wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:53 PM GMT

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

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

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

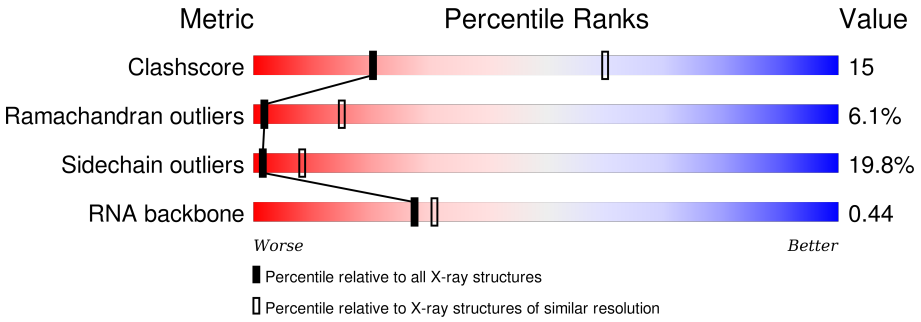
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	FAILED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RNA backbone	2183	1079 (3.70-2.70)

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 <=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	36% 41% 18%
1	6	1800	37% 41% 18%
2	S0	251	23% 45% 11% 18%
2	s0	251	61% 20% 18%
3	S1	254	13% 51% 19% 16%
3	s1	254	65% 19% 15%

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Mol	Chain	Length	Quality of chain
4	S2	253	30% 42% 13% • 14%
4	s2	253	64% 20% • 14%
5	S3	239	41% 36% 13% • 7%
5	s3	239	72% 20% • 7%
6	S4	260	32% 51% 16% •
6	s4	260	79% 20% •
7	S5	224	32% 49% 11% • 8%
7	s5	224	67% 23% • 8%
8	S6	236	38% 45% 12% •
8	s6	236	73% 19% 8%
9	S7	189	27% 49% 20% • •
9	s7	189	75% 21% • •
10	S8	200	31% 51% 12% • 6%
10	s8	200	75% 19% • 6%
11	S9	196	30% 46% 17% • 6%
11	s9	196	76% 17% • 6%
12	C0	105	23% 56% 11% • 9%
13	C1	155	39% 46% 13% •
13	c1	155	77% 15% • 6%
14	C2	142	29% 40% 15% • 13%
14	c2	142	56% 29% • 13%
15	C3	150	39% 47% 11% •
15	c3	150	78% 20% •
16	C4	136	35% 41% 14% • 7%
16	c4	136	67% 26% • 6%

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Mol	Chain	Length	Quality of chain
17	C5	141	30% 43% 13% 12%
17	c5	141	67% 26%
18	C6	142	30% 51% 15%
18	c6	142	78% 20%
19	C7	136	26% 47% 13% 12%
19	c7	136	60% 25% 14%
20	C8	145	32% 49% 14%
20	c8	145	76% 21%
21	C9	143	35% 49% 13%
21	c9	143	81% 17%
22	D0	120	20% 57% 13% 11%
22	d0	120	57% 33% 8%
23	D1	87	31% 48% 20%
23	d1	87	80% 18%
24	D2	129	33% 51% 14%
24	d2	129	86% 13%
25	D3	144	33% 52% 11%
25	d3	144	78% 19%
26	D4	134	35% 51% 11%
26	d4	134	78% 21%
27	D5	107	13% 33% 17% 35%
27	d5	107	47% 17% 36%
28	D6	97	25% 52% 19% 5%
28	d6	97	72% 25%
29	D7	81	36% 43% 17%

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Mol	Chain	Length	Quality of chain
29	d7	81	80% 17% •
30	D8	66	21% 55% 15% 5% 5%
30	d8	66	67% 27% • 5%
31	D9	55	38% 44% 13% • •
31	d9	55	67% 29% •
32	E0	60	45% 45% 8% •
33	E1	76	16% 46% 28% • 7%
34	SR	318	32% 55% 12% •
34	sR	318	89% 10% •
35	SM	273	31% 20% 7% 42%
35	sM	273	29% 8% • 62%
36	1	3396	34% 39% 17% • 7%
36	5	3396	34% 39% 17% • 7%
37	3	121	51% 42% 7%
37	7	121	39% 42% 17% •
38	4	158	41% 41% 18% •
38	8	158	30% 53% 16% •
39	L2	253	40% 46% 11% •
39	l2	253	80% 19%
40	L3	386	39% 49% 12% •
40	l3	386	82% 16% •
41	L4	361	38% 47% 13% •
41	l4	361	80% 19% •
42	L5	296	43% 42% 15% •
42	l5	296	80% 18% ••

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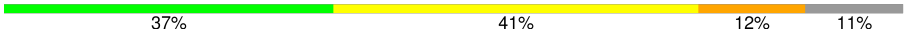
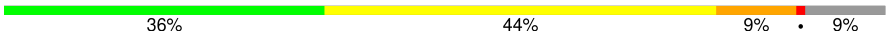
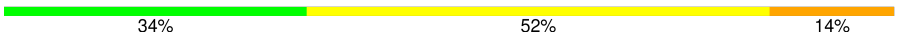
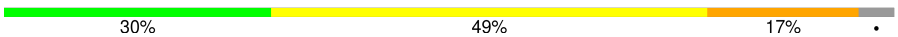
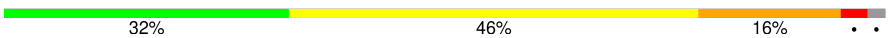
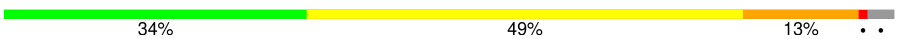
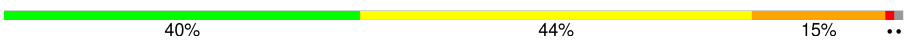
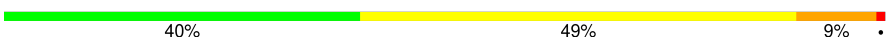
Mol	Chain	Length	Quality of chain
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	
53	m7	183	
54	M8	185	
54	m8	185	
55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

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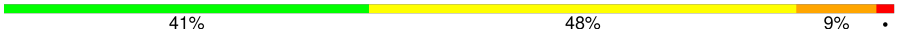
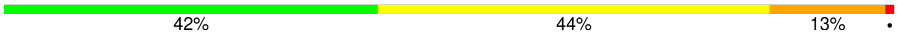
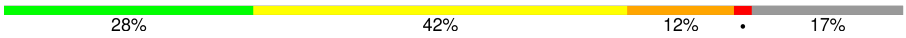
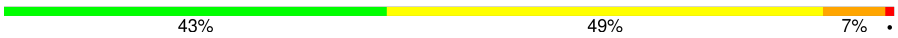
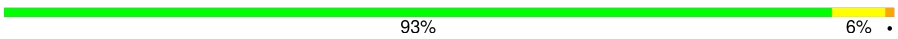
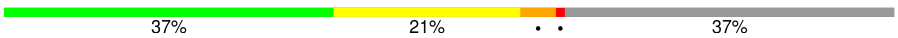
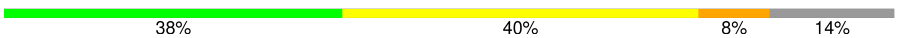
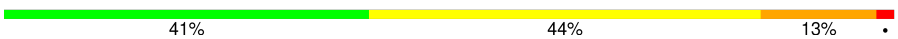
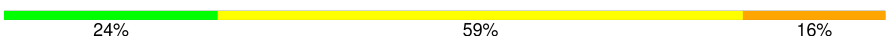
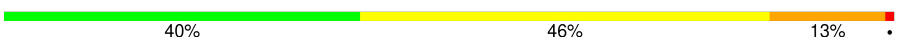
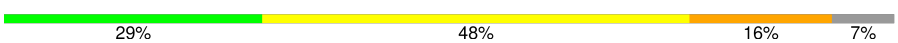
Mol	Chain	Length	Quality of chain
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	104	
66	o0	104	
67	O1	112	
67	o1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

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Mol	Chain	Length	Quality of chain
68	O2	129	36% 51% 12%
68	o2	129	78% 19%
69	O3	106	43% 49% 7%
69	o3	106	83% 15%
70	O4	119	40% 42% 11% 6%
70	o4	119	79% 15% 6%
71	O5	119	39% 41% 18%
71	o5	119	79% 20%
72	O6	99	33% 48% 15%
72	o6	99	74% 23%
73	O7	87	41% 48% 9%
73	o7	87	77% 21%
74	O8	77	27% 51% 22%
74	o8	77	81% 19%
75	O9	50	44% 34% 22%
75	o9	50	84% 16%
76	Q0	52	42% 42% 13%
76	q0	52	75% 25%
77	Q1	25	24% 64% 12%
77	q1	25	72% 28%
78	Q2	105	40% 46% 12%
78	q2	105	75% 23%
79	Q3	91	38% 52% 9%
79	q3	91	82% 18%
80	c0	105	68% 21% 9%

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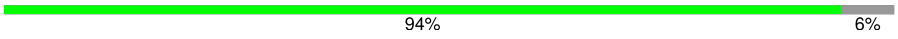
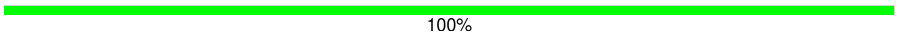
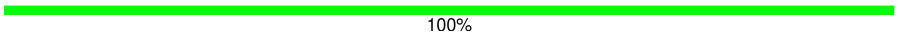
Mol	Chain	Length	Quality of chain
81	e0	62	
82	e1	76	
83	m2	160	
84	p0	311	
85	p1	47	
86	p2	46	

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

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 411288 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	E1	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	SM	159	Total 1104	C 652	N 221	O 231	0	0	0
35	sM	104	Total 680	C 403	N 140	O 137	0	0	0

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

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

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

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

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

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

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

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

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

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

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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	0	0	0
			796	516	131	149			
58	n2	98	Total	C	N	O	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	0	0	0
			612	391	115	106			
74	o8	77	Total	C	N	O	0	0	0
			608	388	114	106			

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

- Molecule 83 is a protein called UNKNOWN PROTEIN m2.

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

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

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

- Molecule 85 is a protein called UNKNOWN PROTEIN p1.

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

- Molecule 86 is a protein called UNKNOWN PROTEIN p2.

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

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

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

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

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

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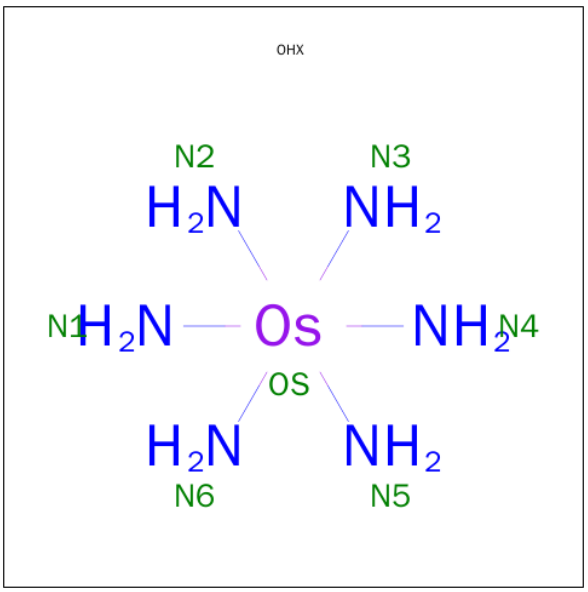
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	s8	3	Total Mg 3 3	0	0
87	c7	2	Total Mg 2 2	0	0
87	7	15	Total Mg 15 15	0	0
87	n3	2	Total Mg 2 2	0	0
87	q1	1	Total Mg 1 1	0	0
87	L3	3	Total Mg 3 3	0	0
87	O5	1	Total Mg 1 1	0	0
87	l2	1	Total Mg 1 1	0	0
87	8	16	Total Mg 16 16	0	0
87	M6	1	Total Mg 1 1	0	0
87	N0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

- Molecule 88 is osmium (III) hexammine (three-letter code: OHX) (formula: $H_{12}N_6Os$).



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	L4	1	Total N Os 7 6 1	0	0
88	M0	1	Total N Os 7 6 1	0	0
88	M5	1	Total N Os 7 6 1	0	0
88	M7	1	Total N Os 7 6 1	0	0
88	M7	1	Total N Os 7 6 1	0	0
88	M8	1	Total N Os 7 6 1	0	0
88	M9	1	Total N Os 7 6 1	0	0
88	N9	1	Total N Os 7 6 1	0	0
88	O3	1	Total N Os 7 6 1	0	0
88	O7	1	Total N Os 7 6 1	0	0
88	O7	1	Total N Os 7 6 1	0	0
88	6	1	Total N Os 7 6 1	0	0
88	6	1	Total N Os 7 6 1	0	0
88	6	1	Total N Os 7 6 1	0	0
88	6	1	Total N Os 7 6 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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88	c1	1	Total N Os 7 6 1	0	0
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88	c5	1	Total N Os 7 6 1	0	0
88	c8	1	Total N Os 7 6 1	0	0
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88	d9	1	Total N Os 7 6 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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88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	l3	1	Total	N	Os	0	0
			7	6	1		
88	l3	1	Total	N	Os	0	0
			7	6	1		
88	l3	1	Total	N	Os	0	0
			7	6	1		

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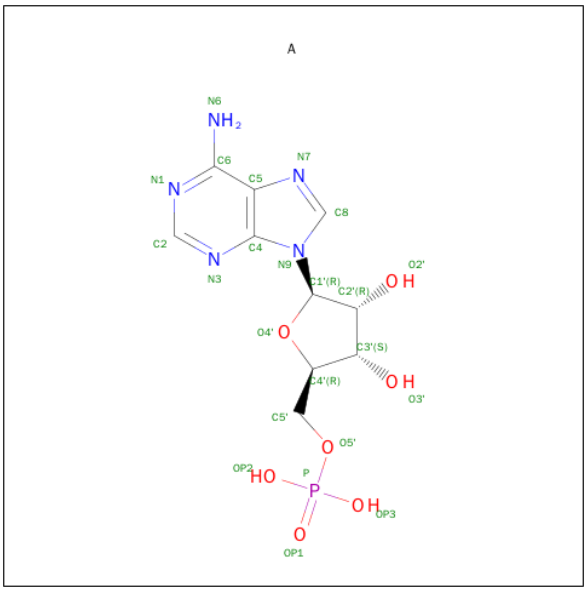
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	l4	1	Total N Os 7 6 1	0	0
88	l4	1	Total N Os 7 6 1	0	0
88	l5	1	Total N Os 7 6 1	0	0
88	l5	1	Total N Os 7 6 1	0	0
88	l5	1	Total N Os 7 6 1	0	0
88	l5	1	Total N Os 7 6 1	0	0
88	l9	1	Total N Os 7 6 1	0	0
88	m0	1	Total N Os 7 6 1	0	0
88	m0	1	Total N Os 7 6 1	0	0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

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

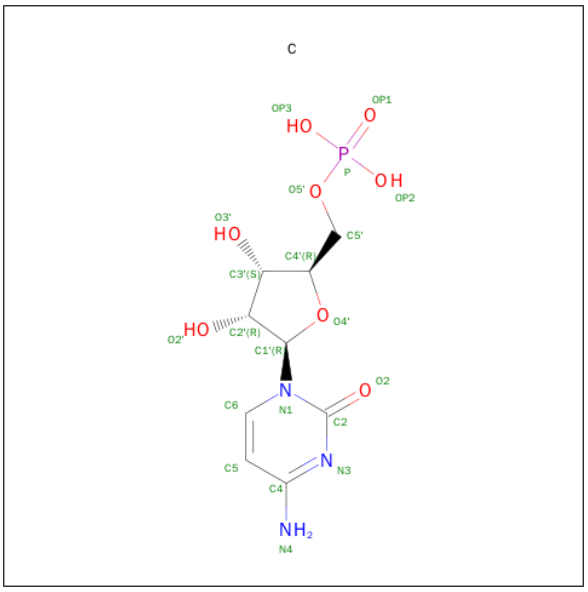
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
89	q0	1	Total Zn 1 1	0	0
89	D6	1	Total Zn 1 1	0	0
89	Q2	1	Total Zn 1 1	0	0
89	e1	1	Total Zn 1 1	0	0
89	Q3	1	Total Zn 1 1	0	0
89	D9	1	Total Zn 1 1	0	0
89	E1	1	Total Zn 1 1	0	0
89	Q0	1	Total Zn 1 1	0	0
89	d7	1	Total Zn 1 1	0	0
89	q3	1	Total Zn 1 1	0	0
89	d9	1	Total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

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



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

- Molecule 91 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C) (formula: $C_9H_{14}N_3O_8P$).



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

Continued on next page...

Continued from previous page...

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

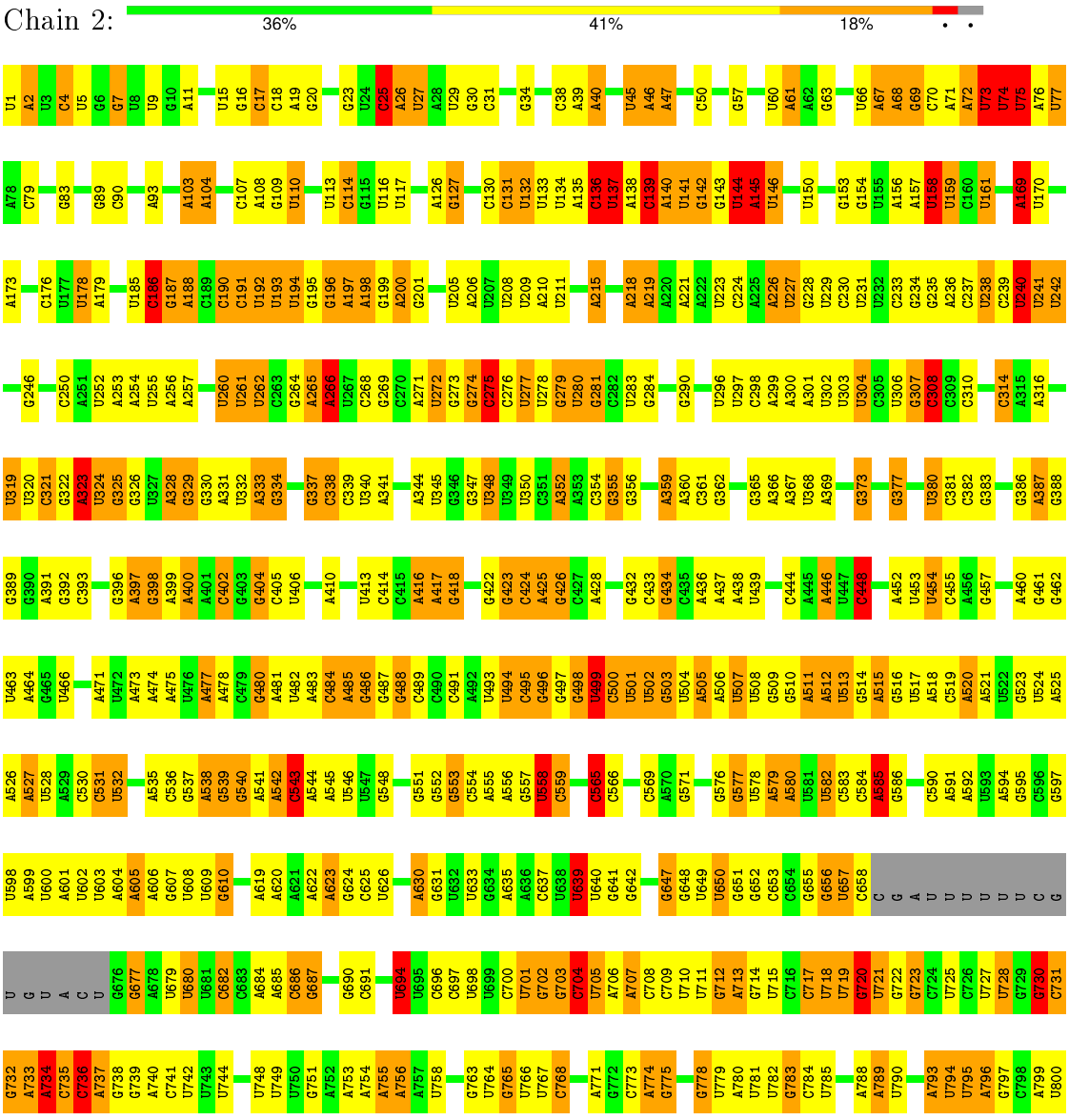
3 Residue-property plots (i)

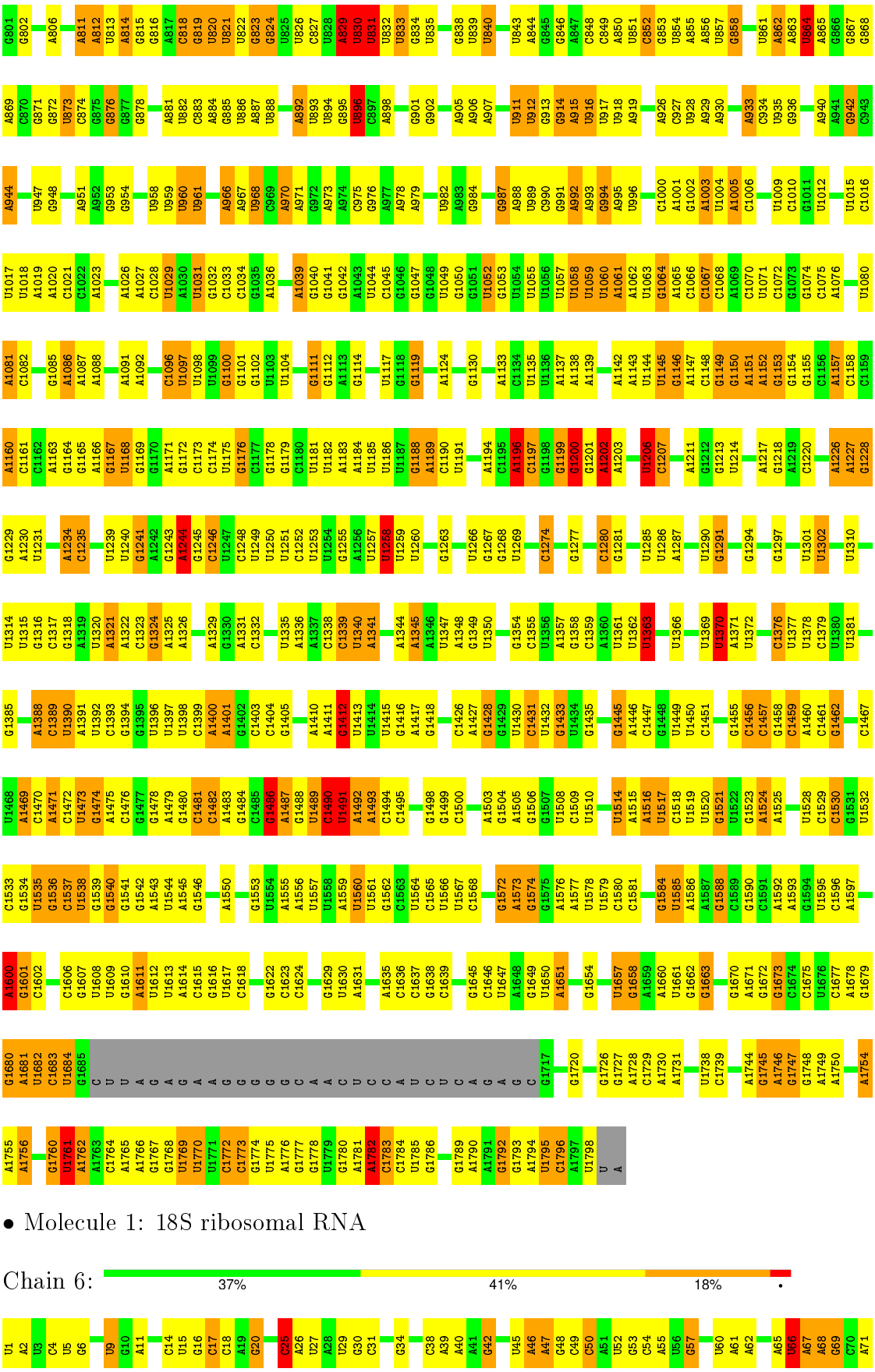
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 (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

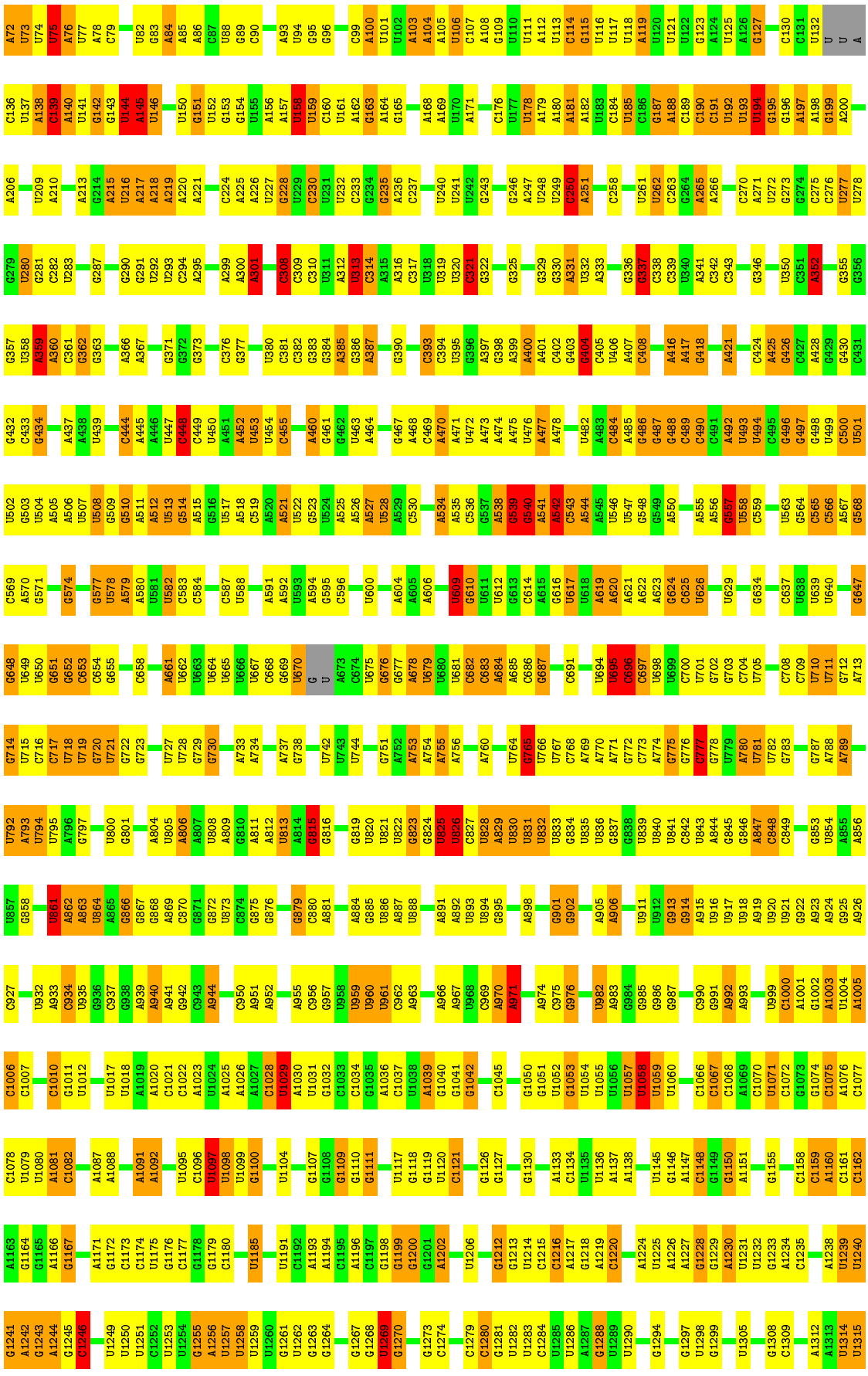
Chain 2:

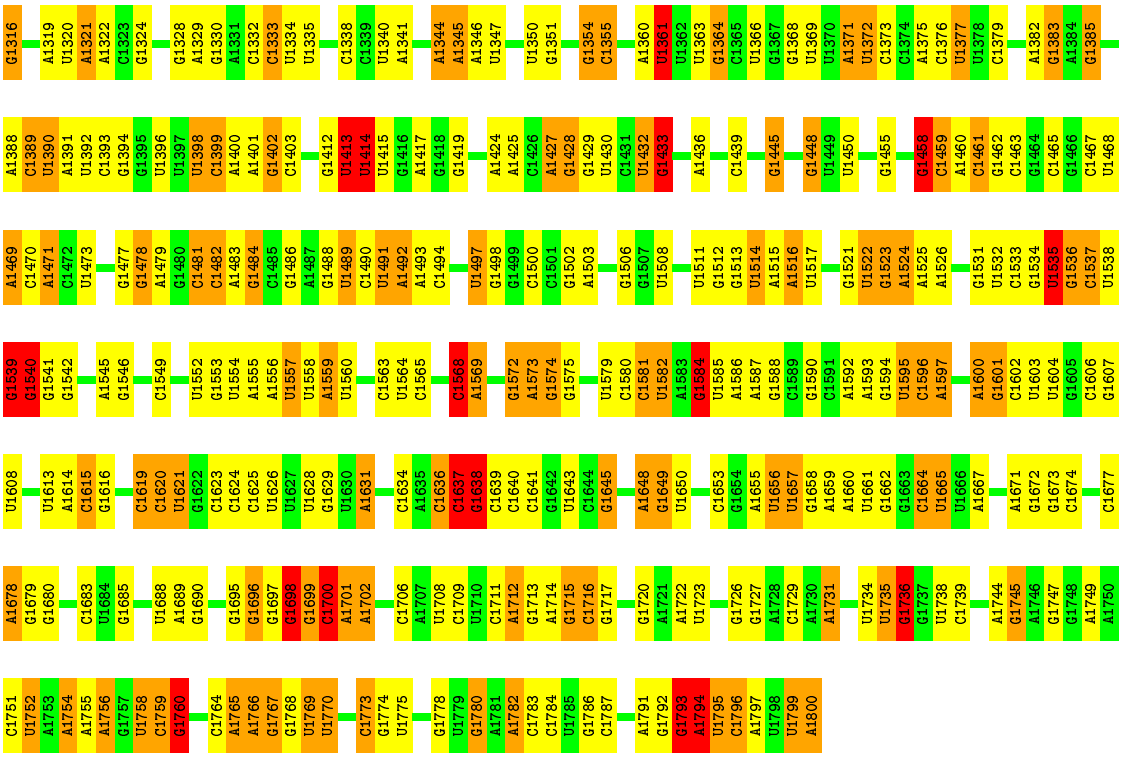




• Molecule 1: 18S ribosomal RNA

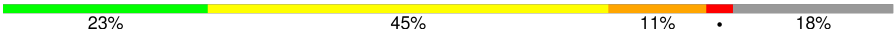
Chain 6:

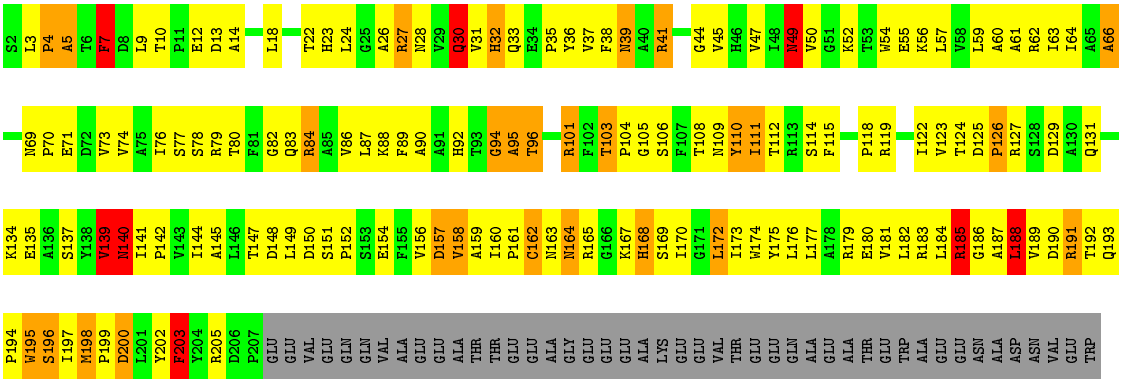




- Molecule 2: 40S ribosomal protein S0-A

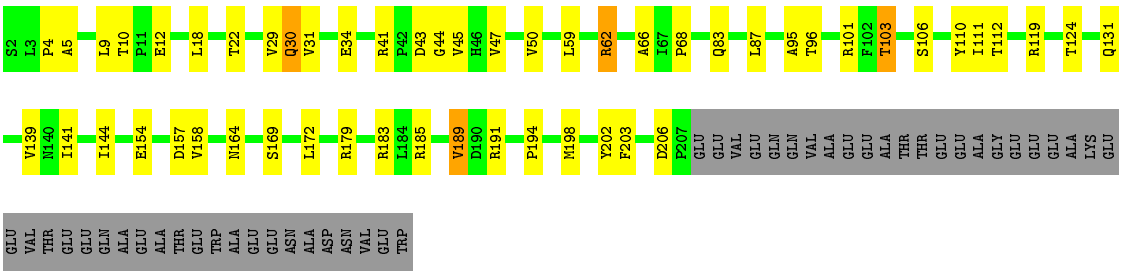
Chain S0:





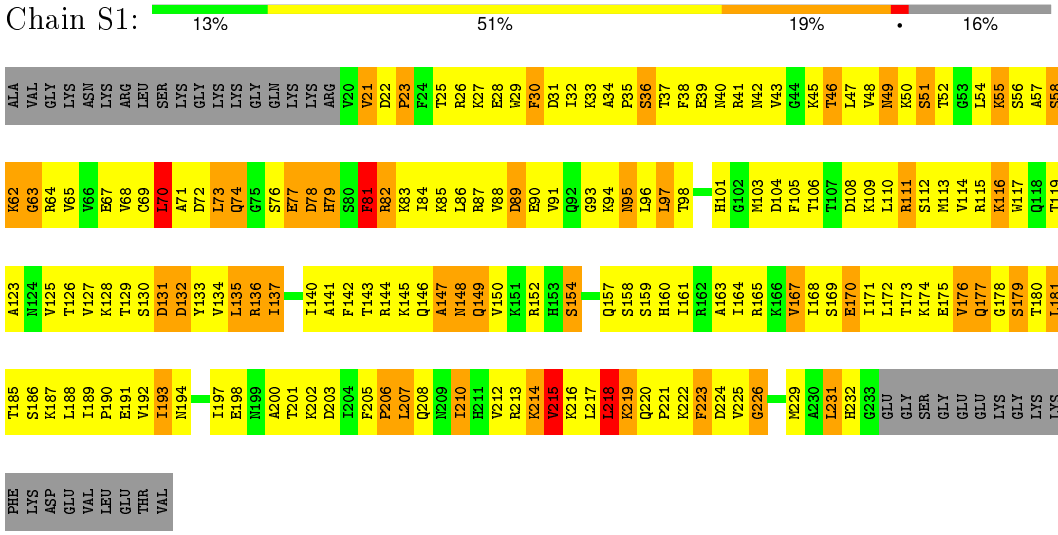
- Molecule 2: 40S ribosomal protein S0-A

Chain s0:



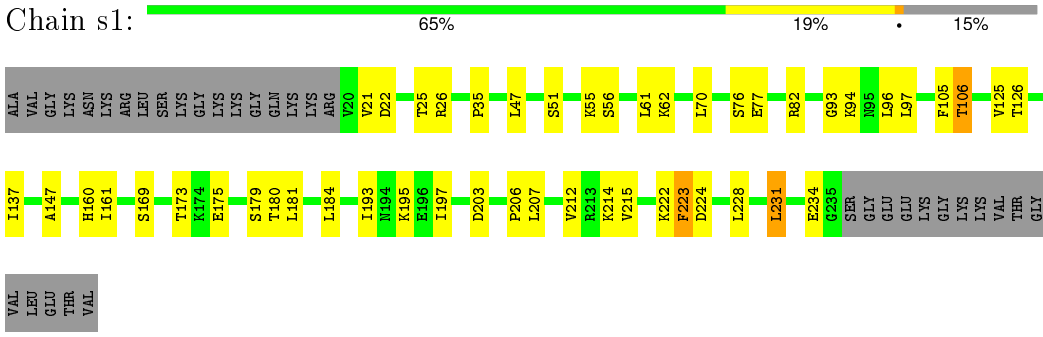
• Molecule 3: 40S ribosomal protein S1-A

Chain S1:



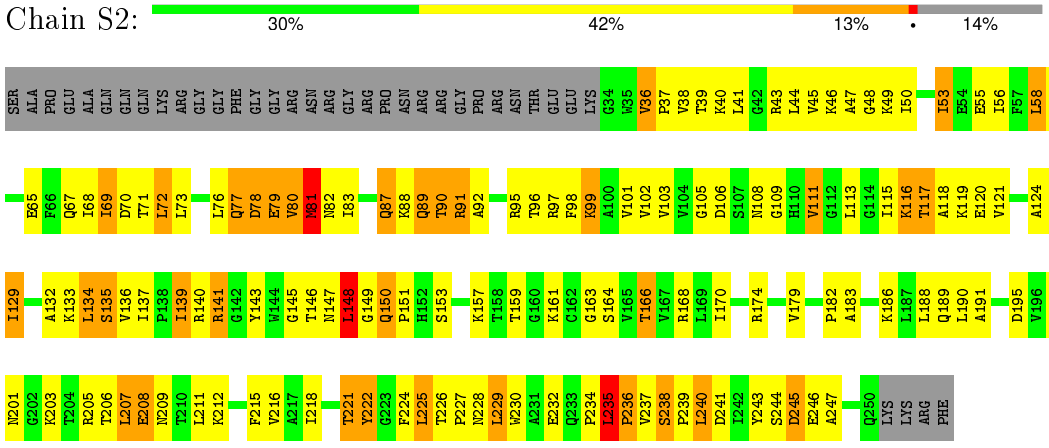
• Molecule 3: 40S ribosomal protein S1-A

Chain s1:



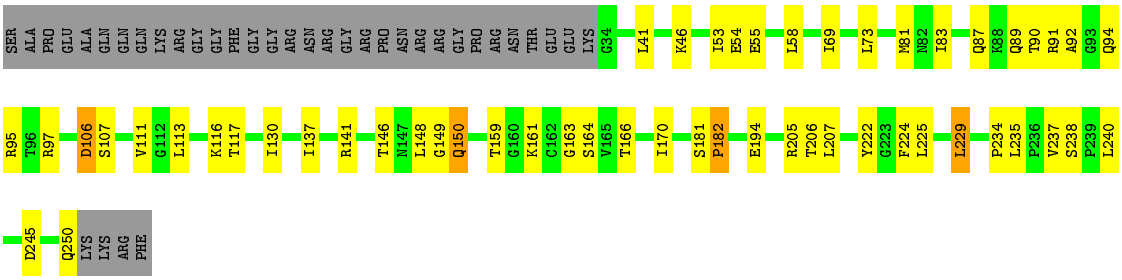
• Molecule 4: 40S ribosomal protein S2

Chain S2:



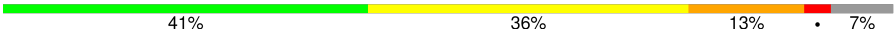
• Molecule 4: 40S ribosomal protein S2

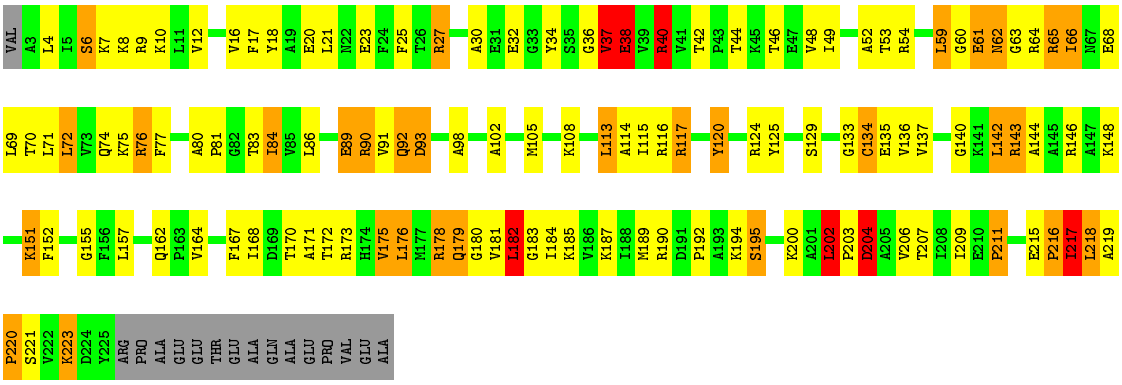
Chain s2:



• Molecule 5: 40S ribosomal protein S3

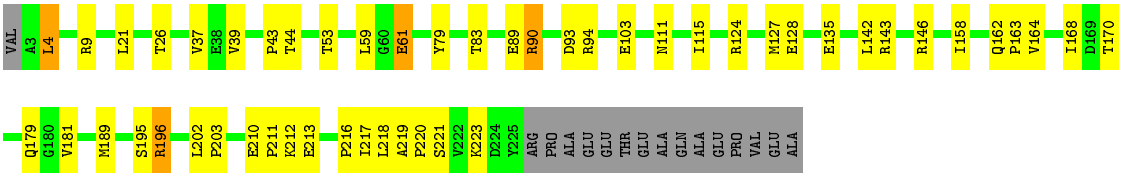
Chain S3:





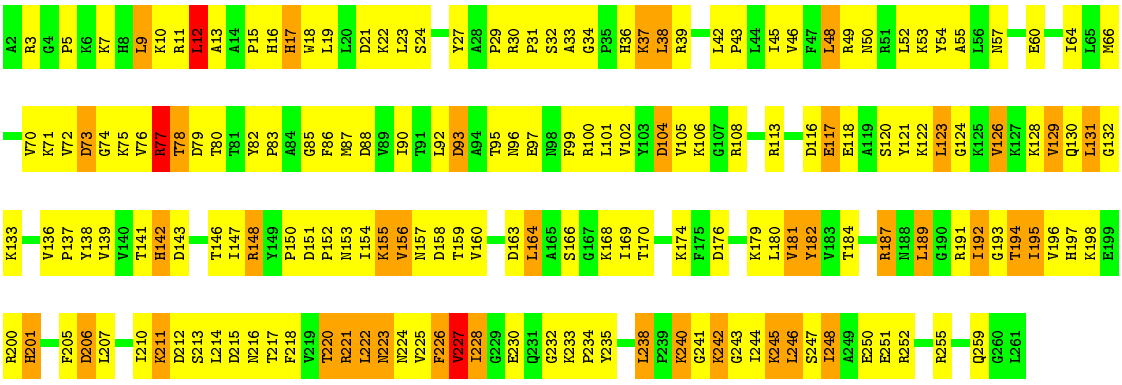
• Molecule 5: 40S ribosomal protein S3

Chain s3:



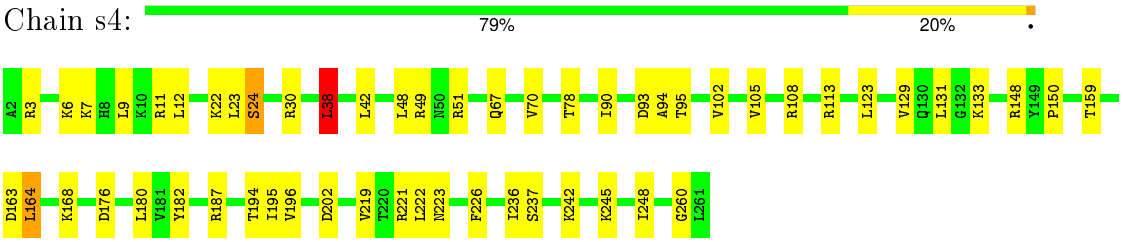
• Molecule 6: 40S ribosomal protein S4-A

Chain S4:



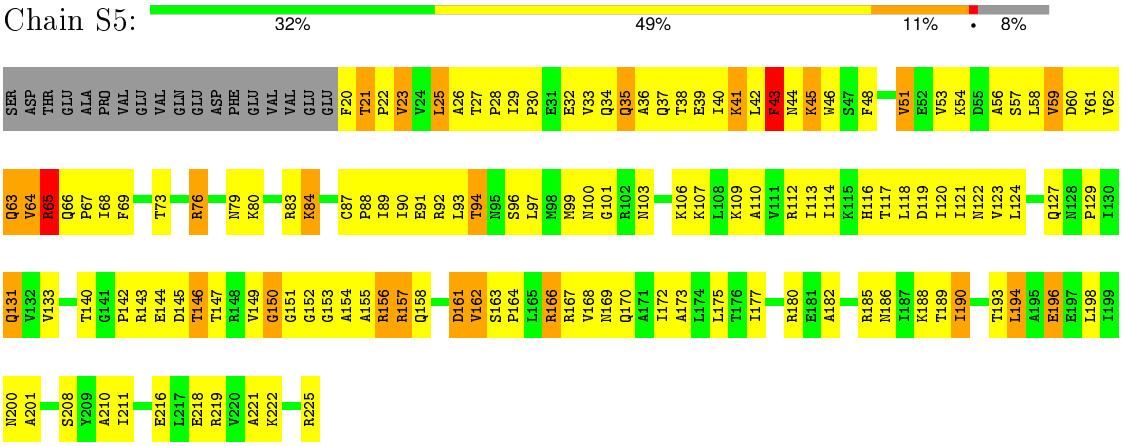
• Molecule 6: 40S ribosomal protein S4-A

Chain s4:



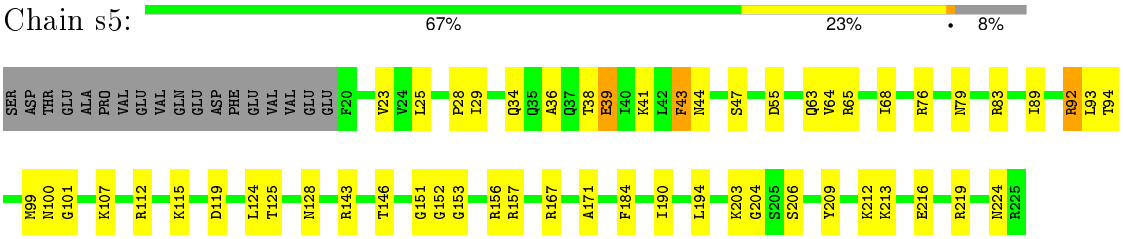
• Molecule 7: 40S ribosomal protein S5

Chain S5:



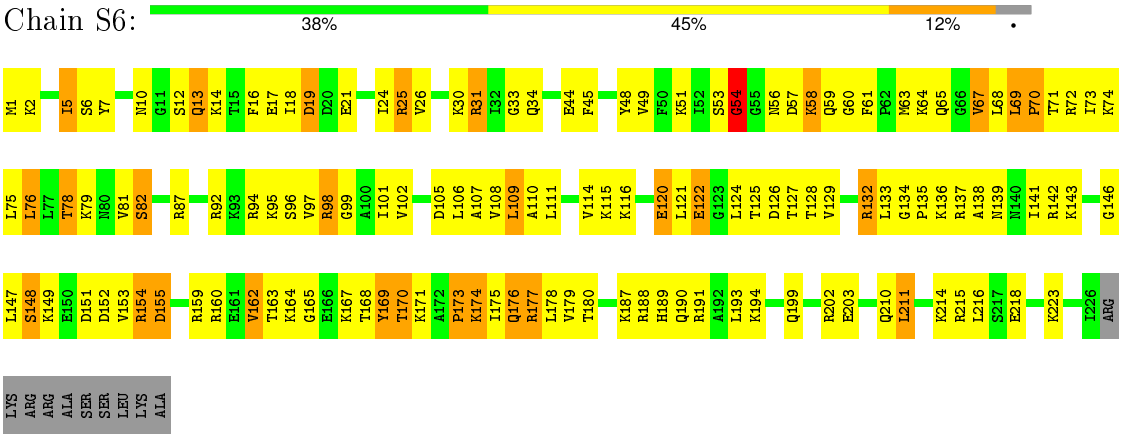
• Molecule 7: 40S ribosomal protein S5

Chain s5:



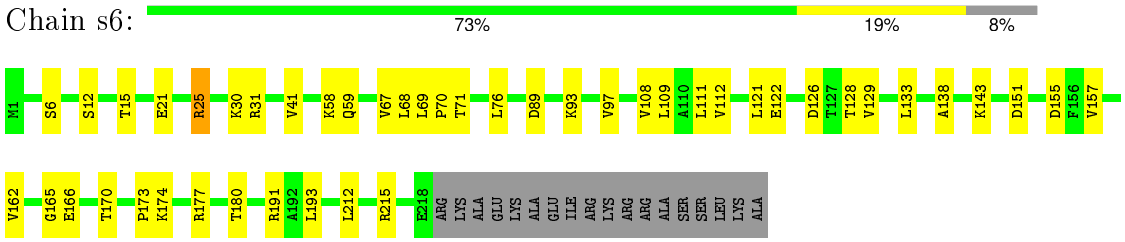
• Molecule 8: 40S ribosomal protein S6-A

Chain S6:



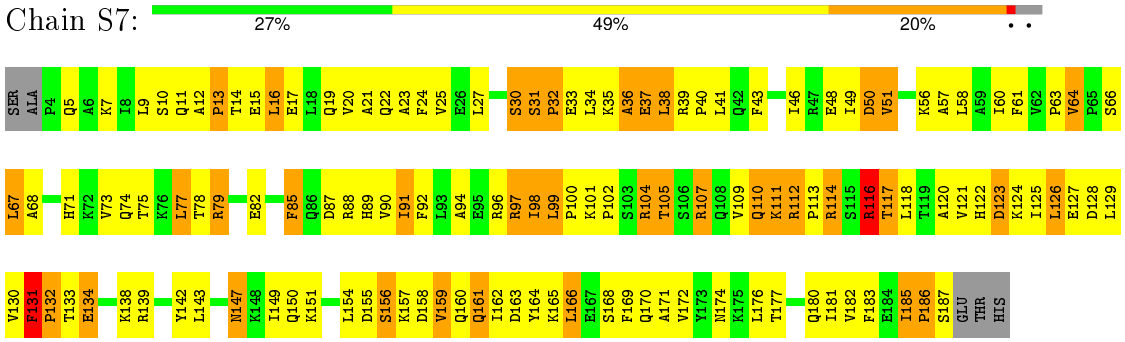
• Molecule 8: 40S ribosomal protein S6-A

Chain s6:



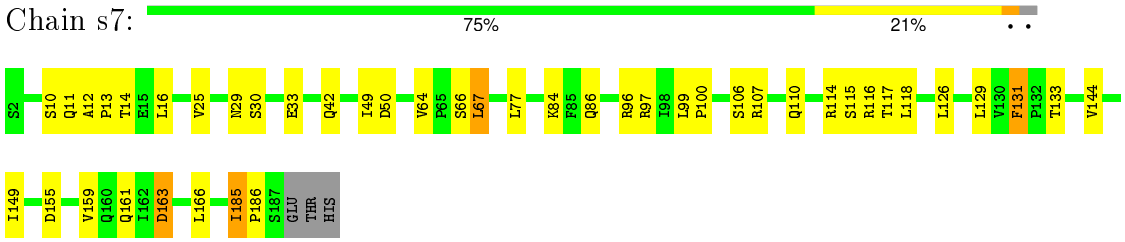
- Molecule 9: 40S ribosomal protein S7-A

Chain S7:



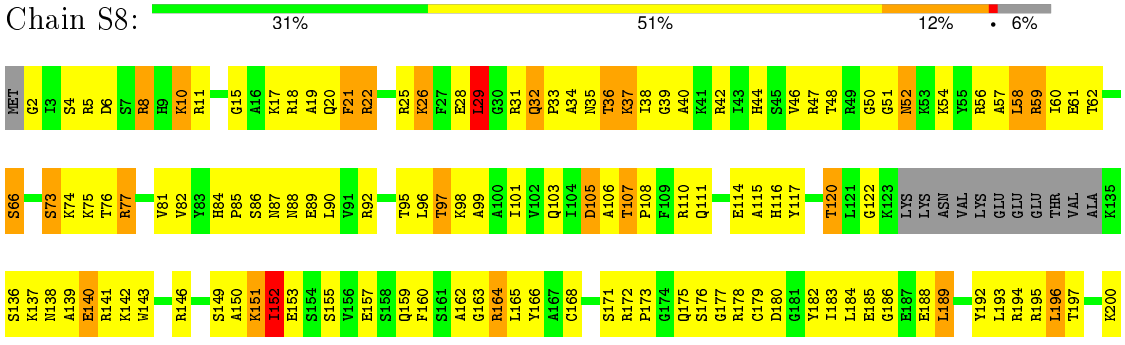
- Molecule 9: 40S ribosomal protein S7-A

Chain s7:



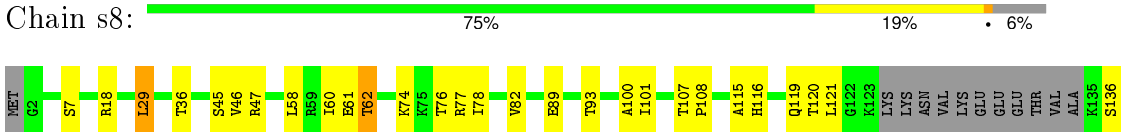
- Molecule 10: 40S ribosomal protein S8-A

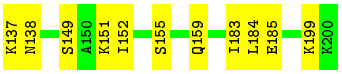
Chain S8:



- Molecule 10: 40S ribosomal protein S8-A

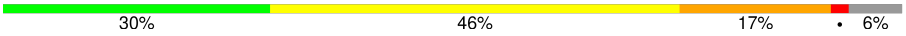
Chain s8:

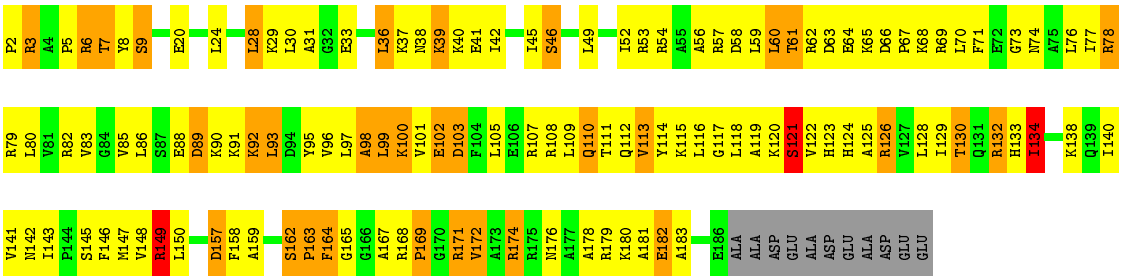




• Molecule 11: 40S ribosomal protein S9-A

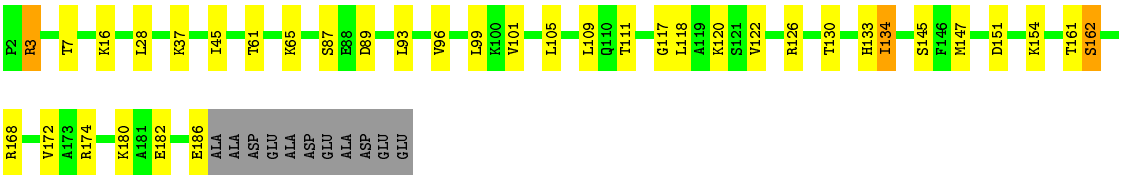
Chain S9:





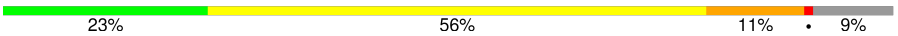
• Molecule 11: 40S ribosomal protein S9-A

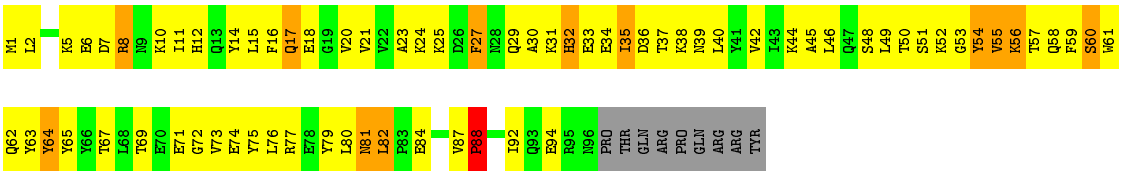
Chain s9:



• Molecule 12: 40S ribosomal protein S10-A

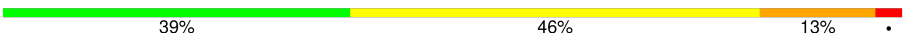
Chain C0:





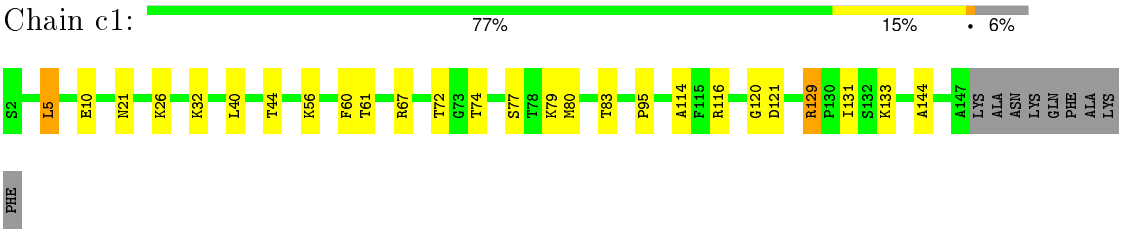
• Molecule 13: 40S ribosomal protein S11-A

Chain C1:



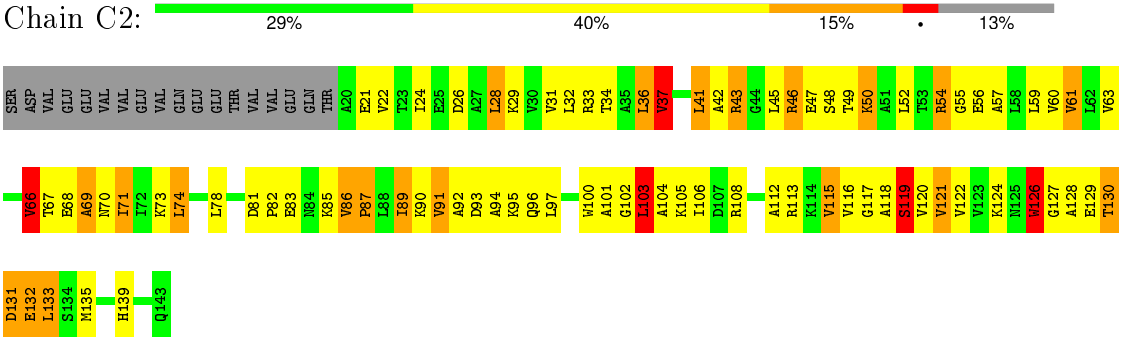
• Molecule 13: 40S ribosomal protein S11-A

Chain c1:



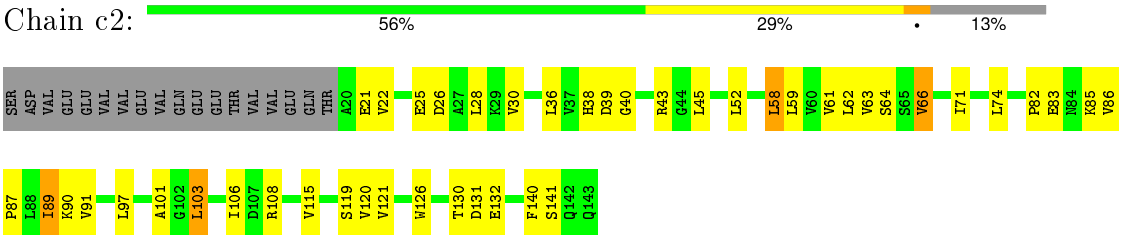
• Molecule 14: 40S ribosomal protein S12

Chain C2:



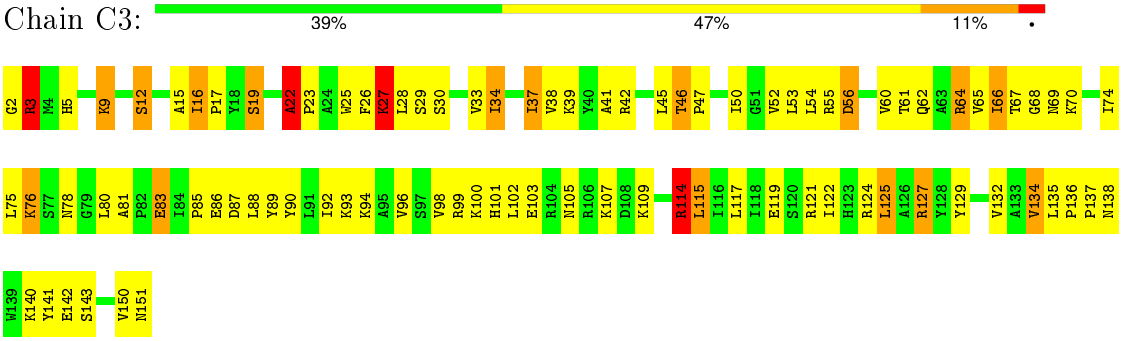
• Molecule 14: 40S ribosomal protein S12

Chain c2:



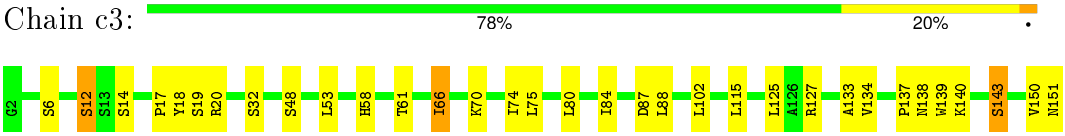
• Molecule 15: 40S ribosomal protein S13

Chain C3:



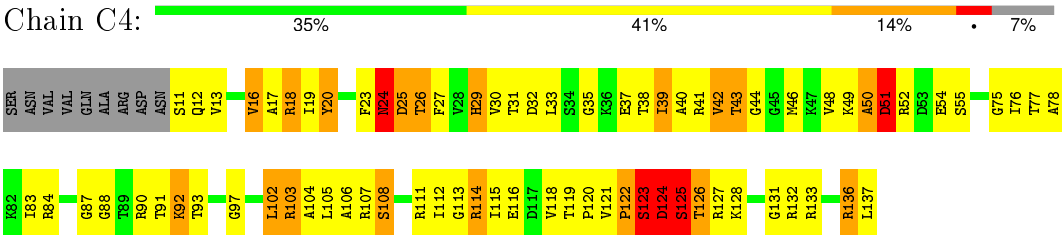
• Molecule 15: 40S ribosomal protein S13

Chain c3:



• Molecule 16: 40S ribosomal protein S14-A

Chain C4:



- Molecule 16: 40S ribosomal protein S14-A

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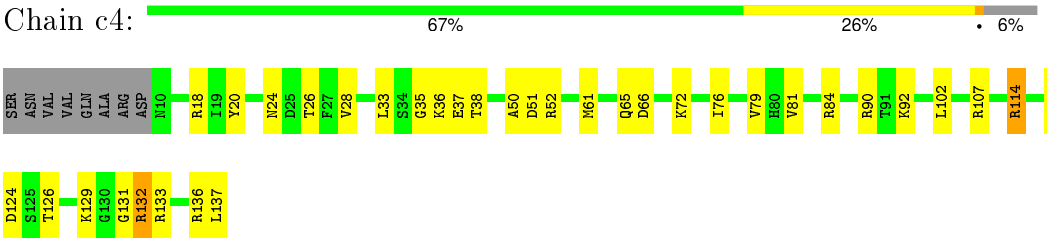
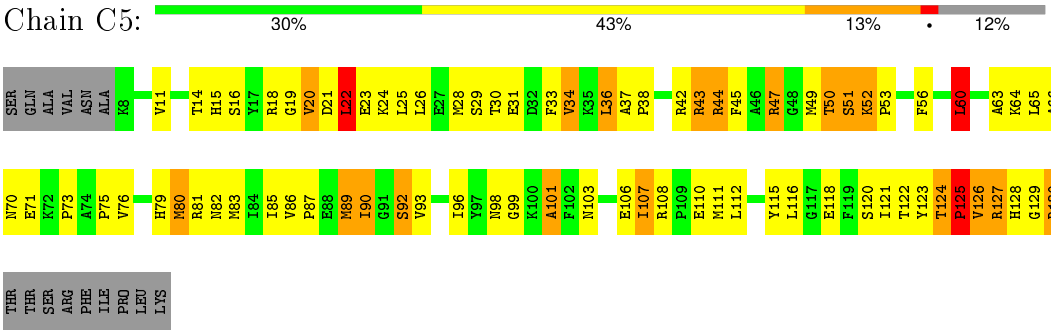


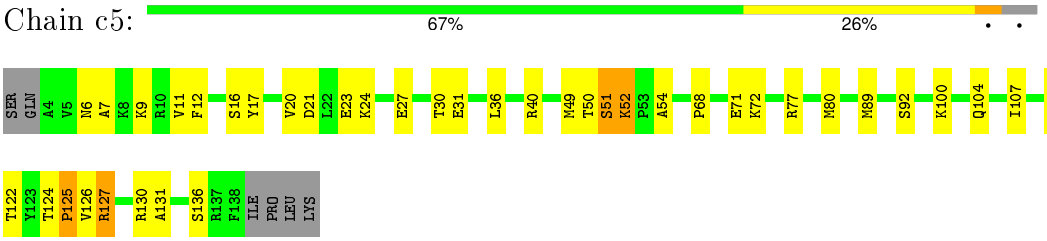
- Molecule 17: 40S ribosomal protein S15

Chain C5:



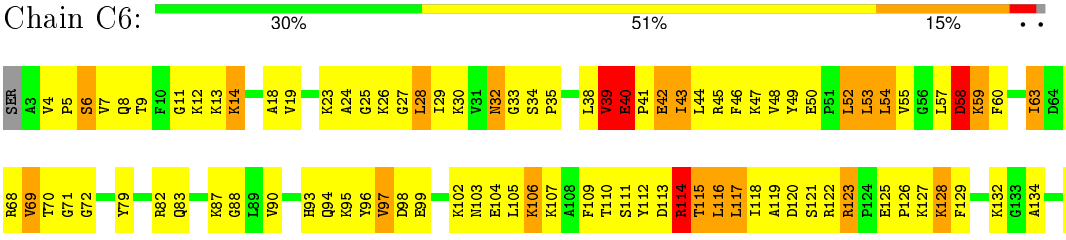
- Molecule 17: 40S ribosomal protein S15

Chain c5:



- Molecule 18: 40S ribosomal protein S16-A

Chain C6:

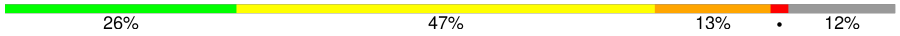


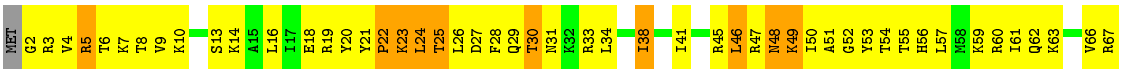
• Molecule 18: 40S ribosomal protein S16-A

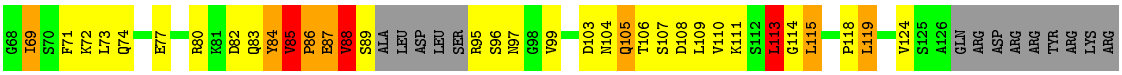
Chain c6:

• Molecule 19: 40S ribosomal protein S17-A

Chain C7:

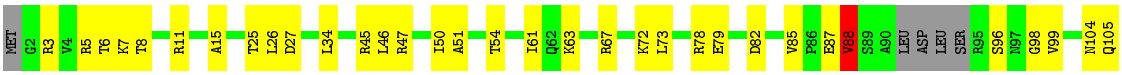






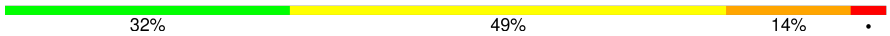
• Molecule 19: 40S ribosomal protein S17-A

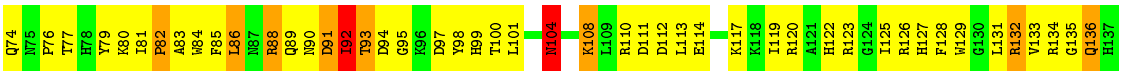
Chain c7:



• Molecule 20: 40S ribosomal protein S18-A

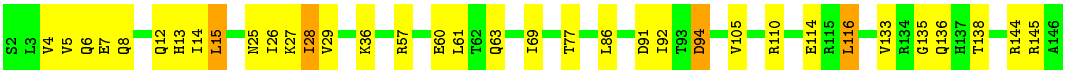
Chain C8:





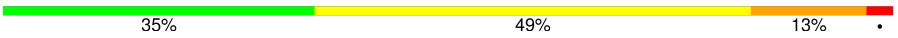
• Molecule 20: 40S ribosomal protein S18-A

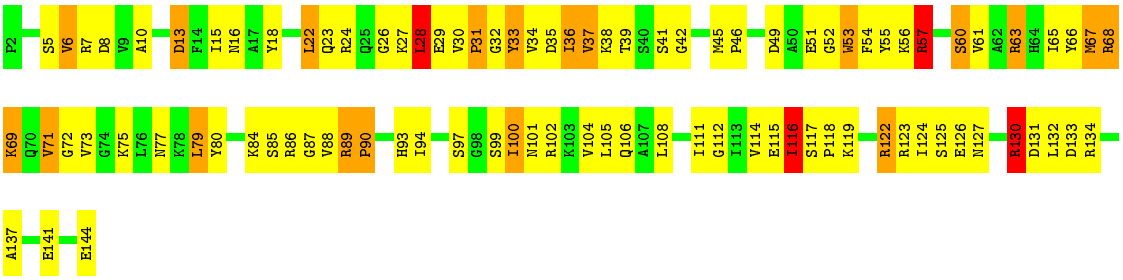
Chain c8:



• Molecule 21: 40S ribosomal protein S19-A

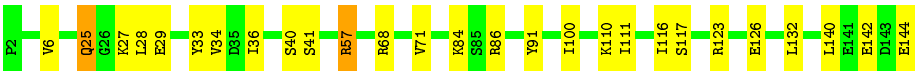
Chain C9:





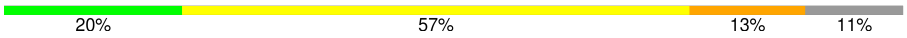
• Molecule 21: 40S ribosomal protein S19-A

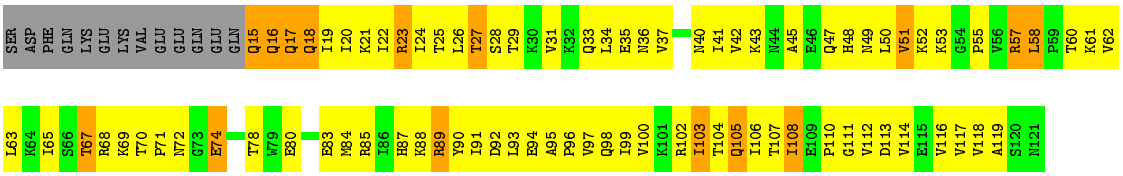
Chain c9:



• Molecule 22: 40S ribosomal protein S20

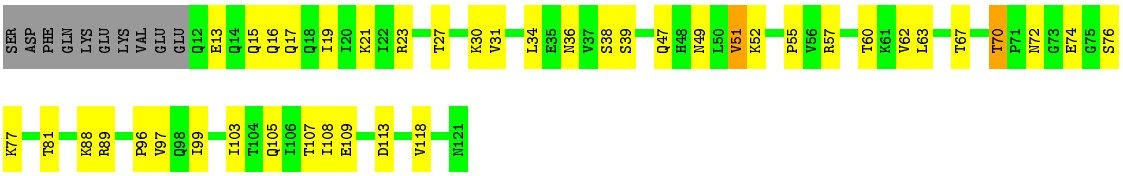
Chain D0:





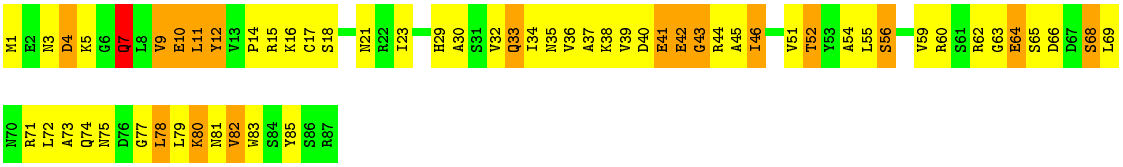
• Molecule 22: 40S ribosomal protein S20

Chain d0:



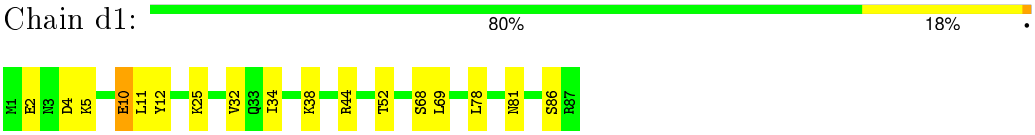
• Molecule 23: 40S ribosomal protein S21-A

Chain D1:



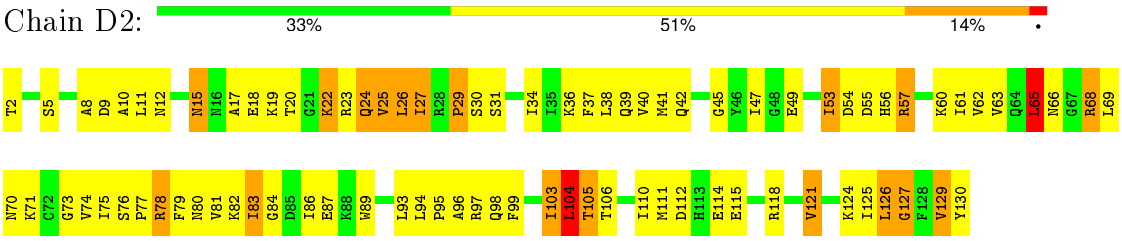
• Molecule 23: 40S ribosomal protein S21-A

Chain d1:



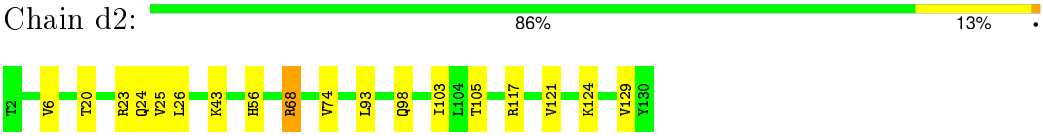
• Molecule 24: 40S ribosomal protein S22-A

Chain D2:



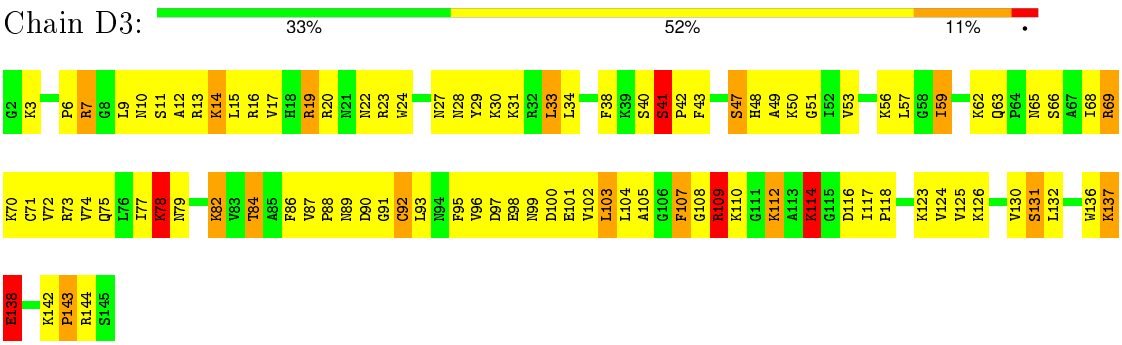
• Molecule 24: 40S ribosomal protein S22-A

Chain d2:



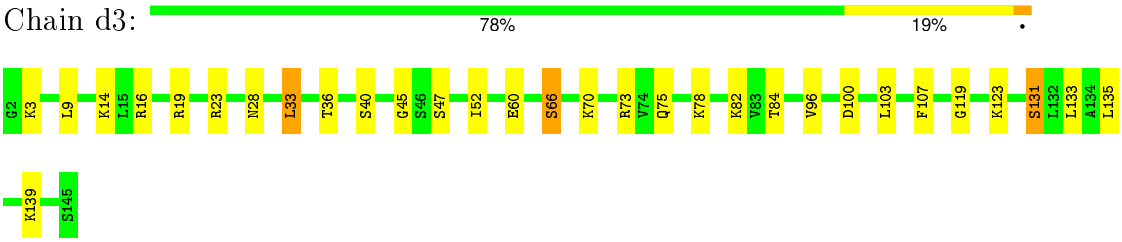
• Molecule 25: 40S ribosomal protein S23-A

Chain D3:



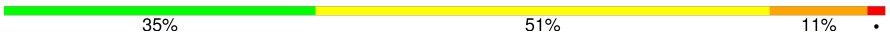
• Molecule 25: 40S ribosomal protein S23-A

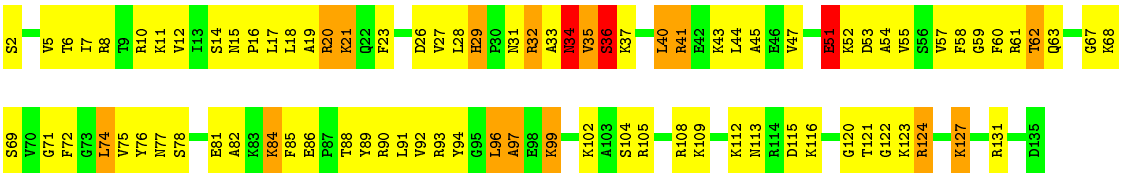
Chain d3:



• Molecule 26: 40S ribosomal protein S24-A

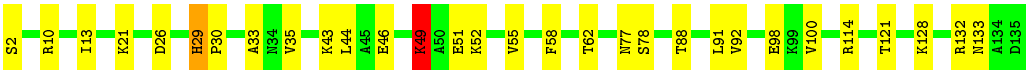
Chain D4:





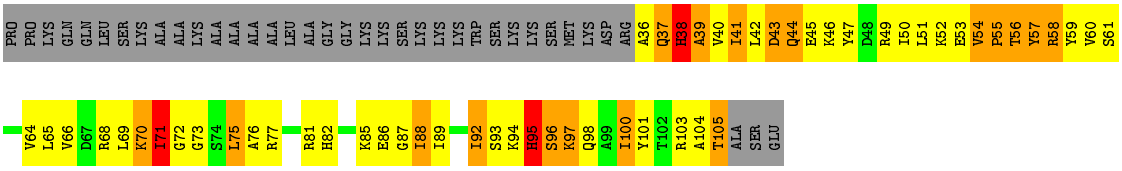
• Molecule 26: 40S ribosomal protein S24-A

Chain d4:



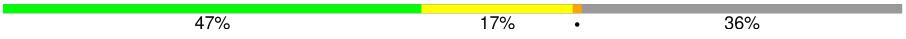
• Molecule 27: 40S ribosomal protein S25-A

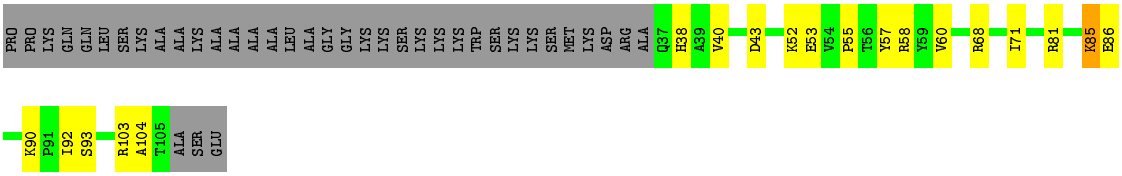
Chain D5:



• Molecule 27: 40S ribosomal protein S25-A

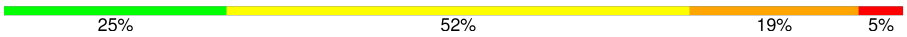
Chain d5:

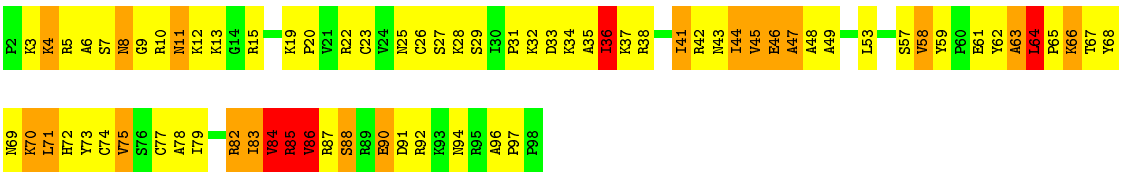




• Molecule 28: 40S ribosomal protein S26-B

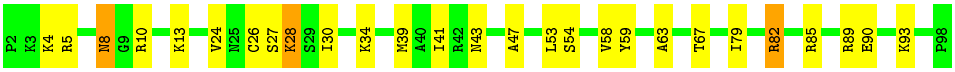
Chain D6:





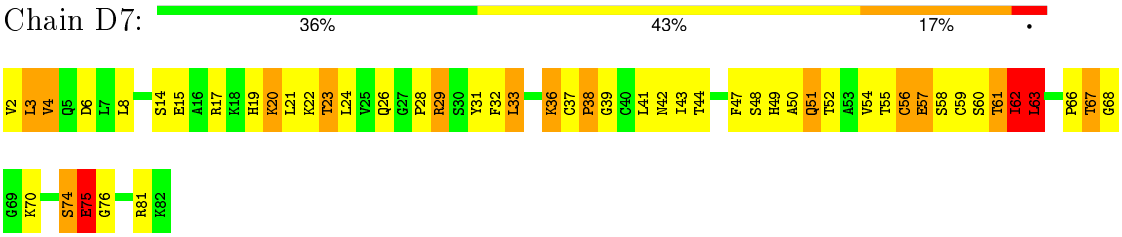
• Molecule 28: 40S ribosomal protein S26-B

Chain d6:



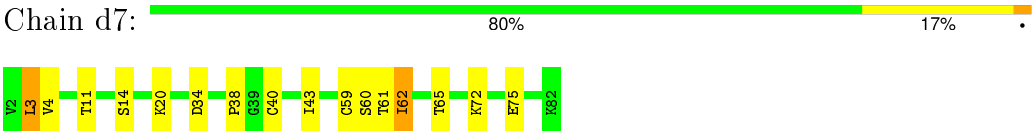
• Molecule 29: 40S ribosomal protein S27-A

Chain D7:



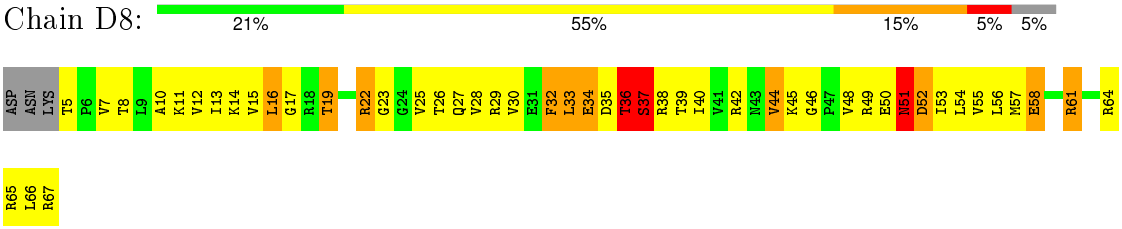
• Molecule 29: 40S ribosomal protein S27-A

Chain d7:



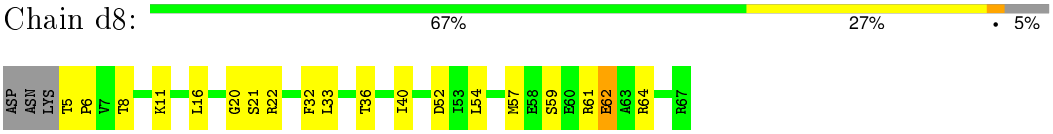
• Molecule 30: 40S ribosomal protein S28-A

Chain D8:



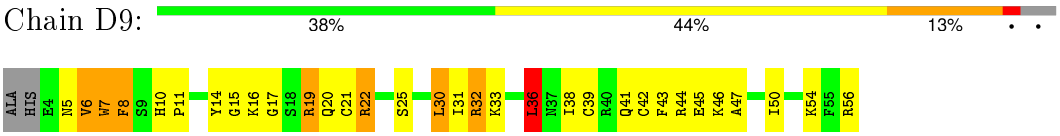
• Molecule 30: 40S ribosomal protein S28-A

Chain d8:



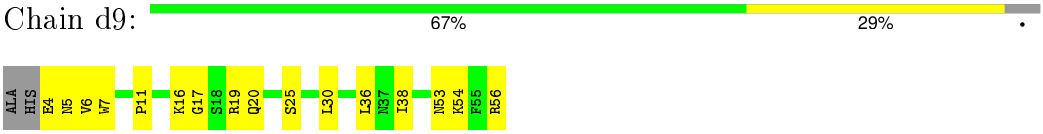
• Molecule 31: 40S ribosomal protein S29-A

Chain D9:



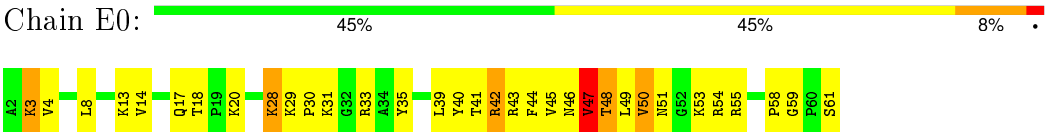
• Molecule 31: 40S ribosomal protein S29-A

Chain d9:



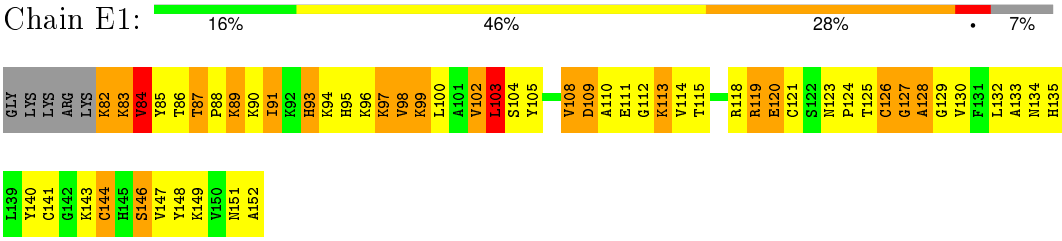
• Molecule 32: 40S ribosomal protein S30-A

Chain E0:



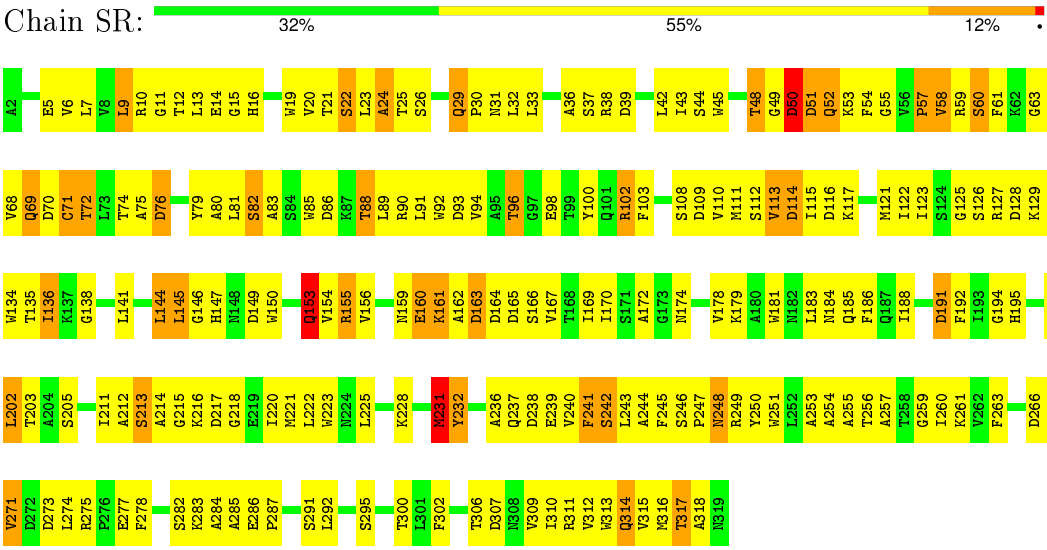
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:



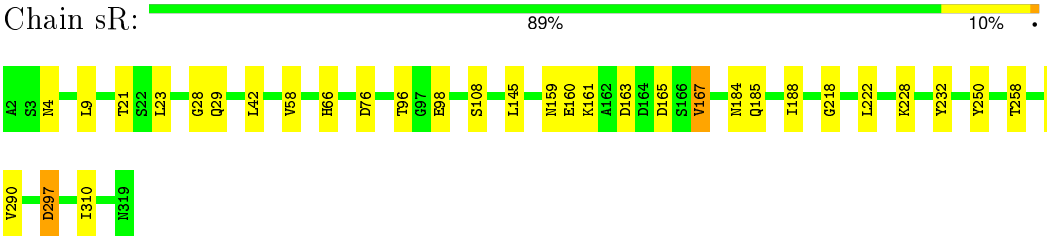
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:



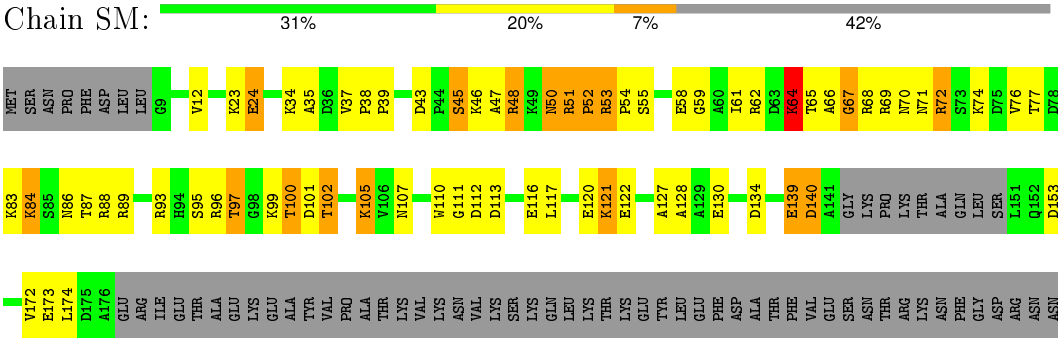
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:



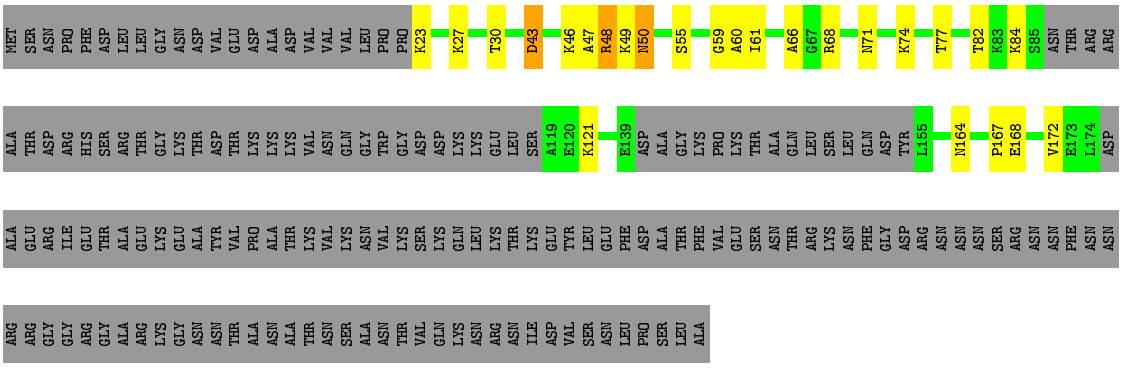
- Molecule 35: Suppressor protein STM1

Chain SM:



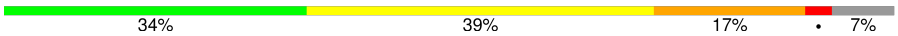
- Molecule 35: Suppressor protein STM1

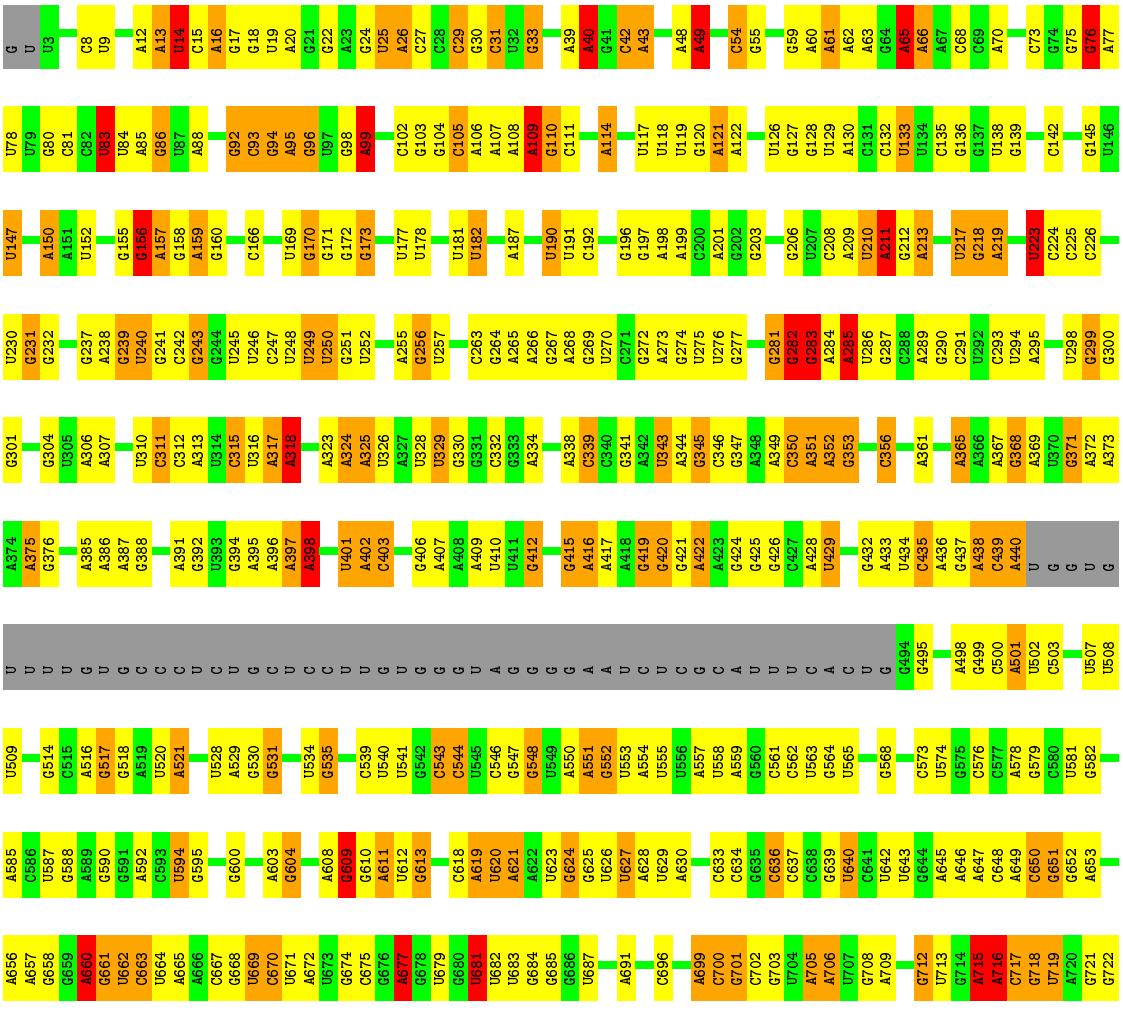
Chain sM:



- Molecule 36: 25S ribosomal RNA

Chain 1:





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A808 G809 A810 U811 G812 G815 A816 A817 C818 U819 A820 C824 U825 G826 A827 A828 U829 A830 G835 A836 A837 G838 A841 A846 A847 A848 C849 U850 C851 U852 G853 G854 U855 G856 G857 A858 G859 G860 C861 U862 C863 G864 G867 C868 U871 U872 C873 U874 G875 G878 U879 G880
A883 A884 U885 C886 G887 A888 U889 C890 C893 G894 A895 A896 U897 U898 U899 G900 G901 A906 G907 G908 G909 G910 C911 G912 A913 A914 A915 G916 A917 C918 U919 A920 A921 U922 C923 G924 A925 A926 A929 U930 C931 G934 U935 A936 G937 C938 U939 G940 G941 U942 U943 C944 C945 U946 G947
C948 C949 G950 A951 A952 G953 U954 U955 U956 C957 C958 C959 U960 C961 A962 G963 G964 A965 U966 A967 G968 C969 A970 G971 A972 C975 U976 C977 G978 U979 A980 U981 C982 A983 G984 U988 G991 A992 G993 G994 U995 A996 A997 A998 G999 C1000 G1001 A1002 A1006 A1009 G1010 A1011 G1012 G1013 U1014
U1015 C1016 C1017 G1018 G1019 G1020 G1024 A1025 U1028 G1029 A1030 U1033 U1034 G1035 A1036 C1037 C1038 U1039 A1040 A970 U1041 U1042 C1045 A1046 A1047 A1048 C1049 U1050 U1051 A1054 A1057 U1058 G1059 U1060 A1061 A1062 G1063 A1064 A1065 G1066 U1067 C1068 C1069 U1070 U1071 G1072 U1073 U1074 A1075 C1076 U1077 U1078 A1079 A1080 U1081
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C1416 G1417 A1418 A1419 C1420 G1421 U1425 C1426 U1427 A1428 G1429 U1430 G1431 C1432 A1433 G1434 A1435 U1436 C1437 G1441 U1442 G1443 G1444 U1445 A1446 G1447 G1450 A1454 U1455 A1456 U1457 U1458 C1459 A1460 A1461 A1462 U1463 G1464 A1465 G1466 A1467 U1470 U1471 U1472 G1476 A1477 G1480 A1481 A1482 G1483 U1484 G1485
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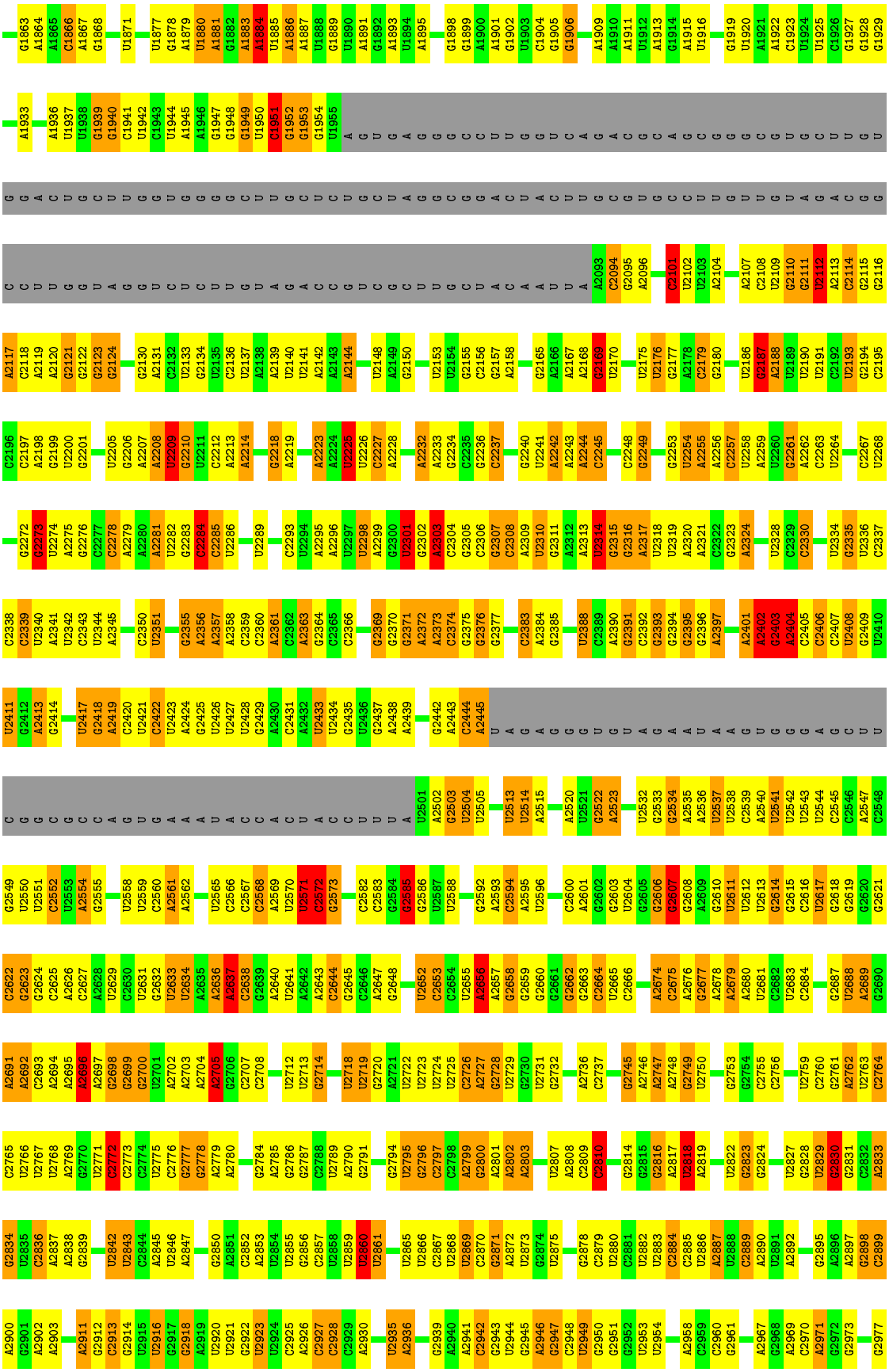
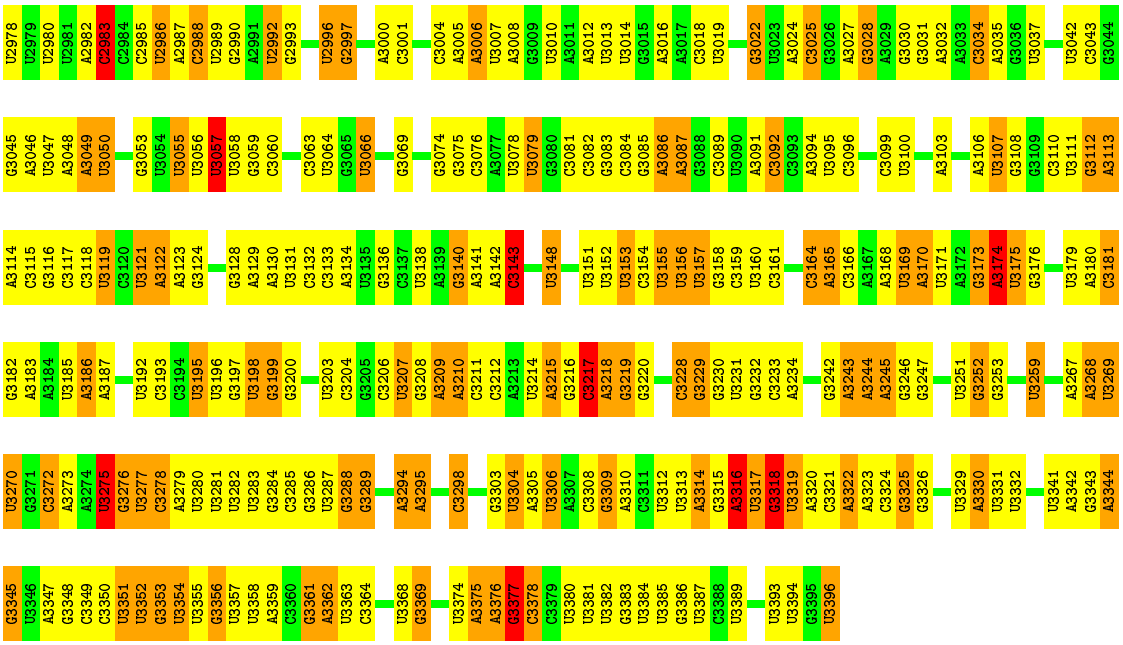
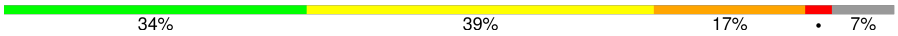
C1792 U1795 G1796 A1797 A1798 A1799 A1804 C1805 A1806 G1807 G1808 A1809 A1810 A1813 A1814 U1815 A1816 G1817 U1818 U1819 U1820 U1821 C1822 A1823 U1824 G1825 C1826 C1827 G1830 U1831 C1832 G1833 U1834 A1835 G1838 A1839 U1840 A1841 A1842 C1843 C1844 G1845 C1846 A1847 G1848 C1849 A1850 G1851 U1855 C1856 C1857 A1858 A1859 G1860

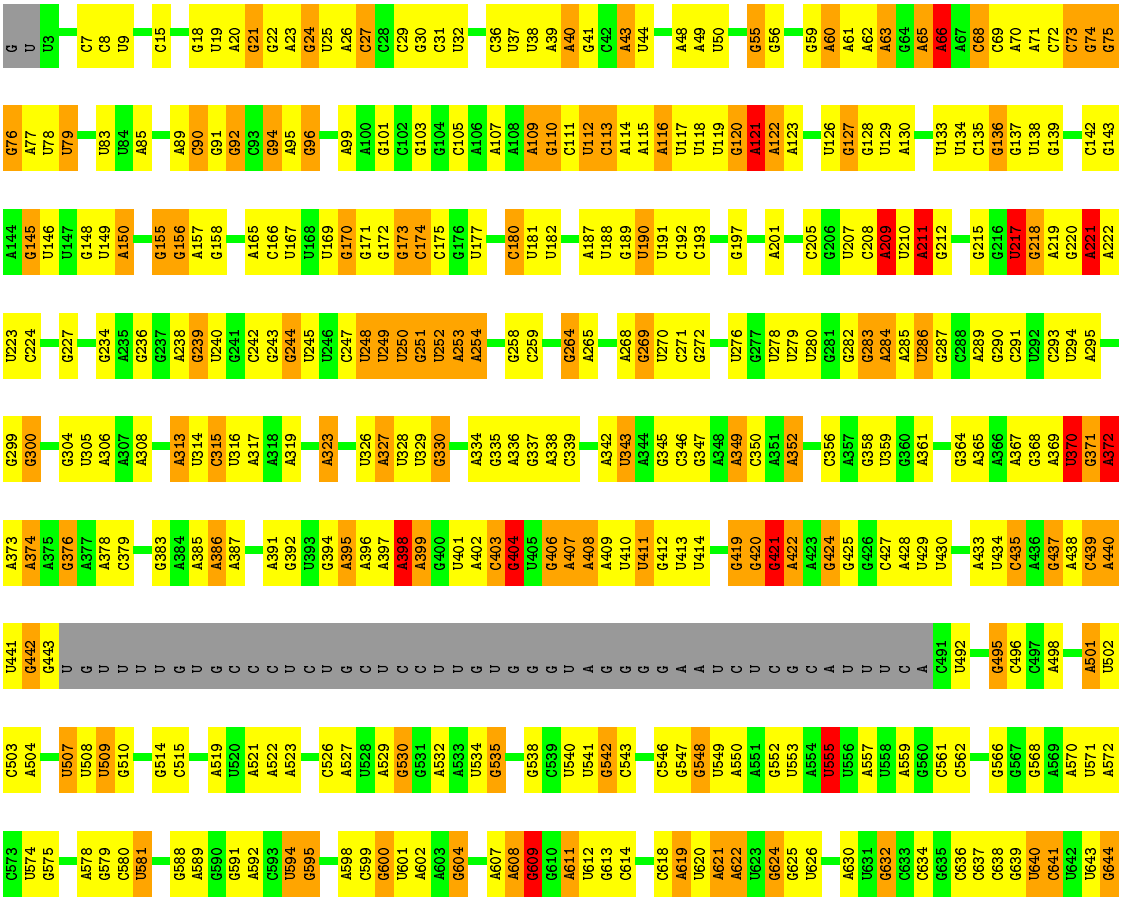


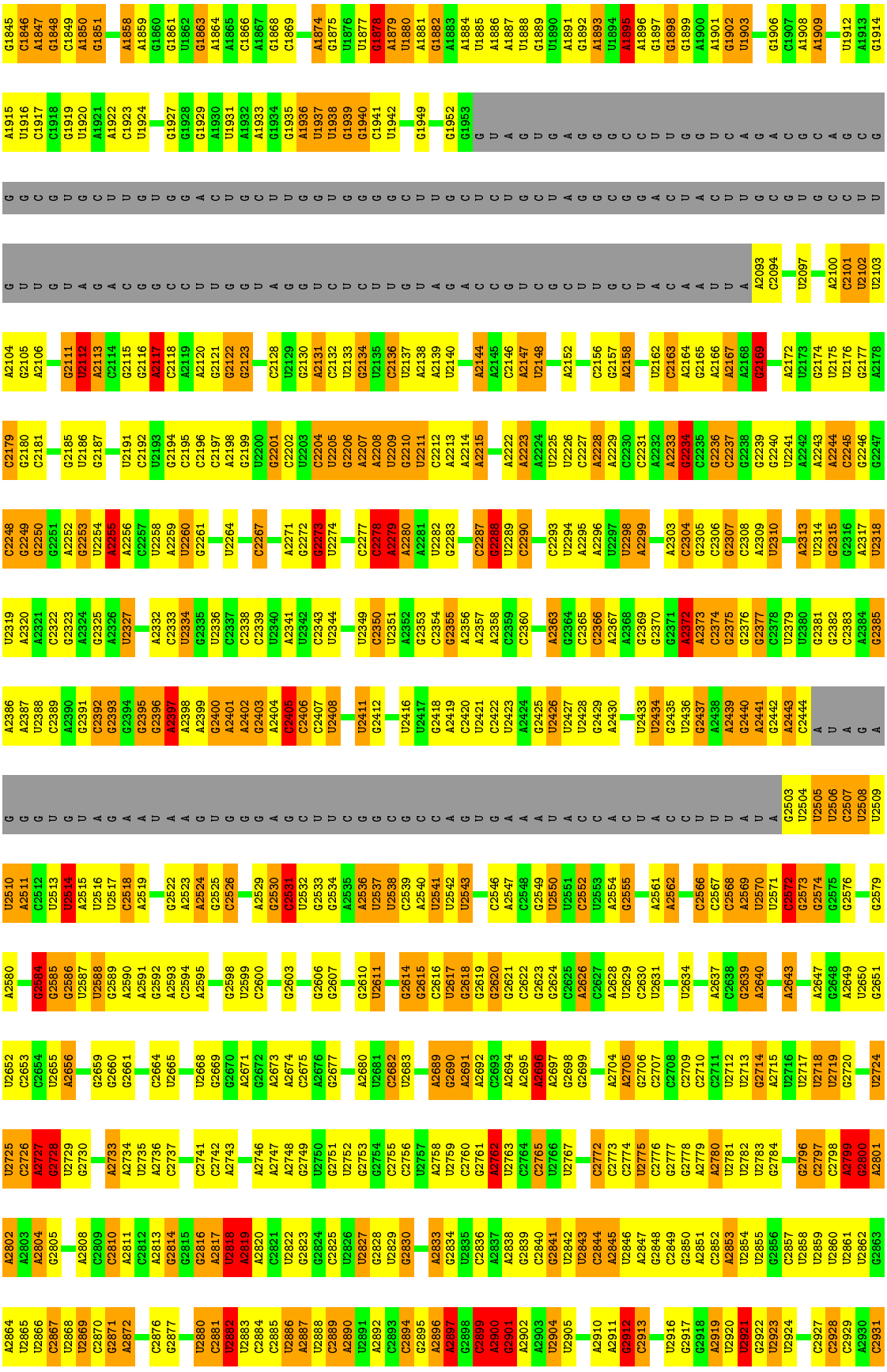


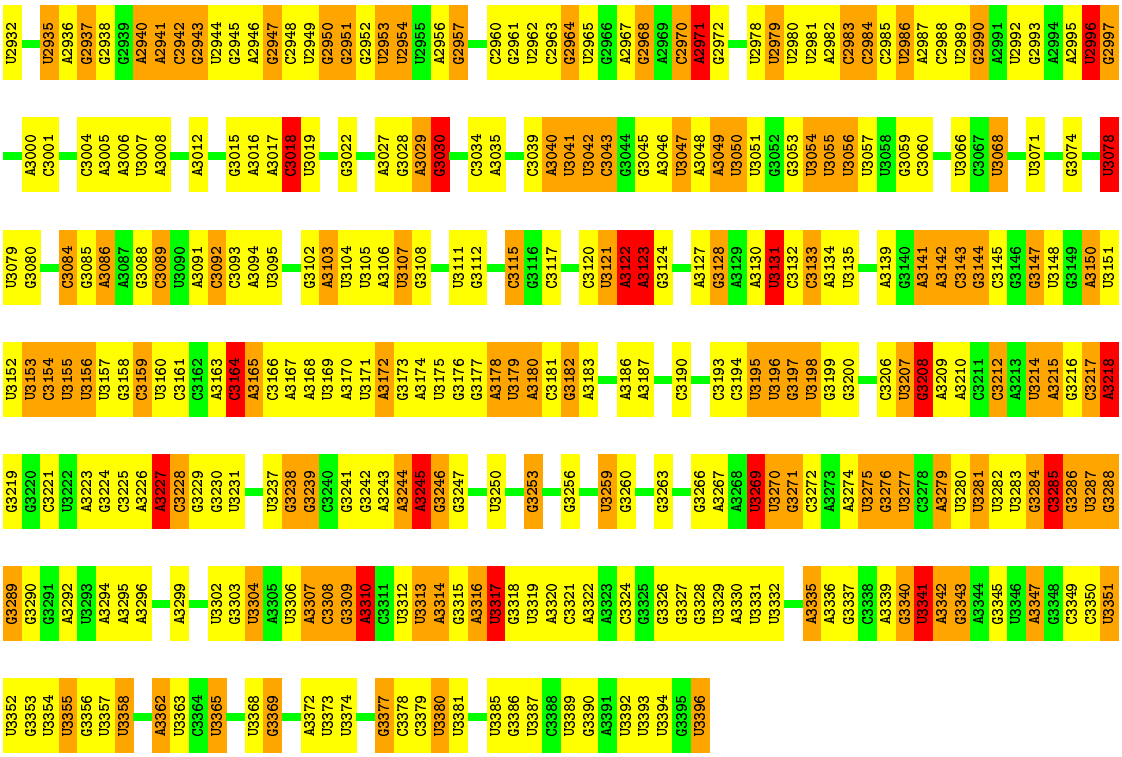
• Molecule 36: 25S ribosomal RNA

Chain 5:



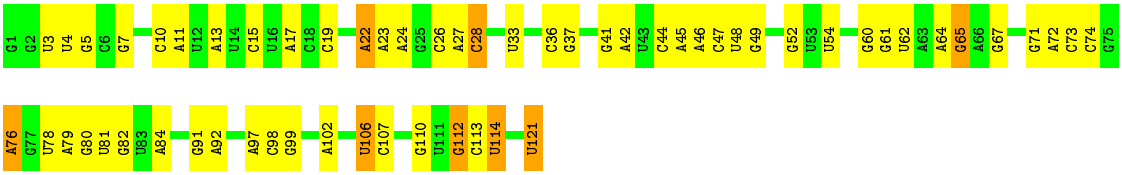






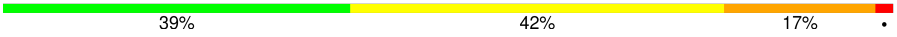
• Molecule 37: 5S ribosomal RNA

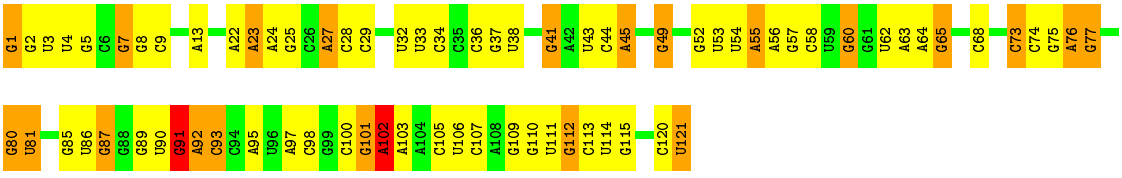
Chain 3:



• Molecule 37: 5S ribosomal RNA

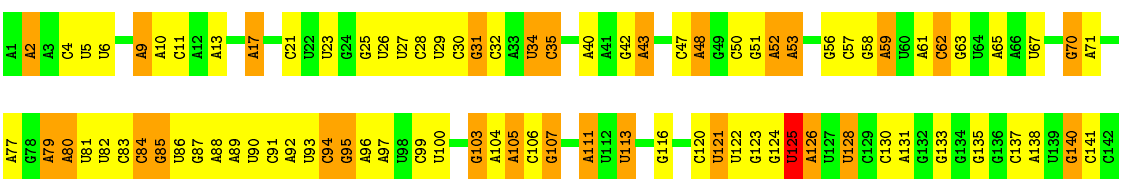
Chain 7:





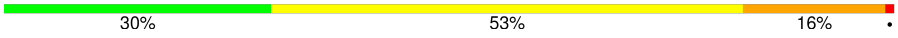
• Molecule 38: 5.8S ribosomal RNA

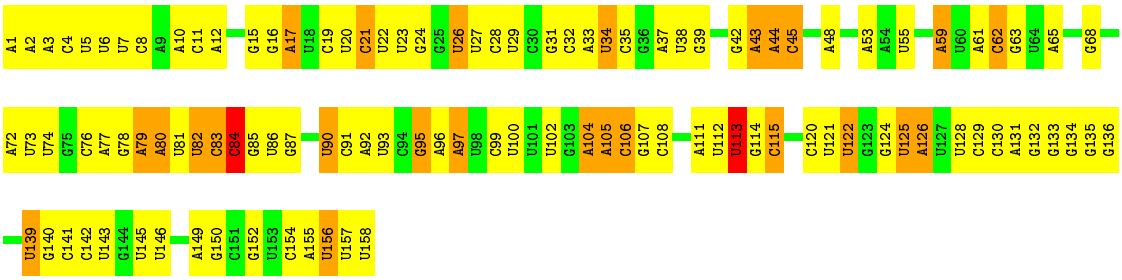
Chain 4:



• Molecule 38: 5.8S ribosomal RNA

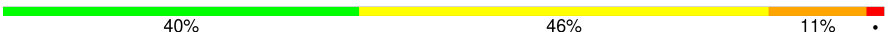
Chain 8:

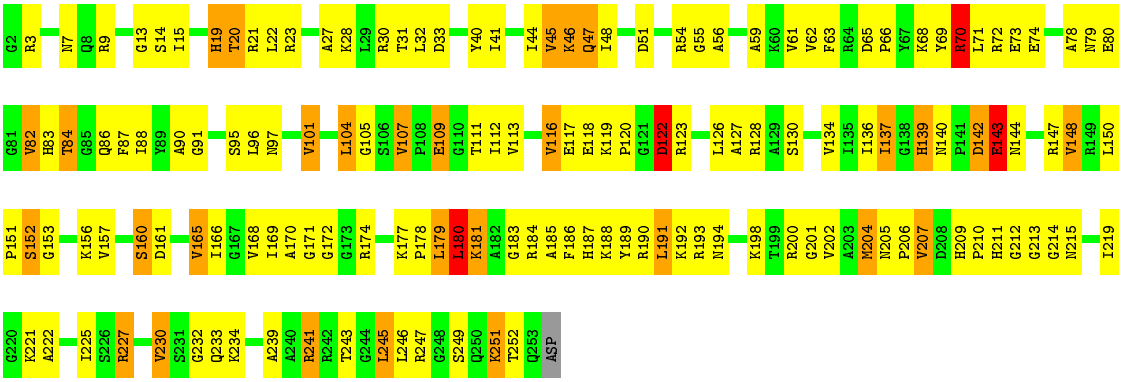




• Molecule 39: 60S ribosomal protein L2-A

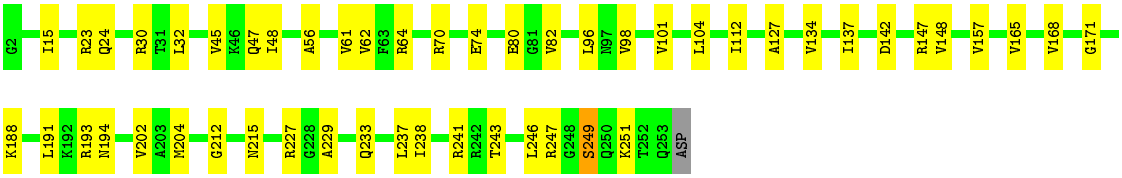
Chain L2:





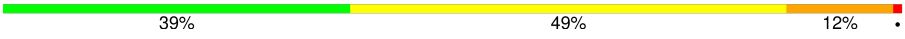
• Molecule 39: 60S ribosomal protein L2-A

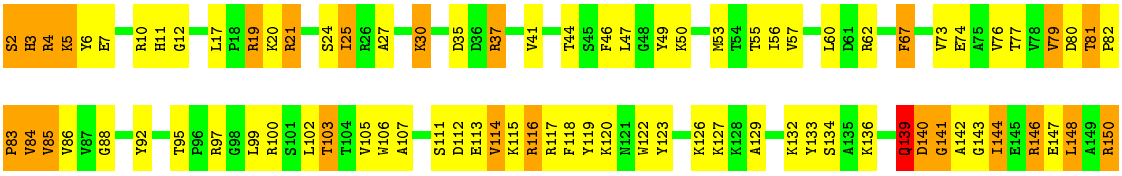
Chain l2:

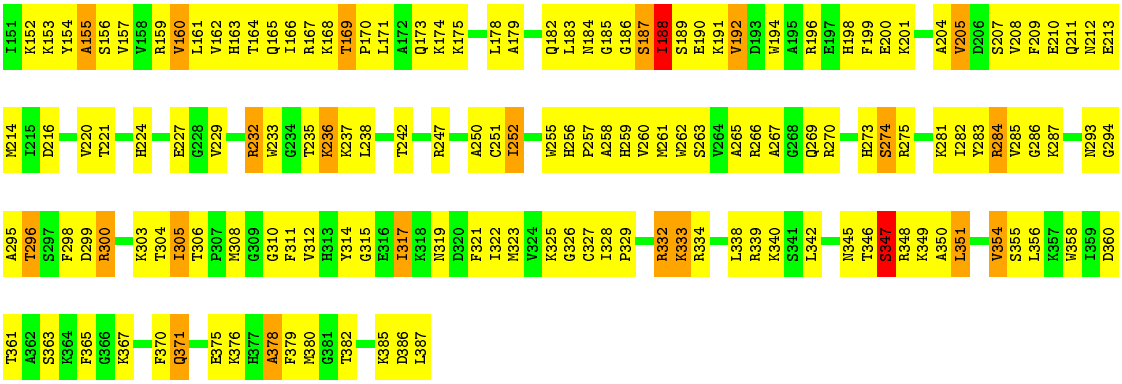


• Molecule 40: 60S ribosomal protein L3

Chain L3:

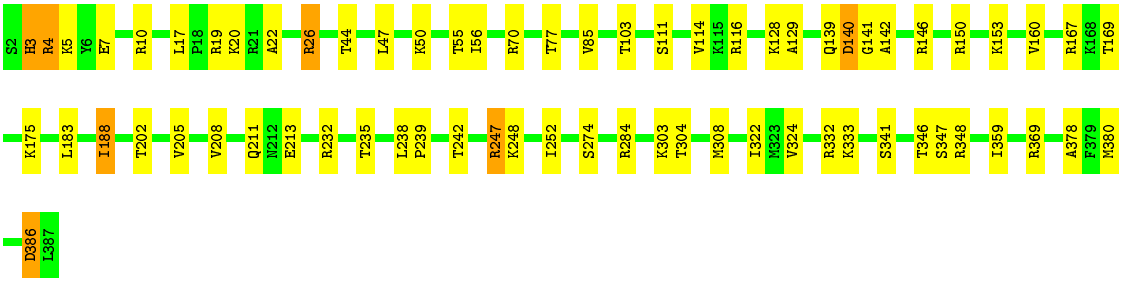






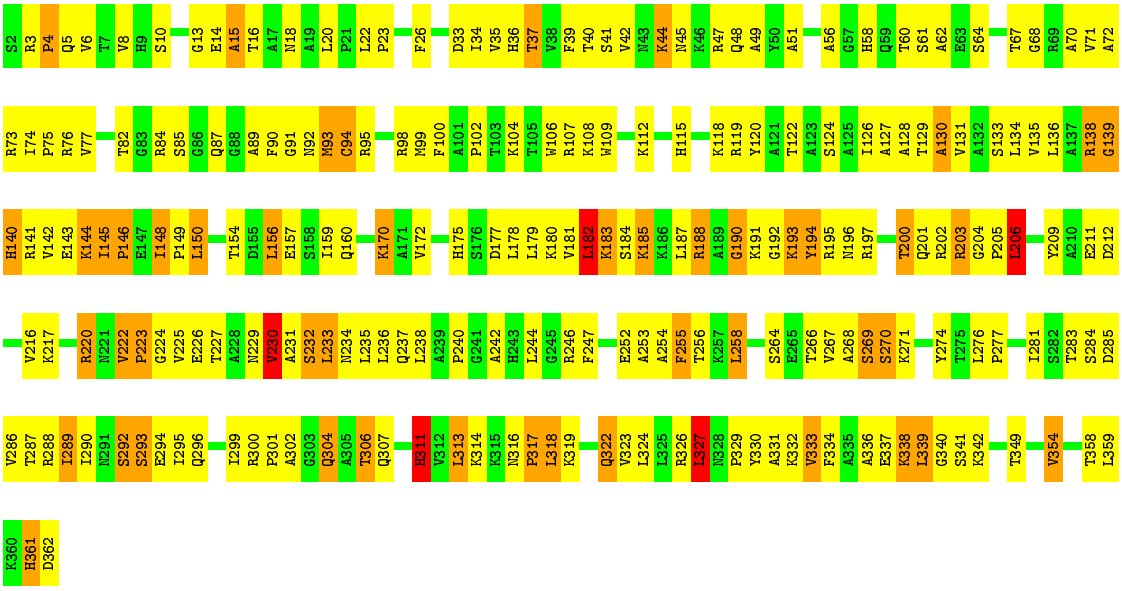
• Molecule 40: 60S ribosomal protein L3

Chain l3:



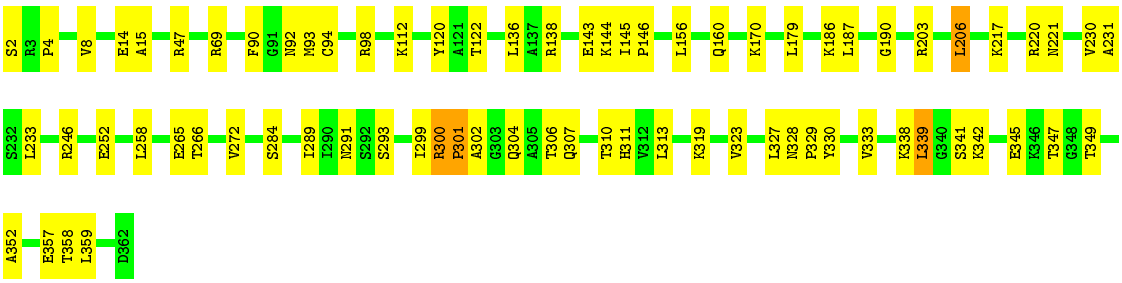
• Molecule 41: 60S ribosomal protein L4-A

Chain L4:



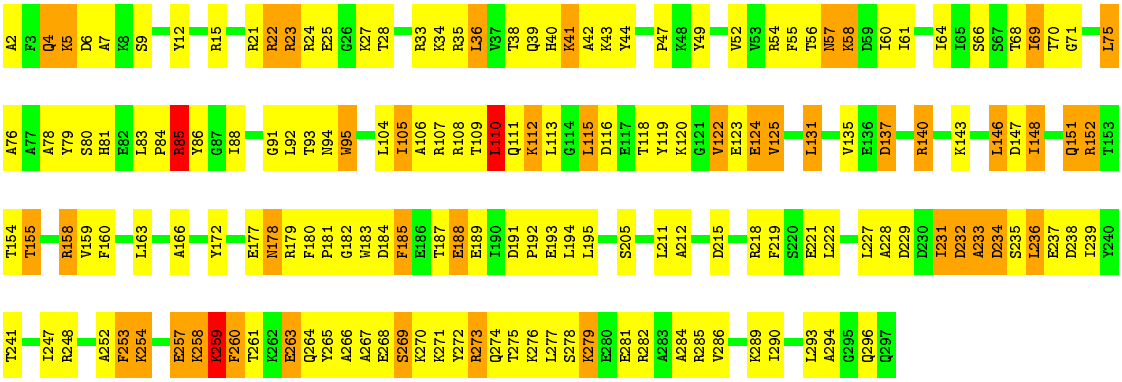
• Molecule 41: 60S ribosomal protein L4-A

Chain l4:



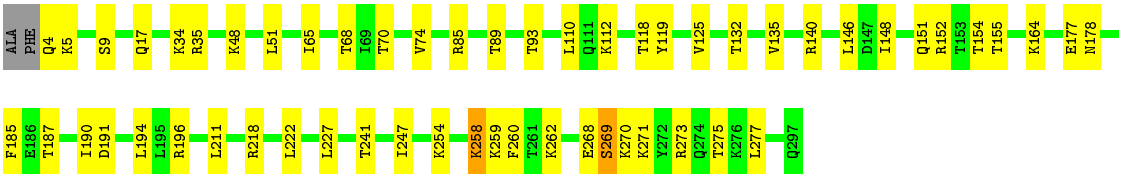
• Molecule 42: 60S ribosomal protein L5

Chain L5:



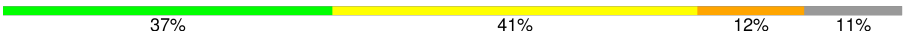
• Molecule 42: 60S ribosomal protein L5

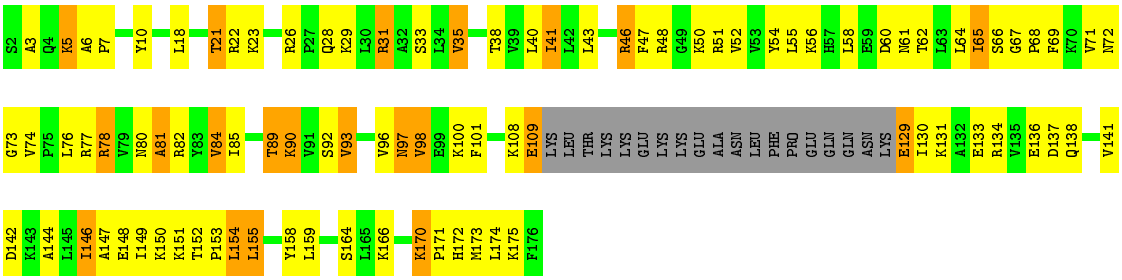
Chain l5:



• Molecule 43: 60S ribosomal protein L6-A

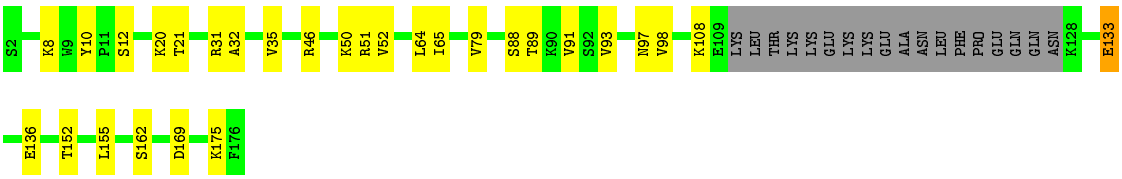
Chain L6:





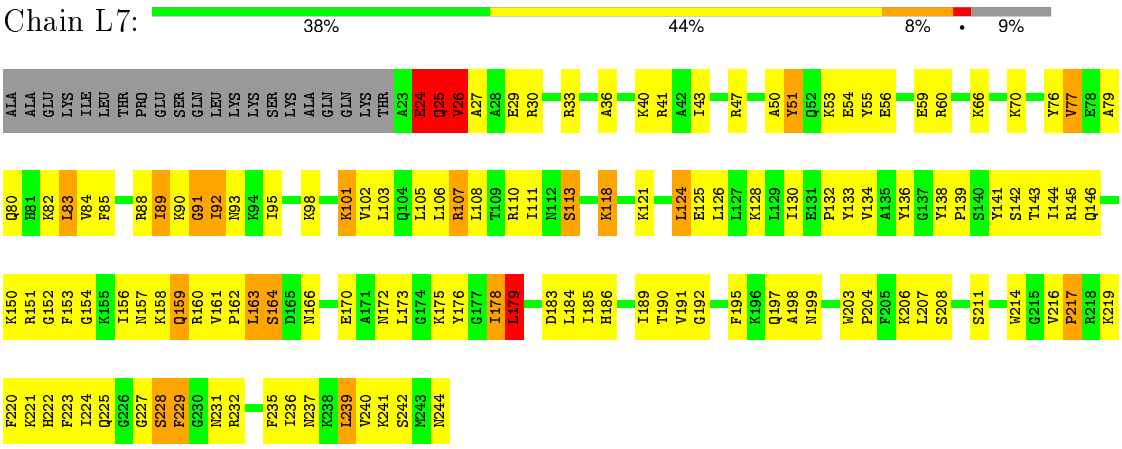
• Molecule 43: 60S ribosomal protein L6-A

Chain l6:



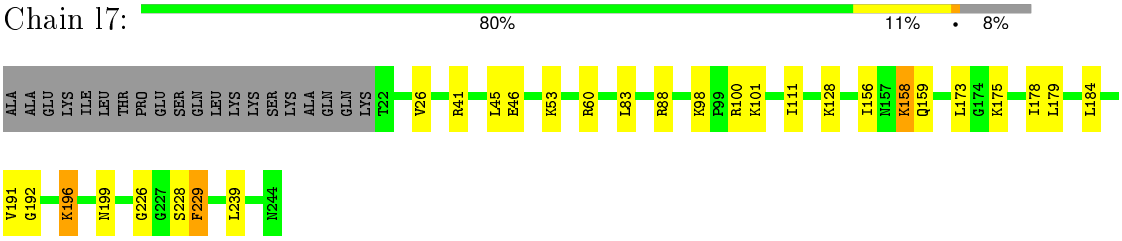
• Molecule 44: 60S ribosomal protein L7-A

Chain L7:



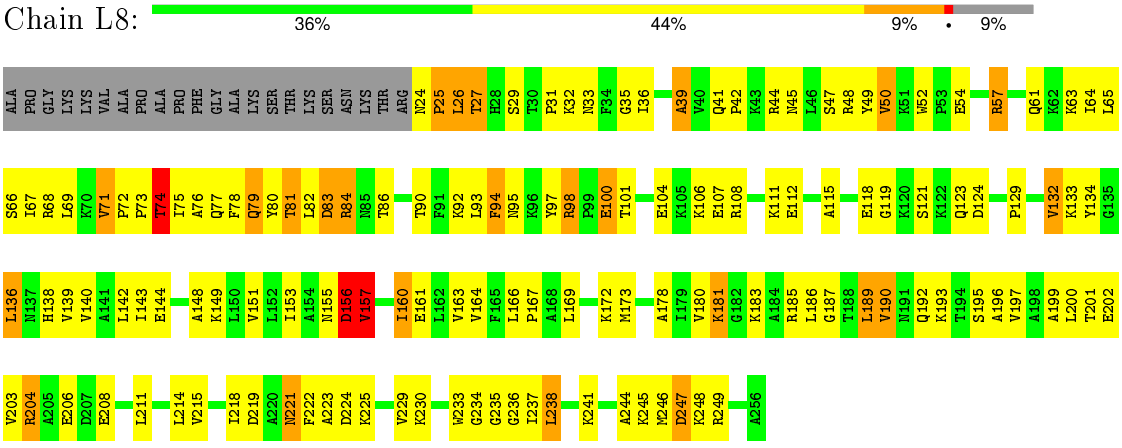
• Molecule 44: 60S ribosomal protein L7-A

Chain l7:



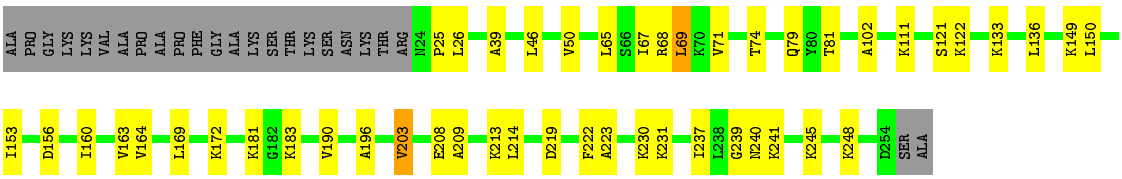
• Molecule 45: 60S ribosomal protein L8-A

Chain L8:



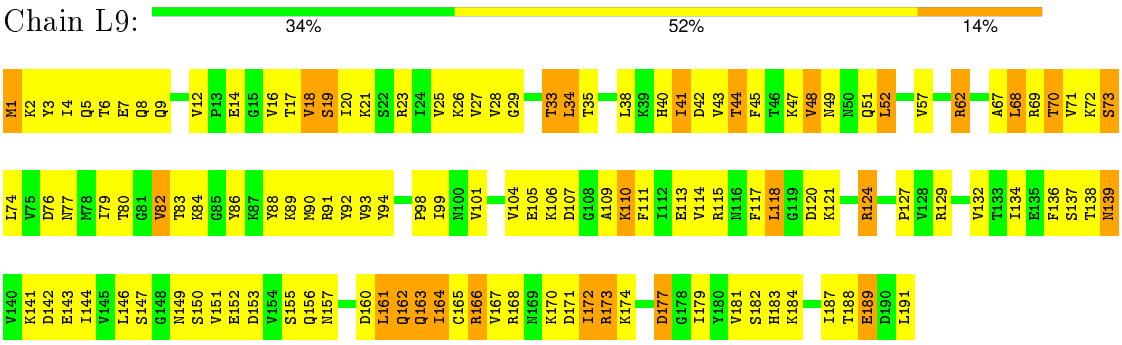
• Molecule 45: 60S ribosomal protein L8-A

Chain l8:



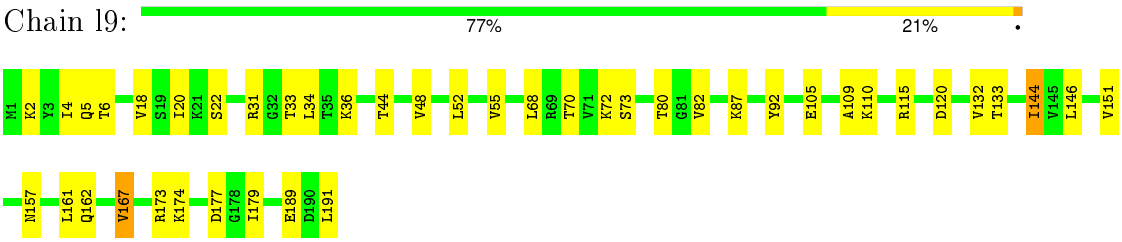
• Molecule 46: 60S ribosomal protein L9-A

Chain L9:



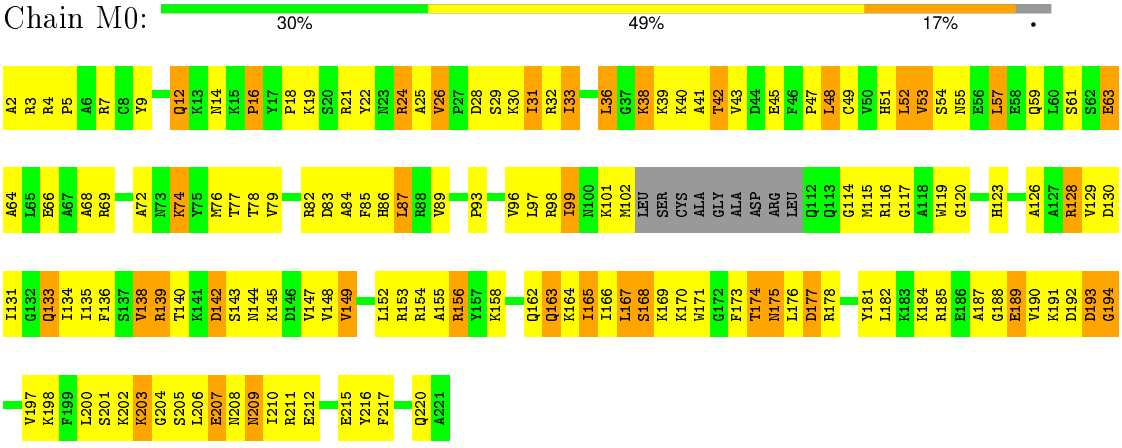
• Molecule 46: 60S ribosomal protein L9-A

Chain l9:



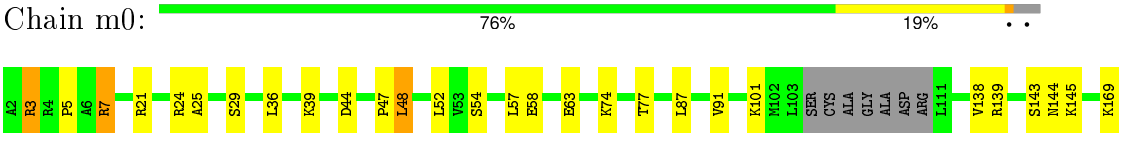
• Molecule 47: 60S ribosomal protein L10

Chain M0:



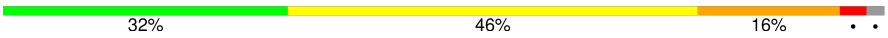
• Molecule 47: 60S ribosomal protein L10

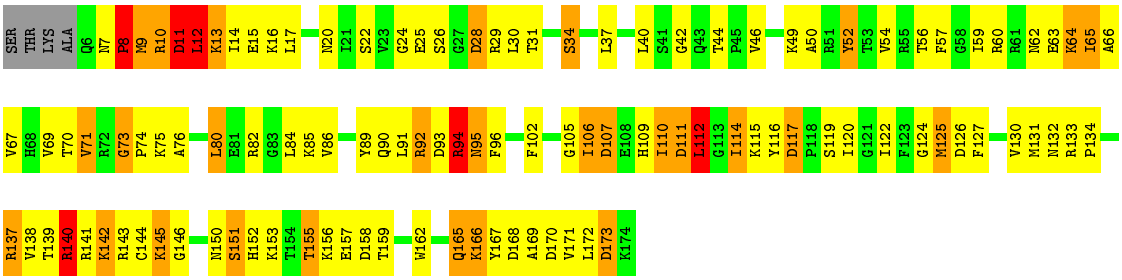
Chain m0:



- Molecule 48: 60S ribosomal protein L11-B

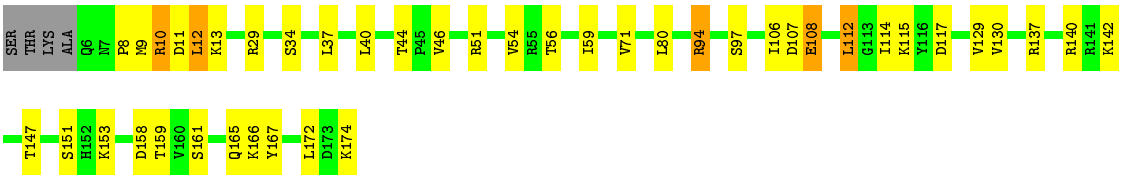
Chain M1:





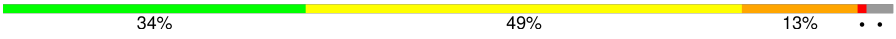
- Molecule 48: 60S ribosomal protein L11-B

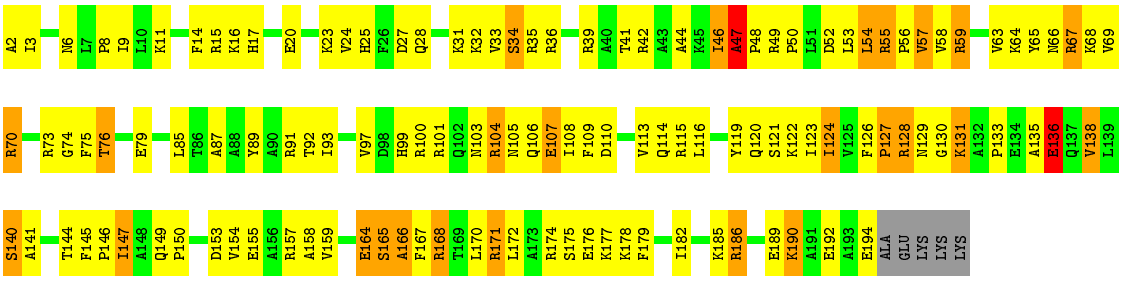
Chain m1:



- Molecule 49: 60S ribosomal protein L13-A

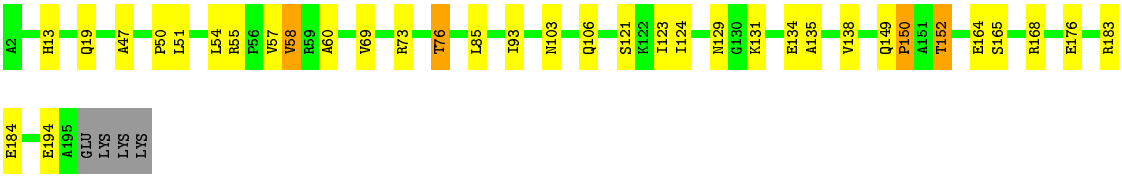
Chain M3:





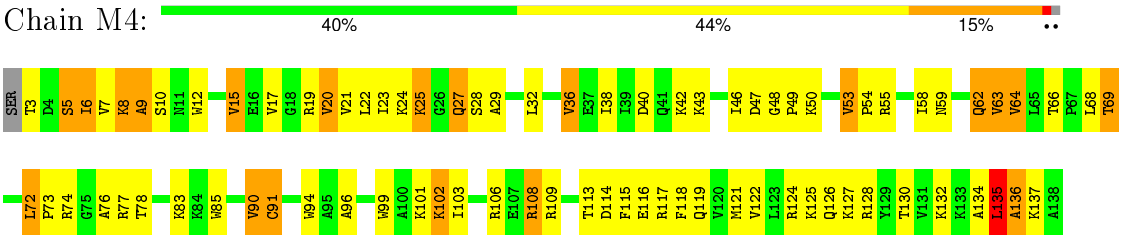
- Molecule 49: 60S ribosomal protein L13-A

Chain m3:



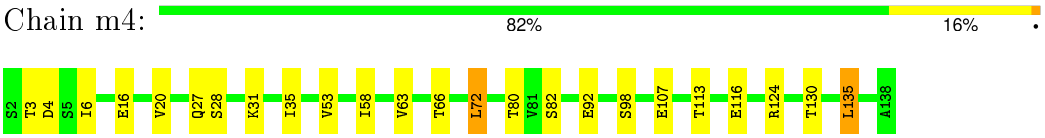
- Molecule 50: 60S ribosomal protein L14-A

Chain M4:



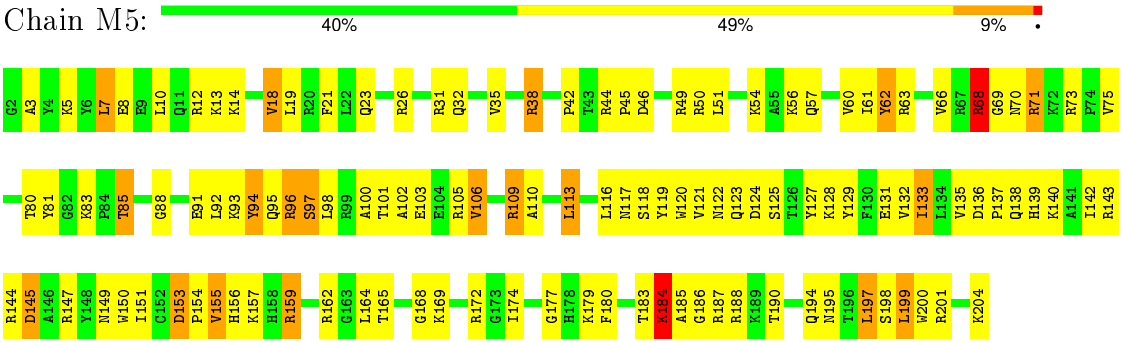
• Molecule 50: 60S ribosomal protein L14-A

Chain m4:



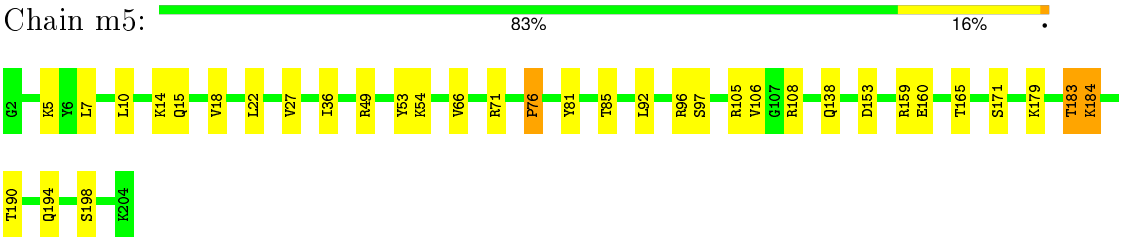
• Molecule 51: 60S ribosomal protein L15-A

Chain M5:



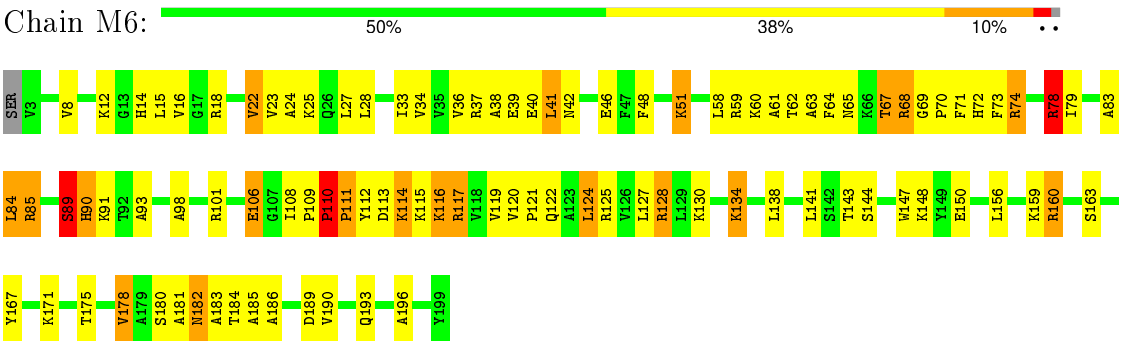
• Molecule 51: 60S ribosomal protein L15-A

Chain m5:



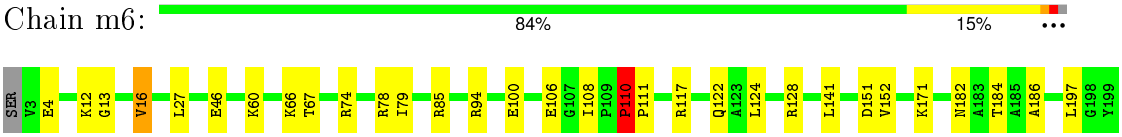
• Molecule 52: 60S ribosomal protein L16-A

Chain M6:



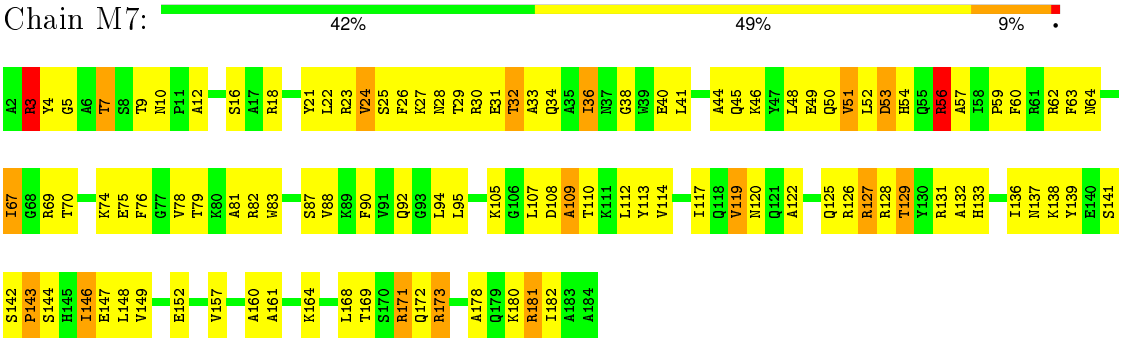
- Molecule 52: 60S ribosomal protein L16-A

Chain m6:



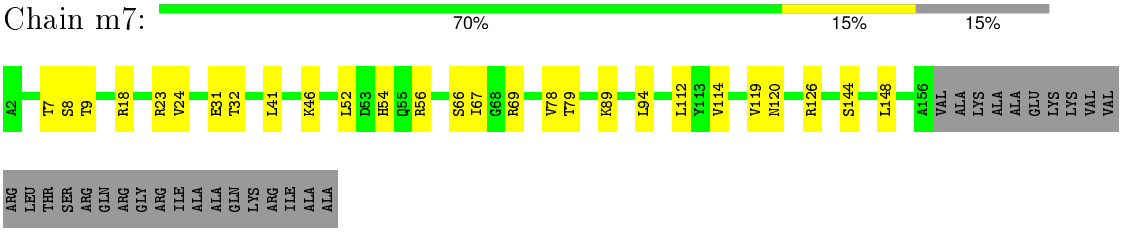
- Molecule 53: 60S ribosomal protein L17-A

Chain M7:



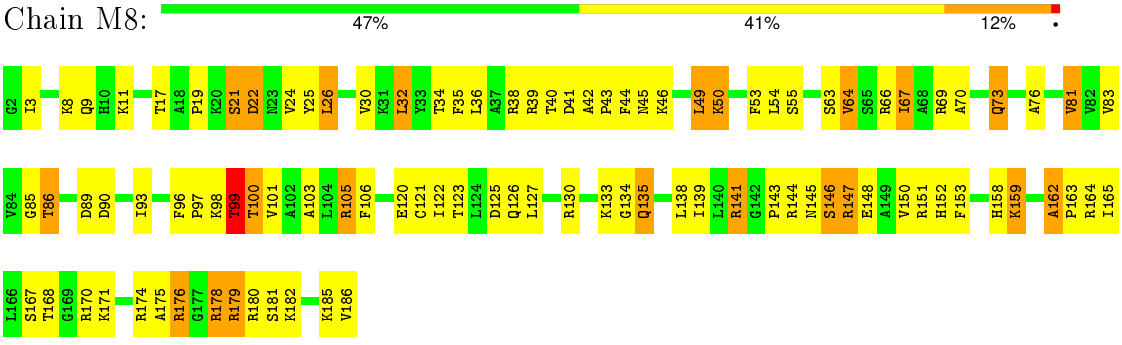
- Molecule 53: 60S ribosomal protein L17-A

Chain m7:



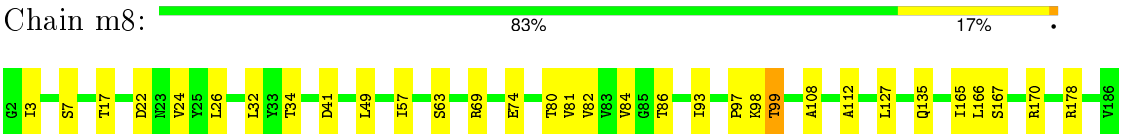
- Molecule 54: 60S ribosomal protein L18-A

Chain M8:



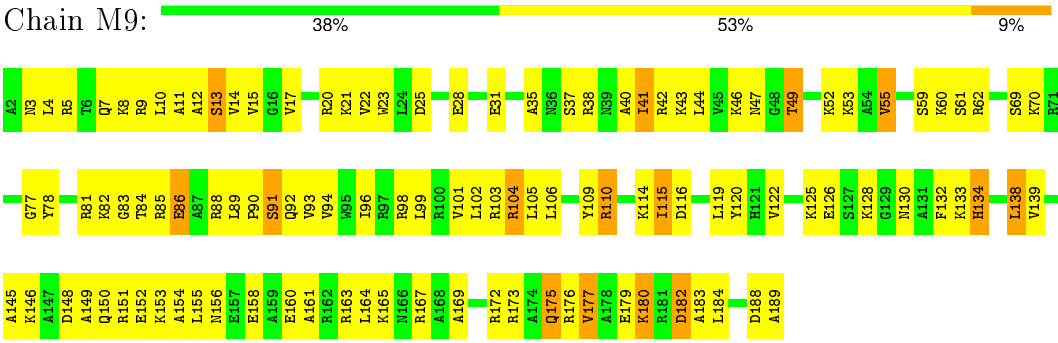
- Molecule 54: 60S ribosomal protein L18-A

Chain m8:



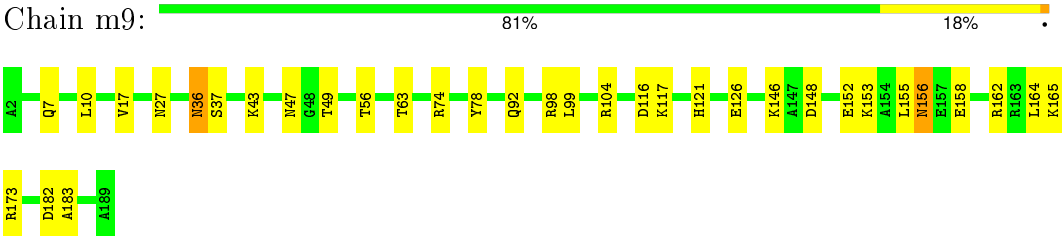
- Molecule 55: 60S ribosomal protein L19-A

Chain M9:



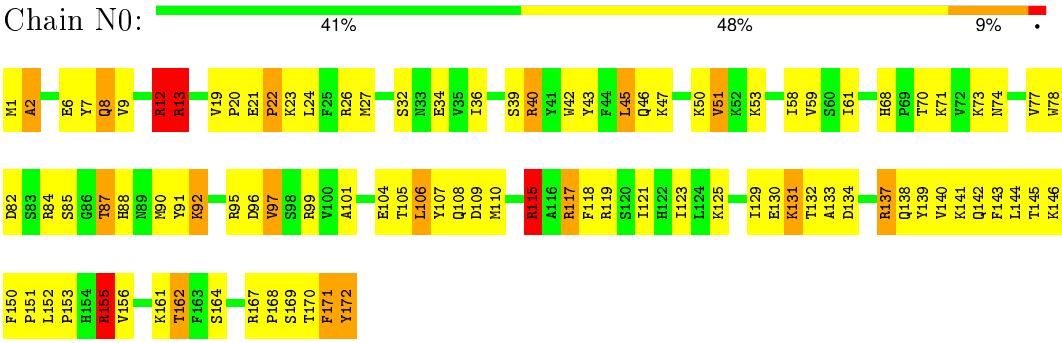
• Molecule 55: 60S ribosomal protein L19-A

Chain m9:



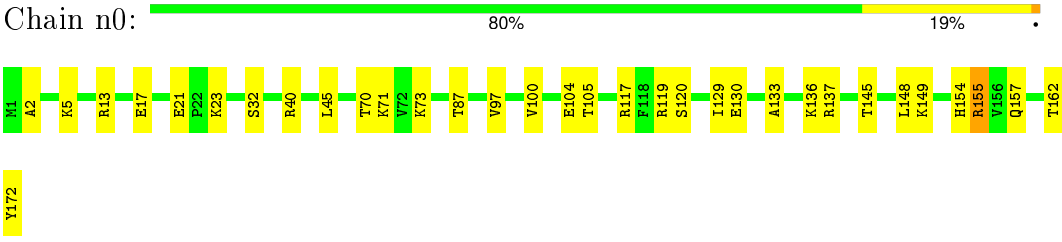
• Molecule 56: 60S ribosomal protein L20-A

Chain N0:



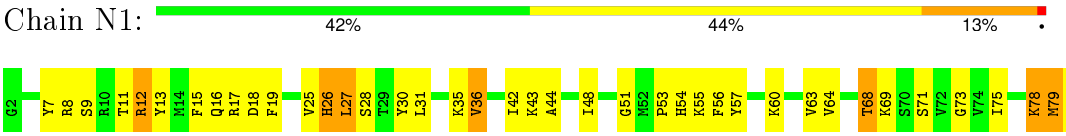
• Molecule 56: 60S ribosomal protein L20-A

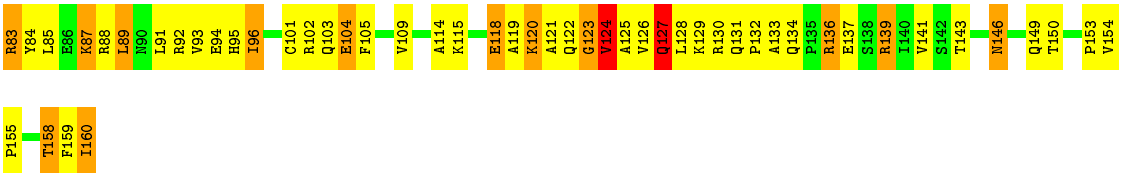
Chain n0:



• Molecule 57: 60S ribosomal protein L21-A

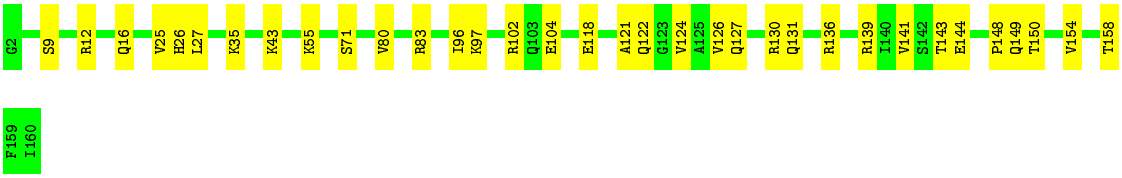
Chain N1:





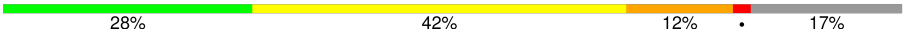
• Molecule 57: 60S ribosomal protein L21-A

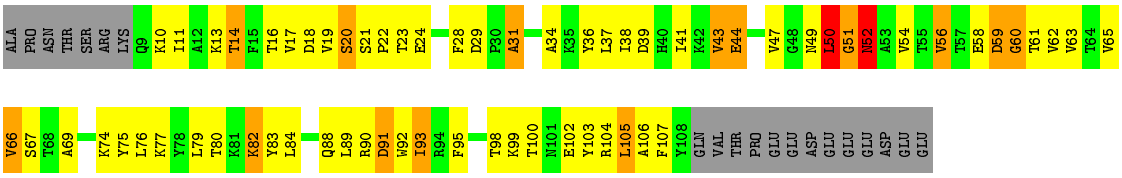
Chain n1:



• Molecule 58: 60S ribosomal protein L22-A

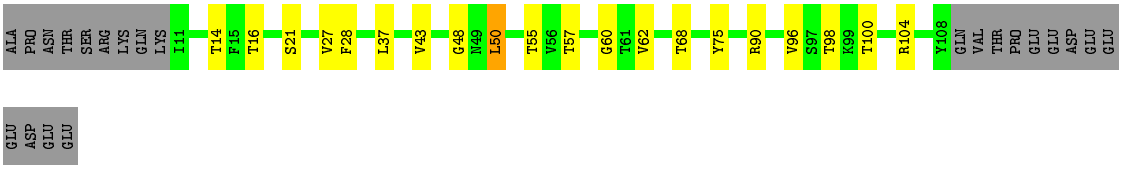
Chain N2:





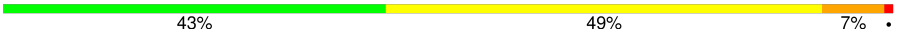
• Molecule 58: 60S ribosomal protein L22-A

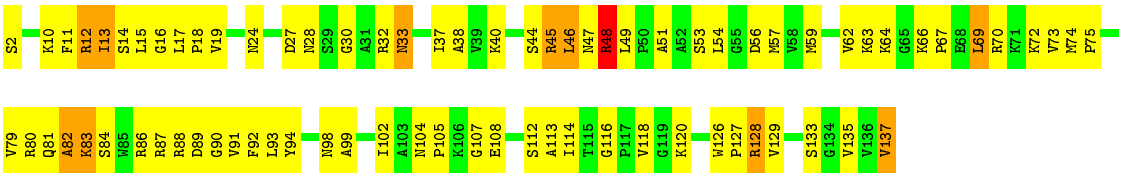
Chain n2:



• Molecule 59: 60S ribosomal protein L23-A

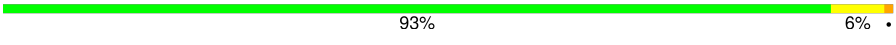
Chain N3:

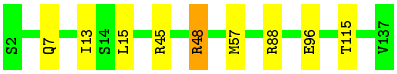




• Molecule 59: 60S ribosomal protein L23-A

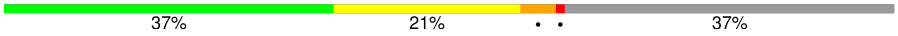
Chain n3:

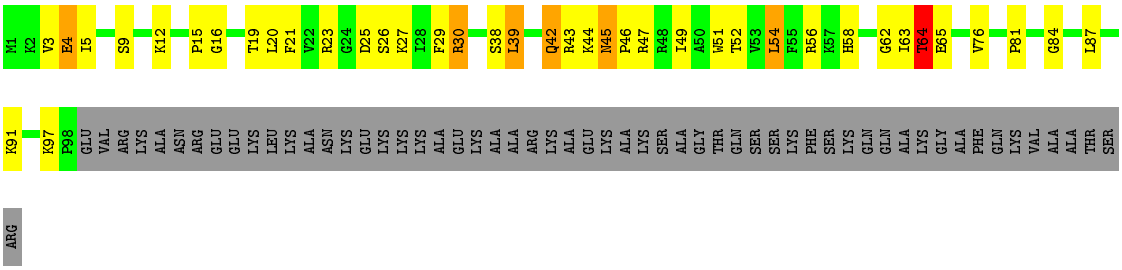




• Molecule 60: 60S ribosomal protein L24-A

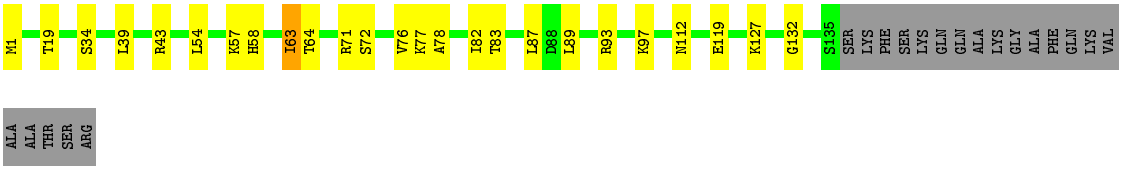
Chain N4:





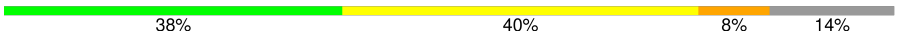
• Molecule 60: 60S ribosomal protein L24-A

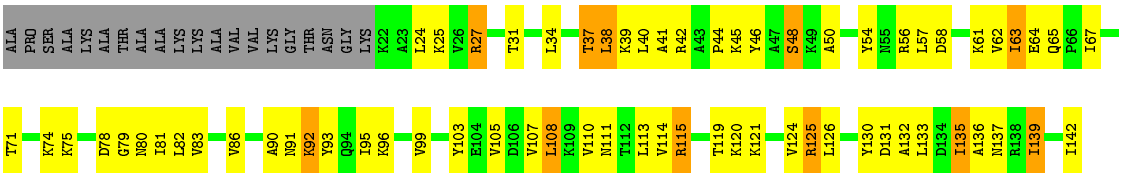
Chain n4:



• Molecule 61: 60S ribosomal protein L25

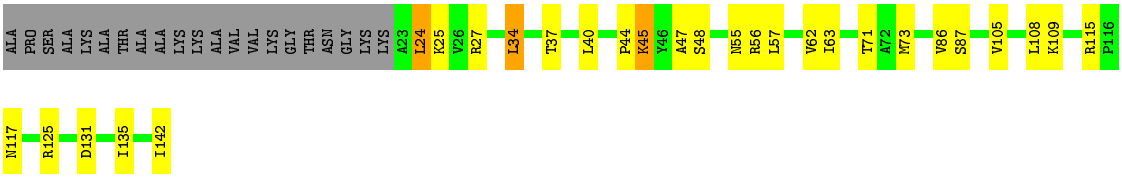
Chain N5:





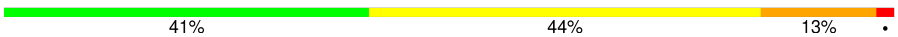
• Molecule 61: 60S ribosomal protein L25

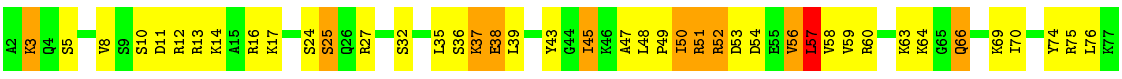
Chain n5:



• Molecule 62: 60S ribosomal protein L26-A

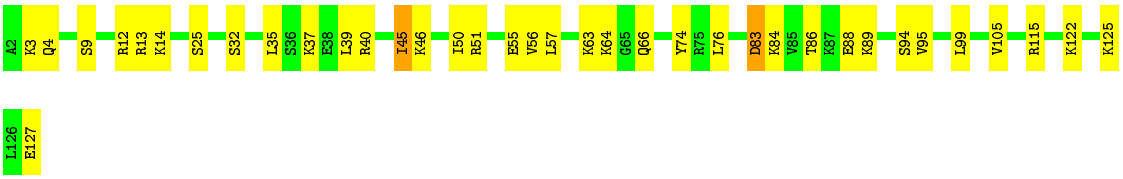
Chain N6:





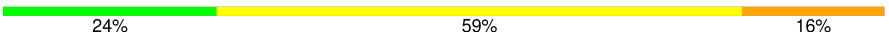
• Molecule 62: 60S ribosomal protein L26-A

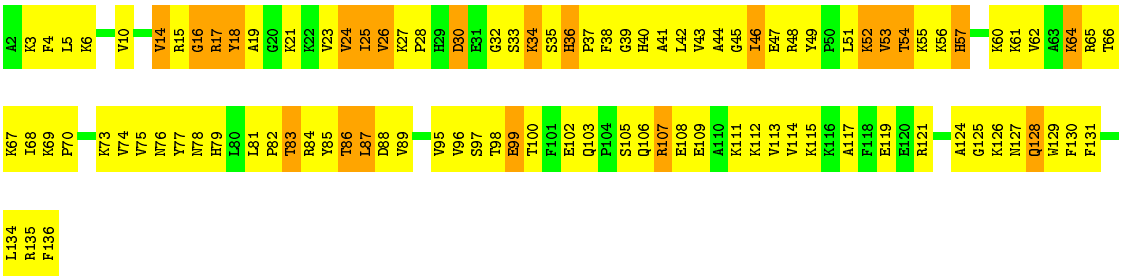
Chain n6:



• Molecule 63: 60S ribosomal protein L27-A

Chain N7:



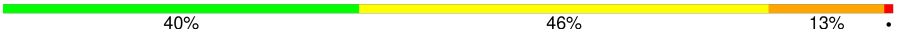


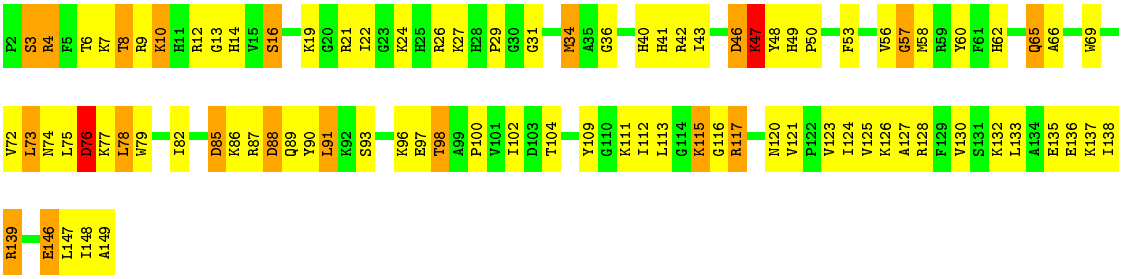
• Molecule 63: 60S ribosomal protein L27-A

Chain n7:

• Molecule 64: 60S ribosomal protein L28

Chain N8:





• Molecule 64: 60S ribosomal protein L28

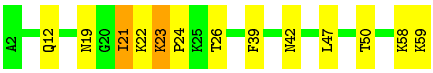
Chain n8:

• Molecule 65: 60S ribosomal protein L29

Chain N9:

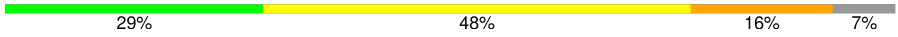
• Molecule 65: 60S ribosomal protein L29

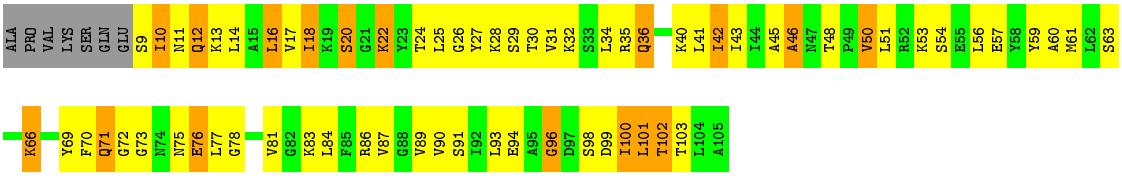
Chain n9:



• Molecule 66: 60S ribosomal protein L30

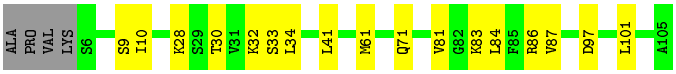
Chain O0:





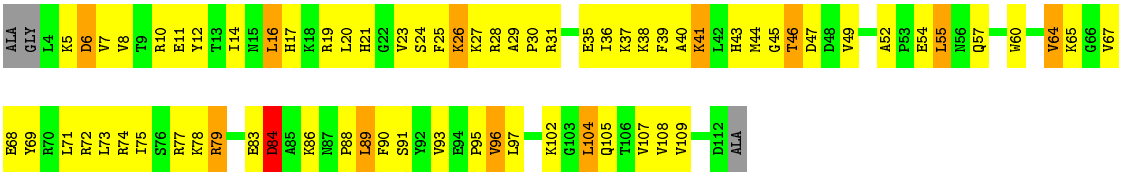
• Molecule 66: 60S ribosomal protein L30

Chain o0:



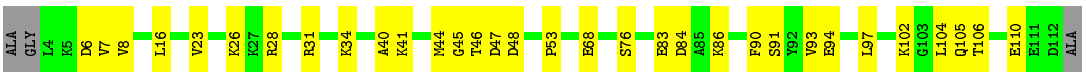
• Molecule 67: 60S ribosomal protein L31-A

Chain O1:



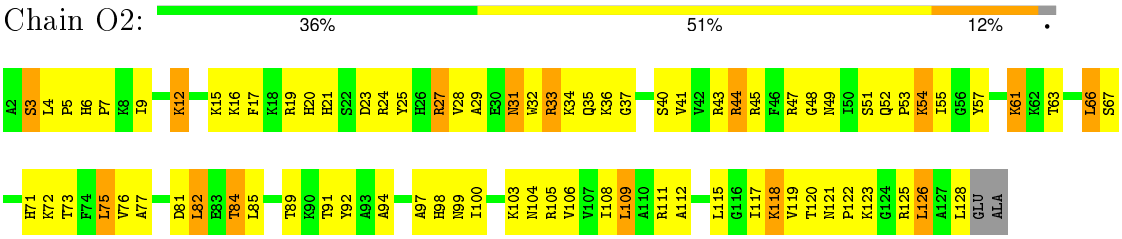
• Molecule 67: 60S ribosomal protein L31-A

Chain o1:



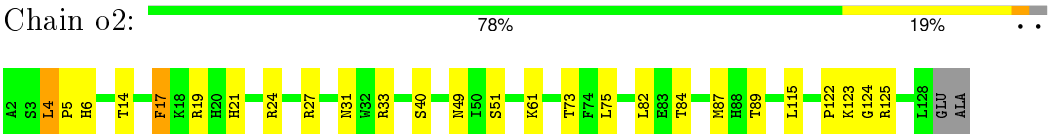
• Molecule 68: 60S ribosomal protein L32

Chain O2:



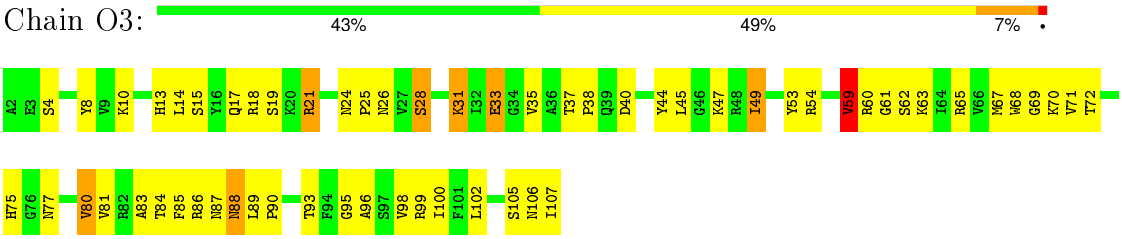
- Molecule 68: 60S ribosomal protein L32

Chain o2:



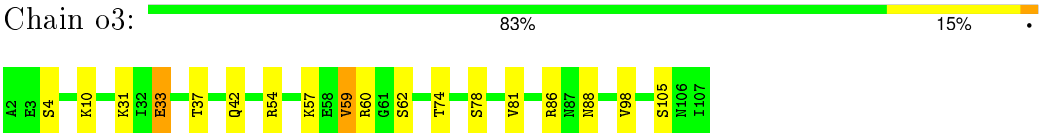
- Molecule 69: 60S ribosomal protein L33-A

Chain O3:



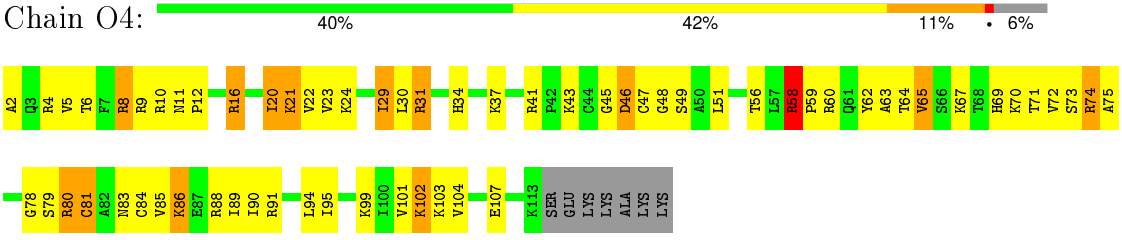
- Molecule 69: 60S ribosomal protein L33-A

Chain o3:



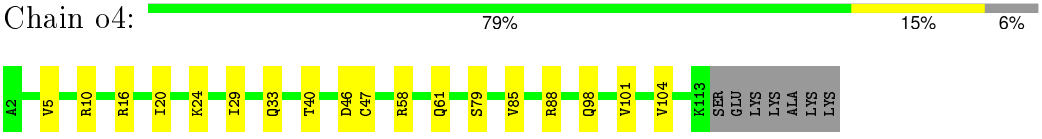
- Molecule 70: 60S ribosomal protein L34-A

Chain O4:



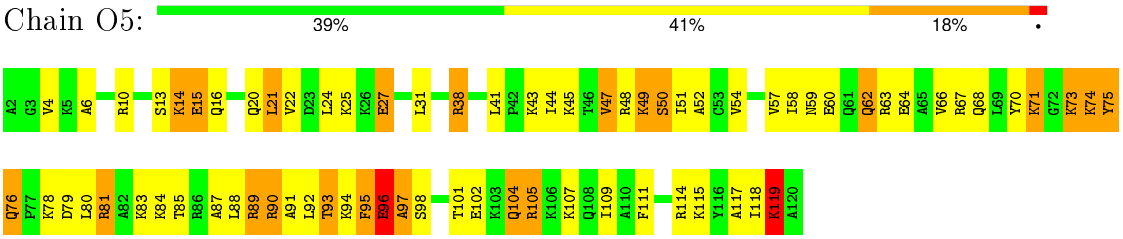
- Molecule 70: 60S ribosomal protein L34-A

Chain o4:



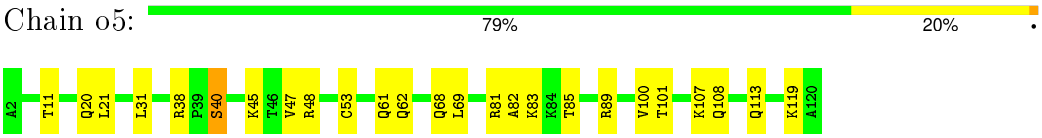
- Molecule 71: 60S ribosomal protein L35-A

Chain O5:



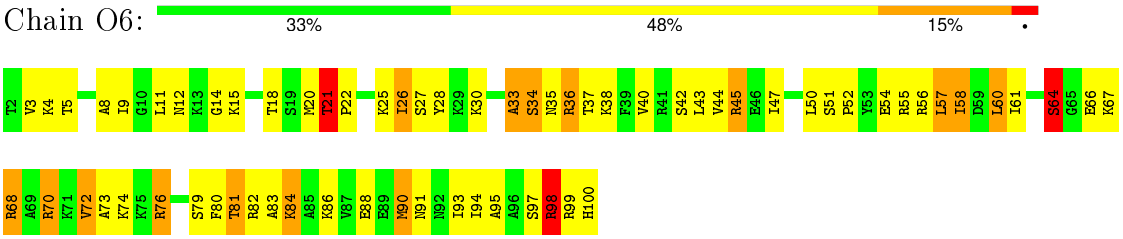
- Molecule 71: 60S ribosomal protein L35-A

Chain o5:



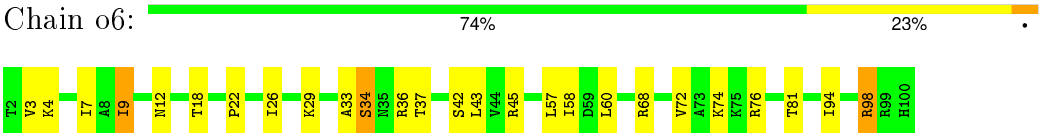
- Molecule 72: 60S ribosomal protein L36-A

Chain O6:



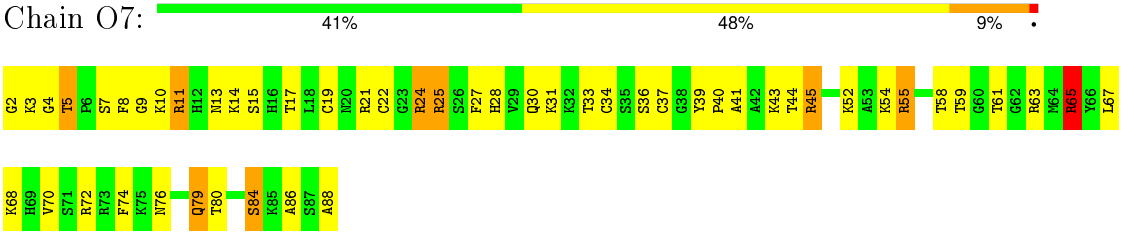
- Molecule 72: 60S ribosomal protein L36-A

Chain o6:



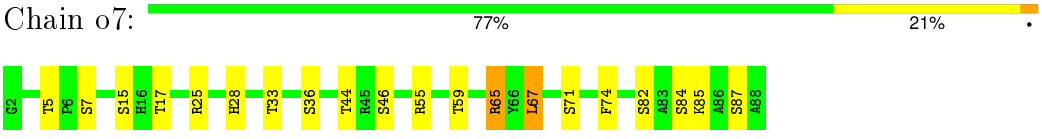
- Molecule 73: 60S ribosomal protein L37-A

Chain O7:



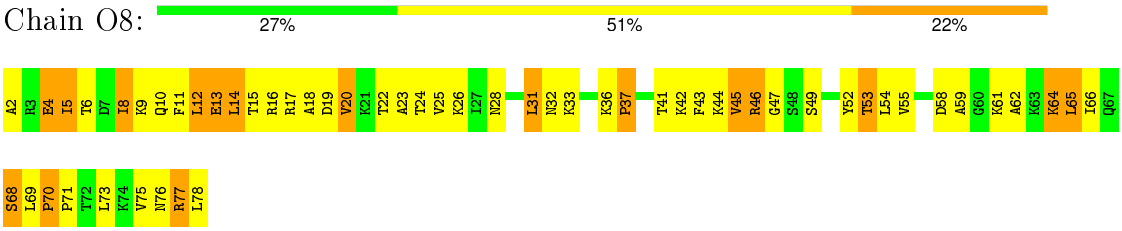
- Molecule 73: 60S ribosomal protein L37-A

Chain o7:



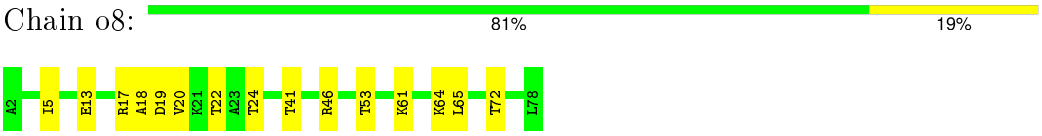
- Molecule 74: 60S ribosomal protein L38

Chain O8:



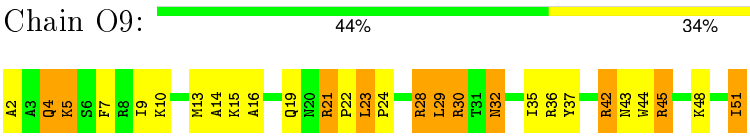
• Molecule 74: 60S ribosomal protein L38

Chain o8:



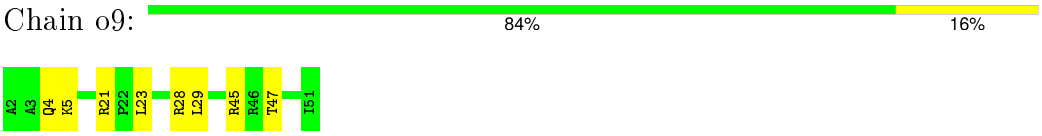
• Molecule 75: 60S ribosomal protein L39

Chain O9:



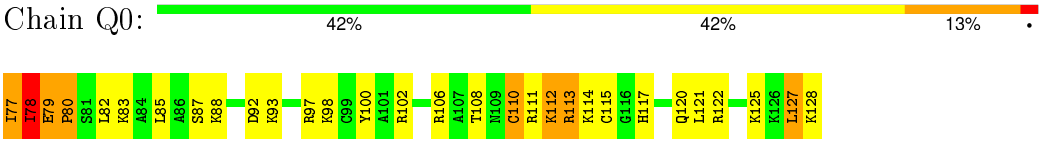
• Molecule 75: 60S ribosomal protein L39

Chain o9:



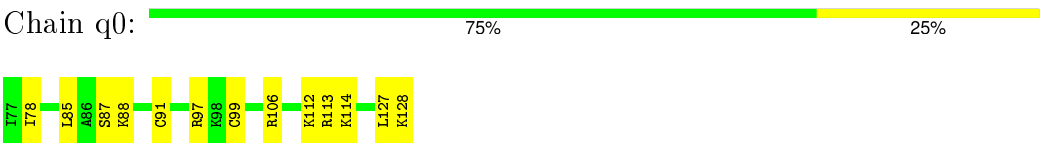
• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:



• Molecule 77: 60S ribosomal protein L41-A

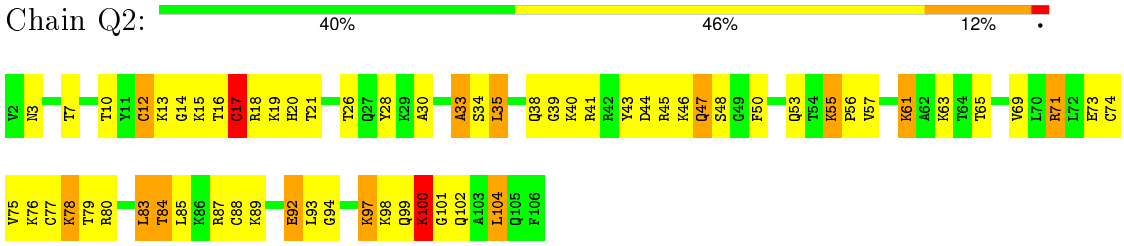
Chain Q1:

• Molecule 77: 60S ribosomal protein L41-A

Chain q1:

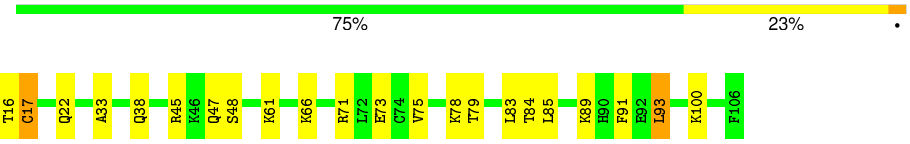
• Molecule 78: 60S ribosomal protein L42-A

Chain Q2:



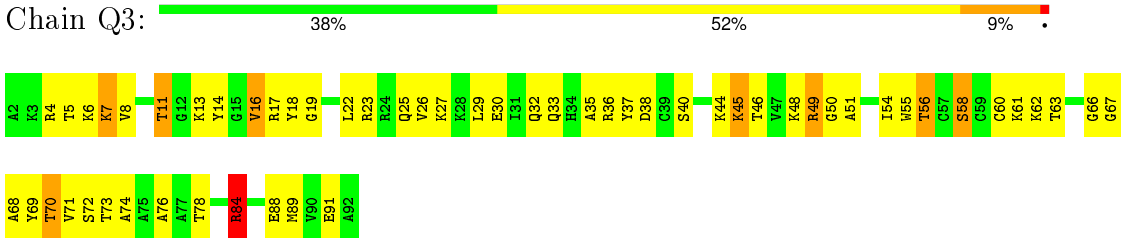
• Molecule 78: 60S ribosomal protein L42-A

Chain q2:



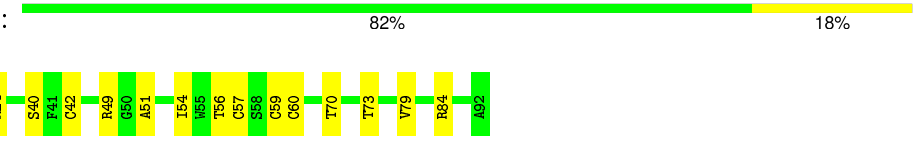
• Molecule 79: 60S ribosomal protein L43-A

Chain Q3:



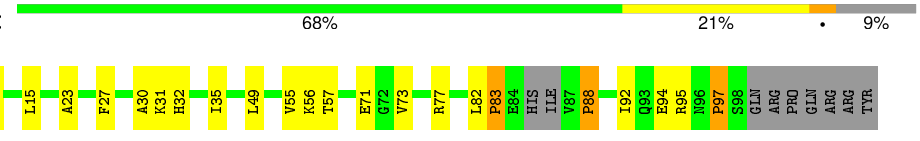
• Molecule 79: 60S ribosomal protein L43-A

Chain q3:



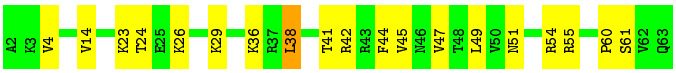
• Molecule 80: 40S ribosomal protein S10-A

Chain c0:



• Molecule 81: 40S ribosomal protein S30-A

Chain e0:

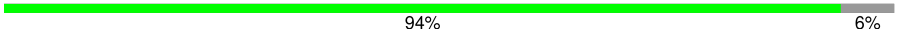


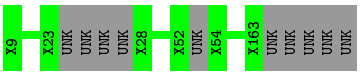
• Molecule 82: Ubiquitin-40S ribosomal protein S31

Chain e1:

• Molecule 83: UNKNOWN PROTEIN m2

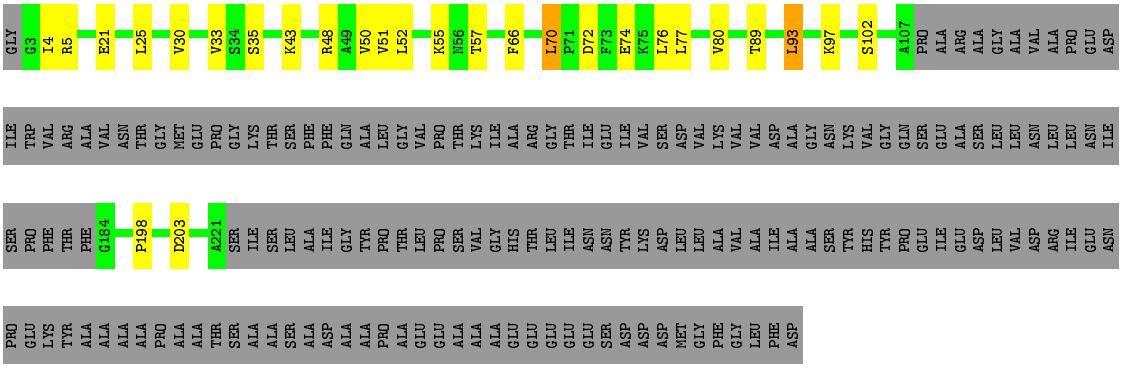
Chain m2:





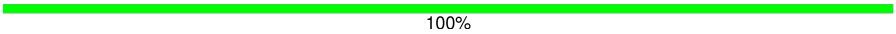
• Molecule 84: 60S acidic ribosomal protein P0

Chain p0:



• Molecule 85: UNKNOWN PROTEIN p1

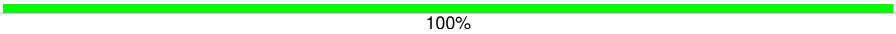
Chain p1:



There are no outlier residues recorded for this chain.

• Molecule 86: UNKNOWN PROTEIN p2

Chain p2:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

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	436.02Å 287.59Å 304.52Å 90.00° 99.02° 90.00°	Depositor
Resolution (Å)	49.82 – 3.20	Depositor
% Data completeness (in resolution range)	100.0 (49.82-3.20)	Depositor
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.181 , 0.237	Depositor
Wilson B-factor (Å^2)	70.5	Xtriage
Anisotropy	0.157	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 1214488 reflections (0.000%)	Xtriage
Total number of atoms	411288	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, OHX, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

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

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

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

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

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

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

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

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

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

There are no chirality outliers.

5 of 52 planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37283	0	18758	895	0
1	6	38238	0	19240	845	0
2	S0	1577	0	1567	166	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	187	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	119	0

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

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

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

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

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 10031 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L3:41:VAL:HA	40:L3:185:GLY:HA3	1.56	1.11
40:L3:296:THR:HG22	40:L3:298:PHE:H	2.66	1.06
1:6:1636:C:H4'	1:6:1637:C:H5'	1.34	1.05
28:D6:26:CYS:SG	28:D6:77:CYS:SG	3.43	1.01
36:5:3274:A:H3'	36:5:3275:U:H5"	1.42	1.01

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	S0	204/251 (81%)	143 (70%)	34 (17%)	27 (13%)	0 1
2	s0	204/251 (81%)	152 (74%)	33 (16%)	19 (9%)	1 5
3	S1	212/254 (84%)	141 (66%)	38 (18%)	33 (16%)	0 1
3	s1	214/254 (84%)	171 (80%)	30 (14%)	13 (6%)	2 15
4	S2	215/253 (85%)	173 (80%)	27 (13%)	15 (7%)	1 10
4	s2	215/253 (85%)	184 (86%)	21 (10%)	10 (5%)	3 22
5	S3	221/239 (92%)	182 (82%)	24 (11%)	15 (7%)	1 11
5	s3	221/239 (92%)	174 (79%)	31 (14%)	16 (7%)	1 10
6	S4	258/260 (99%)	206 (80%)	34 (13%)	18 (7%)	1 10
6	s4	258/260 (99%)	210 (81%)	28 (11%)	20 (8%)	1 8
7	S5	204/224 (91%)	154 (76%)	34 (17%)	16 (8%)	1 8
7	s5	204/224 (91%)	154 (76%)	35 (17%)	15 (7%)	1 9
8	S6	224/236 (95%)	197 (88%)	15 (7%)	12 (5%)	2 19
8	s6	216/236 (92%)	184 (85%)	22 (10%)	10 (5%)	3 23
9	S7	182/189 (96%)	136 (75%)	25 (14%)	21 (12%)	0 3
9	s7	184/189 (97%)	141 (77%)	28 (15%)	15 (8%)	1 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	S8	184/200 (92%)	148 (80%)	23 (12%)	13 (7%)	1 10
10	s8	184/200 (92%)	155 (84%)	16 (9%)	13 (7%)	1 10
11	S9	183/196 (93%)	147 (80%)	26 (14%)	10 (6%)	2 18
11	s9	183/196 (93%)	148 (81%)	28 (15%)	7 (4%)	4 28
12	C0	94/105 (90%)	68 (72%)	17 (18%)	9 (10%)	1 5
13	C1	153/155 (99%)	114 (74%)	24 (16%)	15 (10%)	1 4
13	c1	144/155 (93%)	122 (85%)	16 (11%)	6 (4%)	3 26
14	C2	122/142 (86%)	67 (55%)	34 (28%)	21 (17%)	0 0
14	c2	122/142 (86%)	67 (55%)	32 (26%)	23 (19%)	0 0
15	C3	148/150 (99%)	122 (82%)	20 (14%)	6 (4%)	3 27
15	c3	148/150 (99%)	120 (81%)	18 (12%)	10 (7%)	1 11
16	C4	125/136 (92%)	90 (72%)	19 (15%)	16 (13%)	0 2
16	c4	126/136 (93%)	96 (76%)	19 (15%)	11 (9%)	1 5
17	C5	122/141 (86%)	88 (72%)	22 (18%)	12 (10%)	1 4
17	c5	133/141 (94%)	94 (71%)	20 (15%)	19 (14%)	0 1
18	C6	139/142 (98%)	117 (84%)	11 (8%)	11 (8%)	1 8
18	c6	140/142 (99%)	120 (86%)	12 (9%)	8 (6%)	2 17
19	C7	116/136 (85%)	87 (75%)	21 (18%)	8 (7%)	1 10
19	c7	113/136 (83%)	84 (74%)	19 (17%)	10 (9%)	1 5
20	C8	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1 6
20	c8	143/145 (99%)	115 (80%)	18 (13%)	10 (7%)	1 10
21	C9	141/143 (99%)	120 (85%)	14 (10%)	7 (5%)	3 21
21	c9	141/143 (99%)	114 (81%)	21 (15%)	6 (4%)	3 25
22	D0	105/120 (88%)	82 (78%)	19 (18%)	4 (4%)	4 28
22	d0	108/120 (90%)	87 (81%)	10 (9%)	11 (10%)	1 4
23	D1	85/87 (98%)	64 (75%)	12 (14%)	9 (11%)	0 3
23	d1	85/87 (98%)	72 (85%)	10 (12%)	3 (4%)	4 31
24	D2	127/129 (98%)	112 (88%)	12 (9%)	3 (2%)	7 43
24	d2	127/129 (98%)	112 (88%)	14 (11%)	1 (1%)	24 69
25	D3	142/144 (99%)	109 (77%)	19 (13%)	14 (10%)	1 4
25	d3	142/144 (99%)	119 (84%)	18 (13%)	5 (4%)	4 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
26	D4	132/134 (98%)	106 (80%)	18 (14%)	8 (6%)	2 15
26	d4	132/134 (98%)	106 (80%)	16 (12%)	10 (8%)	1 9
27	D5	68/107 (64%)	44 (65%)	11 (16%)	13 (19%)	0 0
27	d5	67/107 (63%)	49 (73%)	11 (16%)	7 (10%)	1 4
28	D6	95/97 (98%)	62 (65%)	19 (20%)	14 (15%)	0 1
28	d6	95/97 (98%)	67 (70%)	18 (19%)	10 (10%)	1 4
29	D7	79/81 (98%)	63 (80%)	9 (11%)	7 (9%)	1 5
29	d7	79/81 (98%)	60 (76%)	12 (15%)	7 (9%)	1 5
30	D8	61/66 (92%)	49 (80%)	6 (10%)	6 (10%)	1 4
30	d8	61/66 (92%)	43 (70%)	13 (21%)	5 (8%)	1 7
31	D9	51/55 (93%)	41 (80%)	8 (16%)	2 (4%)	4 28
31	d9	51/55 (93%)	36 (71%)	9 (18%)	6 (12%)	0 3
32	E0	58/60 (97%)	47 (81%)	10 (17%)	1 (2%)	11 52
33	E1	69/76 (91%)	38 (55%)	12 (17%)	19 (28%)	0 0
34	SR	316/318 (99%)	244 (77%)	45 (14%)	27 (8%)	1 6
34	sR	316/318 (99%)	261 (83%)	42 (13%)	13 (4%)	3 27
35	SM	155/273 (57%)	111 (72%)	27 (17%)	17 (11%)	0 3
35	sM	98/273 (36%)	57 (58%)	28 (29%)	13 (13%)	0 1
39	L2	250/253 (99%)	224 (90%)	17 (7%)	9 (4%)	4 30
39	l2	250/253 (99%)	214 (86%)	23 (9%)	13 (5%)	2 19
40	L3	384/386 (100%)	322 (84%)	45 (12%)	17 (4%)	3 24
40	l3	384/386 (100%)	339 (88%)	32 (8%)	13 (3%)	5 31
41	L4	359/361 (99%)	297 (83%)	34 (10%)	28 (8%)	1 8
41	l4	359/361 (99%)	299 (83%)	38 (11%)	22 (6%)	2 15
42	L5	294/296 (99%)	237 (81%)	35 (12%)	22 (8%)	1 9
42	l5	292/296 (99%)	253 (87%)	32 (11%)	7 (2%)	7 43
43	L6	152/175 (87%)	134 (88%)	12 (8%)	6 (4%)	4 28
43	l6	153/175 (87%)	130 (85%)	17 (11%)	6 (4%)	4 28
44	L7	220/243 (90%)	184 (84%)	26 (12%)	10 (4%)	3 24
44	l7	221/243 (91%)	189 (86%)	27 (12%)	5 (2%)	8 44
45	L8	231/255 (91%)	189 (82%)	31 (13%)	11 (5%)	3 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
45	l8	229/255 (90%)	188 (82%)	23 (10%)	18 (8%)	1 8
46	L9	189/191 (99%)	166 (88%)	21 (11%)	2 (1%)	17 62
46	l9	189/191 (99%)	166 (88%)	17 (9%)	6 (3%)	5 33
47	M0	207/220 (94%)	171 (83%)	28 (14%)	8 (4%)	4 28
47	m0	209/220 (95%)	172 (82%)	23 (11%)	14 (7%)	1 12
48	M1	167/173 (96%)	122 (73%)	29 (17%)	16 (10%)	1 5
48	m1	167/173 (96%)	141 (84%)	15 (9%)	11 (7%)	1 12
49	M3	191/198 (96%)	154 (81%)	26 (14%)	11 (6%)	2 17
49	m3	192/198 (97%)	150 (78%)	28 (15%)	14 (7%)	1 9
50	M4	134/137 (98%)	113 (84%)	12 (9%)	9 (7%)	1 12
50	m4	135/137 (98%)	118 (87%)	16 (12%)	1 (1%)	26 72
51	M5	201/203 (99%)	183 (91%)	14 (7%)	4 (2%)	9 48
51	m5	201/203 (99%)	181 (90%)	16 (8%)	4 (2%)	9 48
52	M6	195/198 (98%)	176 (90%)	12 (6%)	7 (4%)	4 30
52	m6	195/198 (98%)	179 (92%)	10 (5%)	6 (3%)	5 34
53	M7	181/183 (99%)	144 (80%)	27 (15%)	10 (6%)	2 18
53	m7	153/183 (84%)	132 (86%)	18 (12%)	3 (2%)	9 48
54	M8	183/185 (99%)	154 (84%)	24 (13%)	5 (3%)	6 39
54	m8	183/185 (99%)	151 (82%)	26 (14%)	6 (3%)	5 32
55	M9	186/188 (99%)	172 (92%)	13 (7%)	1 (0%)	34 78
55	m9	186/188 (99%)	167 (90%)	14 (8%)	5 (3%)	6 39
56	N0	170/172 (99%)	154 (91%)	13 (8%)	3 (2%)	11 51
56	n0	170/172 (99%)	160 (94%)	7 (4%)	3 (2%)	11 51
57	N1	157/159 (99%)	139 (88%)	11 (7%)	7 (4%)	3 24
57	n1	157/159 (99%)	140 (89%)	12 (8%)	5 (3%)	5 33
58	N2	98/120 (82%)	72 (74%)	15 (15%)	11 (11%)	0 3
58	n2	96/120 (80%)	78 (81%)	15 (16%)	3 (3%)	5 34
59	N3	134/136 (98%)	120 (90%)	12 (9%)	2 (2%)	13 55
59	n3	134/136 (98%)	124 (92%)	10 (8%)	0	100 100
60	N4	96/155 (62%)	78 (81%)	13 (14%)	5 (5%)	2 19
60	n4	133/155 (86%)	109 (82%)	15 (11%)	9 (7%)	1 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
61	N5	119/141 (84%)	106 (89%)	11 (9%)	2 (2%)	11 52
61	n5	118/141 (84%)	98 (83%)	11 (9%)	9 (8%)	1 9
62	N6	124/126 (98%)	104 (84%)	14 (11%)	6 (5%)	3 22
62	n6	124/126 (98%)	112 (90%)	8 (6%)	4 (3%)	5 33
63	N7	133/135 (98%)	111 (84%)	11 (8%)	11 (8%)	1 7
63	n7	133/135 (98%)	101 (76%)	21 (16%)	11 (8%)	1 7
64	N8	146/148 (99%)	121 (83%)	18 (12%)	7 (5%)	3 22
64	n8	146/148 (99%)	119 (82%)	22 (15%)	5 (3%)	5 31
65	N9	56/58 (97%)	47 (84%)	6 (11%)	3 (5%)	2 19
65	n9	56/58 (97%)	44 (79%)	7 (12%)	5 (9%)	1 5
66	O0	95/104 (91%)	76 (80%)	15 (16%)	4 (4%)	3 26
66	o0	98/104 (94%)	85 (87%)	13 (13%)	0	100 100
67	O1	107/112 (96%)	91 (85%)	8 (8%)	8 (8%)	1 9
67	o1	107/112 (96%)	85 (79%)	13 (12%)	9 (8%)	1 6
68	O2	125/129 (97%)	108 (86%)	17 (14%)	0	100 100
68	o2	125/129 (97%)	109 (87%)	9 (7%)	7 (6%)	2 18
69	O3	104/106 (98%)	92 (88%)	9 (9%)	3 (3%)	6 36
69	o3	104/106 (98%)	96 (92%)	4 (4%)	4 (4%)	4 28
70	O4	110/119 (92%)	94 (86%)	14 (13%)	2 (2%)	11 51
70	o4	110/119 (92%)	100 (91%)	9 (8%)	1 (1%)	21 67
71	O5	117/119 (98%)	99 (85%)	10 (8%)	8 (7%)	1 11
71	o5	117/119 (98%)	95 (81%)	17 (14%)	5 (4%)	3 25
72	O6	97/99 (98%)	78 (80%)	13 (13%)	6 (6%)	2 14
72	o6	97/99 (98%)	76 (78%)	15 (16%)	6 (6%)	2 14
73	O7	85/87 (98%)	74 (87%)	8 (9%)	3 (4%)	4 31
73	o7	85/87 (98%)	70 (82%)	11 (13%)	4 (5%)	3 22
74	O8	75/77 (97%)	65 (87%)	7 (9%)	3 (4%)	4 27
74	o8	75/77 (97%)	60 (80%)	12 (16%)	3 (4%)	4 27
75	O9	48/50 (96%)	40 (83%)	6 (12%)	2 (4%)	3 26
75	o9	48/50 (96%)	43 (90%)	5 (10%)	0	100 100
76	Q0	50/52 (96%)	39 (78%)	9 (18%)	2 (4%)	4 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
76	q0	50/52 (96%)	49 (98%)	0	1 (2%)	9 48
77	Q1	23/25 (92%)	19 (83%)	4 (17%)	0	100 100
77	q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	3 25
78	Q2	103/105 (98%)	84 (82%)	13 (13%)	6 (6%)	2 17
78	q2	103/105 (98%)	92 (89%)	9 (9%)	2 (2%)	10 50
79	Q3	89/91 (98%)	76 (85%)	10 (11%)	3 (3%)	5 31
79	q3	89/91 (98%)	81 (91%)	7 (8%)	1 (1%)	17 62
80	c0	92/105 (88%)	59 (64%)	16 (17%)	17 (18%)	0 0
81	e0	60/62 (97%)	43 (72%)	10 (17%)	7 (12%)	0 3
82	e1	74/76 (97%)	34 (46%)	21 (28%)	19 (26%)	0 0
84	p0	139/311 (45%)	116 (84%)	16 (12%)	7 (5%)	3 21
All	All	22333/24141 (92%)	18253 (82%)	2722 (12%)	1358 (6%)	2 15

5 of 1358 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	S0	164/209 (78%)	136 (83%)	28 (17%)	2 12
2	s0	165/209 (79%)	127 (77%)	38 (23%)	1 4
3	S1	191/223 (86%)	151 (79%)	40 (21%)	1 7
3	s1	192/223 (86%)	153 (80%)	39 (20%)	1 7
4	S2	176/204 (86%)	130 (74%)	46 (26%)	0 2

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

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
55	m9	153/153 (100%)	121 (79%)	32 (21%)	1 7
56	N0	156/156 (100%)	125 (80%)	31 (20%)	1 8
56	n0	156/156 (100%)	127 (81%)	29 (19%)	2 10
57	N1	136/136 (100%)	104 (76%)	32 (24%)	1 4
57	n1	136/136 (100%)	107 (79%)	29 (21%)	1 7
58	N2	87/106 (82%)	72 (83%)	15 (17%)	2 12
58	n2	85/106 (80%)	67 (79%)	18 (21%)	1 7
59	N3	104/104 (100%)	85 (82%)	19 (18%)	2 10
59	n3	104/104 (100%)	95 (91%)	9 (9%)	13 45
60	N4	57/129 (44%)	47 (82%)	10 (18%)	2 12
60	n4	100/129 (78%)	84 (84%)	16 (16%)	3 14
61	N5	104/117 (89%)	88 (85%)	16 (15%)	3 16
61	n5	104/117 (89%)	83 (80%)	21 (20%)	1 7
62	N6	109/109 (100%)	87 (80%)	22 (20%)	1 7
62	n6	109/109 (100%)	75 (69%)	34 (31%)	0 1
63	N7	115/115 (100%)	96 (84%)	19 (16%)	3 13
63	n7	115/115 (100%)	89 (77%)	26 (23%)	1 5
64	N8	118/118 (100%)	90 (76%)	28 (24%)	1 4
64	n8	118/118 (100%)	96 (81%)	22 (19%)	2 10
65	N9	46/46 (100%)	37 (80%)	9 (20%)	1 9
65	n9	46/46 (100%)	38 (83%)	8 (17%)	2 12
66	O0	81/87 (93%)	62 (76%)	19 (24%)	1 4
66	o0	84/87 (97%)	67 (80%)	17 (20%)	1 7
67	O1	92/96 (96%)	75 (82%)	17 (18%)	2 10
67	o1	94/96 (98%)	71 (76%)	23 (24%)	1 3
68	O2	109/110 (99%)	82 (75%)	27 (25%)	1 3
68	o2	109/110 (99%)	89 (82%)	20 (18%)	2 10
69	O3	90/90 (100%)	75 (83%)	15 (17%)	3 13
69	o3	90/90 (100%)	74 (82%)	16 (18%)	2 11
70	O4	95/101 (94%)	76 (80%)	19 (20%)	1 8
70	o4	95/101 (94%)	78 (82%)	17 (18%)	2 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
71	O5	104/104 (100%)	79 (76%)	25 (24%)	1 3
71	o5	103/104 (99%)	82 (80%)	21 (20%)	1 7
72	O6	81/81 (100%)	60 (74%)	21 (26%)	0 2
72	o6	80/81 (99%)	57 (71%)	23 (29%)	0 1
73	O7	70/70 (100%)	57 (81%)	13 (19%)	2 10
73	o7	70/70 (100%)	53 (76%)	17 (24%)	1 3
74	O8	68/68 (100%)	50 (74%)	18 (26%)	0 2
74	o8	67/68 (98%)	55 (82%)	12 (18%)	2 11
75	O9	45/45 (100%)	34 (76%)	11 (24%)	1 3
75	o9	45/45 (100%)	37 (82%)	8 (18%)	2 11
76	Q0	47/47 (100%)	35 (74%)	12 (26%)	1 2
76	q0	47/47 (100%)	36 (77%)	11 (23%)	1 4
77	Q1	23/23 (100%)	19 (83%)	4 (17%)	2 12
77	q1	23/23 (100%)	18 (78%)	5 (22%)	1 6
78	Q2	90/90 (100%)	68 (76%)	22 (24%)	1 3
78	q2	90/90 (100%)	65 (72%)	25 (28%)	0 1
79	Q3	71/71 (100%)	59 (83%)	12 (17%)	2 13
79	q3	71/71 (100%)	56 (79%)	15 (21%)	1 7
80	c0	73/98 (74%)	65 (89%)	8 (11%)	8 33
81	e0	53/53 (100%)	40 (76%)	13 (24%)	1 3
82	e1	66/66 (100%)	45 (68%)	21 (32%)	0 0
84	p0	105/253 (42%)	84 (80%)	21 (20%)	1 8
All	All	18727/20239 (92%)	15017 (80%)	3710 (20%)	1 8

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

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

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

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

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	488 (27%)	56 (3%)
1	6	1792/1800 (99%)	474 (26%)	57 (3%)
36	1	3145/3396 (92%)	688 (21%)	83 (2%)
36	5	3145/3396 (92%)	687 (21%)	76 (2%)
37	3	120/121 (99%)	14 (11%)	0
37	7	120/121 (99%)	24 (20%)	1 (0%)
38	4	157/158 (99%)	38 (24%)	2 (1%)
38	8	157/158 (99%)	37 (23%)	2 (1%)
All	All	10383/10950 (94%)	2450 (23%)	277 (2%)

5 of 2450 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A

5 of 277 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	3169	U
1	6	417	A
36	5	2896	A
36	1	3228	C
38	4	125	U

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, 1424 are monoatomic - leaving 1139 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	A	1	3401	-	15,24,25	0.62	0	16,35,38	1.05	2 (12%)
88	OHX	1	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3880	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3888	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3889	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3890	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3891	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3898	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	1	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3941	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	1	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3984	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	1	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4027	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	1	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4070	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	1	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4113	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	1	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4156	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	1	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4199	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	1	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4218	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4219	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4220	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4221	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4222	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4223	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4224	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4225	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4226	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2081	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	2	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2124	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	2	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2167	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	2	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	215	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	216	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	217	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	218	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	219	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	220	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	221	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	222	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	223	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	224	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	225	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	220	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	221	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	222	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	223	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	224	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	225	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	226	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	227	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	228	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	229	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	230	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	231	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	232	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	233	-	0,6,6	0.00	-	0,15,15	0.00	-
90	A	5	3401	-	15,24,25	0.63	0	16,35,38	0.82	0
88	OHX	5	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3904	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	5	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3947	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	5	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3990	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	5	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4033	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	5	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4076	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	5	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4119	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	5	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4162	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	5	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4205	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	5	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4218	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4219	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4220	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4221	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4222	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4223	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4224	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4225	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4226	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4227	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4228	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4229	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4230	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4231	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4232	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4233	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4234	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4235	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4236	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4237	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4238	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4239	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4240	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4241	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4242	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4243	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4244	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4245	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4246	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4247	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4248	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	5	4249	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4250	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4251	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4252	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4253	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4254	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4255	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4256	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4257	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4258	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2076	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	6	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2105	1	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2119	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	6	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2162	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	6	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2182	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2183	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2184	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2185	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2186	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2187	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2188	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2189	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2190	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2191	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2192	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2193	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2194	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2195	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2196	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2197	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2198	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2199	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2200	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	215	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	216	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	217	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	7	218	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	219	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	220	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	221	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	222	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	223	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	224	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	225	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	226	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	217	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	221	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	222	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	223	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	224	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	225	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	226	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	227	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	228	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	229	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	230	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	C3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	C5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	C8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	D3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	D9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	L3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	L3	405	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	L3	406	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	L4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M7	205	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	N9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	O3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	O7	103	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	O7	104	-	0,6,6	0.00	-	0,15,15	0.00	-
91	C	Q2	502	-	12,21,22	0.82	0	16,30,33	1.13	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
91	C	Q2	503	-	12,21,22	0.78	0	16,30,33	1.20	2 (12%)
88	OHX	S8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	c1	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	c8	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	d4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	d9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l3	405	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l3	406	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l4	404	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l5	305	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l5	306	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l9	600	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m0	301	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m1	203	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m5	306	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m6	203	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	n3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	n3	204	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	n9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	o3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	o7	502	-	0,6,6	0.00	-	0,15,15	0.00	-
91	C	q2	502	-	12,21,22	0.71	0	16,30,33	1.10	1 (6%)
91	C	q2	503	-	12,21,22	0.80	0	16,30,33	0.98	1 (6%)
88	OHX	q2	504	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	s1	302	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	s1	303	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	s8	304	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	sR	401	-	0,6,6	0.00	-	0,15,15	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	A	1	3401	-	-	0/3/25/26	0/3/3/3
88	OHX	1	3873	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3874	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3875	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3876	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3877	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3878	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3879	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3880	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3881	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3882	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3883	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3884	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3885	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3886	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3887	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3888	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3889	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3890	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3891	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3892	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3893	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3894	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3895	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3896	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3897	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3898	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3899	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3900	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3901	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3902	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3903	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3904	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3905	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3906	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3907	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3908	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3909	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3910	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3911	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3912	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3913	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3914	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	3915	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3916	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3917	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3918	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3919	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3920	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3921	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3922	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3923	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3924	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3925	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3926	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3927	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3928	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3929	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3930	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3931	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3932	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3933	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3934	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3935	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3936	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3937	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3938	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3939	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3940	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3941	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3942	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3943	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3944	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3945	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3946	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3947	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3948	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3949	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3950	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3951	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3952	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3953	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3954	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3955	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3956	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	3957	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3958	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3959	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3960	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3961	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3962	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3963	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3964	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3965	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3966	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3967	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3968	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3969	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3970	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3971	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3972	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3973	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3974	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3975	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3976	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3977	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3978	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3979	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3980	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3981	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3982	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3983	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3984	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3985	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3986	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3987	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3988	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3989	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3990	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3991	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3992	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3993	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3994	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3995	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3996	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3997	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3998	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	3999	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4000	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4001	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4002	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4003	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4004	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4005	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4006	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4007	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4008	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4009	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4010	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4011	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4012	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4013	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4014	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4015	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4016	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4017	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4018	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4019	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4020	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4021	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4022	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4023	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4024	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4025	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4026	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4027	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4028	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4029	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4030	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4031	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4032	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4033	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4034	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4035	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4036	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4037	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4038	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4039	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4040	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	4041	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4042	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4043	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4044	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4045	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4046	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4047	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4048	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4049	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4050	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4051	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4052	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4053	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4054	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4055	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4056	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4057	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4058	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4059	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4060	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4061	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4062	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4063	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4064	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4065	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4066	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4067	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4068	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4069	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4070	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4071	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4072	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4073	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4074	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4075	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4076	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4077	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4078	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4079	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4080	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4081	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4082	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	4083	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4084	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4085	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4086	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4087	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4088	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4089	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4090	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4091	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4092	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4093	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4094	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4095	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4096	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4097	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4098	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4099	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4100	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4101	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4102	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4103	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4104	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4105	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4106	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4107	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4108	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4109	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4110	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4111	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4112	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4113	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4114	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4115	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4116	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4117	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4118	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4119	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4120	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4121	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4122	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4123	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4124	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	4125	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4126	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4127	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4128	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4129	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4130	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4131	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4132	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4133	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4134	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4135	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4136	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4137	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4138	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4139	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4140	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4141	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4142	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4143	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4144	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4145	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4146	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4147	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4148	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4149	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4150	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4151	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4152	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4153	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4154	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4155	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4156	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4157	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4158	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4159	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4160	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4161	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4162	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4163	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4164	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4165	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4166	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	4167	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4168	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4169	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4170	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4171	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4172	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4173	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4174	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4175	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4176	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4177	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4178	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4179	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4180	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4181	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4182	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4183	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4184	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4185	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4186	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4187	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4188	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4189	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4190	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4191	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4192	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4193	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4194	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4195	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4196	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4197	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4198	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4199	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4200	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4201	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4202	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4203	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4204	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4205	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4206	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4207	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4208	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	4209	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4210	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4211	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4212	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4213	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4214	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4215	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4216	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4217	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4218	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4219	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4220	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4221	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4222	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4223	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4224	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4225	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4226	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2023	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2024	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2025	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2029	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2030	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2031	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2032	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2033	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2034	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2035	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2036	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2037	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2038	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2039	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2040	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2041	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2042	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2043	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2044	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2045	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2046	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	2	2047	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2048	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2049	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2050	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2051	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2052	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2053	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2054	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2055	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2056	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2057	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2058	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2059	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2060	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2061	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2062	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2063	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2064	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2065	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2066	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2067	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2068	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2069	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2070	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2071	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2072	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2073	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2074	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2075	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2076	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2077	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2078	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2079	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2080	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2081	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2082	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2083	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2084	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2085	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2086	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2087	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2088	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	2	2089	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2090	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2091	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2092	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2093	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2094	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2095	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2096	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2097	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2098	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2099	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2100	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2101	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2102	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2103	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2104	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2105	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2106	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2107	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2108	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2109	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2110	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2111	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2112	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2113	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2114	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2115	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2116	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2117	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2118	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2119	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2120	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2121	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2122	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2123	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2124	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2125	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2126	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2127	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2128	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2129	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2130	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	2	2131	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2132	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2133	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2134	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2135	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2136	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2137	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2138	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2139	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2140	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2141	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2142	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2143	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2144	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2145	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2146	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2147	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2148	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2149	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2150	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2151	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2152	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2153	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2154	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2155	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2156	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2157	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2158	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2159	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2160	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2161	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2162	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2163	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2164	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2165	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2166	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2167	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2168	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2169	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2170	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2171	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2172	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	2	2173	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2174	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2175	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2176	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2177	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2178	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2179	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2180	-	-	0/0/0/0	0/0/0/0
88	OHX	3	215	-	-	0/0/0/0	0/0/0/0
88	OHX	3	216	-	-	0/0/0/0	0/0/0/0
88	OHX	3	217	-	-	0/0/0/0	0/0/0/0
88	OHX	3	218	-	-	0/0/0/0	0/0/0/0
88	OHX	3	219	-	-	0/0/0/0	0/0/0/0
88	OHX	3	220	-	-	0/0/0/0	0/0/0/0
88	OHX	3	221	-	-	0/0/0/0	0/0/0/0
88	OHX	3	222	-	-	0/0/0/0	0/0/0/0
88	OHX	3	223	-	-	0/0/0/0	0/0/0/0
88	OHX	3	224	-	-	0/0/0/0	0/0/0/0
88	OHX	3	225	-	-	0/0/0/0	0/0/0/0
88	OHX	4	220	-	-	0/0/0/0	0/0/0/0
88	OHX	4	221	-	-	0/0/0/0	0/0/0/0
88	OHX	4	222	-	-	0/0/0/0	0/0/0/0
88	OHX	4	223	-	-	0/0/0/0	0/0/0/0
88	OHX	4	224	-	-	0/0/0/0	0/0/0/0
88	OHX	4	225	-	-	0/0/0/0	0/0/0/0
88	OHX	4	226	-	-	0/0/0/0	0/0/0/0
88	OHX	4	227	-	-	0/0/0/0	0/0/0/0
88	OHX	4	228	-	-	0/0/0/0	0/0/0/0
88	OHX	4	229	-	-	0/0/0/0	0/0/0/0
88	OHX	4	230	-	-	0/0/0/0	0/0/0/0
88	OHX	4	231	-	-	0/0/0/0	0/0/0/0
88	OHX	4	232	-	-	0/0/0/0	0/0/0/0
88	OHX	4	233	-	-	0/0/0/0	0/0/0/0
90	A	5	3401	-	-	0/3/25/26	0/3/3/3
88	OHX	5	3901	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3902	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3903	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3904	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3905	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3906	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3907	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3908	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	3909	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3910	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3911	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3912	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3913	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3914	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3915	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3916	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3917	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3918	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3919	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3920	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3921	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3922	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3923	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3924	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3925	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3926	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3927	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3928	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3929	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3930	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3931	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3932	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3933	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3934	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3935	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3936	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3937	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3938	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3939	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3940	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3941	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3942	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3943	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3944	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3945	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3946	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3947	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3948	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3949	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3950	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	3951	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3952	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3953	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3954	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3955	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3956	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3957	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3958	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3959	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3960	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3961	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3962	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3963	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3964	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3965	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3966	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3967	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3968	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3969	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3970	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3971	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3972	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3973	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3974	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3975	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3976	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3977	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3978	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3979	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3980	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3981	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3982	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3983	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3984	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3985	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3986	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3987	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3988	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3989	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3990	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3991	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3992	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	3993	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3994	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3995	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3996	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3997	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3998	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3999	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4000	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4001	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4002	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4003	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4004	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4005	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4006	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4007	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4008	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4009	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4010	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4011	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4012	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4013	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4014	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4015	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4016	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4017	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4018	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4019	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4020	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4021	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4022	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4023	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4024	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4025	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4026	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4027	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4028	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4029	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4030	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4031	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4032	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4033	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4034	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4035	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4036	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4037	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4038	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4039	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4040	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4041	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4042	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4043	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4044	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4045	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4046	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4047	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4048	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4049	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4050	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4051	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4052	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4053	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4054	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4055	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4056	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4057	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4058	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4059	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4060	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4061	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4062	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4063	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4064	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4065	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4066	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4067	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4068	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4069	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4070	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4071	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4072	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4073	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4074	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4075	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4076	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4077	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4078	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4079	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4080	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4081	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4082	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4083	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4084	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4085	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4086	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4087	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4088	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4089	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4090	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4091	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4092	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4093	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4094	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4095	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4096	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4097	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4098	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4099	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4100	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4101	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4102	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4103	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4104	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4105	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4106	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4107	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4108	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4109	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4110	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4111	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4112	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4113	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4114	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4115	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4116	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4117	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4118	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4119	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4120	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4121	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4122	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4123	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4124	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4125	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4126	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4127	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4128	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4129	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4130	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4131	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4132	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4133	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4134	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4135	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4136	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4137	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4138	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4139	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4140	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4141	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4142	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4143	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4144	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4145	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4146	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4147	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4148	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4149	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4150	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4151	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4152	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4153	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4154	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4155	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4156	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4157	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4158	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4159	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4160	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4161	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4162	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4163	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4164	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4165	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4166	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4167	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4168	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4169	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4170	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4171	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4172	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4173	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4174	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4175	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4176	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4177	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4178	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4179	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4180	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4181	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4182	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4183	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4184	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4185	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4186	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4187	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4188	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4189	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4190	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4191	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4192	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4193	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4194	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4195	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4196	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4197	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4198	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4199	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4200	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4201	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4202	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4203	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4204	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4205	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4206	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4207	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4208	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4209	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4210	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4211	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4212	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4213	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4214	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4215	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4216	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4217	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4218	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4219	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4220	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4221	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4222	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4223	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4224	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4225	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4226	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4227	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4228	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4229	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4230	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4231	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4232	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4233	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4234	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4235	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4236	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4237	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4238	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4239	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4240	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4241	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4242	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4243	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4244	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4245	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4246	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4247	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4248	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4249	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4250	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4251	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4252	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4253	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4254	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4255	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4256	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4257	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4258	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2044	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2045	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2046	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2047	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2049	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2050	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2051	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2052	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2053	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2054	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2055	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2056	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2057	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2058	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2059	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2060	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2061	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2062	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2063	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2064	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2065	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2066	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2067	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2068	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2069	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2070	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2071	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	6	2072	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2073	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2074	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2075	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2076	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2077	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2078	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2079	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2080	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2081	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2082	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2083	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2084	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2085	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2086	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2087	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2088	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2089	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2090	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2091	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2092	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2093	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2094	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2095	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2096	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2097	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2098	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2099	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2100	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2101	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2102	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2103	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2104	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2105	1	-	0/0/0/0	0/0/0/0
88	OHX	6	2106	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2107	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2108	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2109	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2110	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2111	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2112	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2113	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	6	2114	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2115	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2116	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2117	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2118	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2119	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2120	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2121	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2122	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2123	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2124	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2125	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2126	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2127	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2128	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2129	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2130	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2131	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2132	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2133	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2134	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2135	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2136	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2137	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2138	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2139	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2140	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2141	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2142	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2143	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2144	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2145	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2146	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2147	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2148	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2149	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2150	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2151	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2152	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2153	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2154	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2155	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	6	2156	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2157	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2158	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2159	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2160	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2161	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2162	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2163	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2164	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2165	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2166	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2167	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2168	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2169	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2170	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2171	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2172	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2173	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2174	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2175	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2176	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2177	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2178	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2179	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2180	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2181	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2182	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2183	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2184	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2185	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2186	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2187	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2188	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2189	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2190	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2191	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2192	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2193	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2194	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2195	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2196	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2197	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	6	2198	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2199	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2200	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2201	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2202	-	-	0/0/0/0	0/0/0/0
88	OHX	7	215	-	-	0/0/0/0	0/0/0/0
88	OHX	7	216	-	-	0/0/0/0	0/0/0/0
88	OHX	7	217	-	-	0/0/0/0	0/0/0/0
88	OHX	7	218	-	-	0/0/0/0	0/0/0/0
88	OHX	7	219	-	-	0/0/0/0	0/0/0/0
88	OHX	7	220	-	-	0/0/0/0	0/0/0/0
88	OHX	7	221	-	-	0/0/0/0	0/0/0/0
88	OHX	7	222	-	-	0/0/0/0	0/0/0/0
88	OHX	7	223	-	-	0/0/0/0	0/0/0/0
88	OHX	7	224	-	-	0/0/0/0	0/0/0/0
88	OHX	7	225	-	-	0/0/0/0	0/0/0/0
88	OHX	7	226	-	-	0/0/0/0	0/0/0/0
88	OHX	8	217	-	-	0/0/0/0	0/0/0/0
88	OHX	8	218	-	-	0/0/0/0	0/0/0/0
88	OHX	8	219	-	-	0/0/0/0	0/0/0/0
88	OHX	8	220	-	-	0/0/0/0	0/0/0/0
88	OHX	8	221	-	-	0/0/0/0	0/0/0/0
88	OHX	8	222	-	-	0/0/0/0	0/0/0/0
88	OHX	8	223	-	-	0/0/0/0	0/0/0/0
88	OHX	8	224	-	-	0/0/0/0	0/0/0/0
88	OHX	8	225	-	-	0/0/0/0	0/0/0/0
88	OHX	8	226	-	-	0/0/0/0	0/0/0/0
88	OHX	8	227	-	-	0/0/0/0	0/0/0/0
88	OHX	8	228	-	-	0/0/0/0	0/0/0/0
88	OHX	8	229	-	-	0/0/0/0	0/0/0/0
88	OHX	8	230	-	-	0/0/0/0	0/0/0/0
88	OHX	C3	201	-	-	0/0/0/0	0/0/0/0
88	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
88	OHX	C8	201	-	-	0/0/0/0	0/0/0/0
88	OHX	D3	202	-	-	0/0/0/0	0/0/0/0
88	OHX	D9	102	-	-	0/0/0/0	0/0/0/0
88	OHX	L3	404	-	-	0/0/0/0	0/0/0/0
88	OHX	L3	405	-	-	0/0/0/0	0/0/0/0
88	OHX	L3	406	-	-	0/0/0/0	0/0/0/0
88	OHX	L4	402	-	-	0/0/0/0	0/0/0/0
88	OHX	M0	303	-	-	0/0/0/0	0/0/0/0
88	OHX	M5	303	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	M7	205	-	-	0/0/0/0	0/0/0/0
88	OHX	M7	206	-	-	0/0/0/0	0/0/0/0
88	OHX	M8	201	-	-	0/0/0/0	0/0/0/0
88	OHX	M9	202	-	-	0/0/0/0	0/0/0/0
88	OHX	N9	101	-	-	0/0/0/0	0/0/0/0
88	OHX	O3	201	-	-	0/0/0/0	0/0/0/0
88	OHX	O7	103	-	-	0/0/0/0	0/0/0/0
88	OHX	O7	104	-	-	0/0/0/0	0/0/0/0
91	C	Q2	502	-	-	0/3/25/26	0/2/2/2
91	C	Q2	503	-	-	0/3/25/26	0/2/2/2
88	OHX	S8	302	-	-	0/0/0/0	0/0/0/0
88	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
88	OHX	c1	202	-	-	0/0/0/0	0/0/0/0
88	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
88	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
88	OHX	c8	202	-	-	0/0/0/0	0/0/0/0
88	OHX	d4	202	-	-	0/0/0/0	0/0/0/0
88	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
88	OHX	l3	404	-	-	0/0/0/0	0/0/0/0
88	OHX	l3	405	-	-	0/0/0/0	0/0/0/0
88	OHX	l3	406	-	-	0/0/0/0	0/0/0/0
88	OHX	l4	403	-	-	0/0/0/0	0/0/0/0
88	OHX	l4	404	-	-	0/0/0/0	0/0/0/0
88	OHX	l5	303	-	-	0/0/0/0	0/0/0/0
88	OHX	l5	304	-	-	0/0/0/0	0/0/0/0
88	OHX	l5	305	-	-	0/0/0/0	0/0/0/0
88	OHX	l5	306	-	-	0/0/0/0	0/0/0/0
88	OHX	l9	600	-	-	0/0/0/0	0/0/0/0
88	OHX	m0	301	-	-	0/0/0/0	0/0/0/0
88	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
88	OHX	m1	203	-	-	0/0/0/0	0/0/0/0
88	OHX	m4	201	-	-	0/0/0/0	0/0/0/0
88	OHX	m5	306	-	-	0/0/0/0	0/0/0/0
88	OHX	m6	203	-	-	0/0/0/0	0/0/0/0
88	OHX	n3	203	-	-	0/0/0/0	0/0/0/0
88	OHX	n3	204	-	-	0/0/0/0	0/0/0/0
88	OHX	n9	101	-	-	0/0/0/0	0/0/0/0
88	OHX	o3	202	-	-	0/0/0/0	0/0/0/0
88	OHX	o7	502	-	-	0/0/0/0	0/0/0/0
91	C	q2	502	-	-	0/3/25/26	0/2/2/2
91	C	q2	503	-	-	0/3/25/26	0/2/2/2
88	OHX	q2	504	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	s1	302	-	-	0/0/0/0	0/0/0/0
88	OHX	s1	303	-	-	0/0/0/0	0/0/0/0
88	OHX	s8	304	-	-	0/0/0/0	0/0/0/0
88	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
91	q2	503	C	C5-C4-N4	-2.76	117.08	121.31
91	Q2	503	C	C6-N1-C2	-2.67	116.95	121.28
90	1	3401	A	C4-C5-N7	2.33	111.63	109.48
90	1	3401	A	C1'-N9-C4	2.35	130.49	126.94
91	Q2	503	C	C2-N3-C4	2.57	119.24	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

367 monomers are involved in 490 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	1	3873	OHX	1	0
88	1	3877	OHX	1	0
88	1	3878	OHX	1	0
88	1	3880	OHX	1	0
88	1	3881	OHX	2	0
88	1	3883	OHX	1	0
88	1	3887	OHX	2	0
88	1	3888	OHX	1	0
88	1	3890	OHX	2	0
88	1	3891	OHX	2	0
88	1	3892	OHX	2	0
88	1	3893	OHX	1	0
88	1	3894	OHX	1	0
88	1	3895	OHX	1	0
88	1	3898	OHX	1	0
88	1	3900	OHX	1	0
88	1	3901	OHX	1	0
88	1	3909	OHX	1	0
88	1	3910	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	1	3915	OHX	1	0
88	1	3916	OHX	1	0
88	1	3921	OHX	1	0
88	1	3924	OHX	1	0
88	1	3934	OHX	1	0
88	1	3936	OHX	1	0
88	1	3940	OHX	2	0
88	1	3942	OHX	3	0
88	1	3943	OHX	1	0
88	1	3950	OHX	1	0
88	1	3951	OHX	1	0
88	1	3956	OHX	1	0
88	1	3957	OHX	1	0
88	1	3967	OHX	1	0
88	1	3968	OHX	3	0
88	1	3969	OHX	1	0
88	1	3970	OHX	1	0
88	1	3972	OHX	1	0
88	1	3976	OHX	1	0
88	1	3979	OHX	1	0
88	1	3982	OHX	6	0
88	1	3983	OHX	1	0
88	1	3985	OHX	2	0
88	1	3988	OHX	1	0
88	1	3992	OHX	1	0
88	1	3993	OHX	1	0
88	1	3995	OHX	1	0
88	1	3997	OHX	2	0
88	1	4005	OHX	1	0
88	1	4009	OHX	1	0
88	1	4013	OHX	1	0
88	1	4015	OHX	4	0
88	1	4020	OHX	1	0
88	1	4022	OHX	1	0
88	1	4025	OHX	1	0
88	1	4027	OHX	1	0
88	1	4031	OHX	2	0
88	1	4044	OHX	2	0
88	1	4046	OHX	1	0
88	1	4048	OHX	2	0
88	1	4051	OHX	2	0
88	1	4053	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	1	4056	OHX	3	0
88	1	4057	OHX	3	0
88	1	4060	OHX	2	0
88	1	4061	OHX	1	0
88	1	4069	OHX	2	0
88	1	4071	OHX	1	0
88	1	4073	OHX	1	0
88	1	4079	OHX	1	0
88	1	4087	OHX	1	0
88	1	4088	OHX	1	0
88	1	4093	OHX	1	0
88	1	4095	OHX	1	0
88	1	4097	OHX	1	0
88	1	4098	OHX	2	0
88	1	4100	OHX	1	0
88	1	4101	OHX	1	0
88	1	4108	OHX	1	0
88	1	4109	OHX	1	0
88	1	4111	OHX	1	0
88	1	4112	OHX	1	0
88	1	4122	OHX	1	0
88	1	4131	OHX	1	0
88	1	4133	OHX	1	0
88	1	4138	OHX	1	0
88	1	4141	OHX	1	0
88	1	4145	OHX	1	0
88	1	4146	OHX	1	0
88	1	4148	OHX	1	0
88	1	4152	OHX	3	0
88	1	4155	OHX	1	0
88	1	4157	OHX	2	0
88	1	4158	OHX	1	0
88	1	4160	OHX	1	0
88	1	4161	OHX	1	0
88	1	4164	OHX	1	0
88	1	4170	OHX	6	0
88	1	4174	OHX	1	0
88	1	4178	OHX	3	0
88	1	4179	OHX	1	0
88	1	4182	OHX	1	0
88	1	4183	OHX	1	0
88	1	4186	OHX	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	1	4194	OHX	1	0
88	1	4195	OHX	3	0
88	1	4210	OHX	1	0
88	1	4212	OHX	1	0
88	1	4213	OHX	1	0
88	1	4217	OHX	1	0
88	1	4220	OHX	1	0
88	1	4221	OHX	1	0
88	2	2026	OHX	1	0
88	2	2027	OHX	1	0
88	2	2031	OHX	1	0
88	2	2032	OHX	1	0
88	2	2034	OHX	1	0
88	2	2036	OHX	3	0
88	2	2038	OHX	1	0
88	2	2039	OHX	1	0
88	2	2041	OHX	1	0
88	2	2042	OHX	1	0
88	2	2044	OHX	6	0
88	2	2045	OHX	1	0
88	2	2047	OHX	1	0
88	2	2048	OHX	1	0
88	2	2051	OHX	1	0
88	2	2053	OHX	1	0
88	2	2057	OHX	1	0
88	2	2064	OHX	1	0
88	2	2066	OHX	1	0
88	2	2067	OHX	1	0
88	2	2073	OHX	1	0
88	2	2074	OHX	2	0
88	2	2076	OHX	1	0
88	2	2078	OHX	1	0
88	2	2082	OHX	1	0
88	2	2084	OHX	2	0
88	2	2086	OHX	1	0
88	2	2089	OHX	1	0
88	2	2092	OHX	1	0
88	2	2095	OHX	1	0
88	2	2097	OHX	2	0
88	2	2099	OHX	7	0
88	2	2102	OHX	1	0
88	2	2104	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	2	2105	OHX	1	0
88	2	2106	OHX	1	0
88	2	2110	OHX	1	0
88	2	2111	OHX	2	0
88	2	2115	OHX	1	0
88	2	2121	OHX	2	0
88	2	2123	OHX	1	0
88	2	2129	OHX	1	0
88	2	2130	OHX	1	0
88	2	2131	OHX	2	0
88	2	2132	OHX	1	0
88	2	2141	OHX	1	0
88	2	2144	OHX	1	0
88	2	2145	OHX	2	0
88	2	2148	OHX	1	0
88	2	2149	OHX	1	0
88	2	2154	OHX	2	0
88	2	2155	OHX	1	0
88	2	2156	OHX	1	0
88	2	2157	OHX	2	0
88	2	2159	OHX	1	0
88	2	2165	OHX	1	0
88	2	2166	OHX	1	0
88	3	220	OHX	1	0
88	4	222	OHX	1	0
88	4	223	OHX	1	0
88	4	225	OHX	1	0
88	4	229	OHX	2	0
88	4	231	OHX	1	0
88	5	3901	OHX	1	0
88	5	3903	OHX	1	0
88	5	3906	OHX	1	0
88	5	3907	OHX	2	0
88	5	3909	OHX	2	0
88	5	3915	OHX	2	0
88	5	3918	OHX	1	0
88	5	3919	OHX	2	0
88	5	3922	OHX	1	0
88	5	3924	OHX	1	0
88	5	3925	OHX	2	0
88	5	3927	OHX	3	0
88	5	3941	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	5	3942	OHX	1	0
88	5	3944	OHX	1	0
88	5	3945	OHX	2	0
88	5	3948	OHX	1	0
88	5	3956	OHX	1	0
88	5	3957	OHX	1	0
88	5	3959	OHX	1	0
88	5	3960	OHX	2	0
88	5	3961	OHX	1	0
88	5	3962	OHX	1	0
88	5	3963	OHX	1	0
88	5	3965	OHX	3	0
88	5	3972	OHX	1	0
88	5	3975	OHX	1	0
88	5	3976	OHX	3	0
88	5	3981	OHX	6	0
88	5	3982	OHX	1	0
88	5	3985	OHX	1	0
88	5	3986	OHX	2	0
88	5	3990	OHX	1	0
88	5	3991	OHX	1	0
88	5	3992	OHX	1	0
88	5	3994	OHX	2	0
88	5	3998	OHX	1	0
88	5	3999	OHX	1	0
88	5	4004	OHX	1	0
88	5	4005	OHX	3	0
88	5	4006	OHX	1	0
88	5	4010	OHX	1	0
88	5	4014	OHX	6	0
88	5	4016	OHX	2	0
88	5	4020	OHX	1	0
88	5	4021	OHX	1	0
88	5	4023	OHX	6	0
88	5	4025	OHX	1	0
88	5	4026	OHX	1	0
88	5	4027	OHX	2	0
88	5	4034	OHX	1	0
88	5	4044	OHX	2	0
88	5	4052	OHX	1	0
88	5	4053	OHX	1	0
88	5	4054	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	5	4055	OHX	1	0
88	5	4069	OHX	3	0
88	5	4071	OHX	1	0
88	5	4075	OHX	1	0
88	5	4077	OHX	1	0
88	5	4082	OHX	1	0
88	5	4091	OHX	1	0
88	5	4094	OHX	1	0
88	5	4097	OHX	1	0
88	5	4100	OHX	1	0
88	5	4103	OHX	1	0
88	5	4106	OHX	2	0
88	5	4109	OHX	1	0
88	5	4111	OHX	1	0
88	5	4114	OHX	1	0
88	5	4115	OHX	1	0
88	5	4118	OHX	1	0
88	5	4123	OHX	1	0
88	5	4133	OHX	1	0
88	5	4134	OHX	1	0
88	5	4135	OHX	1	0
88	5	4142	OHX	2	0
88	5	4145	OHX	1	0
88	5	4147	OHX	2	0
88	5	4151	OHX	1	0
88	5	4156	OHX	1	0
88	5	4163	OHX	1	0
88	5	4164	OHX	1	0
88	5	4166	OHX	1	0
88	5	4172	OHX	1	0
88	5	4186	OHX	1	0
88	5	4187	OHX	1	0
88	5	4189	OHX	1	0
88	5	4190	OHX	1	0
88	5	4194	OHX	2	0
88	5	4196	OHX	2	0
88	5	4197	OHX	1	0
88	5	4198	OHX	1	0
88	5	4199	OHX	1	0
88	5	4200	OHX	2	0
88	5	4202	OHX	1	0
88	5	4203	OHX	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	5	4205	OHX	7	0
88	5	4209	OHX	1	0
88	5	4214	OHX	1	0
88	5	4219	OHX	1	0
88	5	4222	OHX	6	0
88	5	4231	OHX	3	0
88	5	4232	OHX	1	0
88	5	4233	OHX	1	0
88	5	4234	OHX	1	0
88	5	4239	OHX	3	0
88	5	4242	OHX	1	0
88	5	4243	OHX	1	0
88	5	4248	OHX	4	0
88	5	4249	OHX	1	0
88	5	4254	OHX	1	0
88	6	2047	OHX	2	0
88	6	2052	OHX	1	0
88	6	2055	OHX	1	0
88	6	2057	OHX	3	0
88	6	2059	OHX	1	0
88	6	2060	OHX	1	0
88	6	2063	OHX	1	0
88	6	2064	OHX	1	0
88	6	2066	OHX	1	0
88	6	2068	OHX	1	0
88	6	2071	OHX	2	0
88	6	2072	OHX	1	0
88	6	2073	OHX	1	0
88	6	2077	OHX	1	0
88	6	2081	OHX	1	0
88	6	2084	OHX	1	0
88	6	2091	OHX	1	0
88	6	2094	OHX	1	0
88	6	2096	OHX	1	0
88	6	2098	OHX	3	0
88	6	2100	OHX	1	0
88	6	2101	OHX	1	0
88	6	2105	OHX	4	0
88	6	2106	OHX	1	0
88	6	2107	OHX	1	0
88	6	2109	OHX	1	0
88	6	2110	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	6	2112	OHX	1	0
88	6	2116	OHX	2	0
88	6	2117	OHX	1	0
88	6	2118	OHX	1	0
88	6	2120	OHX	1	0
88	6	2122	OHX	1	0
88	6	2124	OHX	1	0
88	6	2126	OHX	2	0
88	6	2132	OHX	1	0
88	6	2133	OHX	1	0
88	6	2134	OHX	1	0
88	6	2140	OHX	1	0
88	6	2142	OHX	1	0
88	6	2143	OHX	4	0
88	6	2145	OHX	1	0
88	6	2146	OHX	1	0
88	6	2147	OHX	1	0
88	6	2150	OHX	2	0
88	6	2152	OHX	1	0
88	6	2155	OHX	1	0
88	6	2168	OHX	2	0
88	6	2172	OHX	1	0
88	6	2175	OHX	1	0
88	6	2177	OHX	1	0
88	6	2180	OHX	1	0
88	6	2184	OHX	1	0
88	6	2186	OHX	1	0
88	6	2187	OHX	2	0
88	6	2193	OHX	1	0
88	6	2194	OHX	1	0
88	6	2200	OHX	1	0
88	6	2202	OHX	1	0
88	7	216	OHX	1	0
88	7	218	OHX	2	0
88	7	220	OHX	1	0
88	7	225	OHX	1	0
88	8	217	OHX	1	0
88	8	218	OHX	5	0
88	8	219	OHX	1	0
88	8	221	OHX	1	0
88	8	225	OHX	6	0
88	8	226	OHX	1	0

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.