



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:04 PM GMT

PDB ID : 4U4U
Title : Crystal structure of Lycorine bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : **FAILED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

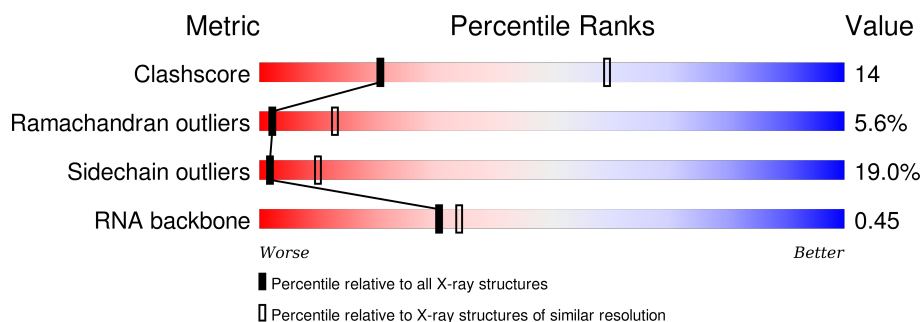
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

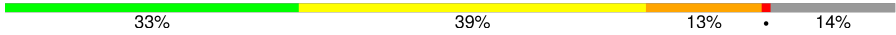



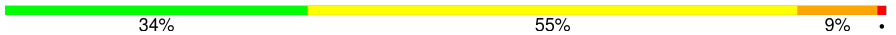

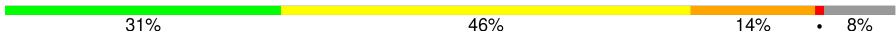

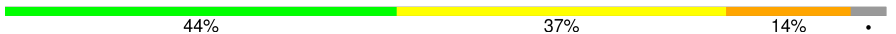

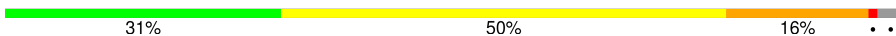

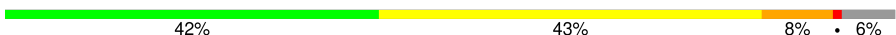







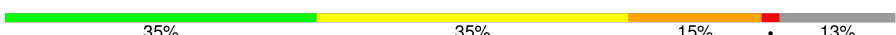




The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey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

Note EDS failed to run properly.

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


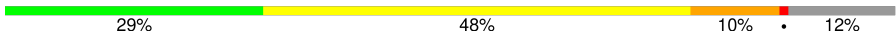



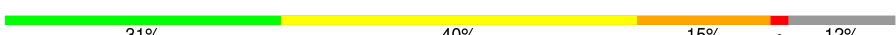

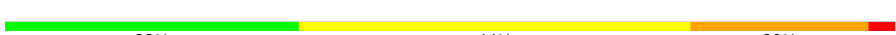



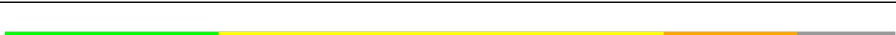

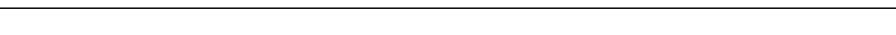
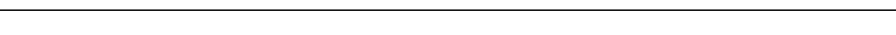
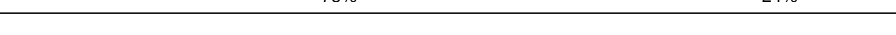

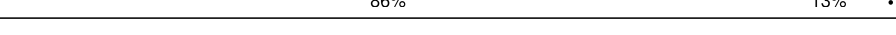






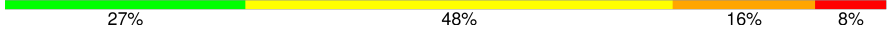
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Mol	Chain	Length	Quality of chain
4	S2	253	
4	s2	253	
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2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







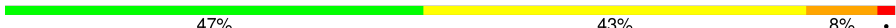


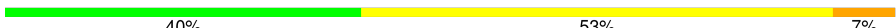


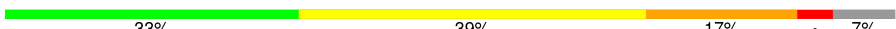
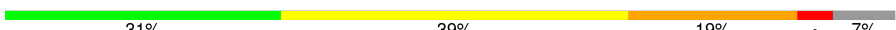


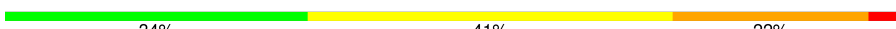
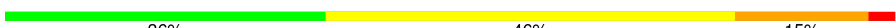


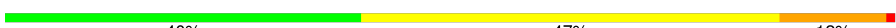

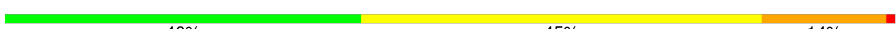


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Mol	Chain	Length	Quality of chain
16	c4	136	
17	C5	141	
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134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






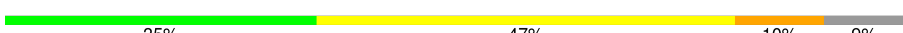





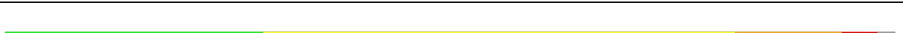













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Mol	Chain	Length	Quality of chain
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	
42	L5	296	







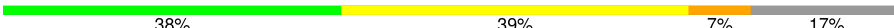



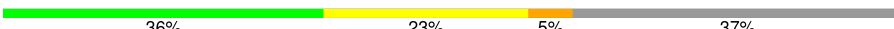





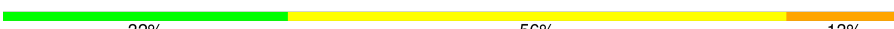





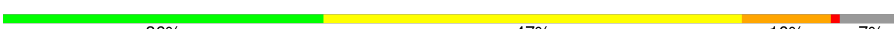


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Mol	Chain	Length	Quality of chain
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	
53	m7	183	
54	M8	185	
54	m8	185	


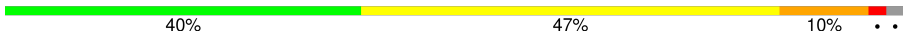



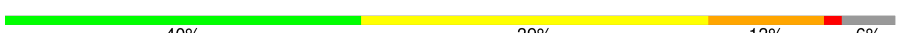





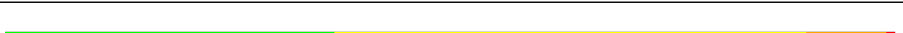













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Mol	Chain	Length	Quality of chain
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	104	
66	o0	104	
67	O1	112	

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Mol	Chain	Length	Quality of chain
67	o1	112	
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	119	
70	o4	119	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	
79	q3	91	

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Mol	Chain	Length	Quality of chain
80	e0	62	
81	sM	273	
82	m2	160	
83	p0	311	
84	p1	47	
85	p2	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	OHX	1	3945	-	-	X	-
87	OHX	1	3964	-	-	X	-
87	OHX	1	3966	-	-	X	-
87	OHX	1	3978	-	-	X	-
87	OHX	1	4009	-	-	X	-
87	OHX	1	4034	-	-	X	-
87	OHX	1	4037	-	-	X	-
87	OHX	1	4042	-	-	X	-
87	OHX	1	4048	-	-	X	-
87	OHX	1	4049	-	-	X	-
87	OHX	1	4060	-	-	X	-
87	OHX	1	4061	-	-	X	-
87	OHX	1	4085	-	-	X	-
87	OHX	1	4089	-	-	X	-
87	OHX	1	4137	-	-	X	-
87	OHX	1	4145	-	-	X	-
87	OHX	1	4151	-	-	X	-
87	OHX	1	4155	-	-	X	-
87	OHX	1	4159	-	-	X	-
87	OHX	1	4161	-	-	X	-
87	OHX	1	4168	-	-	X	-
87	OHX	1	4177	-	-	X	-
87	OHX	1	4186	-	-	X	-
87	OHX	1	4203	-	-	X	-
87	OHX	2	2029	-	-	X	-
87	OHX	2	2042	-	-	X	-
87	OHX	2	2081	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	OHX	2	2083	-	-	X	-
87	OHX	2	2088	-	-	X	-
87	OHX	2	2097	-	-	X	-
87	OHX	2	2109	-	-	X	-
87	OHX	2	2129	-	-	X	-
87	OHX	2	2144	-	-	X	-
87	OHX	5	3943	-	-	X	-
87	OHX	5	3963	-	-	X	-
87	OHX	5	3974	-	-	X	-
87	OHX	5	3979	-	-	X	-
87	OHX	5	4002	-	-	X	-
87	OHX	5	4003	-	-	X	-
87	OHX	5	4011	-	-	X	-
87	OHX	5	4021	-	-	X	-
87	OHX	5	4024	-	-	X	-
87	OHX	5	4056	-	-	X	-
87	OHX	5	4067	-	-	X	-
87	OHX	5	4091	-	-	X	-
87	OHX	5	4092	-	-	X	-
87	OHX	5	4096	-	-	X	-
87	OHX	5	4104	-	-	X	-
87	OHX	5	4144	-	-	X	-
87	OHX	5	4191	-	-	X	-
87	OHX	5	4193	-	-	X	-
87	OHX	5	4200	-	-	X	-
87	OHX	5	4201	-	-	X	-
87	OHX	5	4202	-	-	X	-
87	OHX	5	4215	-	-	X	-
87	OHX	5	4218	-	-	X	-
87	OHX	5	4225	-	-	X	-
87	OHX	5	4235	-	-	X	-
87	OHX	5	4237	-	-	X	-
87	OHX	5	4244	-	-	X	-
87	OHX	6	2063	-	-	X	-
87	OHX	6	2124	-	-	X	-
87	OHX	6	2150	-	-	X	-
87	OHX	6	2162	-	-	X	-
87	OHX	6	2174	-	-	X	-
87	OHX	6	2192	-	-	X	-
87	OHX	8	217	-	-	X	-
87	OHX	8	225	-	-	X	-
87	OHX	C5	201	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	OHX	O7	103	-	-	X	-
88	ZN	Q2	501	-	-	X	-

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 411211 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 81 is a protein called Suppressor protein STM1.

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

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

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

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

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

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

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

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

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

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	L7	2	Total	Mg	0	0
			2	2		
86	m6	1	Total	Mg	0	0
			1	1		
86	n8	5	Total	Mg	0	0
			5	5		
86	o1	2	Total	Mg	0	0
			2	2		
86	N5	1	Total	Mg	0	0
			1	1		
86	6	149	Total	Mg	0	0
			149	149		
86	sM	2	Total	Mg	0	0
			2	2		
86	O4	1	Total	Mg	0	0
			1	1		
86	m5	3	Total	Mg	0	0
			3	3		
86	l3	2	Total	Mg	0	0
			2	2		
86	M1	1	Total	Mg	0	0
			1	1		
86	l4	1	Total	Mg	0	0
			1	1		
86	2	123	Total	Mg	0	0
			123	123		
86	n0	1	Total	Mg	0	0
			1	1		
86	L4	2	Total	Mg	0	0
			2	2		
86	l7	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	M5	1	Total 1	Mg 1	0	0
86	S2	1	Total 1	Mg 1	0	0
86	L8	1	Total 1	Mg 1	0	0
86	D3	1	Total 1	Mg 1	0	0
86	M9	1	Total 1	Mg 1	0	0
86	q0	1	Total 1	Mg 1	0	0
86	SM	1	Total 1	Mg 1	0	0
86	o4	1	Total 1	Mg 1	0	0
86	M0	2	Total 2	Mg 2	0	0
86	c1	1	Total 1	Mg 1	0	0
86	n6	1	Total 1	Mg 1	0	0
86	5	506	Total 506	Mg 506	0	0
86	L5	2	Total 2	Mg 2	0	0
86	O7	1	Total 1	Mg 1	0	0
86	Q2	1	Total 1	Mg 1	0	0
86	1	477	Total 477	Mg 477	0	0
86	D0	1	Total 1	Mg 1	0	0
86	S8	1	Total 1	Mg 1	0	0
86	m1	1	Total 1	Mg 1	0	0
86	M8	1	Total 1	Mg 1	0	0
86	q3	1	Total 1	Mg 1	0	0

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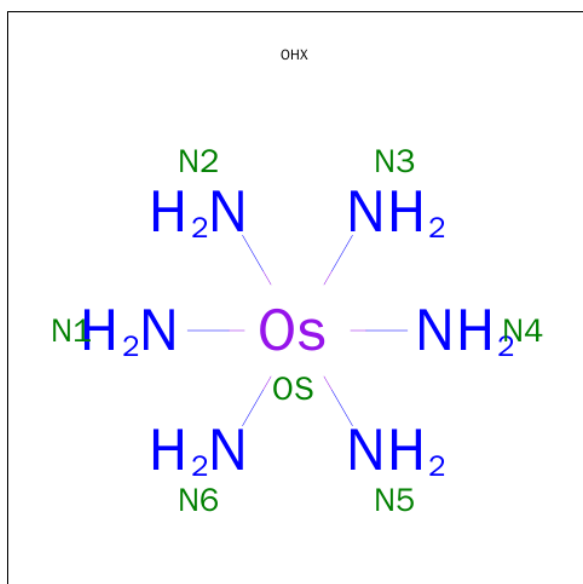
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	o3	2	Total 2	Mg 2	0	0
86	d3	2	Total 2	Mg 2	0	0
86	M3	3	Total 3	Mg 3	0	0
86	N3	3	Total 3	Mg 3	0	0
86	4	21	Total 21	Mg 21	0	0
86	D4	1	Total 1	Mg 1	0	0
86	L2	1	Total 1	Mg 1	0	0
86	l5	2	Total 2	Mg 2	0	0
86	m7	5	Total 5	Mg 5	0	0
86	M7	6	Total 6	Mg 6	0	0
86	N8	3	Total 3	Mg 3	0	0
86	s1	1	Total 1	Mg 1	0	0
86	l9	1	Total 1	Mg 1	0	0
86	s8	2	Total 2	Mg 2	0	0
86	O8	1	Total 1	Mg 1	0	0
86	c7	1	Total 1	Mg 1	0	0
86	7	16	Total 16	Mg 16	0	0
86	n3	2	Total 2	Mg 2	0	0
86	q1	1	Total 1	Mg 1	0	0
86	L3	2	Total 2	Mg 2	0	0
86	d4	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	s4	1	Total 1	Mg 1	0	0
86	l2	2	Total 2	Mg 2	0	0
86	8	14	Total 14	Mg 14	0	0
86	M6	1	Total 1	Mg 1	0	0
86	N0	1	Total 1	Mg 1	0	0
86	3	14	Total 14	Mg 14	0	0

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



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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	S8	1	Total	N	Os	0	0
			7	6	1		
87	C3	1	Total	N	Os	0	0
			7	6	1		
87	C5	1	Total	N	Os	0	0
			7	6	1		
87	C8	1	Total	N	Os	0	0
			7	6	1		
87	D3	1	Total	N	Os	0	0
			7	6	1		
87	D9	1	Total	N	Os	0	0
			7	6	1		
87	SR	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	1	1	Total	N	Os	0	0
			7	6	1		
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	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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87	1	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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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	4	1	Total	N	Os	0	0
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87	L3	1	Total	N	Os	0	0
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87	L3	1	Total	N	Os	0	0
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87	L4	1	Total	N	Os	0	0
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87	M0	1	Total	N	Os	0	0
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87	M5	1	Total	N	Os	0	0
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87	M6	1	Total	N	Os	0	0
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87	M7	1	Total	N	Os	0	0
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87	M7	1	Total	N	Os	0	0
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87	M8	1	Total	N	Os	0	0
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87	M9	1	Total	N	Os	0	0
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87	N1	1	Total	N	Os	0	0
			7	6	1		
87	N9	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	O3	1	Total	N	Os	0	0
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87	O7	1	Total	N	Os	0	0
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87	O7	1	Total	N	Os	0	0
			7	6	1		
87	O9	1	Total	N	Os	0	0
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87	Q2	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	s1	1	Total	N	Os	0	0
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87	s4	1	Total	N	Os	0	0
			7	6	1		
87	s8	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	c1	1	Total 7	N 6	Os 1	0	0
87	c3	1	Total 7	N 6	Os 1	0	0
87	c5	1	Total 7	N 6	Os 1	0	0
87	c8	1	Total 7	N 6	Os 1	0	0
87	d4	1	Total 7	N 6	Os 1	0	0
87	d9	1	Total 7	N 6	Os 1	0	0
87	sR	1	Total 7	N 6	Os 1	0	0
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87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
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87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
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87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	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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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		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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

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

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

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

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

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

- Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

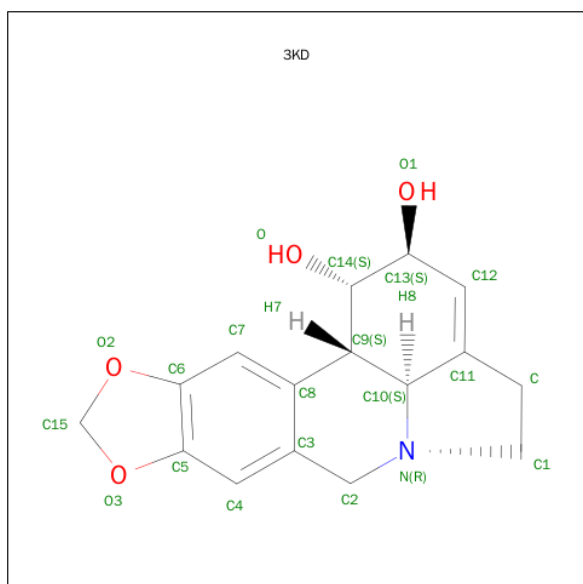
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	q0	1	Total	Zn	0	0
			1	1		
88	D6	1	Total	Zn	0	0
			1	1		
88	Q2	1	Total	Zn	0	0
			1	1		
88	e1	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	Q3	1	Total	Zn	0	0
			1	1		
88	D9	1	Total	Zn	0	0
			1	1		
88	E1	1	Total	Zn	0	0
			1	1		
88	Q0	1	Total	Zn	0	0
			1	1		
88	d7	1	Total	Zn	0	0
			1	1		
88	q3	1	Total	Zn	0	0
			1	1		
88	d9	1	Total	Zn	0	0
			1	1		
88	D7	1	Total	Zn	0	0
			1	1		
88	d6	1	Total	Zn	0	0
			1	1		
88	o7	1	Total	Zn	0	0
			1	1		
88	O7	1	Total	Zn	0	0
			1	1		
88	q2	1	Total	Zn	0	0
			1	1		

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



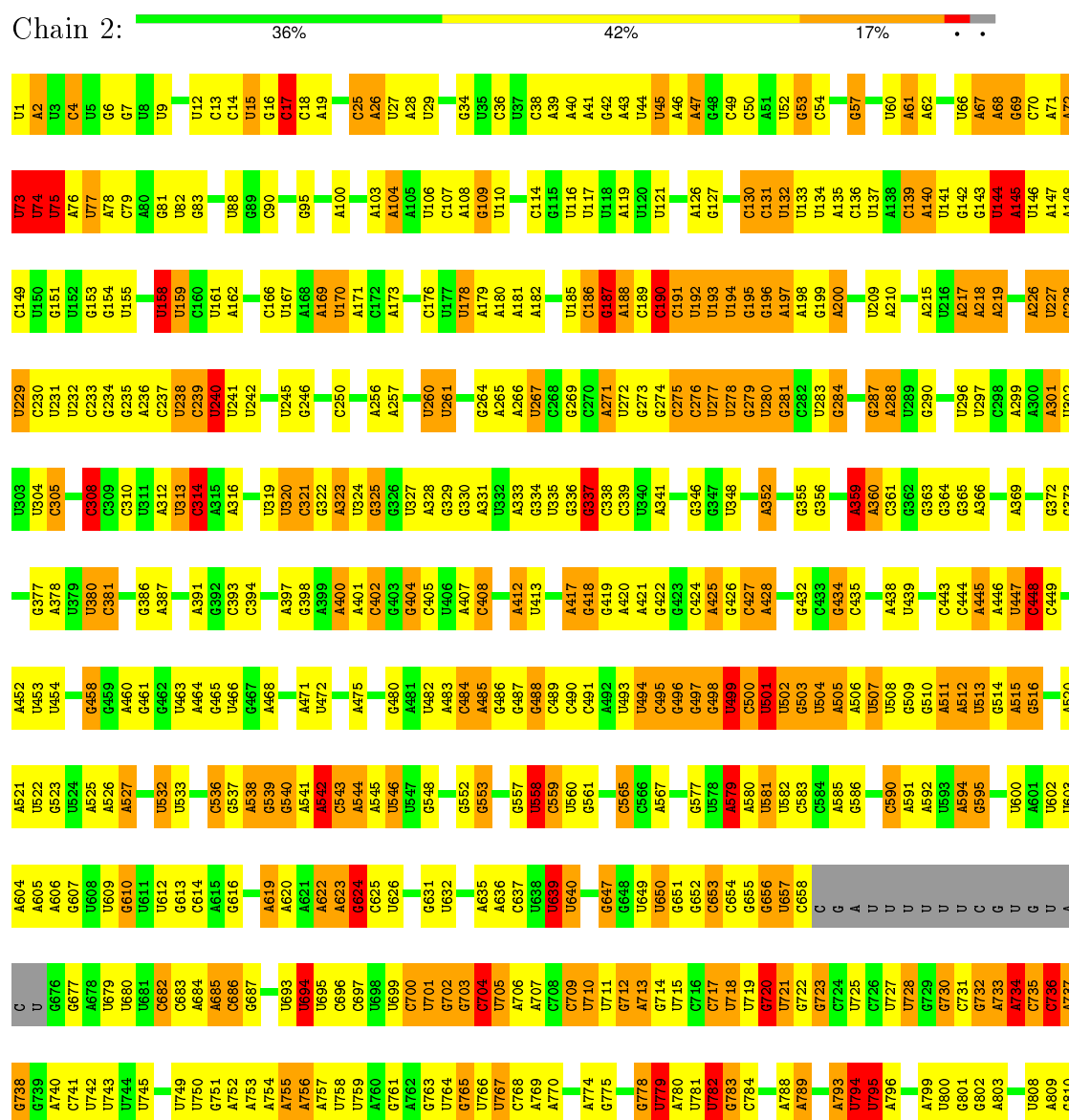
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
89	1	1	Total	C	N	O	0	0
			21	16	1	4		
89	5	1	Total	C	N	O	0	0
			21	16	1	4		

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 errors 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 ($\text{RSRZ} > 2$). 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.

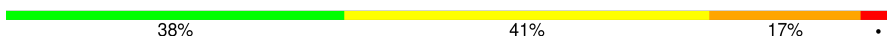
• Molecule 1: 18S ribosomal RNA



A1681	A1753	G1601	G1536	U1473	C1399	A1331	G1255	A1184	G1110	A1026	C943	G875	A811
U1682	A1754	C1602	C1537	G1474	A1400	C1332	A1256	U1185	G1111	A1027	A944	G876	A812
C1683	A1755	U1603	U1538	A1475	A1401	C1333	U1257	U1186	G1112	C1028	A951	G879	U813
U1684	A1756	G1604	G1539	C1476	A1402	U1334	U1258	A1189	A1113	U1029	A952	G880	A814
G1685	G1757	G1605	G1540	A1479	C1403	U1335	G1263	A1190	G1114	A1030	A959	A881	G815
C		C1606	G1541	G1480	A1404	A1336	G1264	U1191	U1115	U1031	U859	U882	G816
U		G1607	G1542	C1481	A1405	C1337	G1265	A1192	A1116	G1032	U860	C883	A817
A		U1608	A1543	G1482	A1406	C1338	G1266	A1193	U1117	C1033	U861	C884	C818
G		G1609	U1544	A1483	A1407	C1339	G1267	A1194	G1118	C1034	C962	G885	G819
G		G1610	A1545	G1484	G1408	U1340	G1268	C1195	G1119	A1039	A966	U886	U820
A		A1611	A1546	A1485	A1409	A1341	G1269	C1196	G1120	G1040	A967	A887	U821
G		A1614	G1548	C1486	A1410	C1342	U1269	A1196	G1121	G1041	A968	U888	U822
A		C1615	A1550	A1487	A1411	U1343	G1270	C1197	C1128	G1042	U868	U889	G823
G		G1616	G1553	G1488	G1412	A1344	G1271	G1198	G1129		C969	C890	G824
G		G1618	U1554	U1489	U1413	A1345	U1272	G1199	U1130	G1046	A970	C891	U825
G		C1620	U1555	A1490	U1414	A1346	G1273	C1200	G1131	A971	A971	A892	U826
C		G1621	A1556	U1491	A1415	U1347	G1274	G1201	A1132	G1051	G972	A893	C827
G		C1622	A1557	A1492	A1416	A1348	U1275	A1202	A1133	U1052	A973	U894	U828
C		C1623	U1558	A1493	A1417	G1349	G1276	A1203	A1138	G1053	A974	C895	A829
A		G1624	U1559	C1494	A1418	U1350	U1277	C1207	A1139	U1058	C975	U896	U830
A		C1625	A1560	A1495	A1419	G1351	G1278	C1208	G1140	U1059	A976	C897	U831
C		U1626	U1561	U1496	A1420	G1354	G1279	C1209	U1145	A1060	A977	A898	U832
U		G1627	G1562	G1498	A1421	C1355	U1280	G1281	U1146	A1061	A978	G899	U833
C		G1628	C1563	C1499	G1428	G1358	U1282	G1212	A1147	A1062	A979	G901	G837
C		G1629	U1564	C1500	A1429	C1359	U1286	G1213	C1148	U1063	G985	G902	G838
A		U1630	C1565	G1501	U1430	A1360	U1287	G1214	G1149	A1064	G986	G913	U839
U		A1631	U1566	G1502	A1431	U1361	U1288	G1215	G1150	A1065	G987	G914	U840
C		A1635	C1567	A1503	A1432	U1362	U1290	A1217	G1151	A1066	A905	A915	U841
C		A1638	C1568	G1504	A1433	U1363	G1291	G1218	A1152	C1066	A932	U916	C842
A		C1639	A1569	A1505	U1434	G1364	G1292	U1225	G1153	C1067	G991	U917	U843
G		G1640	C1570	C1506	G1435	C1365	U1297	A1226	C1156	C1068	A933	U918	U844
A		G1642	U1571	U1507	G1438	U1366	G1299	G1227	A1157	G1073	G994	A919	G845
C		G1646	A1572	C1508	A1446	G1367	A1300	G1228	C1161	A1074	A995	G921	G846
G		U1647	A1573	A1509	U1447	C1368	U1301	G1229	C1162	A1086	G1002	G922	U854
U		G1648	U1574	U1510	C1447	U1369	G1304	A1230	A1163	A1087	G1003	A923	A855
G		G1649	G1575	U1511	U1448	A1370	U1305	U1231	G1164	A1088	U1004	U857	A856
A		U1650	C1580	A1515	U1449	A1371	G1306	U1232	G1165	U1089	A1005	C927	G858
C		A1651	A1583	C1517	A1451	G1375	U1310	A1233	A1166	C1090	C1006	U928	A859
G		C1652	G1584	U1518	G1455	U1378	U1311	G1234	G1167	A1091	U935	A929	U860
A		C1653	U1585	U1519	C1456	U1379	A1312	A1235	U1168	A1092	U936	U861	U861
C		G1654	A1586	G1520	G1457	U1380	U1313	G1236	G1169	A1093	C931	A862	A863
U		U1655	A1587	U1521	C1458	A1381	G1314	U1240	U1170	C1094	U1012	U864	
G		G1656	A1588	U1522	G1459	G1383	G1315	G1241	G1171	A1095	U1013	G867	G867
A		C1657	U1589	G1523	A1460	A1384	G1316	A1244	C1172	C1096	G1014	U937	G868
C		U1658	C1591	A1524	C1461	G1385	G1318	G1245	A1171	U1097	G1015	A930	A869
G		G1659	A1592	U1525	G1462	G1386	A1319	C1246	C1173	U1098	C1016	C937	G870
A		C1660	U1593	U1528	C1463	G1387	U1320	U1247	C1174	A1099	G1017	U1018	G871
C		U1661	G1594	A1529	G1464	A1388	A1321	C1248	U1175	U1099	C1018	A939	G872
G		G1662	U1595	C1530	G1465	C1389	G1322	U1249	G1176	G1100	U1019	A940	G873
A		C1663	G1596	G1531	G1466	U1390	G1324	U1250	G1177	G1101	A1019	G942	G874
C		U1664	U1597	U1532	A1469	A1391	A1325	C1252	G1178	G1107	A1023		
G		G1665	C1598	G1533	C1470	U1392	A1329	U1253	U1182	G1108			
A		C1666	U1599	G1534	A1471	C1393	G1330	U1254	A1183	G1109			
C		U1667	A1600	U1535	C1472	U1398							

• Molecule 1: 18S ribosomal RNA

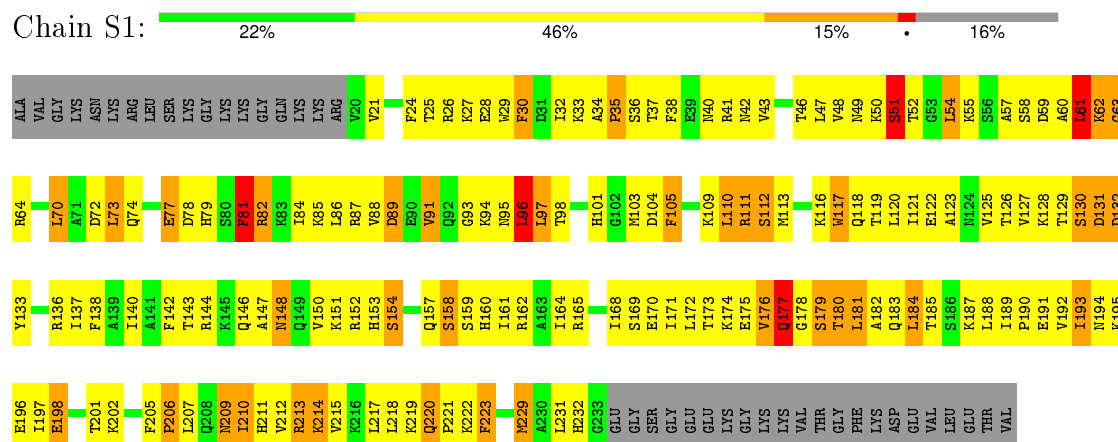
Chain 6:



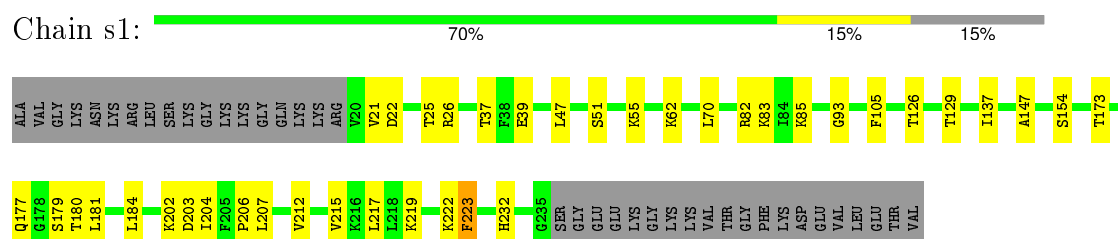
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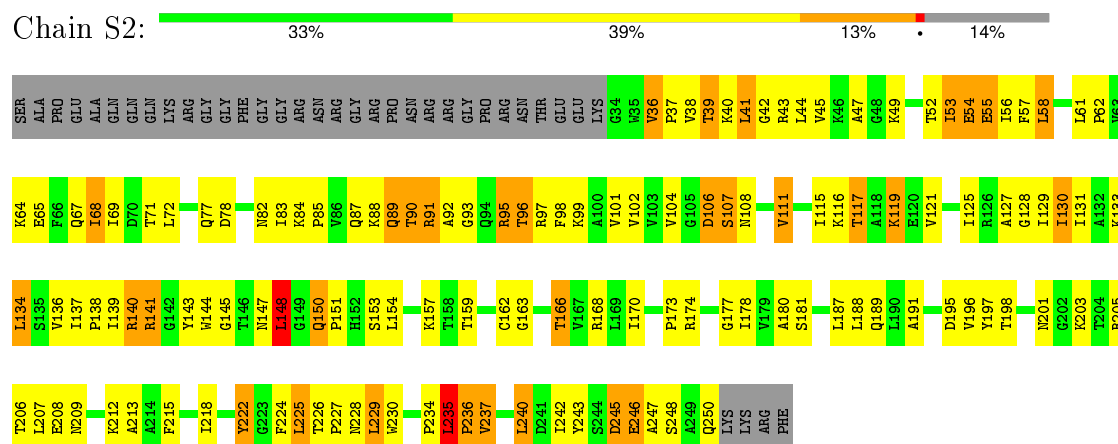
- Molecule 3: 40S ribosomal protein S1-A



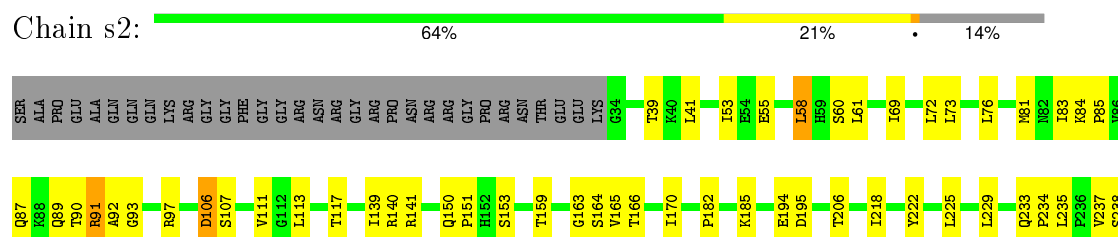
- Molecule 3: 40S ribosomal protein S1-A



- Molecule 4: 40S ribosomal protein S2

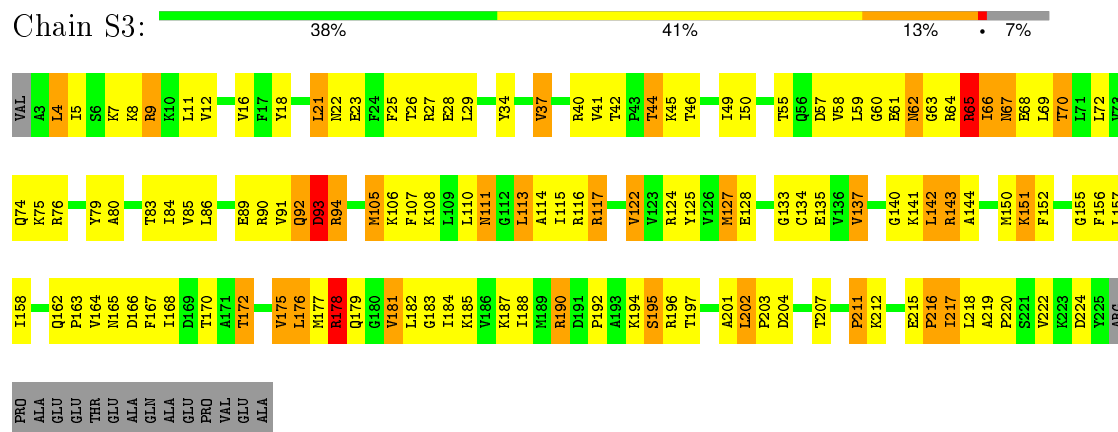


- Molecule 4: 40S ribosomal protein S2

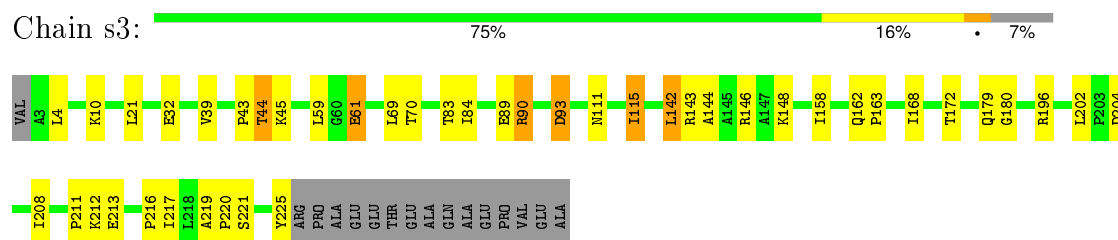




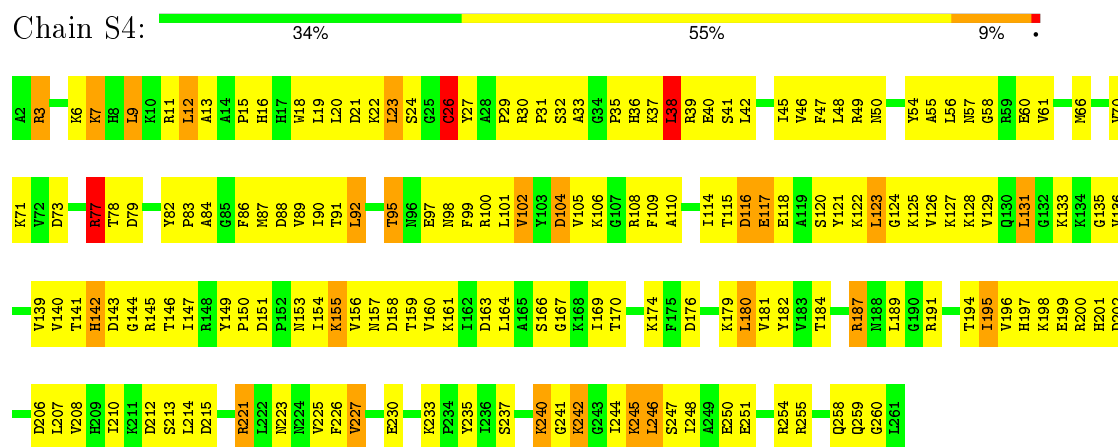
• Molecule 5: 40S ribosomal protein S3



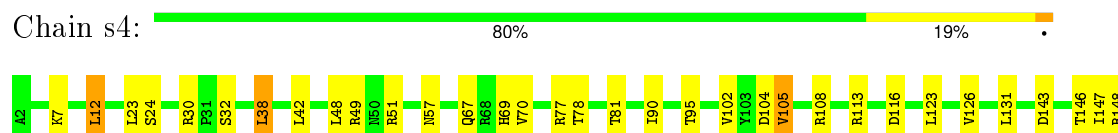
• Molecule 5: 40S ribosomal protein S3



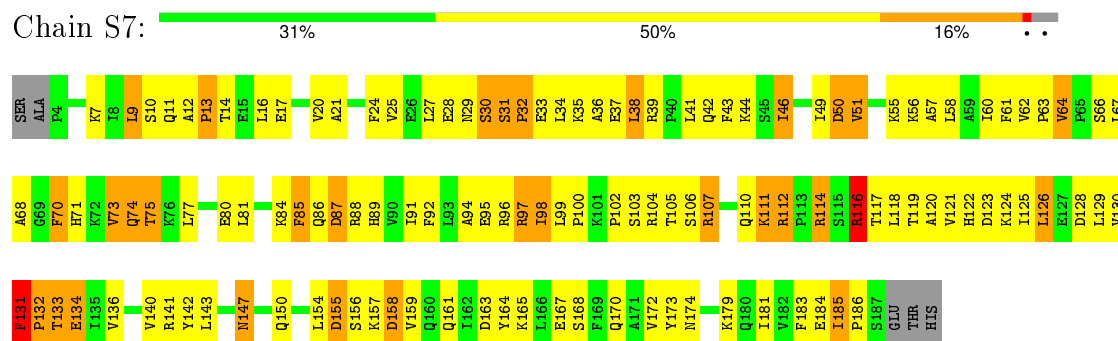
• Molecule 6: 40S ribosomal protein S4-A



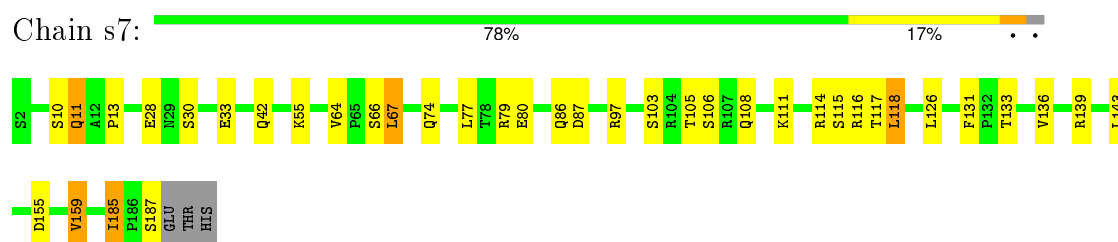
• Molecule 6: 40S ribosomal protein S4-A



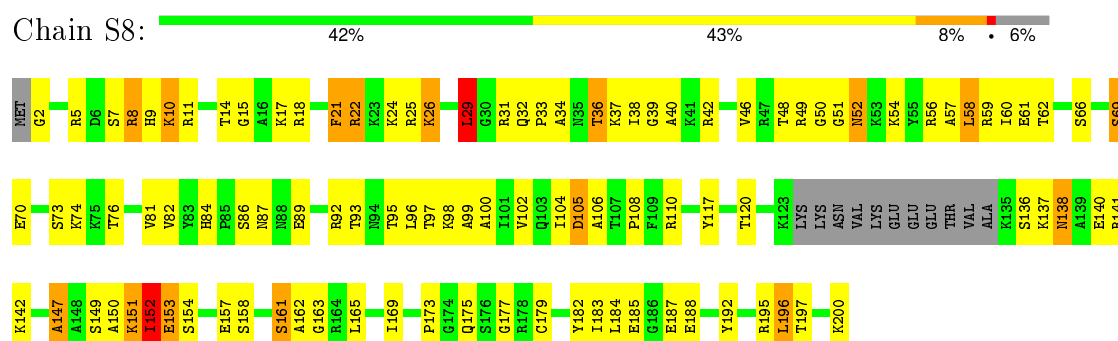
- Molecule 9: 40S ribosomal protein S7-A



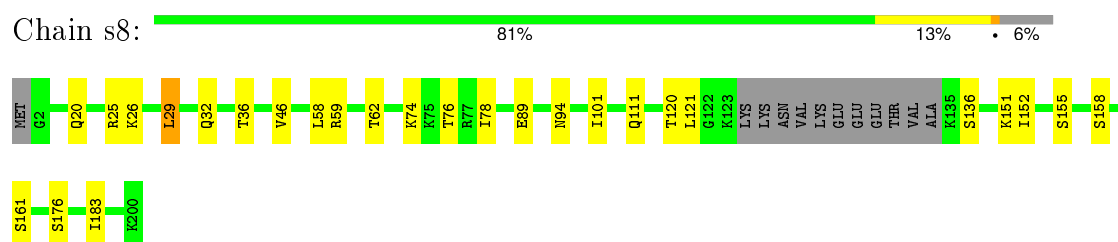
- Molecule 9: 40S ribosomal protein S7-A



- Molecule 10: 40S ribosomal protein S8-A

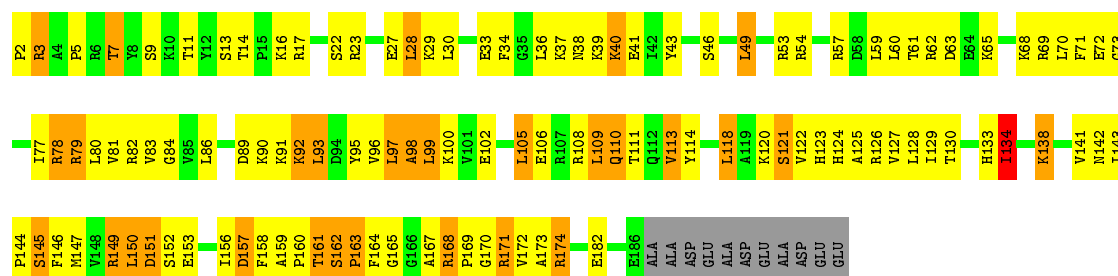


- Molecule 10: 40S ribosomal protein S8-A

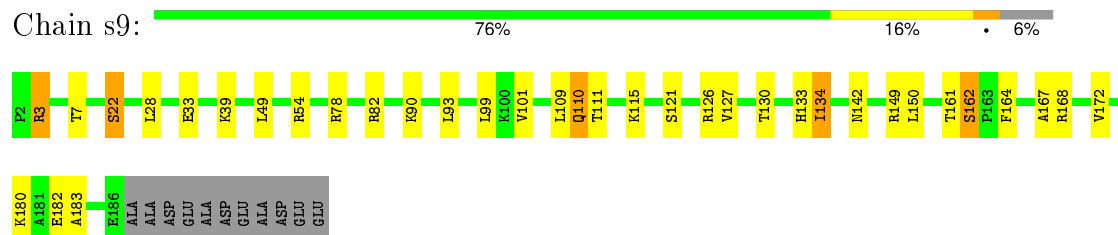


- Molecule 11: 40S ribosomal protein S9-A

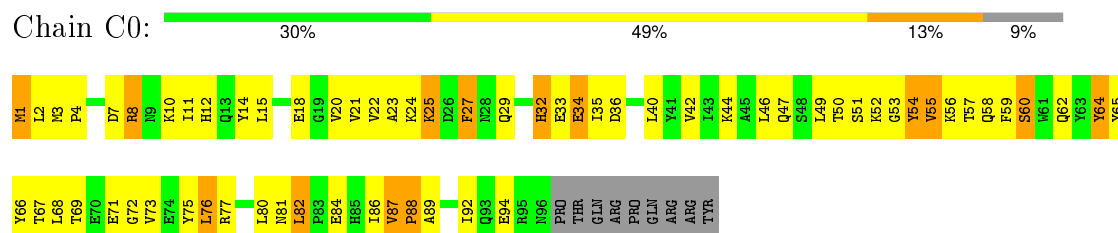




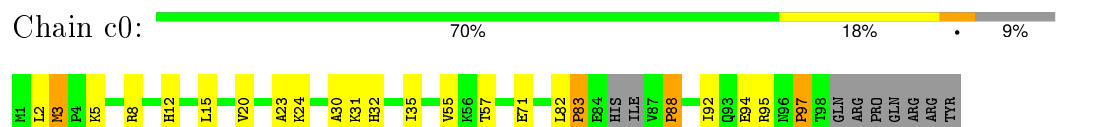
- Molecule 11: 40S ribosomal protein S9-A



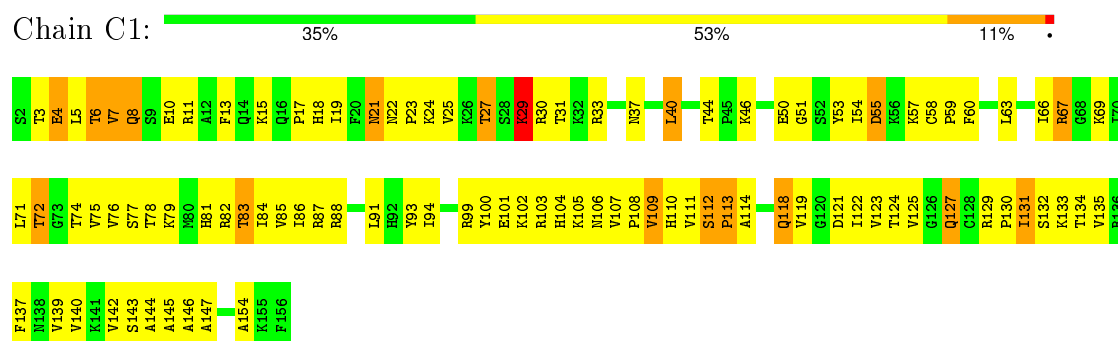
- Molecule 12: 40S ribosomal protein S10-A



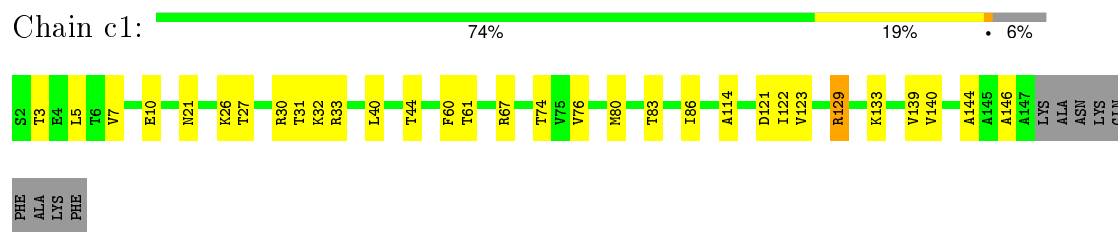
- Molecule 13: 40S ribosomal protein S11-A



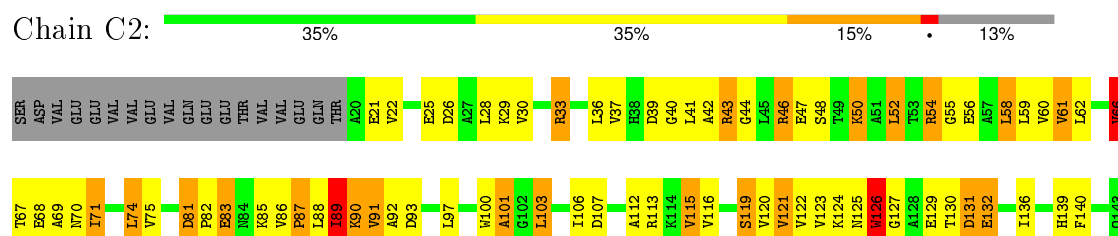
- Molecule 13: 40S ribosomal protein S11-A



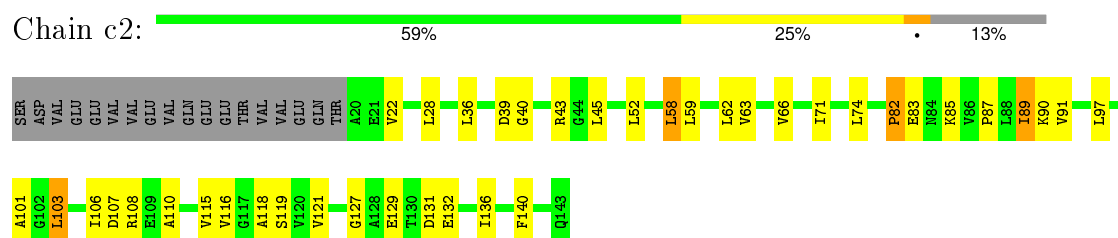
- Molecule 13: 40S ribosomal protein S11-A



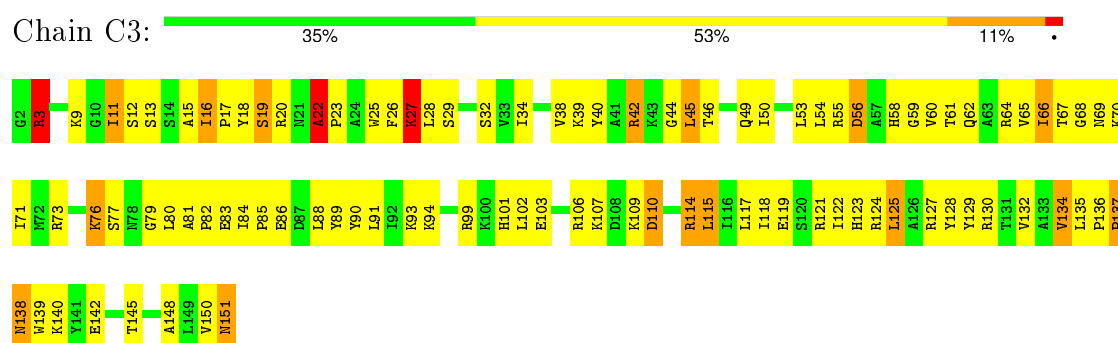
- Molecule 14: 40S ribosomal protein S12



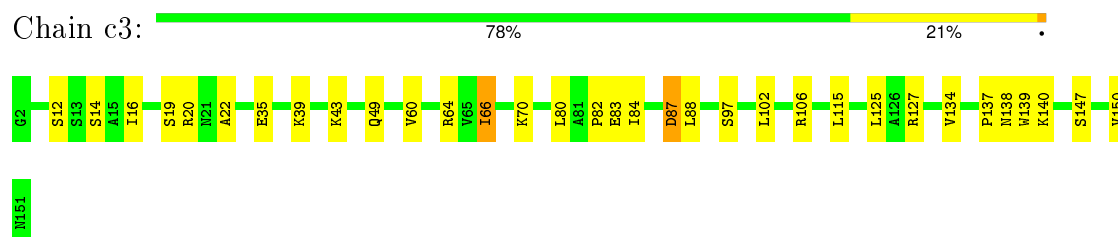
- Molecule 14: 40S ribosomal protein S12



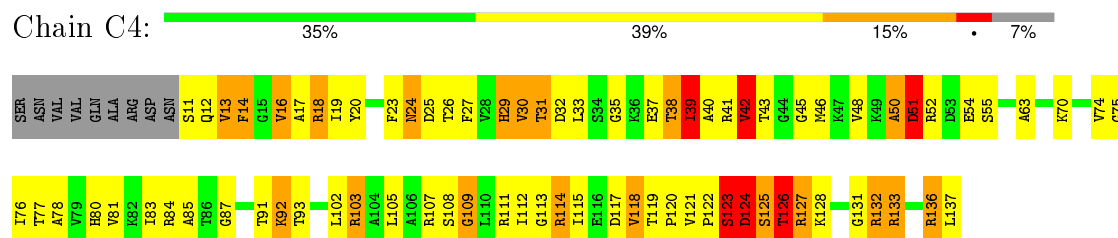
- Molecule 15: 40S ribosomal protein S13



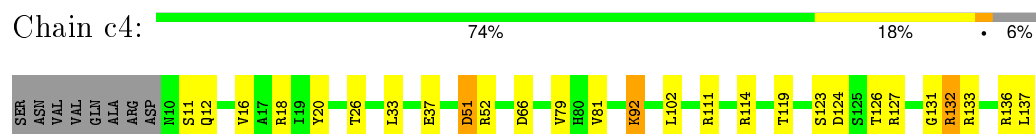
- Molecule 15: 40S ribosomal protein S13



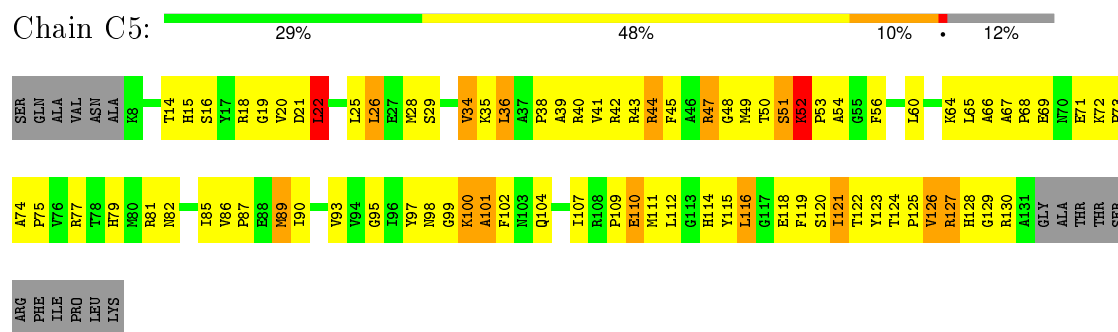
- Molecule 16: 40S ribosomal protein S14-A



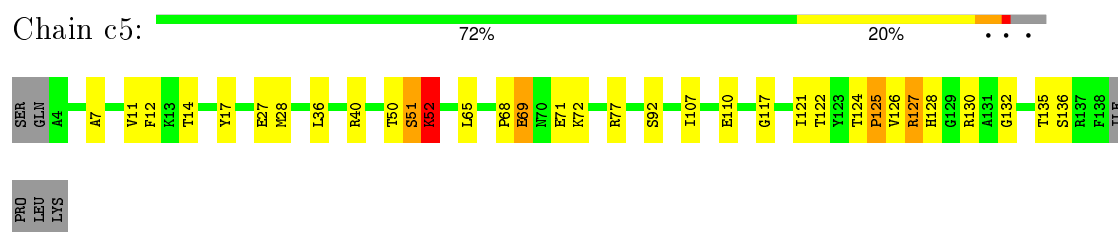
- Molecule 16: 40S ribosomal protein S14-A



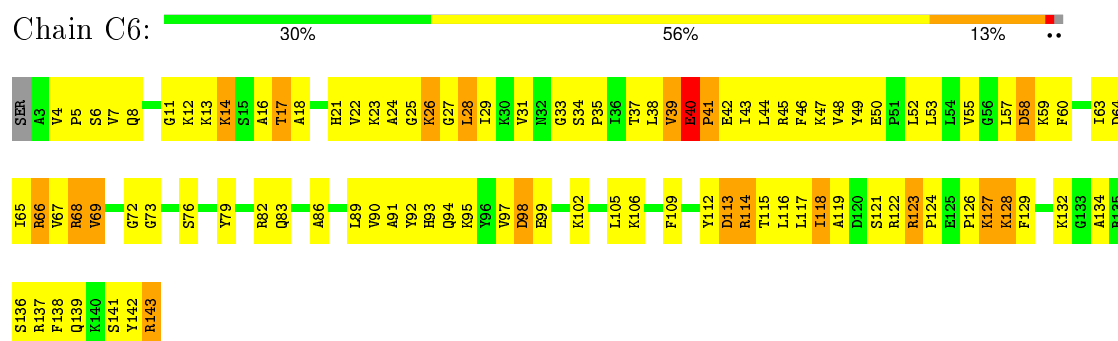
- Molecule 17: 40S ribosomal protein S15




- Molecule 17: 40S ribosomal protein S15



- Molecule 18: 40S ribosomal protein S16-A




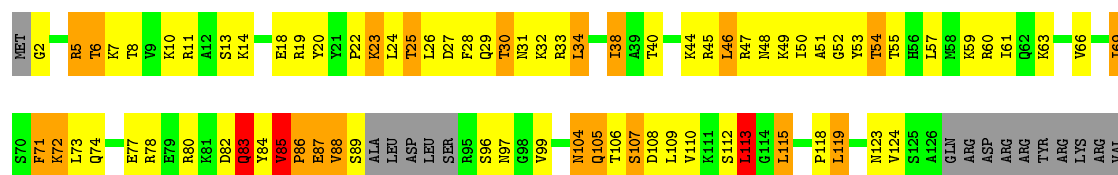
- Molecule 18: 40S ribosomal protein S16-A

Chain c6:  77% 21% •



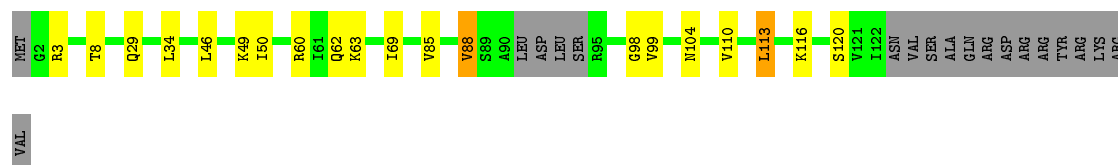
- Molecule 19: 40S ribosomal protein S17-A

Chain C7:  31% 40% 15% 12% •



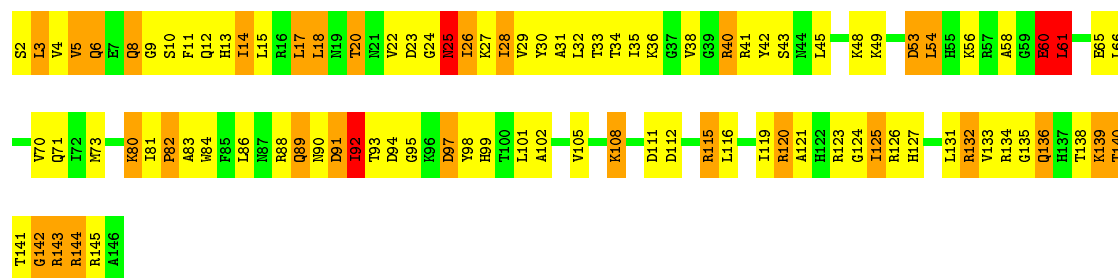
- Molecule 19: 40S ribosomal protein S17-A

Chain c7:  71% 13% 14% •




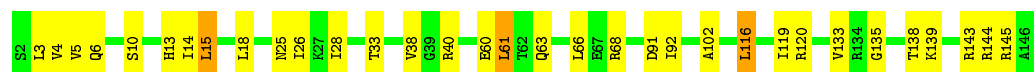
- Molecule 20: 40S ribosomal protein S18-A

Chain C8:  33% 44% 20% •



- Molecule 20: 40S ribosomal protein S18-A

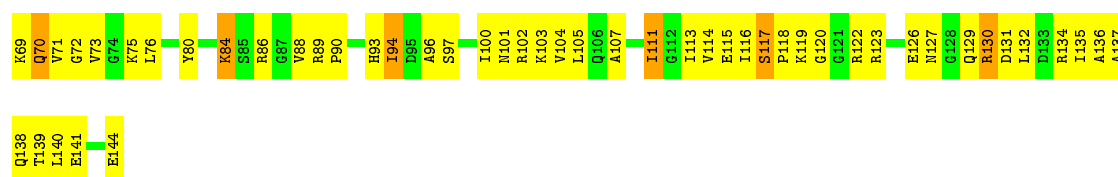
Chain c8:  77% 21% •



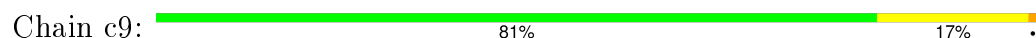
- Molecule 21: 40S ribosomal protein S19-A

Chain C9:  36% 52% 12% •

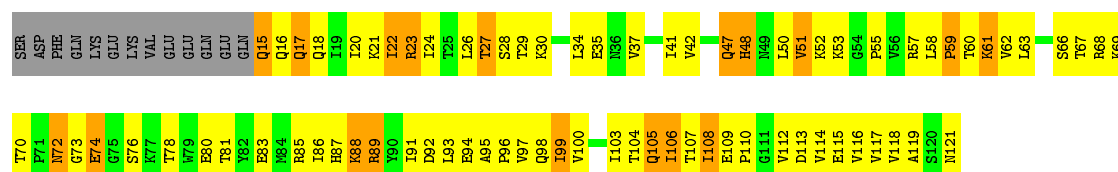




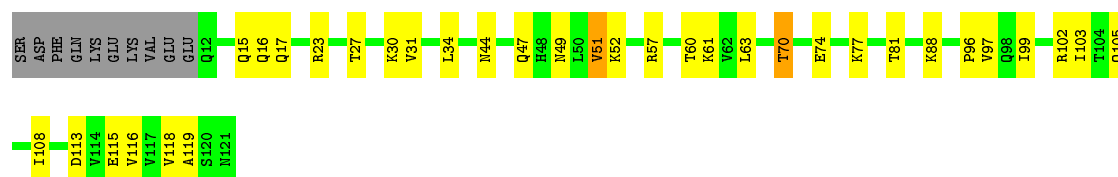
- Molecule 21: 40S ribosomal protein S19-A



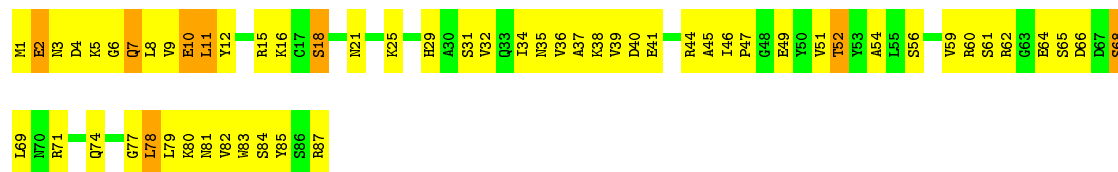
- Molecule 22: 40S ribosomal protein S20



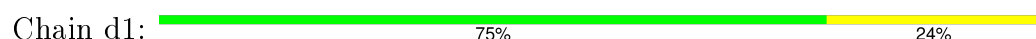
- Molecule 22: 40S ribosomal protein S20



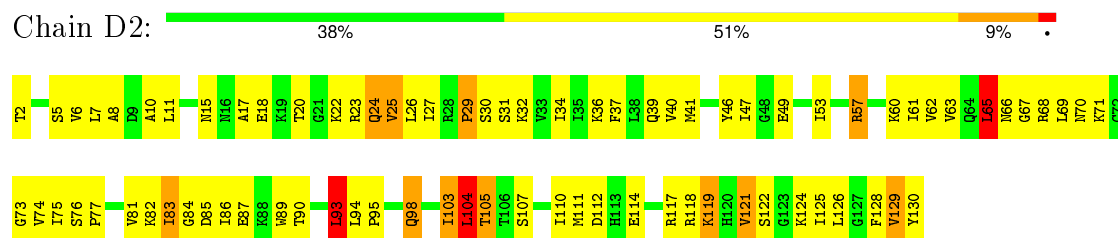
- Molecule 23: 40S ribosomal protein S21-A



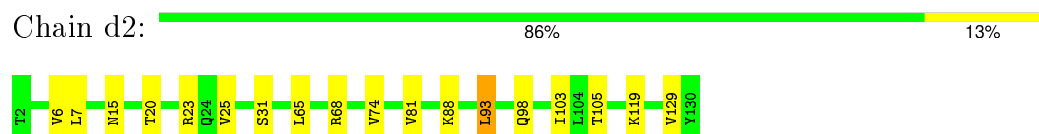
- Molecule 23: 40S ribosomal protein S21-A



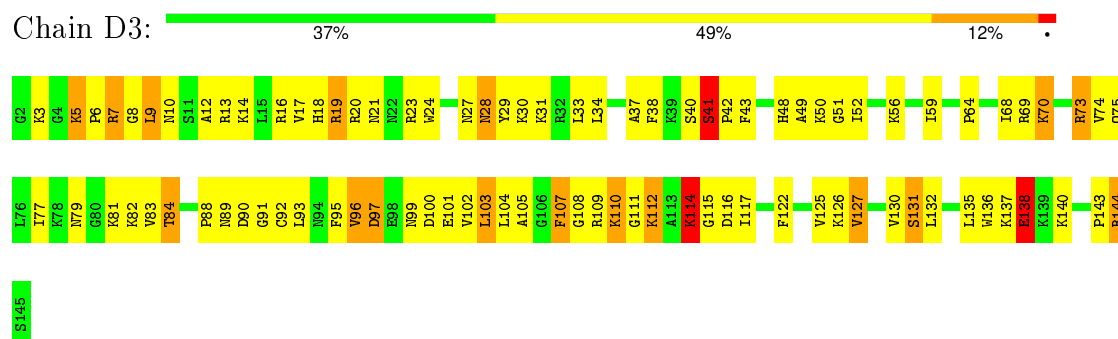
- Molecule 24: 40S ribosomal protein S22-A



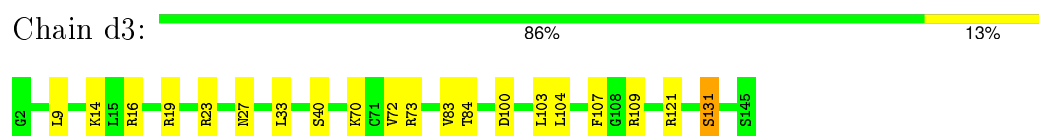
- Molecule 24: 40S ribosomal protein S22-A



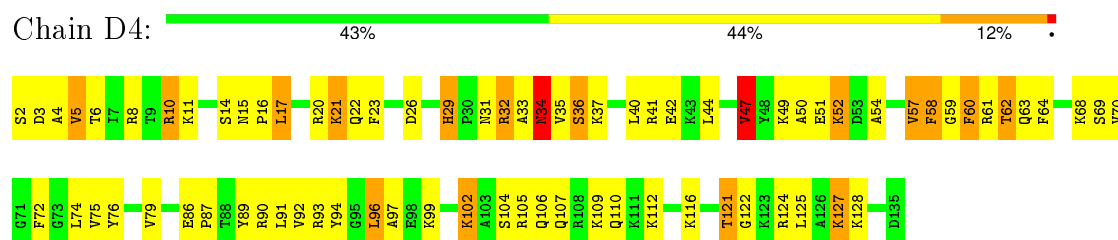
- Molecule 25: 40S ribosomal protein S23-A



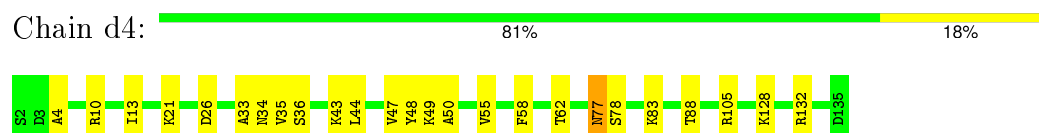
- Molecule 25: 40S ribosomal protein S23-A




- Molecule 26: 40S ribosomal protein S24-A



- Molecule 26: 40S ribosomal protein S24-A



- Chain d7:  80% 19%



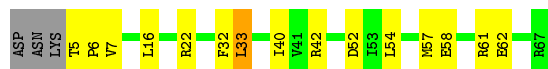
- Molecule 30: 40S ribosomal protein S28-A

Chain D8: 33% 47% 14% 5%



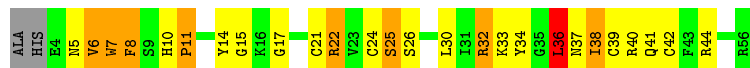
- Molecule 30: 40S ribosomal protein S28-A

Chain d8: 73% 21% 5%



- Molecule 31: 40S ribosomal protein S29-A

Chain D9: 49% 31% 15% 5%



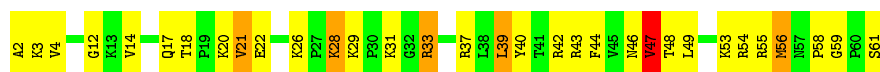
- Molecule 31: 40S ribosomal protein S29-A

Chain d9: 71% 25% 5%



- Molecule 32: 40S ribosomal protein S30-A

Chain E0: 47% 43% 8% 5%



- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1: 24% 37% 33% 7%



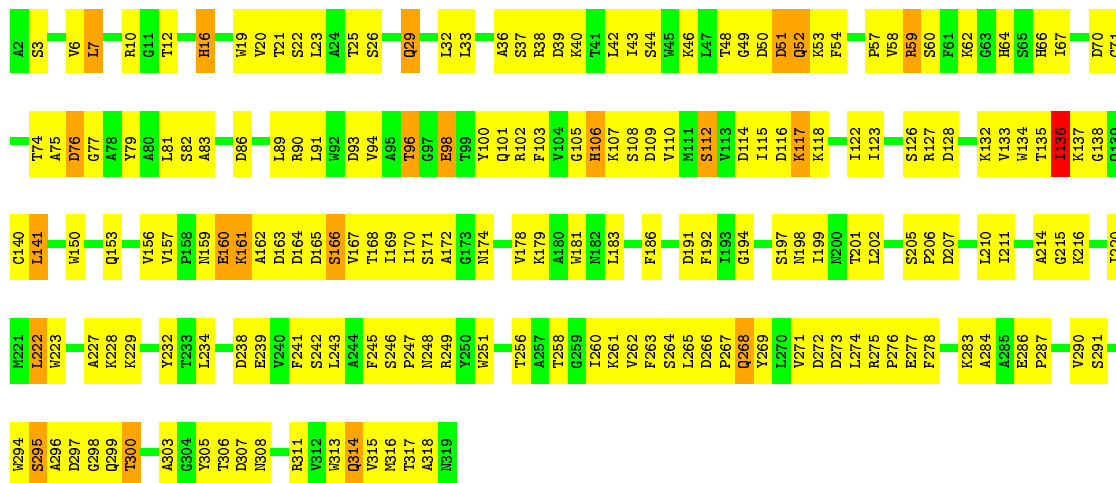
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1: 59% 34% 7%



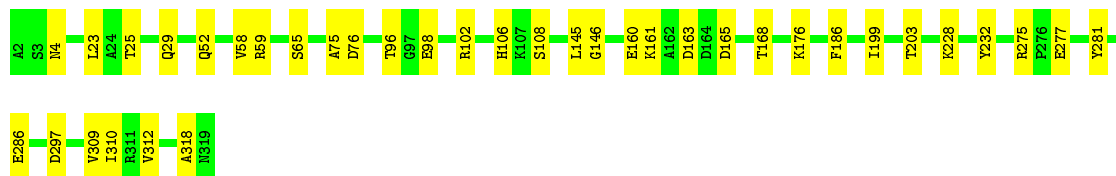
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR: 40% 53% 7%



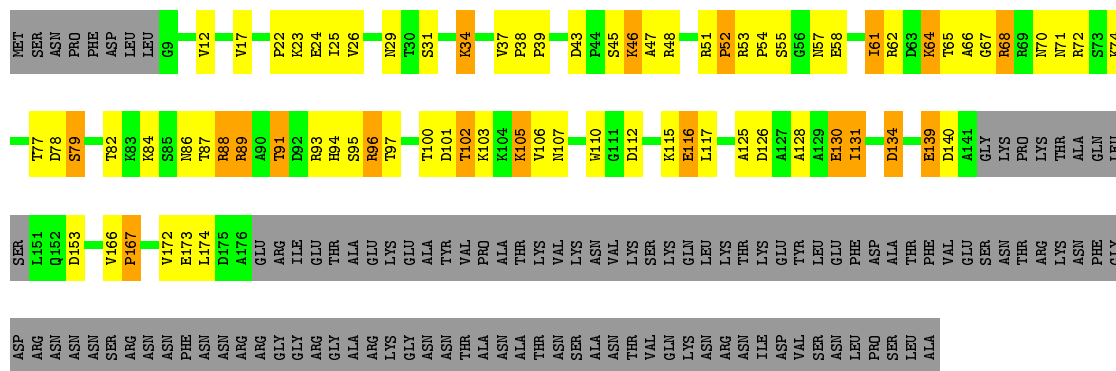
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR: 88% 12%



• Molecule 35: Suppressor protein STM1

Chain SM: 30% 21% 7% 42%



• Molecule 36: 25S ribosomal RNA

Chain 1: 33% 39% 17% 7%

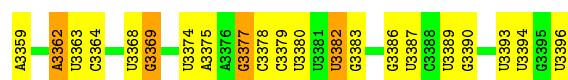
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G1145	A1074	A1003	C838	C863	G792	U707	U639	A572	G	U430	A357	A289	U217	U134	C72	U3
	A1075	U1004	U939	G864	C793	A708	C641	U574	U	U430	G358	G290	G218	U135	C73	U4
G1148	U1078	A1006	G941	G870	U794	A709	C641	C573	G494	C435	U359	C291	G219	G136	G74	G5
G1149	A1079	U1007	U942	U871	U796		G644	G575	A498	A436	A361		A219	G137	G75	A6
A1150	A1080		U943	U872	U797	G712	A645			G437	U362	A295	C220	U138	C7	C8
A1151	U1081	G1010	C873	C873	U798	U713	A646	A578	A498	A438	U363	A296	A221	G139	G76	C9
A1152	U1082	G1013	U874	G875	U799	G714	A647	C580	A501	C439	G363	G297	A222	U140	A77	
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C1155	U1015	U1016	C948	C877	C802	C717	C650	G582	A504	G	A368	G300	C226	G148	U14	
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A1158	U1094	G1018	A951	U880	G805	A720	A653	A585	U508	U	U371		G229	G155	U84	A17
A1159	U1095	G1019	C881	G875	A806	G721	C654	A585		U	A372	A307	U230	U84	G17	A18
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A1165	U1101	U1026	C958	G887	G812	C730	A660	A592	G530	U	A385	C315	A238	G162	G92	G24
G1166	A1102	G1028	C959	A888	G813	G737	A666	C594	A521	C	A386	U316	G239	A157	G93	U25
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G1168	G1104		C961	C890	G815	C743	C663	G595		C	G388	A318	G245	U167	G27	
A1169		U1033	A962		A816	A736	U664	G600	U528	U						
A1170	U1108	U1034	G963	C893	A817	A736	A665	U601	A529	U	A391	G320	G242	G168	G96	C28
G1171	U1109	G1035	G964	G894	G818	C737	A666	A602	G531	C	A392		G243	U169	U97	C29
G1172	U1110	A1036	A965	A895	U819	G737	C667	A603	A532	U	A393		G244	U169	G98	G30
U1173	U1111	C1037	A896	A896	A820	G742	U668	G604	A533	U	G394	A323	U245	G172	A99	G31
A1174	A1112	C1038			U821	C743	U669	U605	A534	U	A396	A325	U249	G173	A100	U32
C1175	U1039	U1039	G969	G900			C670	C906	U534	C	A397	U326	U250	C174	G101	G83
G1176	C1176	A1040	A970	A970	C824	A751	U671	A608	G535	C	A398		G251	C175	A34	
U1177	G1115		G971			U756	A672	A608	A537	U	A399	U329	U252	C180	G103	A35
G1178	G1116	U1043	A972	A906	A827	U756	U673	G610	U541	U	G400	G330		U181	A107	U38
A1179	G1117	U1044	A973	G907	A828	G763	U674	G610	U541	U	U401	G331	G256	U184	A108	A39
A1180	C1118		G974	G909	U829	G763	C675	A811		U	A402	C332			A109	A40
U1181	C1119	A1047	C975	G910	A830	U764	A676	U612	C544	G	C403	G333	C289	A187	G110	G41
A1182	A1120	A1048	U976	C911	G831	C765	A677	G613	U546	U	G404	A334	C290		C111	C42
C1183	U1121	C1049	C977			G678	U678	C614	C546	U	U405	G335	U261	U112	A43	
A1184	U1122	U1050	G978	A914	G835	U767	U679	C618	C547	U	A406	A336	U262	U113	U44	
		U1051	G979	A915	A836	G768	G680		G548	A	A407	G337	U263	U191	U44	
		U1052	A880	G916	A837	C769	U681	A619		U	A408	A338	C264	C182	A49	
		A1053	U881	A917	A838	G770		U620	A551	G	A409	C339	A266	A116	A52	
		A1054	C982	C918	C839	C765	G685	A621	G552	U	U410	G340	A286	G197	U118	G53
		U1056	A983	U919	C840	U776	G686	U622	U553	U	U411	G341		U118	G53	
			G984	A920		U777	U687	U623	A554	A	U412	A342	A289	U119	C54	
				A921	A846	U778	U687	G624	U555	U	U413	U343	U270	A199	G120	
		U1060		U922	A847	G779	A691		U556	U		A344	C271	C200	A57	
		A1061		C923	A848	A780	A692	U627	A557	C	A417	G345	G272	A201	G58	
		A1062	G991		C849	A781	A693	U628	U558	U	A418	C346		A123	G59	
		G1063	A992	U829	C849	U782	C694	A629	U559	C	G419	G347	U276	G206	U124	A60
		A1064	G993	A783		U783	C695	A630	G560	U	G420	A348		U207	C125	A61
		A1065	A994	A784	G854	U631	C696	U631	C561	C	G421	A349	U279	C208	U126	A62
		G1066	C931	G785	U855	G632	A697	C632	C562	A	A422	C350	U280	C209	G127	A63
			U932	A786	G856	C633	U698	C633	U563	U	A423	A351	G281	U210	G128	G54
			A933	G787	G859	C634	A699	G634	G564	U	G424	A352	G282	A211	U129	A65
		C1069	G934	C788	G860	C788	G700	G636	U565	U	G425	G353	G283	G212	A130	A66
		U1071		A789			G701		G566	C	G426	U354	A284	A213	C131	A67

U2274	G2206	C2132	U	A1867	G1784	U1692	C1608	G1543	A1474	G1404	C1342	A1274	U1207
	A2207	U2133	U		U1785	C1693	C1609	G1544	A1475	U1405	A1343	C1275	U1208
	A2208	G2134	G	C1870	G1786	U1694		A1545	G1476	A1406	G1344	G1276	G1209
	A2209		U	C1871	A1787	U1695	A1613	A1546	A1477	A1407	G1345	C1277	U1210
	A2210	A2138	A	U1871	C1788	A1696	C1614	G1547	C1478	G1408	G1346	A1278	U1211
	A2211	A2139	G	A1874	G1789		C1615		U1479	G1409	G1347	G1278	A1212
	C2212	U2140	A		G1790	C1701	U1616	G1551	G1480	U1410	U1348	C1280	G1213
		U2141	C	U1877	C1791	U1702	G1617	G1552	A1481	C1411	G1349		U1214
	A2215	A2142	C	G1878	C1792	U1703	G1618	U1553	A1482	G1412	A1350	G1285	U1215
	G2216	G2143	G	A1879	C1793	U1704	A1619	U1554	G1483	G1413	U1351	A1286	C1216
	U2217	A2144	U	U1880	G1794	U1705	U1620	U1555	U1484	G1414	A1352	A1287	A1217
	G2218		C	U1795	U1795			G1556	G1485	U1415	U1353		U1218
	A2219	U2147	G	A1886	G1796	G1712	G1623	A1557	G1487	G1416	G1354	G1292	
		U2148	C	A1887	A1797				G1488	G1417	A1355	U1293	A1221
			U	U1890	G1798	U1716	U1629	G1560	A1489	A1418	U1356	G1294	G1222
	A2222	A2152	U	A1891	A1799	U1717	U1630	G1561		A1419	G1357	G1295	
	A2223		G	G1892	G1799	G1718	C1631	C1562		G1420	C1358	G1296	A1225
	U2224	G2155	C	U1893	C1802	U1719	A1632	C1563	G1492	G1421	C1359	C1297	G1226
	U2225	C2156	G	A1894	C1803	U1720	C1633	U1564	G1493			U1298	G1227
	U2226	G2157	U	U1895	G1807		G1634	G1565	U1494		G1362	U1299	C1228
	U2227	A2158	C	A1896	G1808	A1723		G1566	U1495	A1428	A1363	G1300	
	A2228	U2159	A	G1897	G1809	U1724	C1639	U1567	G1496	G1429	C1364	A1303	G1230
	A2229	G2160	A	U1898	A1810	C1725		U1568		A1433	G1365	A1304	A1231
	A2233	G2161	U	G1899	A1811		A1642	U1569	G1500	A1434	A1366	U1305	C1232
		U2162	U	A1900	G1812	A1731	C1644	U1570	U1501	A1435	G1367	G1233	
	G2236	C2163	U	A1901	A1813		U1645	A1571	C1502	U1436	U1368	G1234	G1234
	C2237	A2164	A	G1902	A1814	G1735		U1572	A1503	C1437	A1369	G1307	U1235
	G2238	G2165	C	U1903	U1815	U1736	G1645	U1573	A1504	G1440	G1370	A1308	G1236
	G2239	A2166	G	G1904	G1816	A1737	G1655	C1574	C1505	G1441	A1371	G1309	G1237
	G2240	U2167	U	U1905	A1817	U1740	A1656	A1575	A1506	U1442	C1372	G1310	C1238
	U2241	A2168	G	G1906	U1818	U1741	C1657	G1576	G1507	G1443	G1373	G1311	G1239
	A2242	U2170	C	C1907	U1819	U1742	G1658	U1577	C1508	U1444	G1374	C1312	A1240
	A2243		C	U1908	U1820	G1743	U1659	C1578	A1509	G1445	C1375	G1313	U1241
	A2244	U2173	U	A1909	U1821	C1744	G1660	C1579	G1510	A1446	C1376	U1315	G1242
	G2246		U	A1910	C1822	G1745	G1661	A1580		G1447	G1377	U1316	G1243
	G2247	U2176	G				G1662	C1581	G1513	U1448	U1378	A1244	A1245
	C2248	G2177	U	U1916	C1826	A1748	C1663	C1582	G1514	A1449	G1380	A1317	G1246
			U	C1917	G1827	A1749	G1664	A1583	A1515	G1450	A1381	A1318	
			G	C1918	U1834	U1750	C1665	U1584	G1520	C1451	G1382	C1320	U1247
			U	G1919	A1835	G1751		G1585	G1521	A1453	G1383	U1322	G1248
			G	U1920	U1836	A1752	C1669	A1587	U1522	A1454		G1323	G1249
			A	U1921	C1837		C1670	A1588	U1523	U1455	A1386	U1324	
			U	C1923	U1838	C1761		A1589	A1524		U1387		G1255
			U	U1924	G1839	C1762	G1674			C1459	U1388	C1327	U1256
			G	U1925	U1840	U1763	G1675	G1592	G1525	A1460	G1328	A1259	A1260
			C	C1926	U1841	U1764	A1676	A1594	U1526	A1461	C1329	G1261	G1262
			G	G1927	A1842	U1765		U1595	C1527	A1462	A1330	G1263	G1264
			U	A1933	C1843	C1767	G1680	C1596	U1528	U1463	A1331	A1263	
			U	G1934	C1844		U1681	C1597	U1530	G1464	A1332	G1264	
			G	U1935	G1845	G1770	U1682	G1598	C1531	A1465	G1333	U1265	U1265
			U	C1936	U1846	C1771	U1683	G1599	U1532	G1466	C1334	G1266	
			C	U1937	A1847	U1772	C1685		U1533	A1467	C1335	U1267	G1268
			G	G1938	G1848	C1773	U1686	A1534	U1534	U1468	U1336	G1268	
			G	C1941	C1849		U1687	A1602	A1535	C1469	A1337	U1269	
			U	U1942		G1780	U1688	A1603		U1470	C1400	C1338	A1270
			U	G1943		C1781	U1689	G1604	U1539	U1471	A1401	C1339	A1271
			G	C1944		U1782	C1690	A1605	U1540	U1472	C1402	G1340	
			C	A1945		U1783	U1691	U1606		G1473	A1403	U1341	A1273



C2192	C2128	G	U	U1853	G1790	U1695	G1604	U1533	G1464	A1394	G1323	U1241	U1162	G1097
A2198	U2129	G	G	C1856	C1791	A1696	A1605	U1533	G1464	G1395	G1329	G1242	A1098	A1098
A2199	A2130	U	C	C1857	C1792	A1699	U1606	G1536	A1465	C1396	A1330	G1243	A1099	A1099
U2200	A1936	A	U	C1857	C1793	G1700	G1607	G1536	A1466	C1397	A1330	G1244	U1100	U1100
G2201	U2133	G	U	A1858	G1794	C1701	C1608	G1541	A1467	U1398	U1331	G1245	G1101	G1101
G2202	U2134	U	G	A1859	G1795	U1702	C1609	G1542	A1468	A1399	A1332	G1246	A1102	A1102
U2203	G2134	C	U	G1863	G1796		G1610	G1542	A1469	G1400	C1333		A1103	A1103
C2204	U2135	U	U	G1863	G1797			G1547	U1472	G1403	U1334	G1249	A1170	G1104
U2205	C2136	U	G	C1866	A1798	C1710	A1613	G1547	U1472	C1403	U1335	G1250	U1108	U1108
G2206	A2138	C	G	A1867	C1799	C1711	C1614	C1548	G1473	G1404	U1336	A1251	C1175	U1109
A2207	U2139	U	G	G1868	A1800	G1719	C1615	U1549	A1474	U1405	A1337	A1252	G1176	U1110
U2208	G1948	G	C	G1868	U1801	U1717	U1620	U1563	A1475	A1406	C1338	U1253	G1177	U1111
U2209	G1949	U	U	A1874	C1802	G1718	A1621	U1563	A1476	A1407	C1339	C1254	A1112	A1112
G2210	U2142	A	U	G1875	C1803	G1719	U1622	U1564	A1477	G1408	U1258		G1113	G1113
U2211	A2143	G	U	A1876	A1804	U1720	A1638	U1565	C1478	G1409	A1259	A1180	U1181	U1181
C2212	U2144	A	C	G1877	C1805	U1721	A1639	U1566	G1488	U1410	U1336	A1260	G1115	G1115
A2213	A2145	C	U	U1878	A1806	U1722	G1629	G1567	A1489	G1412	U1348	G1261	C1183	G1116
C2214	C2146	C	C	A1879	C1807	A1723	C1631	G1561	A1490	G1413	G1349	G1262	G1117	G1117
A2215	U2147	G	U	U1880	G1808	U1724	A1632	C1562	A1482	G1414	U1350	A1263	A1184	A1184
	A2148	U	U	A1881	A1809	C1725		C1563	G1483	U1415	A1351	A1264	C1187	C1118
G2216	A2149	C	C	G1882	A1810	C1726	A1637	U1564	G1487	G1416	U1352	U1265	U1188	U1120
U2217	G2150	G	U	G1883	C1811	G1727	A1638	G1565	G1488	G1417	U1353	U1266	C1189	U1121
		C	A	A1884	G1812			A1566	A1489	A1418	G1354	U1265	A1190	U1122
U2153	U2153	U	G	U1885	A1813	G1733	G1640	U1567	A1490	A1419	A1355	A1270	U1191	U1123
G2154	G2154	U	G	A1886	A1814	G1734	U1641	U1568	A1491	A1420	U1356	A1271	U1124	U1124
G2155	G2155	G	C	A1887	U1815	G1735	A1642	U1569	G1492	G1421	G1357		U1125	U1125
G2156	G2156	C	C	U1888	A1816	G1736	A1643	U1570	G1493	G1422	G1358	U1276	G1126	G1126
A2158	A2158	U	A	G1889	C1817			A1571	U1494	C1423	C1359		G1127	G1127
G2159	U2159	G	U	A1891	U1818	A1750	U1645	U1572	U1495	C1424		G1289	U1128	U1128
U2160	C2160	C	U	U1892	A1819	G1761		G1573	C1496		G1362	A1290	A1198	A1198
		A	A	U1894	U1820	A1762	G1650	C1574		U1427	G1363		C1199	A1130
C2163	C2163	G	G	A1895	U1821	G1763	U1651	A1575	C1499	A1428	C1364	G1295	A1200	G1131
A2164	A2164	U	C	U1896	C1822	G1764	G1652	G1576	G1500	G1429	G1365	C1296	G1201	G1132
G2165	G2165	U	C	A1897	A1823	C1755		G1577	U1501	U1430	A1366	C1297	A1202	A1133
A2166	A2166	A	U	G1898	U1824	C1756	G1657	C1578	C1502	G1431	G1367	C1298	G1203	G1134
A2167	A2167	G	G	G1902	G1825		G1658	C1579	A1503	C1432	U1368	U1298	A1204	A1135
G2168	G2168	C	A	G1902	G1825	A1760	U1659	A1580	A1504	A1433	A1369	G1300	A1136	A1136
A2169	A2169	G	C	G1906	U1830	C1761	C1660	C1581	C1505	G1434	G1370	A1301	U1208	C1137
U2170	U2170	C	U	C1907	U1831	C1762	G1661	C1582	A1506	A1435	C1371	A1302	G1209	U1138
		C	C	A1910	C1832	U1763	G1662	U1583	G1507	U1436	C1372	A1303		
U2174	A2093	C	U	A1911	G1833	U1764		U1584	C1508	C1437	A1373	A1304	A1212	A1143
U2175	C2094	C	U	A1912	U1834	U1765	A1667	C1585	A1509	U1438	G1374	U1305	G1213	U1144
U2176		U	U	U1912		G1766	G1668	G1586		U1439	C1375	G1306	U1145	U1145
G2177		U	G	G1913	U1837		C1669	A1587	G1513	G1440	G1377	A1308	C1146	C1146
C2178		G	U	G1914	G1838	G1769		A1588	G1514	U1445	U1378	U1309	G1147	G1147
U2179	U2112	U	G	A1915	C1839	C1770	G1677	A1589	A1515	U1446	G1379	A1310	A1221	G1148
G2180	A2113	G	U	U1916	U1840	U1772	G1678	G1591	C1516	A1447	G1380	G1311	G1222	G1149
C2181	C2114	U	U	C1917	A1841	C1773		G1592	U1518	U1448	A1381	C1312	A1150	A1150
A2182	G2115	A	U	C1918	C1842			A1593	G1519	A1449		G1313	G1226	U1151
G2183	G2116	G	G	G1919	C1843	G1778	A1683	A1594	U1519	G1450	C1385	C1314	A1231	G1152
C2185	A2117	A	U	U1920	G1844	C1779	U1684	U1595	G1520	G1451	A1386	U1315	C1232	A1153
U2186	A2120	C	U	U1925	C1846	C1780	G1685	C1596	U1521	A1452	G1387	C1316	C1155	C1155
C2187	G2121	G	G	G1926	A1847	C1781	U1686	C1597	U1522	U1455	U1388	A1317	U1235	C1156
A2188	G2122	C	U	G1927	G1848	U1782	U1687	C1598	A1524	U1456	U1389	A1318	G1236	G1157
U2189	G2123	C	G	G1928	C1849	U1782	U1688	G1599	U1524	A1456	A1390	G1319	G1237	A1158
U2190	G2124	U	C	A1929	U1850	U1785	U1689	G1599	G1528	A1460	A1391	C1320	C1238	A1159
U2191		C	U	A1932	G1851	G1786	U1691	U1601	U1530	A1461	A1393	G1321	C1239	C1160
					G1852	A1787						U1322	A1240	G1161





- Molecule 37: 5S ribosomal RNA

Chain 3: 39% 50% 11% .



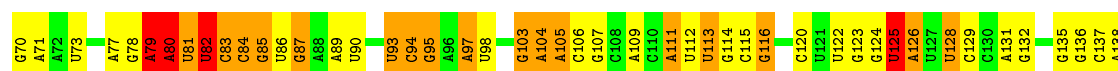
- Molecule 37: 5S ribosomal RNA

Chain 7: 35% 43% 17% 6% .



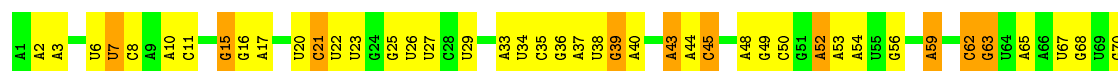
- Molecule 38: 5.8S ribosomal RNA

Chain 4: 34% 41% 22% .



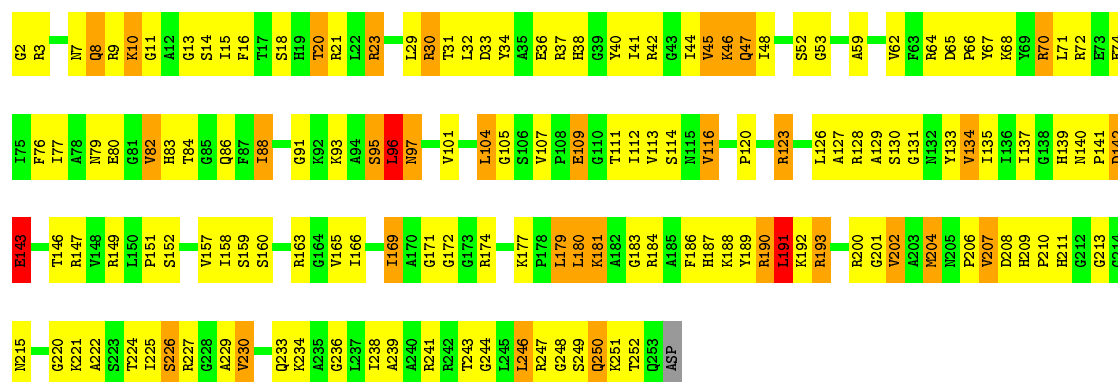
- Molecule 38: 5.8S ribosomal RNA

Chain 8: 36% 46% 15% .

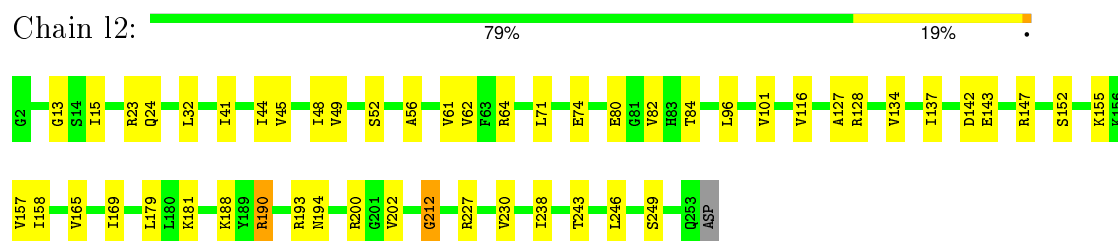


- Molecule 39: 60S ribosomal protein L2-A

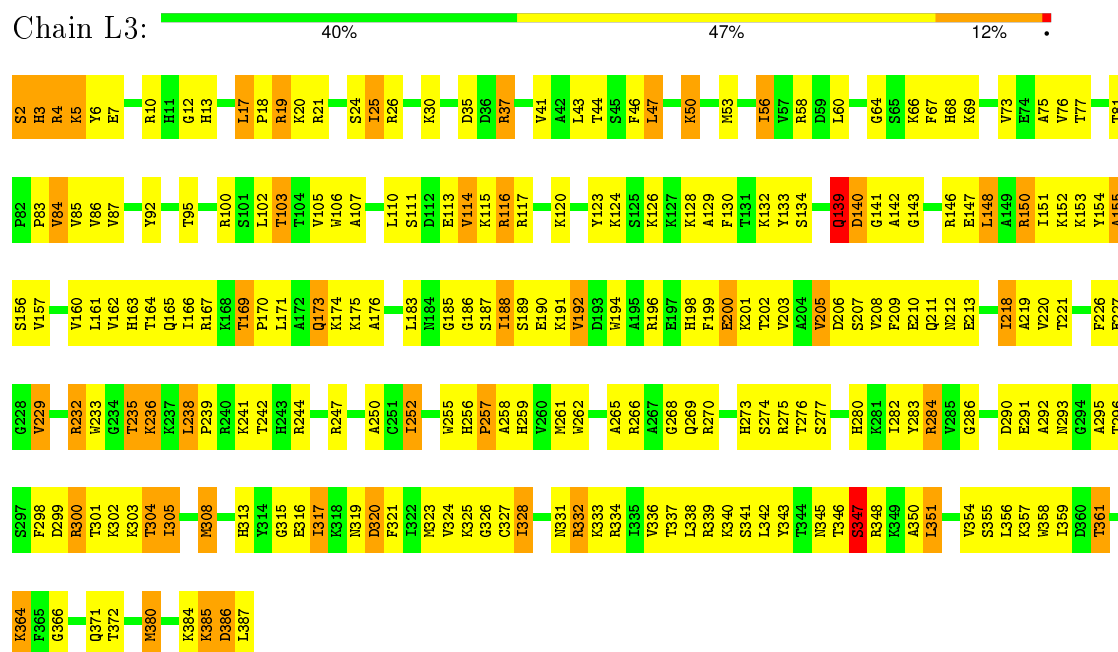
Chain L2: 40% 46% 13% .



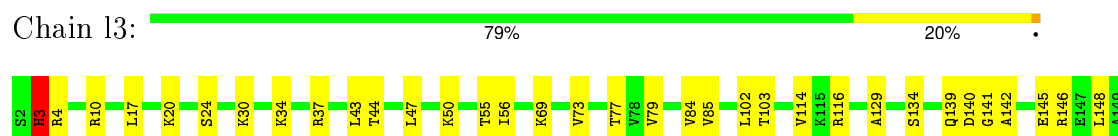
• Molecule 39: 60S ribosomal protein L2-A



• Molecule 40: 60S ribosomal protein L3



• Molecule 40: 60S ribosomal protein L3



G230
N231
R232
E233
E234
F235
I236
I237
K238
L239
SER
GLN
V240
K241
S242
K243
I244

• Molecule 44: 60S ribosomal protein L7-A

Chain 17: 77% 13% 8%

ALA
ALA
GLU
LYS
ILE
LEU
THR
PRO
GLU
SER
GLN
LYS
LYS
LYS
LYS
V26
A32
E39
K40
L45
E54
E59
R60
K82
L83
R88
R100
K121
L124
I130
M157
K158
Q159
L163
L173
G174
K175
I178

L179
S180
I181
L184
V191
G192
K196
K219
F220
K221
G226
F229
E234
L239
I244

• Molecule 45: 60S ribosomal protein L8-A

Chain L8: 35% 47% 10% 9%

ALA
PRO
GLY
LYS
VAL
ALA
PRO
ALA
PRO
PHE
GLY
LYS
SER
THR
ARG
N24
P25
L26
T27
E28
L29
T30
F31
K32
K33
F34
G35
I36
G37
Q38
R44
M45
L46
S47
R48
Y49
V50
K51
M52
P53
E54
Y55
V56
R57
V58
Q59
R60
Q61

K62
K63
L64
L65
S66
I67
R68
L69
K70
V71
I74
I75
A76
Q77
F78
Q79
Y80
T81
L82
D83
R84
E89
L90
T90
F91
R92
L93
F94
N95
R98
P99
E100
T101
E104
K105
K106
E107
R108
L109
K110
T110
K111
E112
A113
A114
A115
V116
A117
E118
P129
Y130
Y131
V132
K133
Y134
L136

N137
H138
V139
V140
L141
L142
I143
E144
M145
K146
K147
L148
A149
L150
I153
A154
N155
D156
V157
D158
P159
I160
E161
L162
V163
V164
F165
L166
L169
K170
K171
K172
V175
P176
Y177
A178
I179
V180
K181
G182
K183
A184
R185
L189
V190
N191
Q192
K193
T194
S195
A196
A199
L200
T201
G202

V203
R204
A205
E206
D207
E208
L211
A212
K213
L214
V215
S216
T217
I218
A223
D224
K225
V229
K230
K231
G236
L237
L238
G239
N240
K241
A242
Q243
A244
K245
D246
D247
K248
D254
S255
A256

• Molecule 45: 60S ribosomal protein L8-A

Chain 18: 72% 17% 9%

ALA
PRO
GLY
LYS
VAL
ALA
PRO
ALA
PRO
PHE
GLY
LYS
SER
THR
ARG
N24
P25
L26
F34
A39
V40
Q41
L65
R68
L69
K70
V71
T74
Q79
Y80
T81
T90
N95
R98
L109
E112
A117
E118
G119
E121

K122
K133
L136
K149
L150
I153
L160
V164
L169
K183
A184
R185
T188
N191
A196
V203
E208
K213
L214
T217
K230
I237
L238
G239
N240
K241
K245
K248
D254
SER
ALA

• Molecule 46: 60S ribosomal protein L9-A

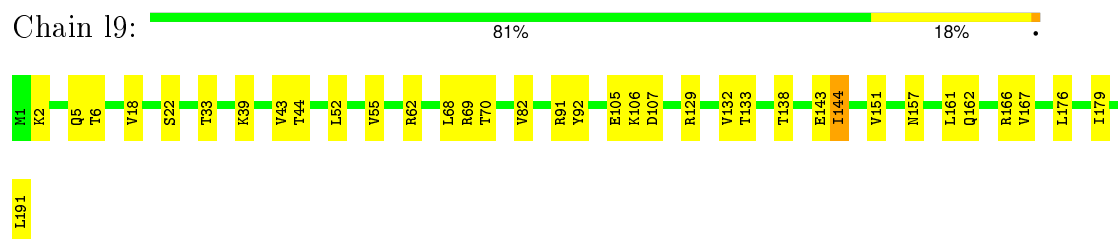
Chain L9: 34% 51% 15%

M1
K2
Y3
I4
Q5
T6
E7
Q8
Q9
I10
E11
V12
P13
V16
T17
V18
S19
I20
K21
S22
R23
I24
V25
K26
V27
G29
T33
L34
T35
A36
N37
L38
K39
H40
I41
D42
T44
K47
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V57
G60
G61
R62
K63
H64
V65
A66
A67

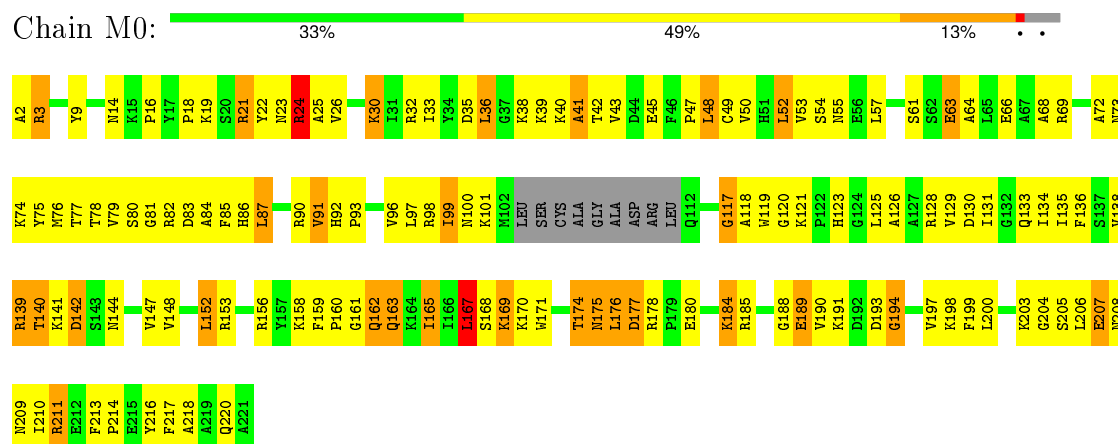
L68
R69
T70
V71
K72
V75
D76
N77
M78
I79
T80
G81
V82
G85
Y86
K87
V88
K89
P90
Y91
I92
Y93
Y94
A95
R96
F97
P98
I103
Y104
E105
K106
D107
G108
A109
K110
I111
I112
E113
V114
R115
D120
I123
R124
N125
V126
P127
R129
V132
T133
I134
E135
F136
S137

T138
M139
V140
K141
D142
E143
I144
V145
L146
S147
V151
E152
Q156
M157
D160
L161
Q162
Q163
I164
C165
R166
V167
R168
D171
R172
R173
K174
F175
L176
D177
G178
I179
Y180
V181
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H183
K184
G185
F186
I187
T188
E189
D190
L191

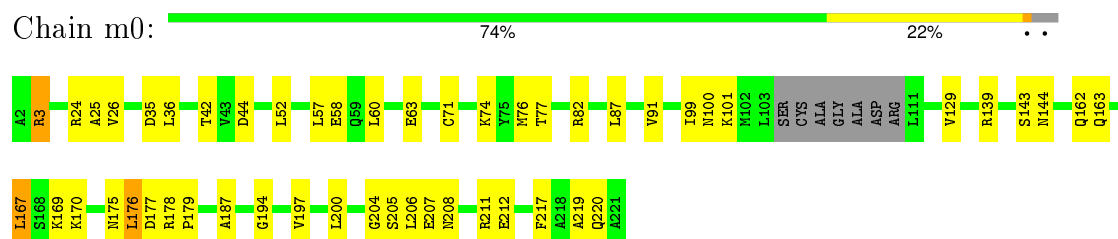
- Molecule 46: 60S ribosomal protein L9-A



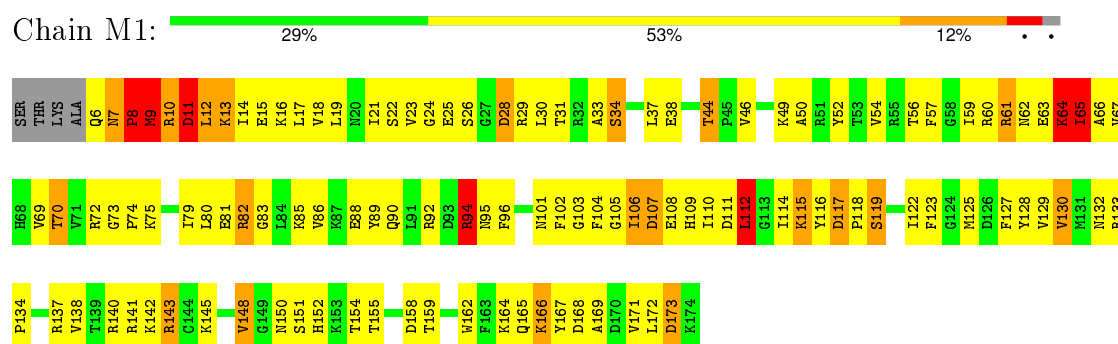
- Molecule 47: 60S ribosomal protein L10



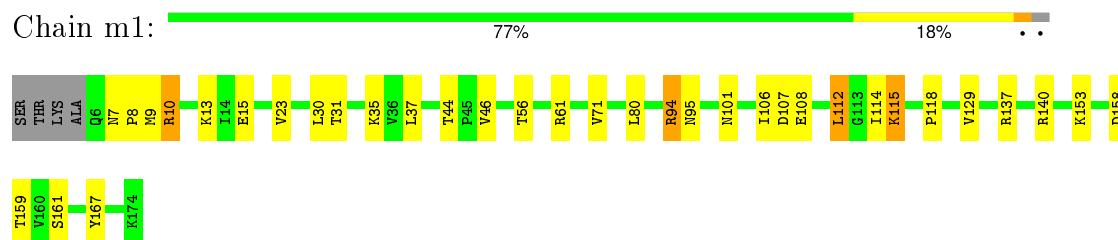
- Molecule 47: 60S ribosomal protein L10



- Molecule 48: 60S ribosomal protein L11-B



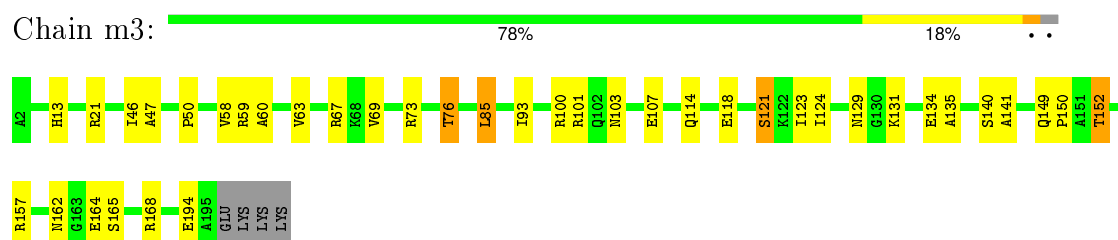
- Molecule 48: 60S ribosomal protein L11-B



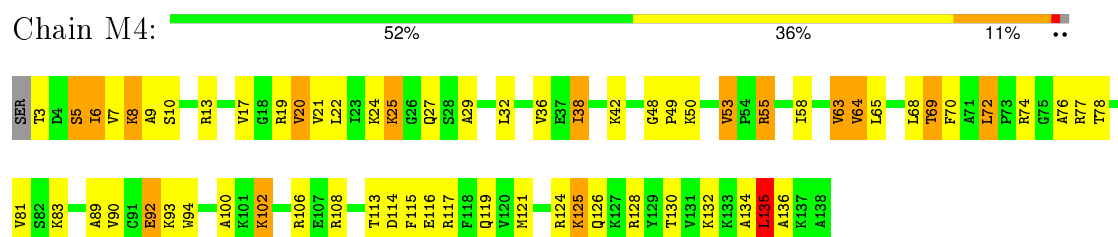
- Molecule 49: 60S ribosomal protein L13-A



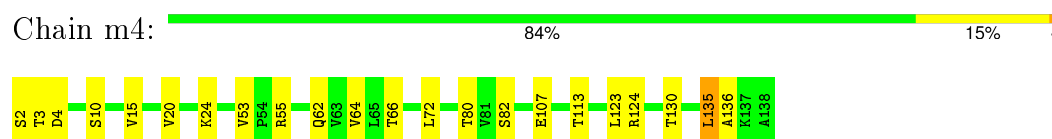
- Molecule 49: 60S ribosomal protein L13-A



- Molecule 50: 60S ribosomal protein L14-A



- Molecule 50: 60S ribosomal protein L14-A



- Molecule 51: 60S ribosomal protein L15-A





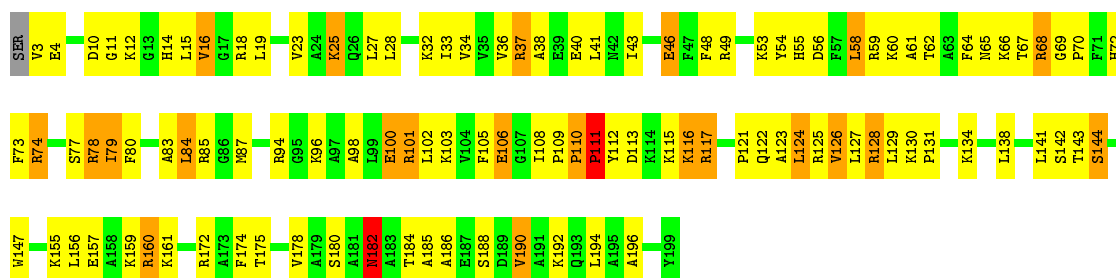
- Molecule 51: 60S ribosomal protein L15-A

Chain m5: 85% 14%



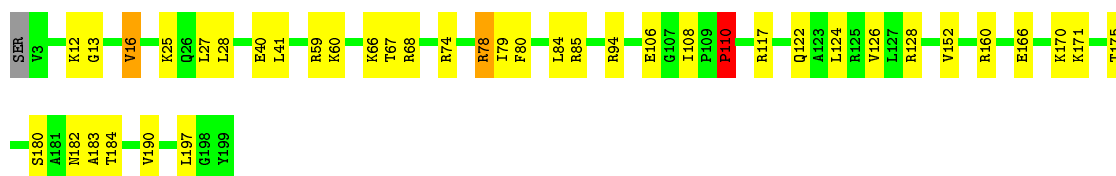
- Molecule 52: 60S ribosomal protein L16-A

Chain M6: 44% 43% 11%



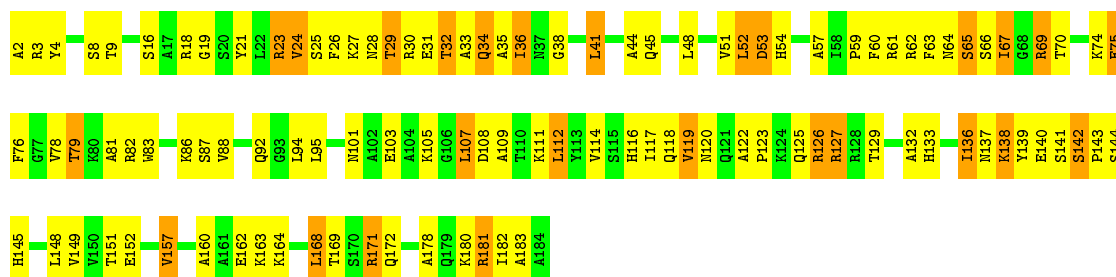
- Molecule 52: 60S ribosomal protein L16-A

Chain m6: 79% 19%

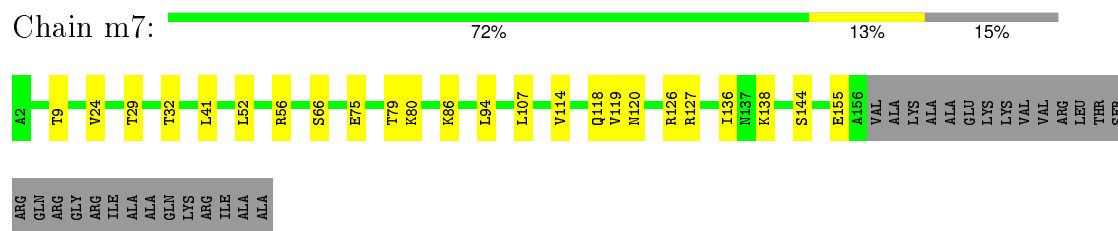


- Molecule 53: 60S ribosomal protein L17-A

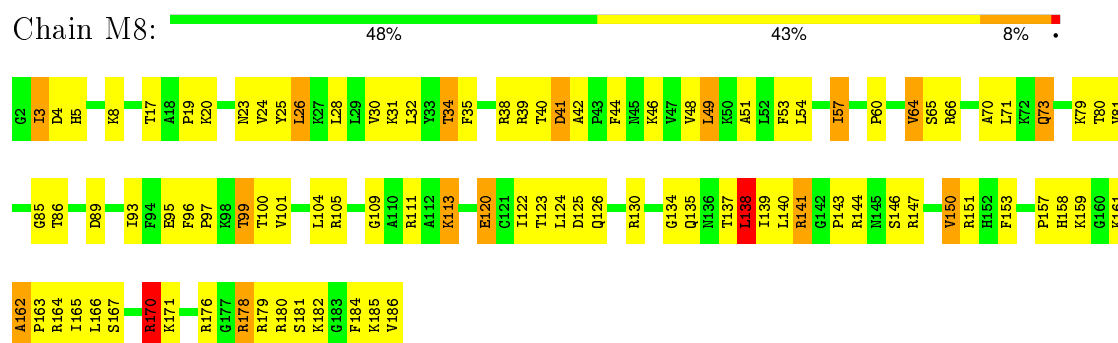
Chain M7: 41% 45% 14%



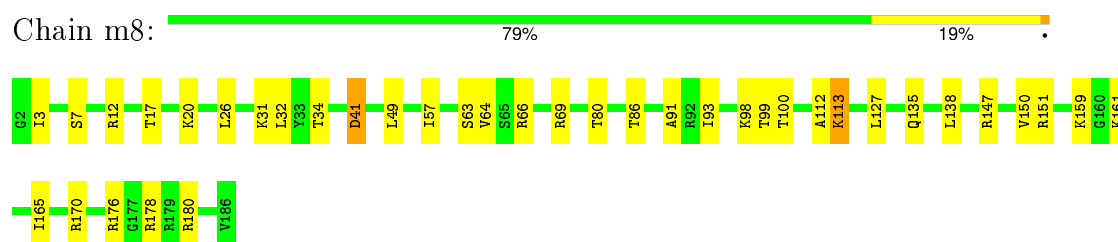
• Molecule 53: 60S ribosomal protein L17-A



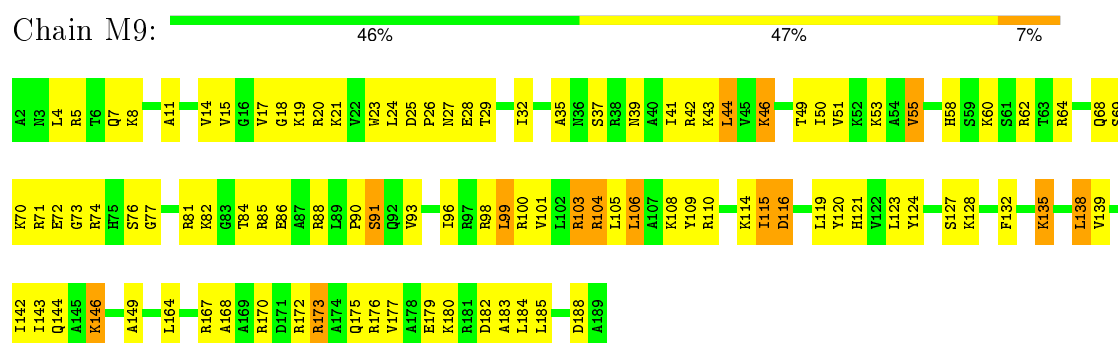
• Molecule 54: 60S ribosomal protein L18-A



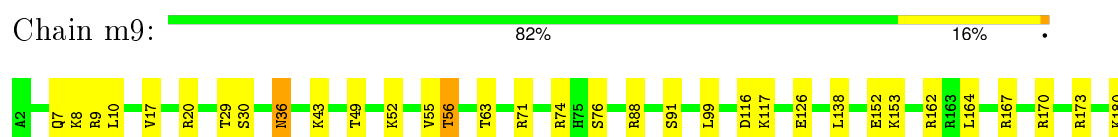
• Molecule 54: 60S ribosomal protein L18-A



• Molecule 55: 60S ribosomal protein L19-A

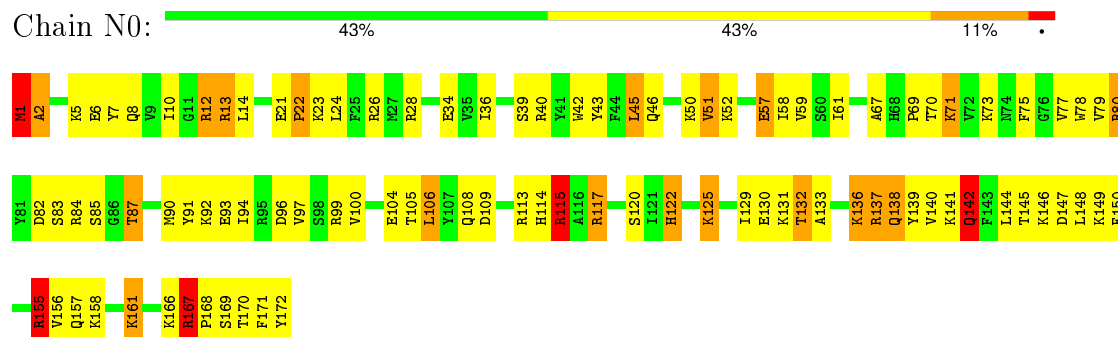


• Molecule 55: 60S ribosomal protein L19-A

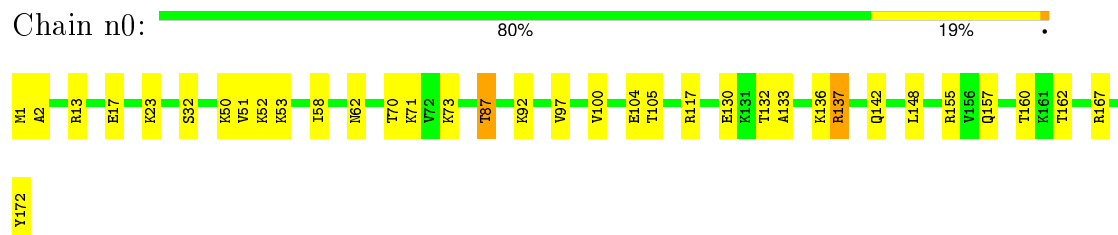




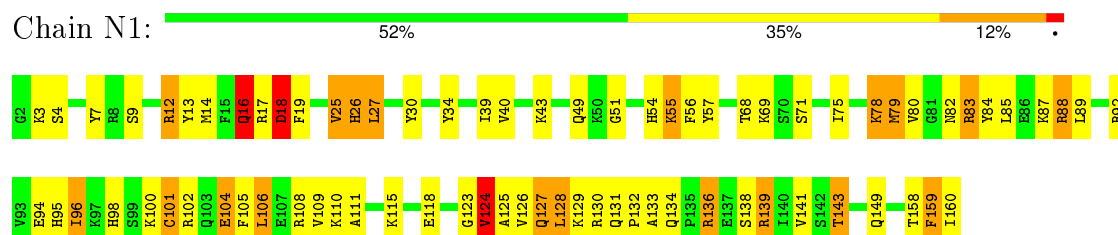
- Molecule 56: 60S ribosomal protein L20-A



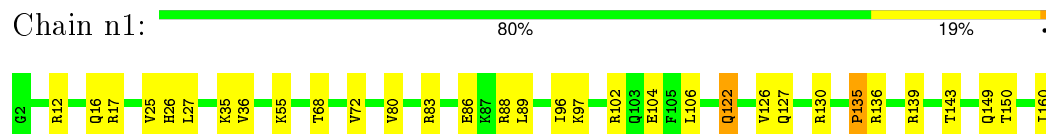
- Molecule 56: 60S ribosomal protein L20-A



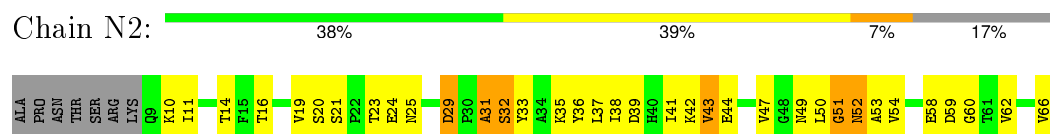
- Molecule 57: 60S ribosomal protein L21-A



- Molecule 57: 60S ribosomal protein L21-A



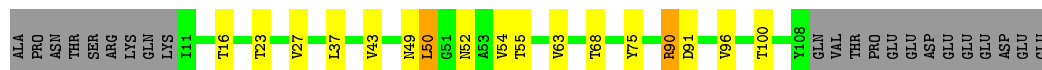
- Molecule 58: 60S ribosomal protein L22-A





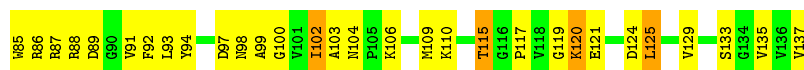
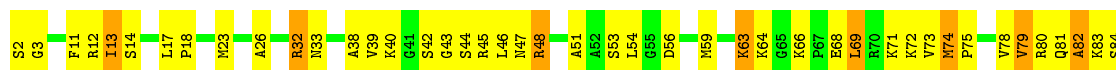
- Molecule 58: 60S ribosomal protein L22-A

Chain n2: 68% 13% 18%



- Molecule 59: 60S ribosomal protein L23-A

Chain N3: 46% 46% 9%



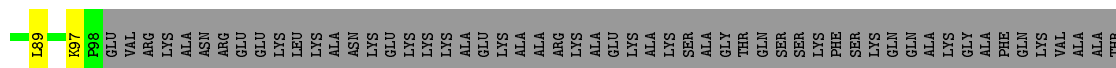
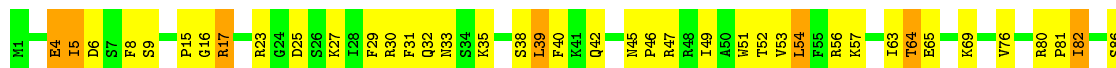
- Molecule 59: 60S ribosomal protein L23-A

Chain n3: 91% 8%



- Molecule 60: 60S ribosomal protein L24-A

Chain N4: 36% 23% 5% 37%

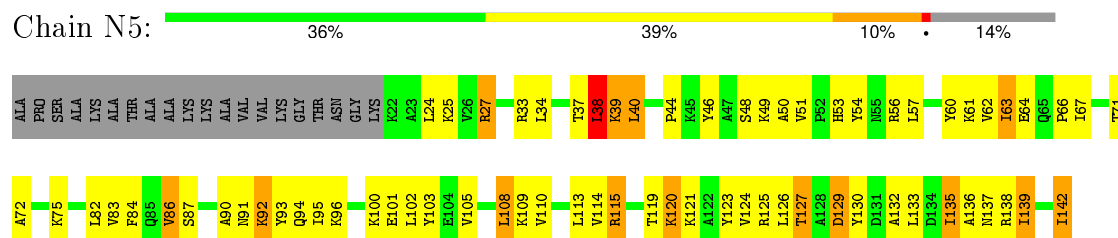


- Molecule 60: 60S ribosomal protein L24-A

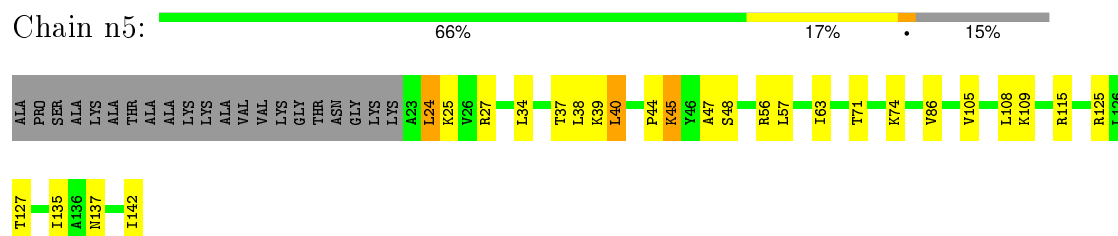
Chain n4: 71% 15% 13%



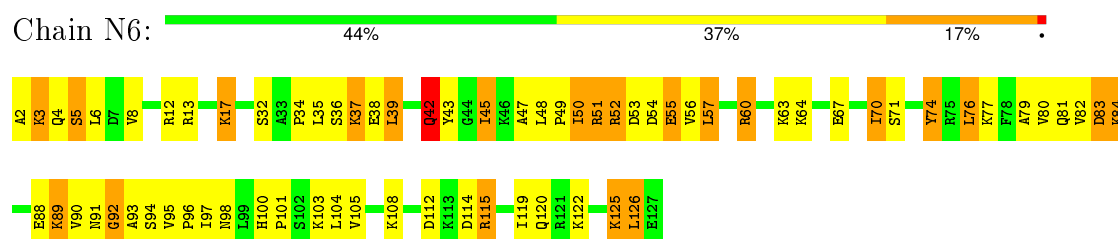
- Molecule 61: 60S ribosomal protein L25



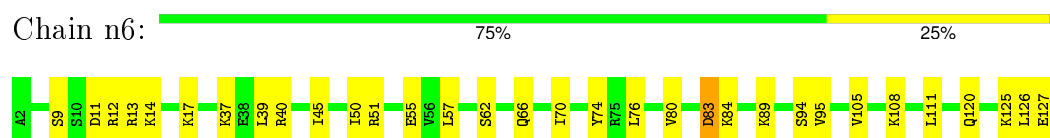
- Molecule 61: 60S ribosomal protein L25



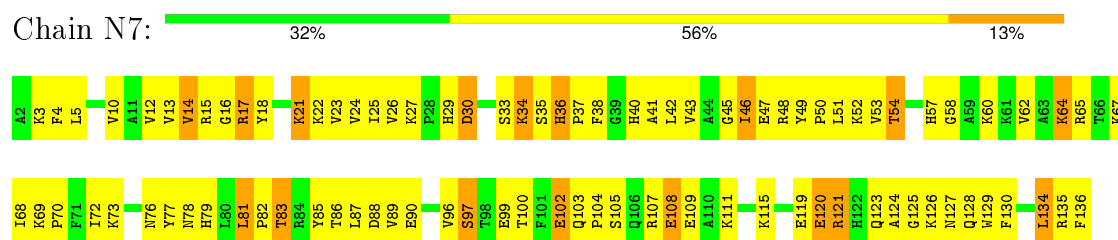
- Molecule 62: 60S ribosomal protein L26-A



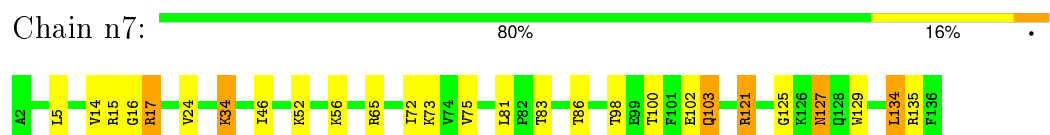
- Molecule 62: 60S ribosomal protein L26-A



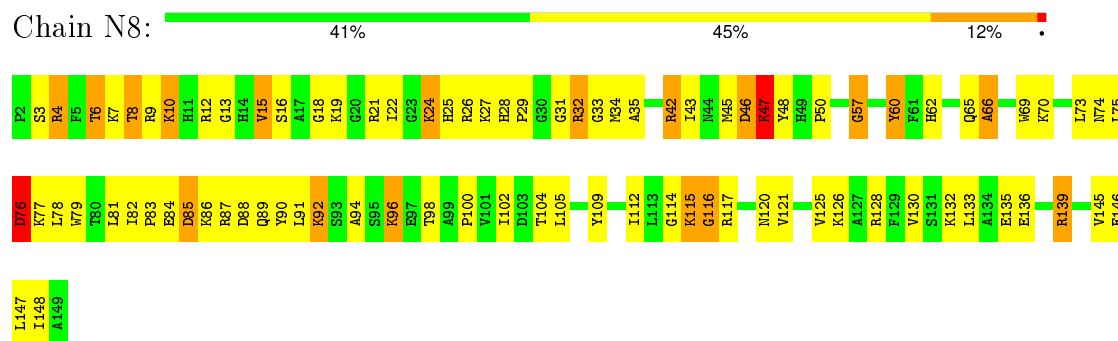
- Molecule 63: 60S ribosomal protein L27-A



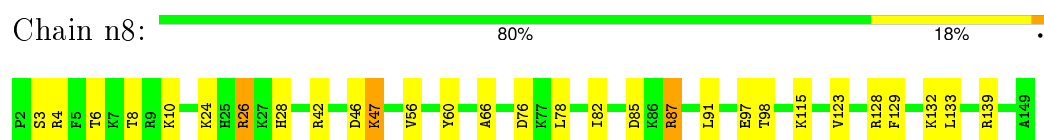
- Molecule 63: 60S ribosomal protein L27-A



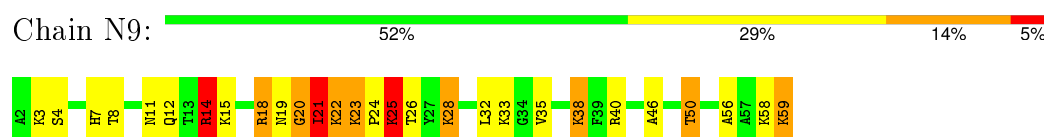
- Molecule 64: 60S ribosomal protein L28



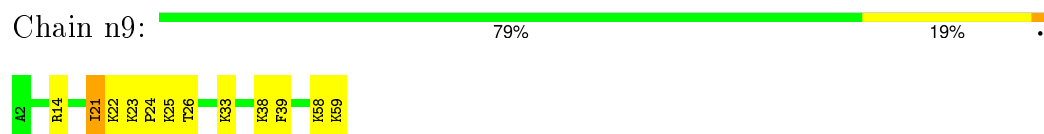
- Molecule 64: 60S ribosomal protein L28



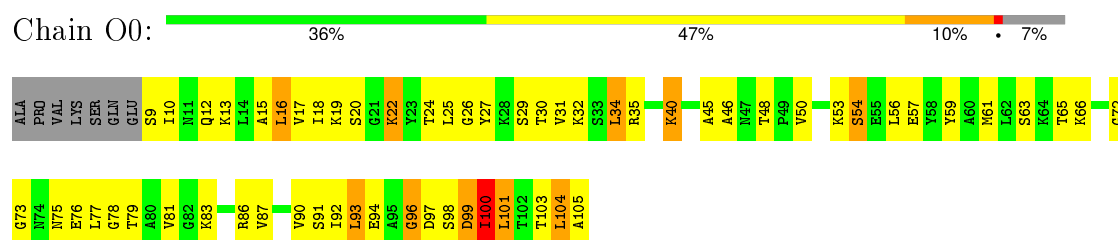
- Molecule 65: 60S ribosomal protein L29



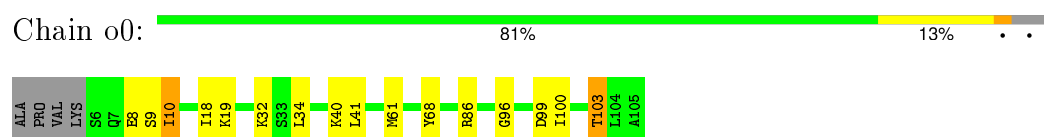
- Molecule 65: 60S ribosomal protein L29



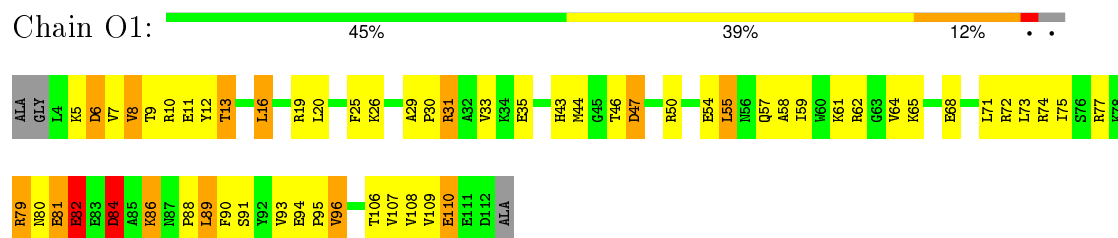
- Molecule 66: 60S ribosomal protein L30



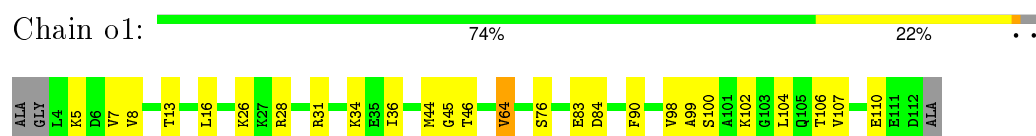
- Molecule 66: 60S ribosomal protein L30



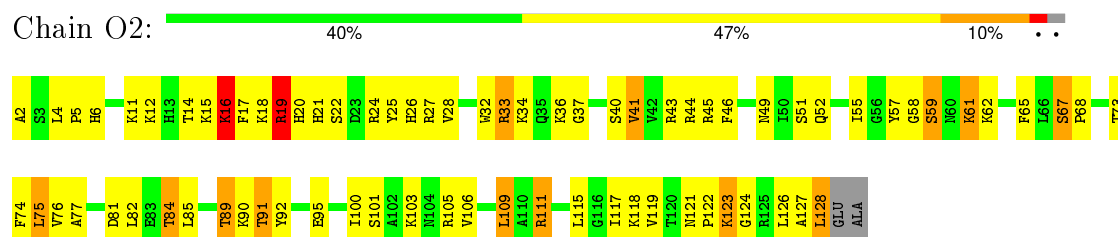
- Molecule 67: 60S ribosomal protein L31-A



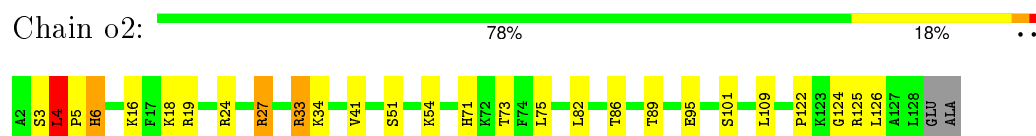
- Molecule 67: 60S ribosomal protein L31-A



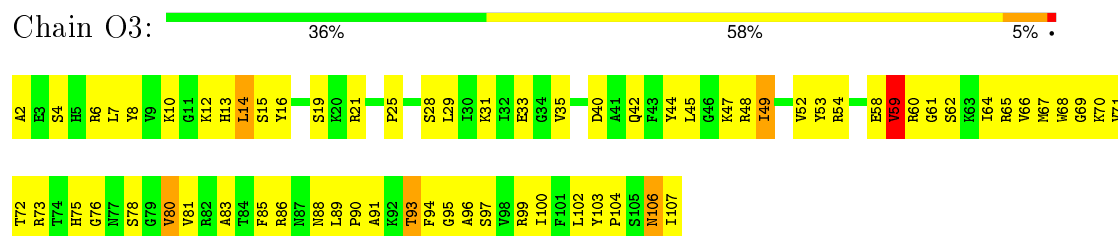
- Molecule 68: 60S ribosomal protein L32



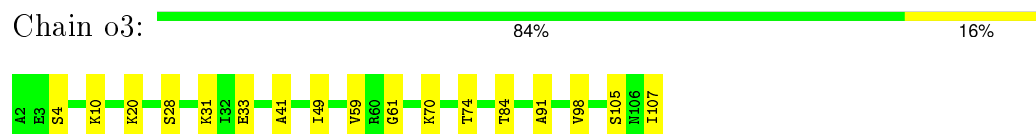
- Molecule 68: 60S ribosomal protein L32



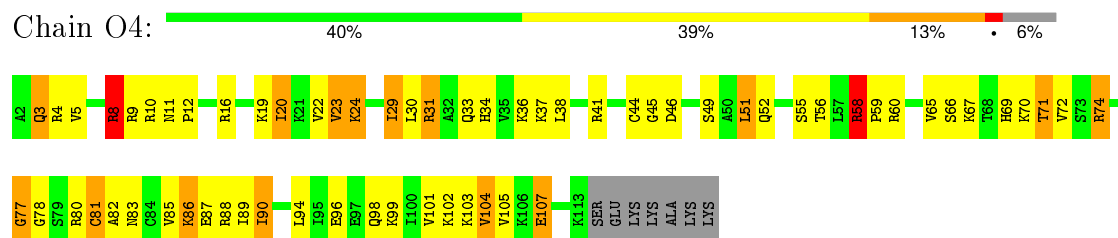
- Molecule 69: 60S ribosomal protein L33-A



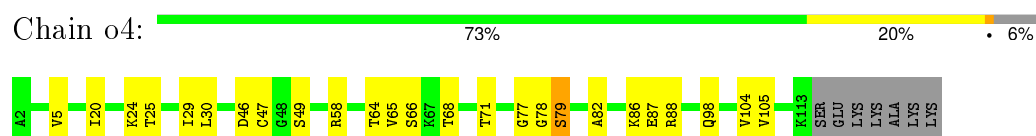
- Molecule 69: 60S ribosomal protein L33-A



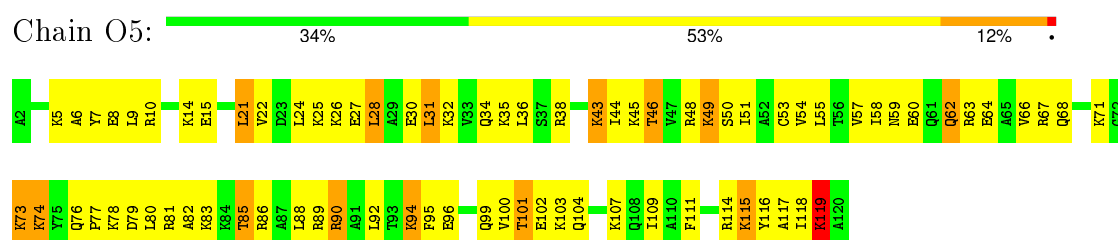
- Molecule 70: 60S ribosomal protein L34-A



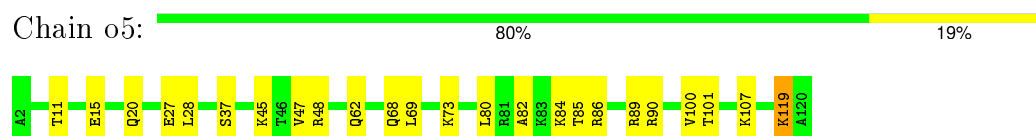
- Molecule 70: 60S ribosomal protein L34-A



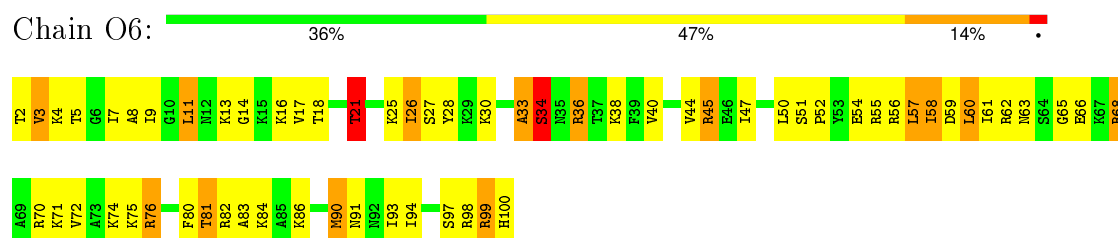
- Molecule 71: 60S ribosomal protein L35-A



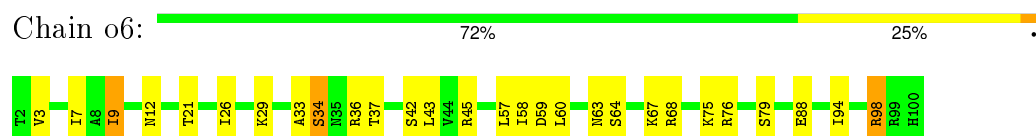
- Molecule 71: 60S ribosomal protein L35-A



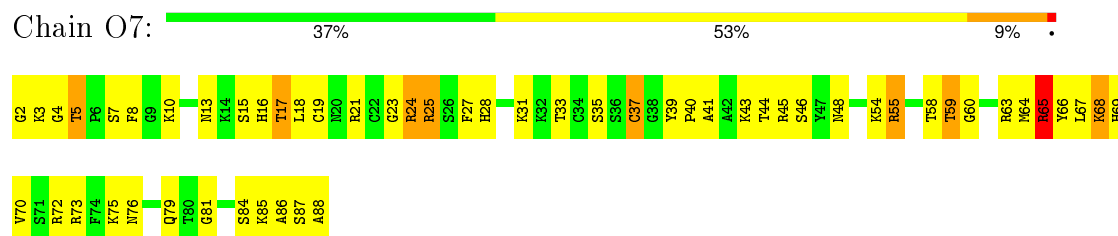
- Molecule 72: 60S ribosomal protein L36-A



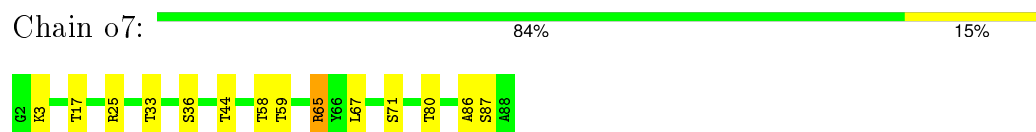
- Molecule 72: 60S ribosomal protein L36-A



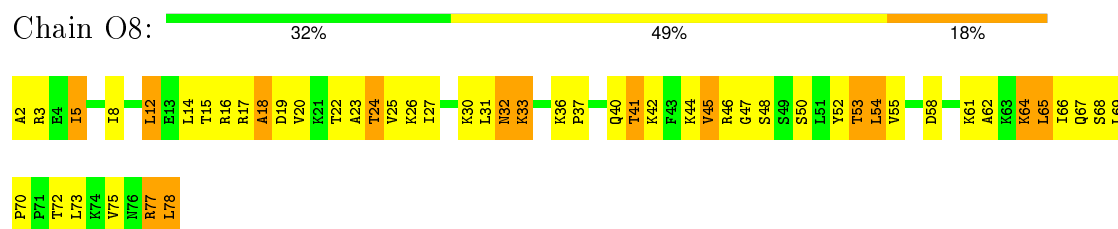
- Molecule 73: 60S ribosomal protein L37-A



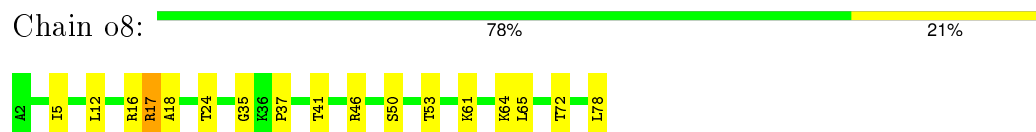
- Molecule 73: 60S ribosomal protein L37-A



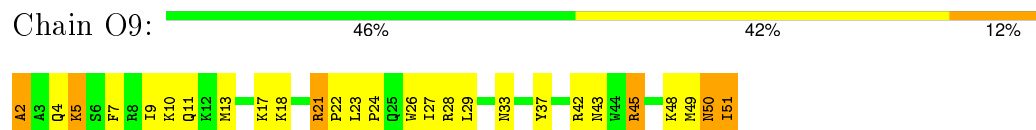
- Molecule 74: 60S ribosomal protein L38



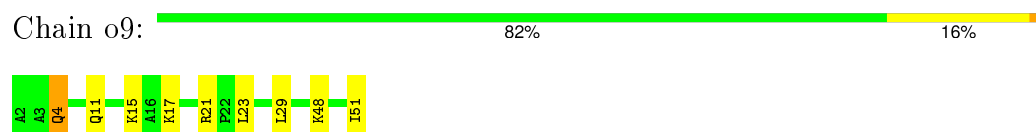
- Molecule 74: 60S ribosomal protein L38



- Molecule 75: 60S ribosomal protein L39

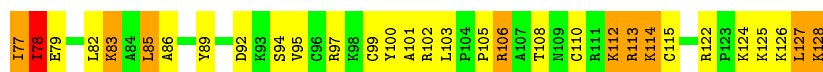


- Molecule 75: 60S ribosomal protein L39



- Molecule 76: Ubiquitin-60S ribosomal protein L40





- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0: 75% 23% .



- Molecule 77: 60S ribosomal protein L41-A

Chain Q1: 12% 64% 20% .



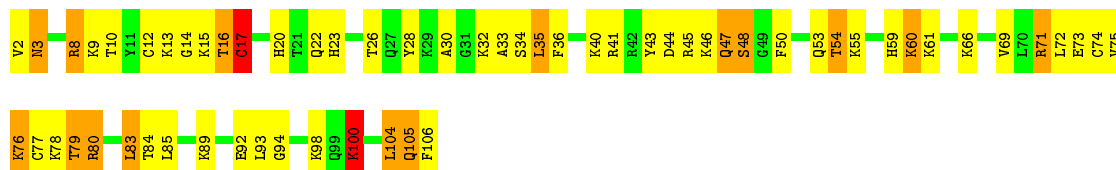
- Molecule 77: 60S ribosomal protein L41-A

Chain q1: 64% 28% 8% .



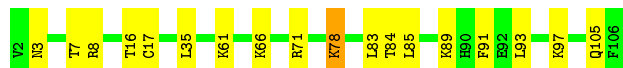
- Molecule 78: 60S ribosomal protein L42-A

Chain Q2: 42% 42% 14% .



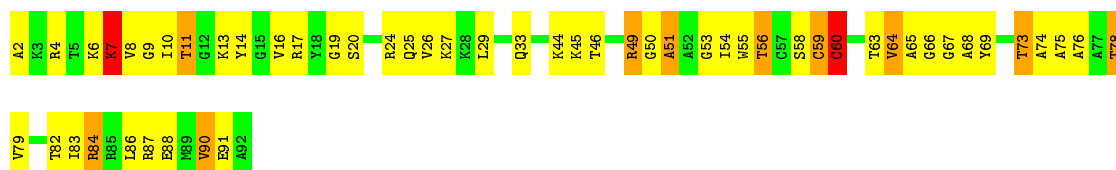
- Molecule 78: 60S ribosomal protein L42-A

Chain q2: 83% 16% .



- Molecule 79: 60S ribosomal protein L43-A

Chain Q3: 41% 46% 11% .



- | | | |
|-----|------|------|
| GLU | ASP | GLY |
| ILE | ILE | G3 |
| SER | PRO | I4 |
| ALA | PHE | R5 |
| ALA | PHE | R6 |
| ALA | PHE | R7 |
| ALA | G184 | E10 |
| ALA | P198 | K14 |
| ALA | A222 | L15 |
| SER | SER | L25 |
| ALA | SER | V23 |
| ALA | SER | R39 |
| ALA | ILE | R42 |
| ALA | GLY | K43 |
| PRO | PRO | E44 |
| ALA | THR | R48 |
| ALA | LEU | V51 |
| GLU | SER | L52 |
| ALA | VAL | K55 |
| ALA | GLY | L67 |
| ALA | ASN | S68 |
| SER | ASN | D69 |
| SER | TTR | L70 |
| ASP | LYS | E74 |
| ASP | ASP | K75 |
| MET | LEU | L76 |
| GLY | LEU | V80 |
| PHE | ALA | R31 |
| PHE | ALA | V84 |
| ASP | ALA | L93 |
| | SER | K97 |
| | TTR | R104 |
| | HIS | A107 |
| | PRO | PRO |
| | ILE | ALA |
| | GLU | ALA |
| | ASP | ARG |
| | LEU | ALA |
| | VAL | GLY |
| | ASP | ALA |
| | ARG | VAL |
| | ILE | ALA |
| | GLU | ASN |
| | GLU | LEU |
| | ASN | GLU |
| | PRO | PRO |

- Molecule 84: unknown protein chain p1

Chain p1:  100%

There are no outlier residues recorded for this chain.

- Molecule 85: unknown protein chain 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 will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	435.26Å 287.54Å 304.02Å 90.00° 98.97° 90.00°	Depositor
Resolution (Å)	73.99 – 3.00	Depositor
% Data completeness (in resolution range)	100.0 (73.99-3.00)	Depositor
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.211 , 0.259	Depositor
Wilson B-factor (Å ²)	64.9	Xtriage
Anisotropy	0.199	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 1468952 reflections	Xtriage
Total number of atoms	411211	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 3KD, 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	0.71	1/41698 (0.0%)	1.27	275/64972 (0.4%)
1	6	0.88	13/42765 (0.0%)	1.38	436/66634 (0.7%)
2	S0	0.43	0/1617	0.66	0/2215
2	s0	0.49	0/1623	0.71	0/2222
3	S1	0.35	0/1735	0.63	1/2335 (0.0%)
3	s1	0.48	0/1748	0.66	0/2352
4	S2	0.49	0/1665	0.67	0/2263
4	s2	0.57	0/1665	0.75	2/2263 (0.1%)
5	S3	0.48	0/1759	0.66	1/2368 (0.0%)
5	s3	0.42	0/1759	0.60	0/2368
6	S4	0.46	0/2109	0.73	1/2839 (0.0%)
6	s4	0.55	0/2109	0.78	1/2839 (0.0%)
7	S5	0.36	0/1629	0.58	0/2202
7	s5	0.44	0/1629	0.64	0/2202
8	S6	0.44	0/1823	0.64	0/2439
8	s6	0.54	0/1779	0.70	0/2379
9	S7	0.42	0/1506	0.65	0/2028
9	s7	0.45	0/1516	0.67	1/2043 (0.0%)
10	S8	0.54	0/1514	0.72	1/2021 (0.0%)
10	s8	0.60	0/1514	0.76	1/2021 (0.0%)
11	S9	0.47	0/1519	0.64	0/2035
11	s9	0.55	0/1519	0.76	2/2035 (0.1%)
12	C0	0.42	0/790	0.70	1/1069 (0.1%)
12	c0	0.36	0/777	0.63	3/1049 (0.3%)
13	C1	0.55	0/1240	0.66	0/1675
13	c1	0.61	0/1194	0.77	0/1610
14	C2	0.38	0/900	0.62	0/1224
14	c2	0.28	0/900	0.56	0/1224
15	C3	0.47	0/1215	0.68	2/1638 (0.1%)
15	c3	0.56	0/1215	0.73	0/1638
16	C4	0.36	0/901	0.63	0/1217
16	c4	0.52	0/960	0.72	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.44	0/998	0.68	0/1341
17	c5	0.45	0/1060	0.66	0/1426
18	C6	0.41	0/1125	0.69	2/1510 (0.1%)
18	c6	0.49	0/1131	0.69	0/1518
19	C7	0.41	0/935	0.62	0/1254
19	c7	0.48	0/914	0.71	0/1224
20	C8	0.42	0/1211	0.63	0/1628
20	c8	0.49	0/1211	0.71	2/1628 (0.1%)
21	C9	0.41	0/1130	0.63	0/1517
21	c9	0.50	0/1130	0.70	2/1517 (0.1%)
22	D0	0.45	0/865	0.64	0/1169
22	d0	0.46	0/892	0.65	0/1205
23	D1	0.44	0/693	0.62	0/935
23	d1	0.54	0/693	0.71	0/935
24	D2	0.48	0/1038	0.73	3/1395 (0.2%)
24	d2	0.59	0/1038	0.74	1/1395 (0.1%)
25	D3	0.60	0/1139	0.77	1/1518 (0.1%)
25	d3	0.70	0/1139	0.89	3/1518 (0.2%)
26	D4	0.44	0/1087	0.63	0/1449
26	d4	0.53	0/1087	0.73	0/1449
27	D5	0.39	0/571	0.68	0/768
27	d5	0.41	0/566	0.63	0/761
28	D6	0.43	0/782	0.67	0/1047
28	d6	0.56	0/782	0.71	0/1047
29	D7	0.42	0/620	0.66	0/838
29	d7	0.46	0/620	0.66	0/838
30	D8	0.35	0/499	0.57	0/670
30	d8	0.44	0/499	0.64	0/670
31	D9	0.50	0/452	0.70	1/600 (0.2%)
31	d9	0.50	0/452	0.64	0/600
32	E0	0.46	0/483	0.63	0/643
33	E1	0.42	0/577	0.78	0/770
33	e1	0.39	0/619	0.72	0/822
34	SR	0.37	0/2494	0.57	0/3393
34	sR	0.38	0/2495	0.56	0/3395
35	SM	0.48	0/1113	0.70	2/1502 (0.1%)
36	1	1.16	153/75394 (0.2%)	1.66	1837/117545 (1.6%)
36	5	1.20	178/75414 (0.2%)	1.67	1863/117575 (1.6%)
37	3	0.95	2/2883 (0.1%)	1.47	39/4491 (0.9%)
37	7	1.16	5/2883 (0.2%)	1.62	57/4491 (1.3%)
38	4	1.13	5/3746 (0.1%)	1.66	86/5832 (1.5%)
38	8	0.98	2/3746 (0.1%)	1.48	42/5832 (0.7%)
39	L2	0.74	0/1948	0.84	3/2617 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	l2	0.71	0/1946	0.86	2/2614 (0.1%)
40	L3	0.74	1/3146 (0.0%)	0.82	1/4228 (0.0%)
40	l3	0.88	1/3146 (0.0%)	0.89	2/4228 (0.0%)
41	L4	0.84	1/2800 (0.0%)	0.94	7/3790 (0.2%)
41	l4	0.74	1/2800 (0.0%)	0.90	6/3790 (0.2%)
42	L5	0.57	0/2425	0.69	1/3271 (0.0%)
42	l5	0.73	0/2408	0.82	1/3248 (0.0%)
43	L6	0.76	0/1260	0.84	0/1694
43	l6	0.78	0/1269	0.84	1/1705 (0.1%)
44	L7	0.78	1/1821 (0.1%)	0.90	2/2451 (0.1%)
44	l7	0.85	1/1828 (0.1%)	0.90	4/2461 (0.2%)
45	L8	0.55	0/1836	0.70	1/2481 (0.0%)
45	l8	0.51	0/1795	0.65	1/2429 (0.0%)
46	L9	0.65	0/1539	0.77	1/2073 (0.0%)
46	l9	0.77	0/1539	0.85	0/2073
47	M0	0.71	0/1741	0.84	3/2335 (0.1%)
47	m0	0.75	0/1758	0.87	2/2358 (0.1%)
48	M1	0.54	0/1374	0.73	1/1842 (0.1%)
48	m1	0.65	0/1374	0.82	2/1842 (0.1%)
49	M3	0.75	0/1568	0.86	0/2106
49	m3	0.69	0/1573	0.85	3/2113 (0.1%)
50	M4	0.73	0/1068	0.80	1/1438 (0.1%)
50	m4	0.82	0/1074	0.85	0/1446
51	M5	0.77	0/1757	0.85	0/2354
51	m5	0.66	0/1757	0.79	0/2354
52	M6	0.86	1/1585 (0.1%)	0.92	3/2128 (0.1%)
52	m6	1.02	5/1585 (0.3%)	0.98	7/2128 (0.3%)
53	M7	0.80	0/1443	0.85	2/1944 (0.1%)
53	m7	0.89	0/1250	0.89	0/1683
54	M8	0.79	0/1465	0.92	3/1965 (0.2%)
54	m8	0.73	0/1465	0.95	2/1965 (0.1%)
55	M9	0.57	0/1538	0.69	0/2050
55	m9	0.61	0/1538	0.70	0/2050
56	N0	0.78	0/1481	0.87	4/1990 (0.2%)
56	n0	0.87	0/1481	0.91	2/1990 (0.1%)
57	N1	0.78	0/1300	0.82	0/1743
57	n1	0.85	1/1300 (0.1%)	0.86	1/1743 (0.1%)
58	N2	0.42	0/812	0.62	0/1099
58	n2	0.51	0/794	0.65	0/1076
59	N3	0.70	0/1018	0.81	0/1369
59	n3	0.87	0/1018	0.98	1/1369 (0.1%)
60	N4	0.56	0/712	0.68	0/958
60	n4	0.69	0/1052	0.75	0/1398

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
61	N5	0.63	0/979	0.80	2/1321 (0.2%)
61	n5	0.65	0/974	0.77	0/1314
62	N6	0.68	0/1004	0.90	1/1341 (0.1%)
62	n6	0.71	1/1004 (0.1%)	0.84	0/1341
63	N7	0.52	0/1118	0.66	0/1497
63	n7	0.46	0/1118	0.63	0/1497
64	N8	0.82	0/1204	0.92	2/1612 (0.1%)
64	n8	0.79	0/1204	0.90	0/1612
65	N9	0.67	0/473	0.83	2/629 (0.3%)
65	n9	0.80	0/473	0.97	0/629
66	O0	0.48	0/751	0.66	0/1008
66	o0	0.49	0/775	0.65	0/1040
67	O1	0.60	0/890	0.72	0/1196
67	o1	0.76	0/897	0.86	0/1205
68	O2	0.85	0/1041	0.89	2/1394 (0.1%)
68	o2	0.82	0/1041	0.94	2/1394 (0.1%)
69	O3	0.95	0/868	0.91	1/1168 (0.1%)
69	o3	0.92	0/868	0.84	0/1168
70	O4	0.58	0/890	0.82	4/1189 (0.3%)
70	o4	0.59	0/890	0.78	0/1189
71	O5	0.70	0/978	0.81	1/1301 (0.1%)
71	o5	0.59	0/974	0.72	0/1297
72	O6	0.64	0/778	0.79	0/1034
72	o6	0.54	0/777	0.73	0/1033
73	O7	0.78	0/696	0.90	1/923 (0.1%)
73	o7	0.75	0/696	0.85	1/923 (0.1%)
74	O8	0.51	0/618	0.64	0/826
74	o8	0.42	0/614	0.61	0/822
75	O9	0.83	1/443 (0.2%)	0.90	0/588
75	o9	0.76	0/443	0.83	0/588
76	Q0	0.73	0/423	0.84	0/562
76	q0	0.95	0/423	1.03	1/562 (0.2%)
77	Q1	0.72	0/234	0.96	1/300 (0.3%)
77	q1	0.82	0/234	1.05	2/300 (0.7%)
78	Q2	0.93	1/860 (0.1%)	0.85	1/1136 (0.1%)
78	q2	0.82	1/860 (0.1%)	0.83	0/1136
79	Q3	0.74	0/701	0.85	0/934
79	q3	0.72	0/701	0.81	0/934
80	e0	0.56	0/499	0.74	0/665
81	sM	0.50	0/684	0.69	1/925 (0.1%)
83	p0	0.46	0/1092	0.61	0/1474
All	All	0.90	376/430075 (0.1%)	1.30	4764/631366 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	s5	0	2
9	S7	0	1
10	S8	0	1
16	C4	0	2
17	c5	0	1
18	c6	0	1
19	C7	0	2
22	d0	0	1
27	D5	0	2
28	D6	0	1
33	E1	0	1
39	l2	0	1
42	l5	0	2
43	L6	0	1
43	l6	0	1
44	l7	0	2
45	L8	0	1
48	M1	0	2
51	M5	0	1
52	M6	0	1
52	m6	0	1
53	M7	0	1
55	m9	0	1
56	N0	0	2
56	n0	0	2
57	N1	0	1
62	n6	0	1
64	N8	0	1
64	n8	0	2
65	N9	0	1
67	O1	0	1
67	o1	0	2
All	All	0	43

The worst 5 of 376 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	15.91	2.09	1.82
36	5	1152	G	N9-C4	-12.55	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	q2	17	CYS	CB-SG	11.87	2.02	1.82
36	1	3181	C	N3-C4	-9.25	1.27	1.33
36	5	2138	A	N7-C5	-8.87	1.33	1.39

The worst 5 of 4764 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-C5	24.25	140.73	128.60
36	5	1152	G	N3-C4-N9	-22.33	112.60	126.00
36	5	1152	G	C2-N3-C4	-20.90	101.45	111.90
36	1	2945	G	O5'-P-OP2	-17.25	90.00	110.70
36	1	1308	A	O5'-P-OP2	-17.00	90.30	110.70

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
16	C4	124	ASP	Peptide
19	C7	22	PRO	Peptide
9	S7	131	PHE	Peptide
10	S8	147	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37283	0	18757	928	0
1	6	38238	0	19240	830	0
2	S0	1577	0	1567	168	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	163	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	128	0
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	125	0
5	s3	1734	0	1817	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	S4	2068	0	2154	150	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	151	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	118	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	117	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	117	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	146	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	62	0
12	c0	762	0	699	0	0
13	C1	1214	0	1259	89	0
13	c1	1168	0	1231	0	0
14	C2	892	0	891	54	0
14	c2	892	0	891	0	0
15	C3	1192	0	1255	93	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	97	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	97	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	116	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	82	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	111	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	87	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	83	0
22	d0	882	0	939	0	0
23	D1	684	0	672	57	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	74	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	89	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	87	0
26	d4	1073	0	1132	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	D5	563	0	603	64	0
27	d5	558	0	598	0	0
28	D6	769	0	814	94	0
28	d6	769	0	814	0	0
29	D7	610	0	630	39	0
29	d7	610	0	631	0	0
30	D8	497	0	535	40	0
30	d8	497	0	535	0	0
31	D9	442	0	428	25	0
31	d9	442	0	428	0	0
32	E0	475	0	525	37	0
33	E1	566	0	601	58	0
33	e1	608	0	657	0	0
34	SR	2441	0	2397	155	0
34	sR	2442	0	2392	0	0
35	SM	1104	0	996	74	0
36	1	67355	0	33845	1266	0
36	5	67376	0	33851	1268	0
37	3	2579	0	1304	51	0
37	7	2579	0	1303	52	0
38	4	3353	0	1695	77	0
38	8	3353	0	1695	71	0
39	L2	1914	0	1981	166	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	242	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	206	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	210	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	62	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	124	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	129	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	121	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1736	127	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	95	0
48	m1	1353	0	1383	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	M3	1543	0	1608	136	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	63	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	130	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	109	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	115	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	92	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	99	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	94	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	84	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	38	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	27	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	63	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	65	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	86	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1214	86	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	35	0
65	n9	462	0	491	0	0
66	O0	743	0	797	53	0
66	o0	767	0	816	0	0
67	O1	876	0	912	52	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	82	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	67	0
69	o3	850	0	880	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	O4	880	0	945	72	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	75	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	64	0
72	o6	770	0	846	0	0
73	O7	681	0	683	52	0
73	o7	681	0	683	0	0
74	O8	612	0	682	44	0
74	o8	608	0	671	0	0
75	O9	436	0	475	36	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	25	0
76	q0	417	0	455	0	0
77	Q1	233	0	284	27	0
77	q1	233	0	284	0	0
78	Q2	847	0	916	59	0
78	q2	847	0	916	0	0
79	Q3	694	0	734	58	0
79	q3	694	0	734	0	0
80	e0	491	0	542	0	0
81	sM	681	0	609	0	0
82	m2	750	0	179	0	0
83	p0	1077	0	1041	0	0
84	p1	235	0	50	0	0
85	p2	230	0	51	0	0
86	1	477	0	0	0	0
86	2	123	0	0	0	0
86	3	14	0	0	0	0
86	4	21	0	0	0	0
86	5	506	0	0	0	0
86	6	149	0	0	0	0
86	7	16	0	0	0	0
86	8	14	0	0	0	0
86	D0	1	0	0	0	0
86	D3	1	0	0	0	0
86	D4	1	0	0	0	0
86	L2	1	0	0	0	0
86	L3	2	0	0	0	0
86	L4	2	0	0	0	0
86	L5	2	0	0	0	0
86	L7	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	L8	1	0	0	0	0
86	M0	2	0	0	0	0
86	M1	1	0	0	0	0
86	M3	3	0	0	0	0
86	M5	1	0	0	0	0
86	M6	1	0	0	0	0
86	M7	6	0	0	0	0
86	M8	1	0	0	0	0
86	M9	1	0	0	0	0
86	N0	1	0	0	0	0
86	N3	3	0	0	0	0
86	N5	1	0	0	0	0
86	N8	3	0	0	0	0
86	O4	1	0	0	0	0
86	O7	1	0	0	0	0
86	O8	1	0	0	0	0
86	Q2	1	0	0	0	0
86	S2	1	0	0	0	0
86	S8	1	0	0	0	0
86	SM	1	0	0	0	0
86	c1	1	0	0	0	0
86	c7	1	0	0	0	0
86	d3	2	0	0	0	0
86	d4	1	0	0	0	0
86	l2	2	0	0	0	0
86	l3	2	0	0	0	0
86	l4	1	0	0	0	0
86	l5	2	0	0	0	0
86	l7	2	0	0	0	0
86	l9	1	0	0	0	0
86	m1	1	0	0	0	0
86	m5	3	0	0	0	0
86	m6	1	0	0	0	0
86	m7	5	0	0	0	0
86	n0	1	0	0	0	0
86	n3	2	0	0	0	0
86	n6	1	0	0	0	0
86	n8	5	0	0	0	0
86	o1	2	0	0	0	0
86	o3	2	0	0	0	0
86	o4	1	0	0	0	0
86	q0	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	q1	1	0	0	0	0
86	q3	1	0	0	0	0
86	s1	1	0	0	0	0
86	s4	1	0	0	0	0
86	s8	2	0	0	0	0
86	sM	2	0	0	0	0
87	1	2436	0	0	267	0
87	2	1106	0	0	125	0
87	3	84	0	0	5	0
87	4	91	0	0	6	0
87	5	2478	0	0	273	0
87	6	1106	0	0	114	0
87	7	77	0	0	6	0
87	8	112	0	0	16	0
87	C3	7	0	0	2	0
87	C5	7	0	0	4	0
87	C8	7	0	0	0	0
87	D3	7	0	0	0	0
87	D9	7	0	0	1	0
87	L3	21	0	0	3	0
87	L4	7	0	0	3	0
87	M0	7	0	0	0	0
87	M5	7	0	0	1	0
87	M6	7	0	0	0	0
87	M7	14	0	0	3	0
87	M8	7	0	0	0	0
87	M9	7	0	0	1	0
87	N1	7	0	0	0	0
87	N9	7	0	0	0	0
87	O2	7	0	0	1	0
87	O3	7	0	0	1	0
87	O7	14	0	0	7	0
87	O9	7	0	0	3	0
87	Q2	7	0	0	3	0
87	S8	7	0	0	0	0
87	SR	7	0	0	0	0
87	c1	7	0	0	0	0
87	c3	7	0	0	0	0
87	c5	7	0	0	0	0
87	c8	7	0	0	0	0
87	d4	7	0	0	0	0
87	d9	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	l3	14	0	0	0	0
87	l4	14	0	0	0	0
87	l5	21	0	0	0	0
87	l9	7	0	0	0	0
87	m0	14	0	0	0	0
87	m1	7	0	0	0	0
87	m4	7	0	0	0	0
87	m5	7	0	0	0	0
87	m6	7	0	0	0	0
87	m7	7	0	0	0	0
87	m8	7	0	0	0	0
87	m9	7	0	0	0	0
87	n3	7	0	0	0	0
87	n6	7	0	0	0	0
87	n9	7	0	0	0	0
87	o2	7	0	0	0	0
87	o3	7	0	0	0	0
87	o7	14	0	0	0	0
87	q2	7	0	0	0	0
87	s1	14	0	0	0	0
87	s4	7	0	0	0	0
87	s8	7	0	0	0	0
87	s9	7	0	0	0	0
87	sR	7	0	0	0	0
88	D6	1	0	0	0	0
88	D7	1	0	0	0	0
88	D9	1	0	0	0	0
88	E1	1	0	0	0	0
88	O7	1	0	0	0	0
88	Q0	1	0	0	0	0
88	Q2	1	0	0	3	0
88	Q3	1	0	0	0	0
88	d6	1	0	0	0	0
88	d7	1	0	0	0	0
88	d9	1	0	0	0	0
88	e1	1	0	0	0	0
88	o7	1	0	0	0	0
88	q0	1	0	0	0	0
88	q2	1	0	0	0	0
88	q3	1	0	0	0	0
89	1	21	0	17	0	0
89	5	21	0	17	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	411211	0	297317	9909	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 14.

The worst 5 of 9909 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)
78:Q2:17:CYS:CB	78:Q2:17:CYS:SG	2.09	1.48
78:Q2:17:CYS:CB	88:Q2:501:ZN:ZN	1.11	1.28
36:1:1481:A:O2'	36:1:1858:A:N3	1.84	1.10
42:L5:152:ARG:HH11	42:L5:152:ARG:HG3	1.87	1.10
40:L3:41:VAL:HA	40:L3:185:GLY:HA3	1.36	1.05

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%)	152 (74%)	31 (15%)	21 (10%)	1	3
2	s0	204/251 (81%)	153 (75%)	26 (13%)	25 (12%)	0	2
3	S1	212/254 (84%)	146 (69%)	39 (18%)	27 (13%)	0	1
3	s1	214/254 (84%)	177 (83%)	26 (12%)	11 (5%)	2	15
4	S2	215/253 (85%)	187 (87%)	17 (8%)	11 (5%)	2	15
4	s2	215/253 (85%)	186 (86%)	16 (7%)	13 (6%)	2	11
5	S3	221/239 (92%)	179 (81%)	29 (13%)	13 (6%)	2	11
5	s3	221/239 (92%)	183 (83%)	19 (9%)	19 (9%)	1	4
6	S4	258/260 (99%)	206 (80%)	41 (16%)	11 (4%)	3	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	s4	258/260 (99%)	216 (84%)	24 (9%)	18 (7%)	1	7
7	S5	204/224 (91%)	158 (78%)	32 (16%)	14 (7%)	1	7
7	s5	204/224 (91%)	164 (80%)	25 (12%)	15 (7%)	1	6
8	S6	224/236 (95%)	194 (87%)	17 (8%)	13 (6%)	2	12
8	s6	216/236 (92%)	189 (88%)	15 (7%)	12 (6%)	2	13
9	S7	182/189 (96%)	137 (75%)	25 (14%)	20 (11%)	0	2
9	s7	184/189 (97%)	148 (80%)	21 (11%)	15 (8%)	1	5
10	S8	184/200 (92%)	154 (84%)	21 (11%)	9 (5%)	3	16
10	s8	184/200 (92%)	163 (89%)	16 (9%)	5 (3%)	6	32
11	S9	183/196 (93%)	151 (82%)	23 (13%)	9 (5%)	3	16
11	s9	183/196 (93%)	140 (76%)	34 (19%)	9 (5%)	3	16
12	C0	94/105 (90%)	68 (72%)	15 (16%)	11 (12%)	0	2
12	c0	92/105 (88%)	64 (70%)	14 (15%)	14 (15%)	0	1
13	C1	153/155 (99%)	126 (82%)	16 (10%)	11 (7%)	1	7
13	c1	144/155 (93%)	118 (82%)	17 (12%)	9 (6%)	2	9
14	C2	122/142 (86%)	70 (57%)	25 (20%)	27 (22%)	0	0
14	c2	122/142 (86%)	68 (56%)	32 (26%)	22 (18%)	0	0
15	C3	148/150 (99%)	123 (83%)	18 (12%)	7 (5%)	3	17
15	c3	148/150 (99%)	120 (81%)	17 (12%)	11 (7%)	1	6
16	C4	125/136 (92%)	94 (75%)	15 (12%)	16 (13%)	0	1
16	c4	126/136 (93%)	101 (80%)	16 (13%)	9 (7%)	1	7
17	C5	122/141 (86%)	88 (72%)	23 (19%)	11 (9%)	1	4
17	c5	133/141 (94%)	92 (69%)	22 (16%)	19 (14%)	0	1
18	C6	139/142 (98%)	116 (84%)	16 (12%)	7 (5%)	3	15
18	c6	140/142 (99%)	116 (83%)	16 (11%)	8 (6%)	2	12
19	C7	116/136 (85%)	91 (78%)	13 (11%)	12 (10%)	1	3
19	c7	113/136 (83%)	87 (77%)	18 (16%)	8 (7%)	1	7
20	C8	143/145 (99%)	115 (80%)	16 (11%)	12 (8%)	1	5
20	c8	143/145 (99%)	114 (80%)	20 (14%)	9 (6%)	2	9
21	C9	141/143 (99%)	115 (82%)	22 (16%)	4 (3%)	6	30
21	c9	141/143 (99%)	119 (84%)	16 (11%)	6 (4%)	3	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	D0	105/120 (88%)	88 (84%)	13 (12%)	4 (4%)	4	22
22	d0	108/120 (90%)	82 (76%)	16 (15%)	10 (9%)	1	4
23	D1	85/87 (98%)	61 (72%)	16 (19%)	8 (9%)	1	4
23	d1	85/87 (98%)	72 (85%)	8 (9%)	5 (6%)	2	11
24	D2	127/129 (98%)	106 (84%)	19 (15%)	2 (2%)	12	48
24	d2	127/129 (98%)	114 (90%)	12 (9%)	1 (1%)	24	66
25	D3	142/144 (99%)	113 (80%)	19 (13%)	10 (7%)	1	7
25	d3	142/144 (99%)	123 (87%)	16 (11%)	3 (2%)	9	40
26	D4	132/134 (98%)	103 (78%)	20 (15%)	9 (7%)	1	7
26	d4	132/134 (98%)	103 (78%)	21 (16%)	8 (6%)	2	11
27	D5	68/107 (64%)	47 (69%)	9 (13%)	12 (18%)	0	1
27	d5	67/107 (63%)	52 (78%)	9 (13%)	6 (9%)	1	4
28	D6	95/97 (98%)	59 (62%)	18 (19%)	18 (19%)	0	0
28	d6	95/97 (98%)	74 (78%)	12 (13%)	9 (10%)	1	3
29	D7	79/81 (98%)	66 (84%)	8 (10%)	5 (6%)	2	9
29	d7	79/81 (98%)	60 (76%)	12 (15%)	7 (9%)	1	4
30	D8	61/66 (92%)	51 (84%)	6 (10%)	4 (7%)	1	8
30	d8	61/66 (92%)	42 (69%)	15 (25%)	4 (7%)	1	8
31	D9	51/55 (93%)	41 (80%)	8 (16%)	2 (4%)	4	21
31	d9	51/55 (93%)	41 (80%)	6 (12%)	4 (8%)	1	6
32	E0	58/60 (97%)	44 (76%)	12 (21%)	2 (3%)	5	25
33	E1	69/76 (91%)	36 (52%)	17 (25%)	16 (23%)	0	0
33	e1	74/76 (97%)	36 (49%)	17 (23%)	21 (28%)	0	0
34	SR	316/318 (99%)	271 (86%)	35 (11%)	10 (3%)	5	27
34	sR	316/318 (99%)	270 (85%)	36 (11%)	10 (3%)	5	27
35	SM	155/273 (57%)	113 (73%)	23 (15%)	19 (12%)	0	2
39	L2	250/253 (99%)	223 (89%)	21 (8%)	6 (2%)	7	35
39	l2	250/253 (99%)	210 (84%)	30 (12%)	10 (4%)	4	21
40	L3	384/386 (100%)	326 (85%)	45 (12%)	13 (3%)	5	25
40	l3	384/386 (100%)	340 (88%)	32 (8%)	12 (3%)	5	28
41	L4	359/361 (99%)	299 (83%)	43 (12%)	17 (5%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	l4	359/361 (99%)	300 (84%)	39 (11%)	20 (6%)	2	13
42	L5	294/296 (99%)	242 (82%)	31 (10%)	21 (7%)	1	7
42	l5	292/296 (99%)	255 (87%)	30 (10%)	7 (2%)	7	35
43	L6	152/175 (87%)	132 (87%)	16 (10%)	4 (3%)	7	33
43	l6	153/175 (87%)	129 (84%)	20 (13%)	4 (3%)	7	33
44	L7	220/243 (90%)	198 (90%)	12 (6%)	10 (4%)	3	18
44	l7	221/243 (91%)	195 (88%)	20 (9%)	6 (3%)	6	32
45	L8	231/255 (91%)	188 (81%)	35 (15%)	8 (4%)	4	24
45	l8	229/255 (90%)	188 (82%)	21 (9%)	20 (9%)	1	4
46	L9	189/191 (99%)	167 (88%)	15 (8%)	7 (4%)	4	23
46	l9	189/191 (99%)	171 (90%)	15 (8%)	3 (2%)	12	48
47	M0	207/220 (94%)	178 (86%)	18 (9%)	11 (5%)	2	14
47	m0	209/220 (95%)	167 (80%)	27 (13%)	15 (7%)	1	7
48	M1	167/173 (96%)	131 (78%)	21 (13%)	15 (9%)	1	4
48	m1	167/173 (96%)	139 (83%)	16 (10%)	12 (7%)	1	7
49	M3	191/198 (96%)	164 (86%)	16 (8%)	11 (6%)	2	12
49	m3	192/198 (97%)	159 (83%)	17 (9%)	16 (8%)	1	5
50	M4	134/137 (98%)	117 (87%)	12 (9%)	5 (4%)	4	23
50	m4	135/137 (98%)	122 (90%)	10 (7%)	3 (2%)	8	38
51	M5	201/203 (99%)	181 (90%)	12 (6%)	8 (4%)	4	21
51	m5	201/203 (99%)	179 (89%)	16 (8%)	6 (3%)	5	29
52	M6	195/198 (98%)	181 (93%)	11 (6%)	3 (2%)	13	50
52	m6	195/198 (98%)	179 (92%)	8 (4%)	8 (4%)	3	20
53	M7	181/183 (99%)	152 (84%)	22 (12%)	7 (4%)	4	21
53	m7	153/183 (84%)	138 (90%)	13 (8%)	2 (1%)	15	53
54	M8	183/185 (99%)	165 (90%)	14 (8%)	4 (2%)	8	38
54	m8	183/185 (99%)	155 (85%)	22 (12%)	6 (3%)	5	26
55	M9	186/188 (99%)	172 (92%)	13 (7%)	1 (0%)	34	76
55	m9	186/188 (99%)	172 (92%)	13 (7%)	1 (0%)	34	76
56	N0	170/172 (99%)	150 (88%)	15 (9%)	5 (3%)	6	29
56	n0	170/172 (99%)	158 (93%)	11 (6%)	1 (1%)	30	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	N1	157/159 (99%)	133 (85%)	18 (12%)	6 (4%)	4	22
57	n1	157/159 (99%)	141 (90%)	12 (8%)	4 (2%)	7	34
58	N2	98/120 (82%)	76 (78%)	17 (17%)	5 (5%)	2	15
58	n2	96/120 (80%)	77 (80%)	13 (14%)	6 (6%)	2	9
59	N3	134/136 (98%)	124 (92%)	9 (7%)	1 (1%)	26	70
59	n3	134/136 (98%)	121 (90%)	11 (8%)	2 (2%)	13	50
60	N4	96/155 (62%)	74 (77%)	13 (14%)	9 (9%)	1	4
60	n4	133/155 (86%)	107 (80%)	17 (13%)	9 (7%)	1	7
61	N5	119/141 (84%)	106 (89%)	12 (10%)	1 (1%)	24	66
61	n5	118/141 (84%)	98 (83%)	11 (9%)	9 (8%)	1	6
62	N6	124/126 (98%)	110 (89%)	8 (6%)	6 (5%)	3	17
62	n6	124/126 (98%)	113 (91%)	7 (6%)	4 (3%)	5	27
63	N7	133/135 (98%)	109 (82%)	18 (14%)	6 (4%)	3	18
63	n7	133/135 (98%)	104 (78%)	18 (14%)	11 (8%)	1	5
64	N8	146/148 (99%)	121 (83%)	15 (10%)	10 (7%)	1	7
64	n8	146/148 (99%)	119 (82%)	22 (15%)	5 (3%)	5	25
65	N9	56/58 (97%)	48 (86%)	6 (11%)	2 (4%)	4	24
65	n9	56/58 (97%)	40 (71%)	12 (21%)	4 (7%)	1	7
66	O0	95/104 (91%)	89 (94%)	4 (4%)	2 (2%)	9	40
66	o0	98/104 (94%)	88 (90%)	6 (6%)	4 (4%)	3	20
67	O1	107/112 (96%)	95 (89%)	7 (6%)	5 (5%)	3	17
67	o1	107/112 (96%)	90 (84%)	12 (11%)	5 (5%)	3	17
68	O2	125/129 (97%)	112 (90%)	10 (8%)	3 (2%)	7	35
68	o2	125/129 (97%)	106 (85%)	13 (10%)	6 (5%)	3	17
69	O3	104/106 (98%)	94 (90%)	7 (7%)	3 (3%)	6	29
69	o3	104/106 (98%)	92 (88%)	8 (8%)	4 (4%)	4	22
70	O4	110/119 (92%)	97 (88%)	12 (11%)	1 (1%)	21	64
70	o4	110/119 (92%)	93 (84%)	11 (10%)	6 (6%)	2	13
71	O5	117/119 (98%)	104 (89%)	12 (10%)	1 (1%)	21	64
71	o5	117/119 (98%)	102 (87%)	13 (11%)	2 (2%)	11	46
72	O6	97/99 (98%)	77 (79%)	15 (16%)	5 (5%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	o6	97/99 (98%)	77 (79%)	13 (13%)	7 (7%)	1	7
73	O7	85/87 (98%)	74 (87%)	8 (9%)	3 (4%)	4	24
73	o7	85/87 (98%)	75 (88%)	8 (9%)	2 (2%)	7	35
74	O8	75/77 (97%)	62 (83%)	11 (15%)	2 (3%)	6	32
74	o8	75/77 (97%)	60 (80%)	11 (15%)	4 (5%)	2	14
75	O9	48/50 (96%)	39 (81%)	8 (17%)	1 (2%)	9	40
75	o9	48/50 (96%)	41 (85%)	6 (12%)	1 (2%)	9	40
76	Q0	50/52 (96%)	46 (92%)	2 (4%)	2 (4%)	4	21
76	q0	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	9	41
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	21 (91%)	1 (4%)	1 (4%)	3	19
78	Q2	103/105 (98%)	84 (82%)	13 (13%)	6 (6%)	2	12
78	q2	103/105 (98%)	92 (89%)	10 (10%)	1 (1%)	19	61
79	Q3	89/91 (98%)	77 (86%)	8 (9%)	4 (4%)	3	18
79	q3	89/91 (98%)	82 (92%)	6 (7%)	1 (1%)	17	58
80	e0	60/62 (97%)	43 (72%)	11 (18%)	6 (10%)	1	3
81	sM	98/273 (36%)	62 (63%)	22 (22%)	14 (14%)	0	1
83	p0	139/311 (45%)	120 (86%)	15 (11%)	4 (3%)	6	29
All	All	22333/24141 (92%)	18562 (83%)	2524 (11%)	1247 (6%)	2	13

5 of 1247 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	39	ASN
2	S0	66	ALA
2	S0	158	VAL
2	S0	191	ARG

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%)	133 (81%)	31 (19%)	2	10
2	s0	165/209 (79%)	131 (79%)	34 (21%)	1	7
3	S1	191/223 (86%)	155 (81%)	36 (19%)	2	10
3	s1	192/223 (86%)	163 (85%)	29 (15%)	3	17
4	S2	176/204 (86%)	142 (81%)	34 (19%)	2	9
4	s2	176/204 (86%)	133 (76%)	43 (24%)	1	4
5	S3	182/194 (94%)	145 (80%)	37 (20%)	1	7
5	s3	182/194 (94%)	151 (83%)	31 (17%)	2	13
6	S4	221/221 (100%)	183 (83%)	38 (17%)	2	12
6	s4	221/221 (100%)	183 (83%)	38 (17%)	2	12
7	S5	173/190 (91%)	142 (82%)	31 (18%)	2	11
7	s5	173/190 (91%)	133 (77%)	40 (23%)	1	5
8	S6	188/201 (94%)	148 (79%)	40 (21%)	1	6
8	s6	187/201 (93%)	151 (81%)	36 (19%)	2	9
9	S7	165/169 (98%)	140 (85%)	25 (15%)	3	16
9	s7	165/169 (98%)	138 (84%)	27 (16%)	3	14
10	S8	150/161 (93%)	130 (87%)	20 (13%)	5	21
10	s8	150/161 (93%)	128 (85%)	22 (15%)	4	18
11	S9	158/165 (96%)	123 (78%)	35 (22%)	1	5
11	s9	158/165 (96%)	128 (81%)	30 (19%)	2	10
12	C0	77/98 (79%)	67 (87%)	10 (13%)	5	22
12	c0	73/98 (74%)	63 (86%)	10 (14%)	4	20
13	C1	129/136 (95%)	107 (83%)	22 (17%)	2	12
13	c1	129/136 (95%)	106 (82%)	23 (18%)	2	11
14	C2	88/118 (75%)	66 (75%)	22 (25%)	1	3
14	c2	88/118 (75%)	66 (75%)	22 (25%)	1	3
15	C3	127/127 (100%)	100 (79%)	27 (21%)	1	6
15	c3	127/127 (100%)	103 (81%)	24 (19%)	2	10
16	C4	81/104 (78%)	60 (74%)	21 (26%)	0	3
16	c4	97/104 (93%)	76 (78%)	21 (22%)	1	6
17	C5	101/117 (86%)	85 (84%)	16 (16%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	c5	103/117 (88%)	84 (82%)	19 (18%)	2	10
18	C6	117/118 (99%)	94 (80%)	23 (20%)	1	9
18	c6	118/118 (100%)	93 (79%)	25 (21%)	1	6
19	C7	94/124 (76%)	72 (77%)	22 (23%)	1	4
19	c7	92/124 (74%)	78 (85%)	14 (15%)	3	16
20	C8	128/128 (100%)	95 (74%)	33 (26%)	0	3
20	c8	128/128 (100%)	103 (80%)	25 (20%)	2	9
21	C9	115/115 (100%)	92 (80%)	23 (20%)	1	8
21	c9	115/115 (100%)	93 (81%)	22 (19%)	2	10
22	D0	100/113 (88%)	78 (78%)	22 (22%)	1	6
22	d0	103/113 (91%)	78 (76%)	25 (24%)	1	4
23	D1	74/74 (100%)	61 (82%)	13 (18%)	2	12
23	d1	74/74 (100%)	56 (76%)	18 (24%)	1	4
24	D2	110/110 (100%)	94 (86%)	16 (14%)	4	18
24	d2	110/110 (100%)	93 (84%)	17 (16%)	3	16
25	D3	119/119 (100%)	98 (82%)	21 (18%)	2	12
25	d3	119/119 (100%)	104 (87%)	15 (13%)	5	24
26	D4	112/112 (100%)	93 (83%)	19 (17%)	2	13
26	d4	112/112 (100%)	94 (84%)	18 (16%)	3	14
27	D5	61/88 (69%)	46 (75%)	15 (25%)	1	4
27	d5	61/88 (69%)	51 (84%)	10 (16%)	3	14
28	D6	83/83 (100%)	67 (81%)	16 (19%)	2	9
28	d6	83/83 (100%)	73 (88%)	10 (12%)	6	26
29	D7	70/70 (100%)	64 (91%)	6 (9%)	13	44
29	d7	70/70 (100%)	60 (86%)	10 (14%)	4	19
30	D8	56/59 (95%)	44 (79%)	12 (21%)	1	6
30	d8	56/59 (95%)	44 (79%)	12 (21%)	1	6
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2	13
31	d9	47/48 (98%)	37 (79%)	10 (21%)	1	6
32	E0	51/51 (100%)	41 (80%)	10 (20%)	1	9
33	E1	62/66 (94%)	46 (74%)	16 (26%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	e1	66/66 (100%)	51 (77%)	15 (23%)	1	5
34	SR	260/261 (100%)	222 (85%)	38 (15%)	4	18
34	sR	260/261 (100%)	233 (90%)	27 (10%)	9	32
35	SM	97/228 (42%)	76 (78%)	21 (22%)	1	6
39	L2	193/195 (99%)	150 (78%)	43 (22%)	1	5
39	l2	192/195 (98%)	152 (79%)	40 (21%)	1	7
40	L3	321/322 (100%)	257 (80%)	64 (20%)	1	8
40	l3	320/322 (99%)	251 (78%)	69 (22%)	1	6
41	L4	288/288 (100%)	228 (79%)	60 (21%)	1	7
41	l4	288/288 (100%)	229 (80%)	59 (20%)	1	7
42	L5	244/244 (100%)	197 (81%)	47 (19%)	2	9
42	l5	243/244 (100%)	196 (81%)	47 (19%)	2	9
43	L6	134/152 (88%)	112 (84%)	22 (16%)	3	14
43	l6	135/152 (89%)	112 (83%)	23 (17%)	2	13
44	L7	186/204 (91%)	162 (87%)	24 (13%)	5	23
44	l7	187/204 (92%)	160 (86%)	27 (14%)	4	18
45	L8	187/207 (90%)	152 (81%)	35 (19%)	2	10
45	l8	177/207 (86%)	147 (83%)	30 (17%)	2	13
46	L9	171/171 (100%)	134 (78%)	37 (22%)	1	6
46	l9	171/171 (100%)	137 (80%)	34 (20%)	1	8
47	M0	177/186 (95%)	143 (81%)	34 (19%)	2	10
47	m0	179/186 (96%)	142 (79%)	37 (21%)	1	7
48	M1	147/150 (98%)	115 (78%)	32 (22%)	1	6
48	m1	147/150 (98%)	122 (83%)	25 (17%)	2	13
49	M3	154/158 (98%)	128 (83%)	26 (17%)	2	13
49	m3	154/158 (98%)	130 (84%)	24 (16%)	3	16
50	M4	107/108 (99%)	84 (78%)	23 (22%)	1	6
50	m4	108/108 (100%)	88 (82%)	20 (18%)	2	10
51	M5	175/175 (100%)	138 (79%)	37 (21%)	1	6
51	m5	175/175 (100%)	149 (85%)	26 (15%)	4	17
52	M6	160/161 (99%)	133 (83%)	27 (17%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	m6	160/161 (99%)	132 (82%)	28 (18%)	2	12
53	M7	140/145 (97%)	109 (78%)	31 (22%)	1	5
53	m7	125/145 (86%)	103 (82%)	22 (18%)	2	12
54	M8	150/150 (100%)	128 (85%)	22 (15%)	4	18
54	m8	150/150 (100%)	118 (79%)	32 (21%)	1	6
55	M9	153/153 (100%)	132 (86%)	21 (14%)	4	20
55	m9	153/153 (100%)	120 (78%)	33 (22%)	1	6
56	N0	156/156 (100%)	121 (78%)	35 (22%)	1	5
56	n0	156/156 (100%)	124 (80%)	32 (20%)	1	7
57	N1	136/136 (100%)	108 (79%)	28 (21%)	1	7
57	n1	136/136 (100%)	108 (79%)	28 (21%)	1	7
58	N2	87/106 (82%)	74 (85%)	13 (15%)	4	17
58	n2	85/106 (80%)	72 (85%)	13 (15%)	3	16
59	N3	104/104 (100%)	86 (83%)	18 (17%)	2	12
59	n3	104/104 (100%)	94 (90%)	10 (10%)	10	38
60	N4	57/129 (44%)	50 (88%)	7 (12%)	6	25
60	n4	100/129 (78%)	82 (82%)	18 (18%)	2	11
61	N5	104/117 (89%)	84 (81%)	20 (19%)	2	10
61	n5	104/117 (89%)	83 (80%)	21 (20%)	1	8
62	N6	109/109 (100%)	83 (76%)	26 (24%)	1	4
62	n6	109/109 (100%)	82 (75%)	27 (25%)	1	3
63	N7	115/115 (100%)	94 (82%)	21 (18%)	2	11
63	n7	115/115 (100%)	93 (81%)	22 (19%)	2	10
64	N8	118/118 (100%)	96 (81%)	22 (19%)	2	10
64	n8	118/118 (100%)	93 (79%)	25 (21%)	1	6
65	N9	46/46 (100%)	35 (76%)	11 (24%)	1	4
65	n9	46/46 (100%)	37 (80%)	9 (20%)	1	9
66	O0	81/87 (93%)	68 (84%)	13 (16%)	3	15
66	o0	84/87 (97%)	70 (83%)	14 (17%)	3	13
67	O1	92/96 (96%)	71 (77%)	21 (23%)	1	5
67	o1	94/96 (98%)	74 (79%)	20 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	O2	109/110 (99%)	87 (80%)	22 (20%)	1	8
68	o2	109/110 (99%)	85 (78%)	24 (22%)	1	6
69	O3	90/90 (100%)	81 (90%)	9 (10%)	9	34
69	o3	90/90 (100%)	77 (86%)	13 (14%)	4	18
70	O4	95/101 (94%)	74 (78%)	21 (22%)	1	5
70	o4	95/101 (94%)	75 (79%)	20 (21%)	1	6
71	O5	104/104 (100%)	80 (77%)	24 (23%)	1	5
71	o5	103/104 (99%)	80 (78%)	23 (22%)	1	5
72	O6	81/81 (100%)	65 (80%)	16 (20%)	1	8
72	o6	80/81 (99%)	56 (70%)	24 (30%)	0	2
73	O7	70/70 (100%)	58 (83%)	12 (17%)	2	12
73	o7	70/70 (100%)	58 (83%)	12 (17%)	2	12
74	O8	68/68 (100%)	52 (76%)	16 (24%)	1	4
74	o8	67/68 (98%)	53 (79%)	14 (21%)	1	7
75	O9	45/45 (100%)	40 (89%)	5 (11%)	8	29
75	o9	45/45 (100%)	36 (80%)	9 (20%)	1	8
76	Q0	47/47 (100%)	35 (74%)	12 (26%)	1	3
76	q0	47/47 (100%)	35 (74%)	12 (26%)	1	3
77	Q1	23/23 (100%)	15 (65%)	8 (35%)	0	1
77	q1	23/23 (100%)	14 (61%)	9 (39%)	0	0
78	Q2	90/90 (100%)	67 (74%)	23 (26%)	0	3
78	q2	90/90 (100%)	73 (81%)	17 (19%)	2	10
79	Q3	71/71 (100%)	56 (79%)	15 (21%)	1	6
79	q3	71/71 (100%)	63 (89%)	8 (11%)	7	28
80	e0	53/53 (100%)	42 (79%)	11 (21%)	1	7
81	sM	54/228 (24%)	40 (74%)	14 (26%)	0	3
83	p0	105/253 (42%)	80 (76%)	25 (24%)	1	4
All	All	18729/20239 (92%)	15175 (81%)	3554 (19%)	2	10

5 of 3554 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
68	O2	61	LYS

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Mol	Chain	Res	Type
7	s5	170	GLN
64	n8	46	ASP
71	O5	28	LEU
2	s0	119	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
42	L5	40	HIS
74	O8	32	ASN
59	n3	33	ASN
42	L5	264	GLN
78	Q2	23	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	451 (25%)	62 (3%)
1	6	1793/1800 (99%)	468 (26%)	56 (3%)
36	1	3145/3396 (92%)	662 (21%)	85 (2%)
36	5	3145/3396 (92%)	673 (21%)	84 (2%)
37	3	120/121 (99%)	16 (13%)	3 (2%)
37	7	120/121 (99%)	21 (17%)	0
38	4	157/158 (99%)	39 (24%)	3 (1%)
38	8	157/158 (99%)	36 (22%)	3 (1%)
All	All	10384/10950 (94%)	2366 (22%)	296 (2%)

5 of 2366 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

5 of 296 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	3121	U

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Mol	Chain	Res	Type
1	6	277	U
36	5	2818	U
36	1	3217	C
38	4	85	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2563 ligands modelled in this entry, 1428 are monoatomic - leaving 1135 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
87	OHX	1	3870	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3871	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3872	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3880	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3883	-	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
87	OHX	1	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3888	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3889	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3890	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3891	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3926	-	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
87	OHX	1	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3969	-	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
87	OHX	1	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4012	-	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
87	OHX	1	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4055	-	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
87	OHX	1	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4098	-	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
87	OHX	1	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4141	-	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
87	OHX	1	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4184	-	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
87	OHX	1	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
89	3KD	1	4218	-	24,25,25	0.76	0	29,39,39	1.19	3 (10%)
87	OHX	2	2021	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2022	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2029	-	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
87	OHX	2	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2072	-	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
87	OHX	2	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2115	-	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
87	OHX	2	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2158	-	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
87	OHX	2	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	227	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	228	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	229	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	230	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	231	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	4	232	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	233	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3940	-	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
87	OHX	5	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3983	-	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
87	OHX	5	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4026	-	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
87	OHX	5	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4069	-	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
87	OHX	5	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4112	-	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
87	OHX	5	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4155	-	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
87	OHX	5	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4198	-	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
87	OHX	5	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4227	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4228	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4229	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4230	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4231	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4232	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4233	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4234	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4235	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4236	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4237	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4238	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4239	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4240	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4241	-	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
87	OHX	5	4242	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4243	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4244	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4245	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4246	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4247	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4248	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4249	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4250	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4251	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4252	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4253	-	0,6,6	0.00	-	0,15,15	0.00	-
89	3KD	5	4254	-	24,25,25	1.00	2 (8%)	29,39,39	1.16	2 (6%)
87	OHX	6	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2079	-	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
87	OHX	6	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2122	-	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
87	OHX	6	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2165	-	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
87	OHX	6	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2182	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2183	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2184	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2185	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2186	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2187	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2188	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2189	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2190	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2191	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2192	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2193	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2194	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2195	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2196	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2197	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2198	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2199	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2200	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2204	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2207	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	217	-	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
87	OHX	7	218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	227	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	227	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	228	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	229	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	230	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	C3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	C5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	C8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	D3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	D9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L3	405	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M5	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M7	207	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M7	208	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M8	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	N1	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
87	OHX	N9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O7	103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O7	104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Q2	503	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	S8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c1	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	d4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	d9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	305	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m0	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m1	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	n3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	n6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	n9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o7	502	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o7	503	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	s1	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	s1	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	s4	302	-	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
87	OHX	s8	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	s9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	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
87	OHX	1	3870	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3871	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3872	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3873	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3874	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3875	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3876	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3877	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3878	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3879	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3880	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3881	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3882	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3883	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3884	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3885	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3886	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3887	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3888	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3889	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3890	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3891	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3892	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3893	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3894	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3895	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3896	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3897	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3898	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3899	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3900	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3901	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3902	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	3903	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3904	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3905	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3906	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3907	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3908	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3909	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3910	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3911	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3912	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3913	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3914	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3915	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3916	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3917	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3918	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3919	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3920	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3921	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3922	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3923	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3924	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3925	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3926	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3927	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3928	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3929	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3930	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3931	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3932	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3933	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3934	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3935	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3936	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3937	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3938	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3939	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3940	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3941	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3942	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3943	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3944	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	3945	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3946	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3947	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3948	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3949	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3950	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3951	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3952	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3953	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3954	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3955	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3956	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3957	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3958	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3959	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3960	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3961	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3962	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3963	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3964	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3965	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3966	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3967	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3968	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3969	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3970	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3971	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3972	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3973	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3974	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3975	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3976	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3977	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3978	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3979	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3980	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3981	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3982	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3983	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3984	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3985	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3986	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	3987	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3988	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3989	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3990	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3991	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3992	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3993	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3994	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3995	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3996	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3997	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3998	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3999	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4000	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4001	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4002	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4003	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4004	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4005	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4006	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4007	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4008	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4009	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4010	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4011	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4012	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4013	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4014	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4015	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4016	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4017	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4018	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4019	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4020	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4021	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4022	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4023	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4024	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4025	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4026	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4027	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4028	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4029	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4030	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4031	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4032	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4033	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4034	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4035	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4036	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4037	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4038	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4039	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4040	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4041	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4042	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4043	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4044	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4045	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4046	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4047	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4048	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4049	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4050	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4051	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4052	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4053	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4054	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4055	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4056	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4057	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4058	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4059	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4060	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4061	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4062	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4063	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4064	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4065	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4066	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4067	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4068	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4069	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4070	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4071	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4072	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4073	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4074	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4075	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4076	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4077	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4078	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4079	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4080	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4081	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4082	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4083	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4084	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4085	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4086	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4087	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4088	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4089	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4090	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4091	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4092	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4093	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4094	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4095	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4096	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4097	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4098	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4099	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4100	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4101	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4102	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4103	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4104	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4105	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4106	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4107	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4108	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4109	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4110	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4111	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4112	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4113	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4114	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4115	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4116	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4117	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4118	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4119	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4120	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4121	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4122	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4123	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4124	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4125	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4126	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4127	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4128	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4129	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4130	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4131	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4132	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4133	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4134	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4135	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4136	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4137	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4138	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4139	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4140	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4141	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4142	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4143	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4144	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4145	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4146	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4147	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4148	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4149	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4150	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4151	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4152	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4153	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4154	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4155	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4156	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4157	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4158	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4159	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4160	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4161	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4162	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4163	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4164	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4165	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4166	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4167	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4168	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4169	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4170	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4171	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4172	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4173	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4174	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4175	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4176	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4177	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4178	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4179	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4180	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4181	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4182	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4183	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4184	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4185	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4186	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4187	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4188	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4189	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4190	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4191	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4192	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4193	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4194	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4195	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4196	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4197	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4198	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4199	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4200	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4201	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4202	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4203	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4204	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4205	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4206	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4207	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4208	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4209	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4210	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4211	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4212	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4213	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4214	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4215	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4216	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4217	-	-	0/0/0/0	0/0/0/0
89	3KD	1	4218	-	-	0/0/43/43	0/5/5/5
87	OHX	2	2021	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2022	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2023	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2024	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2025	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2029	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2030	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2031	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2032	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2033	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2034	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2035	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2036	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2037	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2038	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2039	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2040	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2041	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2042	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2043	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2044	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2045	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2046	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2047	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2048	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2049	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2050	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2051	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2052	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2053	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2054	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2055	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2056	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2057	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2058	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2059	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2060	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2061	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2062	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2063	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2064	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2065	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2066	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2067	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2068	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2069	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2070	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2071	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2072	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2073	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2074	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2075	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2076	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2077	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2078	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2079	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2080	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2081	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2082	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2083	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2084	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2085	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2086	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2087	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2088	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2089	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2090	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2091	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2092	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2093	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2094	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2095	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2096	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2097	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2098	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2099	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2100	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2101	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2102	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2103	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2104	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2105	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2106	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2107	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2108	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2109	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2110	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2111	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2112	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2113	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2114	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2115	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2116	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2117	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2118	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2119	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2120	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2121	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2122	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2123	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2124	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2125	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2126	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2127	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2128	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2129	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2130	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2131	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2132	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2133	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2134	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2135	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2136	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2137	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2138	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2139	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2140	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2141	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2142	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2143	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2144	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2145	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2146	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2147	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2148	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2149	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2150	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2151	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2152	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2153	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2154	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2155	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2156	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2157	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2158	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2159	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2160	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2161	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2162	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2163	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2164	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2165	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2166	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2167	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2168	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2169	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2170	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2171	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2172	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2173	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2174	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2175	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2176	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2177	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2178	-	-	0/0/0/0	0/0/0/0
87	OHX	3	215	-	-	0/0/0/0	0/0/0/0
87	OHX	3	216	-	-	0/0/0/0	0/0/0/0
87	OHX	3	217	-	-	0/0/0/0	0/0/0/0
87	OHX	3	218	-	-	0/0/0/0	0/0/0/0
87	OHX	3	219	-	-	0/0/0/0	0/0/0/0
87	OHX	3	220	-	-	0/0/0/0	0/0/0/0
87	OHX	3	221	-	-	0/0/0/0	0/0/0/0
87	OHX	3	222	-	-	0/0/0/0	0/0/0/0
87	OHX	3	223	-	-	0/0/0/0	0/0/0/0
87	OHX	3	224	-	-	0/0/0/0	0/0/0/0
87	OHX	3	225	-	-	0/0/0/0	0/0/0/0
87	OHX	3	226	-	-	0/0/0/0	0/0/0/0
87	OHX	4	221	-	-	0/0/0/0	0/0/0/0
87	OHX	4	222	-	-	0/0/0/0	0/0/0/0
87	OHX	4	223	-	-	0/0/0/0	0/0/0/0
87	OHX	4	224	-	-	0/0/0/0	0/0/0/0
87	OHX	4	225	-	-	0/0/0/0	0/0/0/0
87	OHX	4	226	-	-	0/0/0/0	0/0/0/0
87	OHX	4	227	-	-	0/0/0/0	0/0/0/0
87	OHX	4	228	-	-	0/0/0/0	0/0/0/0
87	OHX	4	229	-	-	0/0/0/0	0/0/0/0
87	OHX	4	230	-	-	0/0/0/0	0/0/0/0
87	OHX	4	231	-	-	0/0/0/0	0/0/0/0
87	OHX	4	232	-	-	0/0/0/0	0/0/0/0
87	OHX	4	233	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3900	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3901	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3902	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3903	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3904	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	3905	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3906	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3907	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3908	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3909	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3910	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3911	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3912	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3913	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3914	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3915	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3916	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3917	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3918	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3919	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3920	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3921	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3922	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3923	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3924	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3925	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3926	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3927	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3928	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3929	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3930	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3931	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3932	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3933	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3934	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3935	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3936	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3937	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3938	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3939	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3940	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3941	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3942	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3943	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3944	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3945	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3946	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	3947	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3948	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3949	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3950	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3951	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3952	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3953	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3954	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3955	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3956	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3957	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3958	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3959	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3960	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3961	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3962	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3963	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3964	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3965	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3966	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3967	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3968	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3969	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3970	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3971	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3972	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3973	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3974	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3975	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3976	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3977	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3978	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3979	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3980	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3981	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3982	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3983	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3984	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3985	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3986	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3987	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3988	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	3989	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3990	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3991	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3992	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3993	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3994	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3995	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3996	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3997	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3998	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3999	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4000	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4001	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4002	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4003	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4004	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4005	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4006	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4007	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4008	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4009	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4010	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4011	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4012	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4013	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4014	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4015	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4016	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4017	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4018	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4019	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4020	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4021	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4022	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4023	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4024	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4025	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4026	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4027	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4028	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4029	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4030	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4031	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4032	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4033	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4034	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4035	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4036	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4037	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4038	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4039	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4040	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4041	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4042	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4043	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4044	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4045	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4046	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4047	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4048	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4049	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4050	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4051	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4052	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4053	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4054	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4055	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4056	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4057	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4058	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4059	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4060	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4061	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4062	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4063	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4064	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4065	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4066	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4067	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4068	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4069	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4070	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4071	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4072	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4073	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4074	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4075	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4076	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4077	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4078	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4079	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4080	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4081	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4082	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4083	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4084	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4085	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4086	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4087	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4088	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4089	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4090	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4091	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4092	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4093	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4094	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4095	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4096	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4097	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4098	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4099	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4100	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4101	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4102	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4103	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4104	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4105	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4106	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4107	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4108	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4109	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4110	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4111	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4112	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4113	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4114	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4115	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4116	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4117	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4118	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4119	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4120	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4121	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4122	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4123	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4124	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4125	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4126	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4127	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4128	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4129	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4130	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4131	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4132	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4133	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4134	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4135	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4136	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4137	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4138	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4139	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4140	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4141	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4142	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4143	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4144	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4145	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4146	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4147	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4148	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4149	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4150	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4151	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4152	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4153	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4154	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4155	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4156	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4157	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4158	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4159	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4160	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4161	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4162	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4163	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4164	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4165	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4166	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4167	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4168	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4169	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4170	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4171	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4172	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4173	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4174	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4175	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4176	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4177	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4178	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4179	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4180	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4181	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4182	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4183	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4184	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4185	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4186	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4187	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4188	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4189	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4190	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4191	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4192	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4193	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4194	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4195	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4196	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4197	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4198	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4199	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4200	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4201	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4202	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4203	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4204	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4205	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4206	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4207	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4208	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4209	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4210	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4211	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4212	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4213	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4214	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4215	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4216	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4217	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4218	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4219	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4220	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4221	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4222	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4223	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4224	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4225	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4226	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4227	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4228	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4229	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4230	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4231	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4232	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4233	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4234	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4235	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4236	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4237	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4238	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4239	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4240	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4241	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4242	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4243	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4244	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4245	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4246	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4247	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4248	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4249	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4250	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4251	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4252	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4253	-	-	0/0/0/0	0/0/0/0
89	3KD	5	4254	-	-	0/0/43/43	0/5/5/5
87	OHX	6	2050	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2051	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2052	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2053	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2054	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2055	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2056	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2057	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2058	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2059	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2060	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2061	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2062	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2063	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2064	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2065	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2066	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2067	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2068	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2069	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2070	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2071	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2072	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2073	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2074	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2075	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2076	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2077	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2078	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2079	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2080	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2081	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2082	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2083	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2084	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2085	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2086	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2087	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2088	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2089	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2090	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2091	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2092	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2093	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2094	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2095	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2096	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2097	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2098	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2099	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2100	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2101	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2102	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2103	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2104	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2105	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2106	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2107	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2108	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2109	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2110	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2111	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2112	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2113	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2114	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2115	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2116	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2117	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2118	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2119	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2120	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2121	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2122	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2123	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2124	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2125	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2126	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2127	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2128	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2129	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2130	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2131	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2132	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2133	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2134	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2135	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2136	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2137	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2138	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2139	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2140	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2141	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2142	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2143	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2144	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2145	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2146	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2147	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2148	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2149	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2150	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2151	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2152	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2153	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2154	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2155	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2156	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2157	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2158	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2159	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2160	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2161	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2162	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2163	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2164	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2165	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2166	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2167	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2168	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2169	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2170	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2171	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2172	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2173	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2174	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2175	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2176	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2177	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2178	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2179	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2180	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2181	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2182	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2183	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2184	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2185	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2186	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2187	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2188	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2189	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2190	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2191	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2192	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2193	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2194	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2195	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2196	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2197	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2198	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2199	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2200	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2201	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2202	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2203	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2204	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2205	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2206	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2207	-	-	0/0/0/0	0/0/0/0
87	OHX	7	217	-	-	0/0/0/0	0/0/0/0
87	OHX	7	218	-	-	0/0/0/0	0/0/0/0
87	OHX	7	219	-	-	0/0/0/0	0/0/0/0
87	OHX	7	220	-	-	0/0/0/0	0/0/0/0
87	OHX	7	221	-	-	0/0/0/0	0/0/0/0
87	OHX	7	222	-	-	0/0/0/0	0/0/0/0
87	OHX	7	223	-	-	0/0/0/0	0/0/0/0
87	OHX	7	224	-	-	0/0/0/0	0/0/0/0
87	OHX	7	225	-	-	0/0/0/0	0/0/0/0
87	OHX	7	226	-	-	0/0/0/0	0/0/0/0
87	OHX	7	227	-	-	0/0/0/0	0/0/0/0
87	OHX	8	215	-	-	0/0/0/0	0/0/0/0
87	OHX	8	216	-	-	0/0/0/0	0/0/0/0
87	OHX	8	217	-	-	0/0/0/0	0/0/0/0
87	OHX	8	218	-	-	0/0/0/0	0/0/0/0
87	OHX	8	219	-	-	0/0/0/0	0/0/0/0
87	OHX	8	220	-	-	0/0/0/0	0/0/0/0
87	OHX	8	221	-	-	0/0/0/0	0/0/0/0
87	OHX	8	222	-	-	0/0/0/0	0/0/0/0
87	OHX	8	223	-	-	0/0/0/0	0/0/0/0
87	OHX	8	224	-	-	0/0/0/0	0/0/0/0
87	OHX	8	225	-	-	0/0/0/0	0/0/0/0
87	OHX	8	226	-	-	0/0/0/0	0/0/0/0
87	OHX	8	227	-	-	0/0/0/0	0/0/0/0
87	OHX	8	228	-	-	0/0/0/0	0/0/0/0
87	OHX	8	229	-	-	0/0/0/0	0/0/0/0
87	OHX	8	230	-	-	0/0/0/0	0/0/0/0
87	OHX	C3	201	-	-	0/0/0/0	0/0/0/0
87	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
87	OHX	C8	201	-	-	0/0/0/0	0/0/0/0
87	OHX	D3	202	-	-	0/0/0/0	0/0/0/0
87	OHX	D9	102	-	-	0/0/0/0	0/0/0/0
87	OHX	L3	403	-	-	0/0/0/0	0/0/0/0
87	OHX	L3	404	-	-	0/0/0/0	0/0/0/0
87	OHX	L3	405	-	-	0/0/0/0	0/0/0/0
87	OHX	L4	403	-	-	0/0/0/0	0/0/0/0
87	OHX	M0	303	-	-	0/0/0/0	0/0/0/0
87	OHX	M5	302	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	M6	202	-	-	0/0/0/0	0/0/0/0
87	OHX	M7	207	-	-	0/0/0/0	0/0/0/0
87	OHX	M7	208	-	-	0/0/0/0	0/0/0/0
87	OHX	M8	202	-	-	0/0/0/0	0/0/0/0
87	OHX	M9	202	-	-	0/0/0/0	0/0/0/0
87	OHX	N1	201	-	-	0/0/0/0	0/0/0/0
87	OHX	N9	101	-	-	0/0/0/0	0/0/0/0
87	OHX	O2	201	-	-	0/0/0/0	0/0/0/0
87	OHX	O3	201	-	-	0/0/0/0	0/0/0/0
87	OHX	O7	103	-	-	0/0/0/0	0/0/0/0
87	OHX	O7	104	-	-	0/0/0/0	0/0/0/0
87	OHX	O9	101	-	-	0/0/0/0	0/0/0/0
87	OHX	Q2	503	-	-	0/0/0/0	0/0/0/0
87	OHX	S8	302	-	-	0/0/0/0	0/0/0/0
87	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
87	OHX	c1	202	-	-	0/0/0/0	0/0/0/0
87	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
87	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
87	OHX	c8	201	-	-	0/0/0/0	0/0/0/0
87	OHX	d4	202	-	-	0/0/0/0	0/0/0/0
87	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
87	OHX	l3	403	-	-	0/0/0/0	0/0/0/0
87	OHX	l3	404	-	-	0/0/0/0	0/0/0/0
87	OHX	l4	402	-	-	0/0/0/0	0/0/0/0
87	OHX	l4	403	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	303	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	304	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	305	-	-	0/0/0/0	0/0/0/0
87	OHX	l9	202	-	-	0/0/0/0	0/0/0/0
87	OHX	m0	301	-	-	0/0/0/0	0/0/0/0
87	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
87	OHX	m1	202	-	-	0/0/0/0	0/0/0/0
87	OHX	m4	201	-	-	0/0/0/0	0/0/0/0
87	OHX	m5	304	-	-	0/0/0/0	0/0/0/0
87	OHX	m6	202	-	-	0/0/0/0	0/0/0/0
87	OHX	m7	206	-	-	0/0/0/0	0/0/0/0
87	OHX	m8	201	-	-	0/0/0/0	0/0/0/0
87	OHX	m9	201	-	-	0/0/0/0	0/0/0/0
87	OHX	n3	203	-	-	0/0/0/0	0/0/0/0
87	OHX	n6	202	-	-	0/0/0/0	0/0/0/0
87	OHX	n9	101	-	-	0/0/0/0	0/0/0/0
87	OHX	o2	201	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	o3	203	-	-	0/0/0/0	0/0/0/0
87	OHX	o7	502	-	-	0/0/0/0	0/0/0/0
87	OHX	o7	503	-	-	0/0/0/0	0/0/0/0
87	OHX	q2	502	-	-	0/0/0/0	0/0/0/0
87	OHX	s1	302	-	-	0/0/0/0	0/0/0/0
87	OHX	s1	303	-	-	0/0/0/0	0/0/0/0
87	OHX	s4	302	-	-	0/0/0/0	0/0/0/0
87	OHX	s8	303	-	-	0/0/0/0	0/0/0/0
87	OHX	s9	201	-	-	0/0/0/0	0/0/0/0
87	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)
89	5	4254	3KD	C8-C9	-2.16	1.47	1.51
89	5	4254	3KD	C13-C12	3.02	1.54	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	5	4254	3KD	O-C14-C9	-3.43	101.86	109.72
89	1	4218	3KD	O-C14-C9	-2.92	103.05	109.72
89	1	4218	3KD	C1-N-C10	-2.27	103.64	107.15
89	5	4254	3KD	C2-N-C1	2.31	117.37	112.95
89	1	4218	3KD	C2-N-C1	2.96	118.61	112.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

521 monomers are involved in 844 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	3871	OHX	1	0
87	1	3873	OHX	1	0
87	1	3877	OHX	1	0
87	1	3878	OHX	1	0
87	1	3880	OHX	1	0
87	1	3881	OHX	1	0
87	1	3882	OHX	1	0
87	1	3884	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	3886	OHX	1	0
87	1	3887	OHX	2	0
87	1	3889	OHX	3	0
87	1	3890	OHX	2	0
87	1	3891	OHX	1	0
87	1	3892	OHX	2	0
87	1	3894	OHX	1	0
87	1	3896	OHX	1	0
87	1	3897	OHX	1	0
87	1	3898	OHX	1	0
87	1	3899	OHX	1	0
87	1	3904	OHX	1	0
87	1	3905	OHX	1	0
87	1	3906	OHX	2	0
87	1	3912	OHX	1	0
87	1	3913	OHX	2	0
87	1	3915	OHX	1	0
87	1	3918	OHX	1	0
87	1	3920	OHX	1	0
87	1	3926	OHX	1	0
87	1	3931	OHX	1	0
87	1	3933	OHX	2	0
87	1	3937	OHX	2	0
87	1	3939	OHX	2	0
87	1	3940	OHX	1	0
87	1	3945	OHX	7	0
87	1	3947	OHX	2	0
87	1	3949	OHX	1	0
87	1	3953	OHX	1	0
87	1	3954	OHX	1	0
87	1	3957	OHX	2	0
87	1	3959	OHX	1	0
87	1	3960	OHX	1	0
87	1	3963	OHX	2	0
87	1	3964	OHX	7	0
87	1	3966	OHX	5	0
87	1	3968	OHX	1	0
87	1	3970	OHX	1	0
87	1	3972	OHX	1	0
87	1	3973	OHX	1	0
87	1	3975	OHX	1	0
87	1	3978	OHX	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	3979	OHX	1	0
87	1	3981	OHX	1	0
87	1	3982	OHX	1	0
87	1	3983	OHX	2	0
87	1	3984	OHX	1	0
87	1	3986	OHX	1	0
87	1	3987	OHX	1	0
87	1	3988	OHX	1	0
87	1	3989	OHX	2	0
87	1	3992	OHX	1	0
87	1	3993	OHX	1	0
87	1	3998	OHX	1	0
87	1	4002	OHX	1	0
87	1	4003	OHX	1	0
87	1	4007	OHX	1	0
87	1	4008	OHX	1	0
87	1	4009	OHX	6	0
87	1	4012	OHX	2	0
87	1	4014	OHX	1	0
87	1	4019	OHX	1	0
87	1	4021	OHX	1	0
87	1	4023	OHX	1	0
87	1	4025	OHX	3	0
87	1	4029	OHX	2	0
87	1	4033	OHX	2	0
87	1	4034	OHX	4	0
87	1	4035	OHX	1	0
87	1	4037	OHX	7	0
87	1	4039	OHX	1	0
87	1	4042	OHX	4	0
87	1	4043	OHX	2	0
87	1	4044	OHX	1	0
87	1	4045	OHX	3	0
87	1	4047	OHX	1	0
87	1	4048	OHX	5	0
87	1	4049	OHX	7	0
87	1	4050	OHX	2	0
87	1	4052	OHX	2	0
87	1	4055	OHX	2	0
87	1	4057	OHX	1	0
87	1	4060	OHX	6	0
87	1	4061	OHX	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	4062	OHX	3	0
87	1	4066	OHX	2	0
87	1	4067	OHX	1	0
87	1	4068	OHX	1	0
87	1	4070	OHX	1	0
87	1	4071	OHX	1	0
87	1	4072	OHX	1	0
87	1	4075	OHX	1	0
87	1	4080	OHX	1	0
87	1	4081	OHX	1	0
87	1	4085	OHX	4	0
87	1	4089	OHX	7	0
87	1	4090	OHX	1	0
87	1	4092	OHX	1	0
87	1	4093	OHX	2	0
87	1	4095	OHX	2	0
87	1	4096	OHX	1	0
87	1	4099	OHX	1	0
87	1	4100	OHX	1	0
87	1	4101	OHX	1	0
87	1	4103	OHX	1	0
87	1	4104	OHX	1	0
87	1	4112	OHX	1	0
87	1	4114	OHX	1	0
87	1	4119	OHX	1	0
87	1	4123	OHX	2	0
87	1	4124	OHX	2	0
87	1	4127	OHX	2	0
87	1	4130	OHX	1	0
87	1	4136	OHX	1	0
87	1	4137	OHX	4	0
87	1	4138	OHX	2	0
87	1	4140	OHX	3	0
87	1	4144	OHX	3	0
87	1	4145	OHX	5	0
87	1	4146	OHX	1	0
87	1	4148	OHX	2	0
87	1	4149	OHX	1	0
87	1	4151	OHX	5	0
87	1	4152	OHX	1	0
87	1	4154	OHX	1	0
87	1	4155	OHX	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	4159	OHX	5	0
87	1	4160	OHX	2	0
87	1	4161	OHX	7	0
87	1	4163	OHX	1	0
87	1	4165	OHX	1	0
87	1	4168	OHX	6	0
87	1	4169	OHX	2	0
87	1	4170	OHX	1	0
87	1	4172	OHX	3	0
87	1	4173	OHX	3	0
87	1	4177	OHX	8	0
87	1	4179	OHX	2	0
87	1	4184	OHX	1	0
87	1	4185	OHX	1	0
87	1	4186	OHX	5	0
87	1	4188	OHX	1	0
87	1	4193	OHX	2	0
87	1	4196	OHX	1	0
87	1	4198	OHX	1	0
87	1	4200	OHX	1	0
87	1	4201	OHX	1	0
87	1	4202	OHX	1	0
87	1	4203	OHX	6	0
87	1	4204	OHX	1	0
87	1	4206	OHX	1	0
87	1	4208	OHX	2	0
87	1	4209	OHX	1	0
87	1	4210	OHX	1	0
87	1	4212	OHX	1	0
87	1	4214	OHX	1	0
87	2	2021	OHX	1	0
87	2	2024	OHX	1	0
87	2	2029	OHX	8	0
87	2	2030	OHX	1	0
87	2	2031	OHX	2	0
87	2	2032	OHX	1	0
87	2	2033	OHX	1	0
87	2	2034	OHX	3	0
87	2	2036	OHX	1	0
87	2	2037	OHX	2	0
87	2	2040	OHX	1	0
87	2	2042	OHX	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	2	2045	OHX	1	0
87	2	2046	OHX	1	0
87	2	2049	OHX	1	0
87	2	2051	OHX	1	0
87	2	2052	OHX	1	0
87	2	2055	OHX	1	0
87	2	2056	OHX	2	0
87	2	2060	OHX	1	0
87	2	2062	OHX	1	0
87	2	2063	OHX	1	0
87	2	2068	OHX	2	0
87	2	2071	OHX	1	0
87	2	2072	OHX	1	0
87	2	2073	OHX	2	0
87	2	2074	OHX	1	0
87	2	2076	OHX	2	0
87	2	2080	OHX	1	0
87	2	2081	OHX	4	0
87	2	2082	OHX	2	0
87	2	2083	OHX	4	0
87	2	2084	OHX	2	0
87	2	2087	OHX	3	0
87	2	2088	OHX	6	0
87	2	2090	OHX	2	0
87	2	2091	OHX	1	0
87	2	2094	OHX	2	0
87	2	2097	OHX	7	0
87	2	2098	OHX	1	0
87	2	2102	OHX	2	0
87	2	2103	OHX	1	0
87	2	2104	OHX	2	0
87	2	2106	OHX	1	0
87	2	2107	OHX	1	0
87	2	2108	OHX	1	0
87	2	2109	OHX	4	0
87	2	2113	OHX	2	0
87	2	2115	OHX	1	0
87	2	2119	OHX	3	0
87	2	2121	OHX	1	0
87	2	2123	OHX	1	0
87	2	2124	OHX	1	0
87	2	2125	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	2	2127	OHX	1	0
87	2	2129	OHX	9	0
87	2	2130	OHX	1	0
87	2	2134	OHX	2	0
87	2	2136	OHX	1	0
87	2	2138	OHX	1	0
87	2	2139	OHX	1	0
87	2	2141	OHX	1	0
87	2	2143	OHX	2	0
87	2	2144	OHX	6	0
87	2	2146	OHX	1	0
87	2	2147	OHX	1	0
87	2	2150	OHX	1	0
87	2	2152	OHX	1	0
87	2	2153	OHX	1	0
87	2	2154	OHX	1	0
87	2	2155	OHX	3	0
87	2	2157	OHX	1	0
87	2	2158	OHX	1	0
87	2	2160	OHX	2	0
87	2	2163	OHX	1	0
87	2	2164	OHX	1	0
87	2	2165	OHX	1	0
87	2	2171	OHX	1	0
87	2	2172	OHX	1	0
87	3	216	OHX	1	0
87	3	218	OHX	2	0
87	3	221	OHX	1	0
87	3	223	OHX	1	0
87	3	226	OHX	1	0
87	4	221	OHX	1	0
87	4	222	OHX	1	0
87	4	223	OHX	1	0
87	4	225	OHX	1	0
87	4	229	OHX	2	0
87	5	3900	OHX	1	0
87	5	3906	OHX	1	0
87	5	3908	OHX	3	0
87	5	3912	OHX	2	0
87	5	3914	OHX	1	0
87	5	3917	OHX	1	0
87	5	3918	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	3919	OHX	2	0
87	5	3924	OHX	1	0
87	5	3926	OHX	2	0
87	5	3934	OHX	1	0
87	5	3940	OHX	1	0
87	5	3941	OHX	1	0
87	5	3942	OHX	1	0
87	5	3943	OHX	7	0
87	5	3948	OHX	1	0
87	5	3949	OHX	1	0
87	5	3954	OHX	1	0
87	5	3955	OHX	2	0
87	5	3956	OHX	1	0
87	5	3957	OHX	2	0
87	5	3958	OHX	2	0
87	5	3959	OHX	1	0
87	5	3960	OHX	1	0
87	5	3961	OHX	1	0
87	5	3963	OHX	4	0
87	5	3964	OHX	1	0
87	5	3967	OHX	1	0
87	5	3970	OHX	1	0
87	5	3973	OHX	3	0
87	5	3974	OHX	7	0
87	5	3976	OHX	1	0
87	5	3977	OHX	1	0
87	5	3979	OHX	8	0
87	5	3983	OHX	1	0
87	5	3984	OHX	1	0
87	5	3985	OHX	1	0
87	5	3987	OHX	1	0
87	5	3990	OHX	1	0
87	5	3992	OHX	3	0
87	5	4000	OHX	1	0
87	5	4002	OHX	8	0
87	5	4003	OHX	5	0
87	5	4004	OHX	1	0
87	5	4007	OHX	1	0
87	5	4011	OHX	6	0
87	5	4013	OHX	2	0
87	5	4014	OHX	1	0
87	5	4015	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	4016	OHX	1	0
87	5	4021	OHX	8	0
87	5	4023	OHX	1	0
87	5	4024	OHX	4	0
87	5	4025	OHX	2	0
87	5	4027	OHX	1	0
87	5	4028	OHX	1	0
87	5	4030	OHX	1	0
87	5	4031	OHX	1	0
87	5	4032	OHX	1	0
87	5	4035	OHX	1	0
87	5	4040	OHX	2	0
87	5	4042	OHX	2	0
87	5	4047	OHX	1	0
87	5	4050	OHX	1	0
87	5	4052	OHX	1	0
87	5	4056	OHX	6	0
87	5	4057	OHX	1	0
87	5	4060	OHX	1	0
87	5	4062	OHX	1	0
87	5	4066	OHX	3	0
87	5	4067	OHX	7	0
87	5	4068	OHX	1	0
87	5	4069	OHX	1	0
87	5	4073	OHX	1	0
87	5	4075	OHX	3	0
87	5	4077	OHX	3	0
87	5	4078	OHX	1	0
87	5	4079	OHX	1	0
87	5	4080	OHX	1	0
87	5	4081	OHX	1	0
87	5	4089	OHX	1	0
87	5	4090	OHX	1	0
87	5	4091	OHX	6	0
87	5	4092	OHX	4	0
87	5	4093	OHX	1	0
87	5	4094	OHX	2	0
87	5	4095	OHX	2	0
87	5	4096	OHX	6	0
87	5	4098	OHX	1	0
87	5	4099	OHX	1	0
87	5	4101	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	4104	OHX	4	0
87	5	4107	OHX	1	0
87	5	4108	OHX	1	0
87	5	4110	OHX	1	0
87	5	4111	OHX	2	0
87	5	4112	OHX	1	0
87	5	4115	OHX	1	0
87	5	4118	OHX	1	0
87	5	4120	OHX	1	0
87	5	4121	OHX	1	0
87	5	4127	OHX	1	0
87	5	4132	OHX	1	0
87	5	4134	OHX	1	0
87	5	4135	OHX	1	0
87	5	4138	OHX	3	0
87	5	4139	OHX	2	0
87	5	4141	OHX	1	0
87	5	4143	OHX	2	0
87	5	4144	OHX	6	0
87	5	4145	OHX	1	0
87	5	4148	OHX	1	0
87	5	4154	OHX	1	0
87	5	4158	OHX	1	0
87	5	4160	OHX	3	0
87	5	4163	OHX	3	0
87	5	4164	OHX	1	0
87	5	4167	OHX	1	0
87	5	4169	OHX	1	0
87	5	4174	OHX	2	0
87	5	4175	OHX	1	0
87	5	4180	OHX	2	0
87	5	4182	OHX	1	0
87	5	4183	OHX	2	0
87	5	4185	OHX	1	0
87	5	4186	OHX	1	0
87	5	4187	OHX	1	0
87	5	4188	OHX	1	0
87	5	4189	OHX	2	0
87	5	4191	OHX	5	0
87	5	4192	OHX	1	0
87	5	4193	OHX	5	0
87	5	4194	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	4195	OHX	1	0
87	5	4196	OHX	1	0
87	5	4197	OHX	1	0
87	5	4199	OHX	1	0
87	5	4200	OHX	10	0
87	5	4201	OHX	7	0
87	5	4202	OHX	7	0
87	5	4203	OHX	1	0
87	5	4208	OHX	1	0
87	5	4209	OHX	1	0
87	5	4210	OHX	1	0
87	5	4212	OHX	1	0
87	5	4215	OHX	5	0
87	5	4218	OHX	9	0
87	5	4220	OHX	1	0
87	5	4225	OHX	6	0
87	5	4227	OHX	1	0
87	5	4228	OHX	1	0
87	5	4229	OHX	1	0
87	5	4230	OHX	1	0
87	5	4233	OHX	1	0
87	5	4235	OHX	6	0
87	5	4237	OHX	6	0
87	5	4241	OHX	1	0
87	5	4244	OHX	9	0
87	5	4245	OHX	1	0
87	5	4250	OHX	1	0
89	5	4254	3KD	1	0
87	6	2050	OHX	1	0
87	6	2053	OHX	1	0
87	6	2058	OHX	1	0
87	6	2059	OHX	1	0
87	6	2063	OHX	6	0
87	6	2064	OHX	1	0
87	6	2065	OHX	1	0
87	6	2069	OHX	1	0
87	6	2070	OHX	1	0
87	6	2072	OHX	1	0
87	6	2074	OHX	1	0
87	6	2075	OHX	1	0
87	6	2077	OHX	1	0
87	6	2078	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	6	2079	OHX	1	0
87	6	2086	OHX	1	0
87	6	2087	OHX	2	0
87	6	2088	OHX	1	0
87	6	2089	OHX	1	0
87	6	2090	OHX	1	0
87	6	2092	OHX	1	0
87	6	2094	OHX	1	0
87	6	2096	OHX	1	0
87	6	2097	OHX	1	0
87	6	2100	OHX	1	0
87	6	2101	OHX	1	0
87	6	2102	OHX	1	0
87	6	2104	OHX	3	0
87	6	2106	OHX	3	0
87	6	2107	OHX	1	0
87	6	2109	OHX	1	0
87	6	2110	OHX	1	0
87	6	2111	OHX	1	0
87	6	2115	OHX	2	0
87	6	2116	OHX	1	0
87	6	2118	OHX	1	0
87	6	2121	OHX	2	0
87	6	2123	OHX	1	0
87	6	2124	OHX	10	0
87	6	2125	OHX	1	0
87	6	2127	OHX	2	0
87	6	2128	OHX	1	0
87	6	2129	OHX	2	0
87	6	2131	OHX	1	0
87	6	2133	OHX	2	0
87	6	2134	OHX	1	0
87	6	2139	OHX	1	0
87	6	2140	OHX	3	0
87	6	2141	OHX	1	0
87	6	2146	OHX	1	0
87	6	2149	OHX	1	0
87	6	2150	OHX	7	0
87	6	2151	OHX	1	0
87	6	2152	OHX	1	0
87	6	2153	OHX	1	0
87	6	2154	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	6	2157	OHX	2	0
87	6	2158	OHX	1	0
87	6	2162	OHX	4	0
87	6	2163	OHX	1	0
87	6	2164	OHX	1	0
87	6	2165	OHX	1	0
87	6	2174	OHX	8	0
87	6	2178	OHX	1	0
87	6	2179	OHX	1	0
87	6	2181	OHX	1	0
87	6	2182	OHX	1	0
87	6	2185	OHX	1	0
87	6	2186	OHX	1	0
87	6	2187	OHX	2	0
87	6	2191	OHX	2	0
87	6	2192	OHX	4	0
87	6	2195	OHX	1	0
87	6	2196	OHX	1	0
87	6	2197	OHX	1	0
87	6	2202	OHX	1	0
87	6	2205	OHX	1	0
87	6	2207	OHX	1	0
87	7	218	OHX	1	0
87	7	220	OHX	3	0
87	7	222	OHX	1	0
87	7	226	OHX	1	0
87	8	215	OHX	1	0
87	8	217	OHX	7	0
87	8	220	OHX	1	0
87	8	221	OHX	1	0
87	8	222	OHX	1	0
87	8	223	OHX	1	0
87	8	225	OHX	8	0
87	8	226	OHX	1	0
87	8	227	OHX	1	0
87	C3	201	OHX	2	0
87	C5	201	OHX	4	0
87	D9	102	OHX	1	0
87	L3	403	OHX	1	0
87	L3	404	OHX	2	0
87	L4	403	OHX	3	0
87	M5	302	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	M7	207	OHX	2	0
87	M7	208	OHX	1	0
87	M9	202	OHX	1	0
87	O2	201	OHX	1	0
87	O3	201	OHX	1	0
87	O7	103	OHX	6	0
87	O7	104	OHX	1	0
87	O9	101	OHX	3	0
87	Q2	503	OHX	3	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.