



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:55 PM GMT

PDB ID : 4U4O
Title : Crystal structure of Geneticin bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 3.60 Å(reported)

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

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

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

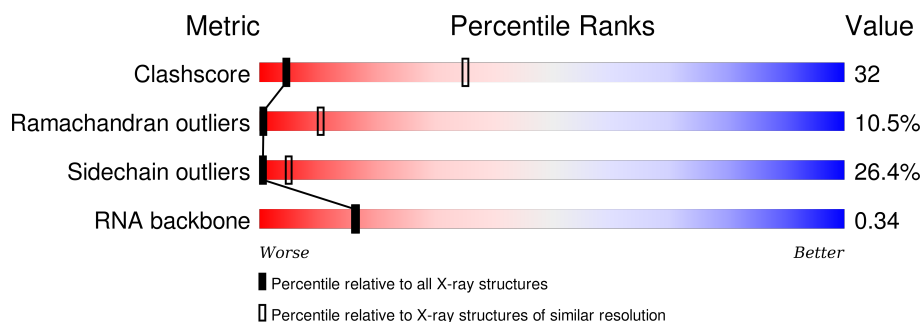
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RNA backbone	2183	1058 (4.40-2.80)

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

Note EDS failed to run properly.

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


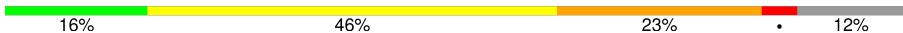



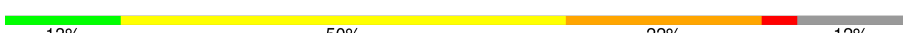





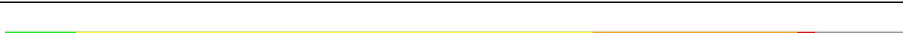








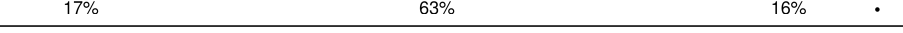




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Mol	Chain	Length	Quality of chain
4	S2	253	
4	s2	253	
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2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

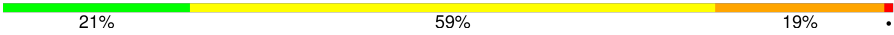



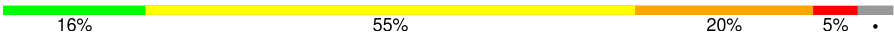

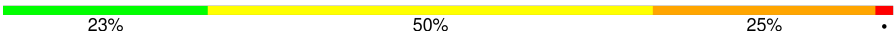
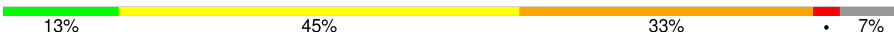
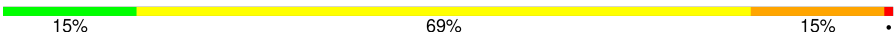















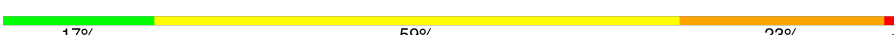
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Mol	Chain	Length	Quality of chain
16	c4	136	
17	C5	141	
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134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








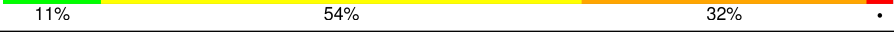


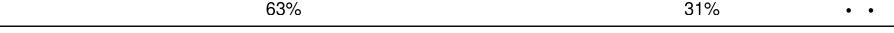
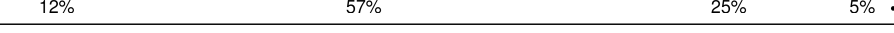
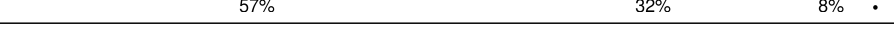


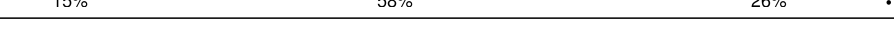

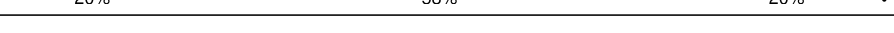







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Mol	Chain	Length	Quality of chain
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3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



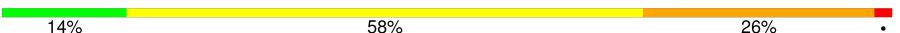



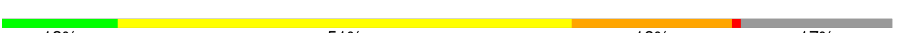










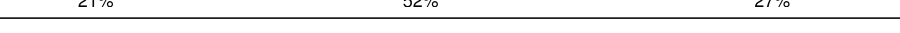







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Mol	Chain	Length	Quality of chain
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6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


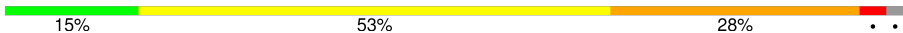

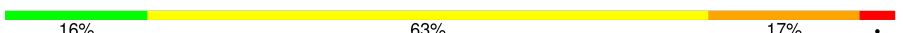

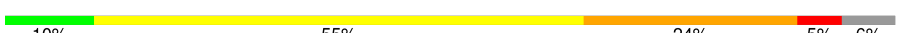





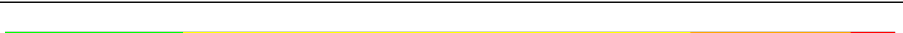













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Mol	Chain	Length	Quality of chain
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8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






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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	OHX	1	3871	-	-	X	-
87	OHX	1	3959	-	-	X	-
87	OHX	1	3965	-	-	X	-
87	OHX	1	3972	-	-	X	-
87	OHX	1	3976	-	-	X	-
87	OHX	1	3993	-	-	X	-
87	OHX	1	4003	-	-	X	-
87	OHX	1	4032	-	-	X	-
87	OHX	1	4044	-	-	X	-
87	OHX	1	4154	-	-	X	-
87	OHX	1	4155	-	-	X	-
87	OHX	1	4171	-	-	X	-
87	OHX	1	4180	-	-	X	-
87	OHX	1	4198	-	-	X	-
87	OHX	2	2031	-	-	X	-
87	OHX	2	2044	-	-	X	-
87	OHX	2	2090	-	-	X	-
87	OHX	2	2095	-	-	X	-
87	OHX	2	2099	-	-	X	-
87	OHX	2	2111	-	-	X	-
87	OHX	2	2131	-	-	X	-
87	OHX	2	2146	-	-	X	-
87	OHX	5	3937	-	-	X	-
87	OHX	5	3973	-	-	X	-
87	OHX	5	4006	-	-	X	-
87	OHX	5	4016	-	-	X	-
87	OHX	5	4028	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	OHX	5	4050	-	-	X	-
87	OHX	5	4061	-	-	X	-
87	OHX	5	4075	-	-	X	-
87	OHX	5	4086	-	-	X	-
87	OHX	5	4097	-	-	X	-
87	OHX	5	4138	-	-	X	-
87	OHX	5	4193	-	-	X	-
87	OHX	5	4194	-	-	X	-
87	OHX	5	4195	-	-	X	-
87	OHX	5	4211	-	-	X	-
87	OHX	5	4228	-	-	X	-
87	OHX	5	4237	-	-	X	-
87	OHX	6	2064	-	-	X	-
87	OHX	6	2125	-	-	X	-
87	OHX	6	2130	-	-	X	-
87	OHX	6	2135	-	-	X	-
87	OHX	6	2152	-	-	X	-
87	OHX	6	2155	-	-	X	-
87	OHX	6	2177	-	-	X	-
87	OHX	6	2189	-	-	X	-
87	OHX	8	220	-	-	X	-
87	OHX	8	229	-	-	X	-
87	OHX	C5	201	-	-	X	-
87	OHX	O1	202	-	-	X	-
89	ZN	Q2	501	-	-	X	-

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 411095 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	1791	Total	C	N	O	P	0	0	0
			38149	17055	6738	12565	1791			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C5	137	SER	ARG	conflict	UNP Q01855
c5	137	SER	ARG	conflict	UNP Q01855

- 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			

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O		0	0	0
			1104	652	221	231				
35	sM	104	Total	C	N	O		0	0	0
			679	402	140	137				

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	12	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	L3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
40	13	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	14	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	15	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	16	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	17	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				

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	N0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			
56	n0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	N2	100	Total	C	N	O	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			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O4	110	GLU	-	expression tag	UNP P87262
O4	111	ALA	-	expression tag	UNP P87262
O4	112	ALA	-	expression tag	UNP P87262

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Chain	Residue	Modelled	Actual	Comment	Reference
O4	113	LYS	-	expression tag	UNP P87262
O4	114	SER	-	expression tag	UNP P87262
O4	115	GLU	-	expression tag	UNP P87262
O4	116	LYS	-	expression tag	UNP P87262
O4	117	LYS	-	expression tag	UNP P87262
O4	118	ALA	-	expression tag	UNP P87262
O4	119	LYS	-	expression tag	UNP P87262
O4	120	LYS	-	expression tag	UNP P87262
o4	110	GLU	-	expression tag	UNP P87262
o4	111	ALA	-	expression tag	UNP P87262
o4	112	ALA	-	expression tag	UNP P87262
o4	113	LYS	-	expression tag	UNP P87262
o4	114	SER	-	expression tag	UNP P87262
o4	115	GLU	-	expression tag	UNP P87262
o4	116	LYS	-	expression tag	UNP P87262
o4	117	LYS	-	expression tag	UNP P87262
o4	118	ALA	-	expression tag	UNP P87262
o4	119	LYS	-	expression tag	UNP P87262
o4	120	LYS	-	expression tag	UNP P87262

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	O6	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			
72	o6	99	Total	C	N	O	S	0	0	0
			770	481	156	131	2			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 S30-A.

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

- Molecule 81 is a protein called Ubiquitin-40S ribosomal protein S31.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
83	p0	143	Total	C	N	O	S	0	0	0
			1076	686	192	195	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	L7	2	Total 2	Mg 2	0	0
86	N9	1	Total 1	Mg 1	0	0
86	n8	2	Total 2	Mg 2	0	0
86	o1	1	Total 1	Mg 1	0	0
86	N5	2	Total 2	Mg 2	0	0
86	6	150	Total 150	Mg 150	0	0
86	n4	1	Total 1	Mg 1	0	0
86	m5	2	Total 2	Mg 2	0	0
86	l3	6	Total 6	Mg 6	0	0
86	M1	1	Total 1	Mg 1	0	0
86	d6	1	Total 1	Mg 1	0	0
86	2	124	Total 124	Mg 124	0	0
86	O3	1	Total 1	Mg 1	0	0
86	L4	2	Total 2	Mg 2	0	0
86	l7	2	Total 2	Mg 2	0	0
86	M5	2	Total 2	Mg 2	0	0
86	o0	1	Total 1	Mg 1	0	0
86	S2	2	Total 2	Mg 2	0	0
86	L8	1	Total 1	Mg 1	0	0
86	D3	1	Total 1	Mg 1	0	0
86	o4	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	M9	1	Total 1	Mg 1	0	0
86	q0	2	Total 2	Mg 2	0	0
86	SM	1	Total 1	Mg 1	0	0
86	c8	1	Total 1	Mg 1	0	0
86	M0	3	Total 3	Mg 3	0	0
86	5	499	Total 499	Mg 499	0	0
86	L5	1	Total 1	Mg 1	0	0
86	O7	1	Total 1	Mg 1	0	0
86	l4	1	Total 1	Mg 1	0	0
86	n9	2	Total 2	Mg 2	0	0
86	1	468	Total 468	Mg 468	0	0
86	s2	1	Total 1	Mg 1	0	0
86	d3	1	Total 1	Mg 1	0	0
86	S8	1	Total 1	Mg 1	0	0
86	l2	1	Total 1	Mg 1	0	0
86	O2	1	Total 1	Mg 1	0	0
86	q3	2	Total 2	Mg 2	0	0
86	o3	2	Total 2	Mg 2	0	0
86	M3	2	Total 2	Mg 2	0	0
86	N3	2	Total 2	Mg 2	0	0
86	N8	4	Total 4	Mg 4	0	0

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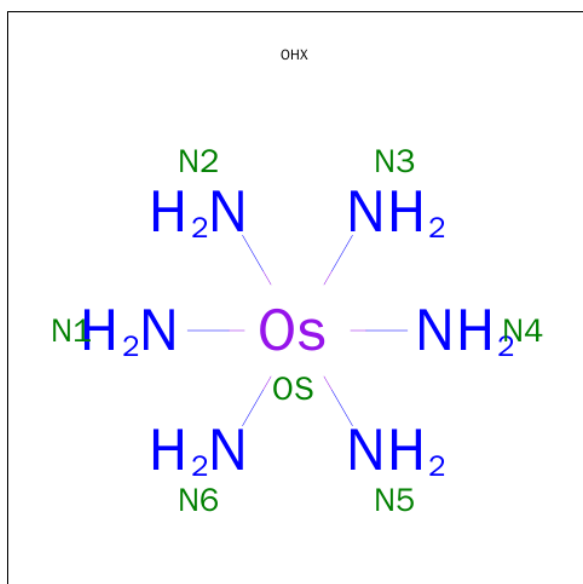
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	4	23	Total 23	Mg 23	0	0
86	D4	1	Total 1	Mg 1	0	0
86	L2	2	Total 2	Mg 2	0	0
86	m1	1	Total 1	Mg 1	0	0
86	l5	3	Total 3	Mg 3	0	0
86	m7	4	Total 4	Mg 4	0	0
86	M7	5	Total 5	Mg 5	0	0
86	m4	1	Total 1	Mg 1	0	0
86	L6	2	Total 2	Mg 2	0	0
86	s1	1	Total 1	Mg 1	0	0
86	l9	1	Total 1	Mg 1	0	0
86	O1	1	Total 1	Mg 1	0	0
86	s8	2	Total 2	Mg 2	0	0
86	o2	1	Total 1	Mg 1	0	0
86	c7	1	Total 1	Mg 1	0	0
86	7	15	Total 15	Mg 15	0	0
86	n3	1	Total 1	Mg 1	0	0
86	q1	1	Total 1	Mg 1	0	0
86	L3	2	Total 2	Mg 2	0	0
86	O5	1	Total 1	Mg 1	0	0
86	m6	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	N6	1	Total	Mg	0	0
			1	1		
86	8	17	Total	Mg	0	0
			17	17		
86	m0	1	Total	Mg	0	0
			1	1		
86	M6	1	Total	Mg	0	0
			1	1		
86	N0	1	Total	Mg	0	0
			1	1		
86	3	14	Total	Mg	0	0
			14	14		

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	3	1	Total	N	Os	0	0
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87	3	1	Total	N	Os	0	0
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87	3	1	Total	N	Os	0	0
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87	3	1	Total	N	Os	0	0
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			7	6	1		
87	3	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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			7	6	1		
87	4	1	Total	N	Os	0	0
			7	6	1		
87	4	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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87	L3	1	Total	N	Os	0	0
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87	L3	1	Total	N	Os	0	0
			7	6	1		
87	L3	1	Total	N	Os	0	0
			7	6	1		
87	L4	1	Total	N	Os	0	0
			7	6	1		
87	M0	1	Total	N	Os	0	0
			7	6	1		
87	M5	1	Total	N	Os	0	0
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87	M6	1	Total	N	Os	0	0
			7	6	1		
87	M7	1	Total	N	Os	0	0
			7	6	1		
87	M9	1	Total	N	Os	0	0
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87	M9	1	Total	N	Os	0	0
			7	6	1		
87	N9	1	Total	N	Os	0	0
			7	6	1		
87	O1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	O3	1	Total	N	Os	0	0
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87	O7	1	Total	N	Os	0	0
			7	6	1		
87	O7	1	Total	N	Os	0	0
			7	6	1		
87	Q2	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	c8	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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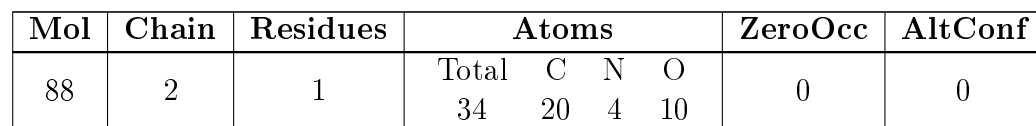
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	8	1	Total	N	Os	0	0
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87	8	1	Total	N	Os	0	0
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87	13	1	Total	N	Os	0	0
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87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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
87	m1	1	Total	N	Os	0	0
			7	6	1		
87	m4	1	Total	N	Os	0	0
			7	6	1		
87	m5	1	Total	N	Os	0	0
			7	6	1		
87	m7	1	Total	N	Os	0	0
			7	6	1		
87	m9	1	Total	N	Os	0	0
			7	6	1		
87	n3	1	Total	N	Os	0	0
			7	6	1		
87	n9	1	Total	N	Os	0	0
			7	6	1		
87	o3	1	Total	N	Os	0	0
			7	6	1		
87	o7	1	Total	N	Os	0	0
			7	6	1		
87	o9	1	Total	N	Os	0	0
			7	6	1		
87	q1	1	Total	N	Os	0	0
			7	6	1		
87	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 88 is GENETICIN (three-letter code: GET) (formula: C₂₀H₄₀N₄O₁₀).



- | 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 |



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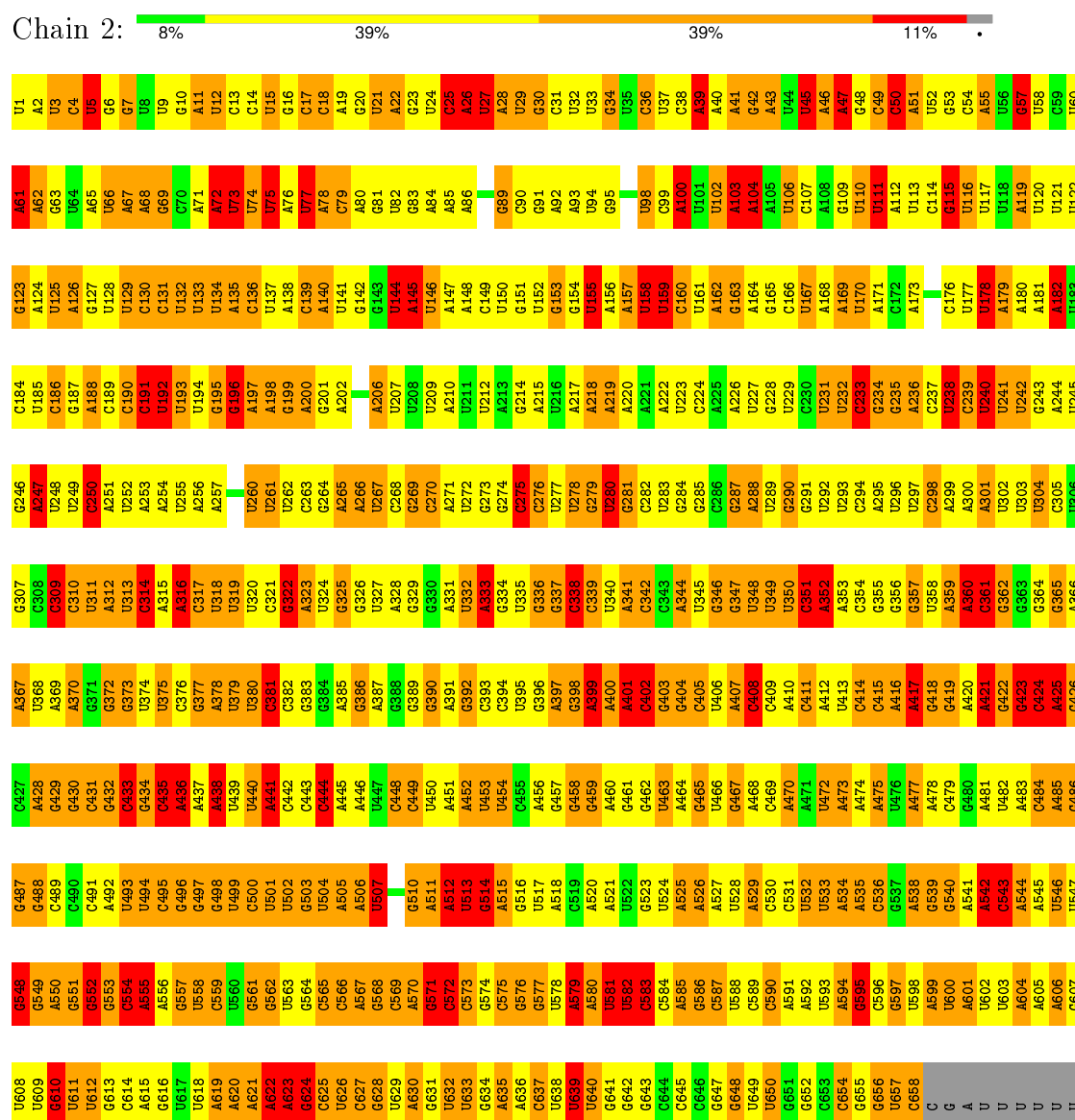
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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89	d6	1	Total 1	Zn 1	0	0
89	o7	1	Total 1	Zn 1	0	0
89	O7	1	Total 1	Zn 1	0	0
89	q2	1	Total 1	Zn 1	0	0

3 Residue-property plots

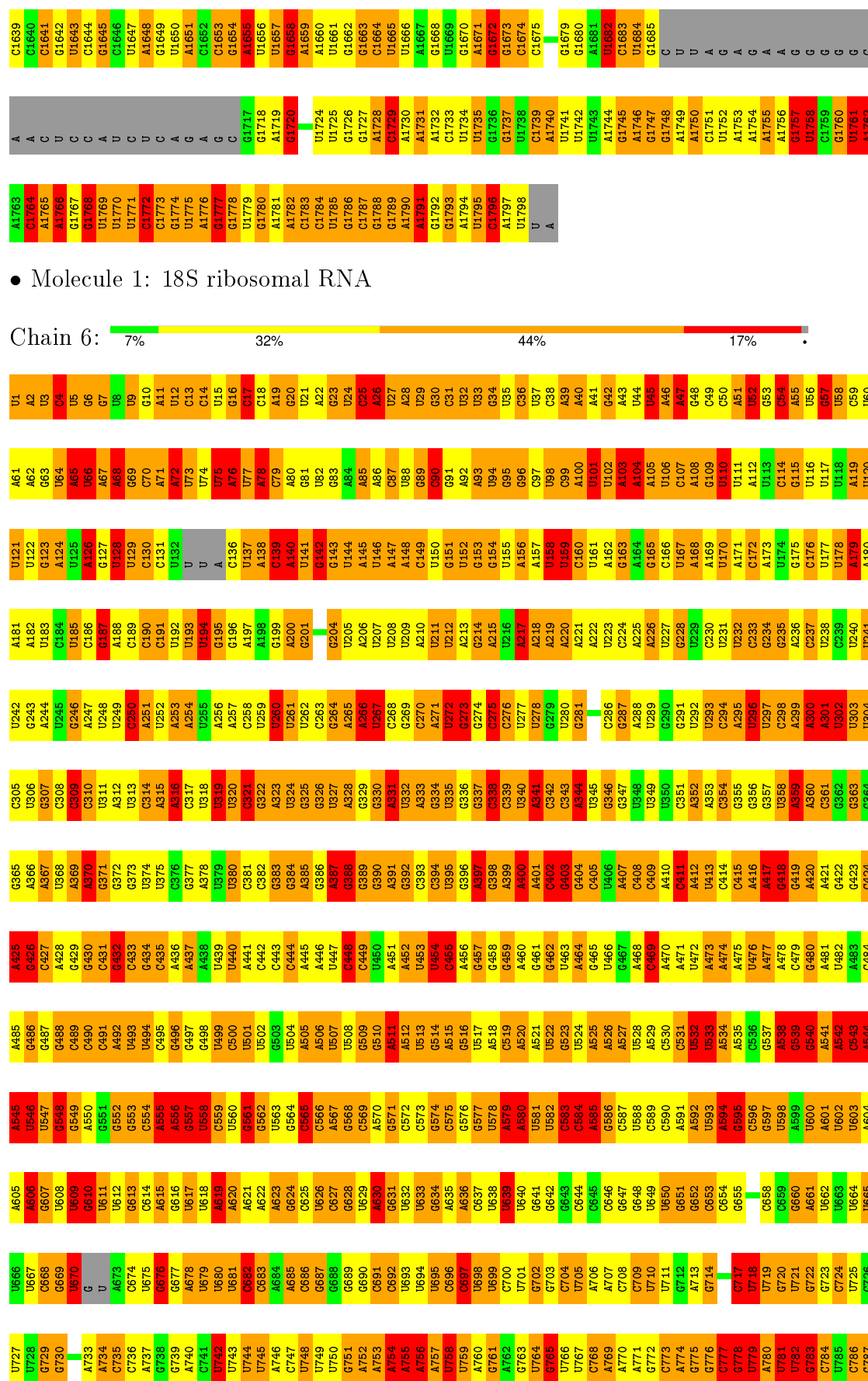
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS failed to run properly.

- Molecule 1: 18S ribosomal RNA

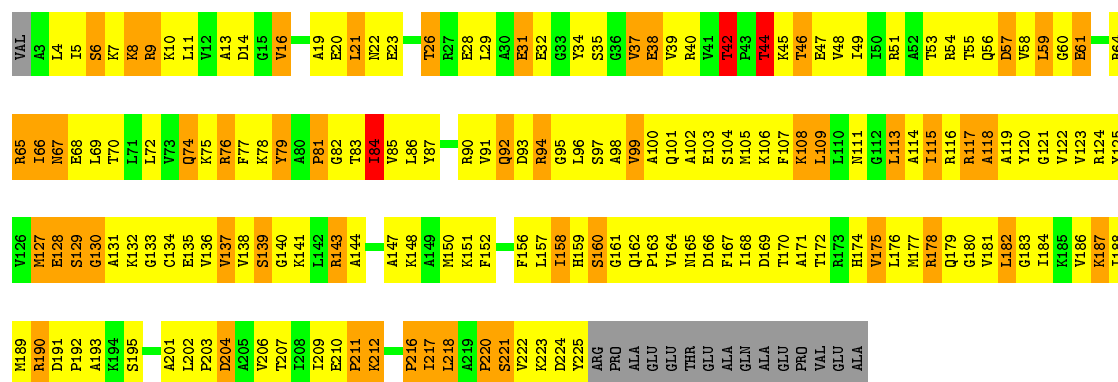


WORLDWIDE
PDB
PROTEIN DATA BANK



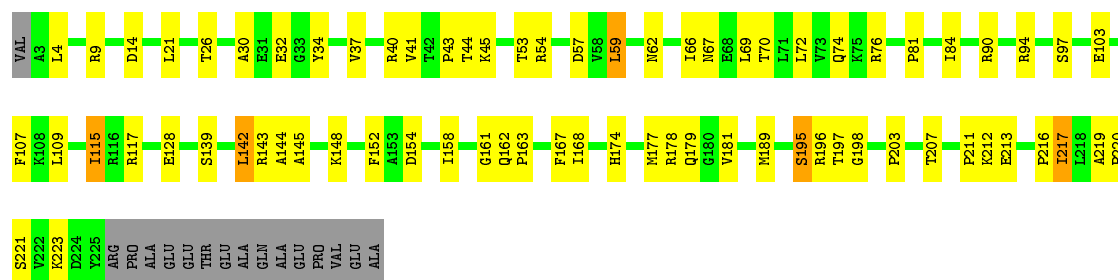
• Molecule 1: 18S ribosomal RNA

G1686	C1636	A1576	A1515	G1395	U1335	C1274	G1212	A1152	A1092	G1032	G972	U912	U851	A788
G1687	C1637	A1577	A1516	U1396	A1336	A1275	G1213	G1153	A1093	C1033	A973	G913	C852	A789
G1688	G1638	U1578	U1517	U1397	A1337	G1276	U1214	G1154	G1094	C1034	A974	G914	G853	A790
G1689	C1639	G1645	C1518	U1398	C1338	G1277		G1155	U1095	G1035	A975	A915		A791
C1700	C1640	C1580	U1519	C1399	C1339	G1278	A1217	A1156	C1096	A1036	G976	U916	A856	U792
A1701	C1641	C1581	U1520	A1400	U1340	C1279	G1218	A1157	U1097	C1037	A977	U917	A857	A793
A1702	G1642	U1582	G1521	A1401	A1341	C1280	A1219	C1158	U1098	U1038	A978	U918	G858	U794
C1703	G1643	A1583	U1522	G1402	C1342	U1281	C1220	A1159	U1099	U1039	A979	A919	A859	U795
U1704	C1644	A1584	G1523	C1403	U1343	U1282	A1221	A1160	U1100	G1040	G980	U920	U860	A796
C1705	G1645	A1585	A1524	G1404	A1344	U1283	G1222	C1161	G1101	G1041	U981	U921	U861	G797
C1706	C1646	A1586	A1525	C1405	A1345	C1284	A1223	C1162	G1102	G1042	U982	U922	A862	C798
A1707	G1647	A1587	A1526	A1406	A1346	U1285	A1226	A1163	U1103	A1043	A983	A923	A863	A799
U1708	A1648	G1588	C1527	U1407	U1347	U1286	A1227	G1164	U1104	U1044	G984	A924	U864	U800
C1709	G1649	C1589	U1528	U1408	A1348	A1287	A1227	G1165	C1105	C1045	G985	G925	A865	G801
U1710	U1650	G1590	C1529	G1409	G1349	U1288	G1228	A1166	U1106	G1046	G986	A926	G866	G802
C1711	A1651	C1591	C1530	A1410	U1350	U1289	G1229	G1167	G1107	G1047	G987	A927	G867	G803
A1712	C1652	A1592	G1531	A1411	G1351	U1290	A1230	U1168	G1108	G1048	A988	U928	G868	A803
G1713	C1653	A1593	U1532	G1412	C1352	G1297	U1231	G1169	G1109	U1049	U989	A929	A869	A804
A1714	G1654	G1594	U1533	U1413	U1353	G1292	U1232	G1170	G1110	G1050	C990	A930	C870	U805
G1715	A1655	U1595	G1534	U1414	U1354	U1293	G1233	A1171	G1111	G1051	G991	G931	G871	U806
C1716	U1656	C1596	U1535	A1415	G1355	G1294	A1234	G1172	G1112	A992	A992	U932	G872	A809
G1717	U1657	A1597	G1536	G1416	U1356	U1295	C1235	C1173	A993	A993	A993	A933	U873	G810
G1718	C1658	U1598	C1537	G1417	A1357	A1296	A1236	C1174	G1114	U1054	G994	C934	C874	A811
A1719	A1659	U1599	U1538	G1418	G1358	G1297	G1237	U1175	U1115	U1055	A995	U935	G875	A812
A1720	A1660	A1600	G1539	G1419	C1359	U1298	A1238	G1176	A1116	U1056	U996	G936	G876	U813
A1721	U1661	G1601	G1540	G1420	A1360	G1299	U1239	C1177	U1117	U1057	G997	G937	G877	A814
A1722	G1662	C1602	G1541	A1421	U1361	A1300	U1240	G1178	G1118	U1058	A998	G938	G878	G815
U1723	G1663	U1603	G1542	U1422	U1362	U1301	A1241	G1179	U1119	U1059	U999	A939	G879	G816
U1724	C1664	A1604	U1543	U1423	U1363	U1302	A1242	A1180	U1120	U1060	C1000	A940	C880	
U1725	U1665	G1605	U1544	A1424	G1364	U1303	G1243	U1181	C1121	A1061	A1001	A941	A881	
G1726	U1666	C1606	A1545	A1425	C1365	G1304	A1244	U1182	G1122	A1062	G1002	G942	U882	U820
G1727	A1667	G1607	G1546	C1426	U1366	U1305	G1245	A1183	C1123	U1063	A1003	C943	C883	
A1728	U1668	U1608	A1547	A1427	G1367	U1306	C1246	A1184	U1004	G1064	A1004	A944	A884	U821
C1729	U1669	G1609	G1548	G1428	U1368	U1307	U1247	U1185	A1125	A1065	A1005	U945	G885	U822
A1730	G1670	G1610	C1549	U1429	U1369	G1308	G1248	U1186	G1126	C1066	A1006	U946	U886	G823
A1731	A1671	A1611	U1550	U1430	U1370	C1309	U1249	U1187	G1127	G1067	C1007	U947	A887	U824
A1732	G1672	U1612	U1551	G1431	A1371	U1310	U1250	G1188	C1128	G1068	G1008	G948	U888	U825
C1733	G1673	U1613	U1552	U1432	U1372	U1311	U1251	A1189	U1129	U1069	U1009	C949	U889	U826
U1734	U1674	A1614	U1553	A1433	C1373	A1312	C1252	C1190	G1130	C1070	C1010	C950	C890	U827
U1735	C1675	C1615	U1554	U1434	C1374	A1313	U1253	U1191	A1131	U1071	G1011	A951	A891	U828
G1736	U1676	G1616	A1555	G1435	A1375	U1314	U1254	C1192	A1132	C1072	G1012	A952	A892	U829
G1737	C1677	U1617	A1556	A1436	C1376	U1315	G1255	A1193	A1133	G1073	A1013	G953	U893	U830
U1738	C1678	C1618	U1557	U1437	U1377	G1316	A1256	A1194	C1134	G1074	G1014	G954	U894	U831
C1739	G1679	U1619	U1558	G1438	U1378	C1317	U1257	C1195	U1145	C1075	U1015	A955	G895	U832
A1740	G1680	C1620	A1559	G1439	C1379	G1318	U1258	A1196	U1136	A1076	G1016	C956	U896	U833
U1741	U1681	G1621	U1560	C1440	U1380	A1319	U1259	C1197	A1137	C1077	U1017	G957	C897	G834
U1742	U1682	G1622		C1441	U1381	U1320	U1260	G1198	A1138	C1078	U1018	U958	A898	U835
U1743	C1683	C1623	U1563	U1442	A1382	A1321	G1261	G1199	A1139	U1079	A1019	U959	G899	U836
A1744	U1684	C1624	U1564	U1443	G1383	A1322	U1262	G1200	G1140	U1080	A1020	U960	A900	G837
G1745	G1685	C1625	C1565	A1444	A1384	C1323	G1263	G1201	G1141	A1081	C1021	U961	A901	G838
A1746	C1686	U1626	U1566	G1445	G1385	G1324	G1264	A1202	A1142	C1082	C1022	C962	G902	
G1747	U1687	U1627	U1567	A1446	G1386	A1325	G1265	A1203	A1143	G1083	A1023	A963	G903	U841
G1748	U1688	U1628	C1568	C1447	G1387	A1326	U1266	A1204	U1144	A1084	U1024	U964	G904	C842
A1749	A1689	G1629	A1569	U1508	A1388	C1327	G1267	C1205	G1085	A1025	A1025	U965	A905	U843
C1750	G1690	A1570	U1569	U1449	G1389	C1328	G1268	U1206	G1146	A1086	A1026	A966	A906	A844
C1751	A1691	A1631	U1570	U1450	U1390	G1330	U1269	U1207	A1147	A1087	A1027	A967	A907	G845
U1752	U1692	G1632	U1571	U1451	A1391	G1330	U1270	A1208	G1148	A1088	C1028	U968	U908	G846
A1753	A1693	C1633	G1572	U1452	A1392	C1332	G1271	A1209	G1149	U1089	U1029	C969	U909	G847
A	A1694	C1634	G1573	G1453	C1393	U1272	U1272	C1210	G1150	U1089	A1030	A970	C910	C848
A	A1695	U1514	G1454	G1454	G1394	U1334	G1273	A1211	A1151	A1091	U1031	A971	U911	A850



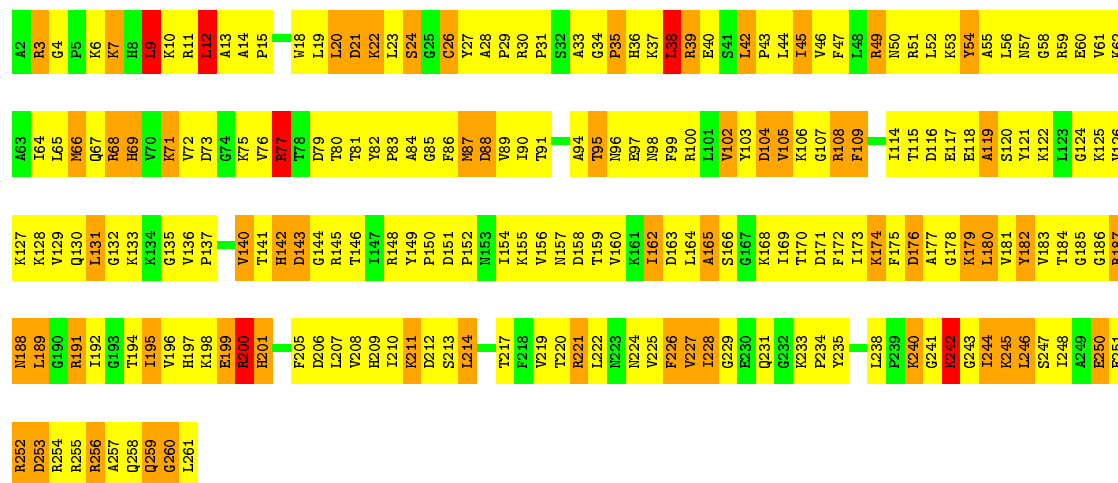
• Molecule 5: 40S ribosomal protein S3

Chain s3: 63% 28% 7%



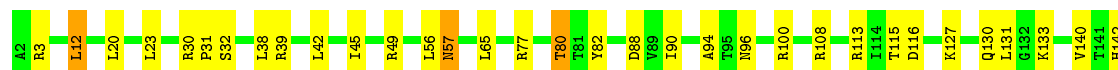
• Molecule 6: 40S ribosomal protein S4-A

Chain S4: 17% 58% 23%



• Molecule 6: 40S ribosomal protein S4-A

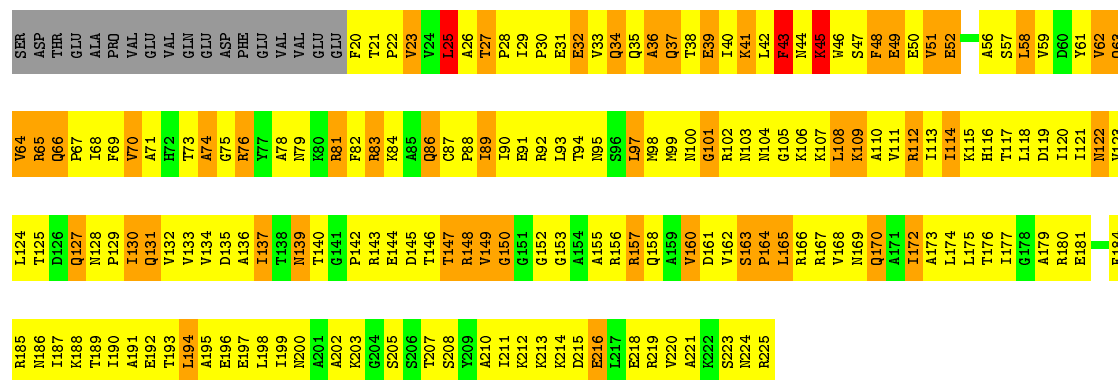
Chain s4: 70% 26%





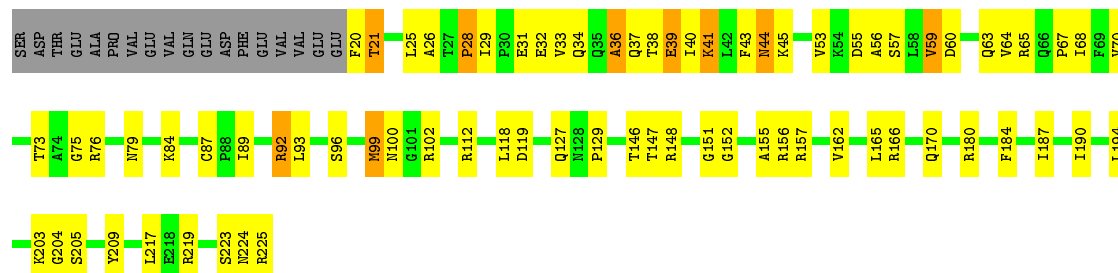
- Molecule 7: 40S ribosomal protein S5

Chain S5: 12% 57% 22% 8%



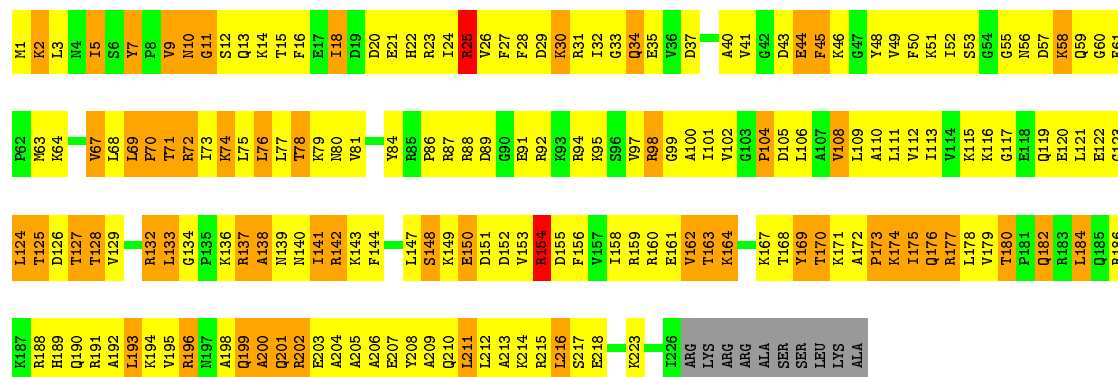
- Molecule 7: 40S ribosomal protein S5

Chain s5: 58% 29% 8%

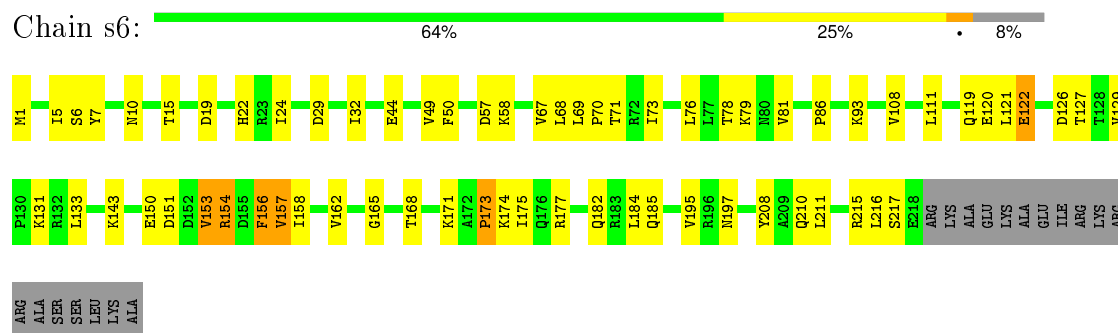


- Molecule 8: 40S ribosomal protein S6-A

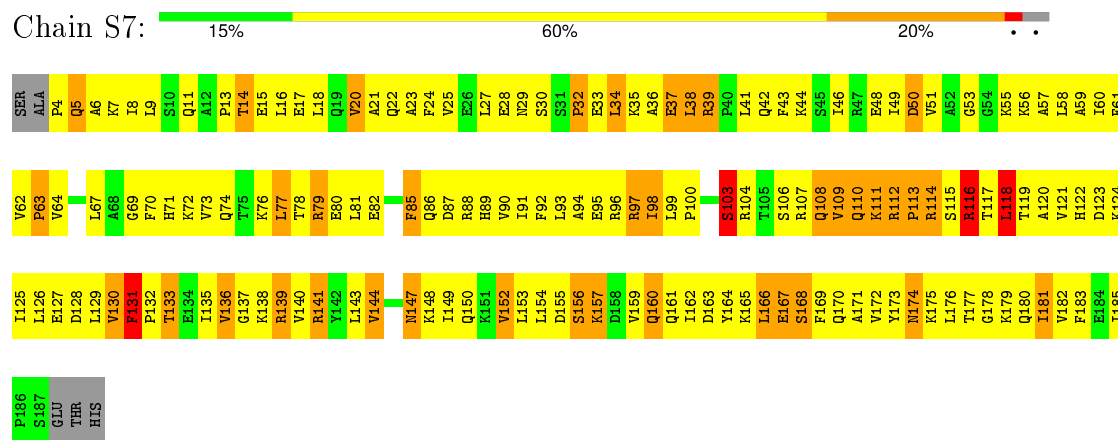
Chain S6: 19% 53% 24%



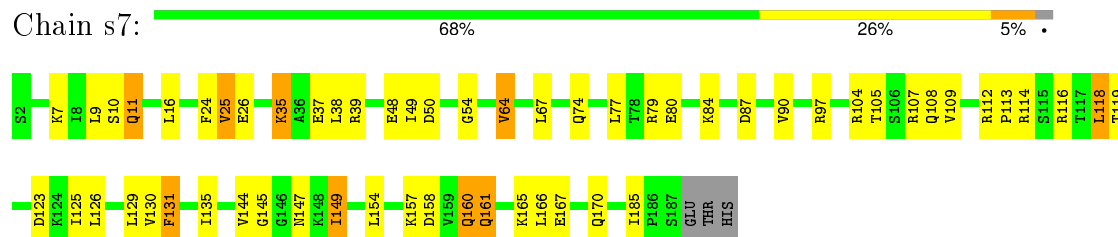
- Molecule 8: 40S ribosomal protein S6-A



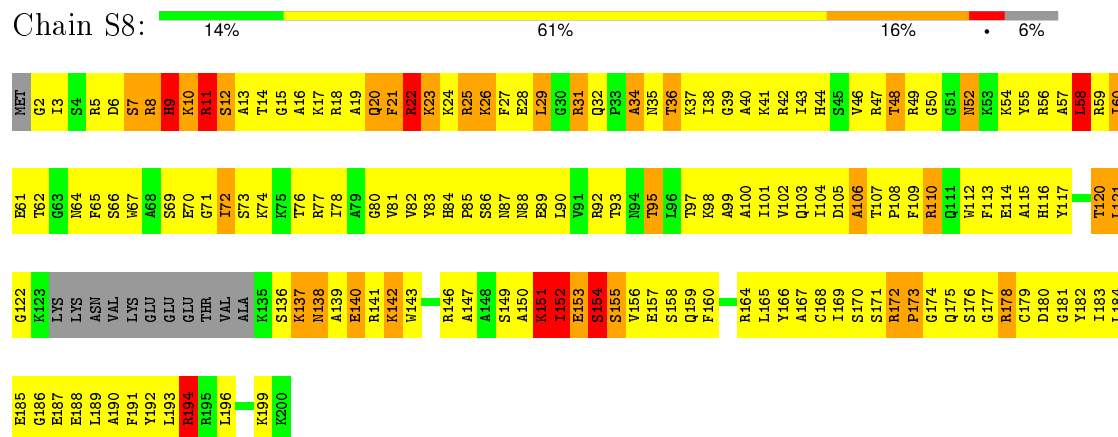
• Molecule 9: 40S ribosomal protein S7-A



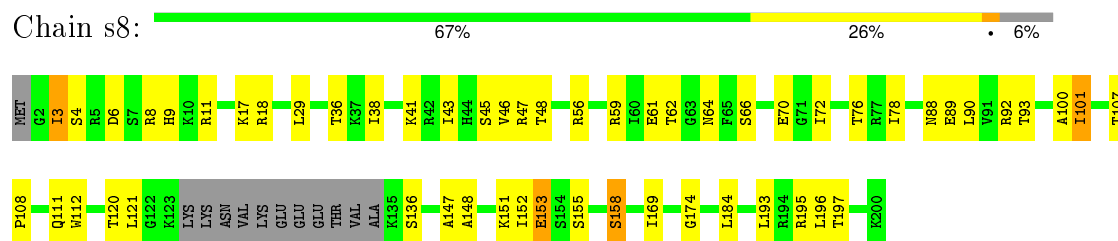
• Molecule 9: 40S ribosomal protein S7-A



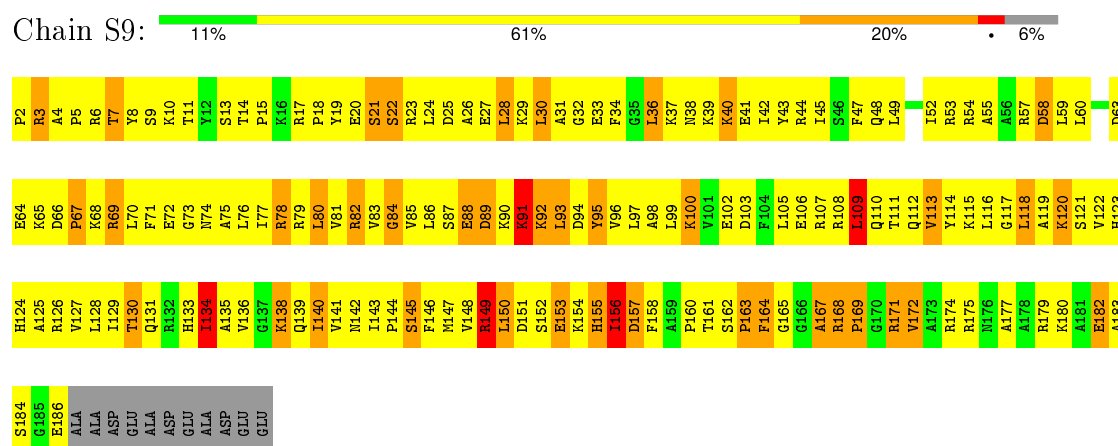
• Molecule 10: 40S ribosomal protein S8-A



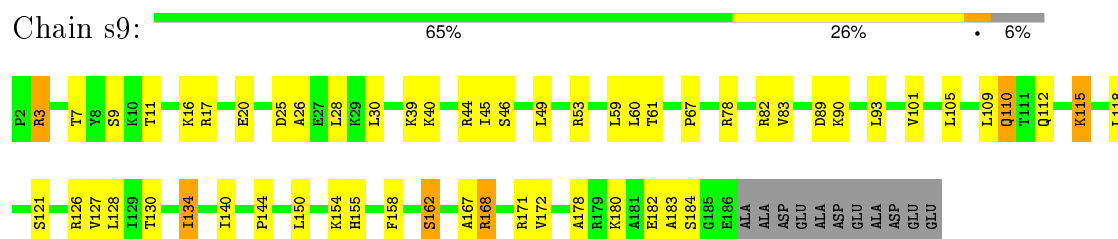
- Molecule 10: 40S ribosomal protein S8-A



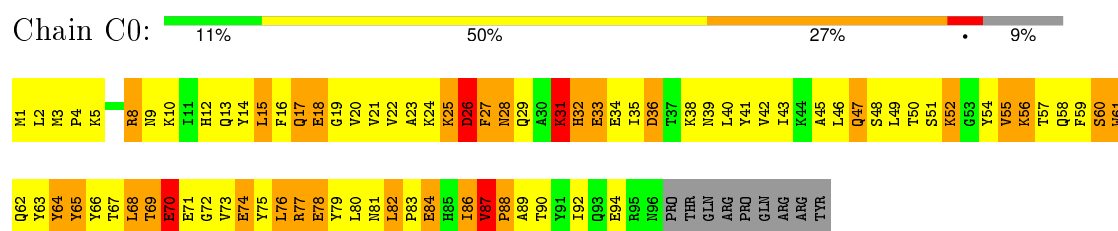
- Molecule 11: 40S ribosomal protein S9-A



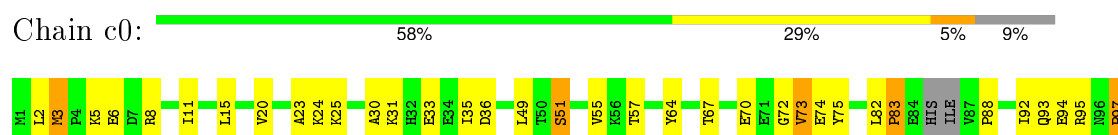
- Molecule 11: 40S ribosomal protein S9-A

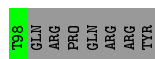


- Molecule 12: 40S ribosomal protein S10-A



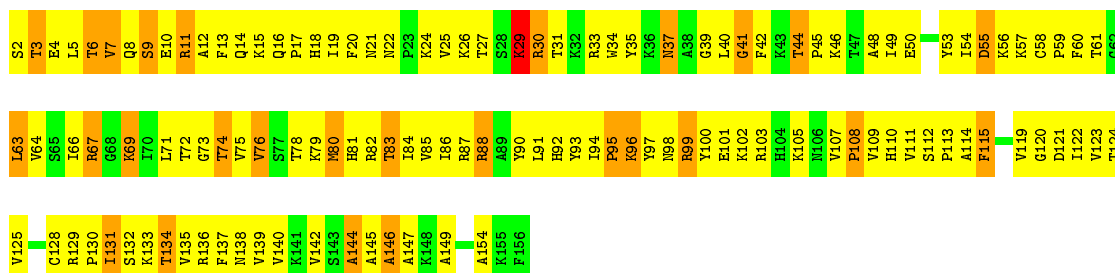
- Molecule 12: 40S ribosomal protein S10-A





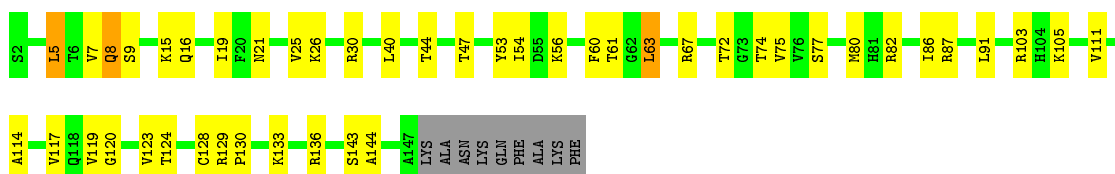
- Molecule 13: 40S ribosomal protein S11-A

Chain C1: 20% 62% 17%



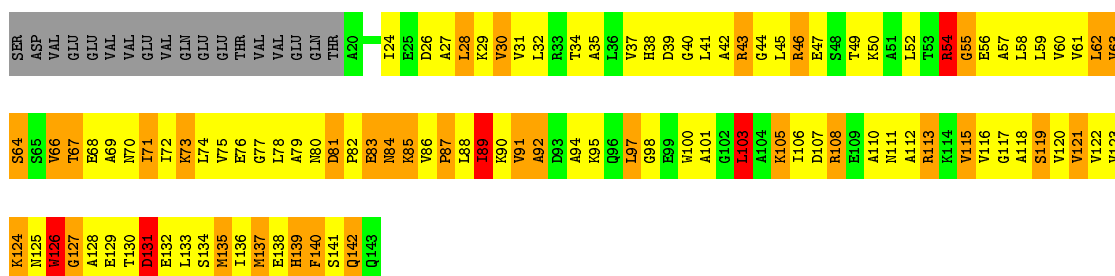
- Molecule 13: 40S ribosomal protein S11-A

Chain c1: 65% 28% 6%



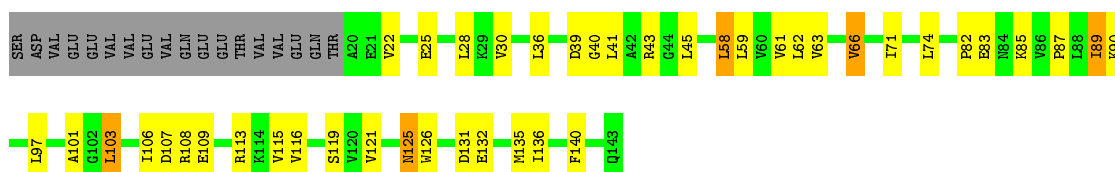
- Molecule 14: 40S ribosomal protein S12

Chain C2: 13% 47% 23% 13%



- Molecule 14: 40S ribosomal protein S12

Chain c2: 57% 27% 13%



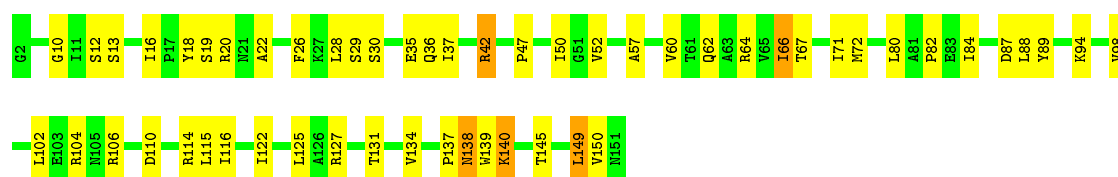
- Molecule 15: 40S ribosomal protein S13

Chain C3: 17% 63% 19%



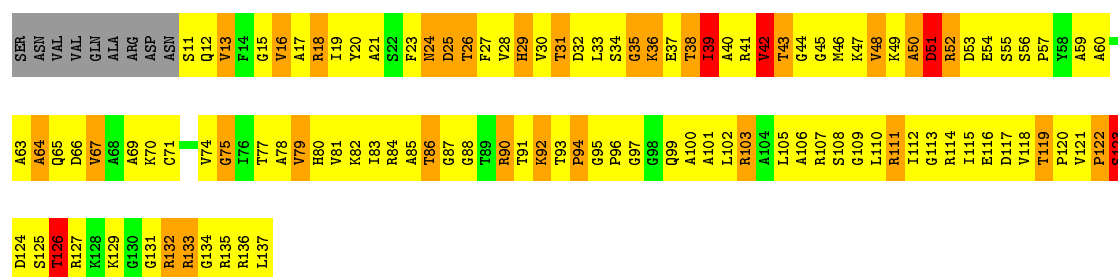
• Molecule 15: 40S ribosomal protein S13

Chain c3: 64% 33%



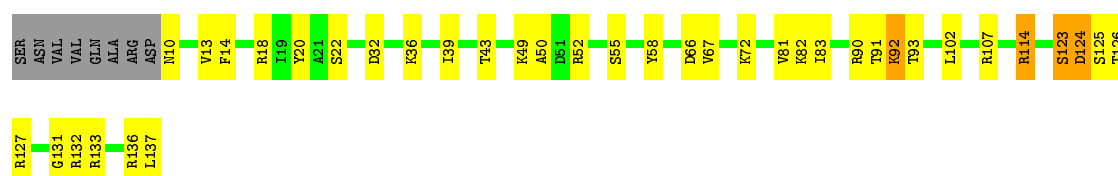
• Molecule 16: 40S ribosomal protein S14-A

Chain C4: 10% 58% 21% 7%



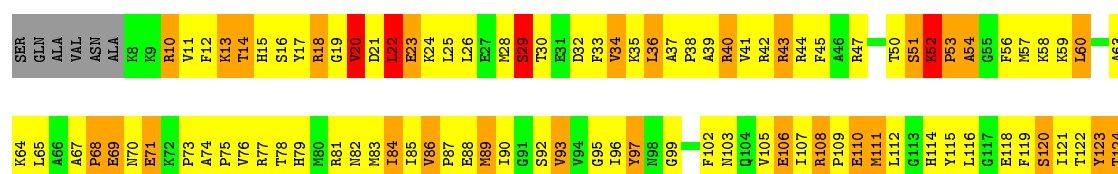
• Molecule 16: 40S ribosomal protein S14-A

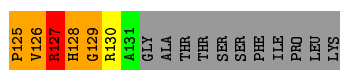
Chain c4: 66% 25% 6%



• Molecule 17: 40S ribosomal protein S15

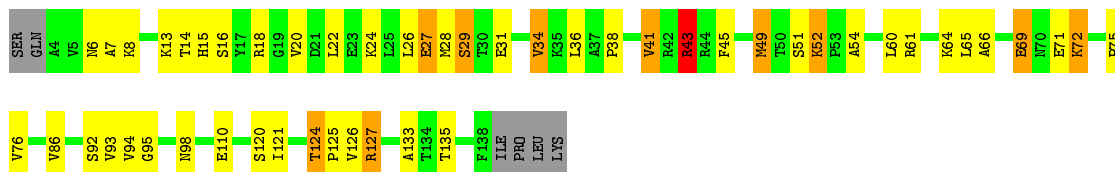
Chain C5: 16% 46% 23% 12%





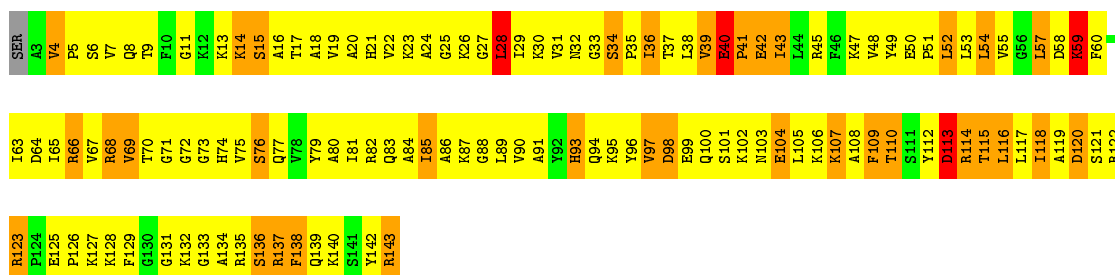
• Molecule 17: 40S ribosomal protein S15

Chain c5: 60% 28% 7% . .



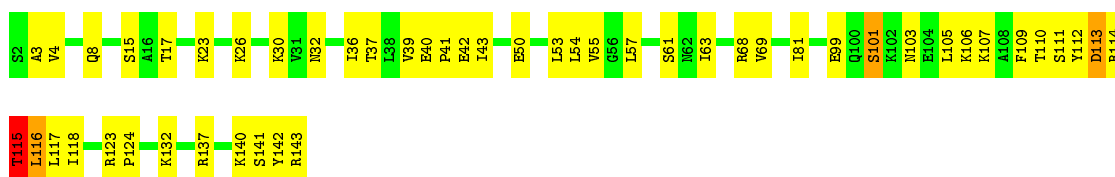
• Molecule 18: 40S ribosomal protein S16-A

Chain C6: 10% 63% 24% . .



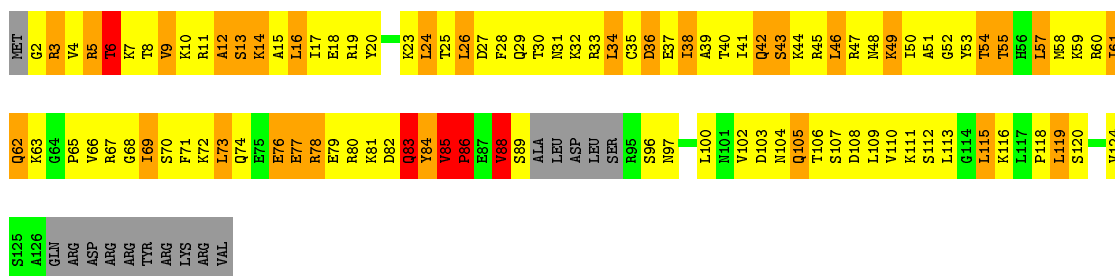
• Molecule 18: 40S ribosomal protein S16-A

Chain c6: 65% 32% . .

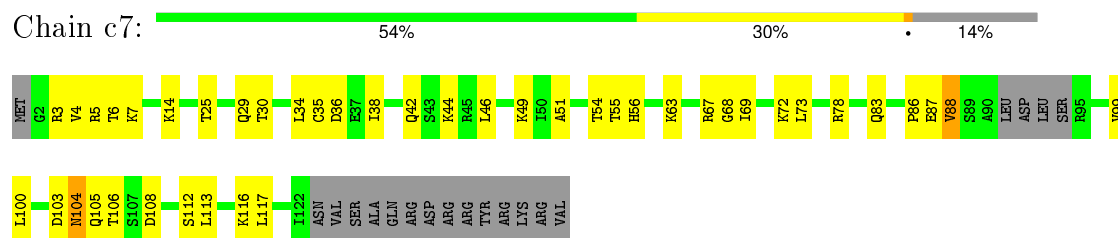


• Molecule 19: 40S ribosomal protein S17-A

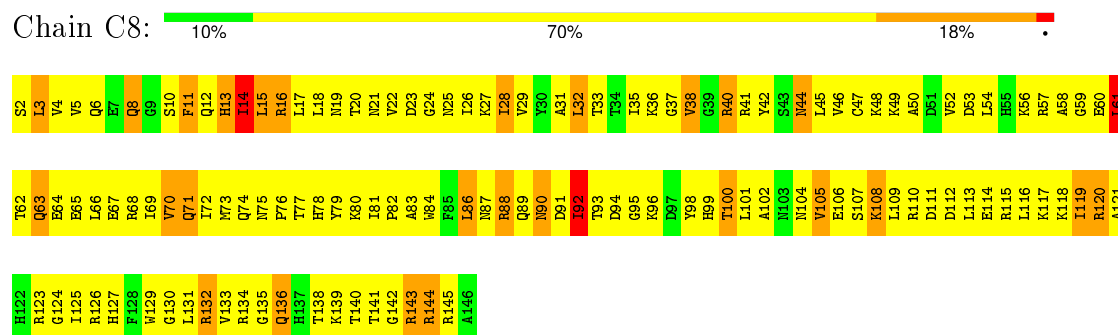
Chain C7: 13% 50% 22% . 12%



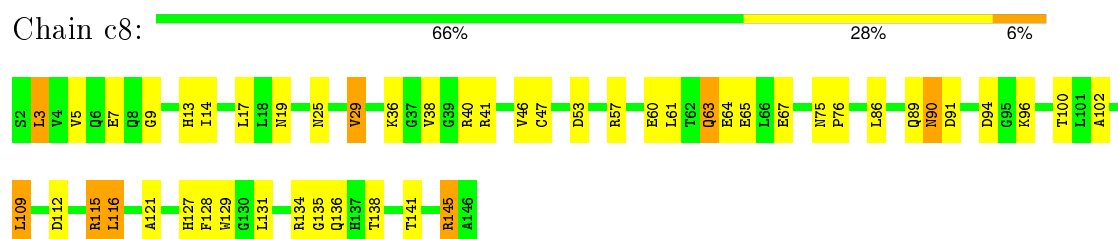
• Molecule 19: 40S ribosomal protein S17-A



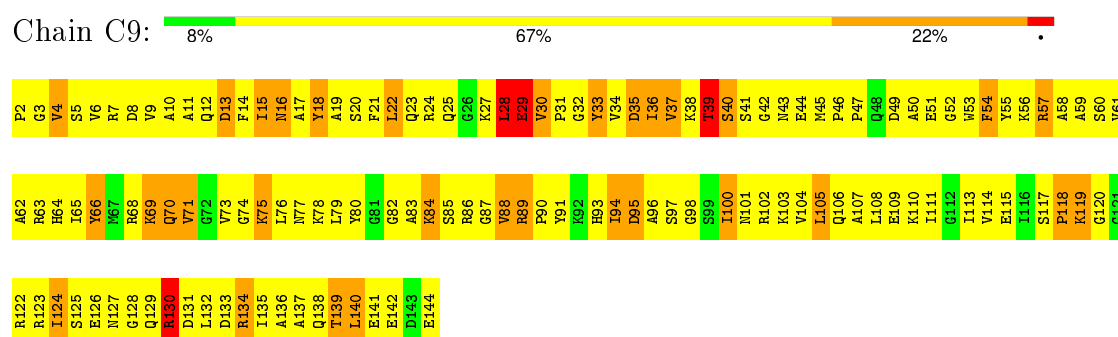
- Molecule 20: 40S ribosomal protein S18-A



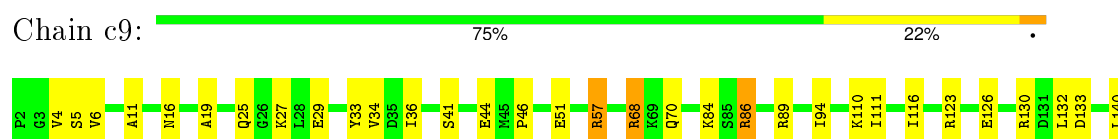
- Molecule 20: 40S ribosomal protein S18-A



- Molecule 21: 40S ribosomal protein S19-A



- Molecule 21: 40S ribosomal protein S19-A



E141
E142
D143
E144

• Molecule 22: 40S ribosomal protein S20

Chain D0: 8% 58% 23% 11%

SER ASP PHE GLN LYS GLU LYS VAL GLU GLN GLN GLN Q15 Q16 Q17 Q18 Q19 I20 K21 I22 I23 I24 I25 I26 L26 L27 S28 S29 T29 K30 K31 K32 K33 L34 E35 N36 N37 V37 S38 S39 N40 I41 I42 V42 K43 K44 N44 A45 E46 Q47 H48 H49 N49 L50 V51 V52 K52 K53 G54 G55 V56 V57 L58 L59 P59 T60 K61

V62 L63 R64 T67 R68 R69 T70 T71 N72 N73 G74 E75 S76 K77 K78 W79 E80 I81 T81 E82 E83 R84 R85 I86 H87 K88 R89 Y90 L94 I91 D92 L93 E94 A95 P96 V97 Q98 I99 V100 K101 R102 I103 T104 T105 I106 T107 I108 E109 P110 G111 V112 D113 V114 E115 V116 V117 V118 A119 N121

• Molecule 22: 40S ribosomal protein S20

Chain d0: 49% 38% 5% 8%

SER ASP PHE GLN LYS GLU LYS VAL GLU GLN Q12 Q13 Q14 Q15 Q16 Q17 Q18 I19 I20 K21 I22 I23 I24 T27 Q33 Q34 E35 S39 K43 K44 A45 E46 H48 H49 L50 V51 V52 K53 V62 L63 S66 T67 R68 R69 T70 T71 G73 E74 K77 T78

E94 A95 P96 V97 Q98 I99 V100 K101 I102 I103 T104 Q105 I106 T107 I108 E109 E115 V116 V117 V118 A119 S120 N121

• Molecule 23: 40S ribosomal protein S21-A

Chain D1: 5% 68% 23% 5%

M1 E2 N3 D4 K5 G6 G7 L8 V9 E10 E11 Y12 Y13 V14 P15 R16 K17 C18 S18 I19 T20 K21 R22 R23 I24 K25 K26 A26 D27 D28 R29 A30 S31 V32 Q33 I34 N35 V36 A37 K38 V39 D40 E41 E42 G43 R44 A45 I46 P47 G48 E49 Y50 V51 T52 Y53 A54 L55 S56 G57 V58 R60

S61 R62 G63 B64 S65 S66 D67 S68 L69 N70 N71 L72 L73 A74 Q75 M76 D76 G77 L78 K80 N81 W82 W83 S84 Y85 S86 R87

• Molecule 23: 40S ribosomal protein S21-A

Chain d1: 70% 26%

M1 E2 N3 D4 K5 G6 G7 L8 V9 E10 E11 Y12 Y13 M21 R22 R23 I24 K25 V32 K38 E41 E42 G43 R44 T52 Y53 S56 S61 R62 D66 D67 N75 L78 S86 R87

• Molecule 24: 40S ribosomal protein S22-A

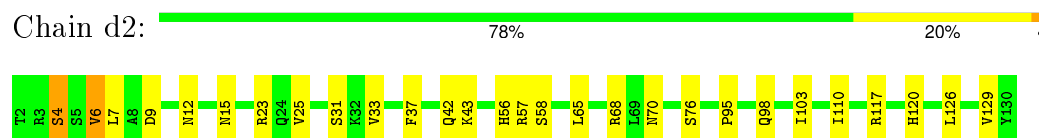
Chain D2: 17% 57% 24%

T2 R3 S4 S5 V6 L7 A8 D9 A10 L11 N12 N13 A14 M15 M16 A17 E18 I19 K20 T21 K22 R23 Q24 V25 L26 I27 R28 P29 S30 I35 K36 F37 L38 Q39 V40 M41 Q42 K43 H44 G45 Y46 I47 G48 E49 F50 E51 Y52 I53 D54 D55 H56 R57 S58 G59 K60 V63 Q64 L65

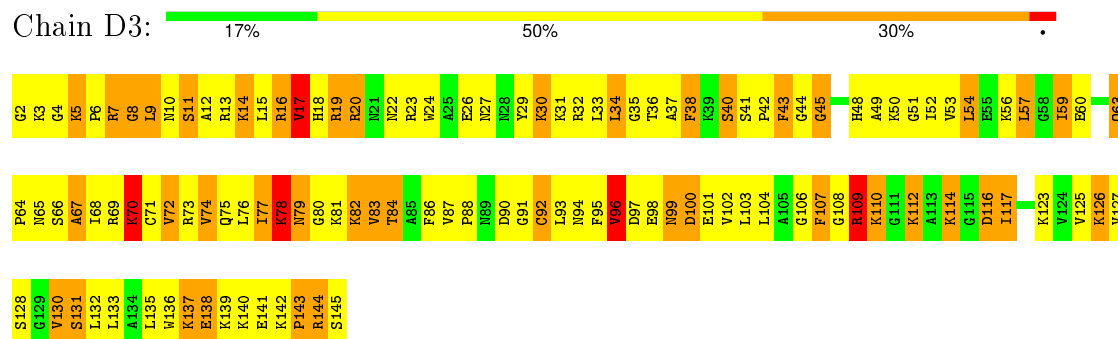
N66 G67 R68 L69 N70 K71 G72 G73 V74 I75 S76 P77 P78 F79 N80 V81 K82 I83 G84 D85 E86 W89 T90 A91 N92 L93 L94 P95 A96 R97 Q98 F99 G100 Y101 V102 I103 I104 T105 S107 A108 G109 I110 M111 D112 H113 E114 E115 A116 R117 R118 K119 H120 S121 V121 S122 G123 K124 I125 L126

G127 F128 Y129 Y130

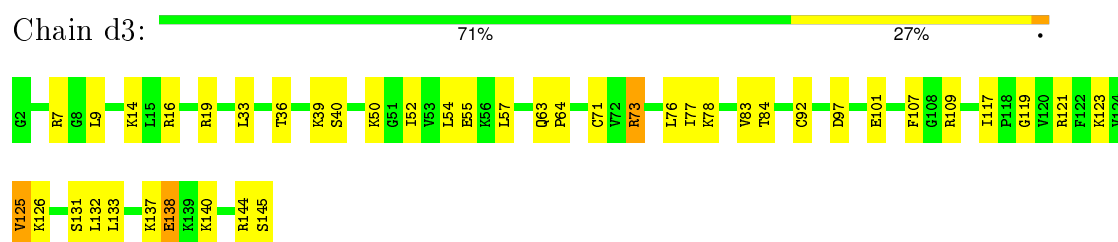
- Molecule 24: 40S ribosomal protein S22-A



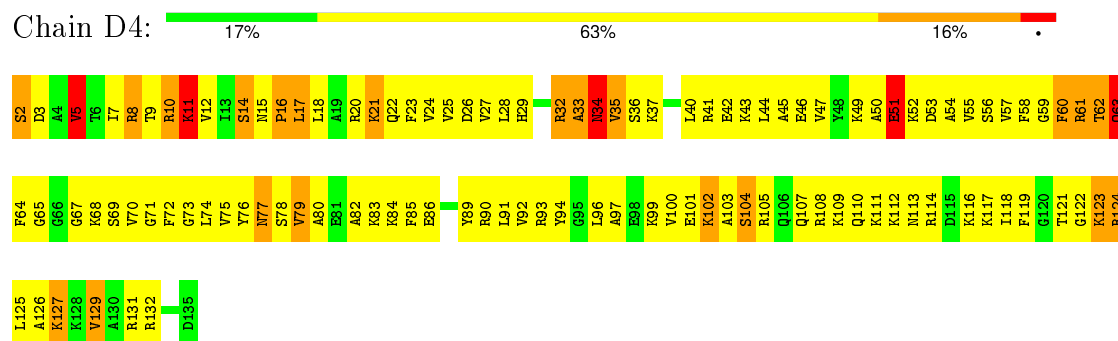
- Molecule 25: 40S ribosomal protein S23-A



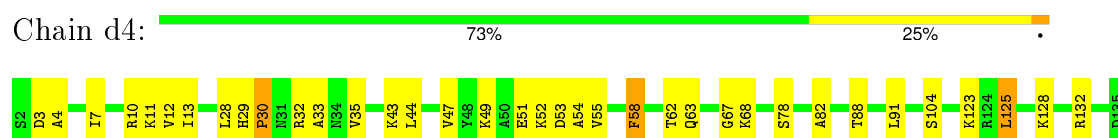
- Molecule 25: 40S ribosomal protein S23-A



- Molecule 26: 40S ribosomal protein S24-A

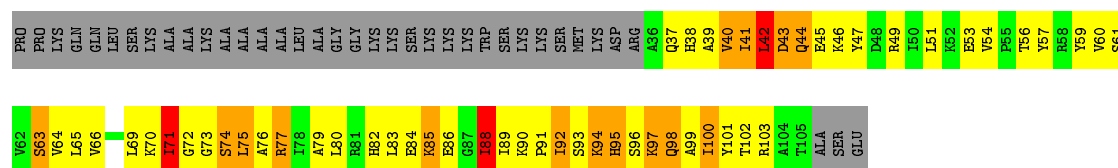


- Molecule 26: 40S ribosomal protein S24-A



- Molecule 27: 40S ribosomal protein S25-A

Chain D5: 

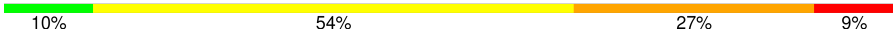


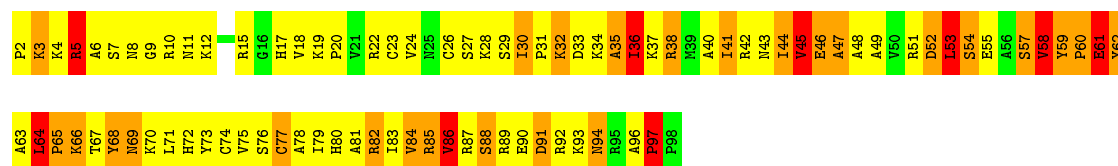
- Molecule 27: 40S ribosomal protein S25-A

Chain d5: 



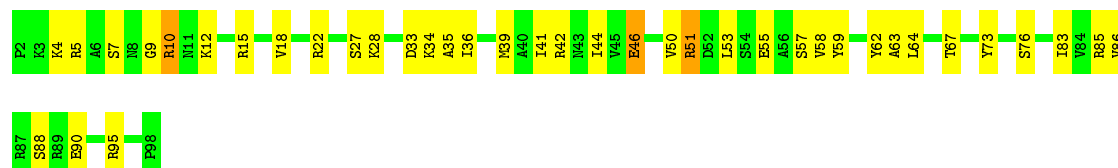
- Molecule 28: 40S ribosomal protein S26-B

Chain D6: 



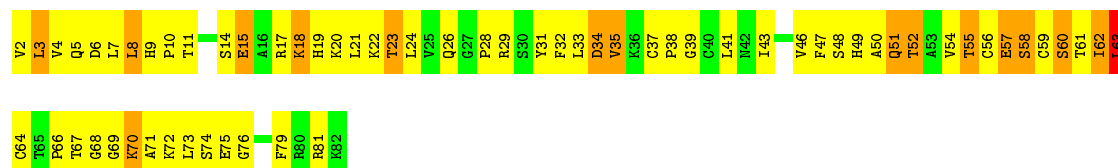
- Molecule 28: 40S ribosomal protein S26-B

Chain d6: 



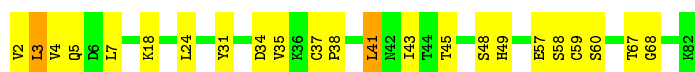
- Molecule 29: 40S ribosomal protein S27-A

Chain D7: 



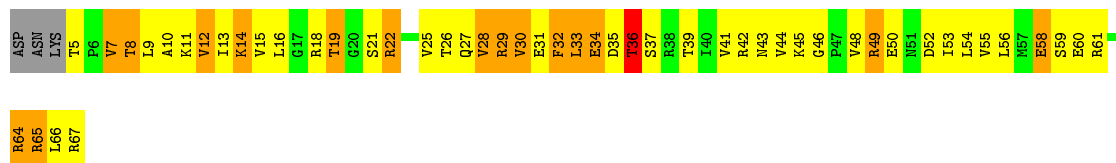
- Molecule 29: 40S ribosomal protein S27-A

Chain d7: 



- Molecule 30: 40S ribosomal protein S28-A

Chain D8: 18% 52% 24% 5%



- Molecule 30: 40S ribosomal protein S28-A

Chain d8: 65% 26% 5% 5%



- Molecule 31: 40S ribosomal protein S29-A

Chain D9: 16% 55% 20% 5%



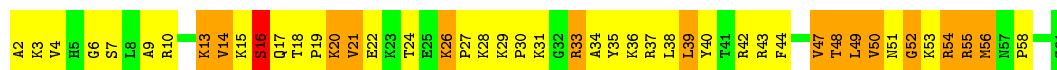
- Molecule 31: 40S ribosomal protein S29-A

Chain d9: 58% 35%



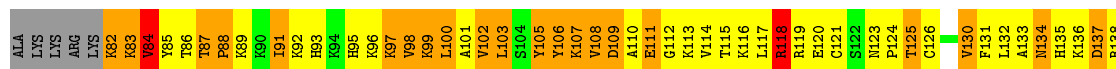
- Molecule 32: 40S ribosomal protein S30-A

Chain E0: 23% 50% 25% 5%



- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1: 13% 45% 33% 7%



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



U1630	C1631	A1632	C1633	C1634	C1635	C1636	C1637	C1638	C1639	C1640	C1641	C1642	C1643	C1644	C1645	C1646	C1647	C1648	C1649	C1650	C1651	C1652	C1653	C1654	C1655	C1656	C1657	C1658	C1659	C1660	C1661	C1662	C1663	C1664	C1665	C1666	C1667	C1668	C1669	C1670	C1671	C1672	C1673	C1674	C1675	C1676	C1677	C1678	C1679	C1680	C1681	C1682	C1683	C1684	C1685	C1686	C1687	C1688	C1689																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
U1570	C1571	A1572	C1573	C1574	C1575	C1576	C1577	C1578	C1579	C1580	C1581	C1582	C1583	C1584	C1585	C1586	C1587	C1588	C1589	C1590	C1591	C1592	C1593	C1594	C1595	C1596	C1597	C1598	C1599	C1600	C1601	C1602	C1603	C1604	C1605	C1606	C1607	C1608	C1609	C1610	C1611	C1612	C1613	C1614	C1615	C1616	C1617	C1618	C1619	C1620	C1621	C1622	C1623	C1624	C1625	C1626	C1627	C1628	C1629																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
G1510	C1511	C1512	C1513	C1514	C1515	C1516	C1517	C1518	C1519	C1520	C1521	C1522	C1523	C1524	C1525	C1526	C1527	C1528	C1529	C1530	C1531	C1532	C1533	C1534	C1535	C1536	C1537	C1538	C1539	C1540	C1541	C1542	C1543	C1544	C1545	C1546	C1547	C1548	C1549	C1550	C1551	C1552	C1553	C1554	C1555	C1556	C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
G1450	C1451	C1452	C1453	C1454	C1455	C1456	C1457	C1458	C1459	C1460	C1461	C1462	C1463	C1464	C1465	C1466	C1467	C1468	C1469	C1470	C1471	C1472	C1473	C1474	C1475	C1476	C1477	C1478	C1479	C1480	C1481	C1482	C1483	C1484	C1485	C1486	C1487	C1488	C1489	C1490	C1491	C1492	C1493	C1494	C1495	C1496	C1497	C1498	C1499	C1500	C1501	C1502	C1503	C1504	C1505	C1506	C1507																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
A1390	C1391	C1392	C1393	C1394	C1395	C1396	C1397	C1398	C1399	C1400	C1401	C1402	C1403	C1404	C1405	C1406	C1407	C1408	C1409	C1410	C1411	C1412	C1413	C1414	C1415	C1416	C1417	C1418	C1419	C1420	C1421	C1422	C1423	C1424	C1425	C1426	C1427	C1428	C1429	C1430	C1431	C1432	C1433	C1434	C1435	C1436	C1437	C1438	C1439	C1440	C1441	C1442	C1443	C1444	C1445	C1446	C1447	C1448	C1449																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
G1269	C1270	C1271	C1272	C1273	C1274	C1275	C1276	C1277	C1278	C1279	C1280	C1281	C1282	C1283	C1284	C1285	C1286	C1287	C1288	C1289	C1290	C1291	C1292	C1293	C1294	C1295	C1296	C1297	C1298	C1299	C1300	C1301	C1302	C1303	C1304	C1305	C1306	C1307	C1308	C1309	C1310	C1311	C1312	C1313	C1314	C1315	C1316	C1317	C1318	C1319	C1320	C1321	C1322	C1323	C1324	C1325	C1326	C1327	C1328	C1329																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
G1209	C1210	C1211	C1212	C1213	C1214	C1215	C1216	C1217	C1218	C1219	C1220	C1221	C1222	C1223	C1224	C1225	C1226	C1227	C1228	C1229	C1230	C1231	C1232	C1233	C1234	C1235	C1236	C1237	C1238	C1239	C1240	C1241	C1242	C1243	C1244	C1245	C1246	C1247	C1248	C1249	C1250	C1251	C1252	C1253	C1254	C1255	C1256	C1257	C1258	C1259	C1260	C1261	C1262	C1263	C1264	C1265	C1266	C1267	C1268	C1269																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
G1149	C1150	C1151	C1152	C1153	C1154	C1155	C1156	C1157	C1158	C1159	C1160	C1161	C1162	C1163	C1164	C1165	C1166	C1167	C1168	C1169	C1170	C1171	C1172	C1173	C1174	C1175	C1176	C1177	C1178	C1179	C1180	C1181	C1182	C1183	C1184	C1185	C1186	C1187	C1188	C1189	C1190	C1191	C1192	C1193	C1194	C1195	C1196	C1197	C1198	C1199	C1200	C1201	C1202	C1203	C1204	C1205	C1206	C1207	C1208	C1209																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
G1087	C1088	C1089	C1090	C1091	C1092	C1093	C1094	C1095	C1096	C1097	C1098	C1099	C1100	C1101	C1102	C1103	C1104	C1105	C1106	C1107	C1108	C1109	C1110	C1111	C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	C1120	C1121	C1122	C1123	C1124	C1125	C1126	C1127	C1128	C1129	C1130	C1131	C1132	C1133	C1134	C1135	C1136	C1137	C1138	C1139	C1140	C1141	C1142	C1143	C1144	C1145	C1146	C1147	C1148	C1149																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
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A2601	G2539	C	A2295	C2235	G2174	C2114	G	G1934	A1874	A1814	G1751	C1690
G2602	A2540	C	A2296	G2236	U2175	G2115	U	G1935	G1875	U1815	A1752	U1691
G2603	A2541	A	U2297	C2237	U2176	G2116	C	A1936	U1876	A1816	U1692	U1692
U2604	G2542	G	U2298	G2238	C2177	A2117	U	U1937	U1877	A1817	G1753	C1693
G2605	C2543	U	A2299	G2239	A2178	C2118	G	G1938	G1878	U1818	G1754	U1694
G2606	G2544	U	A2300	G2240	C2179	A2119	U	G1939	A1879	U1819	U1695	U1695
G2607	A2545	A	U2301	U2241	G2180	A2120	A	G1940	U1880	U1820	A1696	A1696
G2608	C2546	A	G2302	A2242	G2181	G2121	U	C1941	U1881	U1821	G1758	A1697
A2609	U2547	A	A2303	A2243	A2182	G2122	G	U1942	G1882	C1822	C1759	A1698
G2610	G2548	U	C2304	A2244	A2183	G2123	U	C1943	A1883	A1823	A1760	C1699
G2611	C2549	A	G2305	C2245	U2184	G2124	C	U1944	A1884	U1824	C1761	A1699
U2612	U2426	C	C2306	G2246	G2185	A2125	U	A1945	U1885	G1825	C1762	G1700
G2613	C2550	C	G2307	G2247	A2186	A2126	C	U1946	A1886	C1826	U1763	C1701
G2614	A2551	C	A2308	G2248	G2187	U2127	U	G1947	A1887	C1827	U1764	U1702
G2615	G2552	A	C2309	G2249	A2188	C2128	U	G1948	U1888	A1828	U1765	U1703
G2616	U2553	C	A2310	C2250	U2189	G2129	G	C1949	G1889	A1829	G1766	A1704
U2617	A2554	U	G2311	A2251	U2190	A2130	C	U1950	U1890	G1830	C1767	A1707
G2618	C2555	A	A2312	A2252	U2191	A2131	A	C1951	A1891	U1831	U1768	C1708
G2619	U2556	C	G2313	G2253	C2192	C2132	U	G1952	G1892	G1832	G1770	G1709
G2620	C2557	U	U2314	U2254	U2193	U2133	A	U1953	A1893	G1833	C1771	C1710
G2621	U2558	U	G2315	A2255	G2194	G2134	C	G1954	A1894	U1834	U1772	G1711
G2622	C2560	U	G2316	A2256	C2195	U2135	C	U1955	A1895	A1835	C1773	G1712
G2623	G2561	U	A2317	C2257	C2196	C2136	G	A	A1896	C1836	C1774	G1713
G2624	U2562	A	U2318	U2258	C2197	U2137	U	G	G1897	U1837	G1775	A1714
C2625	G2563	U	U2319	A2259	A2198	A2138	C	G	G1898	A1838	U1715	A1715
A2626	U2564	U	A2320	U2260	G2199	A2139	C	U	G1899	A1839	C1779	U1716
G2627	C2565	G	A2321	G2261	U2200	U2140	C	A	A1900	U1840	U1717	U1717
A2628	U2566	U	G2322	A2262	C2201	U2141	U	G	A1901	A1841	G1781	A1708
U2629	C2567	A	C2323	C2263	U2202	A2142	G	G	G1902	U1842	U1782	G1719
C2630	U2568	U	A2324	U2264	U2203	A2143	U	C	U1903	C1843	U1783	U1720
U2631	G2569	A	G2325	C2265	U2204	A2144	C	C	C1904	G1844	G1784	U1721
G2632	A2570	U	A2326	U2266	U2205	A2145	G	C	G1905	C1845	U1785	U1722
G2633	C2571	G	G2327	C2267	G2206	A2146	A	U	U1906	C1846	G1786	A1723
U2634	U2572	A	U2328	U2268	A2207	A2147	C	G	A1907	A1847	U1787	U1724
C2635	G2573	U	C2329	U2269	A2208	U2148	C	U	A1908	G1848	C1788	C1725
A2636	U2574	U	C2330	A2270	U2209	A2149	A	G	A1909	C1849	G1789	C1726
G2637	C2575	G	G2331	A2271	G2210	G2150	U	U	A1910	A1850	G1790	G1727
C2638	U2576	U	A2332	G2272	U2211	C2151	U	C	A1911	G1851	C1791	G1728
G2639	G2579	A	C2333	G2273	C2212	A2152	A	A	U1912	G1852	C1792	A1729
A2640	U2580	G	U2334	U2274	A2213	U2153	C	G	A1913	U1853	C1793	G1730
U2641	C2581	A	G2335	A2275	A2214	U2154	C	A	G1914	C1854	G1794	A1731
A2642	G2582	U	U2336	G2276	A2215	G2155	G	C	A1915	U1855	U1795	U1732
C2643	U2583	A	C2337	C2277	G2216	G2156	U	C	U1916	C1856	G1796	G1733
G2644	C2584	U	G2338	C2278	U2217	G2157	G	C	C1917	C1857	A1797	G1734
G2645	A2585	A	C2339	A2279	G2218	A2158	C	A	C1918	A1858	A1798	G1735
C2646	U2586	G	U2340	A2280	A2219	U2159	C	G	U1919	A1859	A1799	G1736
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G2648	U2588	G	U2342	U2282	G2161	C2161	U	G	A1921	U1861	U1801	C1738
A2649	C2589	C	C2343	G2283	U2262	U2162	G	G	A1922	U1862	C1802	U1739
U2650	G2590	G	U2344	C2284	C2163	U2163	U	C	C1923	G1863	G1803	U1740
G2651	A2591	A	A2345	C2285	A2224	A2164	U	C	U1924	A1864	A1804	A1741
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G2654	A2594	U	A2348	G2288	A2228	A2167	A	G	G1927	A1867	G1807	G1744
U2655	G2595	U	U2349	U2289	A2229	A2168	C	C	G1928	G1868	G1808	C1745
A2656	U2596	C	C2350	C2290	C2230	G2169	A	U	G1929	C1869	A1809	U1746
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C2658	U2598	C	G2352	U2292	A2232	G2171	G	G	U1931	U1871	G1811	G1748
U2659	G2599	U	C2353	C2293	A2233	A2172	U	U	A1932	C1872	C1812	A1749
G2660	C2600	G	C2354	U2294	G2234	U2173	C	G	A1933	U1873	A1813	A1750

● Molecule 36: 25S ribosomal RNA									
Chain 5: <div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> 5% 26% 44% 17% 7%									
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A63	U3386	G3265	C3205	C3145	G3085	U3024	C2964	U2904	C2844
G64	U3387	G3266	C3206	G3146	A3086	G3025	U2965	U2905	A2845
A65	U3388	G3267	U3207	G3147	G3087	G3026	C2966	C2906	U2846
A66	G3328	A3268	G3208	U3148	G3088	A3027	A2967	C2907	G2786
A67	U3329	C3269	A3209	G3149	C3089	G3028	G2968	G2908	C2788
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C69	U3331	C3271	C3211	U3151	C3091	G3030	C2970	A2910	G2729
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G18	U3341	U3281	C3221	C3161	G3101	U3041	U2980	G2800	A2877
U19	A3342	U3282	U3222	G3162	G3102	U3042	U2981	U2860	A2879
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U83	G3346	G3286	A3226	C3166	A3106	A3046	C2985	C2925	U2743
G24	U3347	U3287	A3227	A3167	U3107	U3047	U2986	A2926	C2884
U25	A3348	G3288	G3228	C3168	G3108	A3048	A2987	C2927	C2885
A26	G3349	G3289	G3229	U3169	G3109	A3049	C2988	C2928	A2686
C27	C3350	G3290	G3230	U3170	C3110	U3050	U2989	C2929	U2687
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G92	U3355	A3295	C3235	U3175	C3115	U3055	A2994	A2934	C2812
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A95	U3358	C3298	G3238	A3178	C3118	U3058	G2997	C2937	U2815
G96	A3359	A3299	G3239	U3179	C3119	G3059	G2998	C2938	C2755
U97	U3360	U3300	C3240	A3180	C3120	C3060	U2999	G2939	A2817
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- Molecule 36: 25S ribosomal RNA

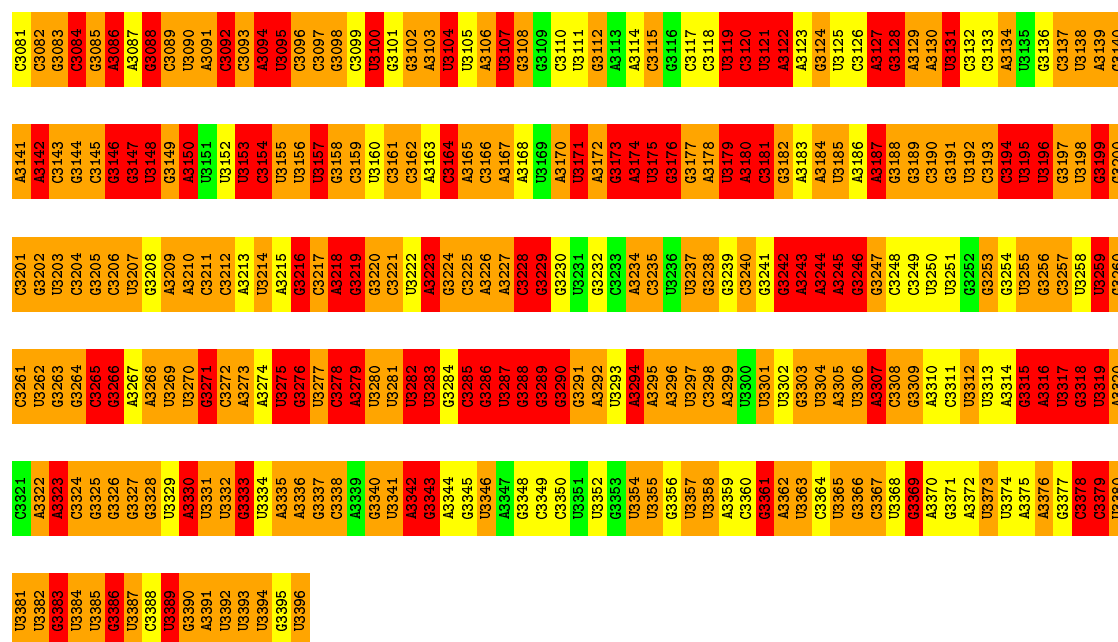
Chain 5: 

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U966	A967	G968	G969	A970	G971	G972	A973	G974	A975	G976	G977	G978	U979	A980	U981	G982	A983	G984	U985	A986	U987	A988	A989	U990	G991	G992	G993	G994	U995	A996	G997	A998	G999	U1000	G1001	A1002	U1003	A1004	G1005	A1006	U1007	U1008	A1009	U1010	A1011	G1012	G1013	U1014	U1015	G1016	U1017	G1018	U1019	G1020	U1021	U1022	G1023	U1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	U1067	U1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	U1078	A1079	U1080	U1081	U1082	G1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	A1144	A1145																																																																																																																																																																																																																																																																																																																																																																																																																																																										
A906	G907	G908	G909	G910	G911	G912	A913	G914	A915	A916	G917	A918	U919	A920	A921	U922	G923	G924	U925	A926	G927	A928	U929	U930	U931	U932	A933	G934	U935	A936	G937	A938	U939	G940	G941	A942	U943	A944	U945	U946	A947	U948	U949	A950	A951	A952	G953	U954	A955	U956	G957	G958	U959	G960	A961	A962	G963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	A1067	A1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	A1144	A1145																																																																																																																																																																																																																																																																																																																																																																																														
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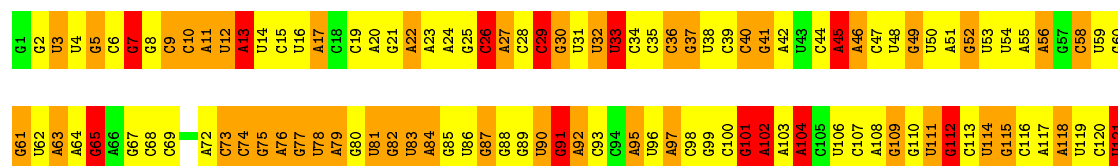


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A3024	U2904	U2844	U2723	G2663	G2603	U2542	U	U2421	A2361	U2301	G2240	G2180	A2120
G3025	U2905	A2845	U2724	G2664	U2604	U2543	G	C2422	C2362	G2302	U2241	C2181	G2121
G3026	G2906	U2846	U2725	G2665	G2605	U2544	A	U2423	A2363	A2242	A2242	A2182	G2122
A3027	G2907	U2847	C2726	G2666	G2606	C2545	A	U2426	G2364	C2304	A2243	A2183	G2123
G3028	U2908	G2848	A2727	G2667	G2607	C2546	A	U2427	C2365	G2305	A2244	U2184	G2124
A3029	G2909	G2849	U2728	G2668	G2608	C2547	U	U2428	C2366	G2306	C2245	G2185	A2125
G3030	G2910	G2850	U2729	G2669	A2609	G2548	A	U2429	A2367	G2307	G2246	U2186	A2126
G3031	A2911	A2851	G2730	G2670	G2610	G2549	C	G2430	A2368	G2308	G2247	G2187	U2127
A3032	G2912	C2852	U2731	A2671	U2611	U2550	C	A2431	G2369	A2309	G2248	A2188	C2128
G3033	C2913	A2853	G2732	G2672	U2612	U2551	A	G2432	G2370	U2310	G2249	U2189	U2129
C3034	G2914	G2854	A2733	A2673	U2613	C2552	C	A2433	G2371	G2311	G2250	G2190	G2130
A3035	U2915	G2855	U2734	A2674	G2614	U2553	U	U2434	A2372	A2312	G2251	U2191	A2131
G3036	U2916	G2856	U2735	G2675	G2615	A2554	A	U2435	A2373	A2313	A2252	C2192	C2132
U3037	G2917	A2857	A2736	A2676	G2616	G2555	C	G2436	C2374	U2314	G2253	U2193	U2133
U3038	U2918	G2858	C2737	G2677	U2617	C2556	C	U2437	G2375	G2315	U2254	G2194	G2134
C3039	A2919	U2859	A2738	A2678	G2618	A2557	U	G2438	G2376	G2316	A2255	C2195	U2135
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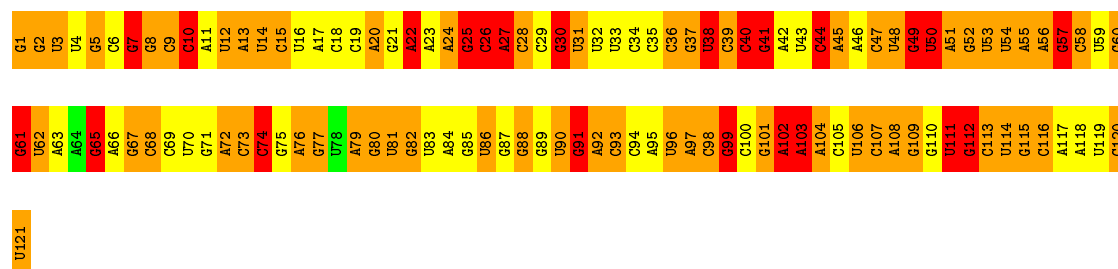
• Molecule 37: 5S ribosomal RNA

Chain 3: 7% 46% 36% 11%



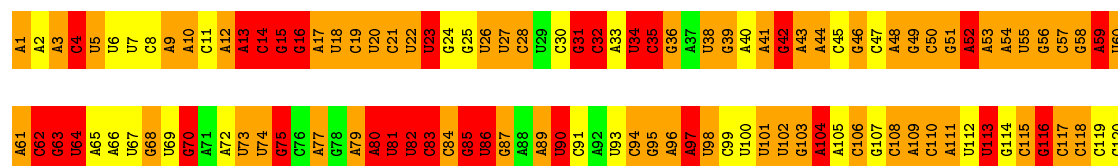
• Molecule 37: 5S ribosomal RNA

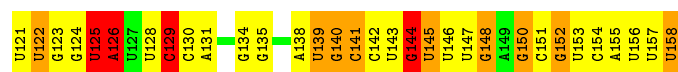
Chain 7: 31% 49% 19%



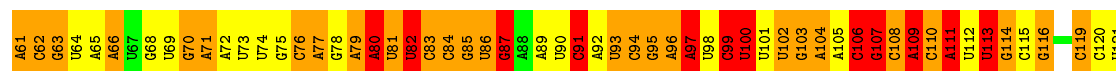
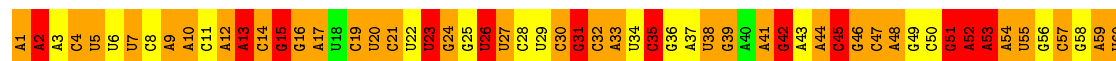
• Molecule 38: 5.8S ribosomal RNA

Chain 4: 8% 29% 42% 21%

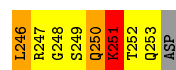
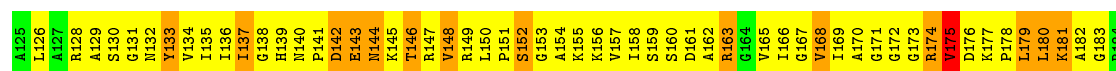
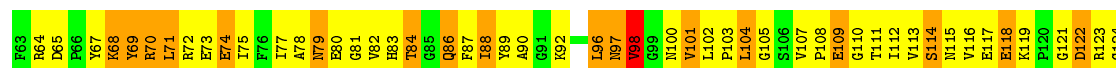
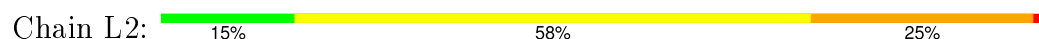




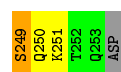
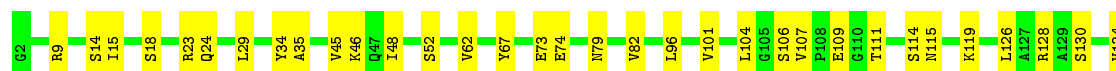
- Molecule 38: 5.8S ribosomal RNA



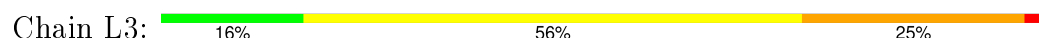
- Molecule 39: 60S ribosomal protein L2-A

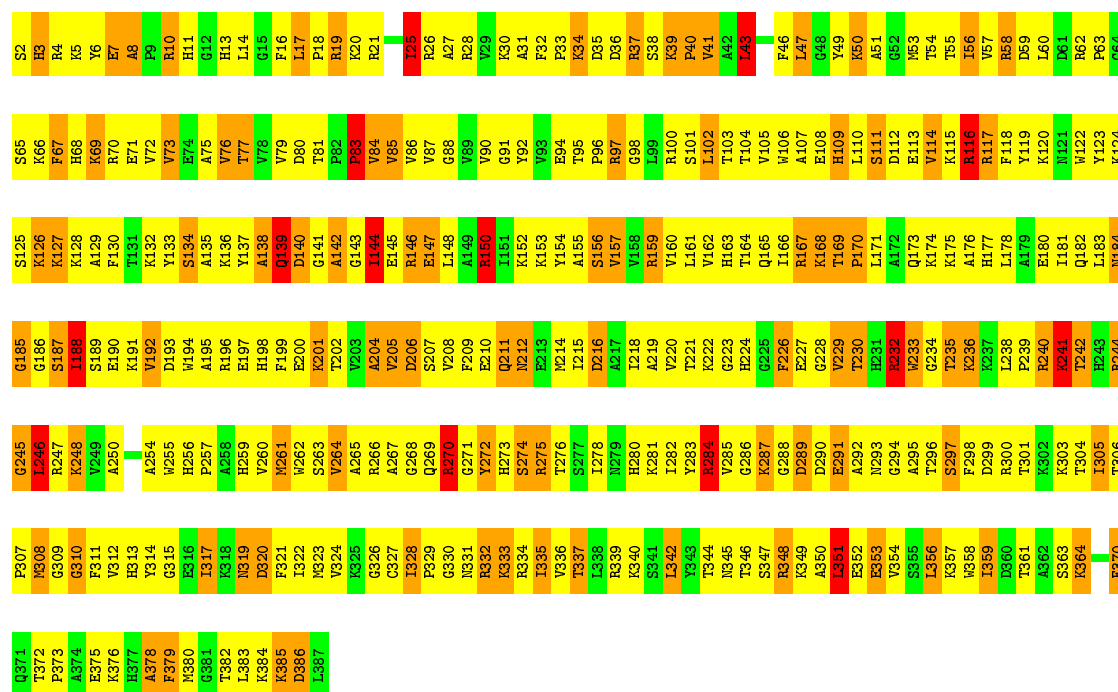


- Molecule 39: 60S ribosomal protein L2-A



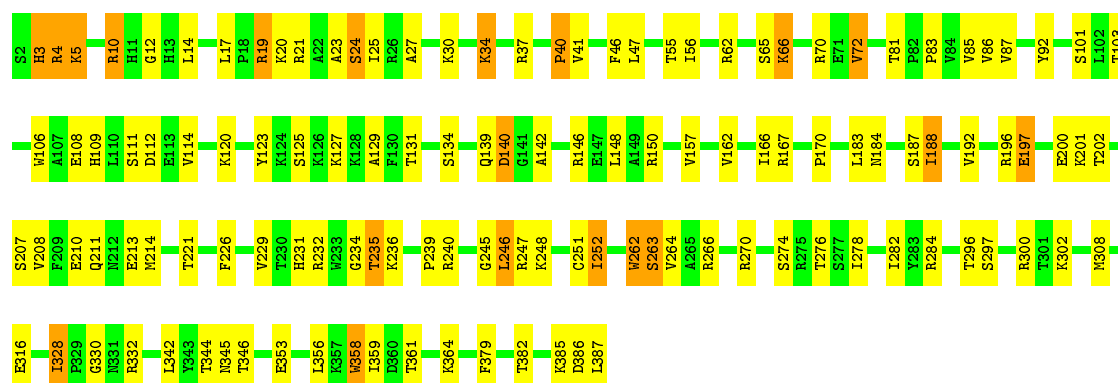
- Molecule 40: 60S ribosomal protein L3





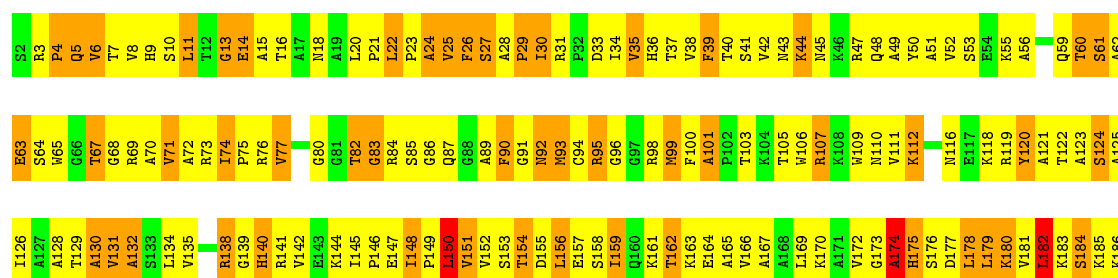
• Molecule 40: 60S ribosomal protein L3

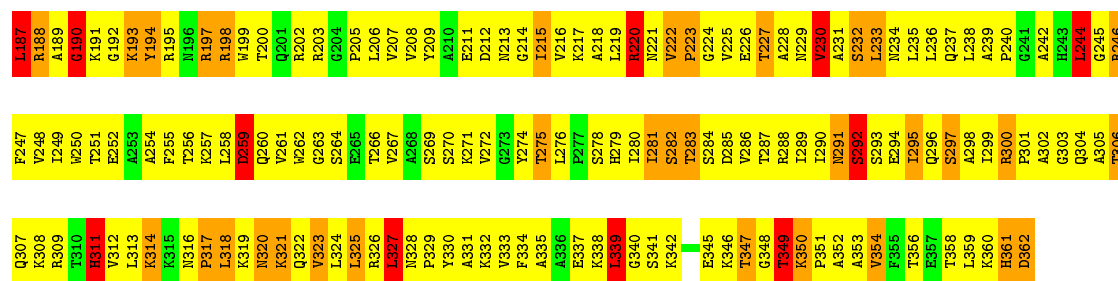
Chain 13: 67% 27% 5%



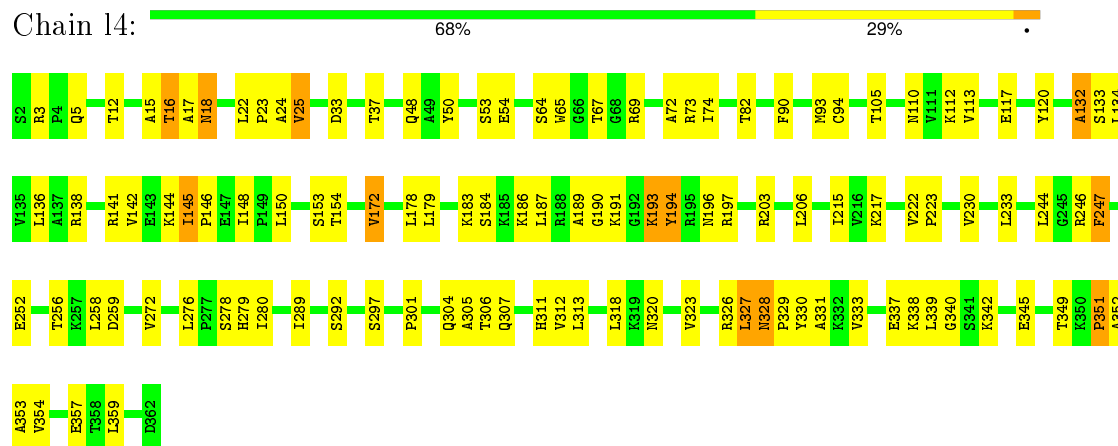
• Molecule 41: 60S ribosomal protein L4-A

Chain L4: 13% 60% 23%

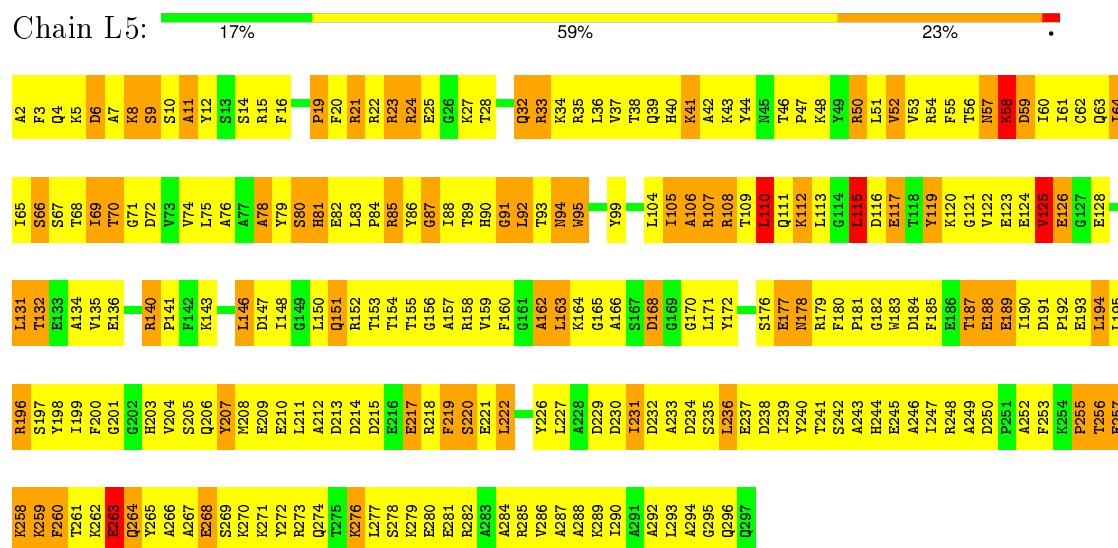




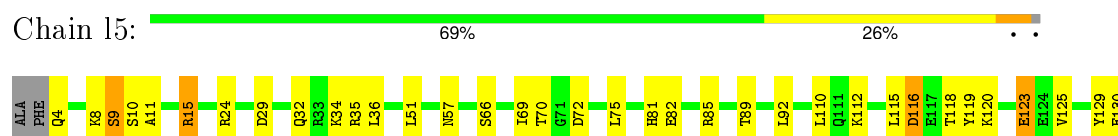
• Molecule 41: 60S ribosomal protein L4-A

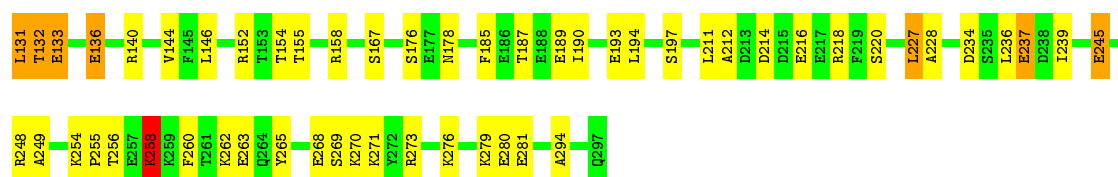


• Molecule 42: 60S ribosomal protein L5



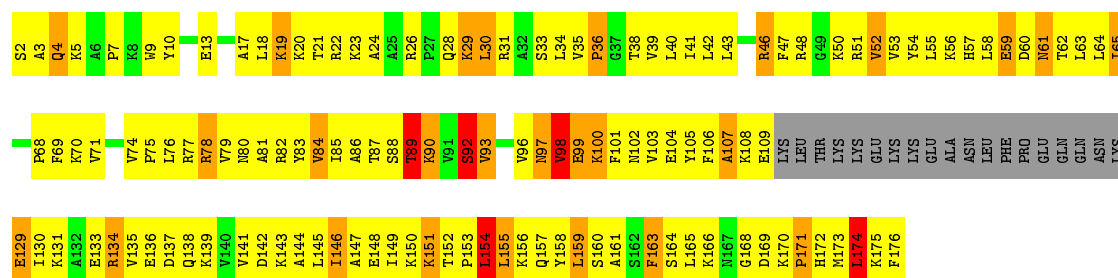
• Molecule 42: 60S ribosomal protein L5





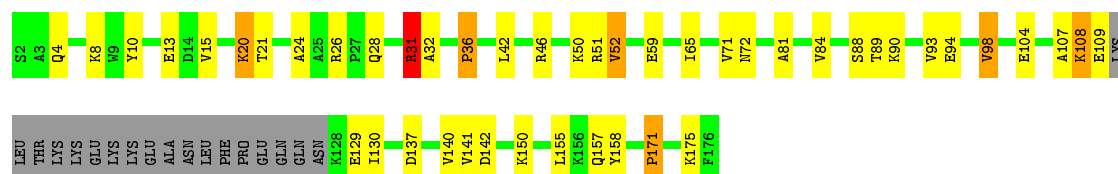
• Molecule 43: 60S ribosomal protein L6-A

Chain L6: 14% 57% 15% • 11%



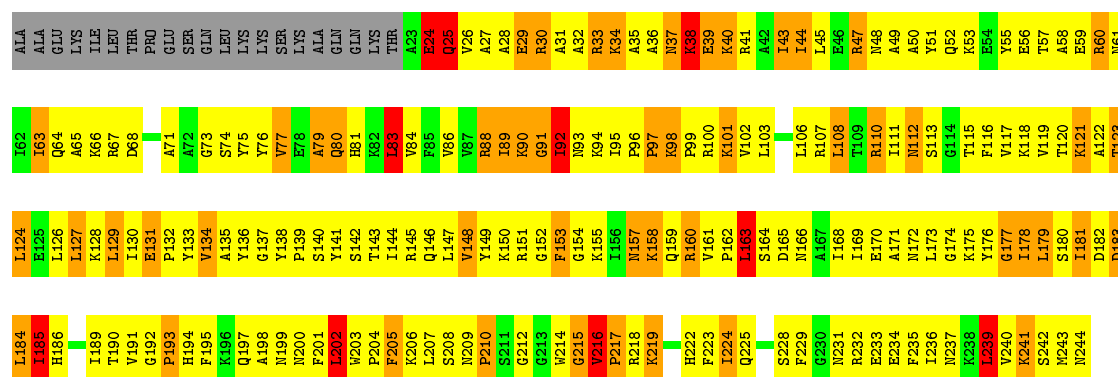
• Molecule 43: 60S ribosomal protein L6-A

Chain l6: 63% 22% • • 10%



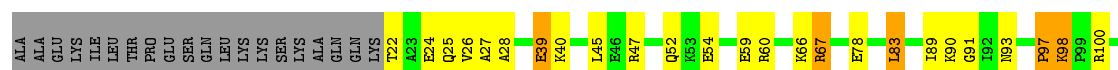
• Molecule 44: 60S ribosomal protein L7-A

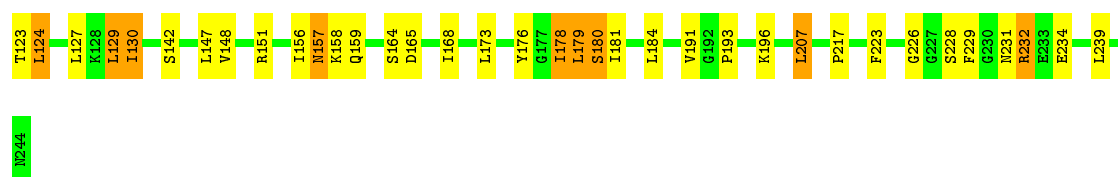
Chain L7: 12% 54% 21% • 9%



• Molecule 44: 60S ribosomal protein L7-A

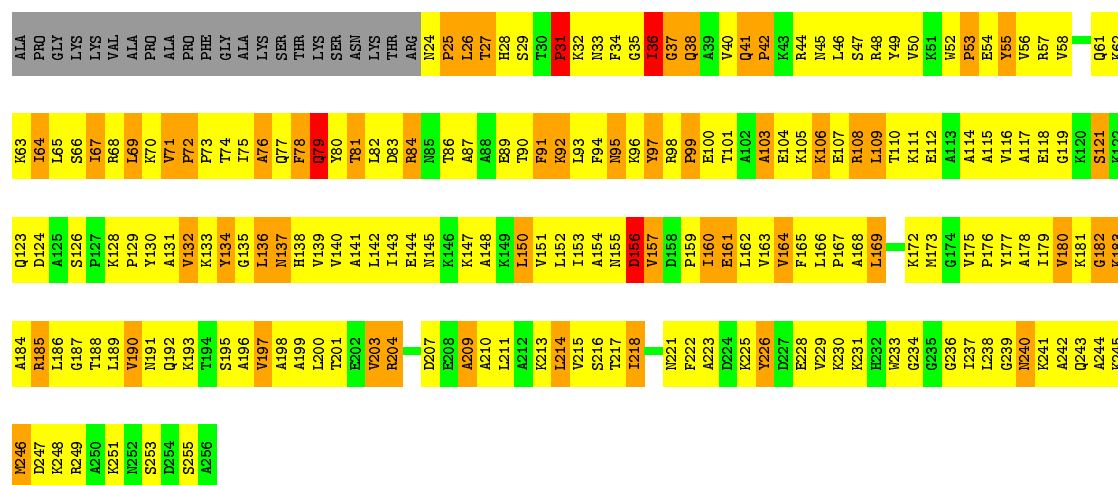
Chain l7: 67% 19% 6% 8%





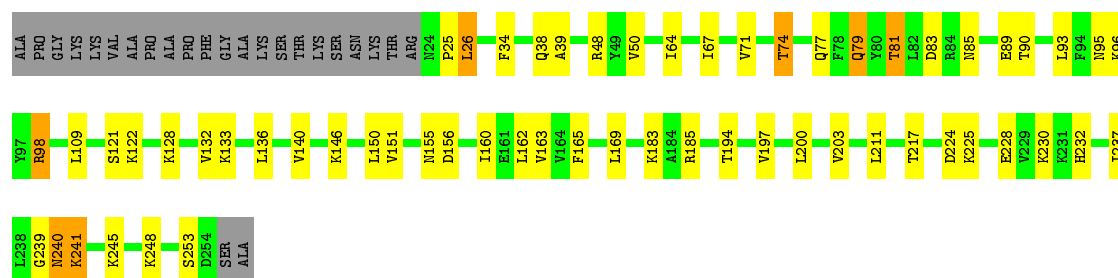
- Molecule 45: 60S ribosomal protein L8-A

Chain L8: 14% 55% 20% 9%



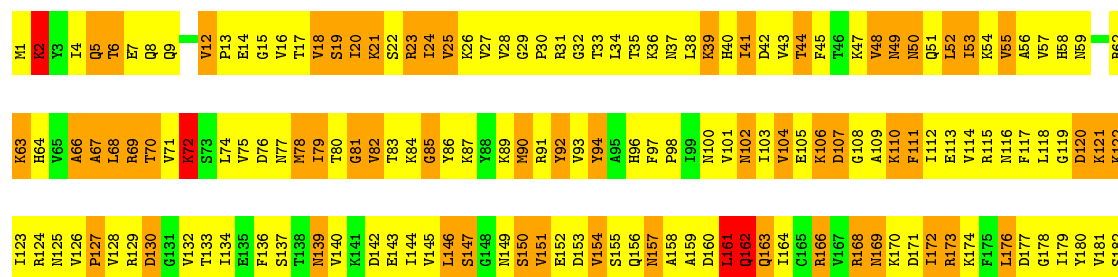
- Molecule 45: 60S ribosomal protein L8-A

Chain l8: 67% 21% 9%



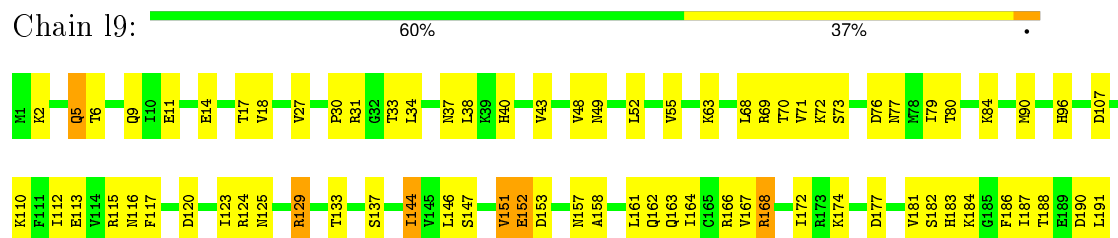
- Molecule 46: 60S ribosomal protein L9-A

Chain L9: 11% 54% 32%

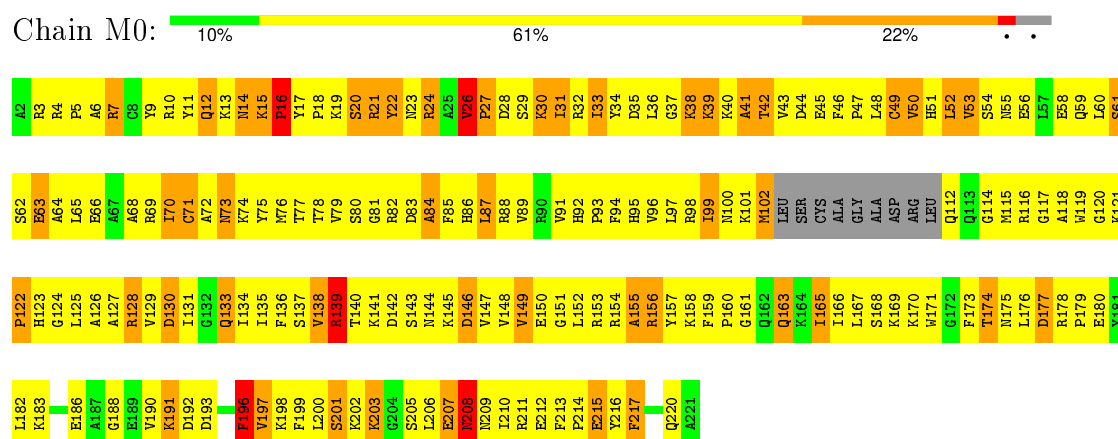




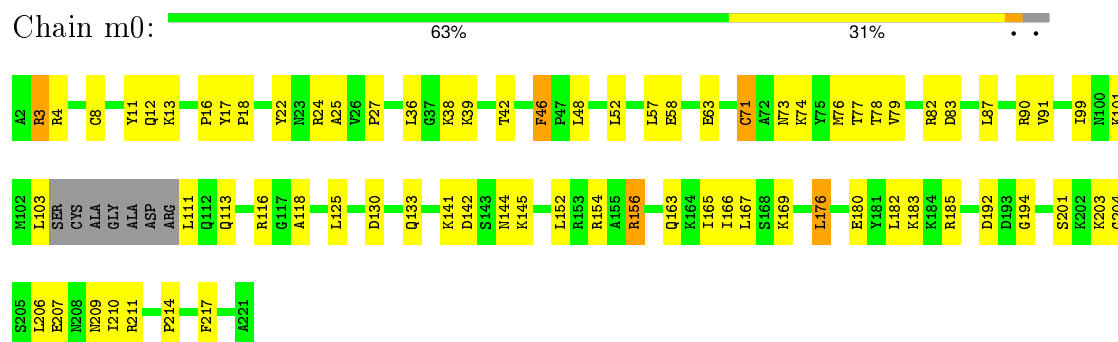
• Molecule 46: 60S ribosomal protein L9-A



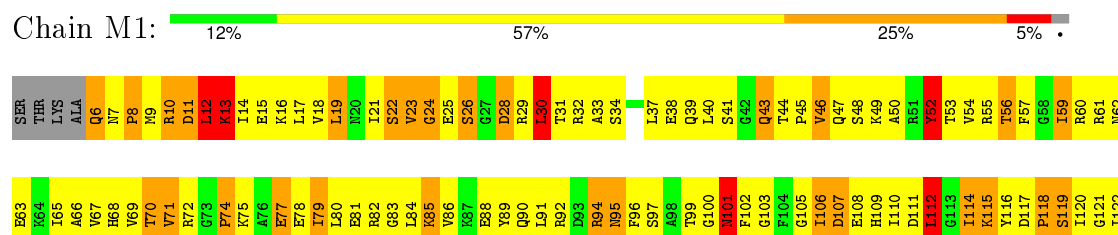
• Molecule 47: 60S ribosomal protein L10

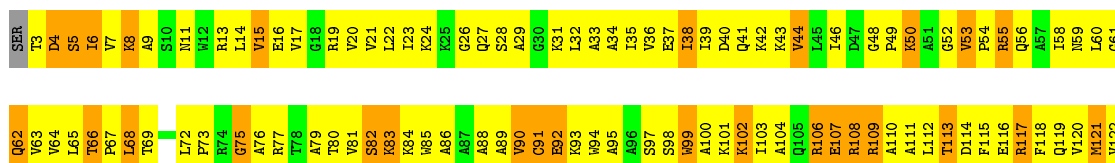


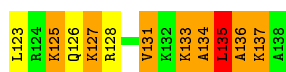
• Molecule 47: 60S ribosomal protein L10



• Molecule 48: 60S ribosomal protein L11-B







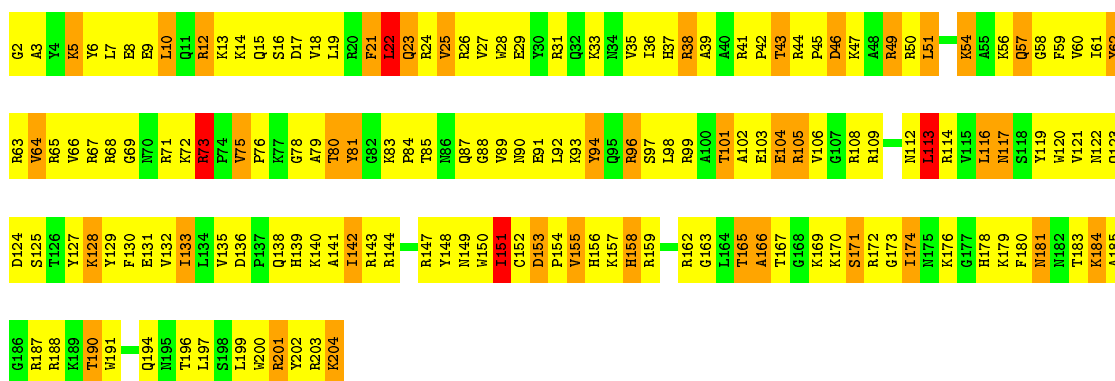
• Molecule 50: 60S ribosomal protein L14-A

Chain m4: 73% 26%



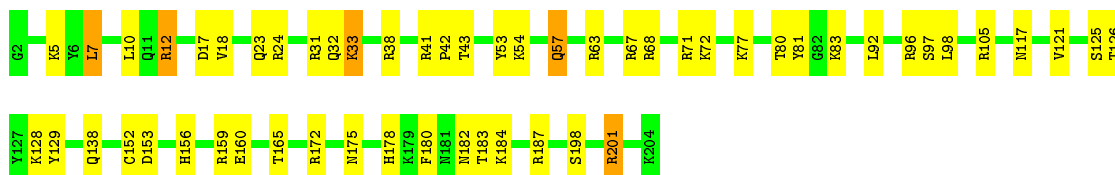
• Molecule 51: 60S ribosomal protein L15-A

Chain M5: 20% 58% 20%



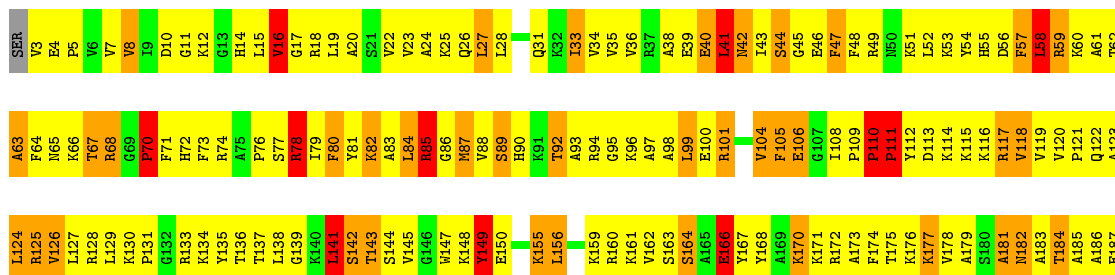
• Molecule 51: 60S ribosomal protein L15-A

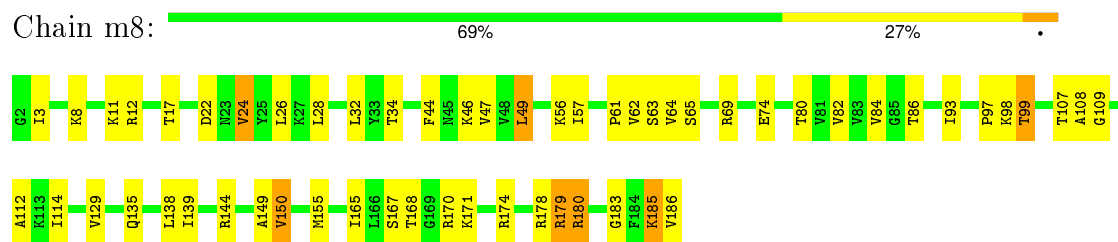
Chain m5: 73% 25%



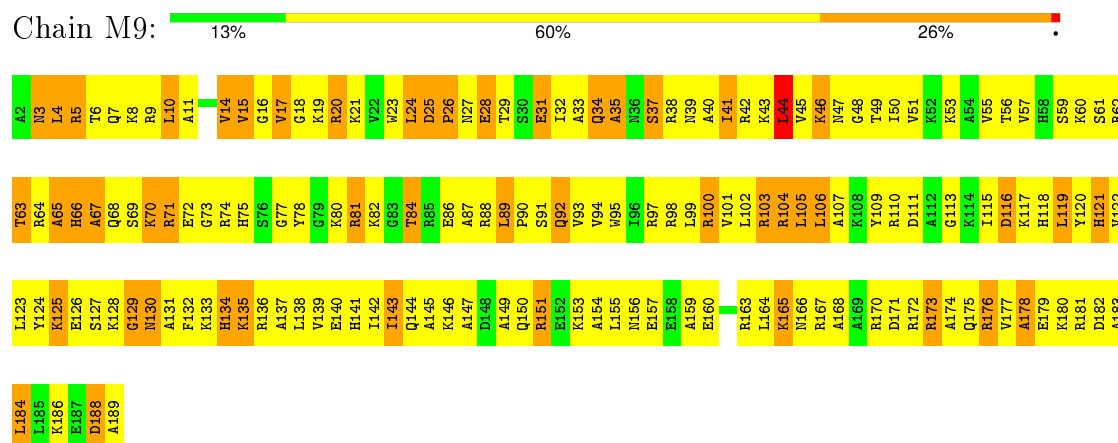
• Molecule 52: 60S ribosomal protein L16-A

Chain M6: 14% 58% 22% 6%

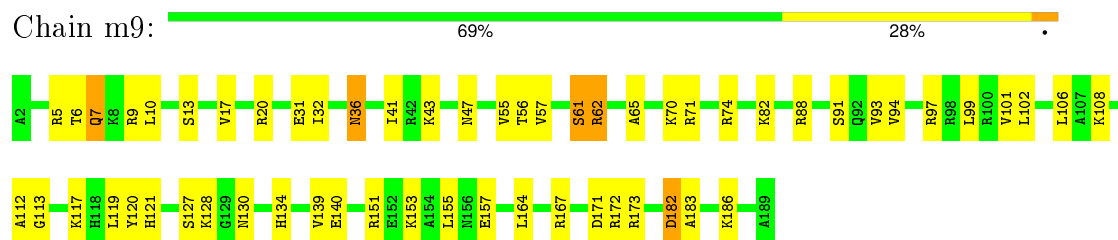




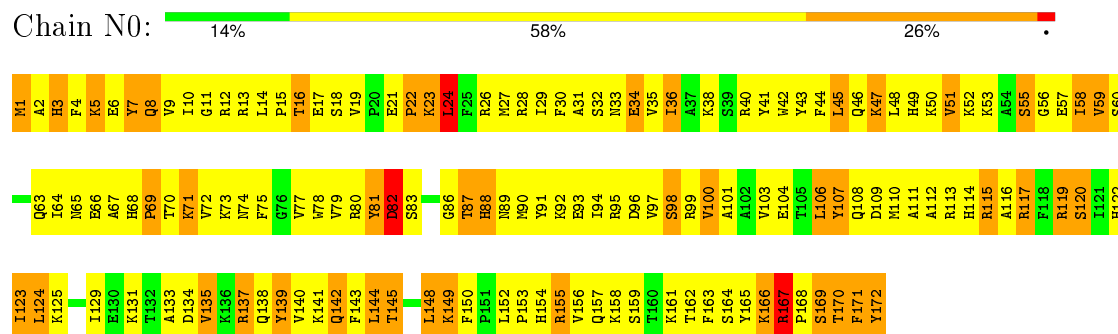
- Molecule 55: 60S ribosomal protein L19-A



- Molecule 55: 60S ribosomal protein L19-A

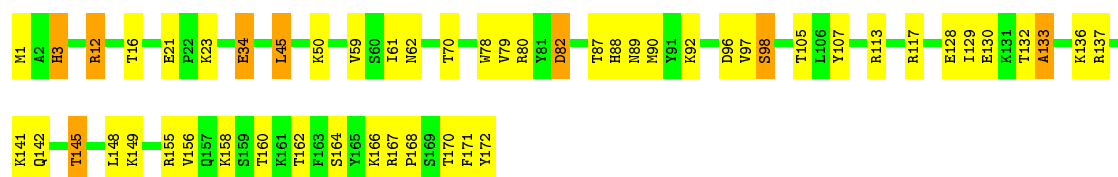


- Molecule 56: 60S ribosomal protein L20-A

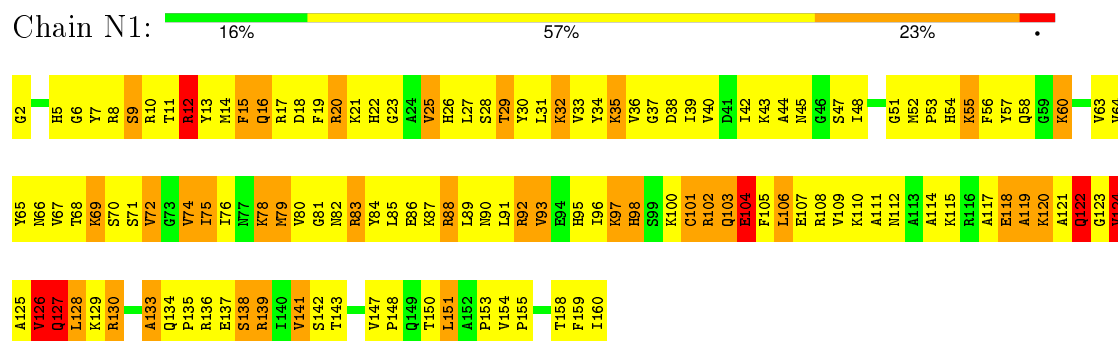


- Molecule 56: 60S ribosomal protein L20-A

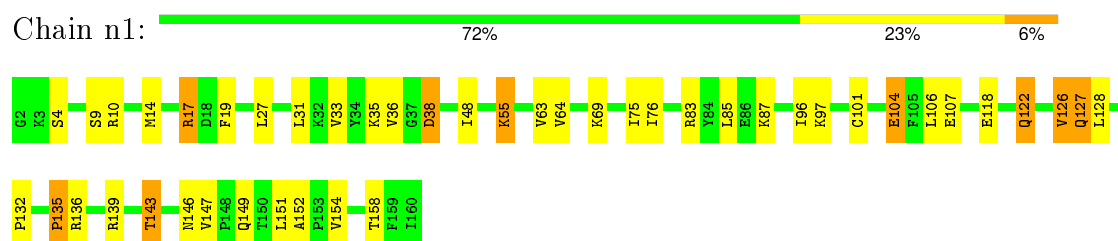




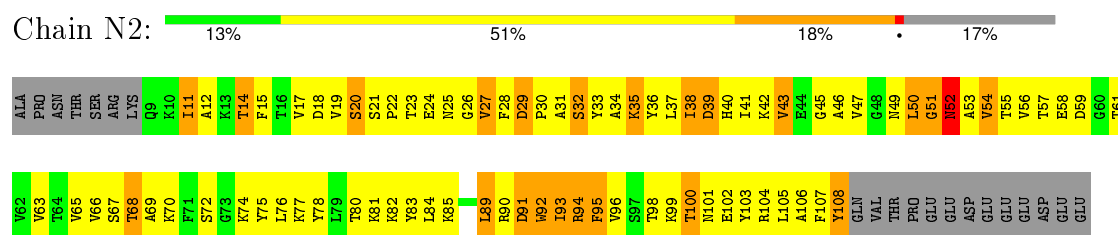
• Molecule 57: 60S ribosomal protein L21-A



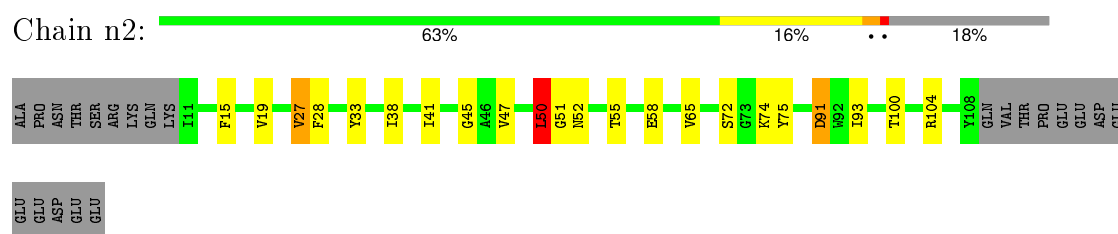
• Molecule 57: 60S ribosomal protein L21-A



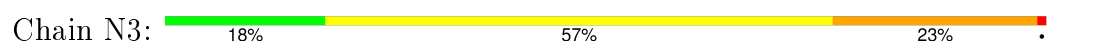
• Molecule 58: 60S ribosomal protein L22-A

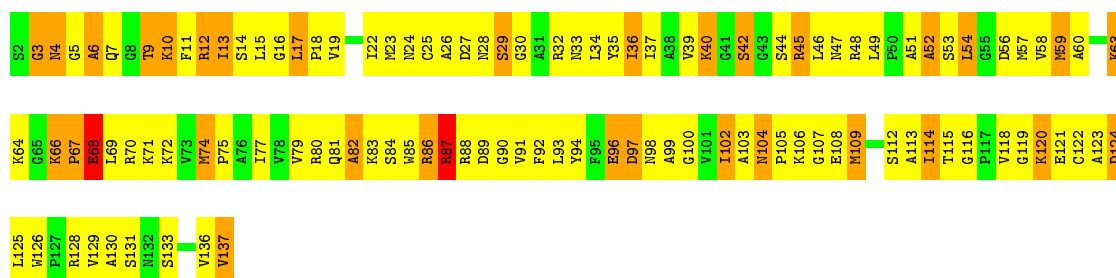


• Molecule 58: 60S ribosomal protein L22-A



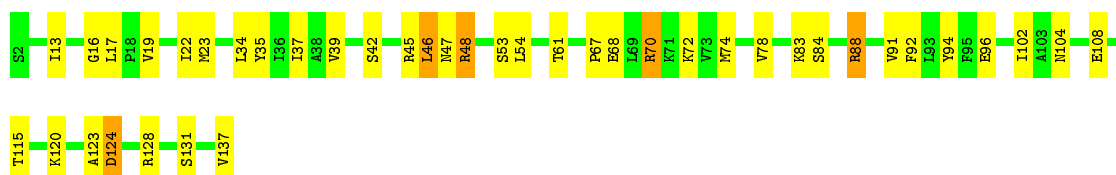
• Molecule 59: 60S ribosomal protein L23-A





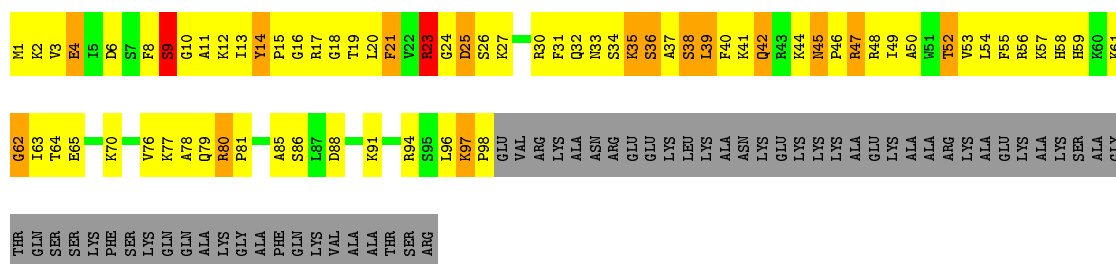
• Molecule 59: 60S ribosomal protein L23-A

Chain n3: 70% 26%



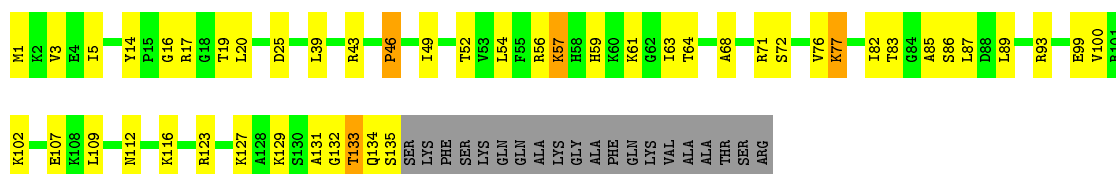
• Molecule 60: 60S ribosomal protein L24-A

Chain N4: 17% 35% 10% 37%



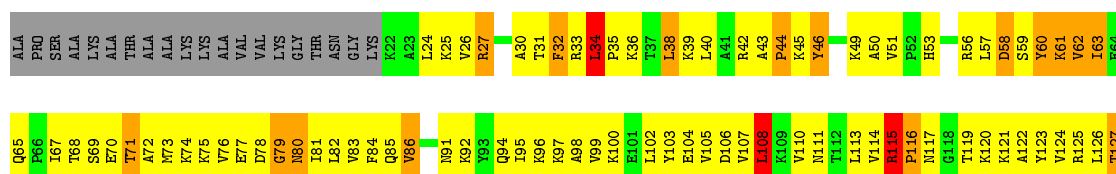
• Molecule 60: 60S ribosomal protein L24-A

Chain n4: 56% 28% 13%



• Molecule 61: 60S ribosomal protein L25

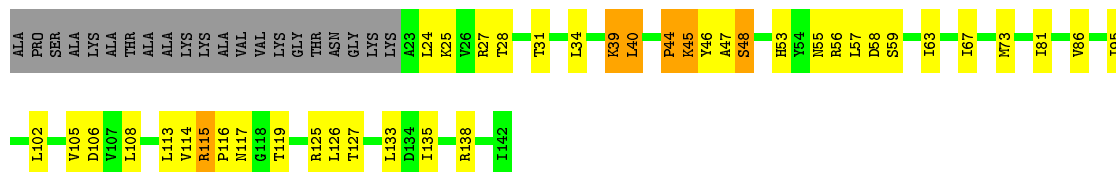
Chain N5: 17% 52% 14% 14%





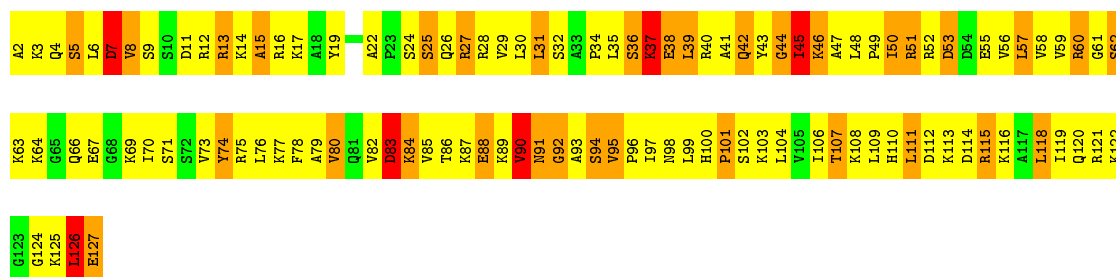
• Molecule 61: 60S ribosomal protein L25

Chain n5: 56% 25% 15%



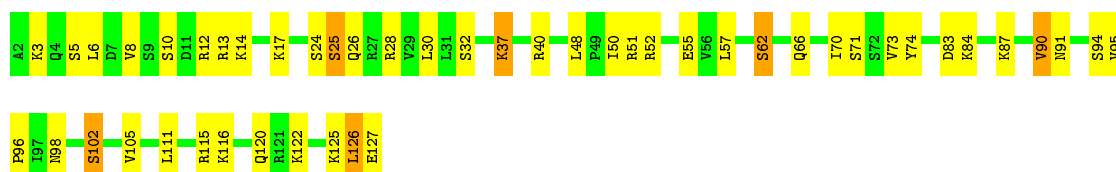
• Molecule 62: 60S ribosomal protein L26-A

Chain N6: 11% 58% 26% 5%



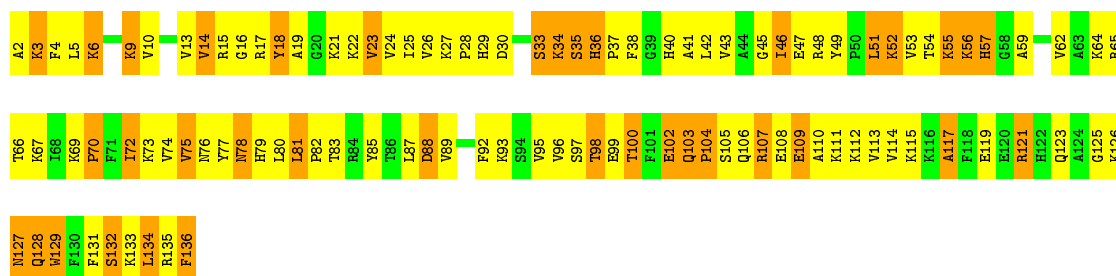
• Molecule 62: 60S ribosomal protein L26-A

Chain n6: 62% 33% 5%

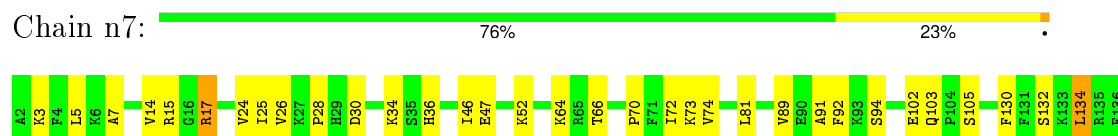


• Molecule 63: 60S ribosomal protein L27-A

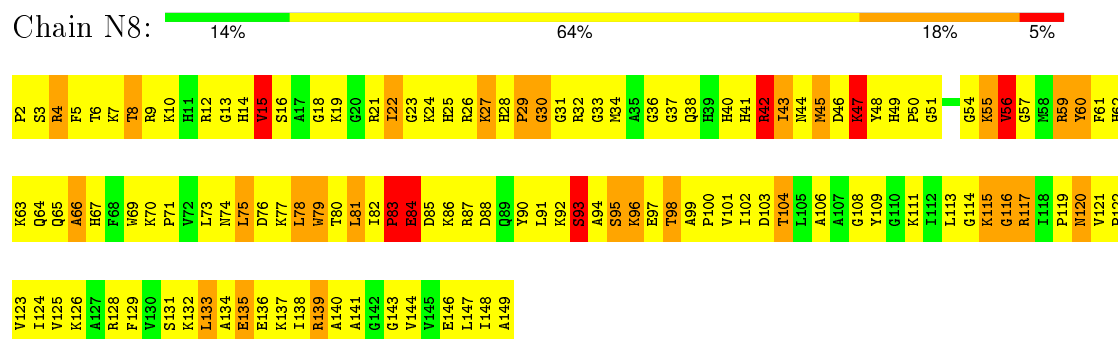
Chain N7: 21% 52% 27%



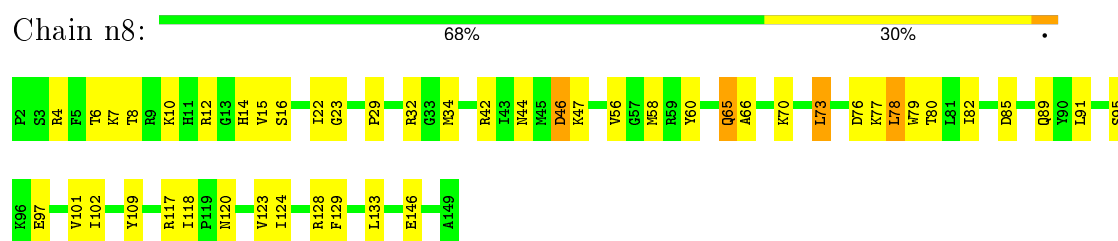
• Molecule 63: 60S ribosomal protein L27-A



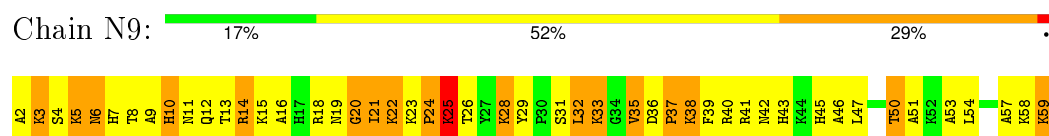
• Molecule 64: 60S ribosomal protein L28



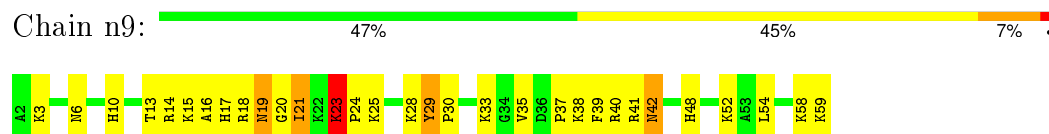
• Molecule 64: 60S ribosomal protein L28



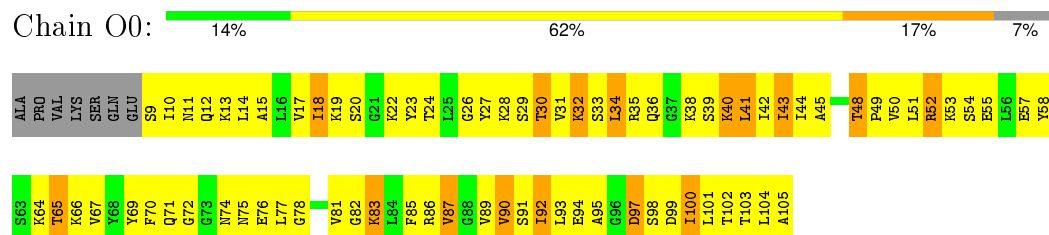
• Molecule 65: 60S ribosomal protein L29



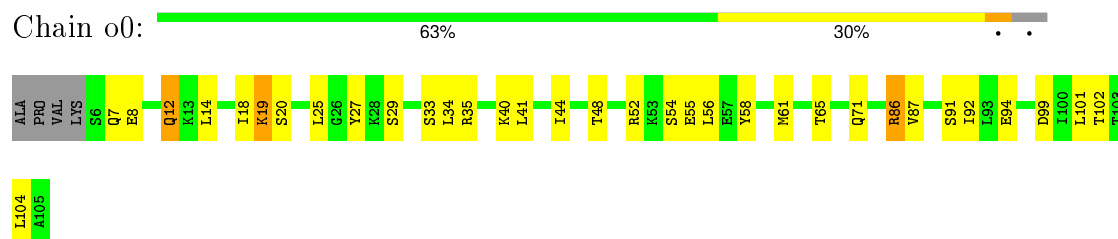
• Molecule 65: 60S ribosomal protein L29



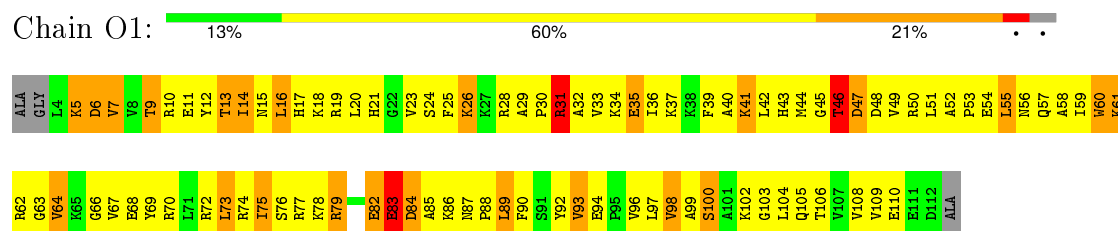
• Molecule 66: 60S ribosomal protein L30



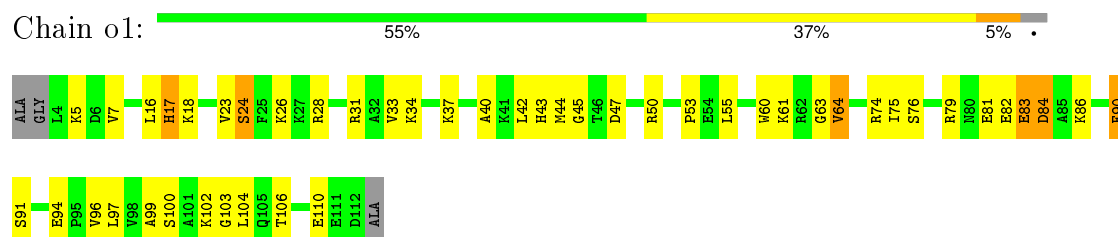
- Molecule 66: 60S ribosomal protein L30



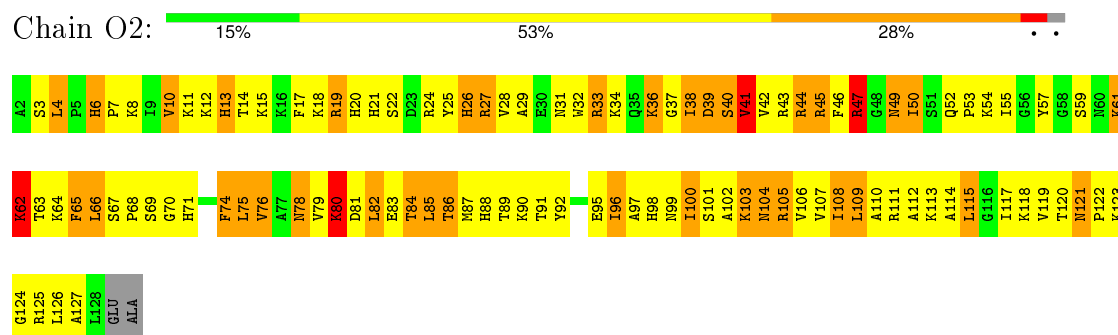
- Molecule 67: 60S ribosomal protein L31-A



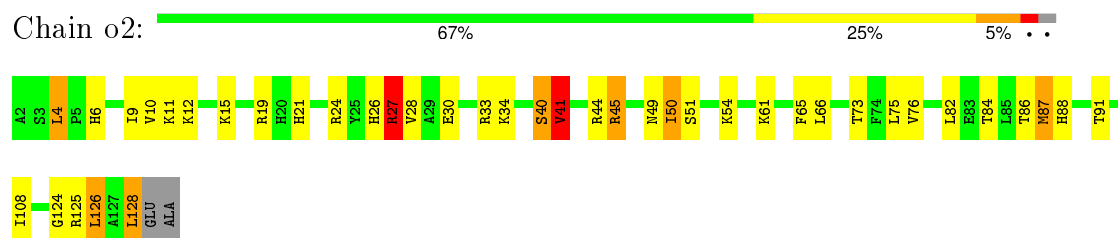
- Molecule 67: 60S ribosomal protein L31-A



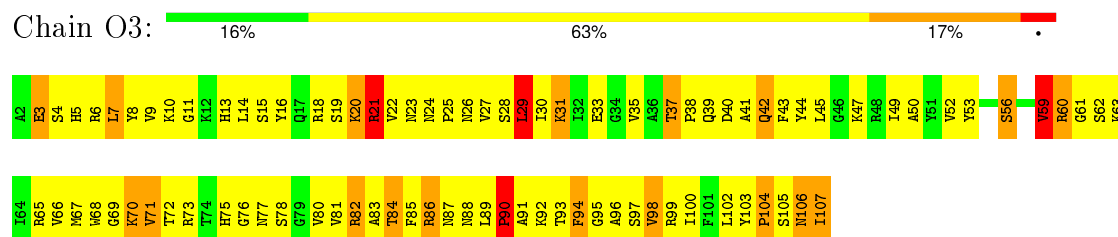
- Molecule 68: 60S ribosomal protein L32



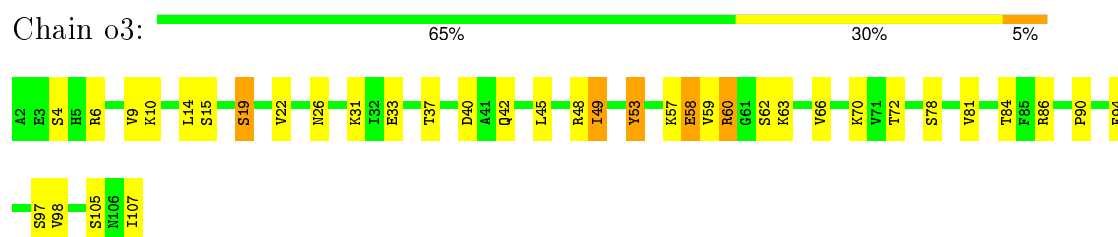
- Molecule 68: 60S ribosomal protein L32



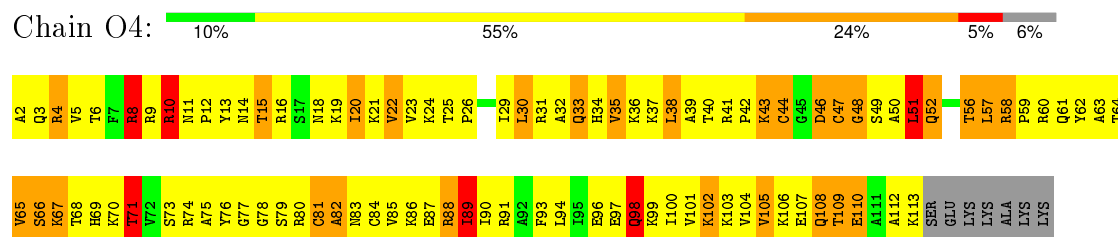
- Molecule 69: 60S ribosomal protein L33-A



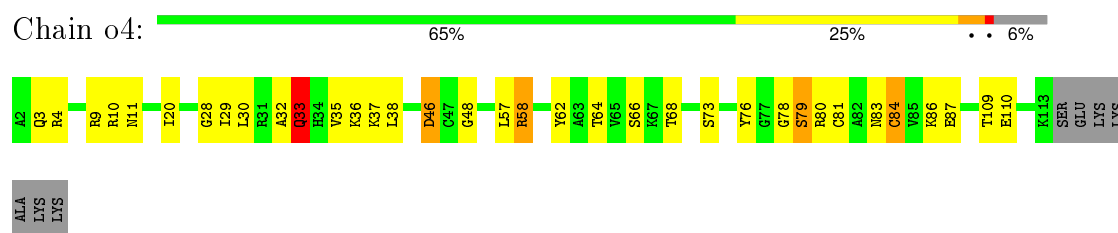
- Molecule 69: 60S ribosomal protein L33-A



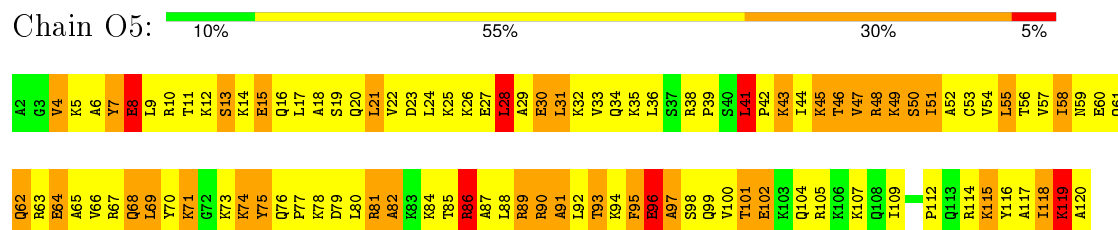
- Molecule 70: 60S ribosomal protein L34-A



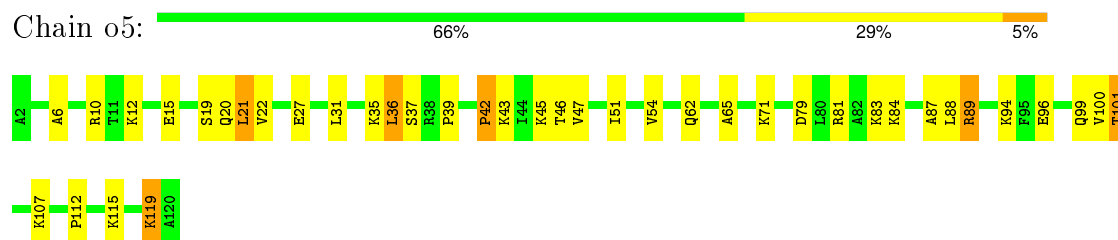
- Molecule 70: 60S ribosomal protein L34-A



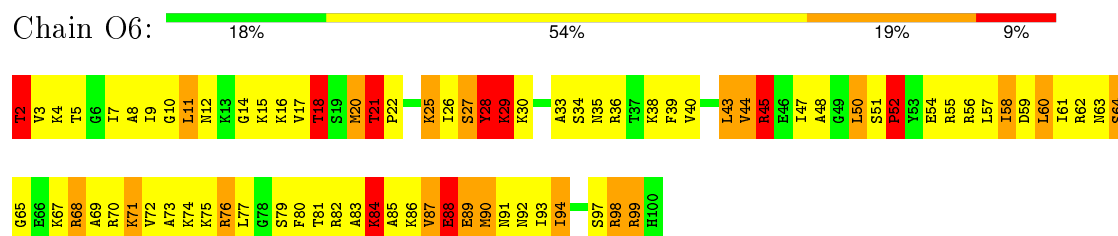
- Molecule 71: 60S ribosomal protein L35-A



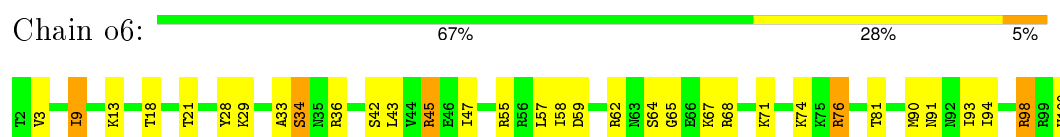
- Molecule 71: 60S ribosomal protein L35-A



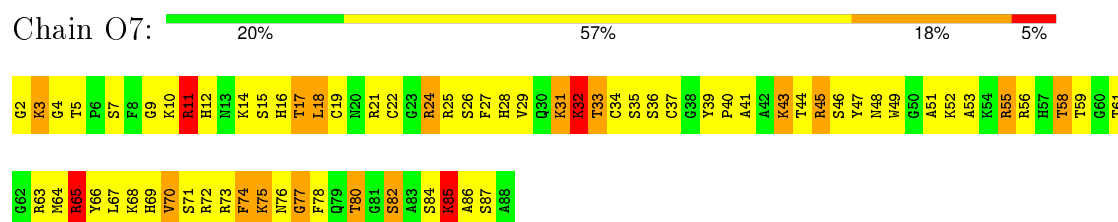
• Molecule 72: 60S ribosomal protein L36-A



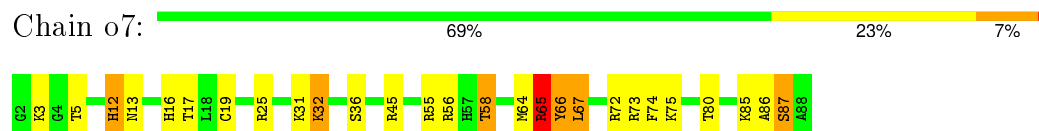
• Molecule 72: 60S ribosomal protein L36-A



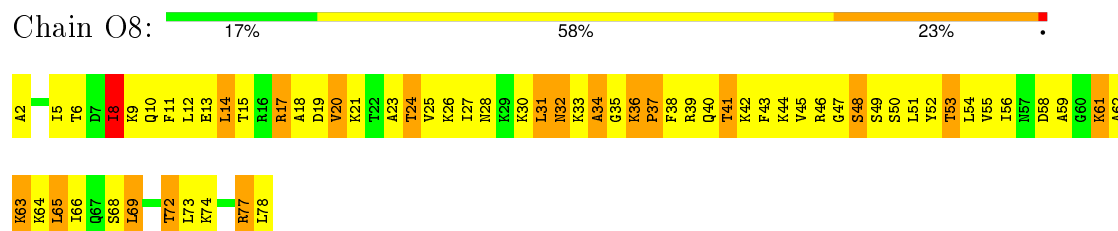
• Molecule 73: 60S ribosomal protein L37-A




• Molecule 73: 60S ribosomal protein L37-A



• Molecule 74: 60S ribosomal protein L38



- Molecule 74: 60S ribosomal protein L38

Chain o8:  77% 22%



- Molecule 75: 60S ribosomal protein L39

Chain O9:  18% 52% 28%




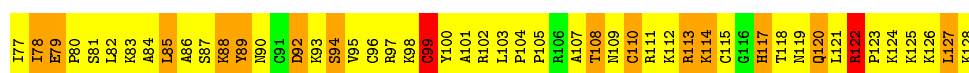
- Molecule 75: 60S ribosomal protein L39

Chain o9:  70% 30%



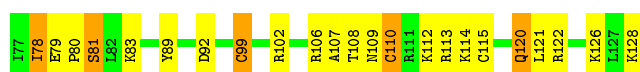
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:  6% 63% 27%



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:  56% 35% 10%



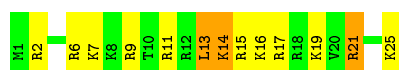
- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:  8% 52% 40%

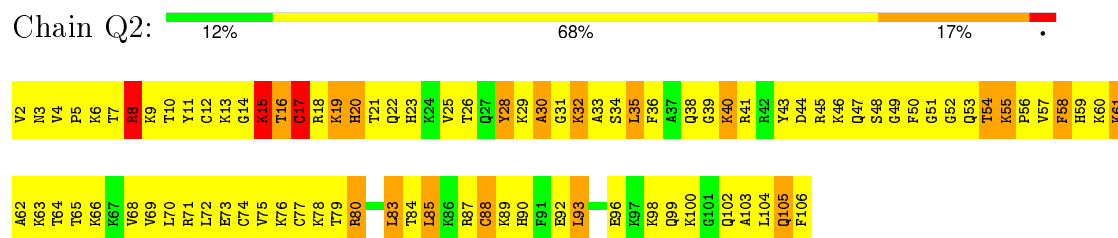


- Molecule 77: 60S ribosomal protein L41-A

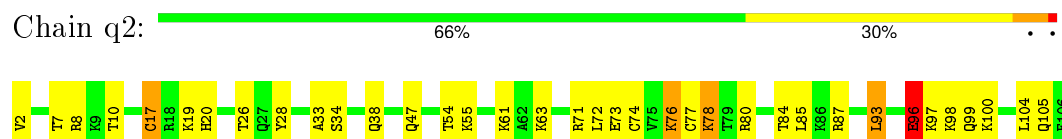
Chain q1:  48% 40% 12%



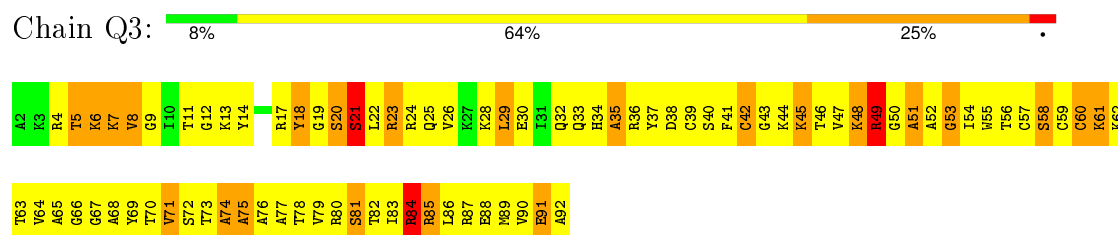
- Molecule 78: 60S ribosomal protein L42-A



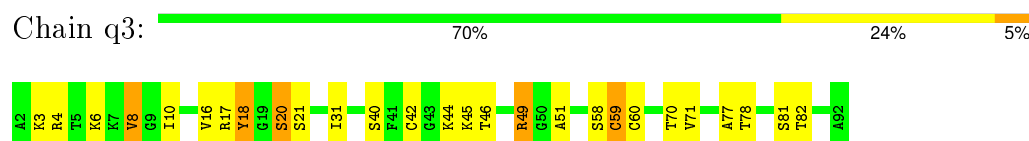
- Molecule 78: 60S ribosomal protein L42-A



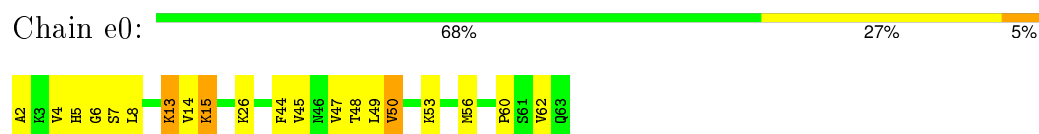
- Molecule 79: 60S ribosomal protein L43-A



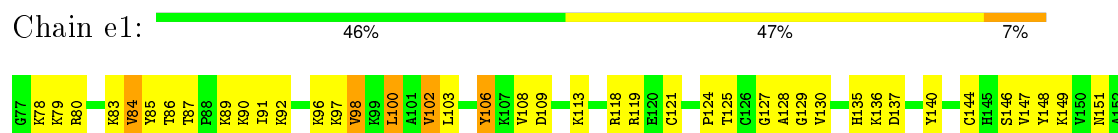
- Molecule 79: 60S ribosomal protein L43-A



- Molecule 80: 40S ribosomal protein S30-A

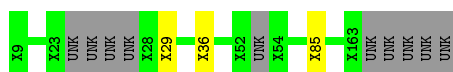


- Molecule 81: Ubiquitin-40S ribosomal protein S31



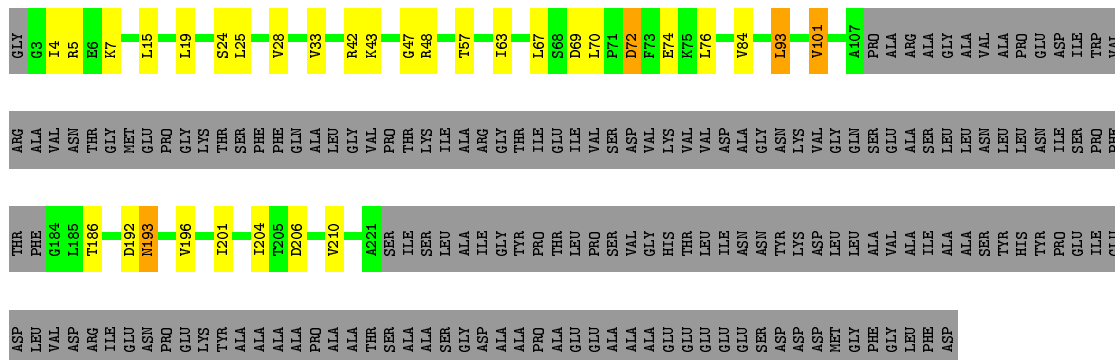
- Molecule 82: unknown protein chain m2





- Molecule 83: 60S acidic ribosomal protein P0

Chain p0: 36% 9% 54%



- Molecule 84: unknown protein chain p1

Chain p1: 100%

There are no outlier residues recorded for this chain.

- Molecule 85: unknown protein chain p2

Chain p2: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	437.00Å 286.75Å 305.18Å 90.00° 99.24° 90.00°	Depositor
Resolution (Å)	135.58 – 3.60	Depositor
% Data completeness (in resolution range)	100.0 (135.58-3.60)	Depositor
R_{merge}	0.52	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.190 , 0.267	Depositor
Wilson B-factor (Å ²)	115.6	Xtriage
Anisotropy	0.083	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 855155 reflections	Xtriage
Total number of atoms	411095	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.08	91/41698 (0.2%)	1.83	1528/64972 (2.4%)
1	6	1.44	367/42663 (0.9%)	2.19	2982/66472 (4.5%)
2	S0	0.60	0/1617	0.83	0/2215
2	s0	0.75	0/1623	0.92	1/2222 (0.0%)
3	S1	0.46	0/1735	0.74	0/2335
3	s1	0.67	0/1748	0.87	3/2352 (0.1%)
4	S2	0.74	2/1665 (0.1%)	0.90	2/2263 (0.1%)
4	s2	0.87	1/1665 (0.1%)	1.01	4/2263 (0.2%)
5	S3	0.72	0/1759	0.86	1/2368 (0.0%)
5	s3	0.72	0/1759	0.89	1/2368 (0.0%)
6	S4	0.65	0/2109	0.86	2/2839 (0.1%)
6	s4	0.77	0/2109	0.90	1/2839 (0.0%)
7	S5	0.54	0/1629	0.76	0/2202
7	s5	0.89	1/1629 (0.1%)	1.02	4/2202 (0.2%)
8	S6	0.64	0/1823	0.79	0/2439
8	s6	0.88	0/1779	0.99	2/2379 (0.1%)
9	S7	0.54	0/1506	0.75	0/2028
9	s7	0.68	0/1516	0.91	2/2043 (0.1%)
10	S8	0.79	0/1514	0.92	1/2021 (0.0%)
10	s8	0.86	0/1514	0.94	1/2021 (0.0%)
11	S9	0.65	0/1519	0.84	1/2035 (0.0%)
11	s9	0.79	0/1519	0.91	2/2035 (0.1%)
12	C0	0.66	0/790	0.86	2/1069 (0.2%)
12	c0	0.56	0/777	0.87	2/1049 (0.2%)
13	C1	0.82	0/1240	0.88	0/1675
13	c1	0.91	0/1194	1.00	2/1610 (0.1%)
14	C2	0.51	0/900	0.80	1/1224 (0.1%)
14	c2	0.46	0/900	0.69	1/1224 (0.1%)
15	C3	0.59	0/1215	0.76	0/1638
15	c3	0.80	0/1215	0.96	2/1638 (0.1%)
16	C4	0.50	0/901	0.79	0/1217
16	c4	0.76	0/960	0.91	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.69	0/998	0.81	0/1341
17	c5	0.89	0/1060	1.05	3/1426 (0.2%)
18	C6	0.60	0/1125	0.89	3/1510 (0.2%)
18	c6	0.93	0/1131	1.06	2/1518 (0.1%)
19	C7	0.59	0/935	0.87	3/1254 (0.2%)
19	c7	0.80	0/914	0.91	1/1224 (0.1%)
20	C8	0.61	0/1211	0.82	0/1628
20	c8	0.92	2/1211 (0.2%)	1.08	5/1628 (0.3%)
21	C9	0.61	0/1130	0.83	0/1517
21	c9	0.94	1/1130 (0.1%)	1.01	2/1517 (0.1%)
22	D0	0.65	0/865	0.83	0/1169
22	d0	0.79	0/892	0.97	1/1205 (0.1%)
23	D1	0.65	0/693	0.88	2/935 (0.2%)
23	d1	0.79	0/693	0.92	0/935
24	D2	0.63	0/1038	0.89	1/1395 (0.1%)
24	d2	0.88	0/1038	0.98	1/1395 (0.1%)
25	D3	0.90	1/1139 (0.1%)	1.04	1/1518 (0.1%)
25	d3	1.17	5/1139 (0.4%)	1.14	4/1518 (0.3%)
26	D4	0.66	0/1087	0.80	0/1449
26	d4	0.77	0/1087	0.92	0/1449
27	D5	0.61	0/571	0.84	0/768
27	d5	0.81	0/566	0.96	0/761
28	D6	0.66	0/782	0.84	0/1047
28	d6	0.81	0/782	0.92	1/1047 (0.1%)
29	D7	0.53	0/620	0.81	1/838 (0.1%)
29	d7	0.67	0/620	0.93	2/838 (0.2%)
30	D8	0.49	0/499	0.74	0/670
30	d8	0.76	0/499	0.97	1/670 (0.1%)
31	D9	0.75	0/452	0.86	0/600
31	d9	0.97	0/452	0.97	0/600
32	E0	0.69	0/483	0.87	0/643
33	E1	0.65	0/577	0.90	0/770
34	SR	0.54	0/2494	0.72	0/3393
34	sR	0.69	0/2495	0.85	2/3395 (0.1%)
35	SM	0.72	0/1113	0.91	2/1502 (0.1%)
35	sM	0.77	0/682	0.98	1/921 (0.1%)
36	1	1.76	1434/75394 (1.9%)	2.53	7929/117545 (6.7%)
36	5	1.87	1867/75414 (2.5%)	2.61	8463/117575 (7.2%)
37	3	1.50	28/2883 (1.0%)	2.28	214/4491 (4.8%)
37	7	2.04	91/2883 (3.2%)	2.85	410/4491 (9.1%)
38	4	1.54	29/3746 (0.8%)	2.42	331/5832 (5.7%)
38	8	1.43	34/3746 (0.9%)	2.16	250/5832 (4.3%)
39	L2	0.98	1/1948 (0.1%)	1.08	2/2617 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	l2	0.96	1/1946 (0.1%)	1.03	4/2614 (0.2%)
40	L3	1.12	3/3146 (0.1%)	1.12	11/4228 (0.3%)
40	l3	1.32	9/3146 (0.3%)	1.24	17/4228 (0.4%)
41	L4	1.03	0/2800	1.15	13/3790 (0.3%)
41	l4	1.02	1/2800 (0.0%)	1.11	5/3790 (0.1%)
42	L5	0.84	1/2425 (0.0%)	0.97	2/3271 (0.1%)
42	l5	1.16	2/2408 (0.1%)	1.08	3/3248 (0.1%)
43	L6	1.15	2/1260 (0.2%)	1.17	4/1694 (0.2%)
43	l6	1.18	2/1269 (0.2%)	1.15	3/1705 (0.2%)
44	L7	1.09	0/1821	1.13	9/2451 (0.4%)
44	l7	1.26	3/1828 (0.2%)	1.17	7/2461 (0.3%)
45	L8	0.74	0/1836	0.91	0/2481
45	l8	0.72	0/1795	0.86	1/2429 (0.0%)
46	L9	0.97	0/1539	1.07	1/2073 (0.0%)
46	l9	1.33	4/1539 (0.3%)	1.23	8/2073 (0.4%)
47	M0	1.02	4/1741 (0.2%)	1.04	1/2335 (0.0%)
47	m0	1.23	5/1758 (0.3%)	1.20	7/2358 (0.3%)
48	M1	0.80	1/1374 (0.1%)	0.93	3/1842 (0.2%)
48	m1	1.09	3/1374 (0.2%)	1.09	5/1842 (0.3%)
49	M3	0.96	2/1568 (0.1%)	1.09	4/2106 (0.2%)
49	m3	0.87	0/1573	1.02	0/2113
50	M4	1.10	0/1068	1.13	1/1438 (0.1%)
50	m4	1.30	1/1074 (0.1%)	1.15	3/1446 (0.2%)
51	M5	0.97	0/1757	1.04	5/2354 (0.2%)
51	m5	0.84	0/1757	0.93	2/2354 (0.1%)
52	M6	1.25	6/1585 (0.4%)	1.28	12/2128 (0.6%)
52	m6	1.54	9/1585 (0.6%)	1.38	14/2128 (0.7%)
53	M7	1.21	3/1443 (0.2%)	1.09	3/1944 (0.2%)
53	m7	1.18	1/1250 (0.1%)	1.19	2/1683 (0.1%)
54	M8	1.03	0/1465	1.12	5/1965 (0.3%)
54	m8	0.98	1/1465 (0.1%)	1.06	3/1965 (0.2%)
55	M9	0.84	0/1538	0.92	3/2050 (0.1%)
55	m9	0.88	1/1538 (0.1%)	0.92	2/2050 (0.1%)
56	N0	1.05	0/1481	1.10	5/1990 (0.3%)
56	n0	1.46	7/1481 (0.5%)	1.21	5/1990 (0.3%)
57	N1	1.09	1/1300 (0.1%)	1.10	4/1743 (0.2%)
57	n1	1.28	6/1300 (0.5%)	1.17	5/1743 (0.3%)
58	N2	0.73	1/812 (0.1%)	0.89	1/1099 (0.1%)
58	n2	0.73	0/794	0.84	1/1076 (0.1%)
59	N3	1.09	2/1018 (0.2%)	1.07	3/1369 (0.2%)
59	n3	1.35	7/1018 (0.7%)	1.28	7/1369 (0.5%)
60	N4	0.90	0/712	0.98	1/958 (0.1%)
60	n4	1.04	0/1052	1.04	0/1398

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
61	N5	0.86	1/979 (0.1%)	1.00	4/1321 (0.3%)
61	n5	0.85	0/974	1.03	2/1314 (0.2%)
62	N6	0.92	0/1004	1.11	6/1341 (0.4%)
62	n6	0.89	0/1004	1.02	5/1341 (0.4%)
63	N7	0.68	0/1118	0.89	1/1497 (0.1%)
63	n7	0.67	0/1118	0.83	0/1497
64	N8	1.05	0/1204	1.10	5/1612 (0.3%)
64	n8	0.98	1/1204 (0.1%)	1.08	2/1612 (0.1%)
65	N9	0.98	0/473	1.07	1/629 (0.2%)
65	n9	1.12	1/473 (0.2%)	1.33	3/629 (0.5%)
66	O0	0.71	0/751	0.87	0/1008
66	o0	0.69	0/775	0.88	2/1040 (0.2%)
67	O1	0.90	0/890	1.00	1/1196 (0.1%)
67	o1	1.13	2/897 (0.2%)	1.20	3/1205 (0.2%)
68	O2	1.21	2/1041 (0.2%)	1.20	4/1394 (0.3%)
68	o2	1.15	2/1041 (0.2%)	1.13	5/1394 (0.4%)
69	O3	1.32	2/868 (0.2%)	1.23	3/1168 (0.3%)
69	o3	1.38	3/868 (0.3%)	1.19	2/1168 (0.2%)
70	O4	0.84	0/890	1.00	4/1189 (0.3%)
70	o4	0.83	1/890 (0.1%)	0.99	2/1189 (0.2%)
71	O5	0.98	2/978 (0.2%)	1.09	2/1301 (0.2%)
71	o5	0.82	0/974	0.89	1/1297 (0.1%)
72	O6	0.84	0/778	0.98	1/1034 (0.1%)
72	o6	0.79	0/777	0.98	1/1033 (0.1%)
73	O7	1.08	0/696	1.20	4/923 (0.4%)
73	o7	0.99	0/696	1.07	3/923 (0.3%)
74	O8	0.72	0/618	0.84	0/826
74	o8	0.66	0/614	0.90	0/822
75	O9	1.05	0/443	1.19	3/588 (0.5%)
75	o9	0.82	0/443	0.99	0/588
76	Q0	1.04	2/423 (0.5%)	1.14	1/562 (0.2%)
76	q0	1.58	3/423 (0.7%)	1.44	5/562 (0.9%)
77	Q1	0.76	0/234	1.11	2/300 (0.7%)
77	q1	1.03	0/234	1.30	3/300 (1.0%)
78	Q2	1.12	1/860 (0.1%)	1.07	2/1136 (0.2%)
78	q2	1.13	2/860 (0.2%)	1.09	2/1136 (0.2%)
79	Q3	1.04	0/701	1.10	3/934 (0.3%)
79	q3	1.07	1/701 (0.1%)	1.05	0/934
80	e0	0.81	0/499	0.95	0/665
81	e1	0.51	0/619	0.87	0/822
83	p0	0.75	0/1091	0.85	0/1472
All	All	1.39	4070/429970 (0.9%)	1.97	22469/631198 (3.6%)

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
2	S0	0	2
2	s0	0	2
3	s1	0	3
5	S3	0	2
5	s3	0	2
6	s4	0	2
7	s5	0	3
9	s7	0	1
11	S9	0	2
11	s9	0	1
12	C0	0	2
15	c3	0	1
16	C4	0	1
17	c5	0	1
18	C6	0	1
18	c6	0	3
19	C7	0	1
19	c7	0	2
20	c8	0	1
21	c9	0	1
22	d0	0	1
23	D1	0	1
24	D2	0	1
24	d2	0	2
25	D3	0	2
26	D4	0	1
26	d4	0	2
27	D5	0	1
27	d5	0	1
28	D6	0	1
28	d6	0	1
33	E1	0	2
35	SM	0	1
39	l2	0	2
40	L3	0	3
40	l3	0	5
41	L4	0	5
41	l4	0	2
42	L5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	l5	0	3
43	L6	0	2
43	l6	0	1
44	L7	0	2
44	l7	0	3
45	l8	0	1
47	M0	0	2
47	m0	0	1
48	m1	0	1
49	m3	0	2
52	M6	0	2
52	m6	0	2
53	M7	0	1
53	m7	0	2
54	m8	0	1
56	n0	0	2
57	N1	0	1
57	n1	0	1
60	n4	0	1
61	n5	0	1
63	N7	0	2
64	N8	0	4
64	n8	0	2
65	N9	0	2
65	n9	0	1
67	o1	0	1
68	o2	0	2
69	O3	0	2
70	O4	0	2
70	o4	0	2
72	O6	0	1
76	q0	0	1
80	e0	0	2
81	e1	0	1
82	m2	0	3
83	p0	0	1
All	All	0	130

The worst 5 of 4070 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	15.17	2.08	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	806	A	N9-C4	-14.79	1.28	1.37
37	7	89	G	C6-O6	14.62	1.37	1.24
36	5	2397	A	N9-C4	-14.38	1.29	1.37
36	5	2875	U	N1-C2	13.97	1.51	1.38

The worst 5 of 22469 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-25.15	110.91	126.00
37	7	44	C	C6-N1-C2	24.27	130.01	120.30
36	5	648	C	N3-C4-C5	-23.62	112.45	121.90
36	5	884	A	N1-C6-N6	23.07	132.44	118.60
38	4	94	C	C6-N1-C2	22.99	129.50	120.30

There are no chirality outliers.

5 of 130 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	S0	29	VAL	Peptide
2	S0	6	THR	Peptide
5	S3	144	ALA	Peptide
5	S3	42	THR	Peptide
11	S9	15	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37283	0	18756	1861	1
1	6	38149	0	19193	1847	0
2	S0	1577	0	1567	285	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	250	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	294	0
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	255	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	301	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	285	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	249	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	204	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	248	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	265	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	130	0
12	c0	762	0	699	0	0
13	C1	1214	0	1259	170	0
13	c1	1168	0	1231	0	0
14	C2	892	0	891	121	0
14	c2	892	0	891	0	0
15	C3	1192	0	1255	184	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	189	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	193	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	215	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	152	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	227	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	199	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	149	0
22	d0	882	0	939	0	1
23	D1	684	0	672	140	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	148	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	190	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	180	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	d4	1073	0	1132	0	0
27	D5	563	0	603	94	0
27	d5	558	0	598	0	0
28	D6	769	0	815	167	0
28	d6	769	0	814	0	0
29	D7	610	0	632	87	0
29	d7	610	0	632	0	0
30	D8	497	0	535	65	0
30	d8	497	0	535	0	0
31	D9	442	0	428	83	0
31	d9	442	0	428	0	0
32	E0	475	0	525	71	0
33	E1	566	0	601	93	0
34	SR	2441	0	2397	334	0
34	sR	2442	0	2392	0	2
35	SM	1104	0	996	156	0
35	sM	679	0	603	0	0
36	1	67355	0	33811	2977	1
36	5	67376	0	33824	2966	0
37	3	2579	0	1304	98	0
37	7	2579	0	1302	119	0
38	4	3353	0	1695	182	0
38	8	3353	0	1695	176	0
39	L2	1914	0	1981	336	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	507	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	484	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	406	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	196	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	321	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	278	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	271	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1736	322	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	221	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	268	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	190	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	279	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	285	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	228	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	236	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	258	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	224	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	232	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	104	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	144	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	90	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	145	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	174	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	166	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	231	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	81	0
65	n9	462	0	491	0	0
66	O0	743	0	797	113	0
66	o0	767	0	816	0	0
67	O1	876	0	912	142	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	157	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	153	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	o3	850	0	880	0	0
70	O4	880	0	945	171	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	177	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	155	0
72	o6	770	0	846	0	0
73	O7	681	0	684	117	0
73	o7	681	0	685	0	0
74	O8	612	0	682	93	0
74	o8	608	0	671	0	0
75	O9	436	0	475	86	0
75	o9	436	0	475	0	0
76	Q0	417	0	456	91	0
76	q0	417	0	456	0	0
77	Q1	233	0	284	44	0
77	q1	233	0	284	0	0
78	Q2	847	0	916	135	0
78	q2	847	0	914	0	0
79	Q3	694	0	734	134	0
79	q3	694	0	734	0	0
80	e0	491	0	542	0	0
81	e1	608	0	656	0	0
82	m2	750	0	175	0	0
83	p0	1076	0	1040	0	0
84	p1	235	0	51	0	0
85	p2	230	0	52	0	0
86	1	468	0	0	0	0
86	2	124	0	0	0	0
86	3	14	0	0	0	0
86	4	23	0	0	0	0
86	5	499	0	0	0	0
86	6	150	0	0	0	0
86	7	15	0	0	0	0
86	8	17	0	0	0	0
86	D3	1	0	0	0	0
86	D4	1	0	0	0	0
86	L2	2	0	0	0	0
86	L3	2	0	0	0	0
86	L4	2	0	0	0	0
86	L5	1	0	0	0	0
86	L6	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	L7	2	0	0	0	0
86	L8	1	0	0	0	0
86	M0	3	0	0	0	0
86	M1	1	0	0	0	0
86	M3	2	0	0	0	0
86	M5	2	0	0	0	0
86	M6	1	0	0	0	0
86	M7	5	0	0	0	0
86	M9	1	0	0	0	0
86	N0	1	0	0	0	0
86	N3	2	0	0	0	0
86	N5	2	0	0	0	0
86	N6	1	0	0	0	0
86	N8	4	0	0	0	0
86	N9	1	0	0	0	0
86	O1	1	0	0	0	0
86	O2	1	0	0	0	0
86	O3	1	0	0	0	0
86	O5	1	0	0	0	0
86	O7	1	0	0	0	0
86	S2	2	0	0	0	0
86	S8	1	0	0	0	0
86	SM	1	0	0	0	0
86	c7	1	0	0	0	0
86	c8	1	0	0	0	0
86	d3	1	0	0	0	0
86	d6	1	0	0	0	0
86	l2	1	0	0	0	0
86	l3	6	0	0	0	0
86	l4	1	0	0	0	0
86	l5	3	0	0	0	0
86	l7	2	0	0	0	0
86	l9	1	0	0	0	0
86	m0	1	0	0	0	0
86	m1	1	0	0	0	0
86	m4	1	0	0	0	0
86	m5	2	0	0	0	0
86	m6	3	0	0	0	0
86	m7	4	0	0	0	0
86	n3	1	0	0	0	0
86	n4	1	0	0	0	0
86	n8	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	n9	2	0	0	0	0
86	o0	1	0	0	0	0
86	o1	1	0	0	0	0
86	o2	1	0	0	0	0
86	o3	2	0	0	0	0
86	o4	1	0	0	0	0
86	q0	2	0	0	0	0
86	q1	1	0	0	0	0
86	q3	2	0	0	0	0
86	s1	1	0	0	0	0
86	s2	1	0	0	0	0
86	s8	2	0	0	0	0
87	1	2429	0	0	266	1
87	2	1099	0	0	117	0
87	3	77	0	0	5	0
87	4	119	0	0	10	0
87	5	2471	0	0	263	0
87	6	1134	0	0	132	0
87	7	77	0	0	4	0
87	8	126	0	0	13	0
87	C3	7	0	0	1	0
87	C5	7	0	0	5	0
87	C8	7	0	0	0	0
87	D3	7	0	0	0	0
87	D9	7	0	0	0	0
87	L3	21	0	0	1	0
87	L4	7	0	0	0	0
87	M0	7	0	0	0	0
87	M5	7	0	0	2	0
87	M6	7	0	0	0	0
87	M7	7	0	0	1	0
87	M9	14	0	0	2	0
87	N9	7	0	0	0	0
87	O1	7	0	0	6	0
87	O2	7	0	0	0	0
87	O3	7	0	0	1	0
87	O7	14	0	0	3	0
87	Q2	7	0	0	3	0
87	S8	7	0	0	1	0
87	SR	7	0	0	0	0
87	c3	7	0	0	0	0
87	c5	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	c8	7	0	0	0	0
87	d4	7	0	0	0	0
87	d9	7	0	0	0	0
87	l3	14	0	0	0	0
87	l4	14	0	0	0	0
87	l5	28	0	0	0	0
87	l9	7	0	0	0	0
87	m0	14	0	0	0	0
87	m1	7	0	0	0	0
87	m4	7	0	0	0	0
87	m5	7	0	0	0	0
87	m7	7	0	0	0	0
87	m9	7	0	0	0	0
87	n3	7	0	0	0	0
87	n9	7	0	0	0	0
87	o3	7	0	0	0	0
87	o7	7	0	0	0	0
87	o9	7	0	0	0	0
87	q1	7	0	0	0	0
87	q2	7	0	0	0	0
87	s1	7	0	0	0	0
87	s8	7	0	0	0	0
87	sR	7	0	0	0	0
88	2	34	0	40	9	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	1	0
89	Q0	1	0	0	1	0
89	Q2	1	0	0	2	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
All	All	411095	0	297211	21971	3

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 32.

The worst 5 of 21971 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)
25:D3:63:GLN:CB	25:D3:63:GLN:CG	1.55	1.57
78:Q2:17:CYS:SG	78:Q2:17:CYS:CB	2.08	1.40
1:2:1754:A:HO2'	32:E0:2:ALA:N	1.52	1.08
78:Q2:17:CYS:SG	78:Q2:77:CYS:HB3	2.80	1.07
36:1:883:A:H5'	53:M7:133:HIS:HA	1.35	1.07

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1491:U:O2'	22:d0:12:GLN:OE1[1_454]	2.02	0.18
36:1:3154:C:N4	34:sR:77:GLY:O[2_656]	2.15	0.05
34:sR:160:GLU:OE2	87:1:4023:OHX:N4[2_646]	2.17	0.03

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%)	137 (67%)	42 (21%)	25 (12%)	0	8
2	s0	204/251 (81%)	139 (68%)	31 (15%)	34 (17%)	0	4
3	S1	212/254 (84%)	142 (67%)	42 (20%)	28 (13%)	0	6
3	s1	214/254 (84%)	155 (72%)	39 (18%)	20 (9%)	1	13
4	S2	215/253 (85%)	148 (69%)	47 (22%)	20 (9%)	1	13
4	s2	215/253 (85%)	156 (73%)	30 (14%)	29 (14%)	0	6
5	S3	221/239 (92%)	154 (70%)	48 (22%)	19 (9%)	1	14
5	s3	221/239 (92%)	147 (66%)	51 (23%)	23 (10%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	S4	258/260 (99%)	184 (71%)	44 (17%)	30 (12%)	0	9
6	s4	258/260 (99%)	175 (68%)	53 (20%)	30 (12%)	0	9
7	S5	204/224 (91%)	129 (63%)	46 (22%)	29 (14%)	0	5
7	s5	204/224 (91%)	124 (61%)	51 (25%)	29 (14%)	0	5
8	S6	224/236 (95%)	166 (74%)	37 (16%)	21 (9%)	1	12
8	s6	216/236 (92%)	165 (76%)	36 (17%)	15 (7%)	1	20
9	S7	182/189 (96%)	131 (72%)	35 (19%)	16 (9%)	1	14
9	s7	184/189 (97%)	126 (68%)	37 (20%)	21 (11%)	0	9
10	S8	184/200 (92%)	132 (72%)	32 (17%)	20 (11%)	0	9
10	s8	184/200 (92%)	144 (78%)	26 (14%)	14 (8%)	1	17
11	S9	183/196 (93%)	128 (70%)	36 (20%)	19 (10%)	1	11
11	s9	183/196 (93%)	122 (67%)	42 (23%)	19 (10%)	1	11
12	C0	94/105 (90%)	54 (57%)	21 (22%)	19 (20%)	0	2
12	c0	92/105 (88%)	56 (61%)	17 (18%)	19 (21%)	0	2
13	C1	153/155 (99%)	113 (74%)	22 (14%)	18 (12%)	0	8
13	c1	144/155 (93%)	108 (75%)	20 (14%)	16 (11%)	0	9
14	C2	122/142 (86%)	71 (58%)	22 (18%)	29 (24%)	0	1
14	c2	122/142 (86%)	65 (53%)	36 (30%)	21 (17%)	0	3
15	C3	148/150 (99%)	107 (72%)	29 (20%)	12 (8%)	1	15
15	c3	148/150 (99%)	95 (64%)	28 (19%)	25 (17%)	0	3
16	C4	125/136 (92%)	80 (64%)	25 (20%)	20 (16%)	0	4
16	c4	126/136 (93%)	90 (71%)	24 (19%)	12 (10%)	1	12
17	C5	122/141 (86%)	78 (64%)	26 (21%)	18 (15%)	0	5
17	c5	133/141 (94%)	75 (56%)	29 (22%)	29 (22%)	0	1
18	C6	139/142 (98%)	105 (76%)	22 (16%)	12 (9%)	1	14
18	c6	140/142 (99%)	97 (69%)	24 (17%)	19 (14%)	0	6
19	C7	116/136 (85%)	76 (66%)	22 (19%)	18 (16%)	0	4
19	c7	113/136 (83%)	73 (65%)	29 (26%)	11 (10%)	1	12
20	C8	143/145 (99%)	107 (75%)	27 (19%)	9 (6%)	2	23
20	c8	143/145 (99%)	98 (68%)	27 (19%)	18 (13%)	0	7
21	C9	141/143 (99%)	99 (70%)	31 (22%)	11 (8%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	c9	141/143 (99%)	98 (70%)	36 (26%)	7 (5%)	3	29
22	D0	105/120 (88%)	74 (70%)	22 (21%)	9 (9%)	1	14
22	d0	108/120 (90%)	75 (69%)	15 (14%)	18 (17%)	0	4
23	D1	85/87 (98%)	53 (62%)	18 (21%)	14 (16%)	0	4
23	d1	85/87 (98%)	64 (75%)	14 (16%)	7 (8%)	1	15
24	D2	127/129 (98%)	91 (72%)	28 (22%)	8 (6%)	2	23
24	d2	127/129 (98%)	105 (83%)	17 (13%)	5 (4%)	4	36
25	D3	142/144 (99%)	87 (61%)	29 (20%)	26 (18%)	0	3
25	d3	142/144 (99%)	119 (84%)	16 (11%)	7 (5%)	3	29
26	D4	132/134 (98%)	98 (74%)	25 (19%)	9 (7%)	1	21
26	d4	132/134 (98%)	101 (76%)	17 (13%)	14 (11%)	0	10
27	D5	68/107 (64%)	43 (63%)	16 (24%)	9 (13%)	0	6
27	d5	67/107 (63%)	45 (67%)	14 (21%)	8 (12%)	0	8
28	D6	95/97 (98%)	53 (56%)	18 (19%)	24 (25%)	0	1
28	d6	95/97 (98%)	71 (75%)	16 (17%)	8 (8%)	1	15
29	D7	79/81 (98%)	58 (73%)	14 (18%)	7 (9%)	1	13
29	d7	79/81 (98%)	61 (77%)	11 (14%)	7 (9%)	1	13
30	D8	61/66 (92%)	45 (74%)	11 (18%)	5 (8%)	1	15
30	d8	61/66 (92%)	39 (64%)	14 (23%)	8 (13%)	0	7
31	D9	51/55 (93%)	32 (63%)	11 (22%)	8 (16%)	0	4
31	d9	51/55 (93%)	35 (69%)	8 (16%)	8 (16%)	0	4
32	E0	58/60 (97%)	34 (59%)	16 (28%)	8 (14%)	0	6
33	E1	69/76 (91%)	39 (56%)	13 (19%)	17 (25%)	0	1
34	SR	316/318 (99%)	237 (75%)	56 (18%)	23 (7%)	1	18
34	sR	316/318 (99%)	251 (79%)	46 (15%)	19 (6%)	2	24
35	SM	155/273 (57%)	90 (58%)	40 (26%)	25 (16%)	0	4
35	sM	98/273 (36%)	59 (60%)	20 (20%)	19 (19%)	0	2
39	L2	250/253 (99%)	197 (79%)	31 (12%)	22 (9%)	1	14
39	l2	250/253 (99%)	192 (77%)	42 (17%)	16 (6%)	2	23
40	L3	384/386 (100%)	290 (76%)	63 (16%)	31 (8%)	1	15
40	l3	384/386 (100%)	299 (78%)	53 (14%)	32 (8%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	L4	359/361 (99%)	260 (72%)	62 (17%)	37 (10%)	1	11
41	l4	359/361 (99%)	251 (70%)	68 (19%)	40 (11%)	0	9
42	L5	294/296 (99%)	200 (68%)	58 (20%)	36 (12%)	0	8
42	l5	292/296 (99%)	221 (76%)	44 (15%)	27 (9%)	1	13
43	L6	152/175 (87%)	123 (81%)	17 (11%)	12 (8%)	1	16
43	l6	153/175 (87%)	107 (70%)	27 (18%)	19 (12%)	0	8
44	L7	220/243 (90%)	154 (70%)	45 (20%)	21 (10%)	1	12
44	l7	221/243 (91%)	165 (75%)	34 (15%)	22 (10%)	1	11
45	L8	231/255 (91%)	137 (59%)	65 (28%)	29 (13%)	0	7
45	l8	229/255 (90%)	155 (68%)	52 (23%)	22 (10%)	1	12
46	L9	189/191 (99%)	137 (72%)	30 (16%)	22 (12%)	0	9
46	l9	189/191 (99%)	142 (75%)	27 (14%)	20 (11%)	0	10
47	M0	207/220 (94%)	148 (72%)	38 (18%)	21 (10%)	1	11
47	m0	209/220 (95%)	149 (71%)	41 (20%)	19 (9%)	1	13
48	M1	167/173 (96%)	116 (70%)	27 (16%)	24 (14%)	0	5
48	m1	167/173 (96%)	120 (72%)	27 (16%)	20 (12%)	0	8
49	M3	191/198 (96%)	134 (70%)	46 (24%)	11 (6%)	2	25
49	m3	192/198 (97%)	126 (66%)	37 (19%)	29 (15%)	0	5
50	M4	134/137 (98%)	97 (72%)	25 (19%)	12 (9%)	1	13
50	m4	135/137 (98%)	92 (68%)	35 (26%)	8 (6%)	2	24
51	M5	201/203 (99%)	151 (75%)	38 (19%)	12 (6%)	2	24
51	m5	201/203 (99%)	151 (75%)	35 (17%)	15 (8%)	1	17
52	M6	195/198 (98%)	146 (75%)	36 (18%)	13 (7%)	1	21
52	m6	195/198 (98%)	151 (77%)	26 (13%)	18 (9%)	1	13
53	M7	181/183 (99%)	128 (71%)	34 (19%)	19 (10%)	1	10
53	m7	153/183 (84%)	111 (72%)	29 (19%)	13 (8%)	1	14
54	M8	183/185 (99%)	132 (72%)	36 (20%)	15 (8%)	1	15
54	m8	183/185 (99%)	134 (73%)	36 (20%)	13 (7%)	1	19
55	M9	186/188 (99%)	136 (73%)	33 (18%)	17 (9%)	1	13
55	m9	186/188 (99%)	125 (67%)	40 (22%)	21 (11%)	0	9
56	N0	170/172 (99%)	139 (82%)	21 (12%)	10 (6%)	2	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	n0	170/172 (99%)	145 (85%)	16 (9%)	9 (5%)	2	27
57	N1	157/159 (99%)	115 (73%)	28 (18%)	14 (9%)	1	13
57	n1	157/159 (99%)	121 (77%)	27 (17%)	9 (6%)	2	25
58	N2	98/120 (82%)	65 (66%)	26 (26%)	7 (7%)	1	19
58	n2	96/120 (80%)	64 (67%)	24 (25%)	8 (8%)	1	15
59	N3	134/136 (98%)	109 (81%)	16 (12%)	9 (7%)	1	21
59	n3	134/136 (98%)	113 (84%)	12 (9%)	9 (7%)	1	21
60	N4	96/155 (62%)	63 (66%)	16 (17%)	17 (18%)	0	3
60	n4	133/155 (86%)	88 (66%)	25 (19%)	20 (15%)	0	5
61	N5	119/141 (84%)	81 (68%)	30 (25%)	8 (7%)	1	21
61	n5	118/141 (84%)	91 (77%)	17 (14%)	10 (8%)	1	14
62	N6	124/126 (98%)	94 (76%)	18 (14%)	12 (10%)	1	12
62	n6	124/126 (98%)	92 (74%)	17 (14%)	15 (12%)	0	8
63	N7	133/135 (98%)	98 (74%)	19 (14%)	16 (12%)	0	8
63	n7	133/135 (98%)	94 (71%)	26 (20%)	13 (10%)	1	12
64	N8	146/148 (99%)	100 (68%)	30 (20%)	16 (11%)	0	9
64	n8	146/148 (99%)	104 (71%)	28 (19%)	14 (10%)	1	12
65	N9	56/58 (97%)	40 (71%)	11 (20%)	5 (9%)	1	13
65	n9	56/58 (97%)	33 (59%)	14 (25%)	9 (16%)	0	4
66	O0	95/104 (91%)	82 (86%)	10 (10%)	3 (3%)	5	42
66	o0	98/104 (94%)	75 (76%)	18 (18%)	5 (5%)	2	28
67	O1	107/112 (96%)	86 (80%)	12 (11%)	9 (8%)	1	15
67	o1	107/112 (96%)	73 (68%)	14 (13%)	20 (19%)	0	3
68	O2	125/129 (97%)	95 (76%)	20 (16%)	10 (8%)	1	16
68	o2	125/129 (97%)	89 (71%)	23 (18%)	13 (10%)	1	11
69	O3	104/106 (98%)	90 (86%)	7 (7%)	7 (7%)	1	21
69	o3	104/106 (98%)	82 (79%)	13 (12%)	9 (9%)	1	14
70	O4	110/119 (92%)	80 (73%)	19 (17%)	11 (10%)	1	11
70	o4	110/119 (92%)	75 (68%)	24 (22%)	11 (10%)	1	11
71	O5	117/119 (98%)	75 (64%)	28 (24%)	14 (12%)	0	8
71	o5	117/119 (98%)	80 (68%)	18 (15%)	19 (16%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	O6	97/99 (98%)	69 (71%)	16 (16%)	12 (12%)	0	8
72	o6	97/99 (98%)	67 (69%)	18 (19%)	12 (12%)	0	8
73	O7	85/87 (98%)	63 (74%)	16 (19%)	6 (7%)	1	19
73	o7	85/87 (98%)	60 (71%)	14 (16%)	11 (13%)	0	7
74	O8	75/77 (97%)	55 (73%)	12 (16%)	8 (11%)	0	10
74	o8	75/77 (97%)	53 (71%)	18 (24%)	4 (5%)	2	27
75	O9	48/50 (96%)	34 (71%)	10 (21%)	4 (8%)	1	15
75	o9	48/50 (96%)	36 (75%)	8 (17%)	4 (8%)	1	15
76	Q0	50/52 (96%)	32 (64%)	12 (24%)	6 (12%)	0	8
76	q0	50/52 (96%)	39 (78%)	6 (12%)	5 (10%)	1	11
77	Q1	23/25 (92%)	18 (78%)	3 (13%)	2 (9%)	1	14
77	q1	23/25 (92%)	16 (70%)	3 (13%)	4 (17%)	0	3
78	Q2	103/105 (98%)	75 (73%)	20 (19%)	8 (8%)	1	16
78	q2	103/105 (98%)	83 (81%)	14 (14%)	6 (6%)	2	25
79	Q3	89/91 (98%)	59 (66%)	16 (18%)	14 (16%)	0	4
79	q3	89/91 (98%)	71 (80%)	9 (10%)	9 (10%)	1	11
80	e0	60/62 (97%)	37 (62%)	14 (23%)	9 (15%)	0	5
81	e1	74/76 (97%)	28 (38%)	26 (35%)	20 (27%)	0	0
83	p0	139/311 (45%)	103 (74%)	27 (19%)	9 (6%)	1	22
All	All	22333/24141 (92%)	15914 (71%)	4073 (18%)	2346 (10%)	1	10

5 of 2346 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	30	GLN
2	S0	39	ASN
2	S0	95	ALA
2	S0	132	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/209 (78%)	117 (71%)	47 (29%)	0	4
2	s0	165/209 (79%)	123 (74%)	42 (26%)	1	6
3	S1	191/223 (86%)	139 (73%)	52 (27%)	0	4
3	s1	192/223 (86%)	147 (77%)	45 (23%)	1	7
4	S2	176/204 (86%)	126 (72%)	50 (28%)	0	4
4	s2	176/204 (86%)	119 (68%)	57 (32%)	0	2
5	S3	182/194 (94%)	133 (73%)	49 (27%)	0	4
5	s3	182/194 (94%)	131 (72%)	51 (28%)	0	4
6	S4	221/221 (100%)	170 (77%)	51 (23%)	1	7
6	s4	221/221 (100%)	165 (75%)	56 (25%)	1	6
7	S5	173/190 (91%)	136 (79%)	37 (21%)	1	9
7	s5	173/190 (91%)	125 (72%)	48 (28%)	0	4
8	S6	188/201 (94%)	139 (74%)	49 (26%)	0	5
8	s6	187/201 (93%)	132 (71%)	55 (29%)	0	3
9	S7	165/169 (98%)	127 (77%)	38 (23%)	1	7
9	s7	165/169 (98%)	122 (74%)	43 (26%)	0	5
10	S8	150/161 (93%)	118 (79%)	32 (21%)	1	10
10	s8	150/161 (93%)	106 (71%)	44 (29%)	0	4
11	S9	158/165 (96%)	121 (77%)	37 (23%)	1	7
11	s9	158/165 (96%)	116 (73%)	42 (27%)	0	5
12	C0	77/98 (79%)	58 (75%)	19 (25%)	1	6
12	c0	73/98 (74%)	54 (74%)	19 (26%)	0	5
13	C1	129/136 (95%)	111 (86%)	18 (14%)	4	28
13	c1	129/136 (95%)	98 (76%)	31 (24%)	1	6
14	C2	88/118 (75%)	66 (75%)	22 (25%)	1	6
14	c2	88/118 (75%)	62 (70%)	26 (30%)	0	3
15	C3	127/127 (100%)	101 (80%)	26 (20%)	1	11
15	c3	127/127 (100%)	96 (76%)	31 (24%)	1	6
16	C4	81/104 (78%)	58 (72%)	23 (28%)	0	4
16	c4	97/104 (93%)	67 (69%)	30 (31%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	C5	101/117 (86%)	72 (71%)	29 (29%)	0	4
17	c5	103/117 (88%)	73 (71%)	30 (29%)	0	4
18	C6	117/118 (99%)	83 (71%)	34 (29%)	0	4
18	c6	118/118 (100%)	87 (74%)	31 (26%)	0	5
19	C7	94/124 (76%)	65 (69%)	29 (31%)	0	3
19	c7	92/124 (74%)	61 (66%)	31 (34%)	0	2
20	C8	128/128 (100%)	101 (79%)	27 (21%)	1	10
20	c8	128/128 (100%)	96 (75%)	32 (25%)	1	6
21	C9	115/115 (100%)	83 (72%)	32 (28%)	0	4
21	c9	115/115 (100%)	85 (74%)	30 (26%)	0	5
22	D0	100/113 (88%)	74 (74%)	26 (26%)	0	5
22	d0	103/113 (91%)	67 (65%)	36 (35%)	0	2
23	D1	74/74 (100%)	59 (80%)	15 (20%)	1	11
23	d1	74/74 (100%)	52 (70%)	22 (30%)	0	3
24	D2	110/110 (100%)	81 (74%)	29 (26%)	0	5
24	d2	110/110 (100%)	88 (80%)	22 (20%)	1	11
25	D3	119/119 (100%)	79 (66%)	40 (34%)	0	2
25	d3	119/119 (100%)	89 (75%)	30 (25%)	1	6
26	D4	112/112 (100%)	88 (79%)	24 (21%)	1	9
26	d4	112/112 (100%)	89 (80%)	23 (20%)	1	11
27	D5	61/88 (69%)	47 (77%)	14 (23%)	1	7
27	d5	61/88 (69%)	47 (77%)	14 (23%)	1	7
28	D6	83/83 (100%)	60 (72%)	23 (28%)	0	4
28	d6	83/83 (100%)	51 (61%)	32 (39%)	0	1
29	D7	70/70 (100%)	57 (81%)	13 (19%)	2	13
29	d7	70/70 (100%)	54 (77%)	16 (23%)	1	8
30	D8	56/59 (95%)	39 (70%)	17 (30%)	0	3
30	d8	56/59 (95%)	42 (75%)	14 (25%)	1	6
31	D9	47/48 (98%)	34 (72%)	13 (28%)	0	4
31	d9	47/48 (98%)	32 (68%)	15 (32%)	0	3
32	E0	51/51 (100%)	35 (69%)	16 (31%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	E1	62/66 (94%)	47 (76%)	15 (24%)	1	6
34	SR	260/261 (100%)	216 (83%)	44 (17%)	2	18
34	sR	260/261 (100%)	213 (82%)	47 (18%)	2	15
35	SM	97/228 (42%)	68 (70%)	29 (30%)	0	3
35	sM	54/228 (24%)	39 (72%)	15 (28%)	0	4
39	L2	193/195 (99%)	138 (72%)	55 (28%)	0	4
39	l2	192/195 (98%)	137 (71%)	55 (29%)	0	4
40	L3	321/322 (100%)	229 (71%)	92 (29%)	0	4
40	l3	321/322 (100%)	235 (73%)	86 (27%)	0	4
41	L4	288/288 (100%)	212 (74%)	76 (26%)	0	5
41	l4	288/288 (100%)	208 (72%)	80 (28%)	0	4
42	L5	244/244 (100%)	195 (80%)	49 (20%)	1	11
42	l5	243/244 (100%)	176 (72%)	67 (28%)	0	4
43	L6	134/152 (88%)	110 (82%)	24 (18%)	2	15
43	l6	135/152 (89%)	105 (78%)	30 (22%)	1	8
44	L7	186/204 (91%)	138 (74%)	48 (26%)	0	5
44	l7	187/204 (92%)	146 (78%)	41 (22%)	1	9
45	L8	187/207 (90%)	144 (77%)	43 (23%)	1	7
45	l8	177/207 (86%)	134 (76%)	43 (24%)	1	6
46	L9	171/171 (100%)	110 (64%)	61 (36%)	0	1
46	l9	171/171 (100%)	119 (70%)	52 (30%)	0	3
47	M0	177/186 (95%)	135 (76%)	42 (24%)	1	7
47	m0	179/186 (96%)	131 (73%)	48 (27%)	0	4
48	M1	147/150 (98%)	111 (76%)	36 (24%)	1	6
48	m1	147/150 (98%)	91 (62%)	56 (38%)	0	1
49	M3	154/158 (98%)	114 (74%)	40 (26%)	0	5
49	m3	154/158 (98%)	102 (66%)	52 (34%)	0	2
50	M4	107/108 (99%)	78 (73%)	29 (27%)	0	4
50	m4	108/108 (100%)	81 (75%)	27 (25%)	1	6
51	M5	175/175 (100%)	143 (82%)	32 (18%)	2	14
51	m5	175/175 (100%)	132 (75%)	43 (25%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	M6	160/161 (99%)	120 (75%)	40 (25%)	1	6
52	m6	160/161 (99%)	119 (74%)	41 (26%)	0	6
53	M7	140/145 (97%)	98 (70%)	42 (30%)	0	3
53	m7	125/145 (86%)	83 (66%)	42 (34%)	0	2
54	M8	150/150 (100%)	115 (77%)	35 (23%)	1	7
54	m8	150/150 (100%)	104 (69%)	46 (31%)	0	3
55	M9	153/153 (100%)	112 (73%)	41 (27%)	0	4
55	m9	153/153 (100%)	113 (74%)	40 (26%)	0	5
56	N0	156/156 (100%)	108 (69%)	48 (31%)	0	3
56	n0	156/156 (100%)	114 (73%)	42 (27%)	0	4
57	N1	136/136 (100%)	100 (74%)	36 (26%)	0	5
57	n1	136/136 (100%)	100 (74%)	36 (26%)	0	5
58	N2	87/106 (82%)	68 (78%)	19 (22%)	1	9
58	n2	85/106 (80%)	68 (80%)	17 (20%)	1	11
59	N3	104/104 (100%)	79 (76%)	25 (24%)	1	6
59	n3	104/104 (100%)	78 (75%)	26 (25%)	1	6
60	N4	57/129 (44%)	45 (79%)	12 (21%)	1	10
60	n4	100/129 (78%)	69 (69%)	31 (31%)	0	3
61	N5	104/117 (89%)	83 (80%)	21 (20%)	1	11
61	n5	104/117 (89%)	70 (67%)	34 (33%)	0	2
62	N6	109/109 (100%)	80 (73%)	29 (27%)	0	5
62	n6	109/109 (100%)	75 (69%)	34 (31%)	0	3
63	N7	115/115 (100%)	92 (80%)	23 (20%)	1	11
63	n7	115/115 (100%)	93 (81%)	22 (19%)	2	12
64	N8	118/118 (100%)	95 (80%)	23 (20%)	2	12
64	n8	118/118 (100%)	85 (72%)	33 (28%)	0	4
65	N9	46/46 (100%)	30 (65%)	16 (35%)	0	2
65	n9	46/46 (100%)	23 (50%)	23 (50%)	0	0
66	O0	81/87 (93%)	62 (76%)	19 (24%)	1	7
66	o0	84/87 (97%)	54 (64%)	30 (36%)	0	1
67	O1	92/96 (96%)	67 (73%)	25 (27%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	o1	94/96 (98%)	67 (71%)	27 (29%)	0	4
68	O2	109/110 (99%)	73 (67%)	36 (33%)	0	2
68	o2	109/110 (99%)	78 (72%)	31 (28%)	0	4
69	O3	90/90 (100%)	71 (79%)	19 (21%)	1	10
69	o3	90/90 (100%)	62 (69%)	28 (31%)	0	3
70	O4	95/101 (94%)	66 (70%)	29 (30%)	0	3
70	o4	95/101 (94%)	70 (74%)	25 (26%)	0	5
71	O5	104/104 (100%)	69 (66%)	35 (34%)	0	2
71	o5	103/104 (99%)	77 (75%)	26 (25%)	1	6
72	O6	81/81 (100%)	56 (69%)	25 (31%)	0	3
72	o6	80/81 (99%)	55 (69%)	25 (31%)	0	3
73	O7	70/70 (100%)	51 (73%)	19 (27%)	0	4
73	o7	70/70 (100%)	48 (69%)	22 (31%)	0	3
74	O8	68/68 (100%)	53 (78%)	15 (22%)	1	8
74	o8	67/68 (98%)	52 (78%)	15 (22%)	1	8
75	O9	45/45 (100%)	35 (78%)	10 (22%)	1	8
75	o9	45/45 (100%)	34 (76%)	11 (24%)	1	6
76	Q0	47/47 (100%)	36 (77%)	11 (23%)	1	7
76	q0	47/47 (100%)	33 (70%)	14 (30%)	0	3
77	Q1	23/23 (100%)	15 (65%)	8 (35%)	0	2
77	q1	23/23 (100%)	14 (61%)	9 (39%)	0	1
78	Q2	90/90 (100%)	65 (72%)	25 (28%)	0	4
78	q2	90/90 (100%)	58 (64%)	32 (36%)	0	1
79	Q3	71/71 (100%)	54 (76%)	17 (24%)	1	6
79	q3	71/71 (100%)	49 (69%)	22 (31%)	0	3
80	e0	53/53 (100%)	41 (77%)	12 (23%)	1	8
81	e1	66/66 (100%)	41 (62%)	25 (38%)	0	1
83	p0	105/253 (42%)	79 (75%)	26 (25%)	1	6
All	All	18730/20239 (92%)	13794 (74%)	4936 (26%)	0	5

5 of 4936 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
72	O6	59	ASP
10	s8	56	ARG
64	n8	102	ILE
76	Q0	127	LEU
5	s3	66	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 122 such sidechains are listed below:

Mol	Chain	Res	Type
5	s3	74	GLN
13	c1	37	ASN
64	n8	25	HIS
5	s3	179	GLN
6	s4	224	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	613 (35%)	71 (4%)
1	6	1787/1800 (99%)	650 (36%)	64 (3%)
36	1	3145/3396 (92%)	1010 (32%)	106 (3%)
36	5	3145/3396 (92%)	1037 (32%)	115 (3%)
37	3	120/121 (99%)	34 (28%)	2 (1%)
37	7	120/121 (99%)	30 (25%)	3 (2%)
38	4	157/158 (99%)	51 (32%)	7 (4%)
38	8	157/158 (99%)	57 (36%)	3 (1%)
All	All	10378/10950 (94%)	3482 (33%)	371 (3%)

5 of 3482 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	5	U
1	2	25	C
1	2	26	A

5 of 371 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	3228	C

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Mol	Chain	Res	Type
1	6	664	U
36	5	3011	A
36	1	3318	G
1	6	103	A

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 2558 ligands modelled in this entry, 1426 are monoatomic - leaving 1132 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
87	OHX	1	3866	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3867	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3868	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3869	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3870	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3871	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3872	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3879	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3880	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3888	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3889	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3890	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3891	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3922	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3965	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3996	36	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4008	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4051	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4094	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4137	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4180	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2077	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2120	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2163	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
88	GET	2	2181	-	33,36,36	0.48	0	43,55,55	1.76	8 (18%)
87	OHX	3	215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	227	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	228	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	229	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	230	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	231	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	232	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	233	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	234	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	235	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	236	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	237	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	4	238	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	239	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	240	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3933	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3976	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4019	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4062	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4105	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4148	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4191	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4227	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4228	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4229	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4230	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4231	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4232	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4233	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4234	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4235	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4236	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4237	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4238	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4239	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4240	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4241	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4242	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4243	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4244	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4245	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4246	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2080	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2123	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2166	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2182	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2183	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2184	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2185	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2186	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2187	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2188	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2189	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2190	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2191	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2192	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2193	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2194	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2195	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2196	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2197	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2198	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2199	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2200	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2204	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2207	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2208	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2209	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	2210	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2211	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	227	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	228	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	229	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	230	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	231	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	232	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	233	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	234	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	235	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	C3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	C5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	C8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	D3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	D9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L3	405	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M0	304	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M6	202	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	M7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M9	203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	N9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O1	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O2	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O7	103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O7	104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	S8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c8	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	d4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	d9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l3	407	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l3	408	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	305	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	306	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	307	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m1	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m7	205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	n3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	n9	103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o7	502	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	q1	102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	s1	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	s8	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	sR	401	-	0,6,6	0.00	-	0,15,15	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	3866	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3867	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3868	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3869	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3870	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3871	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3872	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3873	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3874	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3875	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3876	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3877	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3878	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3879	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3880	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3881	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3882	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3883	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3884	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3885	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3886	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3887	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3888	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3889	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3890	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3891	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3892	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3893	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3894	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3895	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3896	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3897	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3898	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3899	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3900	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3901	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3902	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3903	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3904	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	3905	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3906	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3907	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3908	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3909	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3910	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3911	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3912	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3913	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3914	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3915	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3916	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3917	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3918	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3919	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3920	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3921	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3922	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3923	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3924	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3925	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3926	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3927	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3928	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3929	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3930	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3931	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3932	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3933	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3934	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3935	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3936	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3937	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3938	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3939	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3940	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3941	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3942	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3943	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3944	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3945	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3946	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	3947	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3948	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3949	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3950	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3951	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3952	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3953	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3954	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3955	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3956	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3957	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3958	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3959	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3960	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3961	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3962	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3963	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3964	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3965	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3966	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3967	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3968	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3969	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3970	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3971	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3972	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3973	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3974	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3975	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3976	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3977	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3978	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3979	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3980	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3981	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3982	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3983	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3984	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3985	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3986	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3987	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3988	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	3989	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3990	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3991	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3992	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3993	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3994	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3995	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3996	36	-	0/0/0/0	0/0/0/0
87	OHX	1	3997	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3998	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3999	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4000	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4001	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4002	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4003	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4004	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4005	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4006	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4007	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4008	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4009	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4010	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4011	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4012	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4013	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4014	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4015	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4016	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4017	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4018	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4019	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4020	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4021	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4022	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4023	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4024	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4025	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4026	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4027	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4028	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4029	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4030	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4031	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4032	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4033	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4034	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4035	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4036	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4037	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4038	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4039	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4040	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4041	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4042	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4043	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4044	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4045	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4046	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4047	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4048	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4049	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4050	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4051	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4052	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4053	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4054	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4055	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4056	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4057	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4058	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4059	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4060	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4061	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4062	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4063	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4064	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4065	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4066	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4067	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4068	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4069	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4070	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4071	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4072	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4073	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4074	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4075	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4076	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4077	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4078	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4079	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4080	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4081	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4082	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4083	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4084	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4085	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4086	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4087	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4088	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4089	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4090	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4091	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4092	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4093	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4094	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4095	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4096	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4097	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4098	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4099	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4100	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4101	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4102	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4103	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4104	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4105	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4106	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4107	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4108	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4109	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4110	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4111	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4112	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4113	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4114	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4115	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4116	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4117	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4118	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4119	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4120	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4121	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4122	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4123	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4124	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4125	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4126	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4127	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4128	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4129	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4130	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4131	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4132	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4133	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4134	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4135	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4136	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4137	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4138	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4139	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4140	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4141	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4142	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4143	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4144	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4145	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4146	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4147	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4148	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4149	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4150	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4151	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4152	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4153	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4154	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4155	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4156	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4157	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4158	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4159	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4160	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4161	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4162	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4163	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4164	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4165	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4166	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4167	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4168	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4169	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4170	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4171	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4172	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4173	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4174	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4175	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4176	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4177	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4178	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4179	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4180	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4181	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4182	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4183	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4184	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4185	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4186	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4187	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4188	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4189	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4190	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4191	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4192	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4193	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4194	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4195	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4196	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4197	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4198	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4199	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4200	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4201	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4202	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4203	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4204	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4205	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4206	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4207	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4208	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4209	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4210	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4211	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4212	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2024	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2025	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2029	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2030	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2031	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2032	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2033	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2034	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2035	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2036	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2037	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2038	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2039	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2040	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2041	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2042	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2043	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2044	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2045	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2046	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2047	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2048	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2049	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2050	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2051	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2052	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2053	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2054	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2055	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2056	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2057	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2058	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2059	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2060	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2061	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2062	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2063	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2064	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2065	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2066	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2067	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2068	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2069	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2070	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2071	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2072	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2073	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2074	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2075	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2076	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2077	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2078	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2079	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2080	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2081	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2082	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2083	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2084	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2085	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2086	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2087	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2088	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2089	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2090	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2091	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2092	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2093	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2094	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2095	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2096	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2097	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2098	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2099	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2100	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2101	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2102	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2103	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2104	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2105	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2106	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2107	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2108	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2109	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2110	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2111	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2112	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2113	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2114	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2115	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2116	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2117	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2118	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2119	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2120	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2121	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2122	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2123	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2124	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2125	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2126	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2127	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2128	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2129	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2130	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2131	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2132	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2133	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2134	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2135	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2136	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2137	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2138	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2139	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2140	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2141	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2142	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2143	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2144	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2145	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2146	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2147	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2148	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2149	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2150	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2151	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2152	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2153	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2154	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2155	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2156	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2157	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2158	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2159	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2160	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2161	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2162	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2163	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2164	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2165	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2166	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2167	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2168	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2169	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2170	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2171	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2172	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2173	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2174	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2175	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2176	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2177	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2178	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2179	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2180	-	-	0/0/0/0	0/0/0/0
88	GET	2	2181	-	-	0/13/74/74	0/3/3/3
87	OHX	3	215	-	-	0/0/0/0	0/0/0/0
87	OHX	3	216	-	-	0/0/0/0	0/0/0/0
87	OHX	3	217	-	-	0/0/0/0	0/0/0/0
87	OHX	3	218	-	-	0/0/0/0	0/0/0/0
87	OHX	3	219	-	-	0/0/0/0	0/0/0/0
87	OHX	3	220	-	-	0/0/0/0	0/0/0/0
87	OHX	3	221	-	-	0/0/0/0	0/0/0/0
87	OHX	3	222	-	-	0/0/0/0	0/0/0/0
87	OHX	3	223	-	-	0/0/0/0	0/0/0/0
87	OHX	3	224	-	-	0/0/0/0	0/0/0/0
87	OHX	3	225	-	-	0/0/0/0	0/0/0/0
87	OHX	4	224	-	-	0/0/0/0	0/0/0/0
87	OHX	4	225	-	-	0/0/0/0	0/0/0/0
87	OHX	4	226	-	-	0/0/0/0	0/0/0/0
87	OHX	4	227	-	-	0/0/0/0	0/0/0/0
87	OHX	4	228	-	-	0/0/0/0	0/0/0/0
87	OHX	4	229	-	-	0/0/0/0	0/0/0/0
87	OHX	4	230	-	-	0/0/0/0	0/0/0/0
87	OHX	4	231	-	-	0/0/0/0	0/0/0/0
87	OHX	4	232	-	-	0/0/0/0	0/0/0/0
87	OHX	4	233	-	-	0/0/0/0	0/0/0/0
87	OHX	4	234	-	-	0/0/0/0	0/0/0/0
87	OHX	4	235	-	-	0/0/0/0	0/0/0/0
87	OHX	4	236	-	-	0/0/0/0	0/0/0/0
87	OHX	4	237	-	-	0/0/0/0	0/0/0/0
87	OHX	4	238	-	-	0/0/0/0	0/0/0/0
87	OHX	4	239	-	-	0/0/0/0	0/0/0/0
87	OHX	4	240	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3894	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3895	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3896	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3897	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3898	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3899	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3900	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3901	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3902	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3903	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	3904	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3905	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3906	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3907	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3908	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3909	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3910	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3911	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3912	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3913	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3914	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3915	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3916	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3917	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3918	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3919	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3920	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3921	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3922	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3923	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3924	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3925	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3926	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3927	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3928	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3929	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3930	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3931	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3932	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3933	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3934	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3935	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3936	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3937	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3938	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3939	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3940	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3941	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3942	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3943	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3944	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3945	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	3946	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3947	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3948	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3949	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3950	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3951	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3952	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3953	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3954	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3955	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3956	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3957	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3958	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3959	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3960	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3961	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3962	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3963	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3964	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3965	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3966	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3967	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3968	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3969	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3970	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3971	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3972	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3973	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3974	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3975	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3976	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3977	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3978	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3979	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3980	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3981	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3982	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3983	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3984	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3985	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3986	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3987	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	3988	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3989	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3990	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3991	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3992	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3993	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3994	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3995	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3996	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3997	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3998	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3999	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4000	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4001	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4002	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4003	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4004	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4005	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4006	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4007	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4008	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4009	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4010	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4011	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4012	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4013	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4014	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4015	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4016	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4017	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4018	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4019	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4020	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4021	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4022	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4023	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4024	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4025	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4026	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4027	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4028	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4029	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4030	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4031	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4032	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4033	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4034	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4035	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4036	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4037	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4038	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4039	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4040	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4041	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4042	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4043	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4044	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4045	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4046	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4047	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4048	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4049	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4050	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4051	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4052	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4053	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4054	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4055	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4056	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4057	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4058	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4059	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4060	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4061	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4062	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4063	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4064	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4065	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4066	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4067	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4068	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4069	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4070	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4071	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4072	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4073	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4074	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4075	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4076	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4077	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4078	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4079	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4080	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4081	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4082	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4083	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4084	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4085	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4086	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4087	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4088	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4089	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4090	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4091	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4092	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4093	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4094	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4095	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4096	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4097	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4098	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4099	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4100	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4101	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4102	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4103	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4104	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4105	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4106	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4107	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4108	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4109	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4110	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4111	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4112	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4113	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4114	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4115	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4116	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4117	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4118	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4119	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4120	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4121	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4122	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4123	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4124	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4125	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4126	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4127	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4128	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4129	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4130	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4131	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4132	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4133	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4134	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4135	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4136	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4137	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4138	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4139	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4140	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4141	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4142	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4143	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4144	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4145	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4146	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4147	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4148	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4149	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4150	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4151	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4152	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4153	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4154	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4155	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4156	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4157	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4158	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4159	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4160	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4161	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4162	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4163	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4164	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4165	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4166	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4167	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4168	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4169	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4170	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4171	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4172	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4173	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4174	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4175	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4176	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4177	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4178	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4179	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4180	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4181	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4182	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4183	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4184	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4185	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4186	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4187	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4188	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4189	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4190	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4191	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4192	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4193	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4194	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4195	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4196	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4197	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4198	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4199	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4200	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4201	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4202	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4203	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4204	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4205	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4206	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4207	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4208	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4209	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4210	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4211	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4212	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4213	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4214	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4215	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4216	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4217	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4218	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4219	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4220	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4221	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4222	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4223	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4224	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4225	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4226	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4227	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4228	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4229	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4230	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4231	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4232	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4233	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4234	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4235	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4236	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4237	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4238	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4239	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4240	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4241	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4242	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4243	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4244	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4245	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4246	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2050	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2051	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2052	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2053	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2054	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2055	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2056	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2057	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2058	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2059	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2060	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2061	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2062	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2063	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2064	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2065	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2066	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2067	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2068	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2069	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2070	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2071	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2072	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2073	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2074	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2075	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2076	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2077	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2078	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2079	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2080	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2081	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2082	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2083	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2084	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2085	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2086	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2087	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2088	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2089	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2090	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2091	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2092	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2093	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2094	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2095	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2096	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2097	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2098	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2099	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2100	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2101	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2102	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2103	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2104	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2105	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2106	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2107	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2108	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2109	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2110	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2111	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2112	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2113	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2114	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2115	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2116	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2117	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2118	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2119	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2120	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2121	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2122	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2123	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2124	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2125	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2126	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2127	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2128	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2129	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2130	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2131	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2132	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2133	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2134	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2135	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2136	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2137	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2138	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2139	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2140	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2141	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2142	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2143	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2144	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2145	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2146	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2147	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2148	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2149	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2150	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2151	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2152	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2153	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2154	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2155	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2156	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2157	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2158	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2159	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2160	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2161	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2162	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2163	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2164	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2165	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2166	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2167	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2168	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2169	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2170	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2171	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2172	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2173	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2174	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2175	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2176	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2177	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2178	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2179	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2180	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2181	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2182	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2183	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2184	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2185	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2186	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2187	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2188	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2189	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2190	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2191	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2192	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2193	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2194	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2195	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2196	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2197	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2198	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2199	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2200	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2201	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2202	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2203	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2204	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2205	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2206	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2207	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2208	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2209	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2210	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2211	-	-	0/0/0/0	0/0/0/0
87	OHX	7	216	-	-	0/0/0/0	0/0/0/0
87	OHX	7	217	-	-	0/0/0/0	0/0/0/0
87	OHX	7	218	-	-	0/0/0/0	0/0/0/0
87	OHX	7	219	-	-	0/0/0/0	0/0/0/0
87	OHX	7	220	-	-	0/0/0/0	0/0/0/0
87	OHX	7	221	-	-	0/0/0/0	0/0/0/0
87	OHX	7	222	-	-	0/0/0/0	0/0/0/0
87	OHX	7	223	-	-	0/0/0/0	0/0/0/0
87	OHX	7	224	-	-	0/0/0/0	0/0/0/0
87	OHX	7	225	-	-	0/0/0/0	0/0/0/0
87	OHX	7	226	-	-	0/0/0/0	0/0/0/0
87	OHX	8	218	-	-	0/0/0/0	0/0/0/0
87	OHX	8	219	-	-	0/0/0/0	0/0/0/0
87	OHX	8	220	-	-	0/0/0/0	0/0/0/0
87	OHX	8	221	-	-	0/0/0/0	0/0/0/0
87	OHX	8	222	-	-	0/0/0/0	0/0/0/0
87	OHX	8	223	-	-	0/0/0/0	0/0/0/0
87	OHX	8	224	-	-	0/0/0/0	0/0/0/0
87	OHX	8	225	-	-	0/0/0/0	0/0/0/0
87	OHX	8	226	-	-	0/0/0/0	0/0/0/0
87	OHX	8	227	-	-	0/0/0/0	0/0/0/0
87	OHX	8	228	-	-	0/0/0/0	0/0/0/0
87	OHX	8	229	-	-	0/0/0/0	0/0/0/0
87	OHX	8	230	-	-	0/0/0/0	0/0/0/0
87	OHX	8	231	-	-	0/0/0/0	0/0/0/0
87	OHX	8	232	-	-	0/0/0/0	0/0/0/0
87	OHX	8	233	-	-	0/0/0/0	0/0/0/0
87	OHX	8	234	-	-	0/0/0/0	0/0/0/0
87	OHX	8	235	-	-	0/0/0/0	0/0/0/0
87	OHX	C3	201	-	-	0/0/0/0	0/0/0/0
87	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
87	OHX	C8	201	-	-	0/0/0/0	0/0/0/0
87	OHX	D3	202	-	-	0/0/0/0	0/0/0/0
87	OHX	D9	102	-	-	0/0/0/0	0/0/0/0
87	OHX	L3	403	-	-	0/0/0/0	0/0/0/0
87	OHX	L3	404	-	-	0/0/0/0	0/0/0/0
87	OHX	L3	405	-	-	0/0/0/0	0/0/0/0
87	OHX	L4	403	-	-	0/0/0/0	0/0/0/0
87	OHX	M0	304	-	-	0/0/0/0	0/0/0/0
87	OHX	M5	303	-	-	0/0/0/0	0/0/0/0
87	OHX	M6	202	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	M7	206	-	-	0/0/0/0	0/0/0/0
87	OHX	M9	202	-	-	0/0/0/0	0/0/0/0
87	OHX	M9	203	-	-	0/0/0/0	0/0/0/0
87	OHX	N9	102	-	-	0/0/0/0	0/0/0/0
87	OHX	O1	202	-	-	0/0/0/0	0/0/0/0
87	OHX	O2	202	-	-	0/0/0/0	0/0/0/0
87	OHX	O3	202	-	-	0/0/0/0	0/0/0/0
87	OHX	O7	103	-	-	0/0/0/0	0/0/0/0
87	OHX	O7	104	-	-	0/0/0/0	0/0/0/0
87	OHX	Q2	502	-	-	0/0/0/0	0/0/0/0
87	OHX	S8	302	-	-	0/0/0/0	0/0/0/0
87	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
87	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
87	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
87	OHX	c8	202	-	-	0/0/0/0	0/0/0/0
87	OHX	d4	201	-	-	0/0/0/0	0/0/0/0
87	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
87	OHX	l3	407	-	-	0/0/0/0	0/0/0/0
87	OHX	l3	408	-	-	0/0/0/0	0/0/0/0
87	OHX	l4	402	-	-	0/0/0/0	0/0/0/0
87	OHX	l4	403	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	304	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	305	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	306	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	307	-	-	0/0/0/0	0/0/0/0
87	OHX	l9	202	-	-	0/0/0/0	0/0/0/0
87	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
87	OHX	m0	303	-	-	0/0/0/0	0/0/0/0
87	OHX	m1	202	-	-	0/0/0/0	0/0/0/0
87	OHX	m4	202	-	-	0/0/0/0	0/0/0/0
87	OHX	m5	303	-	-	0/0/0/0	0/0/0/0
87	OHX	m7	205	-	-	0/0/0/0	0/0/0/0
87	OHX	m9	201	-	-	0/0/0/0	0/0/0/0
87	OHX	n3	202	-	-	0/0/0/0	0/0/0/0
87	OHX	n9	103	-	-	0/0/0/0	0/0/0/0
87	OHX	o3	203	-	-	0/0/0/0	0/0/0/0
87	OHX	o7	502	-	-	0/0/0/0	0/0/0/0
87	OHX	o9	101	-	-	0/0/0/0	0/0/0/0
87	OHX	q1	102	-	-	0/0/0/0	0/0/0/0
87	OHX	q2	502	-	-	0/0/0/0	0/0/0/0
87	OHX	s1	302	-	-	0/0/0/0	0/0/0/0
87	OHX	s8	303	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	2	2181	GET	C23-C33-N33	-5.88	94.93	110.78
88	2	2181	GET	O11-C42-C32	-5.51	95.57	108.92
88	2	2181	GET	O62-C62-C12	-3.29	100.96	108.92
88	2	2181	GET	O11-C11-C21	-2.97	102.47	107.96
88	2	2181	GET	O23-C23-C13	-2.67	104.17	110.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

524 monomers are involved in 835 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	3866	OHX	1	0
87	1	3867	OHX	1	0
87	1	3868	OHX	2	0
87	1	3870	OHX	2	0
87	1	3871	OHX	4	0
87	1	3874	OHX	2	0
87	1	3875	OHX	1	0
87	1	3876	OHX	2	0
87	1	3877	OHX	2	0
87	1	3878	OHX	2	0
87	1	3879	OHX	2	0
87	1	3881	OHX	1	0
87	1	3882	OHX	1	0
87	1	3883	OHX	2	0
87	1	3884	OHX	1	0
87	1	3885	OHX	2	0
87	1	3887	OHX	2	0
87	1	3889	OHX	1	0
87	1	3890	OHX	1	0
87	1	3891	OHX	1	0
87	1	3892	OHX	1	0
87	1	3894	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	3895	OHX	1	0
87	1	3897	OHX	1	0
87	1	3900	OHX	1	0
87	1	3901	OHX	1	0
87	1	3902	OHX	2	0
87	1	3905	OHX	2	0
87	1	3907	OHX	1	0
87	1	3910	OHX	1	0
87	1	3911	OHX	2	0
87	1	3912	OHX	1	0
87	1	3913	OHX	2	0
87	1	3916	OHX	2	0
87	1	3917	OHX	1	0
87	1	3921	OHX	1	0
87	1	3926	OHX	1	0
87	1	3927	OHX	1	0
87	1	3928	OHX	2	0
87	1	3932	OHX	1	0
87	1	3934	OHX	3	0
87	1	3935	OHX	2	0
87	1	3936	OHX	1	0
87	1	3937	OHX	1	0
87	1	3938	OHX	1	0
87	1	3940	OHX	1	0
87	1	3941	OHX	1	0
87	1	3944	OHX	1	0
87	1	3945	OHX	1	0
87	1	3952	OHX	1	0
87	1	3958	OHX	1	0
87	1	3959	OHX	5	0
87	1	3960	OHX	1	0
87	1	3963	OHX	1	0
87	1	3964	OHX	1	0
87	1	3965	OHX	4	0
87	1	3966	OHX	2	0
87	1	3968	OHX	1	0
87	1	3969	OHX	2	0
87	1	3971	OHX	1	0
87	1	3972	OHX	6	0
87	1	3973	OHX	1	0
87	1	3975	OHX	2	0
87	1	3976	OHX	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	3977	OHX	1	0
87	1	3979	OHX	1	0
87	1	3981	OHX	2	0
87	1	3982	OHX	1	0
87	1	3983	OHX	1	0
87	1	3984	OHX	2	0
87	1	3986	OHX	1	0
87	1	3988	OHX	1	0
87	1	3993	OHX	6	0
87	1	3996	OHX	3	0
87	1	3997	OHX	1	0
87	1	3998	OHX	1	0
87	1	3999	OHX	1	0
87	1	4000	OHX	1	0
87	1	4001	OHX	1	0
87	1	4003	OHX	5	0
87	1	4005	OHX	1	0
87	1	4006	OHX	3	0
87	1	4007	OHX	1	0
87	1	4008	OHX	1	0
87	1	4010	OHX	1	0
87	1	4013	OHX	1	0
87	1	4023	OHX	2	1
87	1	4024	OHX	2	0
87	1	4025	OHX	1	0
87	1	4030	OHX	1	0
87	1	4032	OHX	5	0
87	1	4033	OHX	2	0
87	1	4034	OHX	1	0
87	1	4035	OHX	1	0
87	1	4037	OHX	3	0
87	1	4038	OHX	1	0
87	1	4039	OHX	2	0
87	1	4041	OHX	1	0
87	1	4042	OHX	1	0
87	1	4043	OHX	3	0
87	1	4044	OHX	7	0
87	1	4045	OHX	1	0
87	1	4046	OHX	1	0
87	1	4051	OHX	1	0
87	1	4054	OHX	1	0
87	1	4055	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	4056	OHX	2	0
87	1	4061	OHX	1	0
87	1	4062	OHX	1	0
87	1	4063	OHX	1	0
87	1	4064	OHX	1	0
87	1	4065	OHX	1	0
87	1	4069	OHX	1	0
87	1	4072	OHX	1	0
87	1	4078	OHX	1	0
87	1	4079	OHX	2	0
87	1	4083	OHX	1	0
87	1	4086	OHX	2	0
87	1	4088	OHX	1	0
87	1	4091	OHX	1	0
87	1	4092	OHX	1	0
87	1	4093	OHX	1	0
87	1	4094	OHX	1	0
87	1	4095	OHX	1	0
87	1	4097	OHX	2	0
87	1	4101	OHX	1	0
87	1	4105	OHX	1	0
87	1	4107	OHX	1	0
87	1	4108	OHX	1	0
87	1	4110	OHX	1	0
87	1	4123	OHX	2	0
87	1	4130	OHX	1	0
87	1	4131	OHX	2	0
87	1	4133	OHX	1	0
87	1	4134	OHX	1	0
87	1	4137	OHX	3	0
87	1	4139	OHX	3	0
87	1	4144	OHX	1	0
87	1	4147	OHX	1	0
87	1	4148	OHX	1	0
87	1	4149	OHX	1	0
87	1	4151	OHX	1	0
87	1	4152	OHX	1	0
87	1	4153	OHX	1	0
87	1	4154	OHX	7	0
87	1	4155	OHX	6	0
87	1	4158	OHX	1	0
87	1	4160	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	4162	OHX	1	0
87	1	4163	OHX	2	0
87	1	4165	OHX	1	0
87	1	4166	OHX	1	0
87	1	4167	OHX	1	0
87	1	4170	OHX	1	0
87	1	4171	OHX	8	0
87	1	4173	OHX	1	0
87	1	4178	OHX	2	0
87	1	4179	OHX	1	0
87	1	4180	OHX	6	0
87	1	4182	OHX	1	0
87	1	4183	OHX	3	0
87	1	4184	OHX	2	0
87	1	4194	OHX	1	0
87	1	4195	OHX	1	0
87	1	4198	OHX	7	0
87	1	4199	OHX	1	0
87	1	4202	OHX	1	0
87	1	4207	OHX	1	0
87	1	4209	OHX	1	0
87	1	4210	OHX	1	0
87	2	2024	OHX	1	0
87	2	2025	OHX	2	0
87	2	2026	OHX	1	0
87	2	2028	OHX	1	0
87	2	2029	OHX	2	0
87	2	2031	OHX	9	0
87	2	2032	OHX	2	0
87	2	2034	OHX	2	0
87	2	2035	OHX	2	0
87	2	2036	OHX	3	0
87	2	2037	OHX	1	0
87	2	2038	OHX	2	0
87	2	2039	OHX	2	0
87	2	2040	OHX	1	0
87	2	2042	OHX	1	0
87	2	2044	OHX	5	0
87	2	2046	OHX	1	0
87	2	2048	OHX	1	0
87	2	2049	OHX	1	0
87	2	2051	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	2	2053	OHX	2	0
87	2	2054	OHX	1	0
87	2	2056	OHX	1	0
87	2	2060	OHX	2	0
87	2	2061	OHX	1	0
87	2	2065	OHX	1	0
87	2	2069	OHX	1	0
87	2	2070	OHX	3	0
87	2	2076	OHX	1	0
87	2	2077	OHX	1	0
87	2	2078	OHX	1	0
87	2	2084	OHX	1	0
87	2	2090	OHX	4	0
87	2	2092	OHX	2	0
87	2	2093	OHX	1	0
87	2	2095	OHX	4	0
87	2	2096	OHX	1	0
87	2	2097	OHX	2	0
87	2	2099	OHX	5	0
87	2	2100	OHX	1	0
87	2	2101	OHX	1	0
87	2	2103	OHX	1	0
87	2	2105	OHX	1	0
87	2	2108	OHX	1	0
87	2	2109	OHX	1	0
87	2	2110	OHX	1	0
87	2	2111	OHX	4	0
87	2	2116	OHX	2	0
87	2	2117	OHX	1	0
87	2	2121	OHX	1	0
87	2	2125	OHX	2	0
87	2	2128	OHX	1	0
87	2	2130	OHX	1	0
87	2	2131	OHX	6	0
87	2	2132	OHX	1	0
87	2	2133	OHX	1	0
87	2	2136	OHX	1	0
87	2	2138	OHX	1	0
87	2	2141	OHX	1	0
87	2	2143	OHX	2	0
87	2	2145	OHX	1	0
87	2	2146	OHX	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	2	2148	OHX	1	0
87	2	2150	OHX	1	0
87	2	2152	OHX	1	0
87	2	2154	OHX	1	0
87	2	2155	OHX	1	0
87	2	2157	OHX	1	0
87	2	2159	OHX	1	0
87	2	2160	OHX	1	0
87	2	2164	OHX	1	0
87	2	2171	OHX	2	0
87	2	2173	OHX	1	0
87	2	2175	OHX	2	0
87	2	2176	OHX	1	0
87	2	2179	OHX	1	0
88	2	2181	GET	9	0
87	3	219	OHX	1	0
87	3	220	OHX	1	0
87	3	222	OHX	3	0
87	4	224	OHX	2	0
87	4	225	OHX	1	0
87	4	227	OHX	1	0
87	4	228	OHX	1	0
87	4	229	OHX	1	0
87	4	231	OHX	1	0
87	4	234	OHX	3	0
87	5	3894	OHX	2	0
87	5	3895	OHX	1	0
87	5	3899	OHX	2	0
87	5	3900	OHX	2	0
87	5	3901	OHX	2	0
87	5	3902	OHX	2	0
87	5	3903	OHX	2	0
87	5	3904	OHX	2	0
87	5	3906	OHX	1	0
87	5	3907	OHX	1	0
87	5	3908	OHX	1	0
87	5	3911	OHX	3	0
87	5	3912	OHX	2	0
87	5	3915	OHX	1	0
87	5	3918	OHX	2	0
87	5	3919	OHX	1	0
87	5	3920	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	3921	OHX	2	0
87	5	3923	OHX	1	0
87	5	3928	OHX	2	0
87	5	3930	OHX	1	0
87	5	3932	OHX	1	0
87	5	3935	OHX	1	0
87	5	3936	OHX	1	0
87	5	3937	OHX	6	0
87	5	3943	OHX	1	0
87	5	3944	OHX	1	0
87	5	3948	OHX	1	0
87	5	3949	OHX	2	0
87	5	3950	OHX	2	0
87	5	3952	OHX	3	0
87	5	3953	OHX	1	0
87	5	3955	OHX	1	0
87	5	3957	OHX	2	0
87	5	3958	OHX	3	0
87	5	3959	OHX	2	0
87	5	3961	OHX	1	0
87	5	3967	OHX	1	0
87	5	3968	OHX	3	0
87	5	3969	OHX	1	0
87	5	3973	OHX	5	0
87	5	3975	OHX	1	0
87	5	3977	OHX	1	0
87	5	3978	OHX	1	0
87	5	3979	OHX	1	0
87	5	3980	OHX	2	0
87	5	3981	OHX	2	0
87	5	3985	OHX	3	0
87	5	3986	OHX	1	0
87	5	3987	OHX	1	0
87	5	3991	OHX	1	0
87	5	3992	OHX	1	0
87	5	3994	OHX	2	0
87	5	3996	OHX	2	0
87	5	3997	OHX	3	0
87	5	3998	OHX	1	0
87	5	4001	OHX	1	0
87	5	4002	OHX	1	0
87	5	4003	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	4006	OHX	6	0
87	5	4007	OHX	1	0
87	5	4008	OHX	1	0
87	5	4009	OHX	1	0
87	5	4013	OHX	1	0
87	5	4014	OHX	1	0
87	5	4015	OHX	1	0
87	5	4016	OHX	8	0
87	5	4018	OHX	1	0
87	5	4019	OHX	1	0
87	5	4021	OHX	1	0
87	5	4023	OHX	1	0
87	5	4024	OHX	1	0
87	5	4027	OHX	1	0
87	5	4028	OHX	6	0
87	5	4029	OHX	2	0
87	5	4034	OHX	1	0
87	5	4039	OHX	2	0
87	5	4041	OHX	1	0
87	5	4044	OHX	1	0
87	5	4046	OHX	2	0
87	5	4049	OHX	1	0
87	5	4050	OHX	6	0
87	5	4059	OHX	1	0
87	5	4060	OHX	2	0
87	5	4061	OHX	7	0
87	5	4062	OHX	1	0
87	5	4063	OHX	1	0
87	5	4067	OHX	1	0
87	5	4074	OHX	2	0
87	5	4075	OHX	6	0
87	5	4080	OHX	1	0
87	5	4081	OHX	1	0
87	5	4083	OHX	1	0
87	5	4084	OHX	2	0
87	5	4085	OHX	1	0
87	5	4086	OHX	4	0
87	5	4087	OHX	3	0
87	5	4091	OHX	1	0
87	5	4092	OHX	2	0
87	5	4094	OHX	1	0
87	5	4096	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	4097	OHX	4	0
87	5	4100	OHX	2	0
87	5	4101	OHX	1	0
87	5	4102	OHX	1	0
87	5	4103	OHX	1	0
87	5	4104	OHX	1	0
87	5	4106	OHX	2	0
87	5	4113	OHX	2	0
87	5	4114	OHX	2	0
87	5	4115	OHX	1	0
87	5	4117	OHX	1	0
87	5	4119	OHX	1	0
87	5	4120	OHX	1	0
87	5	4121	OHX	1	0
87	5	4125	OHX	2	0
87	5	4126	OHX	1	0
87	5	4128	OHX	1	0
87	5	4136	OHX	1	0
87	5	4138	OHX	6	0
87	5	4139	OHX	3	0
87	5	4142	OHX	1	0
87	5	4144	OHX	1	0
87	5	4146	OHX	1	0
87	5	4152	OHX	1	0
87	5	4154	OHX	2	0
87	5	4157	OHX	1	0
87	5	4158	OHX	1	0
87	5	4163	OHX	1	0
87	5	4167	OHX	3	0
87	5	4168	OHX	1	0
87	5	4172	OHX	1	0
87	5	4174	OHX	1	0
87	5	4175	OHX	1	0
87	5	4179	OHX	1	0
87	5	4180	OHX	1	0
87	5	4182	OHX	2	0
87	5	4184	OHX	2	0
87	5	4186	OHX	2	0
87	5	4187	OHX	2	0
87	5	4188	OHX	1	0
87	5	4189	OHX	1	0
87	5	4192	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	4193	OHX	7	0
87	5	4194	OHX	6	0
87	5	4195	OHX	6	0
87	5	4196	OHX	1	0
87	5	4205	OHX	2	0
87	5	4208	OHX	1	0
87	5	4211	OHX	8	0
87	5	4212	OHX	1	0
87	5	4217	OHX	1	0
87	5	4224	OHX	3	0
87	5	4225	OHX	1	0
87	5	4226	OHX	1	0
87	5	4227	OHX	1	0
87	5	4228	OHX	6	0
87	5	4232	OHX	1	0
87	5	4233	OHX	1	0
87	5	4237	OHX	4	0
87	5	4242	OHX	1	0
87	5	4243	OHX	1	0
87	5	4245	OHX	1	0
87	6	2050	OHX	1	0
87	6	2051	OHX	3	0
87	6	2053	OHX	1	0
87	6	2054	OHX	1	0
87	6	2057	OHX	2	0
87	6	2058	OHX	1	0
87	6	2059	OHX	2	0
87	6	2060	OHX	1	0
87	6	2062	OHX	2	0
87	6	2064	OHX	6	0
87	6	2066	OHX	1	0
87	6	2068	OHX	1	0
87	6	2070	OHX	1	0
87	6	2071	OHX	3	0
87	6	2072	OHX	1	0
87	6	2073	OHX	1	0
87	6	2075	OHX	1	0
87	6	2076	OHX	1	0
87	6	2078	OHX	1	0
87	6	2082	OHX	1	0
87	6	2083	OHX	1	0
87	6	2089	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	6	2091	OHX	1	0
87	6	2092	OHX	1	0
87	6	2094	OHX	1	0
87	6	2095	OHX	1	0
87	6	2096	OHX	2	0
87	6	2098	OHX	1	0
87	6	2100	OHX	1	0
87	6	2101	OHX	3	0
87	6	2102	OHX	1	0
87	6	2103	OHX	1	0
87	6	2104	OHX	2	0
87	6	2105	OHX	1	0
87	6	2106	OHX	1	0
87	6	2107	OHX	2	0
87	6	2108	OHX	1	0
87	6	2110	OHX	1	0
87	6	2111	OHX	1	0
87	6	2114	OHX	1	0
87	6	2116	OHX	1	0
87	6	2119	OHX	2	0
87	6	2125	OHX	8	0
87	6	2126	OHX	1	0
87	6	2127	OHX	1	0
87	6	2130	OHX	6	0
87	6	2131	OHX	1	0
87	6	2132	OHX	2	0
87	6	2134	OHX	1	0
87	6	2135	OHX	5	0
87	6	2140	OHX	1	0
87	6	2142	OHX	1	0
87	6	2146	OHX	1	0
87	6	2147	OHX	1	0
87	6	2148	OHX	1	0
87	6	2149	OHX	1	0
87	6	2150	OHX	1	0
87	6	2151	OHX	1	0
87	6	2152	OHX	6	0
87	6	2155	OHX	5	0
87	6	2156	OHX	1	0
87	6	2159	OHX	1	0
87	6	2160	OHX	1	0
87	6	2164	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	6	2165	OHX	1	0
87	6	2167	OHX	1	0
87	6	2171	OHX	1	0
87	6	2172	OHX	1	0
87	6	2177	OHX	8	0
87	6	2179	OHX	1	0
87	6	2180	OHX	1	0
87	6	2181	OHX	1	0
87	6	2183	OHX	1	0
87	6	2184	OHX	2	0
87	6	2186	OHX	1	0
87	6	2187	OHX	1	0
87	6	2189	OHX	5	0
87	6	2191	OHX	1	0
87	6	2195	OHX	2	0
87	6	2196	OHX	1	0
87	6	2199	OHX	3	0
87	6	2200	OHX	1	0
87	6	2201	OHX	3	0
87	6	2209	OHX	1	0
87	7	219	OHX	3	0
87	7	221	OHX	1	0
87	8	218	OHX	2	0
87	8	220	OHX	6	0
87	8	224	OHX	1	0
87	8	225	OHX	1	0
87	8	227	OHX	1	0
87	8	229	OHX	6	0
87	8	234	OHX	2	0
87	C3	201	OHX	1	0
87	C5	201	OHX	5	0
87	L3	405	OHX	1	0
87	M5	303	OHX	2	0
87	M7	206	OHX	1	0
87	M9	202	OHX	2	0
87	O1	202	OHX	6	0
87	O3	202	OHX	1	0
87	O7	103	OHX	3	0
87	Q2	502	OHX	3	0
87	S8	302	OHX	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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