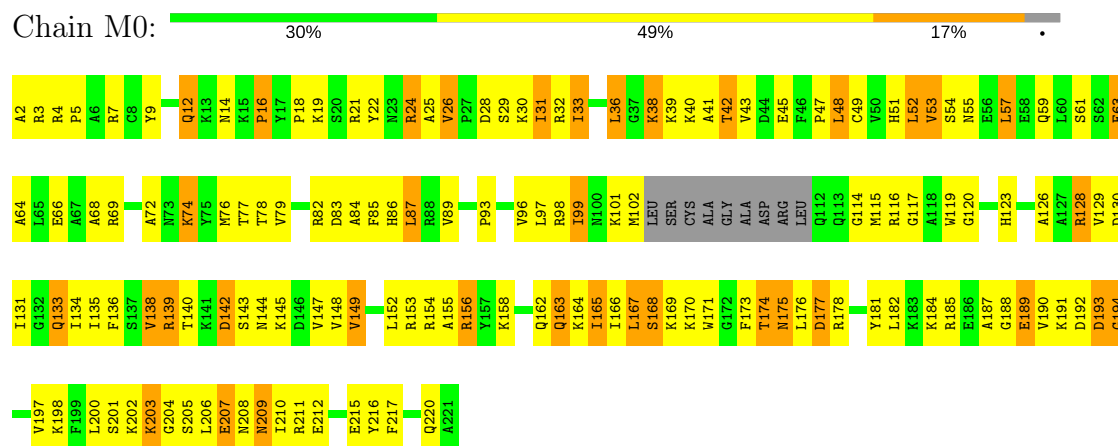
• Molecule 46: 60S ribosomal protein L9-A



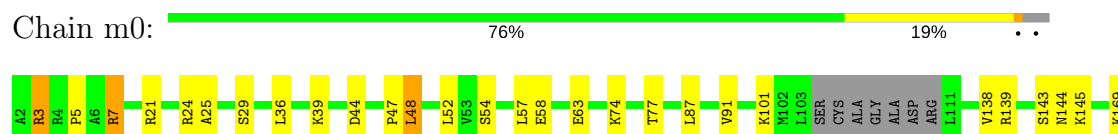
• Molecule 46: 60S ribosomal protein L9-A

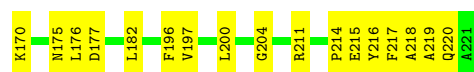


• Molecule 47: 60S ribosomal protein L10



• Molecule 47: 60S ribosomal protein L10





• Molecule 48: 60S ribosomal protein L11-B

Chain M1: 32% 46% 16% . .



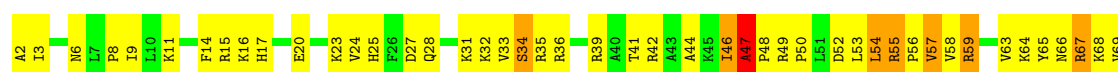
• Molecule 48: 60S ribosomal protein L11-B

Chain m1: 73% 22% . .



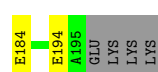
• Molecule 49: 60S ribosomal protein L13-A

Chain M3: 34% 49% 13% . .

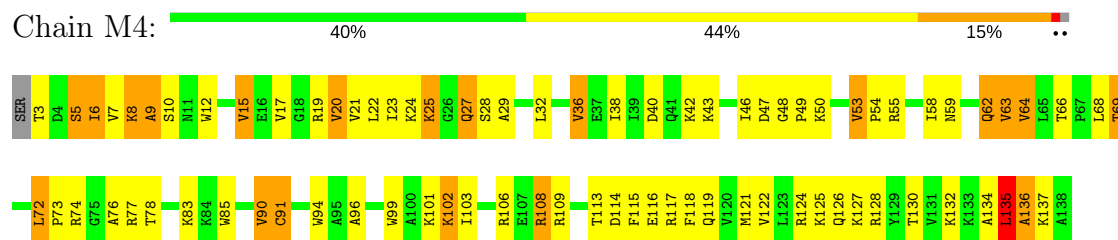


• Molecule 49: 60S ribosomal protein L13-A

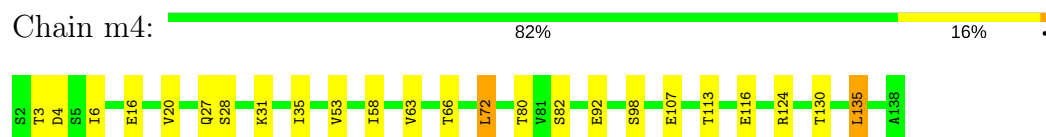
Chain m3: 80% 16% . .



• Molecule 50: 60S ribosomal protein L14-A



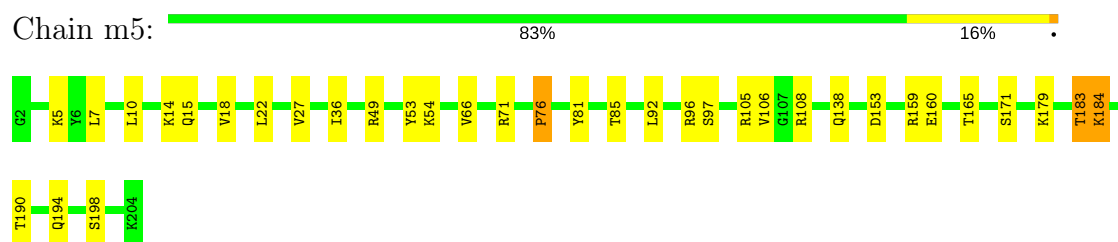
- Molecule 50: 60S ribosomal protein L14-A



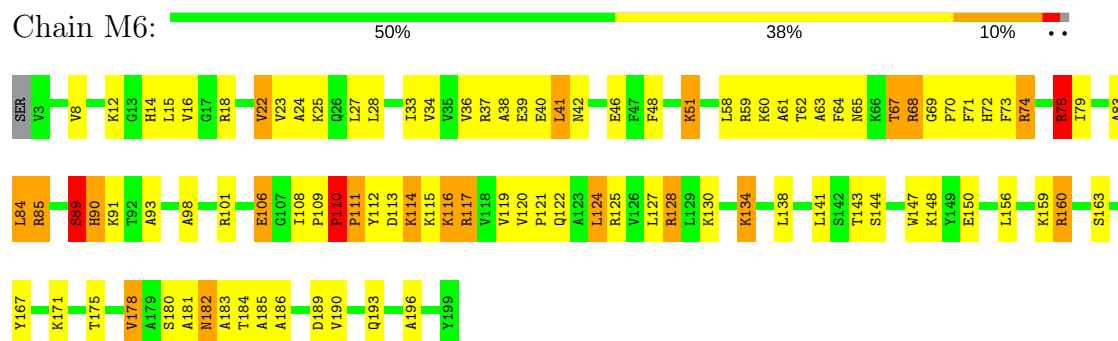
- Molecule 51: 60S ribosomal protein L15-A



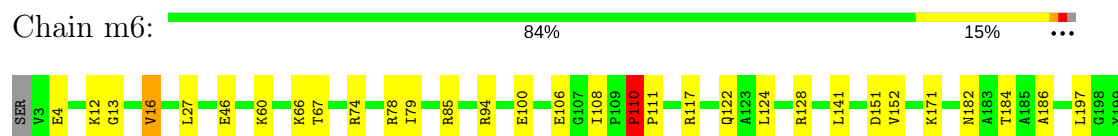
- Molecule 51: 60S ribosomal protein L15-A



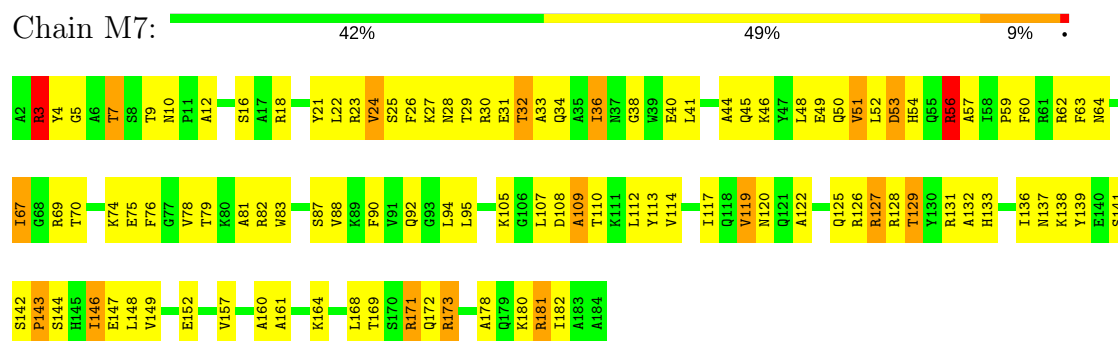
- Molecule 52: 60S ribosomal protein L16-A



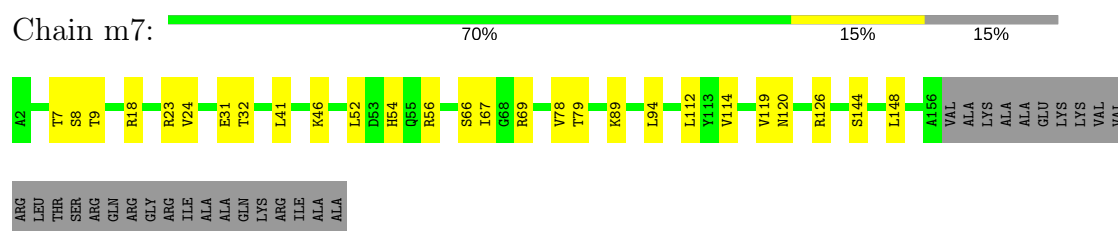
- Molecule 52: 60S ribosomal protein L16-A



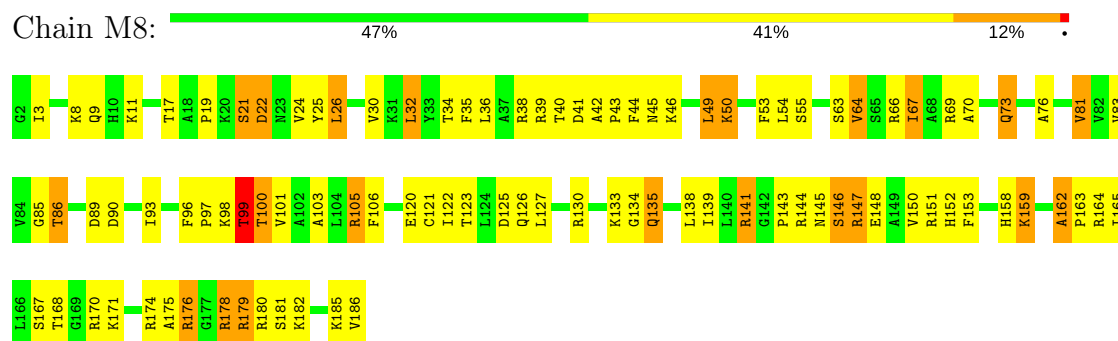
- Molecule 53: 60S ribosomal protein L17-A



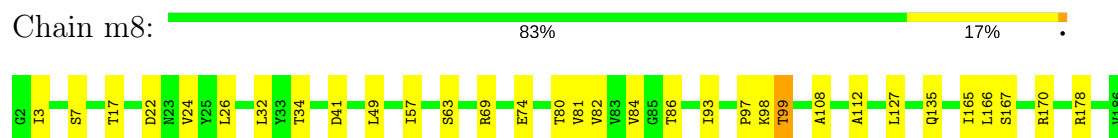
- Molecule 53: 60S ribosomal protein L17-A



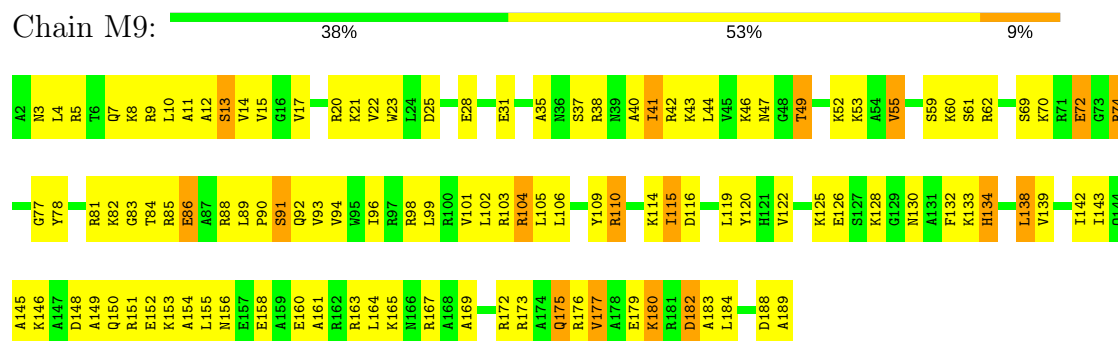
- Molecule 54: 60S ribosomal protein L18-A



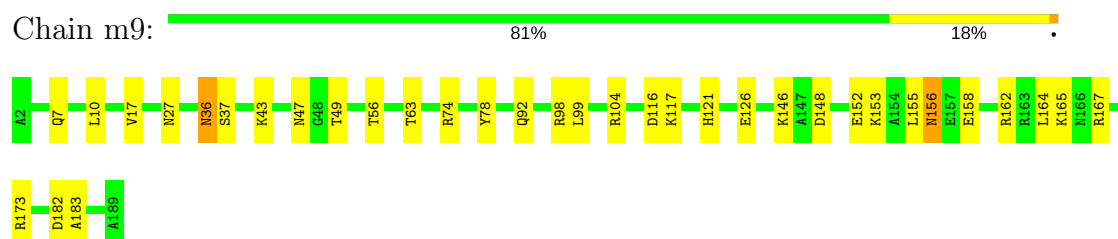
- Molecule 54: 60S ribosomal protein L18-A



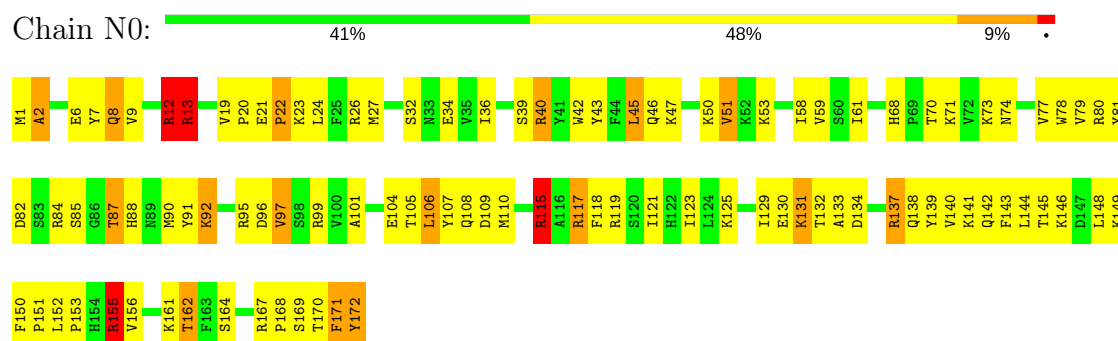
- Molecule 55: 60S ribosomal protein L19-A



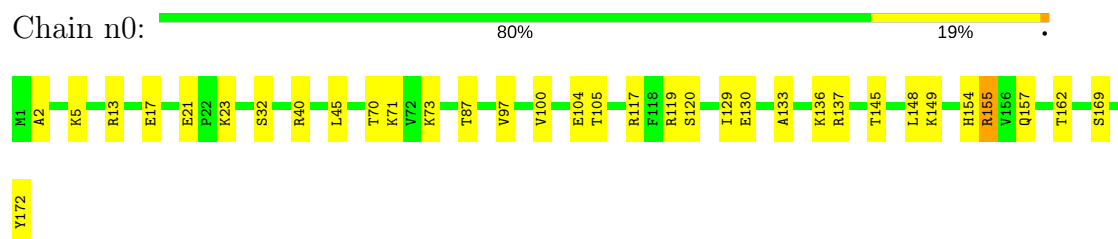
• Molecule 55: 60S ribosomal protein L19-A



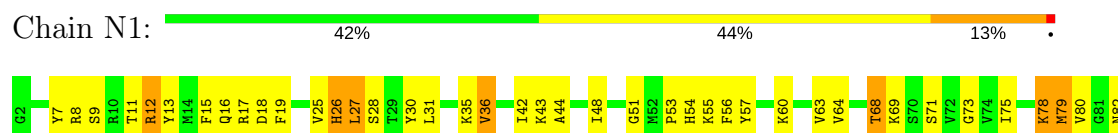
• Molecule 56: 60S ribosomal protein L20-A

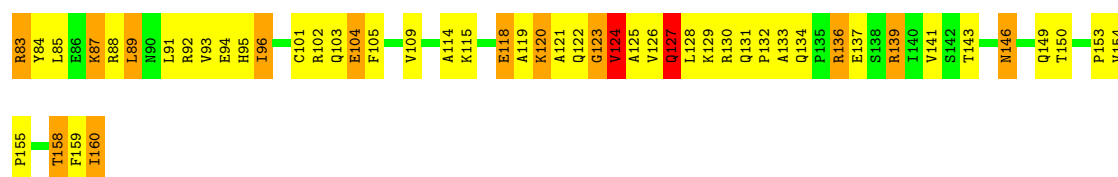


• Molecule 56: 60S ribosomal protein L20-A



• Molecule 57: 60S ribosomal protein L21-A





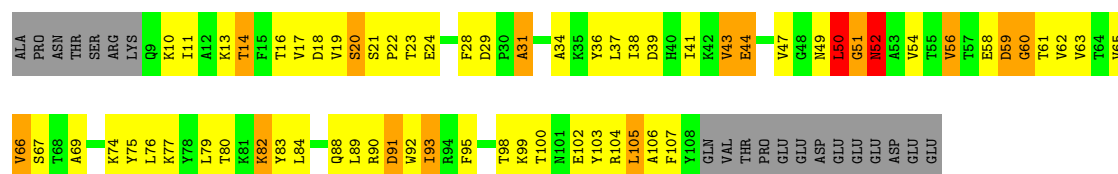
- Molecule 57: 60S ribosomal protein L21-A

Chain n1: 79% 21%



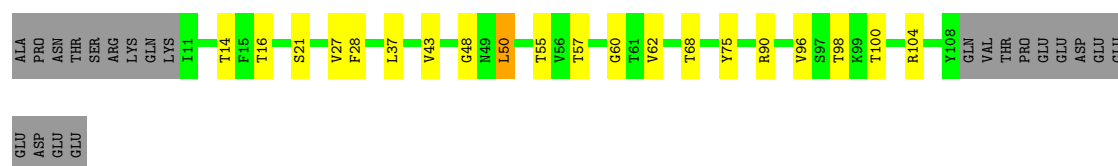
- Molecule 58: 60S ribosomal protein L22-A

Chain N2: 28% 42% 12% 17%



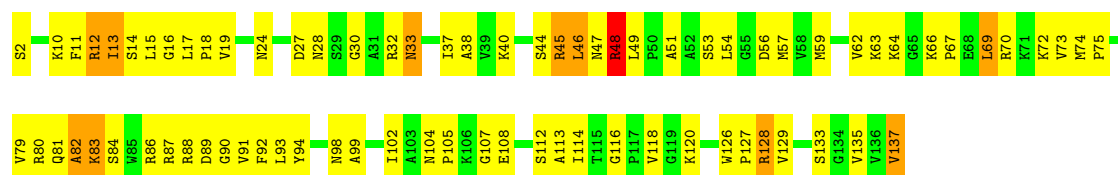
- Molecule 58: 60S ribosomal protein L22-A

Chain n2: 65% 16% 18%



- Molecule 59: 60S ribosomal protein L23-A

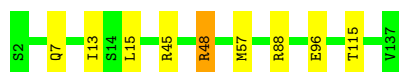
Chain N3: 43% 49% 7%



- Molecule 59: 60S ribosomal protein L23-A

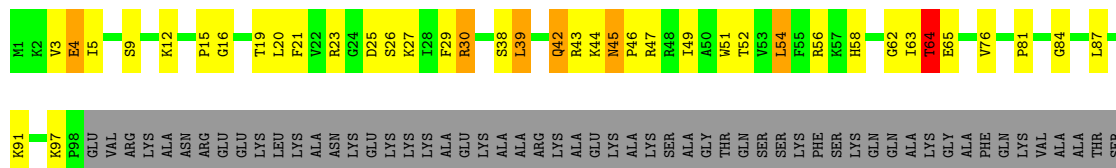
Chain n3: 93% 6%





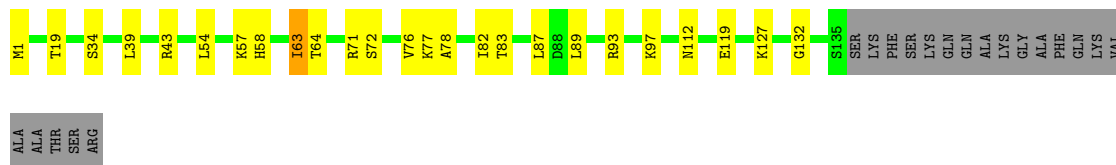
- Molecule 60: 60S ribosomal protein L24-A

Chain N4: 37% 21% 37%



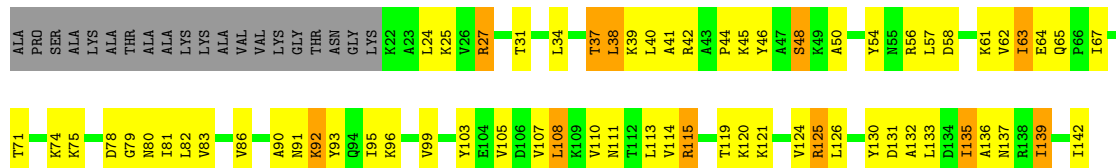
- Molecule 60: 60S ribosomal protein L24-A

Chain n4: 71% 15% 13%



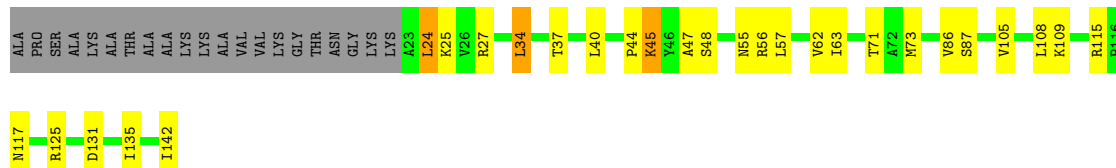
- Molecule 61: 60S ribosomal protein L25

Chain N5: 38% 40% 8% 14%



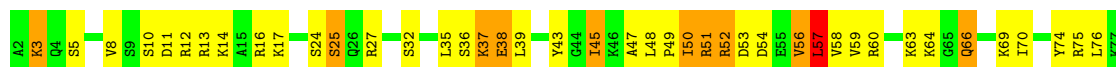
- Molecule 61: 60S ribosomal protein L25

Chain n5: 65% 18% 15%



- Molecule 62: 60S ribosomal protein L26-A

Chain N6: 41% 44% 13%





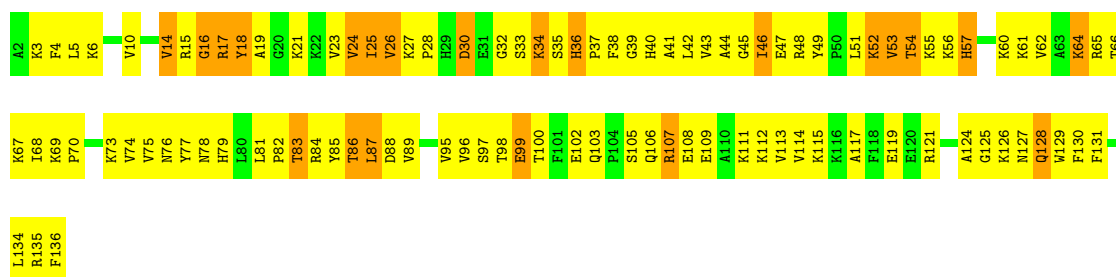
• Molecule 62: 60S ribosomal protein L26-A

Chain n6: 71% 28%



• Molecule 63: 60S ribosomal protein L27-A

Chain N7: 24% 59% 16%



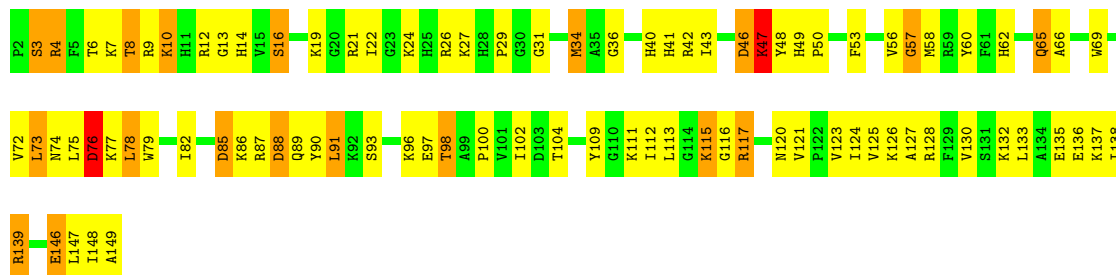
• Molecule 63: 60S ribosomal protein L27-A

Chain n7: 76% 21%



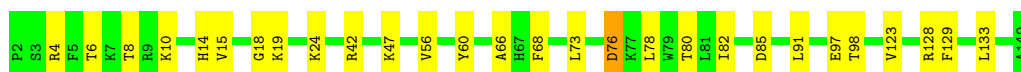
• Molecule 64: 60S ribosomal protein L28

Chain N8: 40% 46% 13%



• Molecule 64: 60S ribosomal protein L28

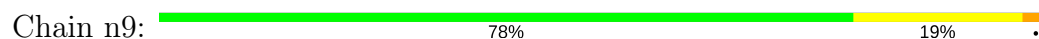
Chain n8: 81% 18%



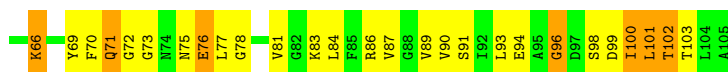
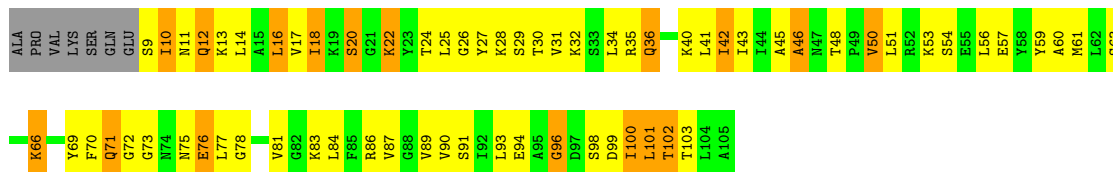
- Molecule 65: 60S ribosomal protein L29



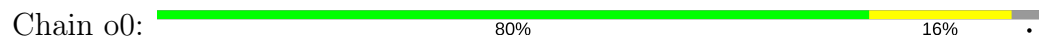
- Molecule 65: 60S ribosomal protein L29



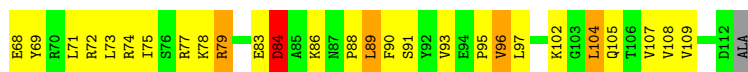
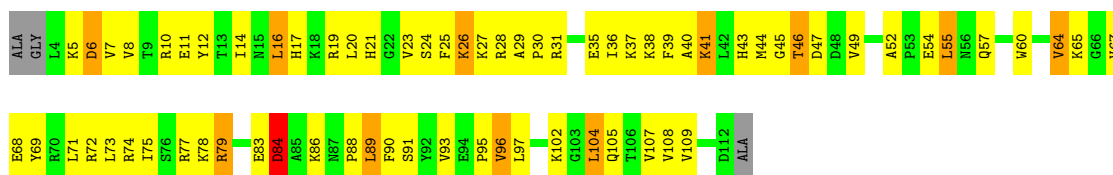
- Molecule 66: 60S ribosomal protein L30



- Molecule 66: 60S ribosomal protein L30



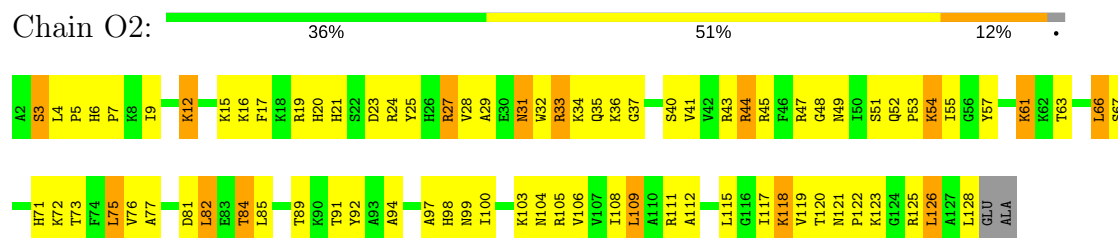
- Molecule 67: 60S ribosomal protein L31-A



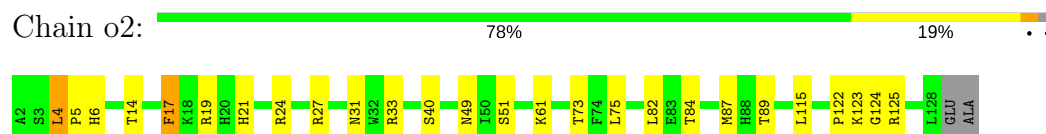
- Molecule 67: 60S ribosomal protein L31-A



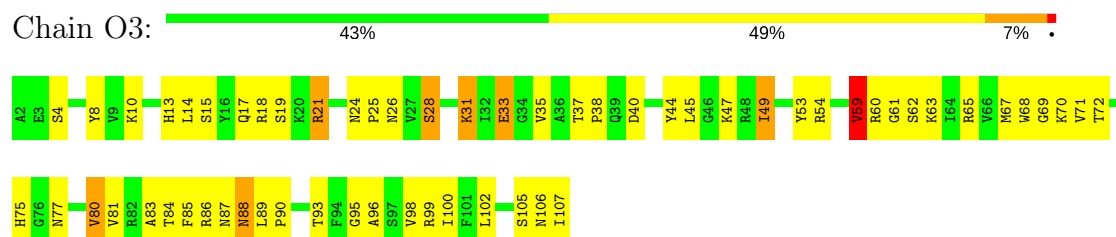
- Molecule 68: 60S ribosomal protein L32



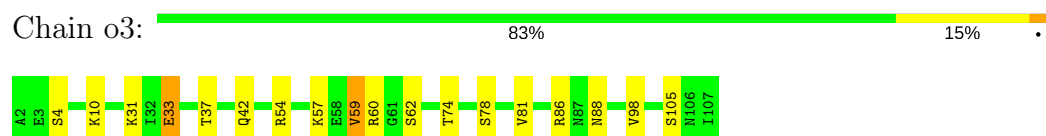
- Molecule 68: 60S ribosomal protein L32



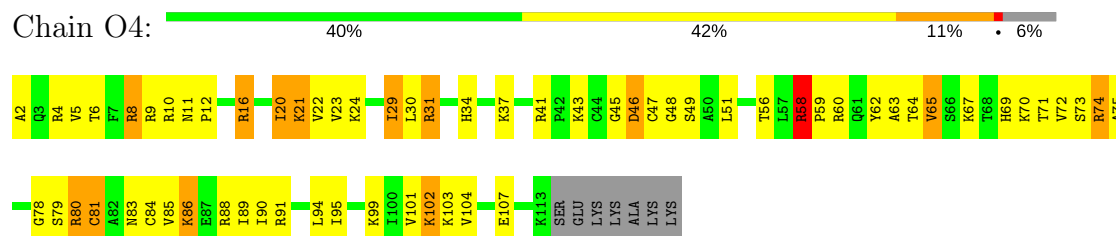
- Molecule 69: 60S ribosomal protein L33-A



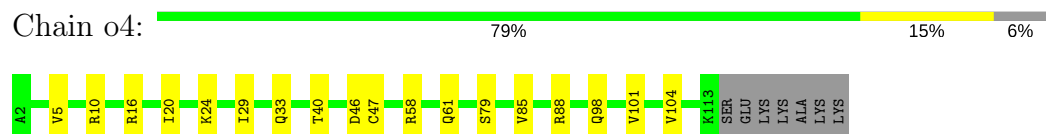
- Molecule 69: 60S ribosomal protein L33-A



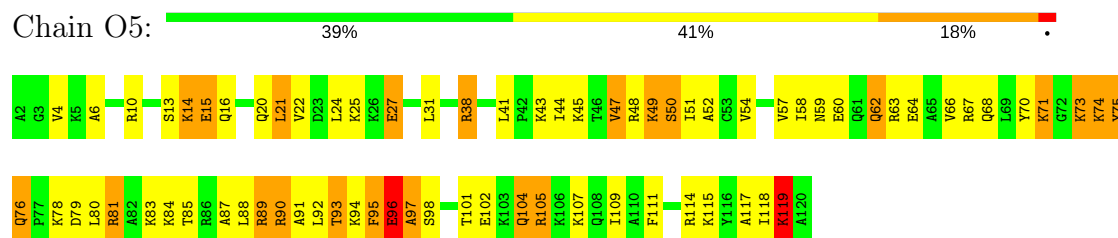
- Molecule 70: 60S ribosomal protein L34-A



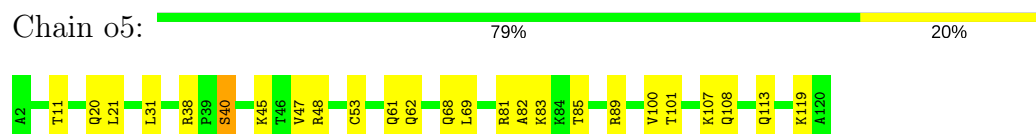
- Molecule 70: 60S ribosomal protein L34-A



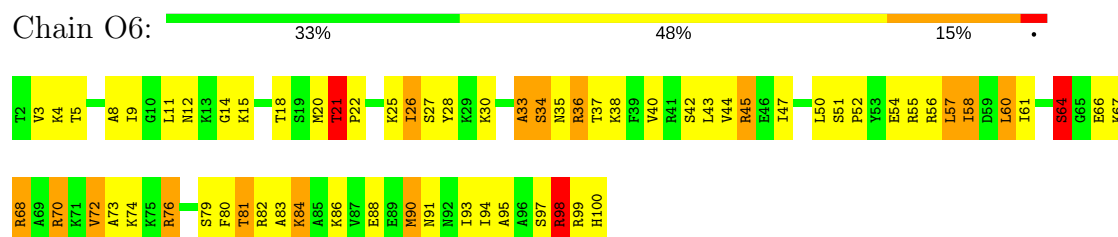
- Molecule 71: 60S ribosomal protein L35-A



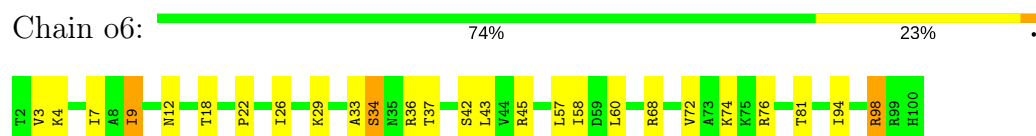
- Molecule 71: 60S ribosomal protein L35-A



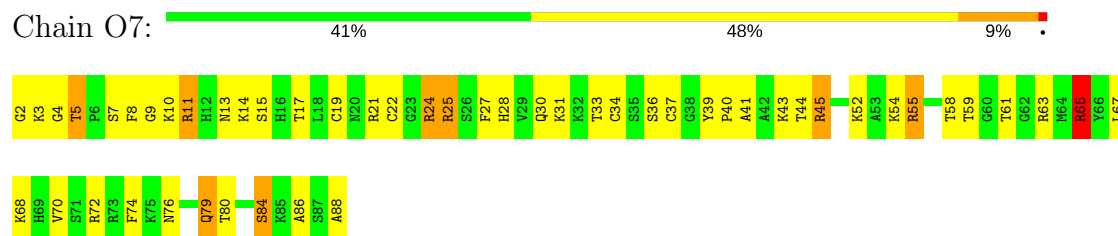
- Molecule 72: 60S ribosomal protein L36-A



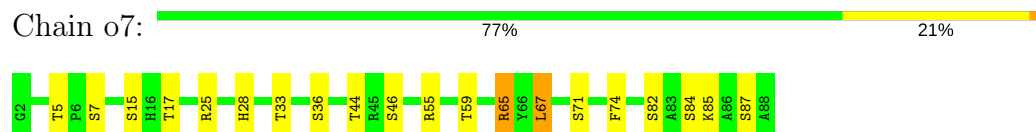
- Molecule 72: 60S ribosomal protein L36-A



- Molecule 73: 60S ribosomal protein L37-A

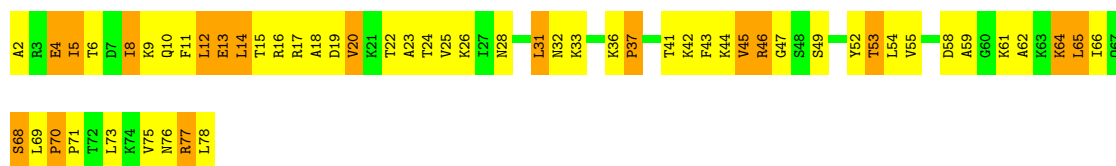


- Molecule 73: 60S ribosomal protein L37-A




- Molecule 74: 60S ribosomal protein L38

Chain O8:  27% 51% 22%



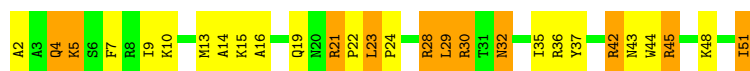
- Molecule 74: 60S ribosomal protein L38

Chain o8:  81% 19%




- Molecule 75: 60S ribosomal protein L39

Chain O9:  44% 34% 22%



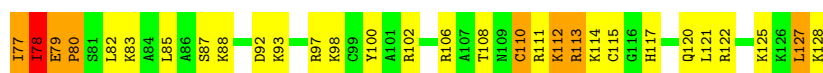
- Molecule 75: 60S ribosomal protein L39

Chain o9:  84% 16%



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:  42% 42% 13% 3%



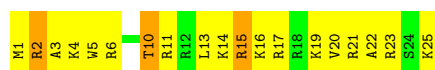
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:  75% 25%



- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:  24% 64% 12%



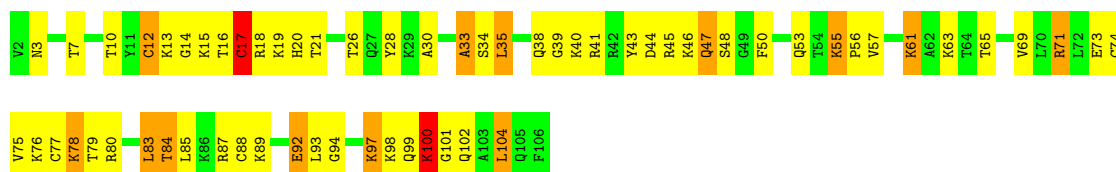
- Molecule 77: 60S ribosomal protein L41-A

Chain q1:  72% 28%




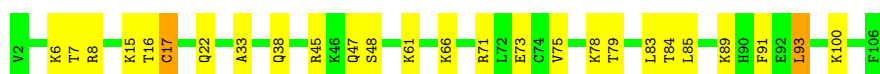
- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:  40% 46% 12%



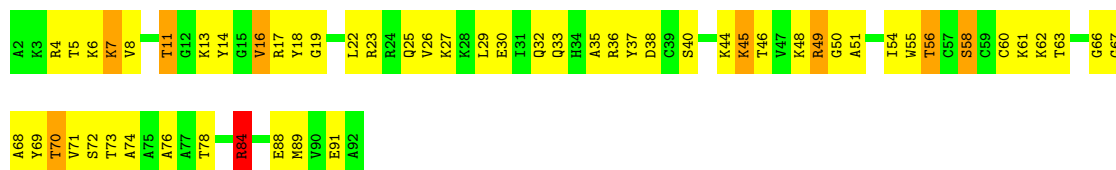
- Molecule 78: 60S ribosomal protein L42-A

Chain q2:  75% 23%




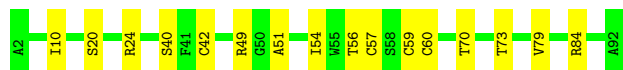
- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:  38% 52% 9%



- Molecule 79: 60S ribosomal protein L43-A

Chain q3:  82% 18%



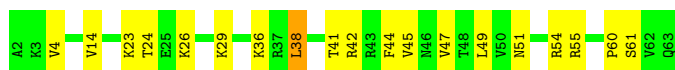
- Molecule 80: 40S ribosomal protein S10-A

Chain c0:  68% 21% 9%



- Molecule 81: 40S ribosomal protein S30-A

Chain e0:  69% 29%



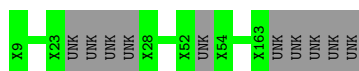
- Molecule 82: Ubiquitin-40S ribosomal protein S31

Chain e1: 55% 36% 8%



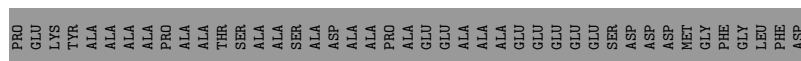
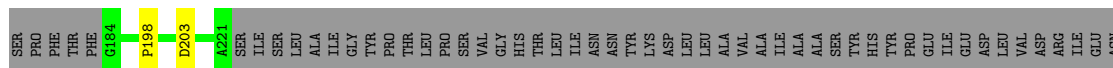
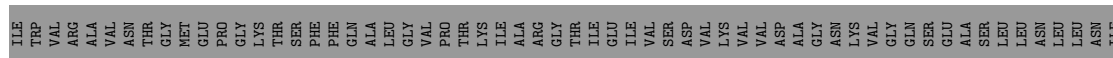
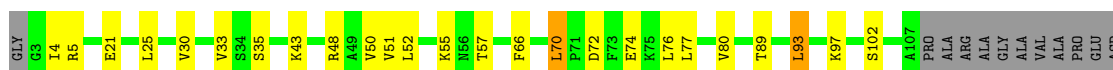
- Molecule 83: UNKNOWN PROTEIN m2

Chain m2: 94% 6%



- Molecule 84: 60S acidic ribosomal protein P0

Chain p0: 37% 8% 54%



- Molecule 85: UNKNOWN PROTEIN p1

Chain p1: 100%

There are no outlier residues recorded for this chain.

- Molecule 86: 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, $\alpha$ , $\beta$ , $\gamma$	436.02Å 287.59Å 304.52Å 90.00° 99.02° 90.00°	Depositor
Resolution (Å)	49.82 – 3.20	Depositor
% Data completeness (in resolution range)	100.0 (49.82-3.20)	Depositor
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.181 , 0.237	Depositor
Wilson B-factor (Å <sup>2</sup> )	70.5	Xtriage
Anisotropy	0.157	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411288	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 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	0.68	1/41698 (0.0%)	1.28	292/64972 (0.4%)
1	6	0.81	13/42765 (0.0%)	1.38	456/66634 (0.7%)
2	S0	0.43	0/1617	0.67	0/2215
2	s0	0.49	0/1623	0.72	0/2222
3	S1	0.37	0/1735	0.69	2/2335 (0.1%)
3	s1	0.51	0/1748	0.70	1/2352 (0.0%)
4	S2	0.45	0/1665	0.65	0/2263
4	s2	0.54	0/1665	0.72	1/2263 (0.0%)
5	S3	0.45	0/1759	0.68	2/2368 (0.1%)
5	s3	0.45	0/1759	0.60	0/2368
6	S4	0.47	0/2109	0.71	0/2839
6	s4	0.52	0/2109	0.75	2/2839 (0.1%)
7	S5	0.38	0/1629	0.60	0/2202
7	s5	0.46	0/1629	0.71	1/2202 (0.0%)
8	S6	0.45	0/1823	0.63	1/2439 (0.0%)
8	s6	0.51	0/1779	0.68	0/2379
9	S7	0.42	0/1506	0.63	0/2028
9	s7	0.44	0/1516	0.70	1/2043 (0.0%)
10	S8	0.51	0/1514	0.76	1/2021 (0.0%)
10	s8	0.59	0/1514	0.77	1/2021 (0.0%)
11	S9	0.43	0/1519	0.65	0/2035
11	s9	0.53	0/1519	0.75	1/2035 (0.0%)
12	C0	0.43	0/790	0.66	1/1069 (0.1%)
13	C1	0.55	0/1240	0.69	0/1675
13	c1	0.60	0/1194	0.80	2/1610 (0.1%)
14	C2	0.35	0/900	0.65	1/1224 (0.1%)
14	c2	0.32	0/900	0.60	1/1224 (0.1%)
15	C3	0.47	0/1215	0.69	3/1638 (0.2%)
15	c3	0.54	0/1215	0.75	1/1638 (0.1%)
16	C4	0.37	0/901	0.64	0/1217
16	c4	0.52	0/960	0.73	0/1290
17	C5	0.44	0/998	0.66	0/1341

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	c5	0.47	0/1060	0.66	0/1426
18	C6	0.43	0/1125	0.69	2/1510 (0.1%)
18	c6	0.48	0/1131	0.71	1/1518 (0.1%)
19	C7	0.40	0/935	0.66	0/1254
19	c7	0.48	0/914	0.72	0/1224
20	C8	0.43	0/1211	0.66	1/1628 (0.1%)
20	c8	0.50	0/1211	0.70	2/1628 (0.1%)
21	C9	0.44	0/1130	0.67	1/1517 (0.1%)
21	c9	0.49	0/1130	0.72	2/1517 (0.1%)
22	D0	0.45	0/865	0.66	0/1169
22	d0	0.49	0/892	0.70	0/1205
23	D1	0.39	0/693	0.59	0/935
23	d1	0.49	0/693	0.70	0/935
24	D2	0.46	0/1038	0.75	2/1395 (0.1%)
24	d2	0.64	0/1038	0.78	1/1395 (0.1%)
25	D3	0.58	0/1139	0.74	0/1518
25	d3	0.64	0/1139	0.82	2/1518 (0.1%)
26	D4	0.41	0/1087	0.59	0/1449
26	d4	0.51	0/1087	0.69	0/1449
27	D5	0.39	0/571	0.77	2/768 (0.3%)
27	d5	0.42	0/566	0.69	0/761
28	D6	0.40	0/782	0.60	0/1047
28	d6	0.53	0/782	0.69	0/1047
29	D7	0.42	0/620	0.68	0/838
29	d7	0.44	0/620	0.68	0/838
30	D8	0.34	0/499	0.62	0/670
30	d8	0.38	0/499	0.64	0/670
31	D9	0.50	0/452	0.74	1/600 (0.2%)
31	d9	0.56	0/452	0.71	0/600
32	E0	0.40	0/483	0.64	0/643
33	E1	0.41	0/577	0.78	0/770
34	SR	0.39	0/2494	0.63	0/3393
34	sR	0.39	0/2495	0.60	0/3395
35	SM	0.45	0/1113	0.68	2/1502 (0.1%)
35	sM	0.41	0/683	0.63	1/923 (0.1%)
36	1	1.01	59/75394 (0.1%)	1.57	1453/117545 (1.2%)
36	5	1.05	74/75414 (0.1%)	1.58	1442/117575 (1.2%)
37	3	0.87	0/2883	1.32	14/4491 (0.3%)
37	7	1.02	1/2883 (0.0%)	1.60	54/4491 (1.2%)
38	4	0.95	1/3746 (0.0%)	1.51	47/5832 (0.8%)
38	8	0.89	0/3746	1.43	43/5832 (0.7%)
39	L2	0.65	0/1948	0.81	2/2617 (0.1%)
39	l2	0.64	0/1946	0.83	0/2614

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
40	L3	0.62	0/3146	0.77	0/4228
40	l3	0.76	0/3146	0.84	3/4228 (0.1%)
41	L4	0.70	1/2800 (0.0%)	0.88	3/3790 (0.1%)
41	l4	0.68	1/2800 (0.0%)	0.85	3/3790 (0.1%)
42	L5	0.51	0/2425	0.67	0/3271
42	l5	0.65	0/2408	0.76	0/3248
43	L6	0.65	0/1260	0.79	0/1694
43	l6	0.66	0/1269	0.76	1/1705 (0.1%)
44	L7	0.68	0/1821	0.85	2/2451 (0.1%)
44	l7	0.74	0/1828	0.80	2/2461 (0.1%)
45	L8	0.51	0/1836	0.69	0/2481
45	l8	0.52	0/1795	0.67	0/2429
46	L9	0.60	0/1539	0.71	0/2073
46	l9	0.70	0/1539	0.80	0/2073
47	M0	0.64	0/1741	0.76	2/2335 (0.1%)
47	m0	0.67	0/1758	0.80	3/2358 (0.1%)
48	M1	0.49	0/1374	0.71	1/1842 (0.1%)
48	m1	0.59	0/1374	0.81	2/1842 (0.1%)
49	M3	0.68	0/1568	0.80	1/2106 (0.0%)
49	m3	0.61	0/1573	0.78	0/2113
50	M4	0.61	0/1068	0.74	0/1438
50	m4	0.68	0/1074	0.80	1/1446 (0.1%)
51	M5	0.65	0/1757	0.79	1/2354 (0.0%)
51	m5	0.64	0/1757	0.77	0/2354
52	M6	0.70	0/1585	0.86	3/2128 (0.1%)
52	m6	0.84	0/1585	0.92	3/2128 (0.1%)
53	M7	0.67	0/1443	0.80	1/1944 (0.1%)
53	m7	0.78	0/1250	0.81	0/1683
54	M8	0.67	0/1465	0.85	2/1965 (0.1%)
54	m8	0.66	0/1465	0.86	2/1965 (0.1%)
55	M9	0.51	0/1538	0.66	0/2050
55	m9	0.57	0/1538	0.65	0/2050
56	N0	0.64	0/1481	0.82	3/1990 (0.2%)
56	n0	0.73	0/1481	0.83	2/1990 (0.1%)
57	N1	0.68	0/1300	0.79	0/1743
57	n1	0.74	0/1300	0.79	0/1743
58	N2	0.44	0/812	0.63	0/1099
58	n2	0.46	0/794	0.62	0/1076
59	N3	0.62	0/1018	0.78	1/1369 (0.1%)
59	n3	0.69	0/1018	0.83	1/1369 (0.1%)
60	N4	0.50	0/712	0.64	0/958
60	n4	0.61	0/1052	0.70	0/1398
61	N5	0.53	0/979	0.74	1/1321 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
61	n5	0.58	0/974	0.74	1/1314 (0.1%)
62	N6	0.63	0/1004	0.82	1/1341 (0.1%)
62	n6	0.57	0/1004	0.78	1/1341 (0.1%)
63	N7	0.49	0/1118	0.66	0/1497
63	n7	0.47	0/1118	0.67	0/1497
64	N8	0.72	0/1204	0.86	1/1612 (0.1%)
64	n8	0.69	0/1204	0.82	0/1612
65	N9	0.60	0/473	0.78	0/629
65	n9	0.63	0/473	0.89	1/629 (0.2%)
66	O0	0.47	0/751	0.64	0/1008
66	o0	0.49	0/775	0.69	0/1040
67	O1	0.60	0/890	0.74	0/1196
67	o1	0.66	0/897	0.81	0/1205
68	O2	0.79	0/1041	0.87	0/1394
68	o2	0.74	0/1041	0.87	2/1394 (0.1%)
69	O3	0.79	0/868	0.85	0/1168
69	o3	0.79	0/868	0.83	0/1168
70	O4	0.59	0/890	0.79	2/1189 (0.2%)
70	o4	0.57	0/890	0.81	0/1189
71	O5	0.62	0/978	0.77	0/1301
71	o5	0.53	0/974	0.67	0/1297
72	O6	0.57	0/778	0.74	0/1034
72	o6	0.55	0/777	0.70	0/1033
73	O7	0.67	0/696	0.94	4/923 (0.4%)
73	o7	0.64	0/696	0.81	1/923 (0.1%)
74	O8	0.48	0/618	0.64	1/826 (0.1%)
74	o8	0.45	0/614	0.64	0/822
75	O9	0.64	0/443	0.83	0/588
75	o9	0.63	0/443	0.76	0/588
76	Q0	0.64	0/423	0.73	0/562
76	q0	0.81	1/423 (0.2%)	0.85	0/562
77	Q1	0.66	0/234	0.84	0/300
77	q1	0.65	0/234	0.98	2/300 (0.7%)
78	Q2	0.74	1/860 (0.1%)	0.83	0/1136
78	q2	0.69	0/860	0.79	1/1136 (0.1%)
79	Q3	0.67	0/701	0.77	0/934
79	q3	0.65	0/701	0.80	0/934
80	c0	0.40	0/777	0.66	3/1049 (0.3%)
81	e0	0.49	0/499	0.72	0/665
82	e1	0.38	0/619	0.74	1/822 (0.1%)
84	p0	0.44	0/1092	0.63	1/1474 (0.1%)
All	All	0.80	153/430074 (0.0%)	1.26	3913/631364 (0.6%)

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
3	s1	0	1
7	s5	0	2
9	S7	0	1
9	s7	0	1
10	s8	0	1
13	C1	0	1
15	c3	0	1
16	C4	0	1
17	c5	0	1
18	C6	0	1
18	c6	0	1
19	C7	0	2
19	c7	0	3
22	d0	0	1
25	D3	0	1
26	d4	0	2
27	D5	0	3
27	d5	0	1
33	E1	0	1
39	L2	0	1
39	l2	0	2
42	l5	0	2
43	l6	0	1
44	l7	0	2
45	L8	0	2
48	M1	0	2
51	m5	0	1
52	M6	0	1
52	m6	0	1
56	N0	0	2
56	n0	0	1
57	N1	0	1
60	n4	0	1
63	n7	0	1
64	n8	0	2
65	N9	0	1
65	n9	0	1
82	e1	0	1
All	All	0	52

The worst 5 of 153 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1152	G	N9-C4	-11.64	1.28	1.38
36	5	3008	A	N9-C4	-8.98	1.32	1.37
36	5	2358	A	N9-C4	-8.04	1.33	1.37
36	1	1114	U	C2-N3	-7.72	1.32	1.37
36	1	2714	G	N9-C4	-7.69	1.31	1.38

The worst 5 of 3913 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-21.84	112.90	126.00
36	5	1152	G	N3-C4-C5	21.63	139.41	128.60
36	5	1152	G	C2-N3-C4	-18.18	102.81	111.90
36	1	2714	G	N3-C4-C5	17.75	137.47	128.60
36	1	1308	A	O5'-P-OP2	-16.96	90.35	110.70

There are no chirality outliers.

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	C1	127	GLN	Peptide
16	C4	124	ASP	Peptide
18	C6	40	GLU	Peptide
19	C7	22	PRO	Peptide
9	S7	131	PHE	Peptide

## 5.2 Too-close contacts [i](#)

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	18758	895	0
1	6	38238	0	19240	845	0
2	S0	1577	0	1567	166	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	187	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	110	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	184	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	153	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	138	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	126	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	131	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	148	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	74	0
13	C1	1214	0	1259	101	0
13	c1	1168	0	1231	0	0
14	C2	892	0	891	65	0
14	c2	892	0	891	0	0
15	C3	1192	0	1255	95	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	94	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	89	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	117	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	94	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	109	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	96	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	88	0
22	d0	882	0	939	0	0
23	D1	684	0	672	78	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	88	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	86	0
25	d3	1121	0	1196	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	D4	1073	0	1132	94	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	70	0
27	d5	558	0	598	0	0
28	D6	769	0	814	99	0
28	d6	769	0	815	0	0
29	D7	610	0	630	51	0
29	d7	610	0	631	0	0
30	D8	497	0	535	47	0
30	d8	497	0	535	0	0
31	D9	442	0	428	32	0
31	d9	442	0	428	0	0
32	E0	475	0	525	37	0
33	E1	566	0	602	58	0
34	SR	2441	0	2397	183	0
34	sR	2442	0	2392	0	0
35	SM	1104	0	996	74	0
35	sM	680	0	607	0	0
36	1	67355	0	33846	1234	0
36	5	67376	0	33861	1200	0
37	3	2579	0	1304	46	0
37	7	2579	0	1304	51	0
38	4	3353	0	1695	60	0
38	8	3353	0	1695	72	0
39	L2	1914	0	1981	157	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	260	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	204	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	182	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	86	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	131	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	126	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	131	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1736	158	0
47	m0	1722	0	1755	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	M1	1353	0	1383	103	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	134	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	89	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	125	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	103	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	100	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	102	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1616	110	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	107	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	105	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	51	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	70	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	25	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	60	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	80	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	103	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	94	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	31	0
65	n9	462	0	491	0	0
66	O0	743	0	797	61	0
66	o0	767	0	816	0	0
67	O1	876	0	912	57	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	88	0
68	o2	1020	0	1090	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	O3	850	0	880	47	0
69	o3	850	0	880	0	0
70	O4	880	0	945	69	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	81	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	66	0
72	o6	770	0	846	0	0
73	O7	681	0	683	47	0
73	o7	681	0	683	0	0
74	O8	612	0	682	49	0
74	o8	608	0	671	0	0
75	O9	436	0	475	32	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	22	0
76	q0	417	0	456	0	0
77	Q1	233	0	284	26	0
77	q1	233	0	284	0	0
78	Q2	847	0	915	56	0
78	q2	847	0	915	0	0
79	Q3	694	0	734	57	0
79	q3	694	0	734	0	0
80	c0	762	0	699	0	0
81	e0	491	0	542	0	0
82	e1	608	0	654	0	0
83	m2	750	0	178	0	0
84	p0	1077	0	1041	0	0
85	p1	235	0	50	0	0
86	p2	230	0	52	0	0
87	1	477	0	0	0	0
87	2	124	0	0	0	0
87	3	14	0	0	0	0
87	4	19	0	0	0	0
87	5	502	0	0	0	0
87	6	144	0	0	0	0
87	7	15	0	0	0	0
87	8	16	0	0	0	0
87	D3	1	0	0	0	0
87	L2	1	0	0	0	0
87	L3	3	0	0	0	0
87	L4	1	0	0	0	0
87	L5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	L7	4	0	0	0	0
87	L8	1	0	0	0	0
87	M0	2	0	0	0	0
87	M1	1	0	0	0	0
87	M3	2	0	0	0	0
87	M5	2	0	0	0	0
87	M6	1	0	0	0	0
87	M7	4	0	0	0	0
87	M9	1	0	0	0	0
87	N0	1	0	0	0	0
87	N3	3	0	0	0	0
87	N5	1	0	0	0	0
87	N8	5	0	0	0	0
87	O2	1	0	0	0	0
87	O4	1	0	0	0	0
87	O5	1	0	0	0	0
87	O7	1	0	0	0	0
87	S4	2	0	0	0	0
87	S8	1	0	0	0	0
87	SM	1	0	0	0	0
87	c1	1	0	0	0	0
87	c7	2	0	0	0	0
87	c8	1	0	0	0	0
87	c9	1	0	0	0	0
87	d3	1	0	0	0	0
87	d4	1	0	0	0	0
87	d6	1	0	0	0	0
87	l2	1	0	0	0	0
87	l3	3	0	0	0	0
87	l4	2	0	0	0	0
87	l5	2	0	0	0	0
87	l7	1	0	0	0	0
87	m1	2	0	0	0	0
87	m5	5	0	0	0	0
87	m6	2	0	0	0	0
87	m7	5	0	0	0	0
87	n0	3	0	0	0	0
87	n3	2	0	0	0	0
87	n6	2	0	0	0	0
87	n8	3	0	0	0	0
87	o1	1	0	0	0	0
87	o3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	o4	1	0	0	0	0
87	q0	1	0	0	0	0
87	q1	1	0	0	0	0
87	q3	2	0	0	0	0
87	s1	1	0	0	0	0
87	s6	1	0	0	0	0
87	s8	3	0	0	0	0
87	sM	1	0	0	0	0
88	1	2478	0	0	145	0
88	2	1106	0	0	73	0
88	3	77	0	0	1	0
88	4	98	0	0	6	0
88	5	2506	0	0	157	0
88	6	1113	0	0	73	0
88	7	84	0	0	5	0
88	8	98	0	0	11	0
88	C3	7	0	0	1	0
88	C5	7	0	0	5	0
88	C8	7	0	0	0	0
88	D3	7	0	0	0	0
88	D9	7	0	0	0	0
88	L3	21	0	0	2	0
88	L4	7	0	0	3	0
88	M0	7	0	0	0	0
88	M5	7	0	0	1	0
88	M7	14	0	0	1	0
88	M8	7	0	0	0	0
88	M9	7	0	0	0	0
88	N9	7	0	0	0	0
88	O3	7	0	0	0	0
88	O7	14	0	0	2	0
88	S8	7	0	0	1	0
88	SR	7	0	0	0	0
88	c1	7	0	0	0	0
88	c3	7	0	0	0	0
88	c5	7	0	0	0	0
88	c8	7	0	0	0	0
88	d4	7	0	0	0	0
88	d9	7	0	0	0	0
88	l3	21	0	0	0	0
88	l4	14	0	0	0	0
88	l5	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	l9	7	0	0	0	0
88	m0	14	0	0	0	0
88	m1	7	0	0	0	0
88	m4	7	0	0	0	0
88	m5	7	0	0	0	0
88	m6	7	0	0	0	0
88	n3	14	0	0	0	0
88	n9	7	0	0	0	0
88	o3	7	0	0	0	0
88	o7	7	0	0	0	0
88	q2	7	0	0	0	0
88	s1	14	0	0	0	0
88	s8	7	0	0	0	0
88	sR	7	0	0	0	0
89	D6	1	0	0	0	0
89	D7	1	0	0	0	0
89	D9	1	0	0	0	0
89	E1	1	0	0	0	0
89	O7	1	0	0	0	0
89	Q0	1	0	0	0	0
89	Q2	1	0	0	0	0
89	Q3	1	0	0	0	0
89	d6	1	0	0	0	0
89	d7	1	0	0	0	0
89	d9	1	0	0	0	0
89	e1	1	0	0	0	0
89	o7	1	0	0	0	0
89	q0	1	0	0	0	0
89	q2	1	0	0	0	0
89	q3	1	0	0	0	0
90	1	22	0	12	0	0
90	5	22	0	12	0	0
91	Q2	40	0	22	3	0
91	q2	40	0	22	0	0
All	All	411288	0	297360	10031	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 15.

The worst 5 of 10031 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)
40:L3:41:VAL:HA	40:L3:185:GLY:HA3	1.56	1.11
40:L3:296:THR:HG22	40:L3:298:PHE:H	2.66	1.06
1:6:1636:C:H4'	1:6:1637:C:H5'	1.34	1.05
28:D6:26:CYS:SG	28:D6:77:CYS:SG	3.43	1.01
36:5:3274:A:H3'	36:5:3275:U:H5''	1.42	1.01

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%)	143 (70%)	34 (17%)	27 (13%)	0	1
2	s0	204/251 (81%)	152 (74%)	33 (16%)	19 (9%)	1	4
3	S1	212/254 (84%)	141 (66%)	38 (18%)	33 (16%)	0	1
3	s1	214/254 (84%)	171 (80%)	30 (14%)	13 (6%)	2	13
4	S2	215/253 (85%)	173 (80%)	27 (13%)	15 (7%)	1	9
4	s2	215/253 (85%)	184 (86%)	21 (10%)	10 (5%)	3	20
5	S3	221/239 (92%)	182 (82%)	24 (11%)	15 (7%)	1	10
5	s3	221/239 (92%)	174 (79%)	31 (14%)	16 (7%)	1	9
6	S4	258/260 (99%)	206 (80%)	34 (13%)	18 (7%)	1	9
6	s4	258/260 (99%)	210 (81%)	28 (11%)	20 (8%)	1	7
7	S5	204/224 (91%)	154 (76%)	34 (17%)	16 (8%)	1	7
7	s5	204/224 (91%)	154 (76%)	35 (17%)	15 (7%)	1	8
8	S6	224/236 (95%)	197 (88%)	15 (7%)	12 (5%)	2	17
8	s6	216/236 (92%)	184 (85%)	22 (10%)	10 (5%)	3	21
9	S7	182/189 (96%)	136 (75%)	25 (14%)	21 (12%)	0	2
9	s7	184/189 (97%)	141 (77%)	28 (15%)	15 (8%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	S8	184/200 (92%)	148 (80%)	23 (12%)	13 (7%)	1	9
10	s8	184/200 (92%)	155 (84%)	16 (9%)	13 (7%)	1	9
11	S9	183/196 (93%)	147 (80%)	26 (14%)	10 (6%)	2	16
11	s9	183/196 (93%)	148 (81%)	28 (15%)	7 (4%)	4	25
12	C0	94/105 (90%)	68 (72%)	17 (18%)	9 (10%)	1	4
13	C1	153/155 (99%)	114 (74%)	24 (16%)	15 (10%)	1	4
13	c1	144/155 (93%)	122 (85%)	16 (11%)	6 (4%)	3	23
14	C2	122/142 (86%)	67 (55%)	34 (28%)	21 (17%)	0	0
14	c2	122/142 (86%)	67 (55%)	32 (26%)	23 (19%)	0	0
15	C3	148/150 (99%)	122 (82%)	20 (14%)	6 (4%)	3	24
15	c3	148/150 (99%)	120 (81%)	18 (12%)	10 (7%)	1	10
16	C4	125/136 (92%)	90 (72%)	19 (15%)	16 (13%)	0	2
16	c4	126/136 (93%)	96 (76%)	19 (15%)	11 (9%)	1	5
17	C5	122/141 (86%)	88 (72%)	22 (18%)	12 (10%)	1	4
17	c5	133/141 (94%)	94 (71%)	20 (15%)	19 (14%)	0	1
18	C6	139/142 (98%)	117 (84%)	11 (8%)	11 (8%)	1	7
18	c6	140/142 (99%)	120 (86%)	12 (9%)	8 (6%)	2	16
19	C7	116/136 (85%)	87 (75%)	21 (18%)	8 (7%)	1	9
19	c7	113/136 (83%)	84 (74%)	19 (17%)	10 (9%)	1	5
20	C8	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	6
20	c8	143/145 (99%)	115 (80%)	18 (13%)	10 (7%)	1	9
21	C9	141/143 (99%)	120 (85%)	14 (10%)	7 (5%)	2	19
21	c9	141/143 (99%)	114 (81%)	21 (15%)	6 (4%)	3	23
22	D0	105/120 (88%)	82 (78%)	19 (18%)	4 (4%)	4	25
22	d0	108/120 (90%)	87 (81%)	10 (9%)	11 (10%)	1	4
23	D1	85/87 (98%)	64 (75%)	12 (14%)	9 (11%)	0	3
23	d1	85/87 (98%)	72 (85%)	10 (12%)	3 (4%)	4	28
24	D2	127/129 (98%)	112 (88%)	12 (9%)	3 (2%)	7	39
24	d2	127/129 (98%)	112 (88%)	14 (11%)	1 (1%)	22	65
25	D3	142/144 (99%)	109 (77%)	19 (13%)	14 (10%)	1	4
25	d3	142/144 (99%)	119 (84%)	18 (13%)	5 (4%)	4	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	D4	132/134 (98%)	106 (80%)	18 (14%)	8 (6%)	2	13
26	d4	132/134 (98%)	106 (80%)	16 (12%)	10 (8%)	1	8
27	D5	68/107 (64%)	44 (65%)	11 (16%)	13 (19%)	0	0
27	d5	67/107 (63%)	49 (73%)	11 (16%)	7 (10%)	0	3
28	D6	95/97 (98%)	62 (65%)	19 (20%)	14 (15%)	0	1
28	d6	95/97 (98%)	67 (70%)	18 (19%)	10 (10%)	0	3
29	D7	79/81 (98%)	63 (80%)	9 (11%)	7 (9%)	1	5
29	d7	79/81 (98%)	60 (76%)	12 (15%)	7 (9%)	1	5
30	D8	61/66 (92%)	49 (80%)	6 (10%)	6 (10%)	1	4
30	d8	61/66 (92%)	43 (70%)	13 (21%)	5 (8%)	1	6
31	D9	51/55 (93%)	41 (80%)	8 (16%)	2 (4%)	3	25
31	d9	51/55 (93%)	36 (71%)	9 (18%)	6 (12%)	0	2
32	E0	58/60 (97%)	47 (81%)	10 (17%)	1 (2%)	11	48
33	E1	69/76 (91%)	38 (55%)	12 (17%)	19 (28%)	0	0
34	SR	316/318 (99%)	244 (77%)	45 (14%)	27 (8%)	1	5
34	sR	316/318 (99%)	261 (83%)	42 (13%)	13 (4%)	3	24
35	SM	155/273 (57%)	111 (72%)	27 (17%)	17 (11%)	0	3
35	sM	98/273 (36%)	57 (58%)	28 (29%)	13 (13%)	0	1
39	L2	250/253 (99%)	224 (90%)	17 (7%)	9 (4%)	4	27
39	l2	250/253 (99%)	214 (86%)	23 (9%)	13 (5%)	2	17
40	L3	384/386 (100%)	322 (84%)	45 (12%)	17 (4%)	3	22
40	l3	384/386 (100%)	339 (88%)	32 (8%)	13 (3%)	4	28
41	L4	359/361 (99%)	297 (83%)	34 (10%)	28 (8%)	1	7
41	l4	359/361 (99%)	299 (83%)	38 (11%)	22 (6%)	2	13
42	L5	294/296 (99%)	237 (81%)	35 (12%)	22 (8%)	1	8
42	l5	292/296 (99%)	253 (87%)	32 (11%)	7 (2%)	7	39
43	L6	152/175 (87%)	134 (88%)	12 (8%)	6 (4%)	3	25
43	l6	153/175 (87%)	130 (85%)	17 (11%)	6 (4%)	3	25
44	L7	220/243 (90%)	184 (84%)	26 (12%)	10 (4%)	3	21
44	l7	221/243 (91%)	189 (86%)	27 (12%)	5 (2%)	7	40
45	L8	231/255 (91%)	189 (82%)	31 (13%)	11 (5%)	2	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	l8	229/255 (90%)	188 (82%)	23 (10%)	18 (8%)	1	7
46	L9	189/191 (99%)	166 (88%)	21 (11%)	2 (1%)	17	58
46	l9	189/191 (99%)	166 (88%)	17 (9%)	6 (3%)	5	30
47	M0	207/220 (94%)	171 (83%)	28 (14%)	8 (4%)	3	25
47	m0	209/220 (95%)	172 (82%)	23 (11%)	14 (7%)	1	10
48	M1	167/173 (96%)	122 (73%)	29 (17%)	16 (10%)	1	4
48	m1	167/173 (96%)	141 (84%)	15 (9%)	11 (7%)	1	11
49	M3	191/198 (96%)	154 (81%)	26 (14%)	11 (6%)	2	15
49	m3	192/198 (97%)	150 (78%)	28 (15%)	14 (7%)	1	8
50	M4	134/137 (98%)	113 (84%)	12 (9%)	9 (7%)	1	10
50	m4	135/137 (98%)	118 (87%)	16 (12%)	1 (1%)	25	68
51	M5	201/203 (99%)	183 (91%)	14 (7%)	4 (2%)	9	44
51	m5	201/203 (99%)	181 (90%)	16 (8%)	4 (2%)	9	44
52	M6	195/198 (98%)	176 (90%)	12 (6%)	7 (4%)	4	27
52	m6	195/198 (98%)	179 (92%)	10 (5%)	6 (3%)	5	31
53	M7	181/183 (99%)	144 (80%)	27 (15%)	10 (6%)	2	16
53	m7	153/183 (84%)	132 (86%)	18 (12%)	3 (2%)	9	44
54	M8	183/185 (99%)	154 (84%)	24 (13%)	5 (3%)	6	35
54	m8	183/185 (99%)	151 (82%)	26 (14%)	6 (3%)	4	29
55	M9	186/188 (99%)	172 (92%)	13 (7%)	1 (0%)	32	74
55	m9	186/188 (99%)	167 (90%)	14 (8%)	5 (3%)	6	35
56	N0	170/172 (99%)	154 (91%)	13 (8%)	3 (2%)	10	47
56	n0	170/172 (99%)	160 (94%)	7 (4%)	3 (2%)	10	47
57	N1	157/159 (99%)	139 (88%)	11 (7%)	7 (4%)	3	21
57	n1	157/159 (99%)	140 (89%)	12 (8%)	5 (3%)	5	30
58	N2	98/120 (82%)	72 (74%)	15 (15%)	11 (11%)	0	3
58	n2	96/120 (80%)	78 (81%)	15 (16%)	3 (3%)	5	31
59	N3	134/136 (98%)	120 (90%)	12 (9%)	2 (2%)	12	51
59	n3	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
60	N4	96/155 (62%)	78 (81%)	13 (14%)	5 (5%)	2	17
60	n4	133/155 (86%)	109 (82%)	15 (11%)	9 (7%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	N5	119/141 (84%)	106 (89%)	11 (9%)	2 (2%)	11	48
61	n5	118/141 (84%)	98 (83%)	11 (9%)	9 (8%)	1	8
62	N6	124/126 (98%)	104 (84%)	14 (11%)	6 (5%)	2	20
62	n6	124/126 (98%)	112 (90%)	8 (6%)	4 (3%)	5	30
63	N7	133/135 (98%)	111 (84%)	11 (8%)	11 (8%)	1	6
63	n7	133/135 (98%)	101 (76%)	21 (16%)	11 (8%)	1	6
64	N8	146/148 (99%)	121 (83%)	18 (12%)	7 (5%)	2	20
64	n8	146/148 (99%)	119 (82%)	22 (15%)	5 (3%)	4	28
65	N9	56/58 (97%)	47 (84%)	6 (11%)	3 (5%)	2	17
65	n9	56/58 (97%)	44 (79%)	7 (12%)	5 (9%)	1	5
66	O0	95/104 (91%)	76 (80%)	15 (16%)	4 (4%)	3	23
66	o0	98/104 (94%)	85 (87%)	13 (13%)	0	100	100
67	O1	107/112 (96%)	91 (85%)	8 (8%)	8 (8%)	1	8
67	o1	107/112 (96%)	85 (79%)	13 (12%)	9 (8%)	1	6
68	O2	125/129 (97%)	108 (86%)	17 (14%)	0	100	100
68	o2	125/129 (97%)	109 (87%)	9 (7%)	7 (6%)	2	16
69	O3	104/106 (98%)	92 (88%)	9 (9%)	3 (3%)	5	33
69	o3	104/106 (98%)	96 (92%)	4 (4%)	4 (4%)	4	25
70	O4	110/119 (92%)	94 (86%)	14 (13%)	2 (2%)	10	47
70	o4	110/119 (92%)	100 (91%)	9 (8%)	1 (1%)	20	64
71	O5	117/119 (98%)	99 (85%)	10 (8%)	8 (7%)	1	10
71	o5	117/119 (98%)	95 (81%)	17 (14%)	5 (4%)	3	23
72	O6	97/99 (98%)	78 (80%)	13 (13%)	6 (6%)	2	13
72	o6	97/99 (98%)	76 (78%)	15 (16%)	6 (6%)	2	13
73	O7	85/87 (98%)	74 (87%)	8 (9%)	3 (4%)	4	28
73	o7	85/87 (98%)	70 (82%)	11 (13%)	4 (5%)	3	20
74	O8	75/77 (97%)	65 (87%)	7 (9%)	3 (4%)	3	24
74	o8	75/77 (97%)	60 (80%)	12 (16%)	3 (4%)	3	24
75	O9	48/50 (96%)	40 (83%)	6 (12%)	2 (4%)	3	23
75	o9	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
76	Q0	50/52 (96%)	39 (78%)	9 (18%)	2 (4%)	3	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
76	q0	50/52 (96%)	49 (98%)	0	1 (2%)	9	44
77	Q1	23/25 (92%)	19 (83%)	4 (17%)	0	100	100
77	q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	3	23
78	Q2	103/105 (98%)	84 (82%)	13 (13%)	6 (6%)	2	15
78	q2	103/105 (98%)	92 (89%)	9 (9%)	2 (2%)	9	46
79	Q3	89/91 (98%)	76 (85%)	10 (11%)	3 (3%)	4	28
79	q3	89/91 (98%)	81 (91%)	7 (8%)	1 (1%)	17	58
80	c0	92/105 (88%)	59 (64%)	16 (17%)	17 (18%)	0	0
81	e0	60/62 (97%)	43 (72%)	10 (17%)	7 (12%)	0	2
82	e1	74/76 (97%)	34 (46%)	21 (28%)	19 (26%)	0	0
84	p0	139/311 (45%)	116 (84%)	16 (12%)	7 (5%)	2	19
All	All	22333/24141 (92%)	18253 (82%)	2722 (12%)	1358 (6%)	2	13

5 of 1358 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	30	GLN
2	S0	39	ASN
2	S0	66	ALA
2	S0	111	ILE

### 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%)	136 (83%)	28 (17%)	2	11
2	s0	165/209 (79%)	127 (77%)	38 (23%)	1	4
3	S1	191/223 (86%)	151 (79%)	40 (21%)	1	6
3	s1	192/223 (86%)	153 (80%)	39 (20%)	1	7
4	S2	176/204 (86%)	130 (74%)	46 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	s2	176/204 (86%)	129 (73%)	47 (27%)	0	2
5	S3	182/194 (94%)	143 (79%)	39 (21%)	1	6
5	s3	182/194 (94%)	143 (79%)	39 (21%)	1	6
6	S4	221/221 (100%)	178 (80%)	43 (20%)	1	8
6	s4	221/221 (100%)	184 (83%)	37 (17%)	2	12
7	S5	173/190 (91%)	145 (84%)	28 (16%)	3	13
7	s5	173/190 (91%)	133 (77%)	40 (23%)	1	4
8	S6	188/201 (94%)	151 (80%)	37 (20%)	1	8
8	s6	187/201 (93%)	150 (80%)	37 (20%)	1	8
9	S7	165/169 (98%)	136 (82%)	29 (18%)	2	10
9	s7	165/169 (98%)	134 (81%)	31 (19%)	2	9
10	S8	150/161 (93%)	122 (81%)	28 (19%)	2	9
10	s8	150/161 (93%)	124 (83%)	26 (17%)	2	11
11	S9	158/165 (96%)	124 (78%)	34 (22%)	1	6
11	s9	158/165 (96%)	126 (80%)	32 (20%)	1	7
12	C0	77/98 (79%)	64 (83%)	13 (17%)	2	11
13	C1	129/136 (95%)	107 (83%)	22 (17%)	2	11
13	c1	129/136 (95%)	109 (84%)	20 (16%)	3	14
14	C2	88/118 (75%)	66 (75%)	22 (25%)	1	2
14	c2	88/118 (75%)	63 (72%)	25 (28%)	0	1
15	C3	127/127 (100%)	100 (79%)	27 (21%)	1	6
15	c3	127/127 (100%)	103 (81%)	24 (19%)	2	9
16	C4	81/104 (78%)	60 (74%)	21 (26%)	0	2
16	c4	97/104 (93%)	69 (71%)	28 (29%)	0	1
17	C5	101/117 (86%)	80 (79%)	21 (21%)	1	6
17	c5	103/117 (88%)	78 (76%)	25 (24%)	1	3
18	C6	117/118 (99%)	89 (76%)	28 (24%)	1	3
18	c6	118/118 (100%)	95 (80%)	23 (20%)	1	8
19	C7	94/124 (76%)	75 (80%)	19 (20%)	1	7
19	c7	92/124 (74%)	66 (72%)	26 (28%)	0	1
20	C8	128/128 (100%)	96 (75%)	32 (25%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	c8	128/128 (100%)	101 (79%)	27 (21%)	1	6
21	C9	115/115 (100%)	83 (72%)	32 (28%)	0	1
21	c9	115/115 (100%)	93 (81%)	22 (19%)	2	9
22	D0	100/113 (88%)	83 (83%)	17 (17%)	2	11
22	d0	103/113 (91%)	71 (69%)	32 (31%)	0	1
23	D1	74/74 (100%)	59 (80%)	15 (20%)	1	7
23	d1	74/74 (100%)	59 (80%)	15 (20%)	1	7
24	D2	110/110 (100%)	88 (80%)	22 (20%)	1	7
24	d2	110/110 (100%)	93 (84%)	17 (16%)	3	14
25	D3	119/119 (100%)	98 (82%)	21 (18%)	2	10
25	d3	119/119 (100%)	92 (77%)	27 (23%)	1	4
26	D4	112/112 (100%)	92 (82%)	20 (18%)	2	10
26	d4	112/112 (100%)	91 (81%)	21 (19%)	2	9
27	D5	61/88 (69%)	50 (82%)	11 (18%)	2	10
27	d5	61/88 (69%)	49 (80%)	12 (20%)	1	8
28	D6	83/83 (100%)	66 (80%)	17 (20%)	1	6
28	d6	83/83 (100%)	63 (76%)	20 (24%)	1	3
29	D7	70/70 (100%)	55 (79%)	15 (21%)	1	6
29	d7	70/70 (100%)	59 (84%)	11 (16%)	3	14
30	D8	56/59 (95%)	40 (71%)	16 (29%)	0	1
30	d8	56/59 (95%)	41 (73%)	15 (27%)	0	2
31	D9	47/48 (98%)	41 (87%)	6 (13%)	5	23
31	d9	47/48 (98%)	37 (79%)	10 (21%)	1	6
32	E0	51/51 (100%)	42 (82%)	9 (18%)	2	10
33	E1	62/66 (94%)	45 (73%)	17 (27%)	0	1
34	SR	260/261 (100%)	214 (82%)	46 (18%)	2	10
34	sR	260/261 (100%)	237 (91%)	23 (9%)	12	42
35	SM	97/228 (42%)	79 (81%)	18 (19%)	2	9
35	sM	54/228 (24%)	40 (74%)	14 (26%)	0	2
39	L2	193/195 (99%)	153 (79%)	40 (21%)	1	6
39	l2	192/195 (98%)	156 (81%)	36 (19%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	L3	320/322 (99%)	260 (81%)	60 (19%)	2	9
40	l3	319/322 (99%)	259 (81%)	60 (19%)	2	9
41	L4	288/288 (100%)	241 (84%)	47 (16%)	3	13
41	l4	288/288 (100%)	236 (82%)	52 (18%)	2	10
42	L5	244/244 (100%)	199 (82%)	45 (18%)	2	9
42	l5	243/244 (100%)	194 (80%)	49 (20%)	1	7
43	L6	134/152 (88%)	113 (84%)	21 (16%)	3	14
43	l6	135/152 (89%)	113 (84%)	22 (16%)	3	13
44	L7	186/204 (91%)	162 (87%)	24 (13%)	5	22
44	l7	187/204 (92%)	163 (87%)	24 (13%)	5	23
45	L8	187/207 (90%)	151 (81%)	36 (19%)	1	9
45	l8	177/207 (86%)	145 (82%)	32 (18%)	2	10
46	L9	171/171 (100%)	135 (79%)	36 (21%)	1	6
46	l9	171/171 (100%)	132 (77%)	39 (23%)	1	4
47	M0	177/186 (95%)	136 (77%)	41 (23%)	1	4
47	m0	179/186 (96%)	148 (83%)	31 (17%)	2	11
48	M1	147/150 (98%)	115 (78%)	32 (22%)	1	6
48	m1	147/150 (98%)	112 (76%)	35 (24%)	1	3
49	M3	154/158 (98%)	124 (80%)	30 (20%)	1	8
49	m3	154/158 (98%)	129 (84%)	25 (16%)	3	13
50	M4	107/108 (99%)	88 (82%)	19 (18%)	2	10
50	m4	108/108 (100%)	84 (78%)	24 (22%)	1	5
51	M5	175/175 (100%)	148 (85%)	27 (15%)	3	15
51	m5	175/175 (100%)	142 (81%)	33 (19%)	2	9
52	M6	160/161 (99%)	134 (84%)	26 (16%)	3	13
52	m6	160/161 (99%)	136 (85%)	24 (15%)	3	16
53	M7	140/145 (97%)	114 (81%)	26 (19%)	2	9
53	m7	125/145 (86%)	101 (81%)	24 (19%)	1	9
54	M8	150/150 (100%)	123 (82%)	27 (18%)	2	10
54	m8	150/150 (100%)	125 (83%)	25 (17%)	2	12
55	M9	153/153 (100%)	130 (85%)	23 (15%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	m9	153/153 (100%)	121 (79%)	32 (21%)	1	6
56	N0	156/156 (100%)	125 (80%)	31 (20%)	1	7
56	n0	156/156 (100%)	127 (81%)	29 (19%)	2	9
57	N1	136/136 (100%)	104 (76%)	32 (24%)	1	4
57	n1	136/136 (100%)	107 (79%)	29 (21%)	1	6
58	N2	87/106 (82%)	72 (83%)	15 (17%)	2	11
58	n2	85/106 (80%)	67 (79%)	18 (21%)	1	6
59	N3	104/104 (100%)	85 (82%)	19 (18%)	2	9
59	n3	104/104 (100%)	95 (91%)	9 (9%)	12	42
60	N4	57/129 (44%)	47 (82%)	10 (18%)	2	11
60	n4	100/129 (78%)	84 (84%)	16 (16%)	3	13
61	N5	104/117 (89%)	88 (85%)	16 (15%)	3	15
61	n5	104/117 (89%)	83 (80%)	21 (20%)	1	7
62	N6	109/109 (100%)	87 (80%)	22 (20%)	1	7
62	n6	109/109 (100%)	75 (69%)	34 (31%)	0	1
63	N7	115/115 (100%)	96 (84%)	19 (16%)	2	12
63	n7	115/115 (100%)	89 (77%)	26 (23%)	1	5
64	N8	118/118 (100%)	90 (76%)	28 (24%)	1	3
64	n8	118/118 (100%)	96 (81%)	22 (19%)	2	9
65	N9	46/46 (100%)	37 (80%)	9 (20%)	1	8
65	n9	46/46 (100%)	38 (83%)	8 (17%)	2	11
66	O0	81/87 (93%)	62 (76%)	19 (24%)	1	4
66	o0	84/87 (97%)	67 (80%)	17 (20%)	1	7
67	O1	92/96 (96%)	75 (82%)	17 (18%)	2	9
67	o1	94/96 (98%)	71 (76%)	23 (24%)	1	2
68	O2	109/110 (99%)	82 (75%)	27 (25%)	1	2
68	o2	109/110 (99%)	89 (82%)	20 (18%)	2	9
69	O3	90/90 (100%)	75 (83%)	15 (17%)	2	12
69	o3	90/90 (100%)	74 (82%)	16 (18%)	2	10
70	O4	95/101 (94%)	76 (80%)	19 (20%)	1	7
70	o4	95/101 (94%)	78 (82%)	17 (18%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	O5	104/104 (100%)	79 (76%)	25 (24%)	1	3
71	o5	103/104 (99%)	82 (80%)	21 (20%)	1	7
72	O6	81/81 (100%)	60 (74%)	21 (26%)	0	2
72	o6	80/81 (99%)	57 (71%)	23 (29%)	0	1
73	O7	70/70 (100%)	57 (81%)	13 (19%)	2	9
73	o7	70/70 (100%)	53 (76%)	17 (24%)	1	3
74	O8	68/68 (100%)	50 (74%)	18 (26%)	0	2
74	o8	67/68 (98%)	55 (82%)	12 (18%)	2	10
75	O9	45/45 (100%)	34 (76%)	11 (24%)	1	3
75	o9	45/45 (100%)	37 (82%)	8 (18%)	2	10
76	Q0	47/47 (100%)	35 (74%)	12 (26%)	0	2
76	q0	47/47 (100%)	36 (77%)	11 (23%)	1	4
77	Q1	23/23 (100%)	19 (83%)	4 (17%)	2	11
77	q1	23/23 (100%)	18 (78%)	5 (22%)	1	6
78	Q2	90/90 (100%)	68 (76%)	22 (24%)	1	3
78	q2	90/90 (100%)	65 (72%)	25 (28%)	0	1
79	Q3	71/71 (100%)	59 (83%)	12 (17%)	2	11
79	q3	71/71 (100%)	56 (79%)	15 (21%)	1	6
80	c0	73/98 (74%)	65 (89%)	8 (11%)	7	30
81	e0	53/53 (100%)	40 (76%)	13 (24%)	1	2
82	e1	66/66 (100%)	45 (68%)	21 (32%)	0	0
84	p0	105/253 (42%)	84 (80%)	21 (20%)	1	7
All	All	18727/20239 (92%)	15017 (80%)	3710 (20%)	1	8

5 of 3710 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
70	O4	8	ARG
8	s6	12	SER
63	n7	135	ARG
72	O6	45	ARG
3	s1	77	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
47	M0	162	GLN
3	s1	149	GLN
53	m7	34	GLN
54	M8	152	HIS
59	N3	33	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	488 (27%)	0
1	6	1792/1800 (99%)	474 (26%)	0
36	1	3145/3396 (92%)	688 (21%)	0
36	5	3145/3396 (92%)	687 (21%)	0
37	3	120/121 (99%)	14 (11%)	0
37	7	120/121 (99%)	24 (20%)	0
38	4	157/158 (99%)	38 (24%)	0
38	8	157/158 (99%)	37 (23%)	0
All	All	10383/10950 (94%)	2450 (23%)	0

5 of 2450 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
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 ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 2563 ligands modelled in this entry, 1424 are monoatomic - leaving 1139 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	$\# Z  > 2$
90	A	1	3401	-	18,24,25	0.82	1 (5%)	17,35,38	1.04	2 (11%)
88	OHX	1	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3880	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3888	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3889	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3890	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3891	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3903	-	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
88	OHX	1	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3946	-	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	$\# Z  > 2$
88	OHX	1	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3989	-	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	$\# Z  > 2$
88	OHX	1	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4032	-	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
88	OHX	1	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4075	-	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
88	OHX	1	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4118	-	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	$\# Z  > 2$
88	OHX	1	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4161	-	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
88	OHX	1	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4204	-	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
88	OHX	1	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4218	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4219	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4220	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4221	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4222	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4223	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4224	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4225	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4226	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2043	-	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
88	OHX	2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2086	-	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
88	OHX	2	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2129	-	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	$\# Z  > 2$
88	OHX	2	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2172	-	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
88	OHX	2	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	215	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	216	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	217	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	218	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	219	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	220	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	221	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	222	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	223	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	224	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	225	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	220	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	221	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	222	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	223	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	224	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	225	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	226	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	227	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	228	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	229	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	230	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	231	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	232	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	233	-	0,6,6	0.00	-	0,15,15	0.00	-
90	A	5	3401	-	18,24,25	0.68	0	17,35,38	0.92	0
88	OHX	5	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3909	-	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	$\# Z  > 2$
88	OHX	5	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3952	-	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
88	OHX	5	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3995	-	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
88	OHX	5	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4038	-	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	$\# Z  > 2$
88	OHX	5	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4081	-	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
88	OHX	5	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4124	-	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
88	OHX	5	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4167	-	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
88	OHX	5	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4210	-	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
88	OHX	5	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4218	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4219	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4220	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4221	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4222	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4223	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4224	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4225	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4226	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4227	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4228	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4229	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4230	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4231	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4232	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4233	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4234	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4235	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4236	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4237	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4238	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4239	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4240	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4241	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4242	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4243	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4244	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4245	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4246	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4247	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4248	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4249	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4250	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4251	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4252	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4253	-	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
88	OHX	5	4254	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4255	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4256	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4257	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4258	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2081	-	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	$\# Z  > 2$
88	OHX	6	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2105	1	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2124	-	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
88	OHX	6	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2167	-	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
88	OHX	6	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2182	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2183	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2184	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2185	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2186	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2187	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2188	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2189	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2190	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2191	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2192	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2193	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2194	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2195	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2196	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2197	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2198	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2199	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2200	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	215	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	216	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	217	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	218	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	219	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	220	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	221	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	222	-	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
88	OHX	7	223	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	224	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	225	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	226	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	217	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	221	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	222	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	223	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	224	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	225	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	226	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	227	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	228	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	229	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	230	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	C3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	C5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	C8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	D3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	D9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	L3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	L3	405	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	L3	406	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	L4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M7	205	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	N9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	O3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	O7	103	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	O7	104	-	0,6,6	0.00	-	0,15,15	0.00	-
91	C	Q2	502	-	15,21,22	0.92	0	16,30,33	0.89	0
91	C	Q2	503	-	15,21,22	0.91	0	16,30,33	1.07	2 (12%)
88	OHX	S8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	c1	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	c3	201	-	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
88	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	c8	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	d4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	d9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l3	405	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l3	406	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l4	404	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l5	305	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l5	306	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l9	600	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m0	301	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m1	203	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m5	306	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m6	203	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	n3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	n3	204	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	n9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	o3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	o7	502	-	0,6,6	0.00	-	0,15,15	0.00	-
91	C	q2	502	-	15,21,22	0.76	0	16,30,33	0.78	0
91	C	q2	503	-	15,21,22	0.93	1 (6%)	16,30,33	0.89	1 (6%)
88	OHX	q2	504	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	s1	302	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	s1	303	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	s8	304	-	0,6,6	0.00	-	0,15,15	0.00	-
88	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
90	A	1	3401	-	-	0/3/25/26	0/3/3/3
88	OHX	1	3873	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3874	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	3875	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3876	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3877	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3878	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3879	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3880	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3881	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3882	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3883	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3884	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3885	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3886	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3887	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3888	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3889	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3890	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3891	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3892	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3893	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3894	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3895	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3896	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3897	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3898	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3899	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3900	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3901	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3902	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3903	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3904	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3905	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3906	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3907	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3908	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3909	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3910	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3911	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3912	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3913	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3914	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3915	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3916	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	3917	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3918	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3919	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3920	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3921	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3922	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3923	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3924	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3925	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3926	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3927	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3928	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3929	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3930	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3931	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3932	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3933	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3934	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3935	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3936	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3937	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3938	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3939	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3940	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3941	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3942	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3943	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3944	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3945	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3946	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3947	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3948	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3949	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3950	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3951	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3952	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3953	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3954	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3955	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3956	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3957	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3958	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	3959	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3960	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3961	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3962	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3963	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3964	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3965	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3966	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3967	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3968	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3969	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3970	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3971	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3972	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3973	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3974	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3975	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3976	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3977	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3978	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3979	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3980	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3981	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3982	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3983	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3984	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3985	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3986	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3987	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3988	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3989	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3990	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3991	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3992	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3993	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3994	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3995	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3996	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3997	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3998	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3999	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4000	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	4001	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4002	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4003	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4004	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4005	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4006	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4007	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4008	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4009	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4010	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4011	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4012	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4013	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4014	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4015	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4016	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4017	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4018	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4019	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4020	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4021	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4022	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4023	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4024	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4025	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4026	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4027	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4028	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4029	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4030	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4031	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4032	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4033	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4034	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4035	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4036	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4037	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4038	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4039	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4040	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4041	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4042	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	4043	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4044	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4045	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4046	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4047	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4048	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4049	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4050	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4051	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4052	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4053	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4054	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4055	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4056	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4057	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4058	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4059	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4060	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4061	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4062	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4063	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4064	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4065	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4066	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4067	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4068	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4069	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4070	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4071	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4072	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4073	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4074	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4075	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4076	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4077	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4078	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4079	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4080	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4081	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4082	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4083	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4084	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	4085	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4086	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4087	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4088	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4089	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4090	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4091	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4092	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4093	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4094	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4095	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4096	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4097	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4098	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4099	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4100	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4101	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4102	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4103	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4104	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4105	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4106	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4107	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4108	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4109	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4110	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4111	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4112	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4113	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4114	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4115	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4116	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4117	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4118	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4119	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4120	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4121	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4122	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4123	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4124	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4125	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4126	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	4127	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4128	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4129	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4130	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4131	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4132	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4133	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4134	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4135	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4136	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4137	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4138	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4139	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4140	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4141	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4142	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4143	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4144	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4145	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4146	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4147	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4148	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4149	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4150	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4151	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4152	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4153	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4154	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4155	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4156	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4157	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4158	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4159	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4160	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4161	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4162	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4163	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4164	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4165	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4166	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4167	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4168	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	4169	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4170	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4171	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4172	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4173	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4174	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4175	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4176	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4177	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4178	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4179	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4180	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4181	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4182	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4183	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4184	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4185	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4186	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4187	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4188	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4189	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4190	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4191	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4192	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4193	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4194	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4195	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4196	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4197	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4198	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4199	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4200	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4201	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4202	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4203	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4204	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4205	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4206	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4207	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4208	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4209	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4210	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	4211	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4212	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4213	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4214	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4215	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4216	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4217	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4218	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4219	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4220	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4221	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4222	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4223	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4224	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4225	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4226	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2023	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2024	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2025	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2029	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2030	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2031	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2032	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2033	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2034	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2035	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2036	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2037	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2038	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2039	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2040	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2041	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2042	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2043	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2044	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2045	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2046	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2047	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2048	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	2	2049	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2050	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2051	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2052	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2053	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2054	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2055	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2056	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2057	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2058	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2059	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2060	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2061	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2062	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2063	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2064	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2065	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2066	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2067	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2068	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2069	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2070	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2071	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2072	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2073	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2074	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2075	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2076	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2077	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2078	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2079	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2080	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2081	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2082	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2083	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2084	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2085	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2086	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2087	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2088	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2089	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2090	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	2	2091	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2092	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2093	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2094	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2095	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2096	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2097	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2098	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2099	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2100	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2101	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2102	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2103	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2104	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2105	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2106	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2107	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2108	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2109	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2110	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2111	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2112	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2113	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2114	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2115	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2116	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2117	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2118	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2119	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2120	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2121	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2122	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2123	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2124	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2125	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2126	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2127	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2128	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2129	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2130	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2131	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2132	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	2	2133	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2134	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2135	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2136	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2137	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2138	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2139	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2140	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2141	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2142	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2143	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2144	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2145	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2146	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2147	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2148	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2149	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2150	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2151	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2152	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2153	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2154	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2155	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2156	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2157	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2158	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2159	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2160	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2161	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2162	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2163	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2164	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2165	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2166	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2167	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2168	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2169	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2170	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2171	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2172	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2173	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2174	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	2	2175	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2176	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2177	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2178	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2179	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2180	-	-	0/0/0/0	0/0/0/0
88	OHX	3	215	-	-	0/0/0/0	0/0/0/0
88	OHX	3	216	-	-	0/0/0/0	0/0/0/0
88	OHX	3	217	-	-	0/0/0/0	0/0/0/0
88	OHX	3	218	-	-	0/0/0/0	0/0/0/0
88	OHX	3	219	-	-	0/0/0/0	0/0/0/0
88	OHX	3	220	-	-	0/0/0/0	0/0/0/0
88	OHX	3	221	-	-	0/0/0/0	0/0/0/0
88	OHX	3	222	-	-	0/0/0/0	0/0/0/0
88	OHX	3	223	-	-	0/0/0/0	0/0/0/0
88	OHX	3	224	-	-	0/0/0/0	0/0/0/0
88	OHX	3	225	-	-	0/0/0/0	0/0/0/0
88	OHX	4	220	-	-	0/0/0/0	0/0/0/0
88	OHX	4	221	-	-	0/0/0/0	0/0/0/0
88	OHX	4	222	-	-	0/0/0/0	0/0/0/0
88	OHX	4	223	-	-	0/0/0/0	0/0/0/0
88	OHX	4	224	-	-	0/0/0/0	0/0/0/0
88	OHX	4	225	-	-	0/0/0/0	0/0/0/0
88	OHX	4	226	-	-	0/0/0/0	0/0/0/0
88	OHX	4	227	-	-	0/0/0/0	0/0/0/0
88	OHX	4	228	-	-	0/0/0/0	0/0/0/0
88	OHX	4	229	-	-	0/0/0/0	0/0/0/0
88	OHX	4	230	-	-	0/0/0/0	0/0/0/0
88	OHX	4	231	-	-	0/0/0/0	0/0/0/0
88	OHX	4	232	-	-	0/0/0/0	0/0/0/0
88	OHX	4	233	-	-	0/0/0/0	0/0/0/0
90	A	5	3401	-	-	0/3/25/26	0/3/3/3
88	OHX	5	3901	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3902	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3903	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3904	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3905	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3906	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3907	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3908	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3909	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3910	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	3911	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3912	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3913	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3914	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3915	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3916	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3917	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3918	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3919	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3920	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3921	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3922	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3923	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3924	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3925	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3926	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3927	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3928	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3929	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3930	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3931	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3932	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3933	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3934	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3935	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3936	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3937	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3938	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3939	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3940	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3941	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3942	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3943	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3944	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3945	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3946	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3947	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3948	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3949	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3950	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3951	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3952	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	3953	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3954	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3955	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3956	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3957	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3958	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3959	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3960	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3961	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3962	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3963	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3964	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3965	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3966	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3967	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3968	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3969	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3970	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3971	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3972	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3973	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3974	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3975	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3976	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3977	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3978	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3979	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3980	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3981	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3982	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3983	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3984	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3985	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3986	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3987	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3988	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3989	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3990	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3991	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3992	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3993	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3994	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	3995	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3996	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3997	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3998	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3999	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4000	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4001	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4002	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4003	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4004	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4005	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4006	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4007	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4008	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4009	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4010	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4011	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4012	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4013	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4014	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4015	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4016	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4017	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4018	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4019	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4020	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4021	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4022	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4023	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4024	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4025	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4026	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4027	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4028	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4029	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4030	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4031	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4032	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4033	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4034	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4035	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4036	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4037	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4038	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4039	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4040	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4041	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4042	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4043	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4044	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4045	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4046	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4047	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4048	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4049	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4050	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4051	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4052	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4053	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4054	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4055	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4056	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4057	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4058	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4059	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4060	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4061	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4062	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4063	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4064	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4065	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4066	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4067	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4068	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4069	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4070	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4071	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4072	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4073	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4074	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4075	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4076	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4077	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4078	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4079	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4080	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4081	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4082	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4083	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4084	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4085	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4086	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4087	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4088	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4089	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4090	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4091	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4092	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4093	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4094	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4095	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4096	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4097	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4098	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4099	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4100	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4101	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4102	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4103	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4104	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4105	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4106	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4107	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4108	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4109	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4110	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4111	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4112	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4113	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4114	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4115	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4116	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4117	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4118	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4119	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4120	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4121	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4122	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4123	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4124	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4125	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4126	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4127	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4128	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4129	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4130	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4131	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4132	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4133	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4134	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4135	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4136	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4137	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4138	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4139	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4140	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4141	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4142	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4143	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4144	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4145	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4146	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4147	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4148	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4149	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4150	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4151	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4152	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4153	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4154	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4155	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4156	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4157	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4158	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4159	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4160	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4161	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4162	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4163	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4164	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4165	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4166	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4167	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4168	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4169	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4170	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4171	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4172	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4173	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4174	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4175	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4176	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4177	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4178	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4179	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4180	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4181	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4182	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4183	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4184	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4185	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4186	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4187	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4188	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4189	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4190	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4191	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4192	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4193	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4194	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4195	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4196	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4197	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4198	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4199	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4200	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4201	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4202	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4203	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4204	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4205	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4206	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4207	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4208	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4209	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4210	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4211	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4212	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4213	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4214	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4215	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4216	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4217	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4218	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4219	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4220	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4221	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4222	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4223	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4224	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4225	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4226	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4227	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4228	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4229	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4230	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4231	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4232	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4233	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4234	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4235	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4236	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4237	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4238	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4239	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4240	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4241	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4242	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4243	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4244	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4245	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4246	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4247	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4248	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4249	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4250	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4251	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4252	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4253	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4254	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4255	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4256	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4257	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4258	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2044	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2045	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2046	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2047	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2049	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2050	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2051	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2052	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2053	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2054	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2055	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2056	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2057	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2058	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2059	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2060	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2061	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2062	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2063	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2064	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2065	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2066	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2067	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2068	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2069	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2070	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2071	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2072	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2073	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	6	2074	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2075	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2076	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2077	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2078	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2079	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2080	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2081	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2082	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2083	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2084	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2085	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2086	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2087	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2088	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2089	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2090	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2091	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2092	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2093	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2094	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2095	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2096	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2097	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2098	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2099	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2100	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2101	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2102	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2103	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2104	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2105	1	-	0/0/0/0	0/0/0/0
88	OHX	6	2106	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2107	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2108	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2109	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2110	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2111	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2112	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2113	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2114	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2115	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	6	2116	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2117	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2118	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2119	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2120	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2121	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2122	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2123	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2124	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2125	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2126	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2127	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2128	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2129	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2130	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2131	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2132	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2133	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2134	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2135	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2136	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2137	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2138	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2139	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2140	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2141	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2142	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2143	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2144	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2145	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2146	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2147	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2148	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2149	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2150	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2151	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2152	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2153	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2154	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2155	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2156	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2157	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	6	2158	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2159	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2160	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2161	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2162	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2163	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2164	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2165	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2166	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2167	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2168	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2169	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2170	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2171	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2172	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2173	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2174	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2175	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2176	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2177	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2178	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2179	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2180	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2181	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2182	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2183	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2184	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2185	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2186	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2187	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2188	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2189	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2190	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2191	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2192	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2193	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2194	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2195	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2196	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2197	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2198	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2199	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	6	2200	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2201	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2202	-	-	0/0/0/0	0/0/0/0
88	OHX	7	215	-	-	0/0/0/0	0/0/0/0
88	OHX	7	216	-	-	0/0/0/0	0/0/0/0
88	OHX	7	217	-	-	0/0/0/0	0/0/0/0
88	OHX	7	218	-	-	0/0/0/0	0/0/0/0
88	OHX	7	219	-	-	0/0/0/0	0/0/0/0
88	OHX	7	220	-	-	0/0/0/0	0/0/0/0
88	OHX	7	221	-	-	0/0/0/0	0/0/0/0
88	OHX	7	222	-	-	0/0/0/0	0/0/0/0
88	OHX	7	223	-	-	0/0/0/0	0/0/0/0
88	OHX	7	224	-	-	0/0/0/0	0/0/0/0
88	OHX	7	225	-	-	0/0/0/0	0/0/0/0
88	OHX	7	226	-	-	0/0/0/0	0/0/0/0
88	OHX	8	217	-	-	0/0/0/0	0/0/0/0
88	OHX	8	218	-	-	0/0/0/0	0/0/0/0
88	OHX	8	219	-	-	0/0/0/0	0/0/0/0
88	OHX	8	220	-	-	0/0/0/0	0/0/0/0
88	OHX	8	221	-	-	0/0/0/0	0/0/0/0
88	OHX	8	222	-	-	0/0/0/0	0/0/0/0
88	OHX	8	223	-	-	0/0/0/0	0/0/0/0
88	OHX	8	224	-	-	0/0/0/0	0/0/0/0
88	OHX	8	225	-	-	0/0/0/0	0/0/0/0
88	OHX	8	226	-	-	0/0/0/0	0/0/0/0
88	OHX	8	227	-	-	0/0/0/0	0/0/0/0
88	OHX	8	228	-	-	0/0/0/0	0/0/0/0
88	OHX	8	229	-	-	0/0/0/0	0/0/0/0
88	OHX	8	230	-	-	0/0/0/0	0/0/0/0
88	OHX	C3	201	-	-	0/0/0/0	0/0/0/0
88	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
88	OHX	C8	201	-	-	0/0/0/0	0/0/0/0
88	OHX	D3	202	-	-	0/0/0/0	0/0/0/0
88	OHX	D9	102	-	-	0/0/0/0	0/0/0/0
88	OHX	L3	404	-	-	0/0/0/0	0/0/0/0
88	OHX	L3	405	-	-	0/0/0/0	0/0/0/0
88	OHX	L3	406	-	-	0/0/0/0	0/0/0/0
88	OHX	L4	402	-	-	0/0/0/0	0/0/0/0
88	OHX	M0	303	-	-	0/0/0/0	0/0/0/0
88	OHX	M5	303	-	-	0/0/0/0	0/0/0/0
88	OHX	M7	205	-	-	0/0/0/0	0/0/0/0
88	OHX	M7	206	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	M8	201	-	-	0/0/0/0	0/0/0/0
88	OHX	M9	202	-	-	0/0/0/0	0/0/0/0
88	OHX	N9	101	-	-	0/0/0/0	0/0/0/0
88	OHX	O3	201	-	-	0/0/0/0	0/0/0/0
88	OHX	O7	103	-	-	0/0/0/0	0/0/0/0
88	OHX	O7	104	-	-	0/0/0/0	0/0/0/0
91	C	Q2	502	-	-	0/3/25/26	0/2/2/2
91	C	Q2	503	-	-	0/3/25/26	0/2/2/2
88	OHX	S8	302	-	-	0/0/0/0	0/0/0/0
88	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
88	OHX	c1	202	-	-	0/0/0/0	0/0/0/0
88	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
88	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
88	OHX	c8	202	-	-	0/0/0/0	0/0/0/0
88	OHX	d4	202	-	-	0/0/0/0	0/0/0/0
88	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
88	OHX	l3	404	-	-	0/0/0/0	0/0/0/0
88	OHX	l3	405	-	-	0/0/0/0	0/0/0/0
88	OHX	l3	406	-	-	0/0/0/0	0/0/0/0
88	OHX	l4	403	-	-	0/0/0/0	0/0/0/0
88	OHX	l4	404	-	-	0/0/0/0	0/0/0/0
88	OHX	l5	303	-	-	0/0/0/0	0/0/0/0
88	OHX	l5	304	-	-	0/0/0/0	0/0/0/0
88	OHX	l5	305	-	-	0/0/0/0	0/0/0/0
88	OHX	l5	306	-	-	0/0/0/0	0/0/0/0
88	OHX	l9	600	-	-	0/0/0/0	0/0/0/0
88	OHX	m0	301	-	-	0/0/0/0	0/0/0/0
88	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
88	OHX	m1	203	-	-	0/0/0/0	0/0/0/0
88	OHX	m4	201	-	-	0/0/0/0	0/0/0/0
88	OHX	m5	306	-	-	0/0/0/0	0/0/0/0
88	OHX	m6	203	-	-	0/0/0/0	0/0/0/0
88	OHX	n3	203	-	-	0/0/0/0	0/0/0/0
88	OHX	n3	204	-	-	0/0/0/0	0/0/0/0
88	OHX	n9	101	-	-	0/0/0/0	0/0/0/0
88	OHX	o3	202	-	-	0/0/0/0	0/0/0/0
88	OHX	o7	502	-	-	0/0/0/0	0/0/0/0
91	C	q2	502	-	-	0/3/25/26	0/2/2/2
91	C	q2	503	-	-	0/3/25/26	0/2/2/2
88	OHX	q2	504	-	-	0/0/0/0	0/0/0/0
88	OHX	s1	302	-	-	0/0/0/0	0/0/0/0
88	OHX	s1	303	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	s8	304	-	-	0/0/0/0	0/0/0/0
88	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	1	3401	A	O5'-C5'	-2.41	1.41	1.44
91	q2	503	C	O5'-C5'	-2.31	1.41	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	Q2	503	C	C6-N1-C2	-2.67	116.95	121.28
91	q2	503	C	C5-C4-N4	-2.33	117.08	121.26
91	Q2	503	C	N4-C4-N3	2.07	120.12	116.64
90	1	3401	A	C1'-N9-C4	2.23	130.49	126.64
90	1	3401	A	C4-C5-N7	2.29	111.63	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

367 monomers are involved in 490 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	1	3873	OHX	1	0
88	1	3877	OHX	1	0
88	1	3878	OHX	1	0
88	1	3880	OHX	1	0
88	1	3881	OHX	2	0
88	1	3883	OHX	1	0
88	1	3887	OHX	2	0
88	1	3888	OHX	1	0
88	1	3890	OHX	2	0
88	1	3891	OHX	2	0
88	1	3892	OHX	2	0
88	1	3893	OHX	1	0
88	1	3894	OHX	1	0
88	1	3895	OHX	1	0
88	1	3898	OHX	1	0
88	1	3900	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	1	3901	OHX	1	0
88	1	3909	OHX	1	0
88	1	3910	OHX	1	0
88	1	3915	OHX	1	0
88	1	3916	OHX	1	0
88	1	3921	OHX	1	0
88	1	3924	OHX	1	0
88	1	3934	OHX	1	0
88	1	3936	OHX	1	0
88	1	3940	OHX	2	0
88	1	3942	OHX	3	0
88	1	3943	OHX	1	0
88	1	3950	OHX	1	0
88	1	3951	OHX	1	0
88	1	3956	OHX	1	0
88	1	3957	OHX	1	0
88	1	3967	OHX	1	0
88	1	3968	OHX	3	0
88	1	3969	OHX	1	0
88	1	3970	OHX	1	0
88	1	3972	OHX	1	0
88	1	3976	OHX	1	0
88	1	3979	OHX	1	0
88	1	3982	OHX	6	0
88	1	3983	OHX	1	0
88	1	3985	OHX	2	0
88	1	3988	OHX	1	0
88	1	3992	OHX	1	0
88	1	3993	OHX	1	0
88	1	3995	OHX	1	0
88	1	3997	OHX	2	0
88	1	4005	OHX	1	0
88	1	4009	OHX	1	0
88	1	4013	OHX	1	0
88	1	4015	OHX	4	0
88	1	4020	OHX	1	0
88	1	4022	OHX	1	0
88	1	4025	OHX	1	0
88	1	4027	OHX	1	0
88	1	4031	OHX	2	0
88	1	4044	OHX	2	0
88	1	4046	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	1	4048	OHX	2	0
88	1	4051	OHX	2	0
88	1	4053	OHX	1	0
88	1	4056	OHX	3	0
88	1	4057	OHX	3	0
88	1	4060	OHX	2	0
88	1	4061	OHX	1	0
88	1	4069	OHX	2	0
88	1	4071	OHX	1	0
88	1	4073	OHX	1	0
88	1	4079	OHX	1	0
88	1	4087	OHX	1	0
88	1	4088	OHX	1	0
88	1	4093	OHX	1	0
88	1	4095	OHX	1	0
88	1	4097	OHX	1	0
88	1	4098	OHX	2	0
88	1	4100	OHX	1	0
88	1	4101	OHX	1	0
88	1	4108	OHX	1	0
88	1	4109	OHX	1	0
88	1	4111	OHX	1	0
88	1	4112	OHX	1	0
88	1	4122	OHX	1	0
88	1	4131	OHX	1	0
88	1	4133	OHX	1	0
88	1	4138	OHX	1	0
88	1	4141	OHX	1	0
88	1	4145	OHX	1	0
88	1	4146	OHX	1	0
88	1	4148	OHX	1	0
88	1	4152	OHX	3	0
88	1	4155	OHX	1	0
88	1	4157	OHX	2	0
88	1	4158	OHX	1	0
88	1	4160	OHX	1	0
88	1	4161	OHX	1	0
88	1	4164	OHX	1	0
88	1	4170	OHX	6	0
88	1	4174	OHX	1	0
88	1	4178	OHX	3	0
88	1	4179	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	1	4182	OHX	1	0
88	1	4183	OHX	1	0
88	1	4186	OHX	4	0
88	1	4194	OHX	1	0
88	1	4195	OHX	3	0
88	1	4210	OHX	1	0
88	1	4212	OHX	1	0
88	1	4213	OHX	1	0
88	1	4217	OHX	1	0
88	1	4220	OHX	1	0
88	1	4221	OHX	1	0
88	2	2026	OHX	1	0
88	2	2027	OHX	1	0
88	2	2031	OHX	1	0
88	2	2032	OHX	1	0
88	2	2034	OHX	1	0
88	2	2036	OHX	3	0
88	2	2038	OHX	1	0
88	2	2039	OHX	1	0
88	2	2041	OHX	1	0
88	2	2042	OHX	1	0
88	2	2044	OHX	6	0
88	2	2045	OHX	1	0
88	2	2047	OHX	1	0
88	2	2048	OHX	1	0
88	2	2051	OHX	1	0
88	2	2053	OHX	1	0
88	2	2057	OHX	1	0
88	2	2064	OHX	1	0
88	2	2066	OHX	1	0
88	2	2067	OHX	1	0
88	2	2073	OHX	1	0
88	2	2074	OHX	2	0
88	2	2076	OHX	1	0
88	2	2078	OHX	1	0
88	2	2082	OHX	1	0
88	2	2084	OHX	2	0
88	2	2086	OHX	1	0
88	2	2089	OHX	1	0
88	2	2092	OHX	1	0
88	2	2095	OHX	1	0
88	2	2097	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	2	2099	OHX	7	0
88	2	2102	OHX	1	0
88	2	2104	OHX	1	0
88	2	2105	OHX	1	0
88	2	2106	OHX	1	0
88	2	2110	OHX	1	0
88	2	2111	OHX	2	0
88	2	2115	OHX	1	0
88	2	2121	OHX	2	0
88	2	2123	OHX	1	0
88	2	2129	OHX	1	0
88	2	2130	OHX	1	0
88	2	2131	OHX	2	0
88	2	2132	OHX	1	0
88	2	2141	OHX	1	0
88	2	2144	OHX	1	0
88	2	2145	OHX	2	0
88	2	2148	OHX	1	0
88	2	2149	OHX	1	0
88	2	2154	OHX	2	0
88	2	2155	OHX	1	0
88	2	2156	OHX	1	0
88	2	2157	OHX	2	0
88	2	2159	OHX	1	0
88	2	2165	OHX	1	0
88	2	2166	OHX	1	0
88	3	220	OHX	1	0
88	4	222	OHX	1	0
88	4	223	OHX	1	0
88	4	225	OHX	1	0
88	4	229	OHX	2	0
88	4	231	OHX	1	0
88	5	3901	OHX	1	0
88	5	3903	OHX	1	0
88	5	3906	OHX	1	0
88	5	3907	OHX	2	0
88	5	3909	OHX	2	0
88	5	3915	OHX	2	0
88	5	3918	OHX	1	0
88	5	3919	OHX	2	0
88	5	3922	OHX	1	0
88	5	3924	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	5	3925	OHX	2	0
88	5	3927	OHX	3	0
88	5	3941	OHX	1	0
88	5	3942	OHX	1	0
88	5	3944	OHX	1	0
88	5	3945	OHX	2	0
88	5	3948	OHX	1	0
88	5	3956	OHX	1	0
88	5	3957	OHX	1	0
88	5	3959	OHX	1	0
88	5	3960	OHX	2	0
88	5	3961	OHX	1	0
88	5	3962	OHX	1	0
88	5	3963	OHX	1	0
88	5	3965	OHX	3	0
88	5	3972	OHX	1	0
88	5	3975	OHX	1	0
88	5	3976	OHX	3	0
88	5	3981	OHX	6	0
88	5	3982	OHX	1	0
88	5	3985	OHX	1	0
88	5	3986	OHX	2	0
88	5	3990	OHX	1	0
88	5	3991	OHX	1	0
88	5	3992	OHX	1	0
88	5	3994	OHX	2	0
88	5	3998	OHX	1	0
88	5	3999	OHX	1	0
88	5	4004	OHX	1	0
88	5	4005	OHX	3	0
88	5	4006	OHX	1	0
88	5	4010	OHX	1	0
88	5	4014	OHX	6	0
88	5	4016	OHX	2	0
88	5	4020	OHX	1	0
88	5	4021	OHX	1	0
88	5	4023	OHX	6	0
88	5	4025	OHX	1	0
88	5	4026	OHX	1	0
88	5	4027	OHX	2	0
88	5	4034	OHX	1	0
88	5	4044	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	5	4052	OHX	1	0
88	5	4053	OHX	1	0
88	5	4054	OHX	1	0
88	5	4055	OHX	1	0
88	5	4069	OHX	3	0
88	5	4071	OHX	1	0
88	5	4075	OHX	1	0
88	5	4077	OHX	1	0
88	5	4082	OHX	1	0
88	5	4091	OHX	1	0
88	5	4094	OHX	1	0
88	5	4097	OHX	1	0
88	5	4100	OHX	1	0
88	5	4103	OHX	1	0
88	5	4106	OHX	2	0
88	5	4109	OHX	1	0
88	5	4111	OHX	1	0
88	5	4114	OHX	1	0
88	5	4115	OHX	1	0
88	5	4118	OHX	1	0
88	5	4123	OHX	1	0
88	5	4133	OHX	1	0
88	5	4134	OHX	1	0
88	5	4135	OHX	1	0
88	5	4142	OHX	2	0
88	5	4145	OHX	1	0
88	5	4147	OHX	2	0
88	5	4151	OHX	1	0
88	5	4156	OHX	1	0
88	5	4163	OHX	1	0
88	5	4164	OHX	1	0
88	5	4166	OHX	1	0
88	5	4172	OHX	1	0
88	5	4186	OHX	1	0
88	5	4187	OHX	1	0
88	5	4189	OHX	1	0
88	5	4190	OHX	1	0
88	5	4194	OHX	2	0
88	5	4196	OHX	2	0
88	5	4197	OHX	1	0
88	5	4198	OHX	1	0
88	5	4199	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	5	4200	OHX	2	0
88	5	4202	OHX	1	0
88	5	4203	OHX	9	0
88	5	4205	OHX	7	0
88	5	4209	OHX	1	0
88	5	4214	OHX	1	0
88	5	4219	OHX	1	0
88	5	4222	OHX	6	0
88	5	4231	OHX	3	0
88	5	4232	OHX	1	0
88	5	4233	OHX	1	0
88	5	4234	OHX	1	0
88	5	4239	OHX	3	0
88	5	4242	OHX	1	0
88	5	4243	OHX	1	0
88	5	4248	OHX	4	0
88	5	4249	OHX	1	0
88	5	4254	OHX	1	0
88	6	2047	OHX	2	0
88	6	2052	OHX	1	0
88	6	2055	OHX	1	0
88	6	2057	OHX	3	0
88	6	2059	OHX	1	0
88	6	2060	OHX	1	0
88	6	2063	OHX	1	0
88	6	2064	OHX	1	0
88	6	2066	OHX	1	0
88	6	2068	OHX	1	0
88	6	2071	OHX	2	0
88	6	2072	OHX	1	0
88	6	2073	OHX	1	0
88	6	2077	OHX	1	0
88	6	2081	OHX	1	0
88	6	2084	OHX	1	0
88	6	2091	OHX	1	0
88	6	2094	OHX	1	0
88	6	2096	OHX	1	0
88	6	2098	OHX	3	0
88	6	2100	OHX	1	0
88	6	2101	OHX	1	0
88	6	2105	OHX	4	0
88	6	2106	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	6	2107	OHX	1	0
88	6	2109	OHX	1	0
88	6	2110	OHX	1	0
88	6	2112	OHX	1	0
88	6	2116	OHX	2	0
88	6	2117	OHX	1	0
88	6	2118	OHX	1	0
88	6	2120	OHX	1	0
88	6	2122	OHX	1	0
88	6	2124	OHX	1	0
88	6	2126	OHX	2	0
88	6	2132	OHX	1	0
88	6	2133	OHX	1	0
88	6	2134	OHX	1	0
88	6	2140	OHX	1	0
88	6	2142	OHX	1	0
88	6	2143	OHX	4	0
88	6	2145	OHX	1	0
88	6	2146	OHX	1	0
88	6	2147	OHX	1	0
88	6	2150	OHX	2	0
88	6	2152	OHX	1	0
88	6	2155	OHX	1	0
88	6	2168	OHX	2	0
88	6	2172	OHX	1	0
88	6	2175	OHX	1	0
88	6	2177	OHX	1	0
88	6	2180	OHX	1	0
88	6	2184	OHX	1	0
88	6	2186	OHX	1	0
88	6	2187	OHX	2	0
88	6	2193	OHX	1	0
88	6	2194	OHX	1	0
88	6	2200	OHX	1	0
88	6	2202	OHX	1	0
88	7	216	OHX	1	0
88	7	218	OHX	2	0
88	7	220	OHX	1	0
88	7	225	OHX	1	0
88	8	217	OHX	1	0
88	8	218	OHX	5	0
88	8	219	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	8	221	OHX	1	0
88	8	225	OHX	6	0
88	8	226	OHX	1	0
88	8	227	OHX	1	0
88	C3	201	OHX	1	0
88	C5	201	OHX	5	0
88	L3	404	OHX	1	0
88	L3	405	OHX	1	0
88	L4	402	OHX	3	0
88	M5	303	OHX	1	0
88	M7	206	OHX	1	0
88	O7	103	OHX	2	0
91	Q2	502	C	1	0
91	Q2	503	C	3	0
88	S8	302	OHX	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 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.