



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 16, 2017 – 10:02 am GMT

PDB ID : 4U3U  
Title : Crystal structure of Cycloheximide bound to the yeast 80S ribosome  
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.  
Deposited on : 2014-07-22  
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

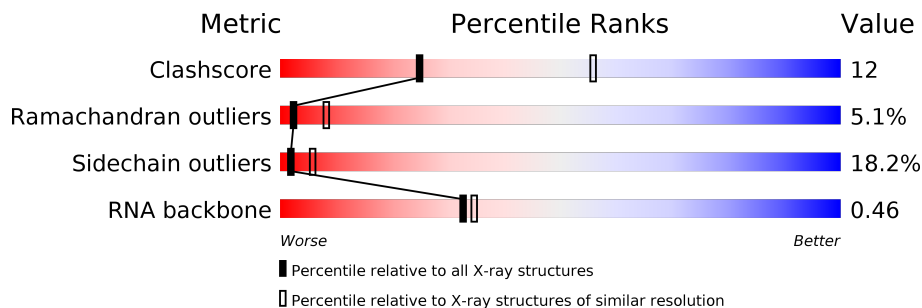
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RNA backbone	2435	1004 (3.20-2.60)





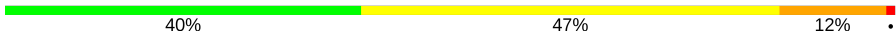

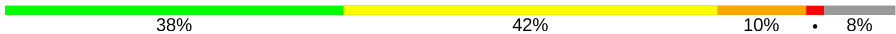

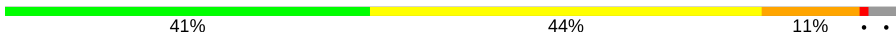

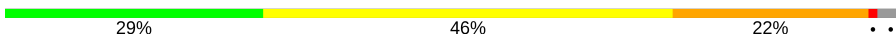

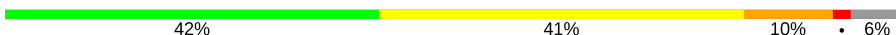







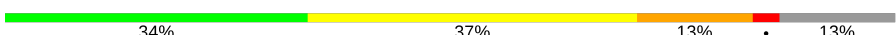




The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria.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

Note EDS failed to run properly.

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






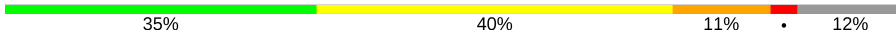

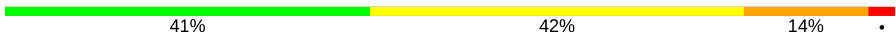

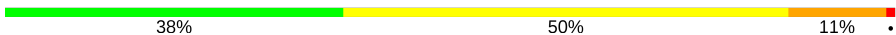

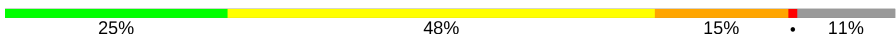













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Mol	Chain	Length	Quality of chain
4	S2	253	
4	s2	253	
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2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



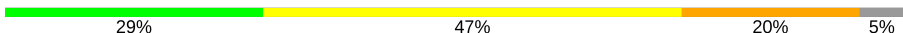











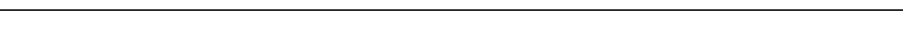




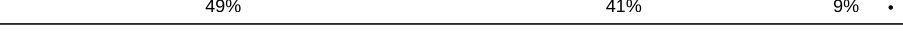

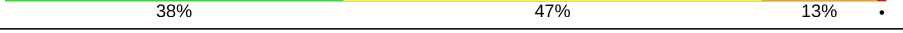



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Mol	Chain	Length	Quality of chain
16	c4	136	
17	C5	141	
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134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






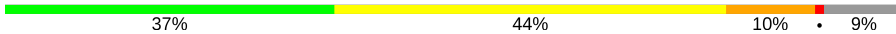

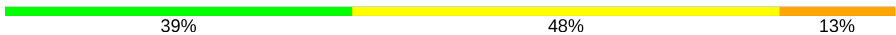

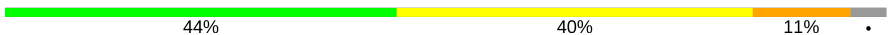

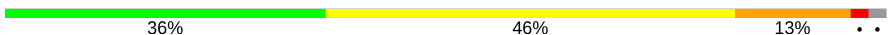













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Mol	Chain	Length	Quality of chain
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3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







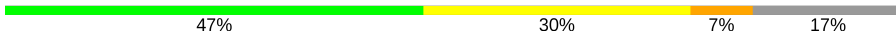



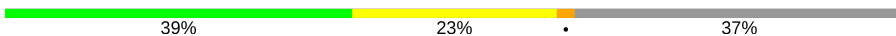














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Mol	Chain	Length	Quality of chain
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6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









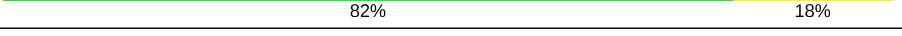


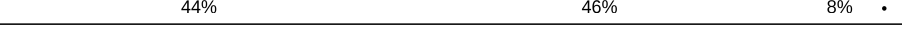

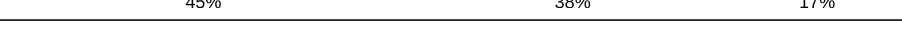


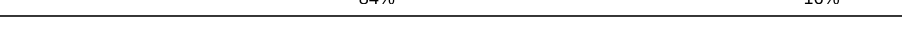

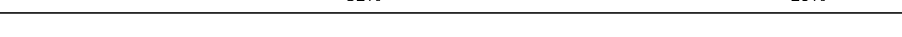
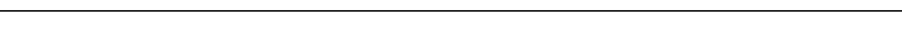

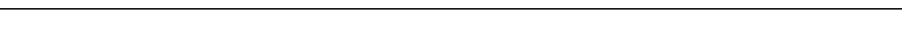
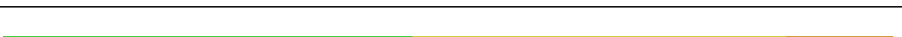


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Mol	Chain	Length	Quality of chain
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	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	3937	-	-	X	-
87	OHX	1	3957	-	-	X	-
87	OHX	1	3959	-	-	X	-
87	OHX	1	3971	-	-	X	-
87	OHX	1	3975	-	-	X	-
87	OHX	1	4003	-	-	X	-
87	OHX	1	4019	-	-	X	-
87	OHX	1	4028	-	-	X	-
87	OHX	1	4032	-	-	X	-
87	OHX	1	4037	-	-	X	-
87	OHX	1	4044	-	-	X	-
87	OHX	1	4052	-	-	X	-
87	OHX	1	4056	-	-	X	-
87	OHX	1	4057	-	-	X	-
87	OHX	1	4067	-	-	X	-
87	OHX	1	4080	-	-	X	-
87	OHX	1	4084	-	-	X	-
87	OHX	1	4114	-	-	X	-
87	OHX	1	4132	-	-	X	-
87	OHX	1	4133	-	-	X	-
87	OHX	1	4140	-	-	X	-
87	OHX	1	4146	-	-	X	-
87	OHX	1	4150	-	-	X	-
87	OHX	1	4155	-	-	X	-
87	OHX	1	4156	-	-	X	-
87	OHX	1	4160	-	-	X	-
87	OHX	1	4168	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	OHX	1	4172	-	-	X	-
87	OHX	1	4198	-	-	X	-
87	OHX	2	2030	-	-	X	-
87	OHX	2	2043	-	-	X	-
87	OHX	2	2074	-	-	X	-
87	OHX	2	2089	-	-	X	-
87	OHX	2	2095	-	-	X	-
87	OHX	2	2098	-	-	X	-
87	OHX	2	2108	-	-	X	-
87	OHX	2	2115	-	-	X	-
87	OHX	2	2130	-	-	X	-
87	OHX	2	2145	-	-	X	-
87	OHX	2	2156	-	-	X	-
87	OHX	2	2161	-	-	X	-
87	OHX	5	3943	-	-	X	-
87	OHX	5	3963	-	-	X	-
87	OHX	5	3974	-	-	X	-
87	OHX	5	3979	-	-	X	-
87	OHX	5	4001	-	-	X	-
87	OHX	5	4002	-	-	X	-
87	OHX	5	4012	-	-	X	-
87	OHX	5	4021	-	-	X	-
87	OHX	5	4034	-	-	X	-
87	OHX	5	4035	-	-	X	-
87	OHX	5	4056	-	-	X	-
87	OHX	5	4067	-	-	X	-
87	OHX	5	4082	-	-	X	-
87	OHX	5	4090	-	-	X	-
87	OHX	5	4093	-	-	X	-
87	OHX	5	4118	-	-	X	-
87	OHX	5	4143	-	-	X	-
87	OHX	5	4192	-	-	X	-
87	OHX	5	4198	-	-	X	-
87	OHX	5	4199	-	-	X	-
87	OHX	5	4200	-	-	X	-
87	OHX	5	4203	-	-	X	-
87	OHX	5	4216	-	-	X	-
87	OHX	5	4233	-	-	X	-
87	OHX	5	4242	-	-	X	-
87	OHX	6	2061	-	-	X	-
87	OHX	6	2122	-	-	X	-
87	OHX	6	2127	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	OHX	6	2129	-	-	X	-
87	OHX	6	2148	-	-	X	-
87	OHX	6	2160	-	-	X	-
87	OHX	6	2172	-	-	X	-
87	OHX	7	217	-	-	X	-
87	OHX	7	226	-	-	X	-
87	OHX	8	216	-	-	X	-
87	OHX	8	223	-	-	X	-
87	OHX	8	224	-	-	X	-
87	OHX	C5	201	-	-	X	-
87	OHX	D9	102	-	-	X	-
87	OHX	O7	103	-	-	X	-
87	OHX	O9	101	-	-	X	-

## 2 Entry composition [i](#)

There are 89 unique types of molecules in this entry. The entry contains 411205 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	l8	231	Total	C	N	O	S	0	0	0
			1764	1131	316	314	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 81 is a protein called 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 m2.

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

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

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

- Molecule 84 is a protein called UNKNOWN PROTEIN 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 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	3	Total	Mg	0	0
			3	3		
86	m7	4	Total	Mg	0	0
			4	4		
86	n8	3	Total	Mg	0	0
			3	3		
86	o1	2	Total	Mg	0	0
			2	2		
86	N5	1	Total	Mg	0	0
			1	1		
86	6	147	Total	Mg	0	0
			147	147		
86	sM	2	Total	Mg	0	0
			2	2		
86	O4	2	Total	Mg	0	0
			2	2		
86	m5	2	Total	Mg	0	0
			2	2		
86	l3	1	Total	Mg	0	0
			1	1		
86	M1	1	Total	Mg	0	0
			1	1		
86	n0	2	Total	Mg	0	0
			2	2		
86	d6	1	Total	Mg	0	0
			1	1		
86	2	122	Total	Mg	0	0
			122	122		
86	O3	1	Total	Mg	0	0
			1	1		
86	L4	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	l7	1	Total 1	Mg 1	0	0
86	M5	2	Total 2	Mg 2	0	0
86	l4	2	Total 2	Mg 2	0	0
86	S2	1	Total 1	Mg 1	0	0
86	L8	1	Total 1	Mg 1	0	0
86	D3	1	Total 1	Mg 1	0	0
86	o4	2	Total 2	Mg 2	0	0
86	M9	1	Total 1	Mg 1	0	0
86	q0	1	Total 1	Mg 1	0	0
86	SM	1	Total 1	Mg 1	0	0
86	c8	2	Total 2	Mg 2	0	0
86	M0	2	Total 2	Mg 2	0	0
86	c1	1	Total 1	Mg 1	0	0
86	5	505	Total 505	Mg 505	0	0
86	L5	1	Total 1	Mg 1	0	0
86	O7	1	Total 1	Mg 1	0	0
86	s6	1	Total 1	Mg 1	0	0
86	Q2	1	Total 1	Mg 1	0	0
86	1	471	Total 471	Mg 471	0	0
86	c4	1	Total 1	Mg 1	0	0
86	D0	1	Total 1	Mg 1	0	0

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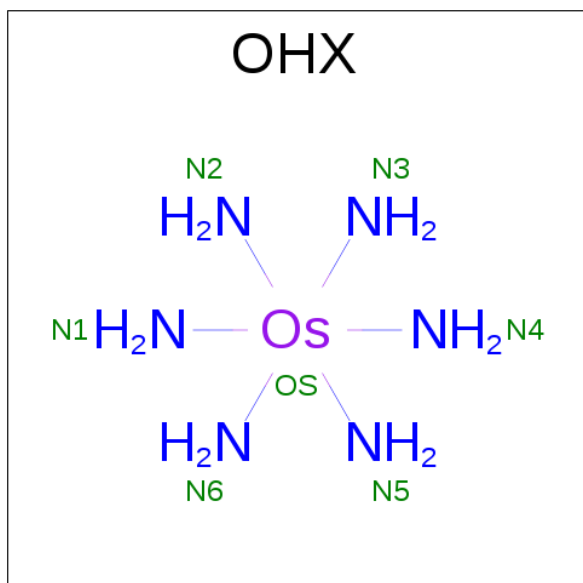
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	S8	1	Total 1	Mg 1	0	0
86	m1	2	Total 2	Mg 2	0	0
86	d3	1	Total 1	Mg 1	0	0
86	q3	2	Total 2	Mg 2	0	0
86	o3	1	Total 1	Mg 1	0	0
86	M3	4	Total 4	Mg 4	0	0
86	N3	3	Total 3	Mg 3	0	0
86	4	22	Total 22	Mg 22	0	0
86	n6	2	Total 2	Mg 2	0	0
86	S4	1	Total 1	Mg 1	0	0
86	L2	1	Total 1	Mg 1	0	0
86	o7	1	Total 1	Mg 1	0	0
86	l5	2	Total 2	Mg 2	0	0
86	C3	1	Total 1	Mg 1	0	0
86	M7	6	Total 6	Mg 6	0	0
86	N8	4	Total 4	Mg 4	0	0
86	s1	1	Total 1	Mg 1	0	0
86	m6	1	Total 1	Mg 1	0	0
86	O1	1	Total 1	Mg 1	0	0
86	s8	1	Total 1	Mg 1	0	0
86	l8	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	c7	2	Total	Mg	0	0
			2	2		
86	7	15	Total	Mg	0	0
			15	15		
86	n3	2	Total	Mg	0	0
			2	2		
86	L3	3	Total	Mg	0	0
			3	3		
86	d4	1	Total	Mg	0	0
			1	1		
86	l2	2	Total	Mg	0	0
			2	2		
86	8	13	Total	Mg	0	0
			13	13		
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		

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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		
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
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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		

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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	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		

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

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

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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
			7	6	1		

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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
			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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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
			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
			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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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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			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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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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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
			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
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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		

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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
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		

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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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			7	6	1		
87	3	1	Total	N	Os	0	0
			7	6	1		
87	3	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	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
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	M7	1	Total	N	Os	0	0
			7	6	1		
87	M9	1	Total	N	Os	0	0
			7	6	1		
87	N1	1	Total	N	Os	0	0
			7	6	1		
87	N9	1	Total	N	Os	0	0
			7	6	1		
87	O2	1	Total	N	Os	0	0
			7	6	1		
87	O3	1	Total	N	Os	0	0
			7	6	1		
87	O7	1	Total	N	Os	0	0
			7	6	1		
87	O7	1	Total	N	Os	0	0
			7	6	1		
87	O9	1	Total	N	Os	0	0
			7	6	1		
87	Q2	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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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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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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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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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 7	N 6	Os 1	0	0
87	s1	1	Total 7	N 6	Os 1	0	0
87	s4	1	Total 7	N 6	Os 1	0	0
87	s8	1	Total 7	N 6	Os 1	0	0
87	s9	1	Total 7	N 6	Os 1	0	0
87	c1	1	Total 7	N 6	Os 1	0	0
87	c3	1	Total 7	N 6	Os 1	0	0
87	c5	1	Total 7	N 6	Os 1	0	0
87	c8	1	Total 7	N 6	Os 1	0	0
87	d4	1	Total 7	N 6	Os 1	0	0
87	d9	1	Total 7	N 6	Os 1	0	0
87	sR	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0

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

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

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

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

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

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

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

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

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

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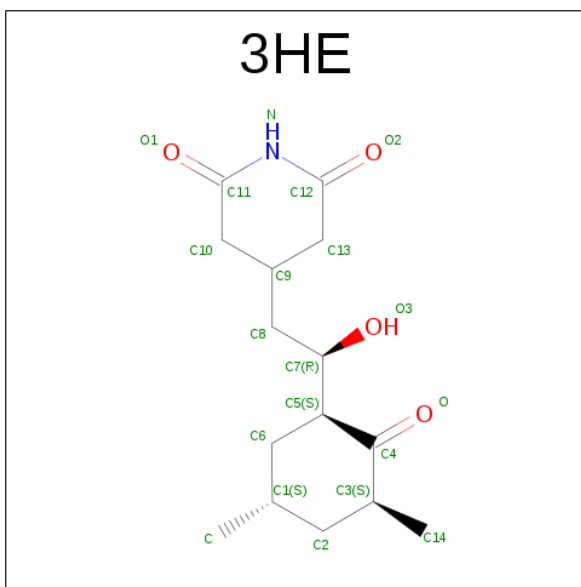
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	l5	1	Total	N	Os	0	0
			7	6	1		
87	l5	1	Total	N	Os	0	0
			7	6	1		
87	l5	1	Total	N	Os	0	0
			7	6	1		
87	l9	1	Total	N	Os	0	0
			7	6	1		
87	m0	1	Total	N	Os	0	0
			7	6	1		
87	m0	1	Total	N	Os	0	0
			7	6	1		
87	m1	1	Total	N	Os	0	0
			7	6	1		
87	m4	1	Total	N	Os	0	0
			7	6	1		
87	m5	1	Total	N	Os	0	0
			7	6	1		
87	m6	1	Total	N	Os	0	0
			7	6	1		
87	m7	1	Total	N	Os	0	0
			7	6	1		
87	m8	1	Total	N	Os	0	0
			7	6	1		
87	n3	1	Total	N	Os	0	0
			7	6	1		
87	n9	1	Total	N	Os	0	0
			7	6	1		
87	o2	1	Total	N	Os	0	0
			7	6	1		
87	o3	1	Total	N	Os	0	0
			7	6	1		
87	o7	1	Total	N	Os	0	0
			7	6	1		
87	o9	1	Total	N	Os	0	0
			7	6	1		
87	q2	1	Total	N	Os	0	0
			7	6	1		

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

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

- Molecule 89 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (three-letter code: 3HE) (formula: C<sub>15</sub>H<sub>23</sub>NO<sub>4</sub>).



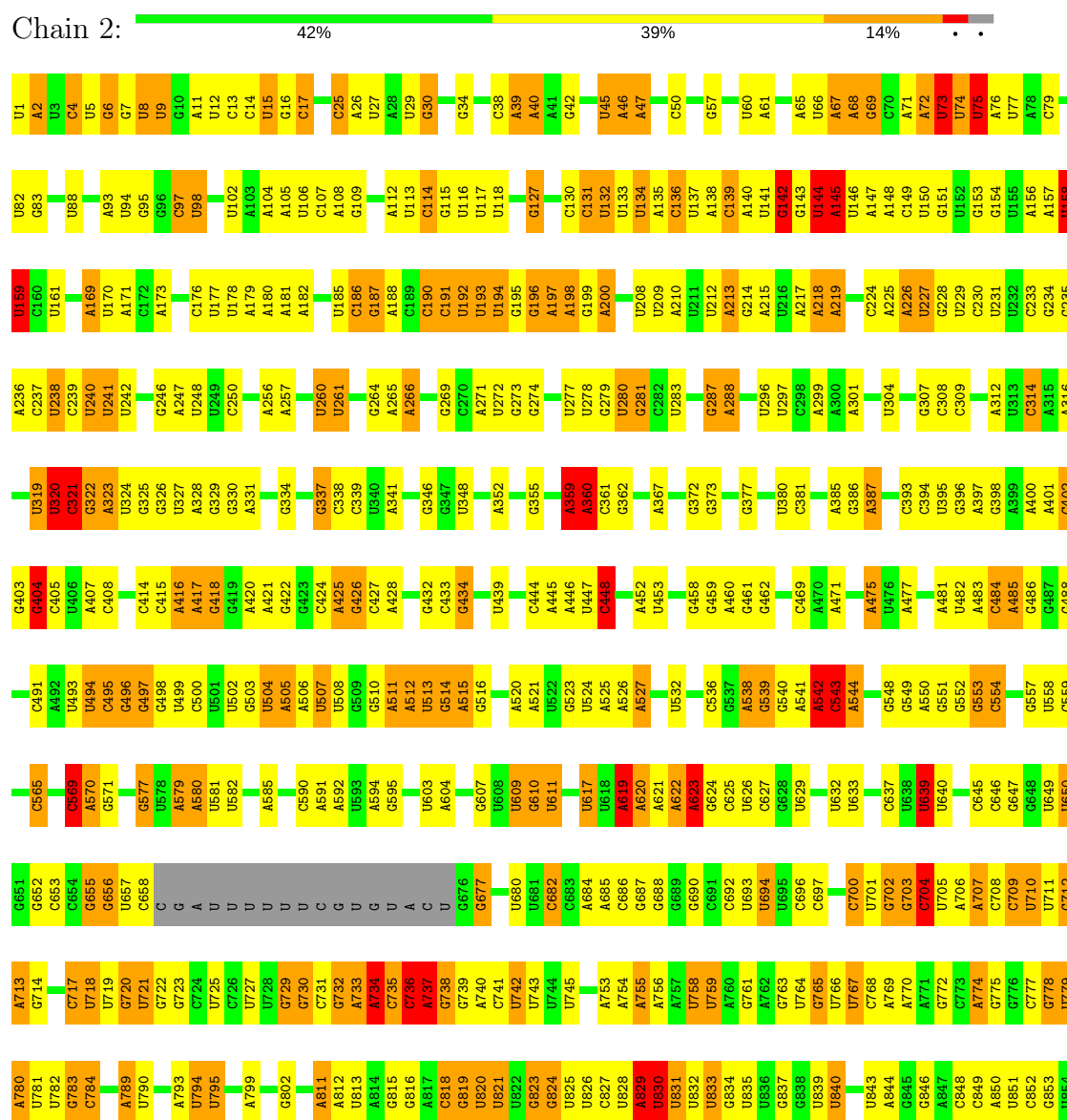
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
89	1	1	Total	C	N	O	0	0
			20	15	1	4		
89	5	1	Total	C	N	O	0	0
			20	15	1	4		

### 3 Residue-property plots

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

Note EDS failed to run properly.

#### • Molecule 1: 18S ribosomal RNA





C1729	G1658	U1517	C1447	U1366	G1278	U1185	A1091	U1015	U928	A855
A1730	U1661	C1518	G1448	G1367	C1279	U1186	A1092	U1016	A929	A856
A1732	G1662	U1520	U1450	U1370	C1280	U1187	C1096	U1017	A930	A857
U1735	G1663	G1521	C1451	U1371	G1281	U1188	U1097	U1018	A833	G585
G1736	C1664	U1522	G1454	U1372	U1282	A1189	G1100	A1019	C934	A862
U1737	U1595	G1523	G1455	A1375	U1283	U1190	G1101	C1021	U935	A863
U1738	C1596	A1525	C1456	U1378	U1286	U1191	G1102	A1026	A939	A864
C1739	A1597	U1528	C1457	U1379	U1290	A1194	G1111	A1027	A940	A865
G1745	C1599	C1529	G1458	C1379	G1291	C1195	G1112	C1028	A941	G666
A1746	A1600	C1530	C1459	U1380	G1292	A1196	A1113	U1029	G942	G667
G1747	G1601	U1531	A1460	U1381	C1292	C1197	G1114	C1028	G943	G668
G1748	C1602	C1533	C1461	A1382	C1309	G1198	G1119	U1030	A944	
A1749	U1603	G1534	G1462	G1385	C1309	G1199	G1119	U1031	G872	
G1750	G1604	U1535	C1463	U1310	U1310	G1200	G1120	C1032	G948	
A1750	U1604	G1536	G1464	G1386	U1311	G1201	U1120	C1033	C949	
C1751	G1605	C1536	G1465	G1387	A1312	A1202	C1121	C1034	C950	
U1754	C1606	C1537	A1471	A1388	U1313	A1203	U1129	G1035	A951	
A1754	G1607	U1538	C1472	C1389	U1314	C1207	U1136	A1039	U959	A881
A1755	U1608	G1539	G1473	U1390	U1315	A1208	U1137	G1040	U960	A882
U1756	U1609	G1540	U1474	A1391	G1316	C1317	A1138	G1041	U961	A883
G1757	G1610	G1541	C1475	U1392	C1317		U1144	G1042		A884
U1758	A1611	G1542	C1476	U1397	U1320	U1214	U1145	G1043	A966	A885
C1759	U1612	G1548	G1477	U1398	A1321	A1217	U1146	A1043	A970	A886
G1760	A1613	C1549	G1478	C1399	A1322	G1218	G1147	U1052	A973	A887
A1761	C1615	A1550	A1480	U1400	C1323	U1227	G1148	U1053	A978	A888
A1762	G1616	A1551	A1401	A1401	G1324	A1227	G1149	U1054	A979	A889
A1765	U1617	G1553	C1482	G1402	A1325	A1227	G1150	U1055	U981	A890
A1766	C1618	U1554	A1483	U1407	C1326	A1234	G1151	U1058	A982	A891
A1767	G1619	A1555	G1484	U1408	G1327	C1235	G1152	U1059	A987	A892
G1768	C1620	A1556	C1485	G1409	G1328	G1236	G1153	U1060	G987	A893
U1769	U1621	U1557	G1486	G1409	G1328	G1237	A1157	A1061	U989	A894
U1773	C1622	U1558	A1487	A1410	A1331	G1237	C1158	A1062	U989	A895
C1773	G1623	A1559	G1488	A1411	C1332	A1337	C1159	U1063	G991	A896
G1774	C1624	U1560	U1489	G1412	A1337	U1239	A1160	G1064	A982	A906
U1775	A1625	U1561	C1490	U1413	C1338	U1240	G1162	A1065	A993	A907
A1776	U1626	C1562	U1491	U1414	C1338	G1241	G1163	C1066	G994	A908
G1777	C1627	C1563	A1492	U1415	C1339	G1241	A1166	A1068	U996	U911
U1778	G1629	U1564	G1493	G1416	U1340	A1341	G1167	C1070	G997	U912
U1779	C1630	C1565	A1497	A1417	A1341		A1171	U1071	A998	G913
G1780	A1631	C1568	G1498	A1424	A1344		G1172	C1072	U999	G914
A1781	C1636	A1569	C1500	A1424	A1345		G1173	G1073	A1001	A915
A1782	C1637	U1570	C1501	A1427	A1346		G1174	C1074	A1002	U916
G1783	G1638	C1571	G1502	G1428	U1347		G1175	U1079	A1003	U917
C1784	C1638	C1572	A1503	G1429	A1348		G1176	U1080	A1004	A918
U1785	G1642	A1573	G1506	U1430	U1349		G1177	A1081	U1005	A919
G1789	C1646	G1574	G1507	U1432	C1431		G1178	C1082	C1006	U920
G1792	C1647	C1578	C1508	U1432	U1432		G1179	A1086		A924
G1793	A1648	U1579	U1509	U1434	G1433		U1175	U1087	C1010	G925
A1794	G1649	C1580	U1510	G1435	U1434		G1176	A1087	G1011	A926
U1795	U1650	C1581	U1511	A1436	A1360		G1177		G1012	C927
C1796	A1651	G1582	G1512	U1437	U1361		G1178		A1003	
A1797	G1654	U1584	G1513	G1438	U1362		G1179		U1004	
U1798	G1654	U1585	U1514	U1438	U1363		G1180		A1005	
U1799	U1657	A1586	A1515	G1445	U1364		G1181		C1010	
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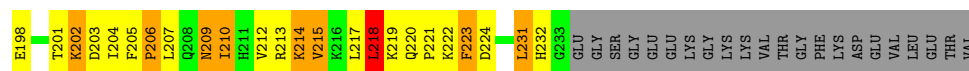
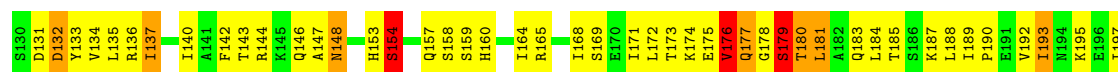
• Molecule 1: 18S ribosomal RNA

Chain 6:  45% 37% 16%

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U77	A78	C79	U82	G83	A84	A85	A86	C87	A92	A93	U94	G95	G96	C99	A100	U101	U102	A103	A104	U105	U106	C107	A108	G109	C114	G115	U116	A119	G127	C130	C131	U132	U	U	A	C136	U137	A138	C139	A140	U141	A142	G143	U144	A145	U146	C149	U150	G151	U152	A153		

G1435	G1351	G1255	G1172	U1097	U920	U843	G768	U694	U617	U546	C479	U319	C233
A1436	G1354	A1256	U1175	U1098	A926	A844	A769	U695	U618	U547	G480	U320	G234
U1437	G1176	U1257	G1016	G1100	A926	G845	A770	C896	A619	G548	A481	C321	G235
A1444	U1259	U1258	G1017	G1101	A933	G846	C697	C697	A620	C549	C484	G322	A236
U1362	C1180	C1182	U1018	G1102	C934	A847	A773	U698	A621	G553	A485	A323	U240
A1446	U1181	U1182	A1019	U1103	C934	C848	A774	U699	A622	C552	G486	U324	U241
C1447	U1182	G1263	A1019	U1104	U935	C849	G775	C700	A623	C552	G487	G325	U242
G1448	A1183	G1264	A1020	G1105	G938	A850	G778	U701	G624	A555	C488	G326	G243
U1449	U1184	G1265	C1021	U1106	G938	U854	G779	G702	C625	A556	G489	A401	G244
U1450	U1185	G1266	A1026	G1107	G942	A855	A780	U705	U626	C557	C490	A328	U245
C1451	U1186	U1269	A1027	G1108	C943	A856	U781	A706	C577	U558	G491	G329	G246
U1452	U1187	G1270	C1028	G1109	A944	U857	U782	A707	C627	C559	C492	A331	A247
G1455	C1190	C1274	U1029	G1114	U945	G858	G783	A707	U629	C560	U493	U332	U246
A1456	U1275	U1275	A1030	G1117	C950	A859	G787	U710	A630	G562	U494	A333	U249
C1457	U1276	U1276	U1031	U1117	C950	G787	G787	U711	C637	U563	C407	A408	C250
G1458	G1277	G1277	A1193	G1118	A951	A863	A788	U712	U638	C564	C495	G334	A251
C1459	G1278	G1278	G1032	G1119	A952	U864	A789	A713	U639	C565	G496	U335	G261
A1460	C1279	C1279	C1034	U1119	G953	A865	A793	G714	U640	C566	G497	G336	U262
G1385	A1196	G1280	G1039	C1121	C956	G866	A793	U718	C645	C569	U498	G337	G263
A1388	G1199	G1281	G1040	C1122	G957	G868	U795	U719	C646	C570	C500	C338	G264
C1389	G1200	G1282	G1041	G1123	U958	U870	A799	G720	G647	C571	U501	U340	A265
A1390	A1124	G1283	G1042	A1124	U959	G872	U800	G721	G648	C574	G503	A341	A266
G1391	G1127	U1284	G1050	G1127	U960	C874	G801	G722	G652	C577	U504	U348	A271
U1392	G1130	A1208	G1051	U1052	U961	G875	U808	G723	C653	C577	A505	U349	U272
C1393	G1212	G1212	G1052	G1053	A963	G876	A809	G724	C654	U578	A506	U350	G273
U1396	A1133	G1304	G1053	U964	U964	C880	G810	U728	G655	A579	U508	C351	G274
U1397	C1134	U1305	U1057	U965	A966	C880	G811	G730	C658	U581	G509	A352	C275
U1398	A1217	C1306	U1058	A966	A966	A884	A812	G730	C659	U582	G510	G354	C276
C1399	G1218	G1218	U1059	C969	C969	G885	U813	A733	G660	C583	A511	U358	U277
A1400	C1220	C1220	A1060	A970	A971	U886	A814	A734	A661	C584	A512	A359	G279
G1402	A1226	U1311	A1062	G972	A973	A891	G816	G736	U665	C587	G514	A360	U280
C1403	A1227	A1312	U1063	A973	A973	A892	A817	A737	U666	U588	A515	C361	G281
G1404	G1228	A1313	G1064	U1145	G1065	U893	C818	G738	U667	C588	G516	G362	C282
U1405	G1229	U1314	A1065	G1146	C1066	U894	G819	G739	U670	A594	U517	G363	U283
A1406	A1230	G1315	C1066	G1146	A977	G895	U820	A740	U670	C595	A518	G364	G287
G1410	U1231	G1316	C1067	G1150	G986	A898	U821	C741	G	C597	C519	A366	G287
U1413	A1234	U1320	C1070	A1151	G987	G901	U822	U742	U	U600	G523	A369	G291
U1414	G1237	A1321	U1071	G1152	G987	G902	G823	G751	A673	U601	U524	A370	U292
U1415	A1238	A1322	C1072	G1153	C990	G903	U825	A752	G676	A602	A525	G371	U293
G1416	U1239	G1330	C1077	G1155	A991	U904	U826	A753	G677	U603	A526	C376	U297
A1417	U1240	G1331	C1078	C1156	A992	G904	C827	A754	A678	U604	A460	G377	C298
G1418	G1241	C1332	U1079	A1157	A993	A905	U828	A755	A679	A605	G461	A378	A299
C1419	A1242	C1333	U1080	C1159	G997	A906	A829	A756	U679	A606	G462	A379	A300
G1420	G1243	U1334	U1081	A1160	G997	C910	U830	A757	U680	G607	U532	U379	A301
U1427	A1244	U1335	C1082	C1161	C1000	U911	U831	U758	U681	G608	U533	C381	C305
G1428	G1245	A1336	U1089	G1162	A1001	U912	U832	U759	C682	U609	A538	C382	C308
U1508	A1344	A1344	C1090	A1163	G1002	G913	U833	A760	C683	G610	G539	G383	C309
C1509	G1429	A1345	C1091	G1164	U1003	A915	G834	G761	A684	U611	G540	G384	C310
U1514	U1251	A1346	A1091	G1165	U1004	G916	U835	A762	C685	U612	A541	A385	G314
A1516	U1252	U1347	A1092	G1166	A1005	U916	U836	G763	C686	G613	A542	G386	A315
U1433	U1253	U1347	A1096	G1167	C1010	U917	G837	U764	C687	C514	C543	A387	A316
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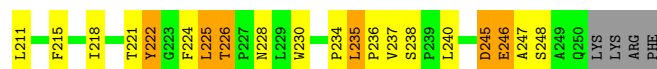
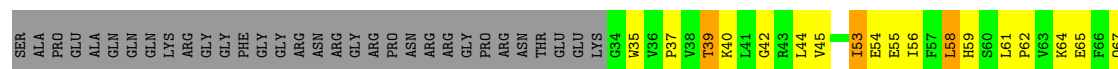




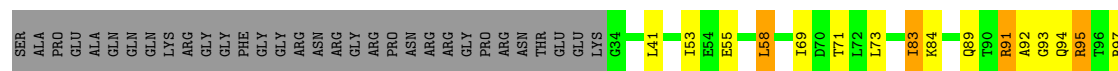
• Molecule 3: 40S ribosomal protein S1-A



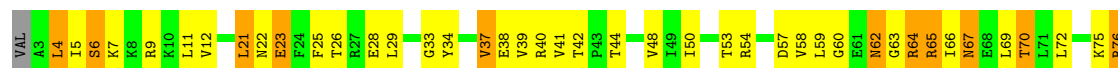
• Molecule 4: 40S ribosomal protein S2

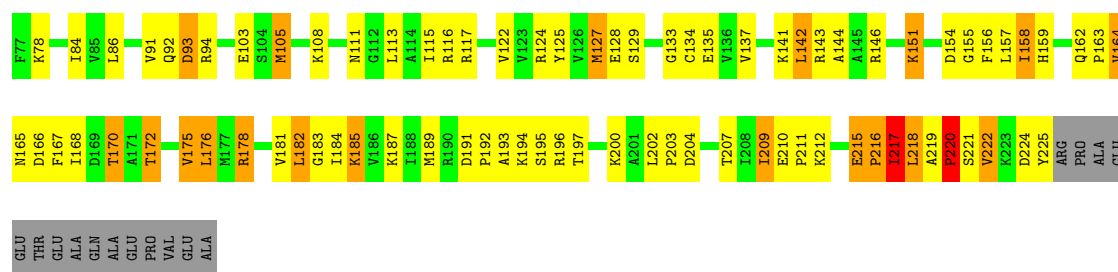


• Molecule 4: 40S ribosomal protein S2



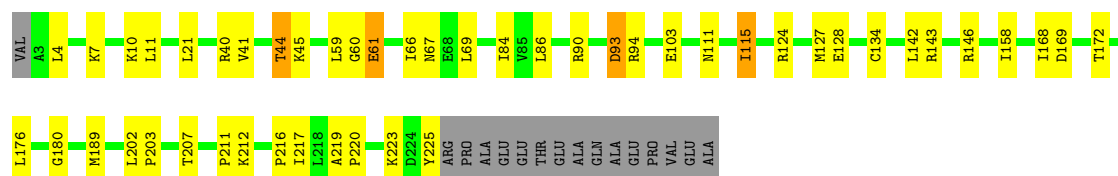
• Molecule 5: 40S ribosomal protein S3





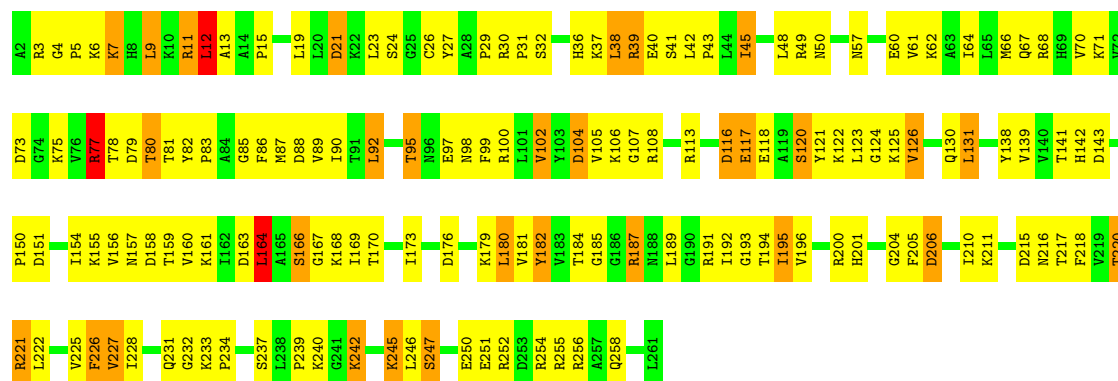
• Molecule 5: 40S ribosomal protein S3

Chain s3: 73% 18% 7%



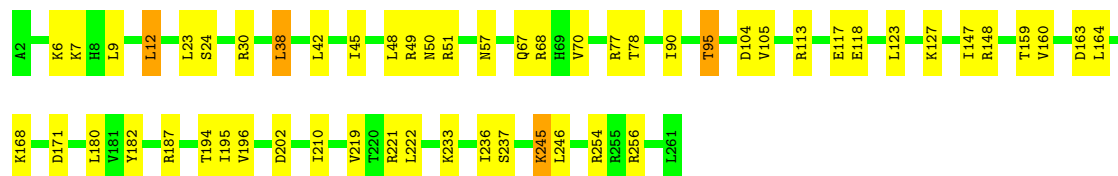
• Molecule 6: 40S ribosomal protein S4-A

Chain S4: 40% 47% 12%



• Molecule 6: 40S ribosomal protein S4-A

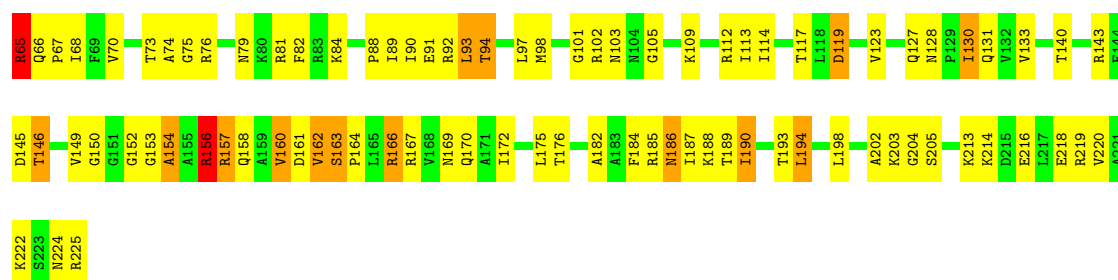
Chain s4: 79% 20%



• Molecule 7: 40S ribosomal protein S5

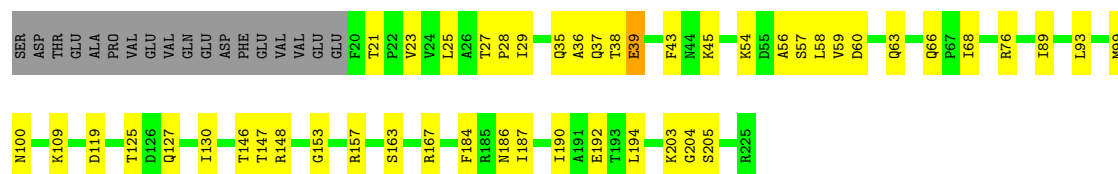
Chain S5: 38% 42% 10% 8%





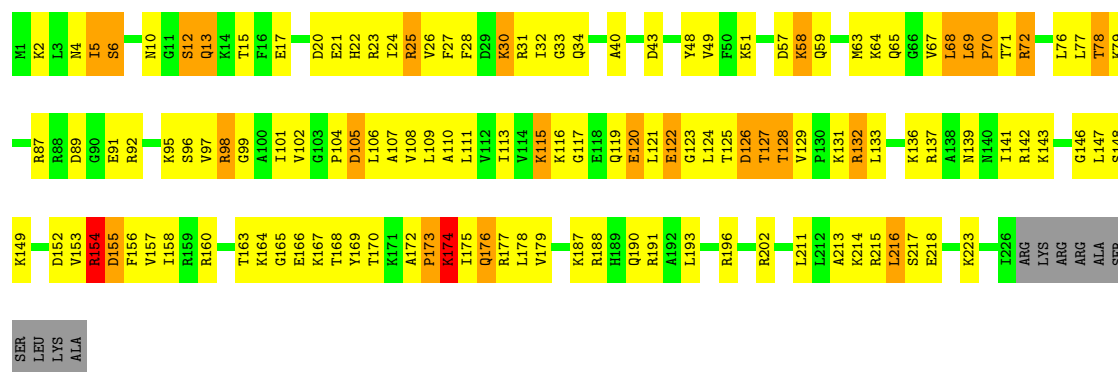
• Molecule 7: 40S ribosomal protein S5

Chain s5: 71% 21% 8%



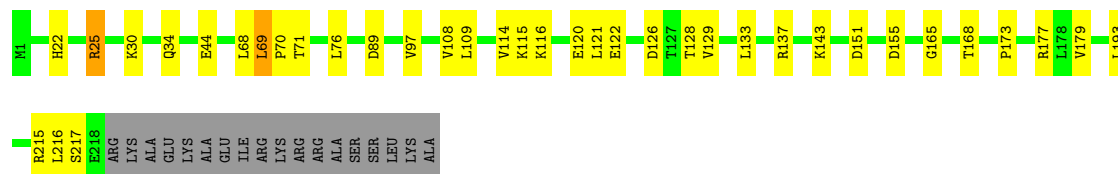
• Molecule 8: 40S ribosomal protein S6-A

Chain S6: 41% 44% 11%



• Molecule 8: 40S ribosomal protein S6-A

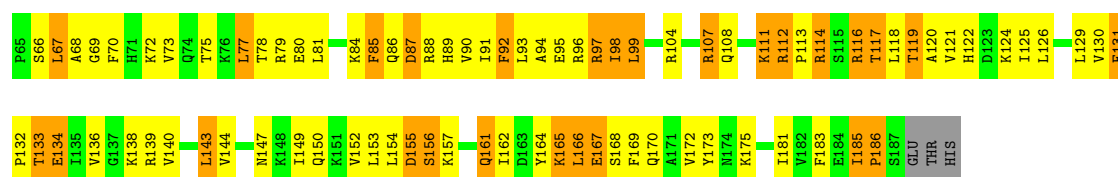
Chain s6: 77% 15% 8%



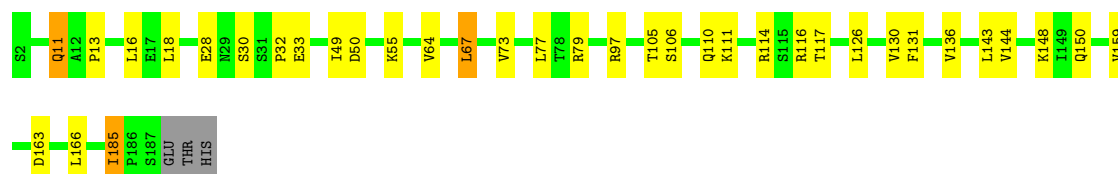
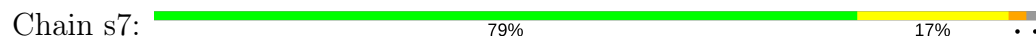
• Molecule 9: 40S ribosomal protein S7-A

Chain S7: 29% 46% 22%

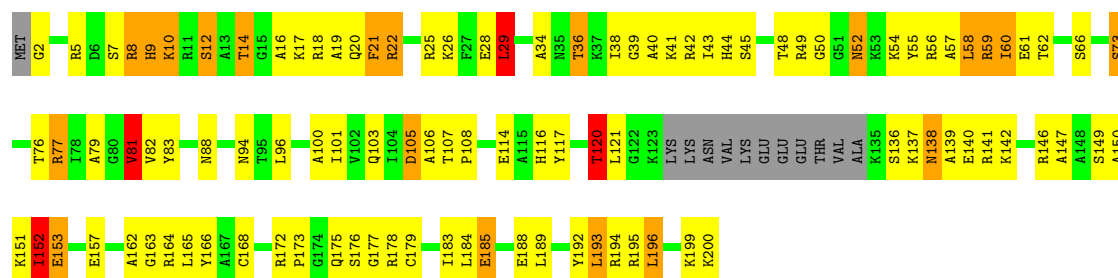




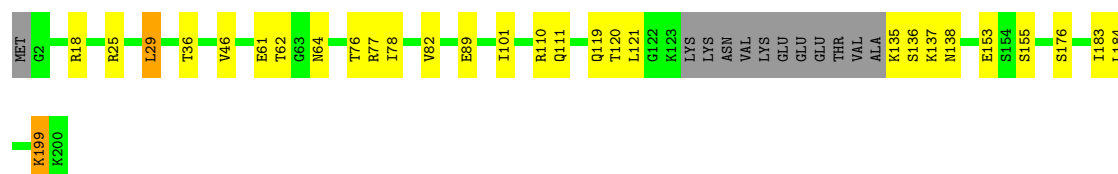
• Molecule 9: 40S ribosomal protein S7-A



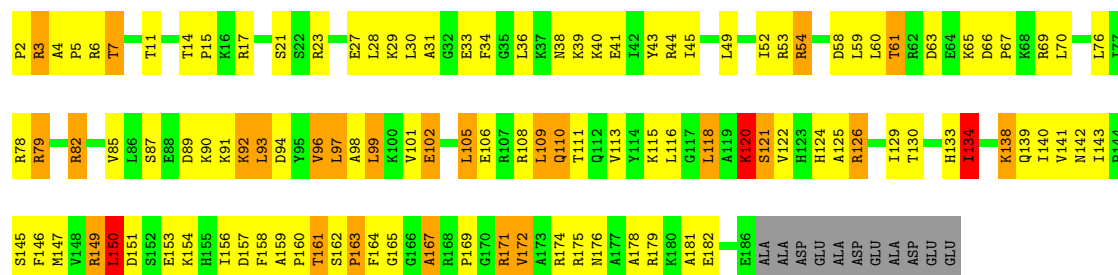
• Molecule 10: 40S ribosomal protein S8-A



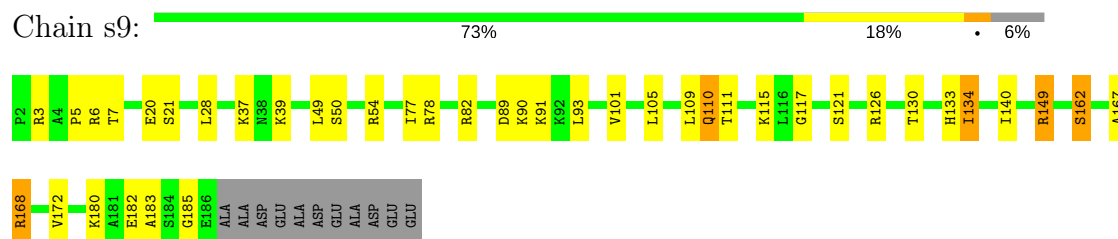
• Molecule 10: 40S ribosomal protein S8-A



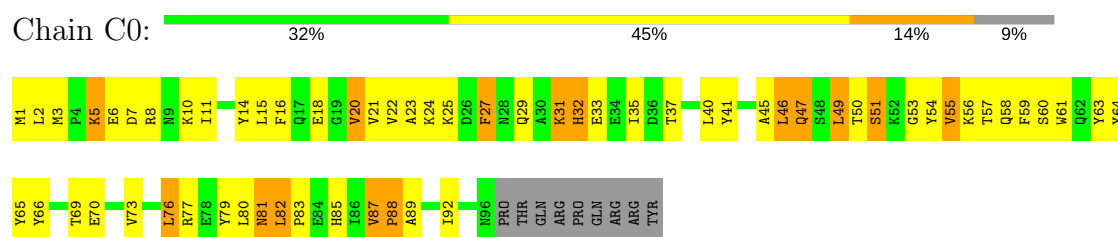
• Molecule 11: 40S ribosomal protein S9-A



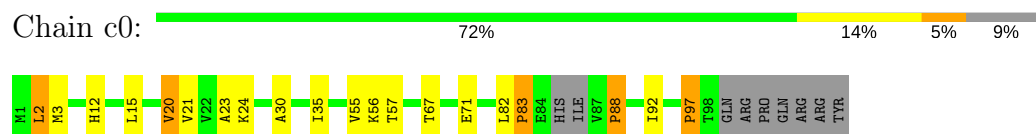
- Molecule 11: 40S ribosomal protein S9-A



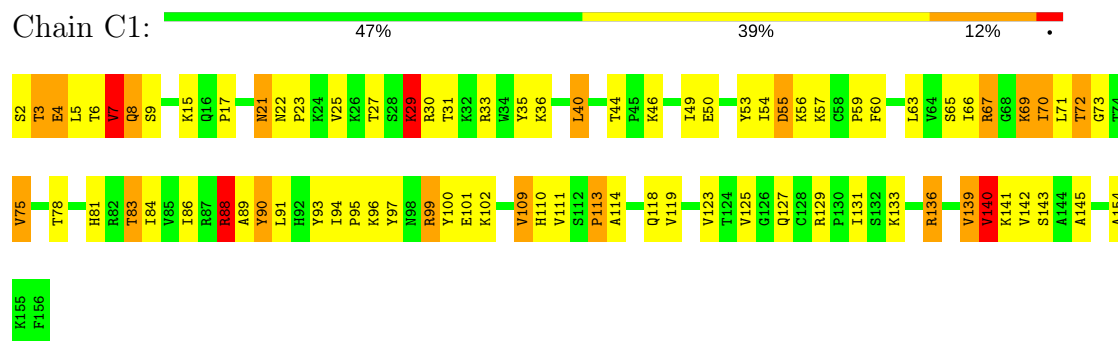
- Molecule 12: 40S ribosomal protein S10-A



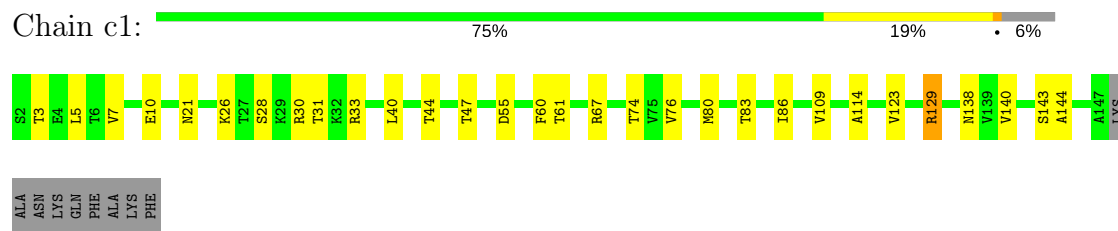
- Molecule 12: 40S ribosomal protein S10-A



- Molecule 13: 40S ribosomal protein S11-A



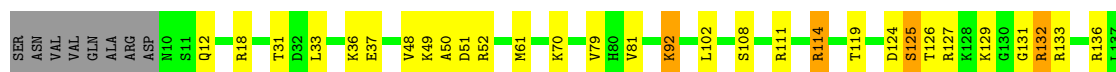
- Molecule 13: 40S ribosomal protein S11-A



- Molecule 14: 40S ribosomal protein S12







- Molecule 17: 40S ribosomal protein S15



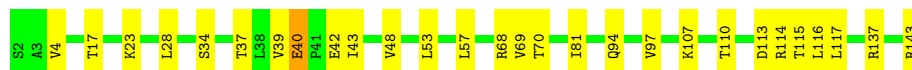
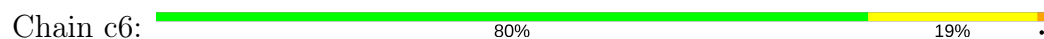
- Molecule 17: 40S ribosomal protein S15



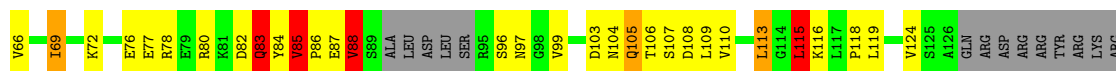
- Molecule 18: 40S ribosomal protein S16-A



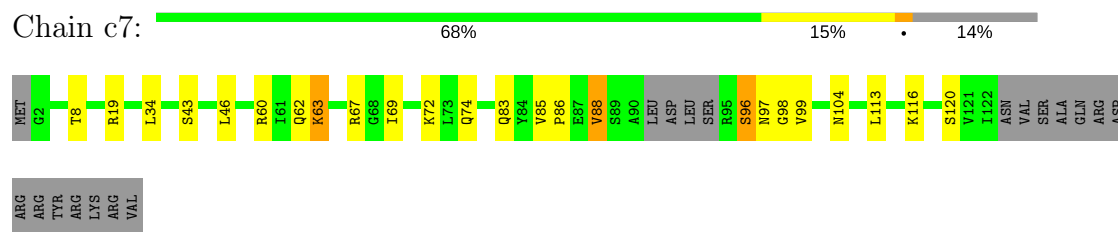
- Molecule 18: 40S ribosomal protein S16-A



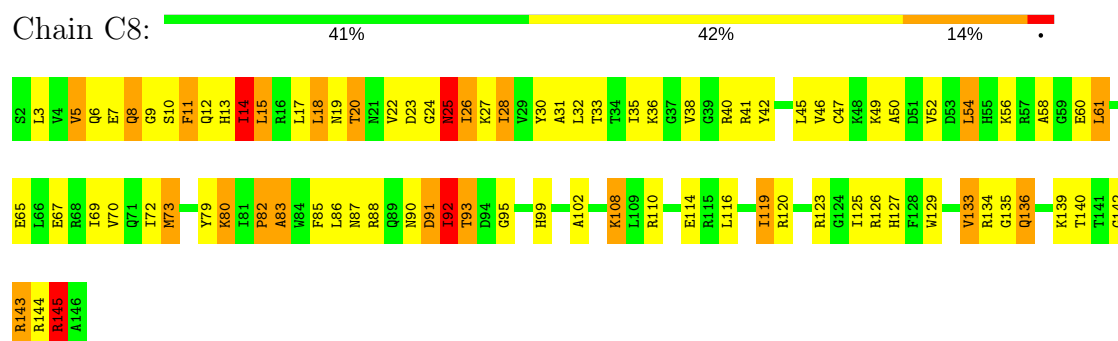
- Molecule 19: 40S ribosomal protein S17-A



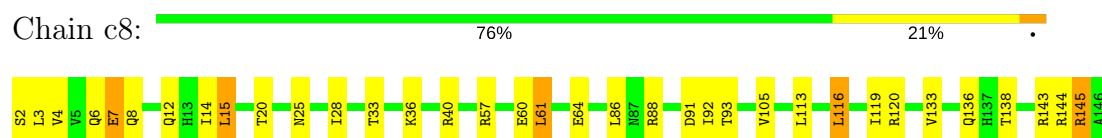
- Molecule 19: 40S ribosomal protein S17-A



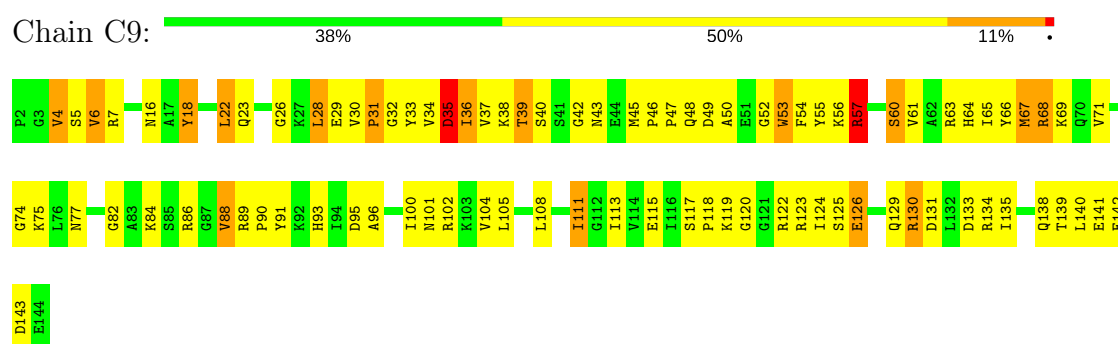
- Molecule 20: 40S ribosomal protein S18-A



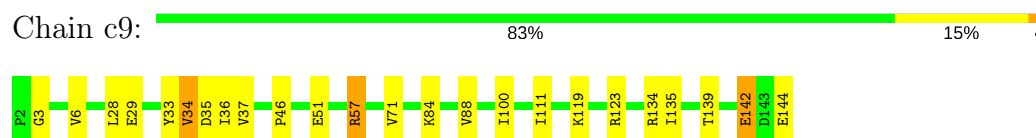
- Molecule 20: 40S ribosomal protein S18-A



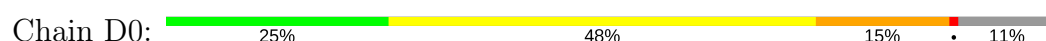
- Molecule 21: 40S ribosomal protein S19-A

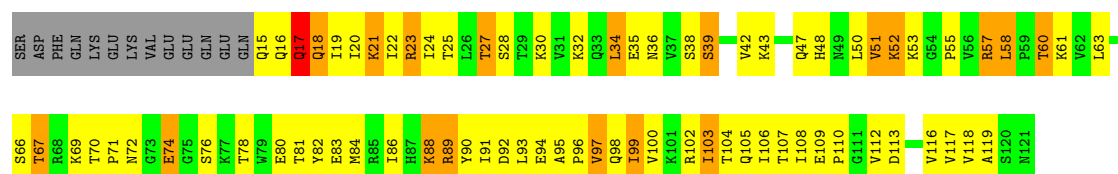


- Molecule 21: 40S ribosomal protein S19-A



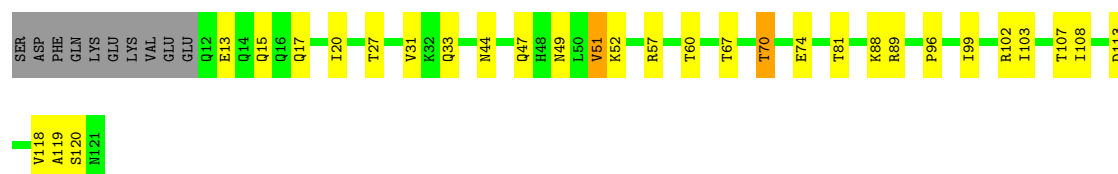
- Molecule 22: 40S ribosomal protein S20





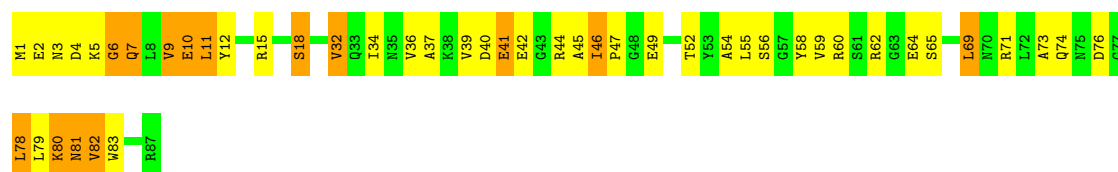
- Molecule 22: 40S ribosomal protein S20

Chain d0: 67% 23% 8%



- Molecule 23: 40S ribosomal protein S21-A

Chain D1: 46% 38% 16%



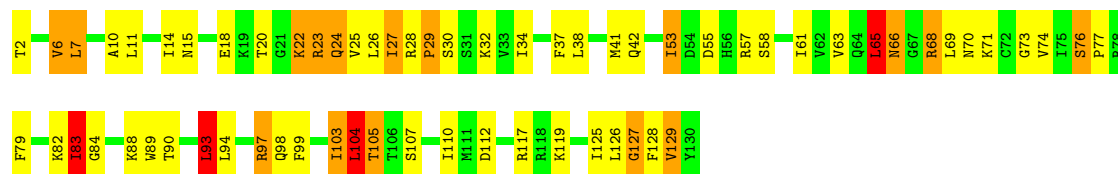
- Molecule 23: 40S ribosomal protein S21-A

Chain d1: 84% 15% 1%



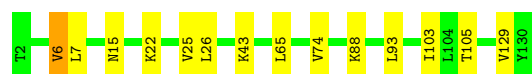
- Molecule 24: 40S ribosomal protein S22-A

Chain D2: 50% 35% 12%

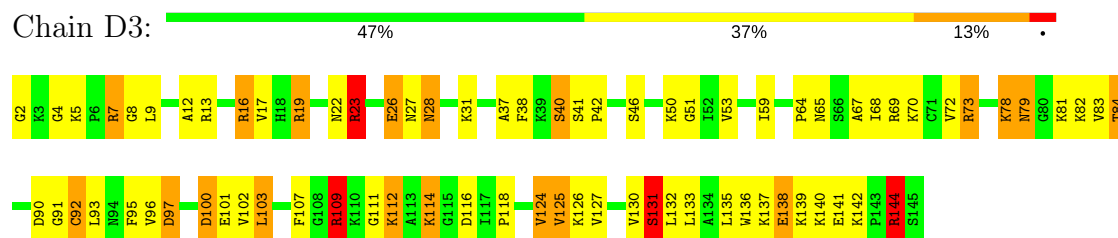


- Molecule 24: 40S ribosomal protein S22-A

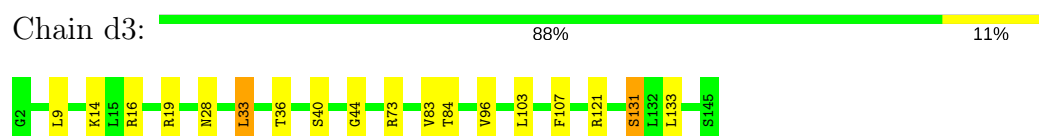
Chain d2: 89% 10% 1%



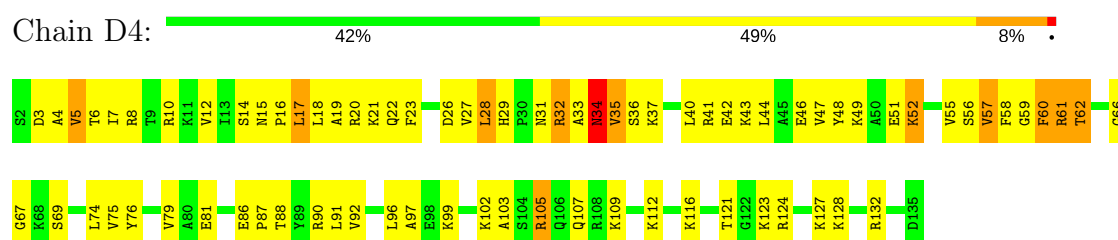
- Molecule 25: 40S ribosomal protein S23-A



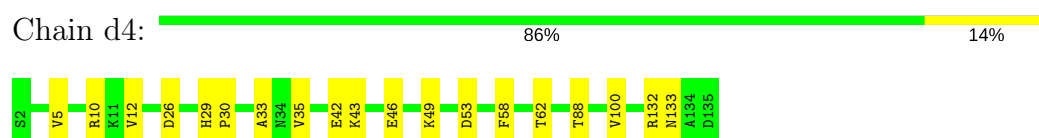
• Molecule 25: 40S ribosomal protein S23-A



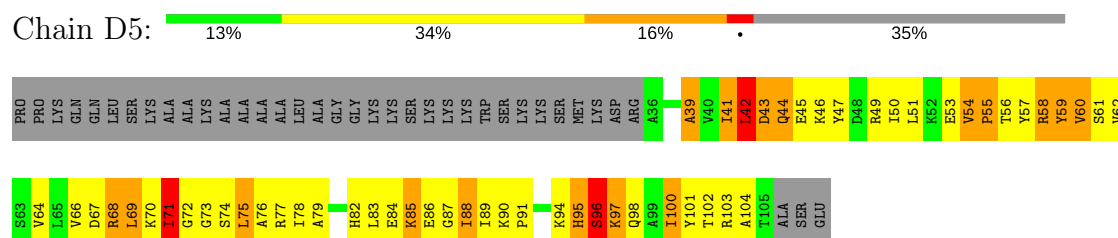
• Molecule 26: 40S ribosomal protein S24-A



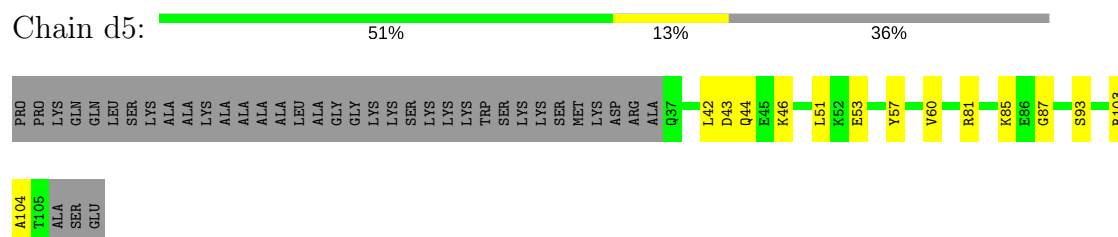
• Molecule 26: 40S ribosomal protein S24-A



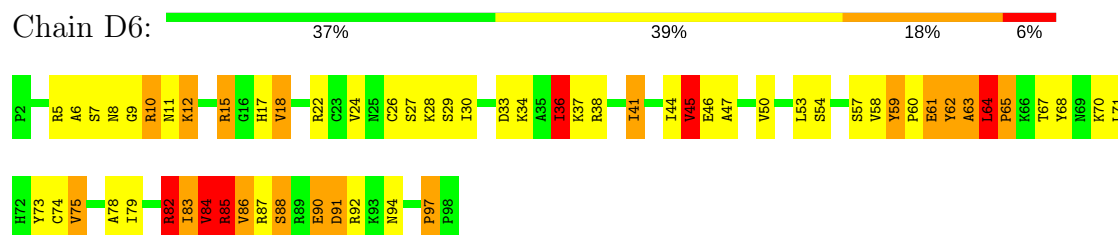
• Molecule 27: 40S ribosomal protein S25-A



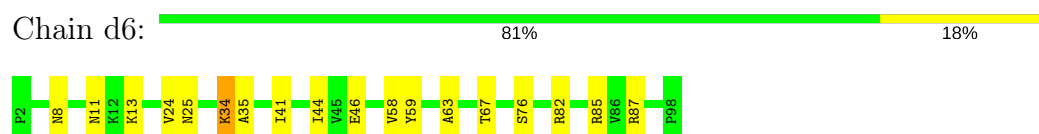
• Molecule 27: 40S ribosomal protein S25-A



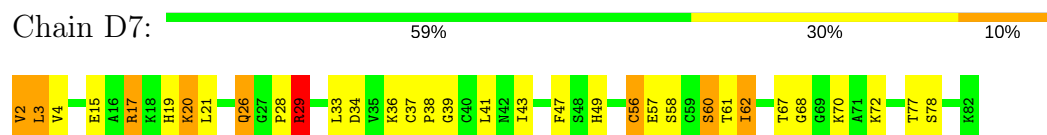
## • Molecule 28: 40S ribosomal protein S26-B



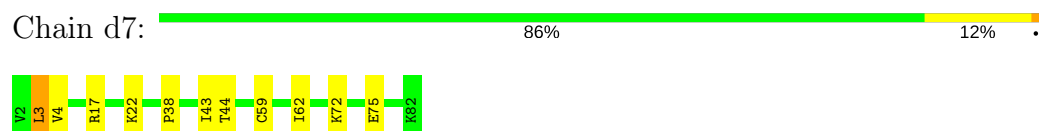
## • Molecule 28: 40S ribosomal protein S26-B



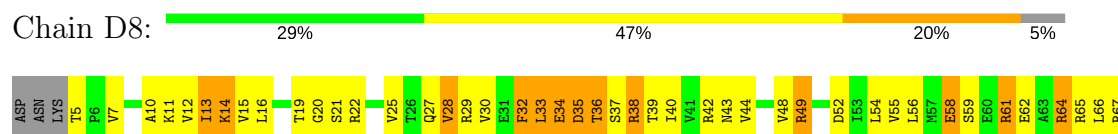
## • Molecule 29: 40S ribosomal protein S27-A



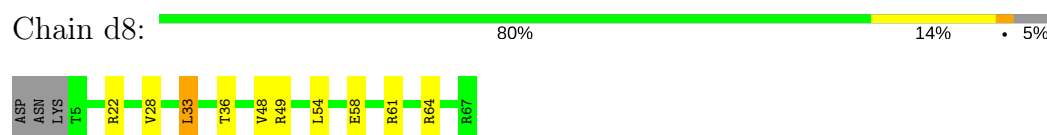
## • Molecule 29: 40S ribosomal protein S27-A



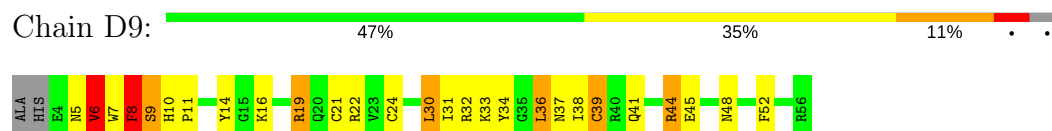
## • Molecule 30: 40S ribosomal protein S28-A



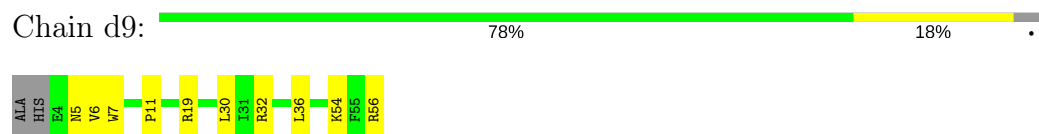
## • Molecule 30: 40S ribosomal protein S28-A



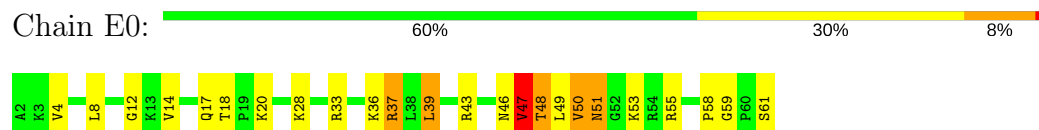
## • Molecule 31: 40S ribosomal protein S29-A



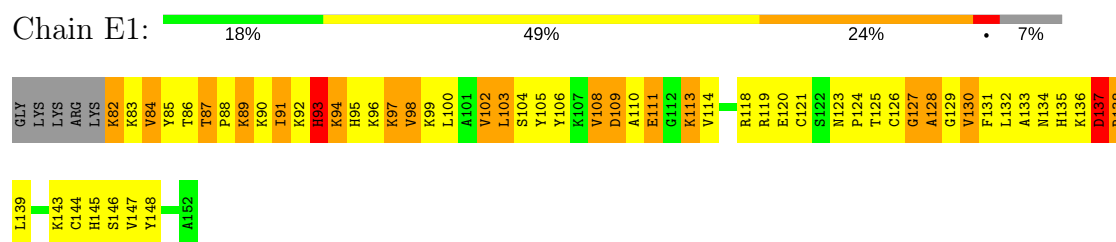
- Molecule 31: 40S ribosomal protein S29-A



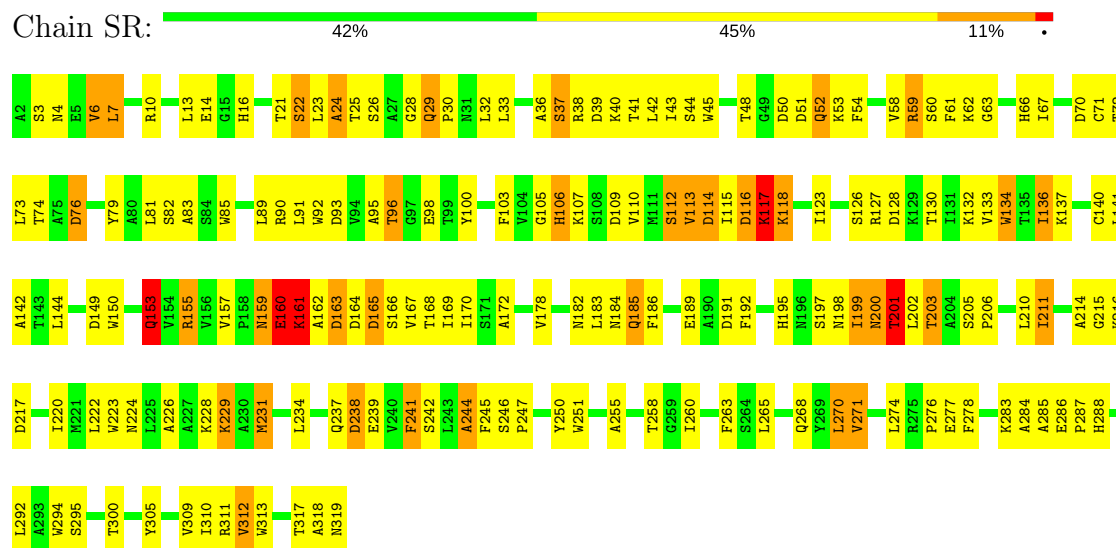
- Molecule 32: 40S ribosomal protein S30-A



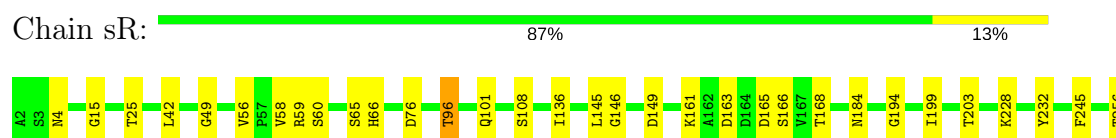
- Molecule 33: Ubiquitin-40S ribosomal protein S31



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



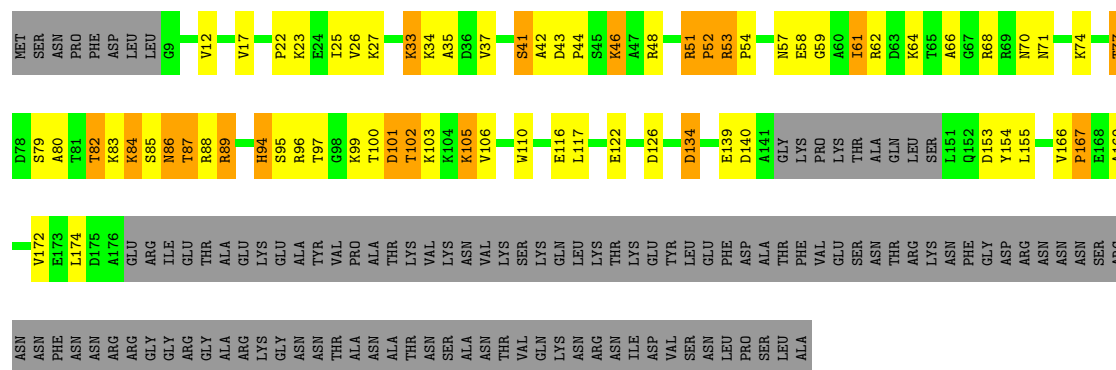
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein





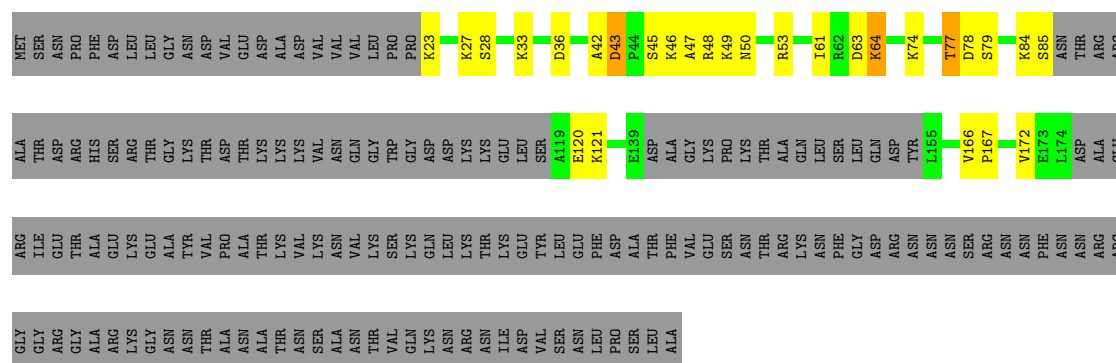
• Molecule 35: Suppressor protein STM1

Chain SM:



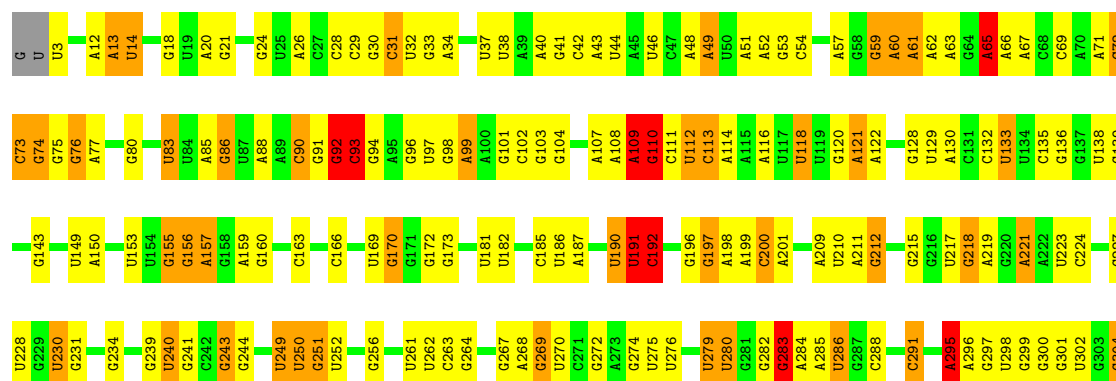
• Molecule 35: Suppressor protein STM1

Chain sM:



• Molecule 36: 25S ribosomal RNA

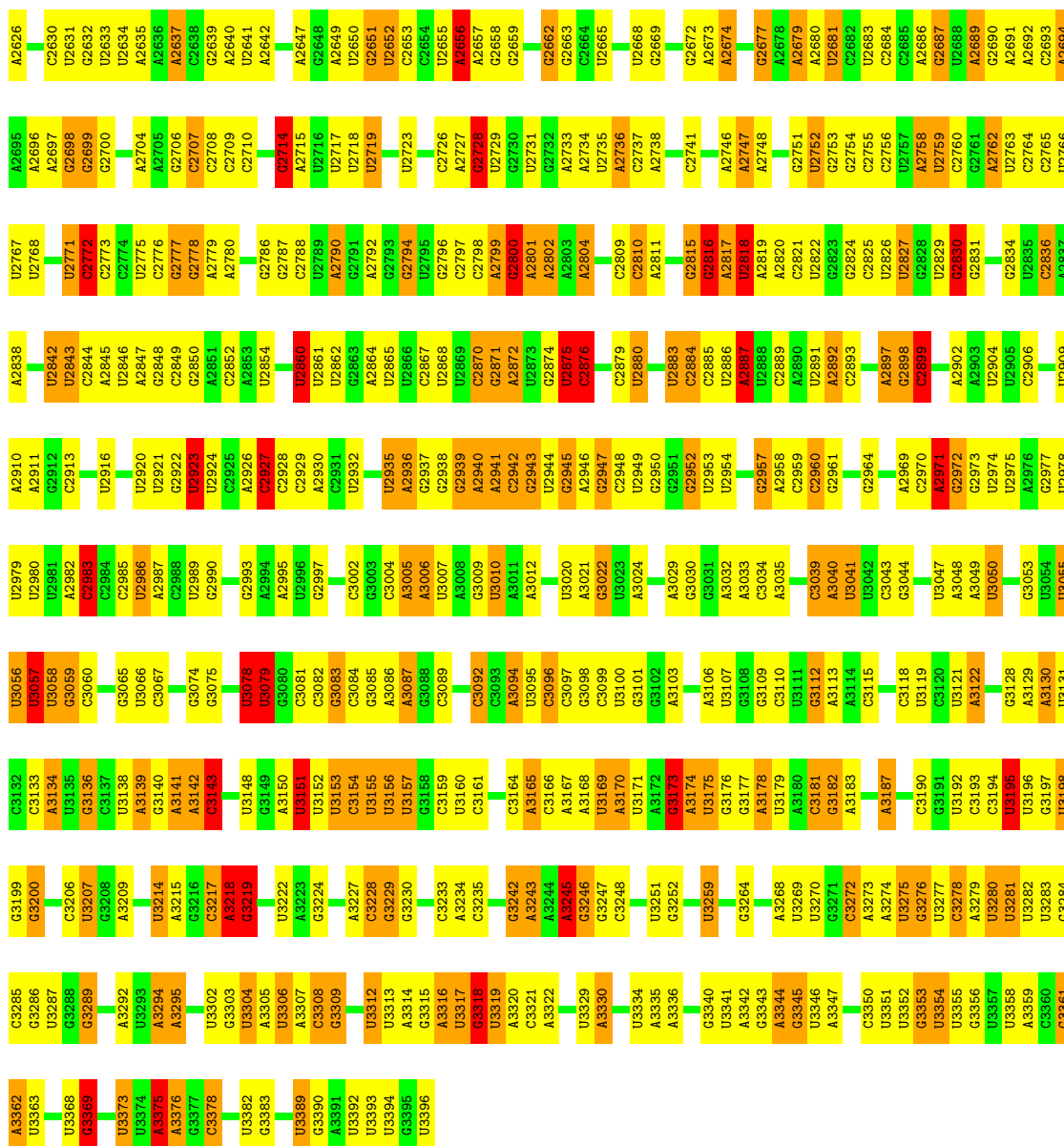
Chain 1:



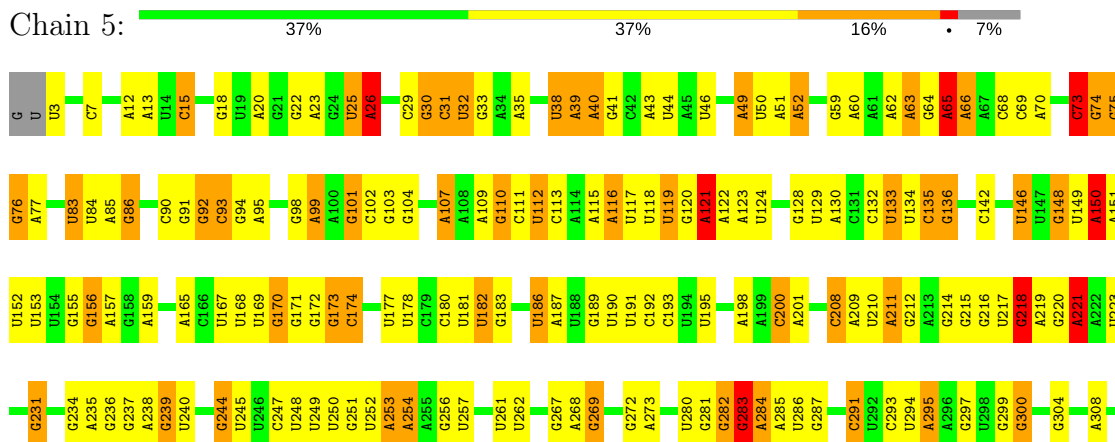






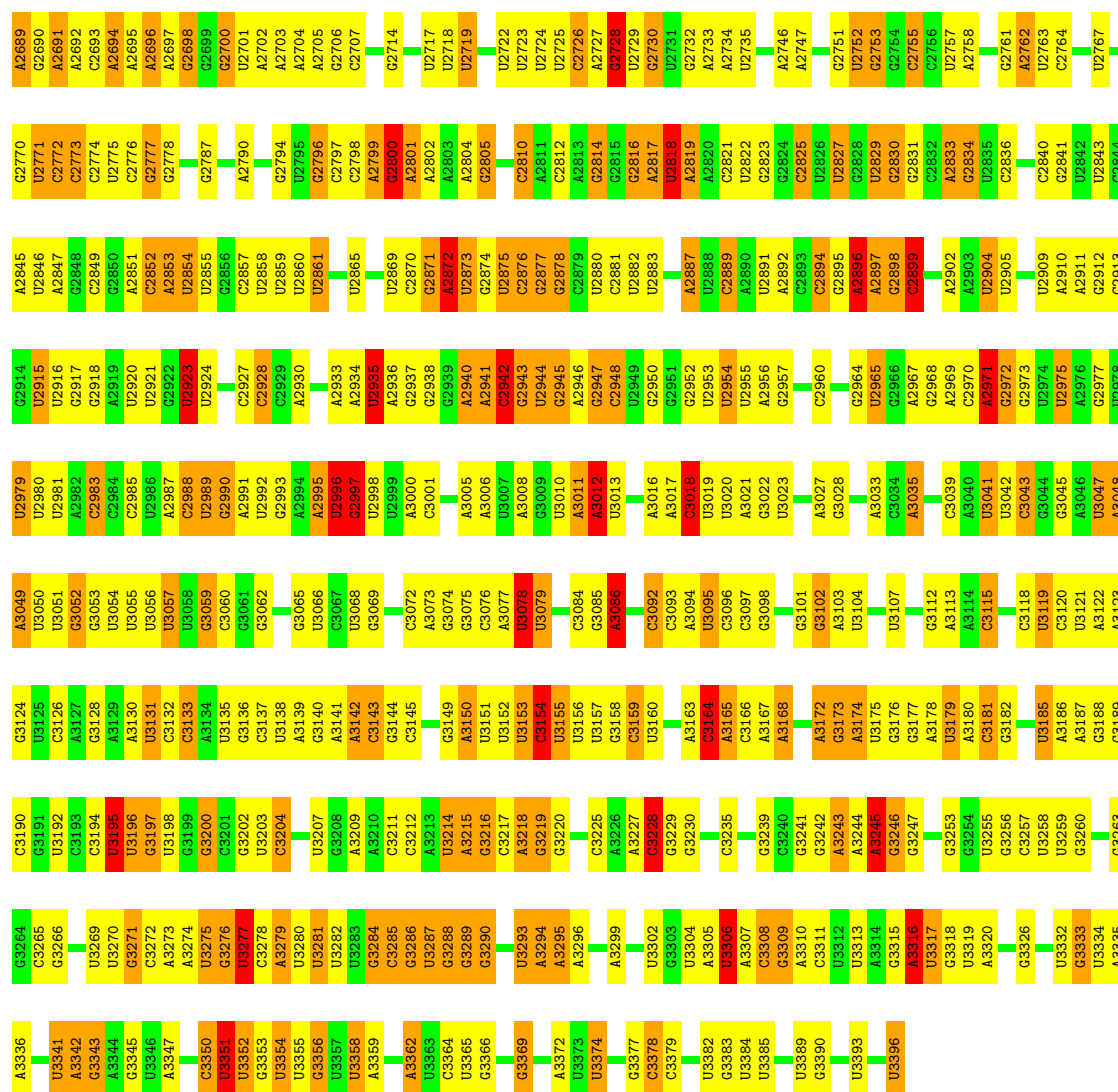


- Molecule 36: 25S ribosomal RNA



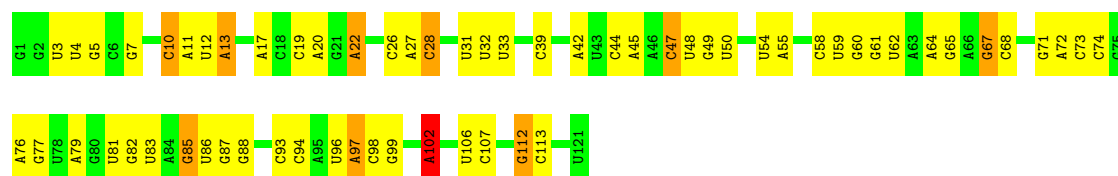
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G1433	G1434	C1364	A1294	G1194	U1128	U1056	U986	A915	A836	A744	C675	U627	A523	C	A396	U314
A1435	G1295	C1195	A1195	A1129	A1129	A1057	U988	G916	A837	U748	A677	A620	U528	U	A397	C315
U1436	C1296	A1197	C1296	A1130	U1058	U1058	A989	A917	G838	C749	A677	A621	G530	C	A398	A529
C1437	G1367	C1198	A1198	G1132	C1132	G1059	U990	C918	C839	C753	U679	U623	G531	C	A399	A319
U1438	U1368	A1199	U1299	A1133	A1133	A1062	G991	A920	C840	C753	G680	U625	C543	C	G400	A323
A1369	A1300	A1200	G1300	G1134	U1063	G1063	A992	A921	A847	C758	U681	G618	U534	U	U401	U328
G1440	A1370	C1201	A1135	A1135	A1064	A1064	G993	U922	A848	C758	U682	A611	G535	C	A402	U329
G1441	A1302	A1202	U1138	U1138	A1065	G1065	G994	G924	G849	G763	U683	G613	G404	U	G403	U328
U1445	A1303	A1205	U1138	U1138	A1066	G1066	A996	A925	U850	G763	G686	C618	C543	U	U405	G330
U1446	U1304	G1206	C1141	C1141	U1069	C1069	A997	A926	U852	U764	G687	A619	C546	G	G406	G337
G1447	G1306	G1207	G1142	G1142	U1070	U1070	A998	C927	G853	U766	G688	A620	G547	G	A407	A338
G1450	U1379	U1208	A1143	A1143	U1071	U1071	G999	C928	G857	U767	U689	A621	G548	U	A408	C340
C1451	G1387	G1209	U1151	U1151	G1072	U1072	C1000	C923	U858	C768	A691	A622	U549	A	U410	U340
A1452	U1380	G1210	C1146	C1146	U1073	U1073	G1001	G924	G859	G769	A692	U623	A550	G	U411	G341
A1453	G1310	A1212	G1147	G1147	U1076	U1076	G1002	C931	G860	G770	A693	U625	A551	G	G412	A342
U1454	C1312	U1214	G1148	G1148	C1077	C1077	A1003	A936	G861	G774	C694	U626	G552	G	U413	U343
A1455	G1313	U1215	A1150	A1150	U1078	U1078	U1004	G937	U862	A775	C695	U627	U553	G	A416	A344
U1457	C1314	G1222	U1151	U1151	U1079	U1079	A1006	C938	G863	U776	C696	A628	U555	A	A417	G345
A1461	U1315	A1231	A1154	A1154	U1081	U1081	U1008	U942	G864	U777	A697	U629	U556	U	A418	A348
A1465	G1316	C1232	C1155	C1155	G1082	G1082	A1009	C944	U869	U778	A699	U631	A557	C	G419	A349
A1468	A1317	A1233	U1156	U1156	U1083	U1083	G1010	C945	G870	U780	G700	G532	U558	U	G420	C350
U1470	C1318	C1232	C1156	C1156	A1084	A1084	G1010	C946	U871	G781	C633	U633	A559	C	G421	A351
U1471	G1319	U1235	G1157	G1157	G1087	G1087	G1013	G947	U872	U782	C634	U634	C562	G	A422	A352
G1472	C1320	G1236	A1158	A1158	U1093	U1093	U1014	C948	C873	U784	G635	U635	U563	U	G423	G353
A1473	U1321	G1237	C1159	C1159	A1094	U1094	U1015	C949	U874	A784	G636	U636	U564	A	G424	U354
G1474	C1322	U1238	G1160	G1160	U1095	U1095	C1016	A952	C877	U786	G708	C637	G566	U	G425	A357
A1475	G1327	C1238	C1161	C1161	U1096	U1096	C1017	G953	C878	U787	A709	G638	G567	U	G426	G358
U1476	C1328	A1240	U1162	U1162	G1097	G1097	U1018	U954	G879	U788	A710	G639	A570	U	C427	G358
U1477	U1241	G1242	A1163	A1163	U1098	U1098	G1019	U955	U879	A789	C641	U641	C570	C	A428	U359
U1478	A1330	G1243	G1164	G1164	A1099	A1099	U1020	U956	G880	U790	A711	U642	C571	A	U429	G360
U1479	C1331	U1244	A1165	A1165	C1099	C1099	G1021	C957	C881	U791	G712	U643	C572	U	U430	A361
U1480	U1334	A1245	G1166	G1166	U1100	U1100	G1024	C958	A882	U796	A715	U644	U574	U	U431	U362
U1481	C1335	G1246	U1167	U1167	G1101	G1101	A1025	C959	A883	U796	A716	G644	G575	U	G493	G363
A1482	U1336	A1246	U1168	U1168	A1102	A1102	A1026	U960	A888	G800	C717	A645	C576	U	G494	G364
G1483	A1337	G1249	A1169	A1169	G1103	G1103	A1027	C961	U889	A801	G718	C648	C577	U	C435	A365
U1484	C1338	U1250	G1170	G1170	U1104	U1104	A1028	A962	U890	C802	U719	A649	A578	U	A436	A366
G1485	U1339	A1251	A1171	A1171	U1108	U1108	G1029	G963	G891	C803	A720	C650	G579	U	A437	A367
U1486	C1340	C1255	U1172	U1172	U1109	U1109	A965	G964	U892	C804	G721	G651	C580	U	A438	G368
U1487	U1341	G1256	G1173	G1173	U1110	U1110	U1032	A966	C893	G805	G725	C654	G584	U	C439	A369
U1488	C1342	U1257	C1175	C1175	U1111	U1111	U1033	U966	G894	A906	G726	C655	A585	U	A440	U370
A1489	A1343	A1258	A1176	A1176	U1112	U1112	U1034	A970	A895	U811	A661	C656	A586	U	U441	G371
G1492	G1344	G1260	G1177	G1177	U1113	U1113	G1035	G971	A896	U812	G728	A657	U587	U	G443	A374
U1493	U1345	G1261	A1179	A1179	U1114	U1114	A1036	A972	U897	G812	G731	G658	G588	U	G	A375
U1494	C1346	G1262	U1180	U1180	U1115	U1115	C1037	A973	G900	G815	U731	G659	A589	U	U506	G376
U1495	U1348	A1263	U1181	U1181	G1116	G1116	A1040	G974	A907	A916	C732	A660	A592	U	U	A377
C1496	G1349	G1264	A1182	A1182	C1118	C1118	U1047	C975	A906	C818	A736	G661	C593	U	U	A378
U1497	U1350	U1265	C1183	C1183	U1121	U1121	A1048	G978	G907	C919	A737	U662	C594	U	U	A385
G1499	A1352	G1266	A1184	A1184	U1122	U1122	C1049	U979	G908	C824	A738	U664	G595	U	G	A386
U1500	U1353	U1267	U1185	U1185	U1123	U1123	U1050	U981	G910	U825	G739	C596	G597	U	A516	A389
A1506	G1354	U1276	C1189	C1189	U1124	U1124	U1051	C982	C911	U830	G740	U669	A598	C	G	G390
G1507	U1355	C1277	U1190	U1190	U1125	U1125	U1051	A983	G912	A830	G741	U673	A599	C	C	A391
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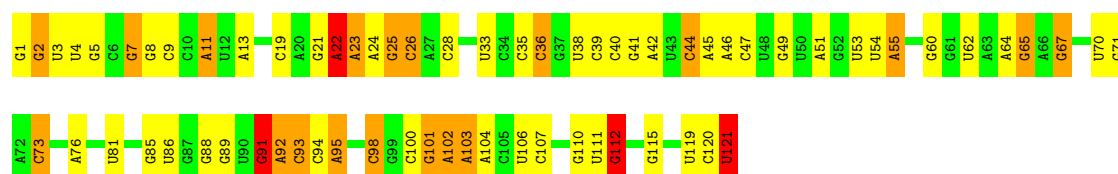
### • Molecule 37: 5S ribosomal RNA

Chain 3: 49% 43% 7%

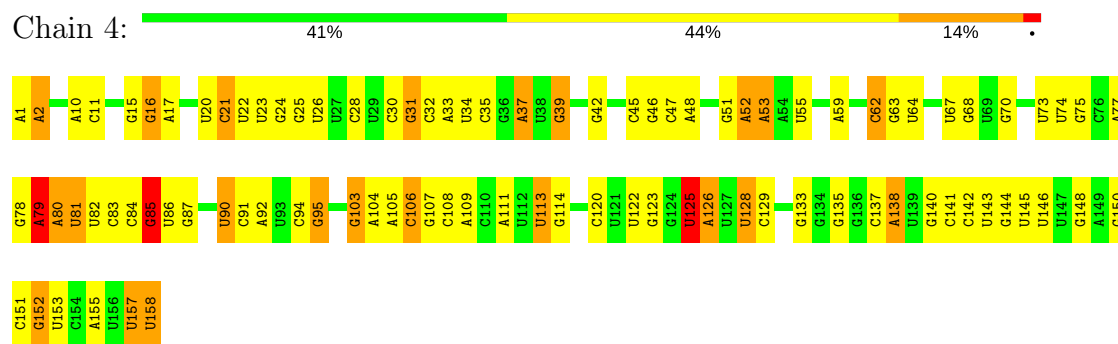


### • Molecule 37: 5S ribosomal RNA

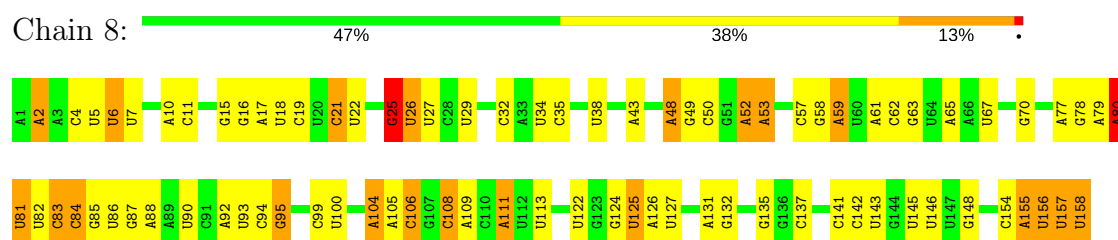
Chain 7: 43% 38% 16%



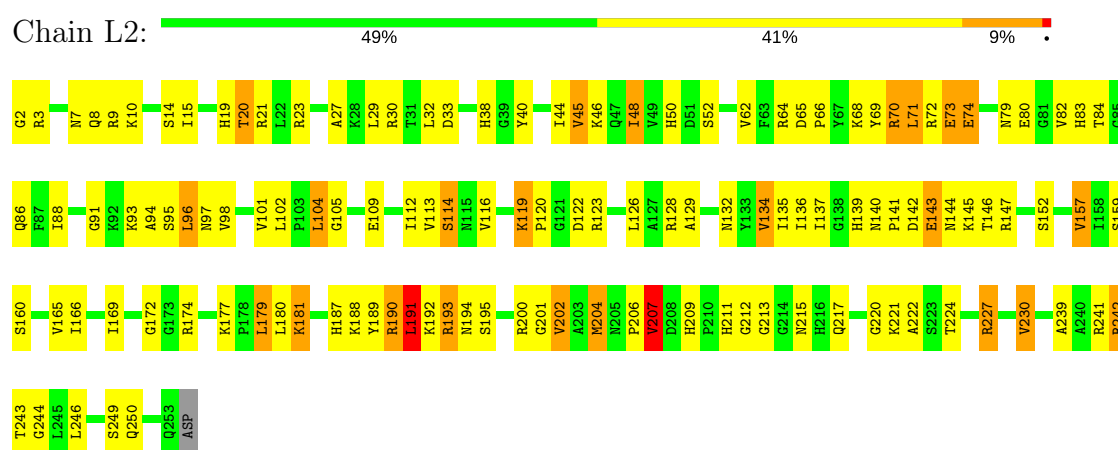
- Molecule 38: 5.8S ribosomal RNA



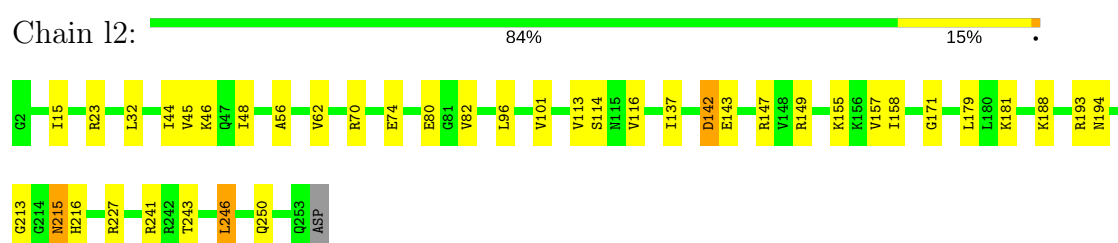
- Molecule 38: 5.8S ribosomal RNA



- Molecule 39: 60S ribosomal protein L2-A

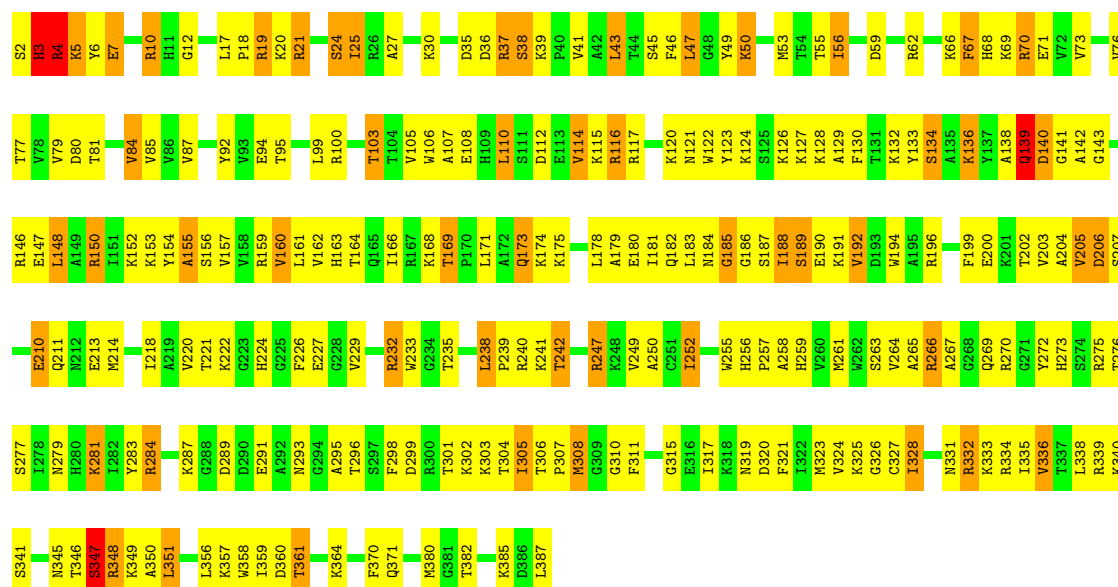


- Molecule 39: 60S ribosomal protein L2-A



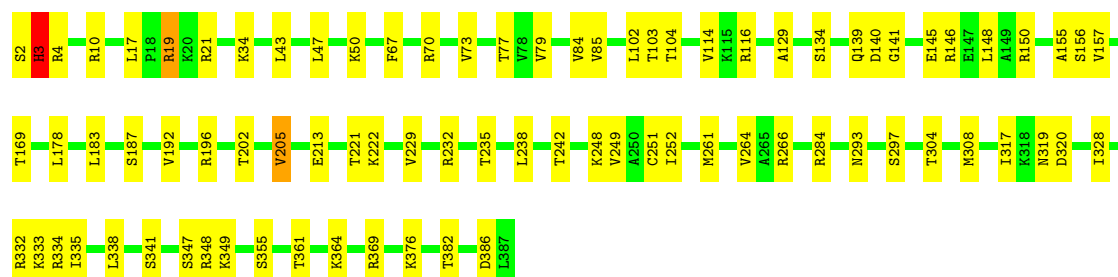
- Molecule 40: 60S ribosomal protein L3





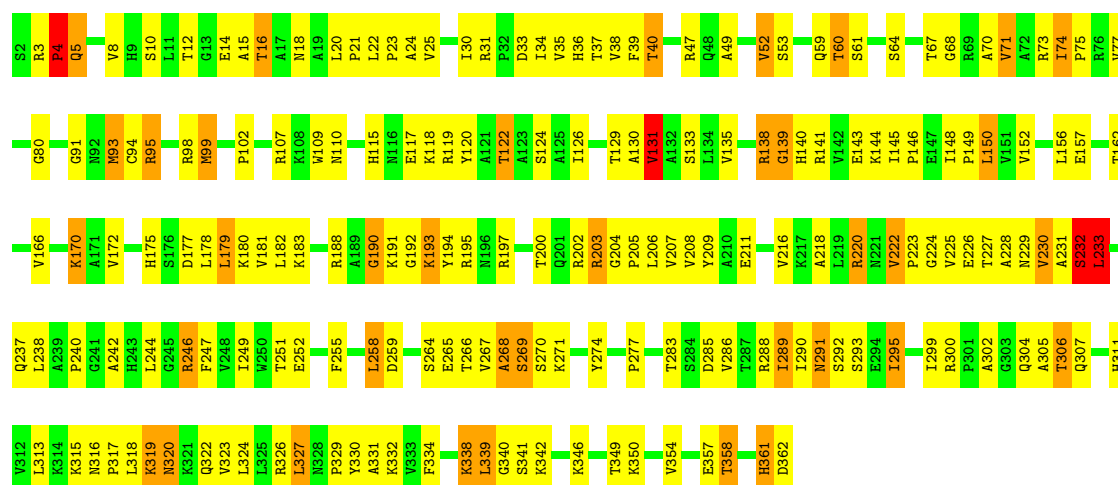
• Molecule 40: 60S ribosomal protein L3

Chain L3: 78% 21%



• Molecule 41: 60S ribosomal protein L4-A

Chain L4: 46% 43% 10%



• Molecule 41: 60S ribosomal protein L4-A



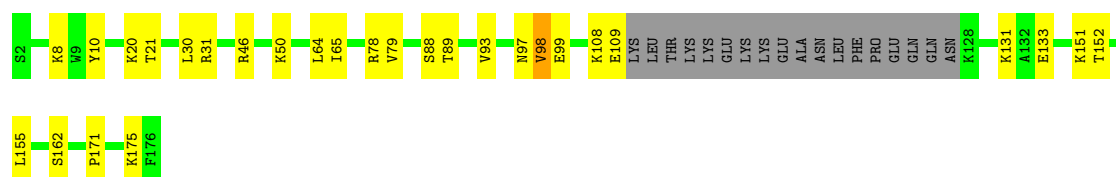
- Molecule 42: 60S ribosomal protein L5

- Molecule 42: 60S ribosomal protein L5

- Molecule 43: 60S ribosomal protein L6-A

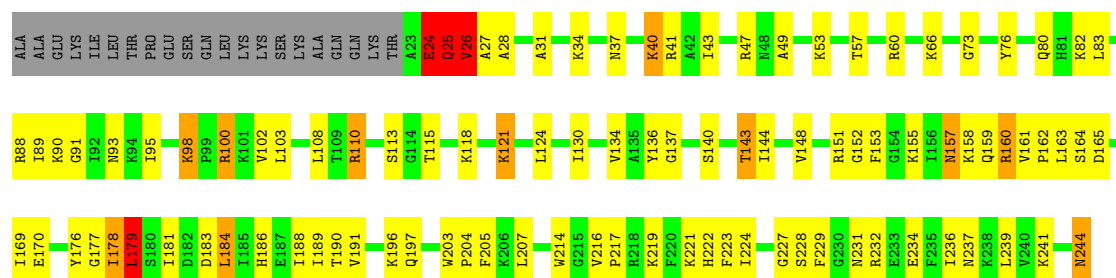
- Molecule 43: 60S ribosomal protein L6-A

Chain 16:  74% 15% • 10%



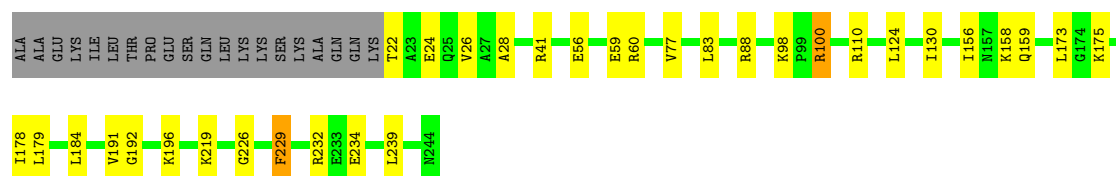
• Molecule 44: 60S ribosomal protein L7-A

Chain L7: 51% 35% 5% 9%



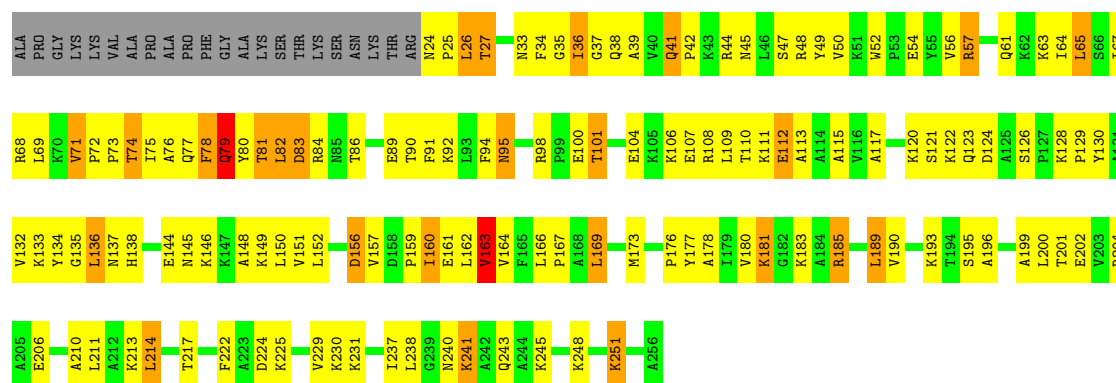
• Molecule 44: 60S ribosomal protein L7-A

Chain L7: 78% 13% 8%



• Molecule 45: 60S ribosomal protein L8-A

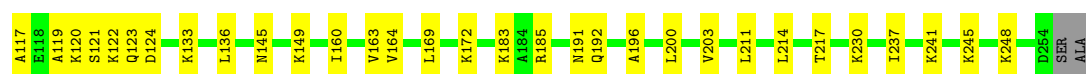
Chain L8: 37% 44% 10% 9%



• Molecule 45: 60S ribosomal protein L8-A

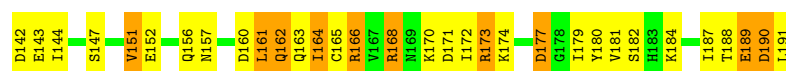
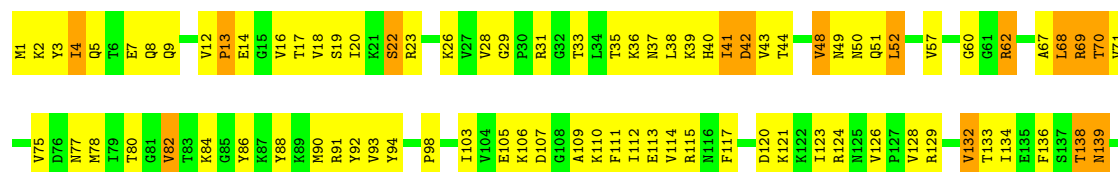
Chain L8: 71% 19% 9%





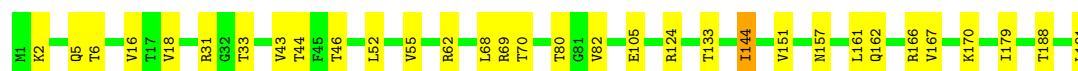
• Molecule 46: 60S ribosomal protein L9-A

Chain L9: 39% 48% 13%



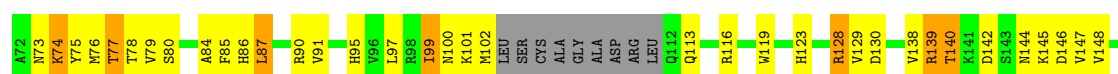
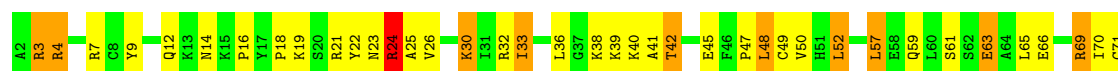
• Molecule 46: 60S ribosomal protein L9-A

Chain l9: 83% 16% •



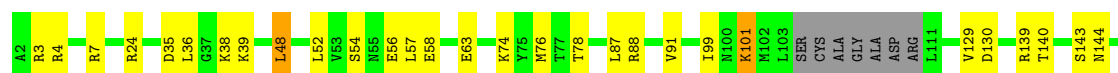
• Molecule 47: 60S ribosomal protein L10

Chain M0: 44% 40% 11% •



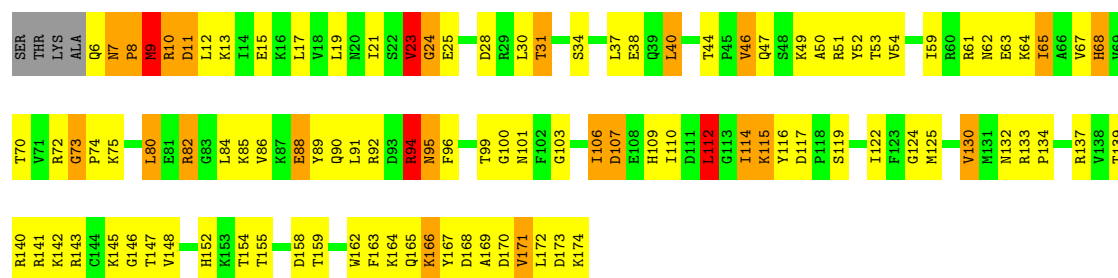
• Molecule 47: 60S ribosomal protein L10

Chain m0: 75% 21% • •



• Molecule 48: 60S ribosomal protein L11-B

Chain M1: 36% 46% 13% • •



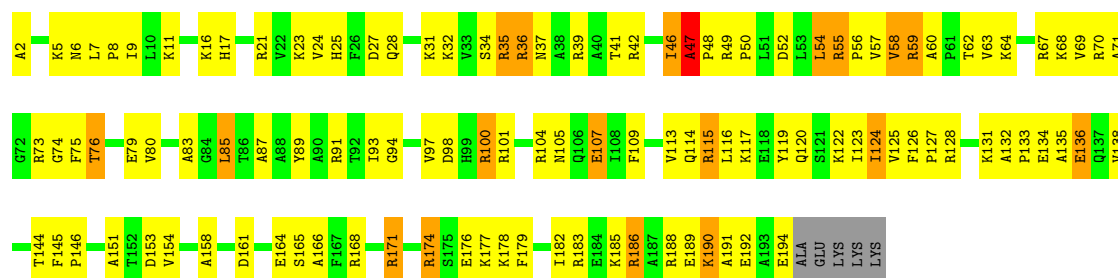
- Molecule 48: 60S ribosomal protein L11-B

Chain m1: 80% 16% ..



- Molecule 49: 60S ribosomal protein L13-A

Chain M3: 39% 48% 9% ..



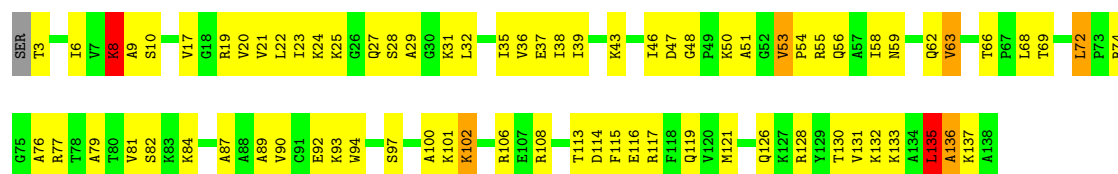
- Molecule 49: 60S ribosomal protein L13-A

Chain m3: 80% 17% ..



- Molecule 50: 60S ribosomal protein L14-A

Chain M4: 44% 50% ..



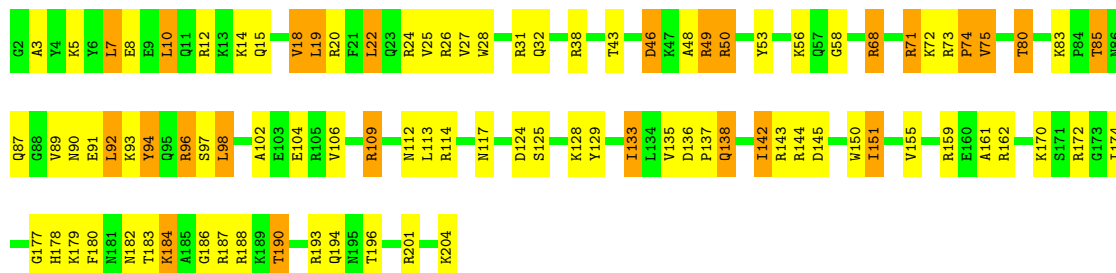
- Molecule 50: 60S ribosomal protein L14-A

Chain m4: 85% 14% ..



• Molecule 51: 60S ribosomal protein L15-A

Chain M5: 54% 33% 12%



• Molecule 51: 60S ribosomal protein L15-A

Chain m5: 84% 14%



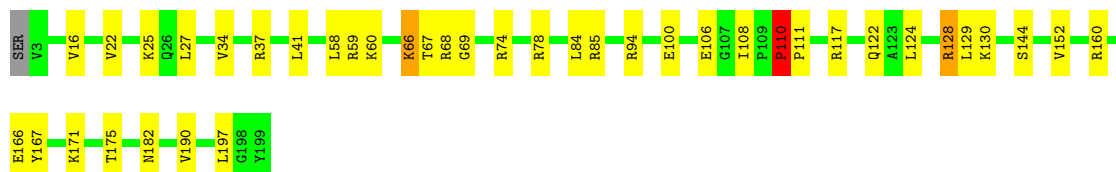
• Molecule 52: 60S ribosomal protein L16-A

Chain M6: 53% 34% 11%



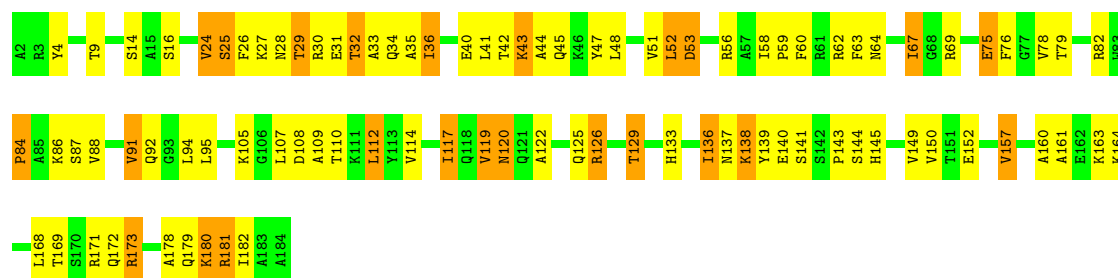
• Molecule 52: 60S ribosomal protein L16-A

Chain m6: 79% 19%



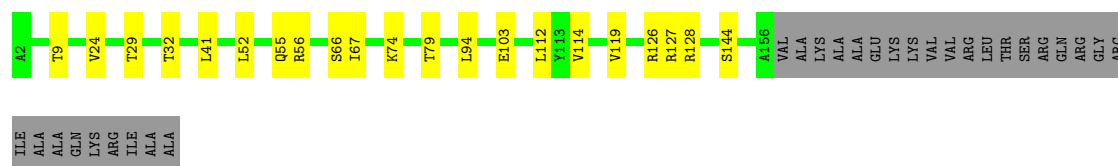
• Molecule 53: 60S ribosomal protein L17-A

Chain M7: 50% 37% 13%



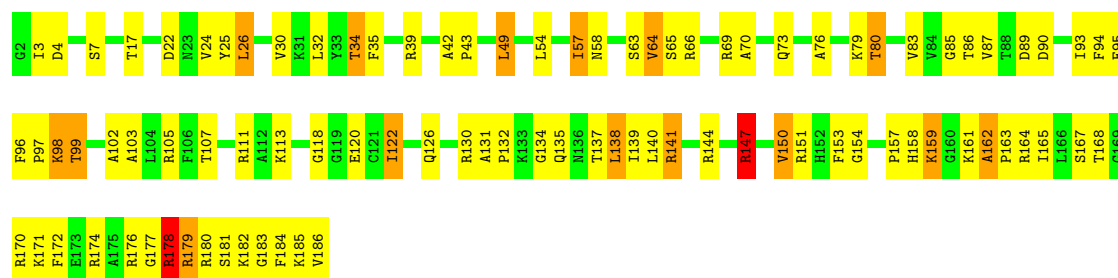
- Molecule 53: 60S ribosomal protein L17-A

Chain m7: 73% 11% 15%



- Molecule 54: 60S ribosomal protein L18-A

Chain M8: 50% 41% 8%



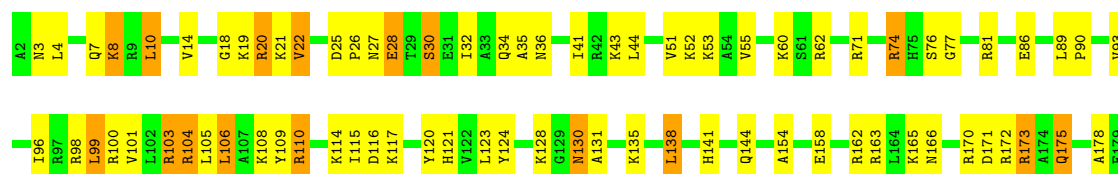
- Molecule 54: 60S ribosomal protein L18-A

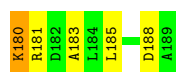
Chain m8: 80% 19%



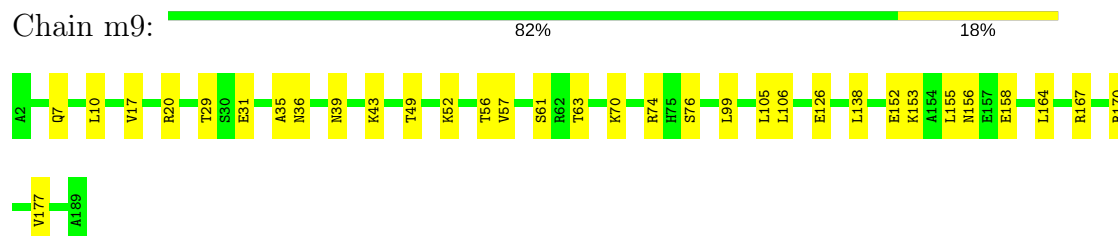
- Molecule 55: 60S ribosomal protein L19-A

Chain M9: 56% 35% 9%

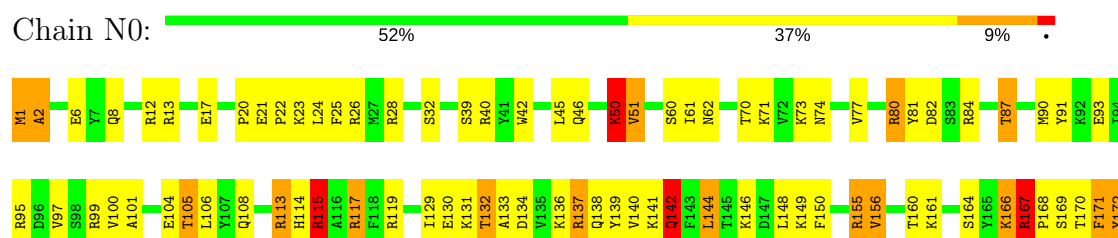




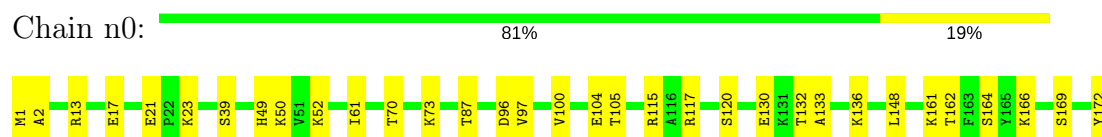
• Molecule 55: 60S ribosomal protein L19-A



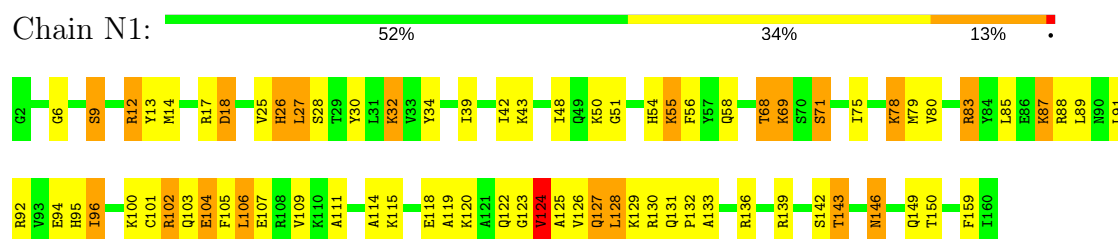
• Molecule 56: 60S ribosomal protein L20-A



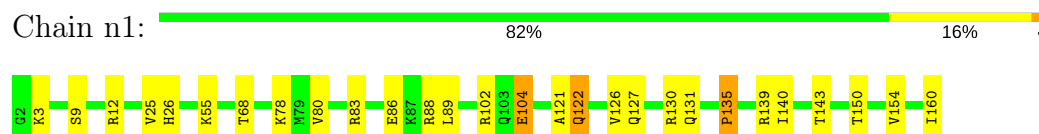
• Molecule 56: 60S ribosomal protein L20-A



• Molecule 57: 60S ribosomal protein L21-A

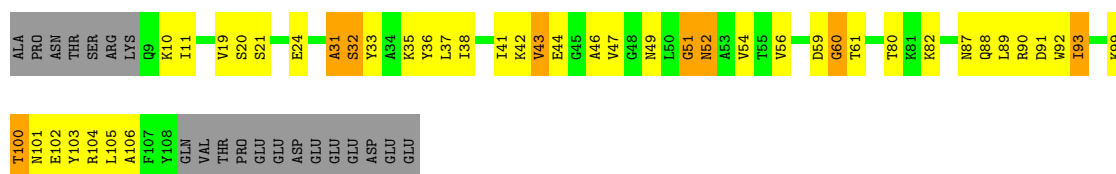


• Molecule 57: 60S ribosomal protein L21-A



• Molecule 58: 60S ribosomal protein L22-A





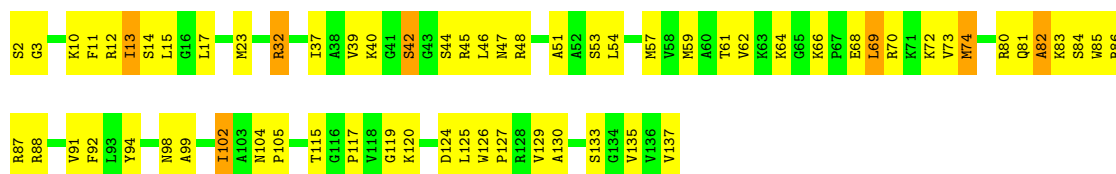
- Molecule 58: 60S ribosomal protein L22-A

Chain n2: 68% 13% 18%



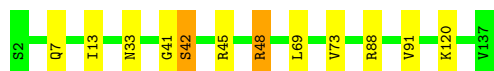
- Molecule 59: 60S ribosomal protein L23-A

Chain N3: 52% 43% 5%



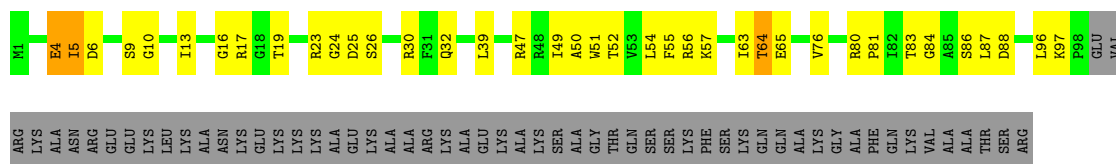
- Molecule 59: 60S ribosomal protein L23-A

Chain n3: 91% 7%



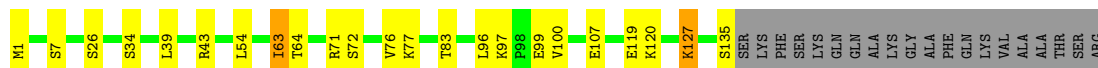
- Molecule 60: 60S ribosomal protein L24-A

Chain N4: 39% 23% 37%



- Molecule 60: 60S ribosomal protein L24-A

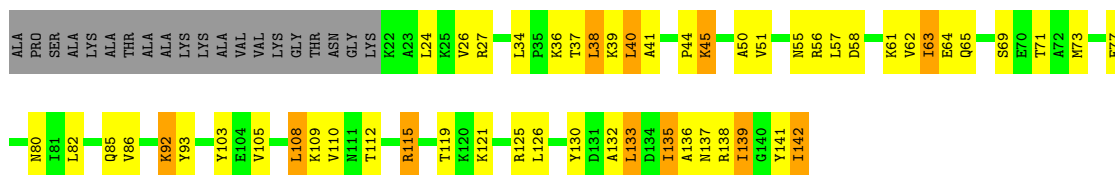
Chain n4: 72% 14% 13%



- Molecule 61: 60S ribosomal protein L25

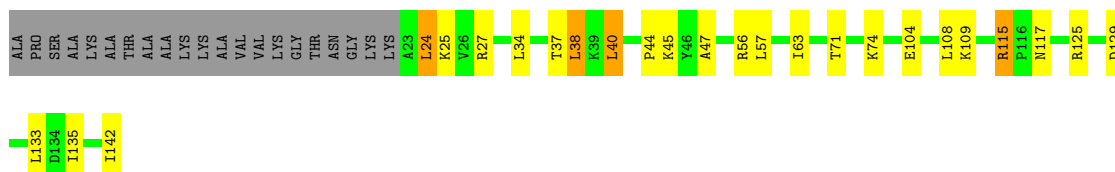
Chain N5: 48% 30% 8% 14%





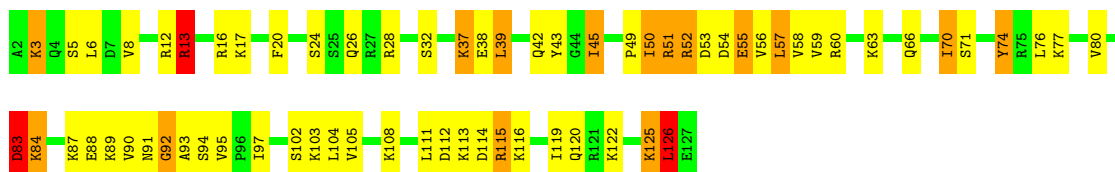
- Molecule 61: 60S ribosomal protein L25

Chain n5: 67% 15% 15%



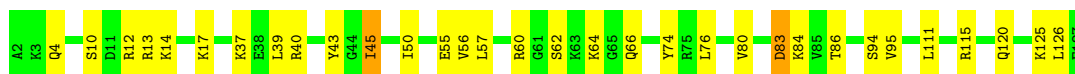
- Molecule 62: 60S ribosomal protein L26-A

Chain N6: 47% 39% 12%



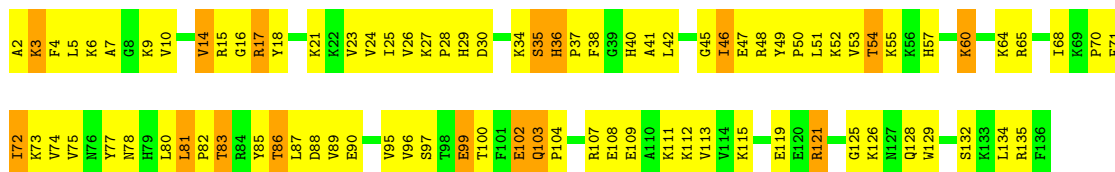
- Molecule 62: 60S ribosomal protein L26-A

Chain n6: 75% 24%



- Molecule 63: 60S ribosomal protein L27-A

Chain N7: 35% 53% 12%

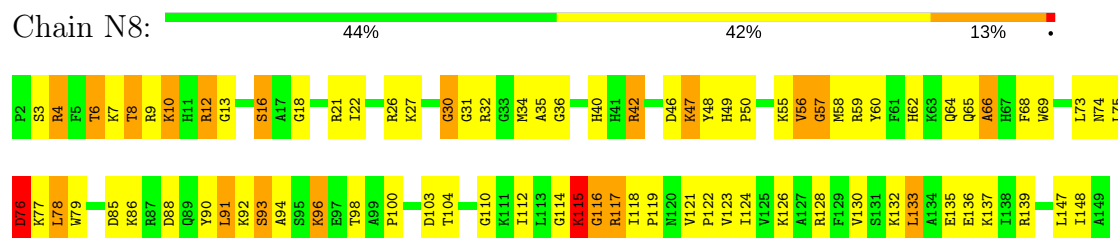


- Molecule 63: 60S ribosomal protein L27-A

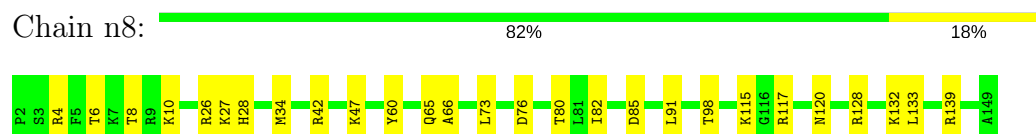
Chain n7: 78% 21%



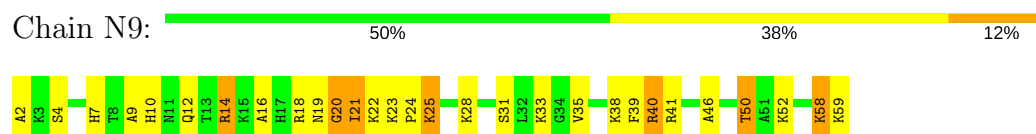
- Molecule 64: 60S ribosomal protein L28



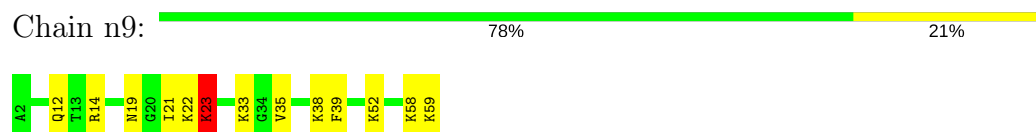
- Molecule 64: 60S ribosomal protein L28



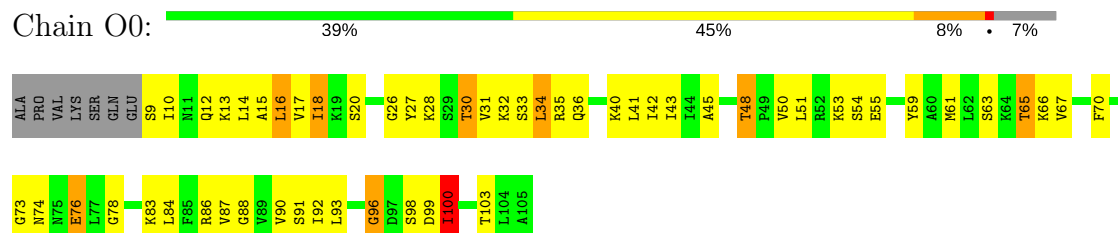
- Molecule 65: 60S ribosomal protein L29



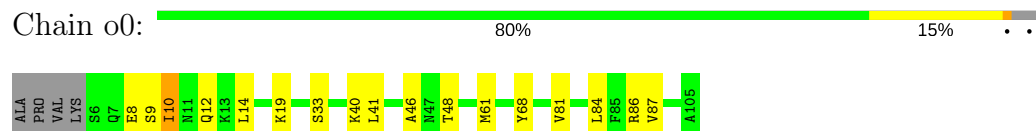
- Molecule 65: 60S ribosomal protein L29



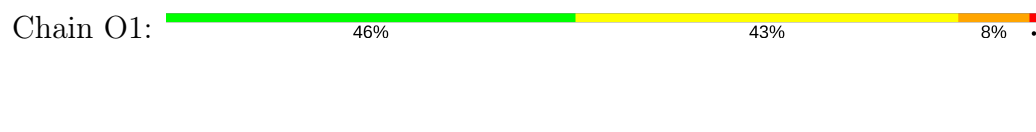
- Molecule 66: 60S ribosomal protein L30

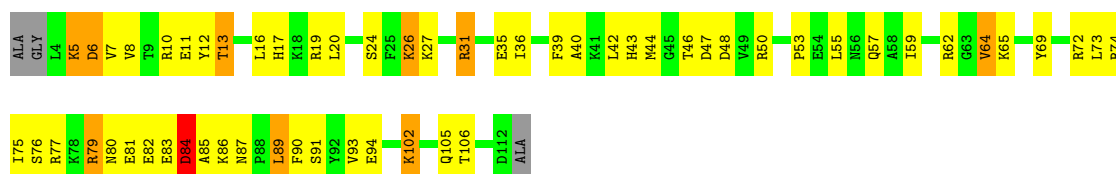


- Molecule 66: 60S ribosomal protein L30



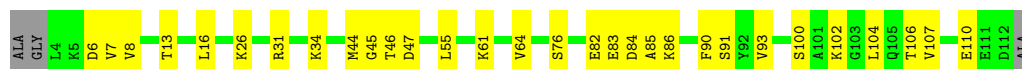
- Molecule 67: 60S ribosomal protein L31-A





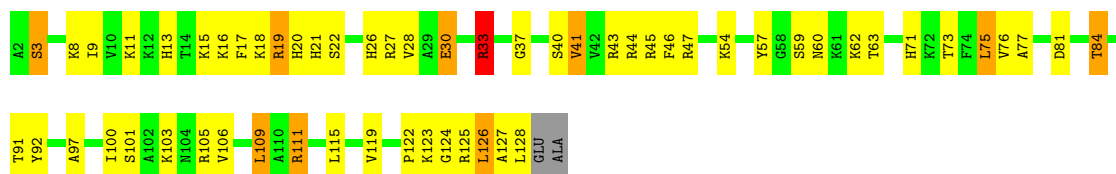
- Molecule 67: 60S ribosomal protein L31-A

Chain o1: 71% 27% .



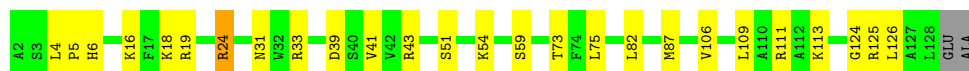
- Molecule 68: 60S ribosomal protein L32

Chain O2: 53% 37% 7% ..



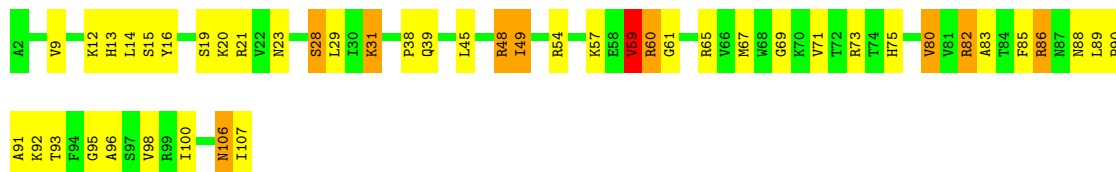
- Molecule 68: 60S ribosomal protein L32

Chain o2: 78% 19% ..



- Molecule 69: 60S ribosomal protein L33-A

Chain O3: 57% 34% 8% .



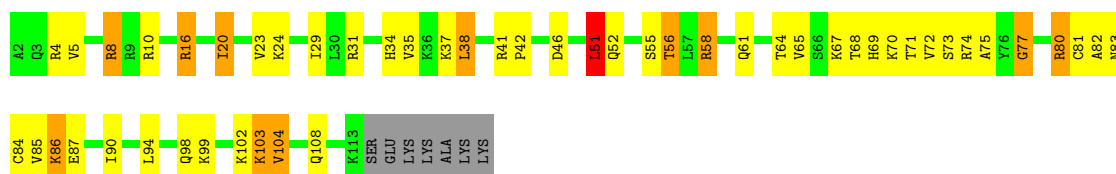
- Molecule 69: 60S ribosomal protein L33-A

Chain o3: 85% 14% .



- Molecule 70: 60S ribosomal protein L34-A

Chain O4: 51% 33% 9% 6%



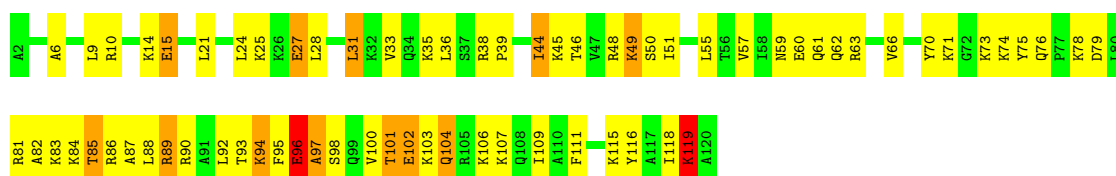
- Molecule 70: 60S ribosomal protein L34-A

Chain o4:    81% 13% 6%



- Molecule 71: 60S ribosomal protein L35-A

Chain O5:    42% 46% 10%



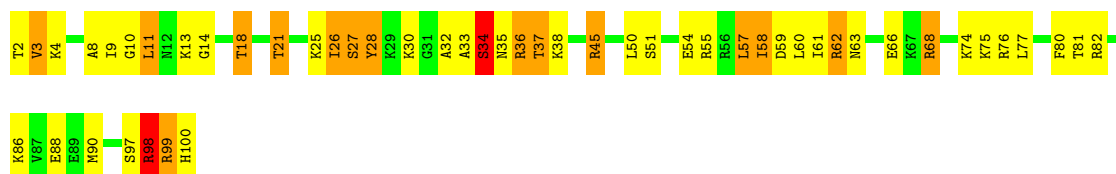
- Molecule 71: 60S ribosomal protein L35-A

Chain o5:   82% 18%



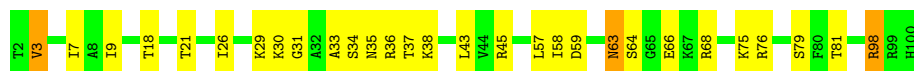
- Molecule 72: 60S ribosomal protein L36-A

Chain O6:    48% 34% 15%



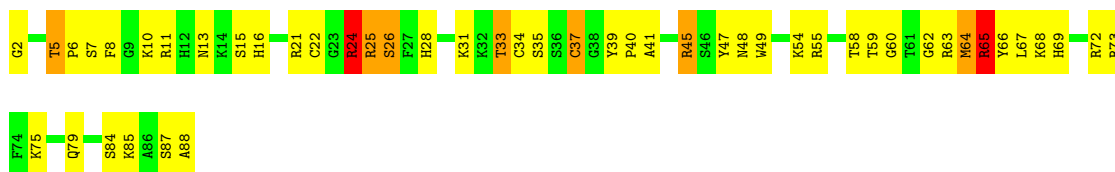
- Molecule 72: 60S ribosomal protein L36-A

Chain o6:   71% 26%



- Molecule 73: 60S ribosomal protein L37-A

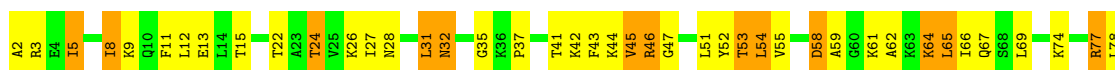
Chain O7:    44% 46% 8%



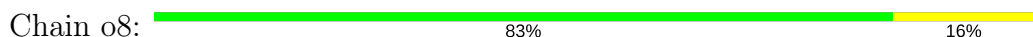
- Molecule 73: 60S ribosomal protein L37-A



- Molecule 74: 60S ribosomal protein L38



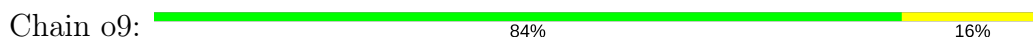
- Molecule 74: 60S ribosomal protein L38



- Molecule 75: 60S ribosomal protein L39



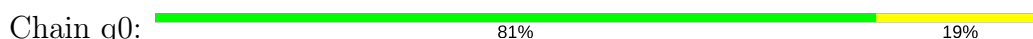
- Molecule 75: 60S ribosomal protein L39



- Molecule 76: Ubiquitin-60S ribosomal protein L40



- Molecule 76: Ubiquitin-60S ribosomal protein L40





- Molecule 77: 60S ribosomal protein L41-A

Chain Q1: 24% 56% 20%



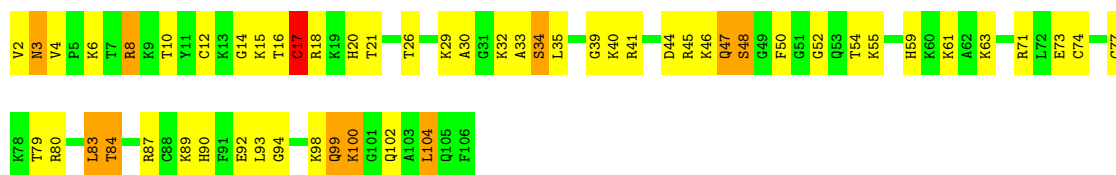
- Molecule 77: 60S ribosomal protein L41-A

Chain q1: 76% 20%



- Molecule 78: 60S ribosomal protein L42-A

Chain Q2: 48% 42% 10%



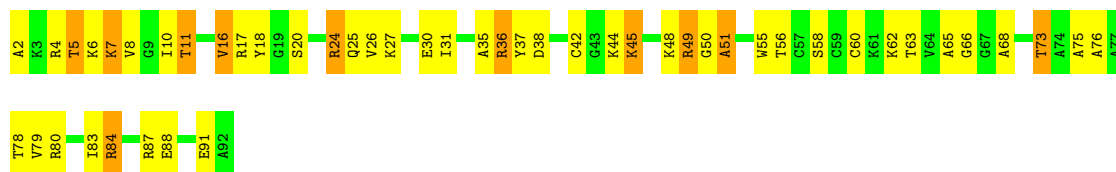
- Molecule 78: 60S ribosomal protein L42-A

Chain q2: 81% 18%



- Molecule 79: 60S ribosomal protein L43-A

Chain Q3: 46% 42% 12%

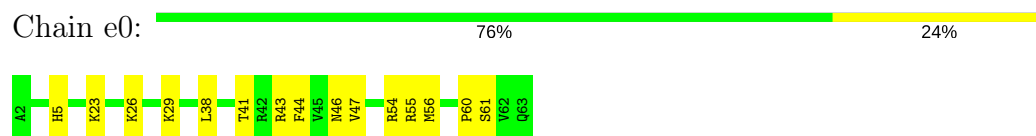


- Molecule 79: 60S ribosomal protein L43-A

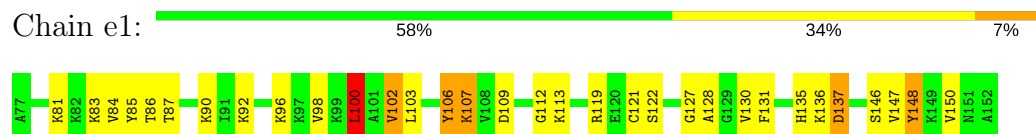
Chain q3: 81% 18%



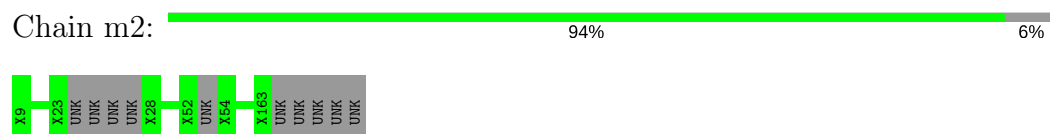
- Molecule 80: 40S ribosomal protein S30-A



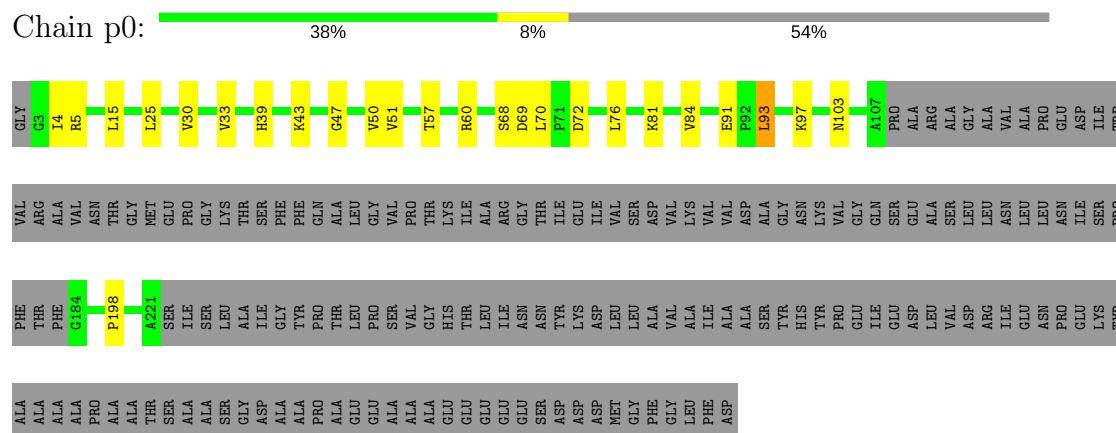
- Molecule 81: Ubiquitin-40S ribosomal protein S31



- Molecule 82: UNKNOWN PROTEIN m2



- Molecule 83: 60S acidic ribosomal protein P0



- Molecule 84: UNKNOWN PROTEIN p1



There are no outlier residues recorded for this chain.

- Molecule 85: UNKNOWN PROTEIN p2



There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	436.43Å 288.22Å 305.08Å 90.00° 98.99° 90.00°	Depositor
Resolution (Å)	267.37 – 2.90	Depositor
% Data completeness (in resolution range)	100.0 (267.37-2.90)	Depositor
$R_{merge}$	0.40	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, $R_{free}$	0.204 , 0.245	Depositor
Wilson B-factor (Å <sup>2</sup> )	66.3	Xtriage
Anisotropy	0.213	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	2	0.69	3/41698 (0.0%)	1.25	259/64972 (0.4%)
1	6	0.83	9/42765 (0.0%)	1.36	416/66634 (0.6%)
2	S0	0.45	0/1617	0.63	0/2215
2	s0	0.50	0/1623	0.70	0/2222
3	S1	0.35	0/1735	0.63	2/2335 (0.1%)
3	s1	0.49	0/1748	0.68	0/2352
4	S2	0.49	0/1665	0.66	1/2263 (0.0%)
4	s2	0.60	0/1665	0.76	2/2263 (0.1%)
5	S3	0.49	0/1759	0.62	0/2368
5	s3	0.47	0/1759	0.60	0/2368
6	S4	0.48	0/2109	0.71	1/2839 (0.0%)
6	s4	0.57	0/2109	0.77	1/2839 (0.0%)
7	S5	0.39	0/1629	0.58	0/2202
7	s5	0.45	0/1629	0.63	0/2202
8	S6	0.45	0/1823	0.64	0/2439
8	s6	0.55	0/1779	0.69	0/2379
9	S7	0.43	0/1506	0.63	0/2028
9	s7	0.49	0/1516	0.68	0/2043
10	S8	0.53	0/1514	0.74	1/2021 (0.0%)
10	s8	0.62	0/1514	0.76	1/2021 (0.0%)
11	S9	0.46	0/1519	0.64	0/2035
11	s9	0.56	0/1519	0.72	1/2035 (0.0%)
12	C0	0.42	0/790	0.67	1/1069 (0.1%)
12	c0	0.39	0/777	0.63	3/1049 (0.3%)
13	C1	0.61	0/1240	0.80	1/1675 (0.1%)
13	c1	0.63	0/1194	0.78	0/1610
14	C2	0.36	0/900	0.63	0/1224
14	c2	0.30	0/900	0.56	0/1224
15	C3	0.46	0/1215	0.66	3/1638 (0.2%)
15	c3	0.56	0/1215	0.73	1/1638 (0.1%)
16	C4	0.36	0/901	0.63	0/1217
16	c4	0.51	0/960	0.72	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	C5	0.46	0/998	0.65	0/1341
17	c5	0.51	0/1060	0.66	1/1426 (0.1%)
18	C6	0.45	0/1125	0.66	2/1510 (0.1%)
18	c6	0.49	0/1131	0.71	0/1518
19	C7	0.43	0/935	0.63	0/1254
19	c7	0.51	0/914	0.73	0/1224
20	C8	0.46	0/1211	0.64	0/1628
20	c8	0.49	0/1211	0.71	2/1628 (0.1%)
21	C9	0.46	0/1130	0.67	1/1517 (0.1%)
21	c9	0.51	0/1130	0.74	2/1517 (0.1%)
22	D0	0.46	0/865	0.65	0/1169
22	d0	0.51	0/892	0.68	0/1205
23	D1	0.43	0/693	0.60	0/935
23	d1	0.54	0/693	0.71	0/935
24	D2	0.53	0/1038	0.73	3/1395 (0.2%)
24	d2	0.62	0/1038	0.74	0/1395
25	D3	0.60	0/1139	0.81	3/1518 (0.2%)
25	d3	0.70	0/1139	0.79	1/1518 (0.1%)
26	D4	0.45	0/1087	0.59	0/1449
26	d4	0.51	0/1087	0.68	0/1449
27	D5	0.40	0/571	0.71	1/768 (0.1%)
27	d5	0.44	0/566	0.63	0/761
28	D6	0.44	0/782	0.67	0/1047
28	d6	0.54	0/782	0.72	0/1047
29	D7	0.43	0/620	0.67	1/838 (0.1%)
29	d7	0.49	0/620	0.68	0/838
30	D8	0.34	0/499	0.55	0/670
30	d8	0.42	0/499	0.66	0/670
31	D9	0.52	0/452	0.73	1/600 (0.2%)
31	d9	0.54	0/452	0.67	0/600
32	E0	0.46	0/483	0.61	0/643
33	E1	0.45	0/577	0.73	0/770
34	SR	0.89	2/2494 (0.1%)	1.42	4/3393 (0.1%)
34	sR	0.41	0/2495	0.58	0/3395
35	SM	0.52	0/1113	0.68	2/1502 (0.1%)
35	sM	0.50	0/683	0.66	1/923 (0.1%)
36	1	1.08	69/75394 (0.1%)	1.60	1618/117545 (1.4%)
36	5	1.10	113/75414 (0.1%)	1.60	1498/117575 (1.3%)
37	3	0.87	1/2883 (0.0%)	1.39	30/4491 (0.7%)
37	7	1.10	5/2883 (0.2%)	1.61	64/4491 (1.4%)
38	4	1.01	0/3746	1.51	61/5832 (1.0%)
38	8	0.87	0/3746	1.37	23/5832 (0.4%)
39	L2	0.72	0/1948	0.87	4/2617 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	l2	0.72	1/1946 (0.1%)	0.86	2/2614 (0.1%)
40	L3	0.73	0/3146	0.83	3/4228 (0.1%)
40	l3	0.82	2/3146 (0.1%)	0.89	7/4228 (0.2%)
41	L4	0.79	0/2800	0.94	6/3790 (0.2%)
41	l4	0.73	0/2800	0.88	3/3790 (0.1%)
42	L5	0.58	0/2425	0.70	0/3271
42	l5	0.71	0/2408	0.76	0/3248
43	L6	0.77	0/1260	0.84	1/1694 (0.1%)
43	l6	0.72	0/1269	0.82	1/1705 (0.1%)
44	L7	0.79	0/1821	0.85	1/2451 (0.0%)
44	l7	0.82	0/1828	0.86	3/2461 (0.1%)
45	L8	0.55	0/1836	0.67	1/2481 (0.0%)
45	l8	0.52	0/1796	0.69	1/2431 (0.0%)
46	L9	0.64	0/1539	0.76	1/2073 (0.0%)
46	l9	0.78	0/1539	0.82	0/2073
47	M0	0.72	0/1741	0.83	3/2335 (0.1%)
47	m0	0.77	1/1758 (0.1%)	0.85	3/2358 (0.1%)
48	M1	0.52	0/1374	0.71	1/1842 (0.1%)
48	m1	0.64	0/1374	0.79	1/1842 (0.1%)
49	M3	0.73	0/1568	0.84	3/2106 (0.1%)
49	m3	0.66	0/1573	0.82	3/2113 (0.1%)
50	M4	0.70	0/1068	0.80	1/1438 (0.1%)
50	m4	0.77	0/1074	0.81	1/1446 (0.1%)
51	M5	0.76	0/1757	0.82	0/2354
51	m5	0.65	0/1757	0.78	1/2354 (0.0%)
52	M6	0.83	1/1585 (0.1%)	0.92	3/2128 (0.1%)
52	m6	0.98	1/1585 (0.1%)	0.98	8/2128 (0.4%)
53	M7	0.78	1/1443 (0.1%)	0.83	0/1944
53	m7	0.84	0/1250	0.81	0/1683
54	M8	0.76	0/1465	0.91	4/1965 (0.2%)
54	m8	0.71	0/1465	0.87	1/1965 (0.1%)
55	M9	0.54	0/1538	0.66	0/2050
55	m9	0.59	0/1538	0.66	0/2050
56	N0	0.76	0/1481	0.83	1/1990 (0.1%)
56	n0	0.86	0/1481	0.83	0/1990
57	N1	0.78	1/1300 (0.1%)	0.81	0/1743
57	n1	0.82	1/1300 (0.1%)	0.81	0/1743
58	N2	0.44	0/812	0.61	0/1099
58	n2	0.51	0/794	0.67	0/1076
59	N3	0.72	0/1018	0.80	0/1369
59	n3	0.83	0/1018	0.94	3/1369 (0.2%)
60	N4	0.60	0/712	0.66	0/958
60	n4	0.66	0/1052	0.75	0/1398

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
61	N5	0.61	0/979	0.77	1/1321 (0.1%)
61	n5	0.62	0/974	0.75	1/1314 (0.1%)
62	N6	0.70	0/1004	0.88	3/1341 (0.2%)
62	n6	0.63	0/1004	0.80	1/1341 (0.1%)
63	N7	0.50	0/1118	0.65	0/1497
63	n7	0.45	0/1118	0.61	0/1497
64	N8	0.82	0/1204	0.92	2/1612 (0.1%)
64	n8	0.76	0/1204	0.95	3/1612 (0.2%)
65	N9	0.73	0/473	0.80	1/629 (0.2%)
65	n9	0.81	0/473	1.00	1/629 (0.2%)
66	O0	0.45	0/751	0.63	0/1008
66	o0	0.49	0/775	0.66	0/1040
67	O1	0.61	0/890	0.72	0/1196
67	o1	0.77	0/897	0.82	0/1205
68	O2	0.83	0/1041	0.92	2/1394 (0.1%)
68	o2	0.82	0/1041	0.92	3/1394 (0.2%)
69	O3	0.89	0/868	0.88	1/1168 (0.1%)
69	o3	0.89	0/868	0.84	0/1168
70	O4	0.59	0/890	0.75	1/1189 (0.1%)
70	o4	0.61	1/890 (0.1%)	0.73	0/1189
71	O5	0.67	0/978	0.78	0/1301
71	o5	0.58	0/974	0.66	0/1297
72	O6	0.63	0/778	0.82	1/1034 (0.1%)
72	o6	0.52	0/777	0.68	0/1033
73	O7	0.81	1/696 (0.1%)	0.95	2/923 (0.2%)
73	o7	0.70	0/696	0.79	0/923
74	O8	0.51	0/618	0.63	0/826
74	o8	0.44	0/614	0.61	0/822
75	O9	0.77	0/443	0.89	0/588
75	o9	0.69	0/443	0.76	1/588 (0.2%)
76	Q0	0.67	0/423	0.76	0/562
76	q0	0.81	0/423	0.90	0/562
77	Q1	0.68	0/234	1.04	0/300
77	q1	0.83	0/234	0.94	1/300 (0.3%)
78	Q2	0.93	1/860 (0.1%)	0.87	2/1136 (0.2%)
78	q2	0.86	1/860 (0.1%)	0.81	0/1136
79	Q3	0.77	0/701	0.82	0/934
79	q3	0.70	0/701	0.85	2/934 (0.2%)
80	e0	0.52	0/499	0.72	0/665
81	e1	0.39	0/619	0.73	1/822 (0.1%)
83	p0	0.43	0/1092	0.60	0/1474
All	All	0.85	215/430075 (0.0%)	1.27	4114/631366 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	s0	0	1
3	s1	0	1
6	s4	0	1
7	s5	0	1
9	S7	0	1
9	s7	0	1
10	S8	0	1
13	C1	0	1
16	C4	0	2
17	c5	0	1
19	C7	0	2
19	c7	0	1
20	c8	0	1
22	d0	0	1
25	d3	0	1
27	D5	0	3
28	D6	0	3
34	SR	0	2
39	L2	0	1
39	l2	0	2
42	l5	0	1
43	L6	0	1
44	L7	0	1
44	l7	0	2
52	M6	0	1
52	m6	0	1
53	M7	0	1
53	m7	0	1
56	n0	0	1
59	n3	0	1
62	n6	0	1
64	N8	0	2
64	n8	0	1
65	N9	0	1
65	n9	0	1
67	O1	0	1
67	o1	0	1
75	o9	0	1
78	Q2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
81	e1	0	1
All	All	0	50

The worst 5 of 215 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	SR	160	GLU	C-N	-30.25	0.64	1.34
34	SR	161	LYS	C-N	-24.97	0.76	1.34
78	Q2	17	CYS	CB-SG	16.00	2.09	1.82
36	5	1152	G	N9-C4	-13.57	1.27	1.38
78	q2	17	CYS	CB-SG	12.94	2.04	1.82

The worst 5 of 4114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	SR	161	LYS	O-C-N	-44.54	51.44	122.70
34	SR	160	GLU	C-N-CA	-39.83	22.12	121.70
34	SR	160	GLU	CA-C-N	-34.85	40.53	117.20
36	5	1152	G	N3-C4-C5	27.52	142.36	128.60
36	5	1152	G	N3-C4-N9	-27.23	109.66	126.00

There are no chirality outliers.

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	C1	88	ARG	Peptide
16	C4	123	SER	Peptide
16	C4	124	ASP	Peptide
9	S7	31	SER	Peptide
10	S8	79	ALA	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37283	0	18757	754	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6	38238	0	19241	711	0
2	S0	1577	0	1567	124	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	143	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	111	0
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	108	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	138	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	134	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	123	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	116	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	102	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	124	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	48	0
12	c0	762	0	699	0	0
13	C1	1214	0	1259	64	0
13	c1	1168	0	1231	0	0
14	C2	892	0	891	56	0
14	c2	892	0	891	0	0
15	C3	1192	0	1255	70	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	84	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	66	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	70	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	64	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	84	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	90	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	d0	882	0	939	0	0
23	D1	684	0	672	55	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	65	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	68	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	70	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	56	0
27	d5	558	0	598	0	0
28	D6	769	0	814	77	0
28	d6	769	0	814	0	0
29	D7	610	0	631	34	0
29	d7	610	0	631	0	0
30	D8	497	0	535	45	0
30	d8	497	0	535	0	0
31	D9	442	0	428	29	0
31	d9	442	0	428	0	0
32	E0	475	0	525	22	0
33	E1	566	0	602	64	0
34	SR	2441	0	2395	134	1
34	sR	2442	0	2392	0	0
35	SM	1104	0	996	58	0
35	sM	680	0	607	0	0
36	1	67355	0	33847	1105	0
36	5	67376	0	33858	1051	1
37	3	2579	0	1304	38	0
37	7	2579	0	1304	37	0
38	4	3353	0	1695	56	1
38	8	3353	0	1695	56	0
39	L2	1914	0	1981	124	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	239	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	170	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	153	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	61	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	l7	1791	0	1869	0	0
45	L8	1804	0	1875	126	0
45	l8	1764	0	1821	0	0
46	L9	1518	0	1587	107	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1736	112	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	87	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	111	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	58	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	104	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	97	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	87	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	88	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	73	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	82	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	68	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	35	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	58	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	20	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	48	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	59	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	79	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	103	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	n9	462	0	491	0	0
66	O0	743	0	797	48	0
66	o0	767	0	816	0	0
67	O1	876	0	912	47	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	51	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	41	0
69	o3	850	0	880	0	0
70	O4	880	0	945	45	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	64	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	50	0
72	o6	770	0	846	0	0
73	O7	681	0	683	50	0
73	o7	681	0	683	0	0
74	O8	612	0	682	32	0
74	o8	608	0	671	0	0
75	O9	436	0	475	36	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	20	0
76	q0	417	0	455	0	0
77	Q1	233	0	284	22	0
77	q1	233	0	284	0	0
78	Q2	847	0	916	45	0
78	q2	847	0	916	0	0
79	Q3	694	0	734	49	0
79	q3	694	0	734	0	0
80	e0	491	0	542	0	0
81	e1	608	0	654	0	0
82	m2	750	0	176	0	0
83	p0	1077	0	1041	0	0
84	p1	235	0	51	0	0
85	p2	230	0	52	0	0
86	1	471	0	0	0	0
86	2	122	0	0	0	0
86	3	14	0	0	0	0
86	4	22	0	0	0	0
86	5	505	0	0	0	0
86	6	147	0	0	0	0
86	7	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	8	13	0	0	0	0
86	C3	1	0	0	0	0
86	D0	1	0	0	0	0
86	D3	1	0	0	0	0
86	L2	1	0	0	0	0
86	L3	3	0	0	0	0
86	L4	1	0	0	0	0
86	L5	1	0	0	0	0
86	L7	3	0	0	0	0
86	L8	1	0	0	0	0
86	M0	2	0	0	0	0
86	M1	1	0	0	0	0
86	M3	4	0	0	0	0
86	M5	2	0	0	0	0
86	M6	1	0	0	0	0
86	M7	6	0	0	0	0
86	M9	1	0	0	0	0
86	N0	1	0	0	0	0
86	N3	3	0	0	0	0
86	N5	1	0	0	0	0
86	N8	4	0	0	0	0
86	O1	1	0	0	0	0
86	O3	1	0	0	0	0
86	O4	2	0	0	0	0
86	O7	1	0	0	0	0
86	Q2	1	0	0	0	0
86	S2	1	0	0	0	0
86	S4	1	0	0	0	0
86	S8	1	0	0	0	0
86	SM	1	0	0	0	0
86	c1	1	0	0	0	0
86	c4	1	0	0	0	0
86	c7	2	0	0	0	0
86	c8	2	0	0	0	0
86	d3	1	0	0	0	0
86	d4	1	0	0	0	0
86	d6	1	0	0	0	0
86	l2	2	0	0	0	0
86	l3	1	0	0	0	0
86	l4	2	0	0	0	0
86	l5	2	0	0	0	0
86	l7	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	l8	1	0	0	0	0
86	m1	2	0	0	0	0
86	m5	2	0	0	0	0
86	m6	1	0	0	0	0
86	m7	4	0	0	0	0
86	n0	2	0	0	0	0
86	n3	2	0	0	0	0
86	n6	2	0	0	0	0
86	n8	3	0	0	0	0
86	o1	2	0	0	0	0
86	o3	1	0	0	0	0
86	o4	2	0	0	0	0
86	o7	1	0	0	0	0
86	q0	1	0	0	0	0
86	q3	2	0	0	0	0
86	s1	1	0	0	0	0
86	s6	1	0	0	0	0
86	s8	1	0	0	0	0
86	sM	2	0	0	0	0
87	1	2457	0	0	251	0
87	2	1106	0	0	121	0
87	3	77	0	0	6	0
87	4	98	0	0	8	0
87	5	2464	0	0	245	0
87	6	1113	0	0	103	0
87	7	91	0	0	11	0
87	8	112	0	0	19	0
87	C3	7	0	0	0	0
87	C5	7	0	0	6	0
87	C8	7	0	0	1	0
87	D3	7	0	0	0	0
87	D9	7	0	0	4	0
87	L3	21	0	0	1	0
87	L4	7	0	0	2	0
87	M0	7	0	0	0	0
87	M5	7	0	0	0	0
87	M7	14	0	0	2	0
87	M9	7	0	0	1	0
87	N1	7	0	0	0	0
87	N9	7	0	0	0	0
87	O2	7	0	0	0	0
87	O3	7	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	O7	14	0	0	6	0
87	O9	7	0	0	4	0
87	Q2	7	0	0	2	0
87	S8	7	0	0	1	0
87	SR	7	0	0	0	0
87	c1	7	0	0	0	0
87	c3	7	0	0	0	0
87	c5	7	0	0	0	0
87	c8	7	0	0	0	0
87	d4	7	0	0	0	0
87	d9	7	0	0	0	0
87	l3	21	0	0	0	0
87	l4	14	0	0	0	0
87	l5	21	0	0	0	0
87	l9	7	0	0	0	0
87	m0	14	0	0	0	0
87	m1	7	0	0	0	0
87	m4	7	0	0	0	0
87	m5	7	0	0	0	0
87	m6	7	0	0	0	0
87	m7	7	0	0	0	0
87	m8	7	0	0	0	0
87	n3	7	0	0	0	0
87	n9	7	0	0	0	0
87	o2	7	0	0	0	0
87	o3	7	0	0	0	0
87	o7	7	0	0	0	0
87	o9	7	0	0	0	0
87	q2	7	0	0	0	0
87	s1	7	0	0	0	0
87	s4	7	0	0	0	0
87	s8	7	0	0	0	0
87	s9	7	0	0	0	0
87	sR	7	0	0	0	0
88	D6	1	0	0	0	0
88	D7	1	0	0	0	0
88	D9	1	0	0	0	0
88	E1	1	0	0	0	0
88	O7	1	0	0	0	0
88	Q0	1	0	0	0	0
88	Q2	1	0	0	0	0
88	Q3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	d6	1	0	0	0	0
88	d7	1	0	0	0	0
88	d9	1	0	0	0	0
88	e1	1	0	0	0	0
88	o7	1	0	0	0	0
88	q0	1	0	0	0	0
88	q2	1	0	0	0	0
88	q3	1	0	0	0	0
89	1	20	0	23	0	0
89	5	20	0	23	2	0
All	All	411205	0	297335	8431	2

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

The worst 5 of 8431 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:M6:66:LYS:NZ	52:M6:66:LYS:CE	1.49	1.52
78:Q2:17:CYS:CB	78:Q2:17:CYS:SG	2.09	1.45
36:1:1481:A:O2'	36:1:1858:A:N3	1.85	1.07
40:L3:41:VAL:HA	40:L3:185:GLY:HA3	1.52	1.03
40:L3:296:THR:HG22	40:L3:298:PHE:H	1.44	0.99

All (2) 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)
1:2:236:A:O2'	38:4:158:U:O2'[2_556]	2.06	0.14
34:SR:137:LYS:NZ	36:5:3293:U:O4[2_546]	2.10	0.10

## 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%)	151 (74%)	36 (18%)	17 (8%)	1	2
2	s0	204/251 (81%)	157 (77%)	30 (15%)	17 (8%)	1	2
3	S1	212/254 (84%)	145 (68%)	35 (16%)	32 (15%)	0	0
3	s1	214/254 (84%)	179 (84%)	21 (10%)	14 (6%)	1	4
4	S2	215/253 (85%)	190 (88%)	17 (8%)	8 (4%)	4	16
4	s2	215/253 (85%)	184 (86%)	20 (9%)	11 (5%)	2	8
5	S3	221/239 (92%)	194 (88%)	19 (9%)	8 (4%)	4	17
5	s3	221/239 (92%)	182 (82%)	24 (11%)	15 (7%)	1	4
6	S4	258/260 (99%)	213 (83%)	34 (13%)	11 (4%)	3	12
6	s4	258/260 (99%)	224 (87%)	19 (7%)	15 (6%)	2	6
7	S5	204/224 (91%)	166 (81%)	20 (10%)	18 (9%)	1	2
7	s5	204/224 (91%)	167 (82%)	18 (9%)	19 (9%)	1	2
8	S6	224/236 (95%)	194 (87%)	19 (8%)	11 (5%)	2	9
8	s6	216/236 (92%)	189 (88%)	20 (9%)	7 (3%)	5	19
9	S7	182/189 (96%)	137 (75%)	26 (14%)	19 (10%)	0	1
9	s7	184/189 (97%)	154 (84%)	21 (11%)	9 (5%)	2	9
10	S8	184/200 (92%)	156 (85%)	13 (7%)	15 (8%)	1	2
10	s8	184/200 (92%)	163 (89%)	15 (8%)	6 (3%)	4	18
11	S9	183/196 (93%)	153 (84%)	21 (12%)	9 (5%)	2	9
11	s9	183/196 (93%)	154 (84%)	19 (10%)	10 (6%)	2	7
12	C0	94/105 (90%)	74 (79%)	13 (14%)	7 (7%)	1	3
12	c0	92/105 (88%)	65 (71%)	15 (16%)	12 (13%)	0	1
13	C1	153/155 (99%)	125 (82%)	14 (9%)	14 (9%)	1	2
13	c1	144/155 (93%)	123 (85%)	14 (10%)	7 (5%)	2	9
14	C2	122/142 (86%)	76 (62%)	24 (20%)	22 (18%)	0	0
14	c2	122/142 (86%)	74 (61%)	30 (25%)	18 (15%)	0	0
15	C3	148/150 (99%)	129 (87%)	13 (9%)	6 (4%)	3	13
15	c3	148/150 (99%)	124 (84%)	14 (10%)	10 (7%)	1	4
16	C4	125/136 (92%)	98 (78%)	16 (13%)	11 (9%)	1	2
16	c4	126/136 (93%)	102 (81%)	12 (10%)	12 (10%)	1	1
17	C5	122/141 (86%)	91 (75%)	21 (17%)	10 (8%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	c5	133/141 (94%)	97 (73%)	22 (16%)	14 (10%)	0	1
18	C6	139/142 (98%)	122 (88%)	11 (8%)	6 (4%)	3	12
18	c6	140/142 (99%)	124 (89%)	10 (7%)	6 (4%)	3	12
19	C7	116/136 (85%)	87 (75%)	20 (17%)	9 (8%)	1	3
19	c7	113/136 (83%)	92 (81%)	10 (9%)	11 (10%)	1	1
20	C8	143/145 (99%)	117 (82%)	14 (10%)	12 (8%)	1	2
20	c8	143/145 (99%)	120 (84%)	16 (11%)	7 (5%)	2	9
21	C9	141/143 (99%)	121 (86%)	14 (10%)	6 (4%)	3	12
21	c9	141/143 (99%)	117 (83%)	17 (12%)	7 (5%)	2	8
22	D0	105/120 (88%)	87 (83%)	14 (13%)	4 (4%)	4	15
22	d0	108/120 (90%)	86 (80%)	13 (12%)	9 (8%)	1	2
23	D1	85/87 (98%)	67 (79%)	11 (13%)	7 (8%)	1	2
23	d1	85/87 (98%)	76 (89%)	8 (9%)	1 (1%)	15	46
24	D2	127/129 (98%)	113 (89%)	11 (9%)	3 (2%)	7	27
24	d2	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	22	57
25	D3	142/144 (99%)	109 (77%)	17 (12%)	16 (11%)	0	1
25	d3	142/144 (99%)	124 (87%)	17 (12%)	1 (1%)	25	60
26	D4	132/134 (98%)	111 (84%)	14 (11%)	7 (5%)	2	7
26	d4	132/134 (98%)	109 (83%)	18 (14%)	5 (4%)	4	15
27	D5	68/107 (64%)	48 (71%)	10 (15%)	10 (15%)	0	0
27	d5	67/107 (63%)	52 (78%)	10 (15%)	5 (8%)	1	3
28	D6	95/97 (98%)	66 (70%)	10 (10%)	19 (20%)	0	0
28	d6	95/97 (98%)	74 (78%)	13 (14%)	8 (8%)	1	2
29	D7	79/81 (98%)	61 (77%)	15 (19%)	3 (4%)	4	15
29	d7	79/81 (98%)	62 (78%)	12 (15%)	5 (6%)	1	4
30	D8	61/66 (92%)	51 (84%)	6 (10%)	4 (7%)	1	4
30	d8	61/66 (92%)	46 (75%)	13 (21%)	2 (3%)	4	18
31	D9	51/55 (93%)	41 (80%)	8 (16%)	2 (4%)	3	14
31	d9	51/55 (93%)	43 (84%)	4 (8%)	4 (8%)	1	3
32	E0	58/60 (97%)	45 (78%)	10 (17%)	3 (5%)	2	8
33	E1	69/76 (91%)	35 (51%)	19 (28%)	15 (22%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	SR	316/318 (99%)	252 (80%)	36 (11%)	28 (9%)	1	2
34	sR	316/318 (99%)	274 (87%)	30 (10%)	12 (4%)	4	15
35	SM	155/273 (57%)	112 (72%)	22 (14%)	21 (14%)	0	0
35	sM	98/273 (36%)	65 (66%)	18 (18%)	15 (15%)	0	0
39	L2	250/253 (99%)	222 (89%)	25 (10%)	3 (1%)	15	46
39	l2	250/253 (99%)	219 (88%)	25 (10%)	6 (2%)	7	27
40	L3	384/386 (100%)	339 (88%)	31 (8%)	14 (4%)	4	17
40	l3	384/386 (100%)	343 (89%)	31 (8%)	10 (3%)	6	24
41	L4	359/361 (99%)	303 (84%)	37 (10%)	19 (5%)	2	7
41	l4	359/361 (99%)	309 (86%)	31 (9%)	19 (5%)	2	7
42	L5	294/296 (99%)	249 (85%)	27 (9%)	18 (6%)	2	5
42	l5	292/296 (99%)	256 (88%)	32 (11%)	4 (1%)	13	41
43	L6	152/175 (87%)	140 (92%)	10 (7%)	2 (1%)	14	43
43	l6	153/175 (87%)	130 (85%)	19 (12%)	4 (3%)	6	24
44	L7	220/243 (90%)	202 (92%)	11 (5%)	7 (3%)	5	19
44	l7	221/243 (91%)	204 (92%)	14 (6%)	3 (1%)	13	41
45	L8	231/255 (91%)	189 (82%)	30 (13%)	12 (5%)	2	8
45	l8	229/255 (90%)	185 (81%)	23 (10%)	21 (9%)	1	2
46	L9	189/191 (99%)	170 (90%)	15 (8%)	4 (2%)	8	30
46	l9	189/191 (99%)	173 (92%)	13 (7%)	3 (2%)	11	37
47	M0	207/220 (94%)	182 (88%)	18 (9%)	7 (3%)	4	18
47	m0	209/220 (95%)	175 (84%)	25 (12%)	9 (4%)	3	12
48	M1	167/173 (96%)	127 (76%)	26 (16%)	14 (8%)	1	2
48	m1	167/173 (96%)	143 (86%)	15 (9%)	9 (5%)	2	7
49	M3	191/198 (96%)	170 (89%)	17 (9%)	4 (2%)	8	30
49	m3	192/198 (97%)	162 (84%)	18 (9%)	12 (6%)	1	4
50	M4	134/137 (98%)	116 (87%)	11 (8%)	7 (5%)	2	8
50	m4	135/137 (98%)	126 (93%)	7 (5%)	2 (2%)	12	39
51	M5	201/203 (99%)	186 (92%)	8 (4%)	7 (4%)	4	17
51	m5	201/203 (99%)	179 (89%)	16 (8%)	6 (3%)	5	20
52	M6	195/198 (98%)	183 (94%)	7 (4%)	5 (3%)	6	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	m6	195/198 (98%)	184 (94%)	8 (4%)	3 (2%)	12	39
53	M7	181/183 (99%)	156 (86%)	17 (9%)	8 (4%)	3	11
53	m7	153/183 (84%)	136 (89%)	16 (10%)	1 (1%)	25	60
54	M8	183/185 (99%)	166 (91%)	12 (7%)	5 (3%)	6	23
54	m8	183/185 (99%)	161 (88%)	15 (8%)	7 (4%)	4	15
55	M9	186/188 (99%)	177 (95%)	7 (4%)	2 (1%)	17	48
55	m9	186/188 (99%)	169 (91%)	14 (8%)	3 (2%)	11	37
56	N0	170/172 (99%)	156 (92%)	10 (6%)	4 (2%)	7	27
56	n0	170/172 (99%)	158 (93%)	11 (6%)	1 (1%)	28	64
57	N1	157/159 (99%)	137 (87%)	14 (9%)	6 (4%)	4	15
57	n1	157/159 (99%)	142 (90%)	12 (8%)	3 (2%)	9	33
58	N2	98/120 (82%)	73 (74%)	19 (19%)	6 (6%)	2	5
58	n2	96/120 (80%)	79 (82%)	13 (14%)	4 (4%)	3	12
59	N3	134/136 (98%)	125 (93%)	8 (6%)	1 (1%)	25	60
59	n3	134/136 (98%)	125 (93%)	7 (5%)	2 (2%)	12	39
60	N4	96/155 (62%)	72 (75%)	15 (16%)	9 (9%)	1	1
60	n4	133/155 (86%)	113 (85%)	11 (8%)	9 (7%)	1	4
61	N5	119/141 (84%)	108 (91%)	9 (8%)	2 (2%)	11	36
61	n5	118/141 (84%)	97 (82%)	15 (13%)	6 (5%)	2	8
62	N6	124/126 (98%)	111 (90%)	7 (6%)	6 (5%)	2	10
62	n6	124/126 (98%)	109 (88%)	10 (8%)	5 (4%)	3	14
63	N7	133/135 (98%)	115 (86%)	11 (8%)	7 (5%)	2	7
63	n7	133/135 (98%)	109 (82%)	11 (8%)	13 (10%)	1	1
64	N8	146/148 (99%)	120 (82%)	18 (12%)	8 (6%)	2	7
64	n8	146/148 (99%)	129 (88%)	16 (11%)	1 (1%)	25	60
65	N9	56/58 (97%)	50 (89%)	4 (7%)	2 (4%)	4	17
65	n9	56/58 (97%)	44 (79%)	9 (16%)	3 (5%)	2	7
66	O0	95/104 (91%)	89 (94%)	4 (4%)	2 (2%)	8	30
66	o0	98/104 (94%)	88 (90%)	8 (8%)	2 (2%)	9	31
67	O1	107/112 (96%)	96 (90%)	7 (6%)	4 (4%)	4	16
67	o1	107/112 (96%)	89 (83%)	10 (9%)	8 (8%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	O2	125/129 (97%)	113 (90%)	11 (9%)	1 (1%)	22	57
68	o2	125/129 (97%)	108 (86%)	14 (11%)	3 (2%)	7	27
69	O3	104/106 (98%)	99 (95%)	4 (4%)	1 (1%)	18	51
69	o3	104/106 (98%)	95 (91%)	6 (6%)	3 (3%)	5	21
70	O4	110/119 (92%)	102 (93%)	7 (6%)	1 (1%)	20	54
70	o4	110/119 (92%)	102 (93%)	5 (4%)	3 (3%)	6	23
71	O5	117/119 (98%)	104 (89%)	9 (8%)	4 (3%)	4	18
71	o5	117/119 (98%)	105 (90%)	10 (8%)	2 (2%)	11	36
72	O6	97/99 (98%)	78 (80%)	13 (13%)	6 (6%)	2	5
72	o6	97/99 (98%)	84 (87%)	5 (5%)	8 (8%)	1	2
73	O7	85/87 (98%)	74 (87%)	11 (13%)	0	100	100
73	o7	85/87 (98%)	74 (87%)	9 (11%)	2 (2%)	7	27
74	O8	75/77 (97%)	65 (87%)	8 (11%)	2 (3%)	6	23
74	o8	75/77 (97%)	67 (89%)	5 (7%)	3 (4%)	3	14
75	O9	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
75	o9	48/50 (96%)	45 (94%)	2 (4%)	1 (2%)	8	30
76	Q0	50/52 (96%)	46 (92%)	2 (4%)	2 (4%)	3	14
76	q0	50/52 (96%)	49 (98%)	0	1 (2%)	9	31
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
78	Q2	103/105 (98%)	89 (86%)	9 (9%)	5 (5%)	2	9
78	q2	103/105 (98%)	94 (91%)	7 (7%)	2 (2%)	9	33
79	Q3	89/91 (98%)	81 (91%)	6 (7%)	2 (2%)	8	29
79	q3	89/91 (98%)	81 (91%)	6 (7%)	2 (2%)	8	29
80	e0	60/62 (97%)	51 (85%)	5 (8%)	4 (7%)	1	4
81	e1	74/76 (97%)	37 (50%)	18 (24%)	19 (26%)	0	0
83	p0	139/311 (45%)	114 (82%)	21 (15%)	4 (3%)	5	21
All	All	22333/24141 (92%)	18964 (85%)	2226 (10%)	1143 (5%)	2	8

5 of 1143 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO

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Mol	Chain	Res	Type
2	S0	30	GLN
2	S0	39	ASN
2	S0	95	ALA
2	S0	158	VAL

### 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%)	130 (79%)	34 (21%)	1	4
2	s0	165/209 (79%)	138 (84%)	27 (16%)	2	8
3	S1	191/223 (86%)	159 (83%)	32 (17%)	2	7
3	s1	192/223 (86%)	162 (84%)	30 (16%)	3	9
4	S2	176/204 (86%)	140 (80%)	36 (20%)	1	4
4	s2	176/204 (86%)	137 (78%)	39 (22%)	1	3
5	S3	182/194 (94%)	142 (78%)	40 (22%)	1	3
5	s3	182/194 (94%)	145 (80%)	37 (20%)	1	4
6	S4	221/221 (100%)	178 (80%)	43 (20%)	1	5
6	s4	221/221 (100%)	179 (81%)	42 (19%)	2	5
7	S5	173/190 (91%)	148 (86%)	25 (14%)	4	11
7	s5	173/190 (91%)	144 (83%)	29 (17%)	2	7
8	S6	188/201 (94%)	150 (80%)	38 (20%)	1	4
8	s6	187/201 (93%)	155 (83%)	32 (17%)	2	7
9	S7	165/169 (98%)	127 (77%)	38 (23%)	1	2
9	s7	165/169 (98%)	136 (82%)	29 (18%)	2	6
10	S8	150/161 (93%)	128 (85%)	22 (15%)	3	11
10	s8	150/161 (93%)	126 (84%)	24 (16%)	3	8
11	S9	158/165 (96%)	122 (77%)	36 (23%)	1	3
11	s9	158/165 (96%)	123 (78%)	35 (22%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	C0	77/98 (79%)	62 (80%)	15 (20%)	1	5
12	c0	73/98 (74%)	63 (86%)	10 (14%)	4	12
13	C1	129/136 (95%)	108 (84%)	21 (16%)	3	8
13	c1	129/136 (95%)	105 (81%)	24 (19%)	2	5
14	C2	88/118 (75%)	67 (76%)	21 (24%)	1	2
14	c2	88/118 (75%)	70 (80%)	18 (20%)	1	4
15	C3	127/127 (100%)	106 (84%)	21 (16%)	2	8
15	c3	127/127 (100%)	103 (81%)	24 (19%)	2	5
16	C4	81/104 (78%)	58 (72%)	23 (28%)	0	1
16	c4	97/104 (93%)	75 (77%)	22 (23%)	1	3
17	C5	101/117 (86%)	86 (85%)	15 (15%)	3	10
17	c5	103/117 (88%)	85 (82%)	18 (18%)	2	6
18	C6	117/118 (99%)	97 (83%)	20 (17%)	2	7
18	c6	118/118 (100%)	95 (80%)	23 (20%)	1	5
19	C7	94/124 (76%)	73 (78%)	21 (22%)	1	3
19	c7	92/124 (74%)	77 (84%)	15 (16%)	3	8
20	C8	128/128 (100%)	102 (80%)	26 (20%)	1	4
20	c8	128/128 (100%)	98 (77%)	30 (23%)	1	2
21	C9	115/115 (100%)	95 (83%)	20 (17%)	2	7
21	c9	115/115 (100%)	96 (84%)	19 (16%)	2	8
22	D0	100/113 (88%)	76 (76%)	24 (24%)	1	2
22	d0	103/113 (91%)	81 (79%)	22 (21%)	1	3
23	D1	74/74 (100%)	61 (82%)	13 (18%)	2	6
23	d1	74/74 (100%)	60 (81%)	14 (19%)	2	5
24	D2	110/110 (100%)	88 (80%)	22 (20%)	1	4
24	d2	110/110 (100%)	96 (87%)	14 (13%)	5	15
25	D3	119/119 (100%)	96 (81%)	23 (19%)	1	5
25	d3	119/119 (100%)	102 (86%)	17 (14%)	4	11
26	D4	112/112 (100%)	95 (85%)	17 (15%)	3	10
26	d4	112/112 (100%)	98 (88%)	14 (12%)	5	16
27	D5	61/88 (69%)	47 (77%)	14 (23%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	d5	61/88 (69%)	52 (85%)	9 (15%)	3	11
28	D6	83/83 (100%)	68 (82%)	15 (18%)	2	6
28	d6	83/83 (100%)	72 (87%)	11 (13%)	4	13
29	D7	70/70 (100%)	59 (84%)	11 (16%)	3	9
29	d7	70/70 (100%)	63 (90%)	7 (10%)	9	27
30	D8	56/59 (95%)	42 (75%)	14 (25%)	1	2
30	d8	56/59 (95%)	47 (84%)	9 (16%)	3	8
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2	7
31	d9	47/48 (98%)	41 (87%)	6 (13%)	5	15
32	E0	51/51 (100%)	44 (86%)	7 (14%)	4	12
33	E1	62/66 (94%)	51 (82%)	11 (18%)	2	6
34	SR	260/261 (100%)	223 (86%)	37 (14%)	4	11
34	sR	260/261 (100%)	230 (88%)	30 (12%)	6	20
35	SM	97/228 (42%)	79 (81%)	18 (19%)	2	5
35	sM	54/228 (24%)	39 (72%)	15 (28%)	0	1
39	L2	193/195 (99%)	156 (81%)	37 (19%)	1	5
39	l2	192/195 (98%)	160 (83%)	32 (17%)	2	7
40	L3	321/322 (100%)	250 (78%)	71 (22%)	1	3
40	l3	319/322 (99%)	250 (78%)	69 (22%)	1	3
41	L4	288/288 (100%)	241 (84%)	47 (16%)	3	8
41	l4	288/288 (100%)	239 (83%)	49 (17%)	2	7
42	L5	244/244 (100%)	206 (84%)	38 (16%)	3	9
42	l5	243/244 (100%)	198 (82%)	45 (18%)	2	5
43	L6	134/152 (88%)	115 (86%)	19 (14%)	4	11
43	l6	135/152 (89%)	111 (82%)	24 (18%)	2	6
44	L7	186/204 (91%)	169 (91%)	17 (9%)	11	32
44	l7	187/204 (92%)	160 (86%)	27 (14%)	4	11
45	L8	187/207 (90%)	152 (81%)	35 (19%)	2	5
45	l8	177/207 (86%)	146 (82%)	31 (18%)	2	6
46	L9	171/171 (100%)	140 (82%)	31 (18%)	2	6
46	l9	171/171 (100%)	141 (82%)	30 (18%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	M0	177/186 (95%)	139 (78%)	38 (22%)	1	3
47	m0	179/186 (96%)	140 (78%)	39 (22%)	1	3
48	M1	147/150 (98%)	117 (80%)	30 (20%)	1	4
48	m1	147/150 (98%)	123 (84%)	24 (16%)	3	8
49	M3	154/158 (98%)	124 (80%)	30 (20%)	1	5
49	m3	154/158 (98%)	132 (86%)	22 (14%)	4	11
50	M4	107/108 (99%)	89 (83%)	18 (17%)	2	7
50	m4	108/108 (100%)	88 (82%)	20 (18%)	2	5
51	M5	175/175 (100%)	145 (83%)	30 (17%)	2	7
51	m5	175/175 (100%)	146 (83%)	29 (17%)	2	8
52	M6	160/161 (99%)	138 (86%)	22 (14%)	4	12
52	m6	160/161 (99%)	127 (79%)	33 (21%)	1	4
53	M7	140/145 (97%)	112 (80%)	28 (20%)	1	4
53	m7	125/145 (86%)	106 (85%)	19 (15%)	3	10
54	M8	150/150 (100%)	126 (84%)	24 (16%)	3	8
54	m8	150/150 (100%)	120 (80%)	30 (20%)	1	4
55	M9	153/153 (100%)	128 (84%)	25 (16%)	3	8
55	m9	153/153 (100%)	123 (80%)	30 (20%)	1	5
56	N0	156/156 (100%)	125 (80%)	31 (20%)	1	4
56	n0	156/156 (100%)	125 (80%)	31 (20%)	1	4
57	N1	136/136 (100%)	104 (76%)	32 (24%)	1	2
57	n1	136/136 (100%)	109 (80%)	27 (20%)	1	4
58	N2	87/106 (82%)	79 (91%)	8 (9%)	11	32
58	n2	85/106 (80%)	72 (85%)	13 (15%)	3	10
59	N3	104/104 (100%)	91 (88%)	13 (12%)	5	16
59	n3	104/104 (100%)	96 (92%)	8 (8%)	15	40
60	N4	57/129 (44%)	52 (91%)	5 (9%)	12	34
60	n4	100/129 (78%)	84 (84%)	16 (16%)	3	8
61	N5	104/117 (89%)	81 (78%)	23 (22%)	1	3
61	n5	104/117 (89%)	82 (79%)	22 (21%)	1	4
62	N6	109/109 (100%)	86 (79%)	23 (21%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	n6	109/109 (100%)	82 (75%)	27 (25%)	1	2
63	N7	115/115 (100%)	93 (81%)	22 (19%)	2	5
63	n7	115/115 (100%)	96 (84%)	19 (16%)	2	8
64	N8	118/118 (100%)	101 (86%)	17 (14%)	4	11
64	n8	118/118 (100%)	96 (81%)	22 (19%)	2	5
65	N9	46/46 (100%)	36 (78%)	10 (22%)	1	3
65	n9	46/46 (100%)	36 (78%)	10 (22%)	1	3
66	O0	81/87 (93%)	70 (86%)	11 (14%)	4	12
66	o0	84/87 (97%)	68 (81%)	16 (19%)	2	5
67	O1	92/96 (96%)	75 (82%)	17 (18%)	2	5
67	o1	94/96 (98%)	73 (78%)	21 (22%)	1	3
68	O2	109/110 (99%)	91 (84%)	18 (16%)	2	8
68	o2	109/110 (99%)	88 (81%)	21 (19%)	1	5
69	O3	90/90 (100%)	78 (87%)	12 (13%)	4	13
69	o3	90/90 (100%)	76 (84%)	14 (16%)	3	9
70	O4	95/101 (94%)	75 (79%)	20 (21%)	1	4
70	o4	95/101 (94%)	82 (86%)	13 (14%)	4	12
71	O5	104/104 (100%)	82 (79%)	22 (21%)	1	4
71	o5	103/104 (99%)	83 (81%)	20 (19%)	1	5
72	O6	81/81 (100%)	63 (78%)	18 (22%)	1	3
72	o6	80/81 (99%)	56 (70%)	24 (30%)	0	1
73	O7	70/70 (100%)	58 (83%)	12 (17%)	2	7
73	o7	70/70 (100%)	55 (79%)	15 (21%)	1	3
74	O8	68/68 (100%)	53 (78%)	15 (22%)	1	3
74	o8	67/68 (98%)	56 (84%)	11 (16%)	2	8
75	O9	45/45 (100%)	39 (87%)	6 (13%)	4	13
75	o9	45/45 (100%)	40 (89%)	5 (11%)	7	21
76	Q0	47/47 (100%)	42 (89%)	5 (11%)	8	24
76	q0	47/47 (100%)	38 (81%)	9 (19%)	2	5
77	Q1	23/23 (100%)	15 (65%)	8 (35%)	0	0
77	q1	23/23 (100%)	17 (74%)	6 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	Q2	90/90 (100%)	74 (82%)	16 (18%)	2	6
78	q2	90/90 (100%)	72 (80%)	18 (20%)	1	4
79	Q3	71/71 (100%)	57 (80%)	14 (20%)	1	5
79	q3	71/71 (100%)	56 (79%)	15 (21%)	1	4
80	e0	53/53 (100%)	42 (79%)	11 (21%)	1	4
81	e1	66/66 (100%)	48 (73%)	18 (27%)	0	1
83	p0	105/253 (42%)	83 (79%)	22 (21%)	1	4
All	All	18728/20239 (92%)	15327 (82%)	3401 (18%)	2	6

5 of 3401 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
68	O2	41	VAL
8	s6	22	HIS
64	n8	26	ARG
71	O5	15	GLU
3	s1	25	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
3	s1	209	ASN
8	s6	197	ASN
51	m5	194	GLN
3	s1	211	HIS
6	s4	231	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	451 (25%)	0
1	6	1792/1800 (99%)	435 (24%)	0
36	1	3145/3396 (92%)	619 (19%)	0
36	5	3145/3396 (92%)	623 (19%)	0
37	3	120/121 (99%)	10 (8%)	0
37	7	120/121 (99%)	17 (14%)	0
38	4	157/158 (99%)	33 (21%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
38	8	157/158 (99%)	38 (24%)	0
All	All	10383/10950 (94%)	2226 (21%)	0

5 of 2226 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	8	U
1	2	17	C
1	2	25	C

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2559 ligands modelled in this entry, 1424 are monoatomic - leaving 1135 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
87	OHX	1	3864	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3865	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3997	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
87	OHX	1	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
89	3HE	1	4215	-	21,21,21	0.51	0	18,30,30	0.52	0
87	OHX	2	2022	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2061	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-
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	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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	4	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	227	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	228	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	229	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	230	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	231	-	0,6,6	0.00	-	0,15,15	0.00	-
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	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	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
87	OHX	5	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	4230	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4231	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4232	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4233	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4234	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4235	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4236	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4237	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4238	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4239	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4240	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4241	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4242	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4243	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4244	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4245	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4246	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4247	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4248	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4249	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4250	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4251	-	0,6,6	0.00	-	0,15,15	0.00	-
89	3HE	5	4252	-	21,21,21	0.86	1 (4%)	18,30,30	0.77	0
87	OHX	6	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2049	-	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	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
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	-
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	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
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	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	7	215	-	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	7	227	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	214	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	227	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	228	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	229	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	C3	202	-	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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	D9	102	-	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	L3	406	-	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	M0	303	-	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	207	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M7	208	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	N1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	N9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O3	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	O9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Q2	503	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	S8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c1	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c8	203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	d4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	d9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l3	402	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l4	404	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	305	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l9	600	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m0	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m1	203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m5	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	-
87	OHX	m7	205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m8	201	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	n3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	n9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o3	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	o9	101	-	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	s4	301	-	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	s9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	sR	401	-	0,6,6	0.00	-	0,15,15	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	3864	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3865	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
87	OHX	1	3989	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3990	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3991	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3992	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3993	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3994	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3995	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3996	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3997	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3998	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3999	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4000	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4001	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4002	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4003	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4004	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4005	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4006	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4007	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4008	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4009	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4010	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4011	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4012	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4013	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
87	OHX	1	4199	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4200	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4201	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4202	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4203	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4204	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4205	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4206	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4207	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4208	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4209	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4210	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4211	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4212	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4213	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4214	-	-	0/0/0/0	0/0/0/0
89	3HE	1	4215	-	-	0/8/36/36	0/2/2/2
87	OHX	2	2022	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2023	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2024	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2025	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2029	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	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	223	-	-	0/0/0/0	0/0/0/0
87	OHX	4	224	-	-	0/0/0/0	0/0/0/0
87	OHX	4	225	-	-	0/0/0/0	0/0/0/0
87	OHX	4	226	-	-	0/0/0/0	0/0/0/0
87	OHX	4	227	-	-	0/0/0/0	0/0/0/0
87	OHX	4	228	-	-	0/0/0/0	0/0/0/0
87	OHX	4	229	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	5	3900	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3901	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3902	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3903	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3904	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	3935	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3936	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3937	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3938	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3939	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3940	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3941	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3942	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3943	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3944	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3945	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3946	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	3977	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3978	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3979	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3980	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3981	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3982	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3983	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3984	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3985	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3986	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3987	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3988	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4019	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4020	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4021	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4022	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4023	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4024	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4025	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4026	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4027	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4028	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4029	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4030	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4061	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4062	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4063	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4064	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4065	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4066	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4067	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4068	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4069	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4070	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4071	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4072	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4103	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4104	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4105	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4106	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4107	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4108	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4109	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4110	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4111	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4112	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4113	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4114	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4145	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4146	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4147	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4148	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4149	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4150	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4151	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4152	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4153	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4154	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4155	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4156	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4187	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4188	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4189	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4190	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4191	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4192	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4193	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4194	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4195	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4196	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4197	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4198	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4229	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4230	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4231	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4232	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4233	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4234	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4235	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4236	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4237	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4238	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4239	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4240	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4241	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4242	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4243	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4244	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4245	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4246	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4247	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4248	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4249	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4250	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4251	-	-	0/0/0/0	0/0/0/0
89	3HE	5	4252	-	-	0/8/36/36	0/2/2/2
87	OHX	6	2047	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2049	-	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	7	215	-	-	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	7	227	-	-	0/0/0/0	0/0/0/0
87	OHX	8	214	-	-	0/0/0/0	0/0/0/0
87	OHX	8	215	-	-	0/0/0/0	0/0/0/0
87	OHX	8	216	-	-	0/0/0/0	0/0/0/0
87	OHX	8	217	-	-	0/0/0/0	0/0/0/0
87	OHX	8	218	-	-	0/0/0/0	0/0/0/0
87	OHX	8	219	-	-	0/0/0/0	0/0/0/0
87	OHX	8	220	-	-	0/0/0/0	0/0/0/0
87	OHX	8	221	-	-	0/0/0/0	0/0/0/0
87	OHX	8	222	-	-	0/0/0/0	0/0/0/0
87	OHX	8	223	-	-	0/0/0/0	0/0/0/0
87	OHX	8	224	-	-	0/0/0/0	0/0/0/0
87	OHX	8	225	-	-	0/0/0/0	0/0/0/0
87	OHX	8	226	-	-	0/0/0/0	0/0/0/0
87	OHX	8	227	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	C3	202	-	-	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	404	-	-	0/0/0/0	0/0/0/0
87	OHX	L3	405	-	-	0/0/0/0	0/0/0/0
87	OHX	L3	406	-	-	0/0/0/0	0/0/0/0
87	OHX	L4	402	-	-	0/0/0/0	0/0/0/0
87	OHX	M0	303	-	-	0/0/0/0	0/0/0/0
87	OHX	M5	303	-	-	0/0/0/0	0/0/0/0
87	OHX	M7	207	-	-	0/0/0/0	0/0/0/0
87	OHX	M7	208	-	-	0/0/0/0	0/0/0/0
87	OHX	M9	202	-	-	0/0/0/0	0/0/0/0
87	OHX	N1	201	-	-	0/0/0/0	0/0/0/0
87	OHX	N9	101	-	-	0/0/0/0	0/0/0/0
87	OHX	O2	201	-	-	0/0/0/0	0/0/0/0
87	OHX	O3	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	O9	101	-	-	0/0/0/0	0/0/0/0
87	OHX	Q2	503	-	-	0/0/0/0	0/0/0/0
87	OHX	S8	302	-	-	0/0/0/0	0/0/0/0
87	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
87	OHX	c1	202	-	-	0/0/0/0	0/0/0/0
87	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
87	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
87	OHX	c8	203	-	-	0/0/0/0	0/0/0/0
87	OHX	d4	202	-	-	0/0/0/0	0/0/0/0
87	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
87	OHX	l3	402	-	-	0/0/0/0	0/0/0/0
87	OHX	l3	403	-	-	0/0/0/0	0/0/0/0
87	OHX	l3	404	-	-	0/0/0/0	0/0/0/0
87	OHX	l4	403	-	-	0/0/0/0	0/0/0/0
87	OHX	l4	404	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	303	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	304	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	305	-	-	0/0/0/0	0/0/0/0
87	OHX	l9	600	-	-	0/0/0/0	0/0/0/0
87	OHX	m0	301	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
87	OHX	m1	203	-	-	0/0/0/0	0/0/0/0
87	OHX	m4	201	-	-	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
87	OHX	m7	205	-	-	0/0/0/0	0/0/0/0
87	OHX	m8	201	-	-	0/0/0/0	0/0/0/0
87	OHX	n3	203	-	-	0/0/0/0	0/0/0/0
87	OHX	n9	101	-	-	0/0/0/0	0/0/0/0
87	OHX	o2	201	-	-	0/0/0/0	0/0/0/0
87	OHX	o3	202	-	-	0/0/0/0	0/0/0/0
87	OHX	o7	103	-	-	0/0/0/0	0/0/0/0
87	OHX	o9	101	-	-	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	s4	301	-	-	0/0/0/0	0/0/0/0
87	OHX	s8	302	-	-	0/0/0/0	0/0/0/0
87	OHX	s9	201	-	-	0/0/0/0	0/0/0/0
87	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	5	4252	3HE	C5-C7	3.22	1.58	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

477 monomers are involved in 786 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	3866	OHX	1	0
87	1	3871	OHX	1	0
87	1	3874	OHX	1	0
87	1	3875	OHX	1	0
87	1	3880	OHX	3	0
87	1	3882	OHX	1	0
87	1	3883	OHX	2	0
87	1	3885	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	3888	OHX	1	0
87	1	3890	OHX	1	0
87	1	3891	OHX	1	0
87	1	3897	OHX	2	0
87	1	3898	OHX	1	0
87	1	3899	OHX	1	0
87	1	3904	OHX	1	0
87	1	3905	OHX	1	0
87	1	3910	OHX	1	0
87	1	3912	OHX	1	0
87	1	3913	OHX	1	0
87	1	3918	OHX	1	0
87	1	3919	OHX	1	0
87	1	3921	OHX	1	0
87	1	3923	OHX	1	0
87	1	3925	OHX	1	0
87	1	3929	OHX	2	0
87	1	3931	OHX	1	0
87	1	3932	OHX	1	0
87	1	3937	OHX	6	0
87	1	3939	OHX	1	0
87	1	3942	OHX	1	0
87	1	3946	OHX	1	0
87	1	3947	OHX	1	0
87	1	3950	OHX	3	0
87	1	3953	OHX	1	0
87	1	3956	OHX	1	0
87	1	3957	OHX	5	0
87	1	3958	OHX	1	0
87	1	3959	OHX	6	0
87	1	3963	OHX	2	0
87	1	3968	OHX	1	0
87	1	3971	OHX	6	0
87	1	3972	OHX	1	0
87	1	3974	OHX	1	0
87	1	3975	OHX	8	0
87	1	3977	OHX	1	0
87	1	3980	OHX	1	0
87	1	3981	OHX	1	0
87	1	3982	OHX	2	0
87	1	3983	OHX	1	0
87	1	3985	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	3993	OHX	3	0
87	1	3997	OHX	1	0
87	1	4001	OHX	1	0
87	1	4002	OHX	2	0
87	1	4003	OHX	7	0
87	1	4006	OHX	2	0
87	1	4008	OHX	1	0
87	1	4010	OHX	1	0
87	1	4012	OHX	1	0
87	1	4013	OHX	2	0
87	1	4017	OHX	1	0
87	1	4019	OHX	7	0
87	1	4027	OHX	1	0
87	1	4028	OHX	6	0
87	1	4030	OHX	1	0
87	1	4032	OHX	6	0
87	1	4034	OHX	1	0
87	1	4037	OHX	4	0
87	1	4038	OHX	2	0
87	1	4039	OHX	1	0
87	1	4040	OHX	1	0
87	1	4042	OHX	1	0
87	1	4043	OHX	3	0
87	1	4044	OHX	6	0
87	1	4045	OHX	1	0
87	1	4047	OHX	2	0
87	1	4050	OHX	1	0
87	1	4052	OHX	6	0
87	1	4055	OHX	3	0
87	1	4056	OHX	5	0
87	1	4057	OHX	7	0
87	1	4060	OHX	1	0
87	1	4061	OHX	3	0
87	1	4066	OHX	1	0
87	1	4067	OHX	5	0
87	1	4070	OHX	1	0
87	1	4072	OHX	2	0
87	1	4073	OHX	1	0
87	1	4074	OHX	1	0
87	1	4078	OHX	1	0
87	1	4080	OHX	7	0
87	1	4082	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	4084	OHX	4	0
87	1	4085	OHX	1	0
87	1	4087	OHX	1	0
87	1	4088	OHX	1	0
87	1	4090	OHX	1	0
87	1	4095	OHX	1	0
87	1	4096	OHX	1	0
87	1	4098	OHX	1	0
87	1	4099	OHX	1	0
87	1	4107	OHX	1	0
87	1	4109	OHX	1	0
87	1	4114	OHX	5	0
87	1	4118	OHX	2	0
87	1	4120	OHX	1	0
87	1	4122	OHX	1	0
87	1	4125	OHX	1	0
87	1	4128	OHX	1	0
87	1	4131	OHX	1	0
87	1	4132	OHX	4	0
87	1	4133	OHX	4	0
87	1	4135	OHX	2	0
87	1	4138	OHX	1	0
87	1	4139	OHX	3	0
87	1	4140	OHX	6	0
87	1	4143	OHX	2	0
87	1	4144	OHX	1	0
87	1	4146	OHX	7	0
87	1	4148	OHX	1	0
87	1	4149	OHX	1	0
87	1	4150	OHX	6	0
87	1	4154	OHX	2	0
87	1	4155	OHX	7	0
87	1	4156	OHX	7	0
87	1	4159	OHX	1	0
87	1	4160	OHX	5	0
87	1	4163	OHX	3	0
87	1	4164	OHX	1	0
87	1	4165	OHX	1	0
87	1	4167	OHX	1	0
87	1	4168	OHX	4	0
87	1	4172	OHX	8	0
87	1	4174	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	4175	OHX	1	0
87	1	4179	OHX	1	0
87	1	4180	OHX	1	0
87	1	4181	OHX	3	0
87	1	4183	OHX	1	0
87	1	4189	OHX	1	0
87	1	4191	OHX	3	0
87	1	4193	OHX	1	0
87	1	4194	OHX	1	0
87	1	4196	OHX	1	0
87	1	4197	OHX	1	0
87	1	4198	OHX	7	0
87	1	4199	OHX	1	0
87	1	4201	OHX	1	0
87	1	4204	OHX	2	0
87	1	4207	OHX	1	0
87	1	4208	OHX	1	0
87	1	4209	OHX	1	0
87	2	2030	OHX	7	0
87	2	2033	OHX	1	0
87	2	2034	OHX	1	0
87	2	2035	OHX	2	0
87	2	2037	OHX	1	0
87	2	2038	OHX	2	0
87	2	2041	OHX	1	0
87	2	2043	OHX	6	0
87	2	2044	OHX	1	0
87	2	2046	OHX	1	0
87	2	2047	OHX	1	0
87	2	2050	OHX	1	0
87	2	2052	OHX	1	0
87	2	2057	OHX	1	0
87	2	2061	OHX	2	0
87	2	2063	OHX	1	0
87	2	2069	OHX	2	0
87	2	2070	OHX	1	0
87	2	2072	OHX	1	0
87	2	2073	OHX	1	0
87	2	2074	OHX	6	0
87	2	2075	OHX	1	0
87	2	2077	OHX	1	0
87	2	2081	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	2	2083	OHX	1	0
87	2	2085	OHX	1	0
87	2	2088	OHX	1	0
87	2	2089	OHX	6	0
87	2	2091	OHX	1	0
87	2	2093	OHX	1	0
87	2	2094	OHX	3	0
87	2	2095	OHX	7	0
87	2	2098	OHX	7	0
87	2	2104	OHX	1	0
87	2	2107	OHX	1	0
87	2	2108	OHX	5	0
87	2	2109	OHX	1	0
87	2	2110	OHX	2	0
87	2	2114	OHX	2	0
87	2	2115	OHX	8	0
87	2	2116	OHX	1	0
87	2	2118	OHX	1	0
87	2	2120	OHX	3	0
87	2	2124	OHX	1	0
87	2	2125	OHX	1	0
87	2	2126	OHX	1	0
87	2	2128	OHX	2	0
87	2	2130	OHX	9	0
87	2	2131	OHX	1	0
87	2	2133	OHX	1	0
87	2	2135	OHX	2	0
87	2	2137	OHX	1	0
87	2	2140	OHX	1	0
87	2	2143	OHX	1	0
87	2	2144	OHX	2	0
87	2	2145	OHX	6	0
87	2	2147	OHX	1	0
87	2	2148	OHX	1	0
87	2	2153	OHX	2	0
87	2	2154	OHX	1	0
87	2	2155	OHX	1	0
87	2	2156	OHX	4	0
87	2	2158	OHX	1	0
87	2	2159	OHX	1	0
87	2	2161	OHX	6	0
87	2	2164	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	2	2165	OHX	3	0
87	2	2166	OHX	1	0
87	2	2168	OHX	1	0
87	2	2170	OHX	2	0
87	2	2171	OHX	2	0
87	2	2172	OHX	1	0
87	2	2178	OHX	1	0
87	3	216	OHX	1	0
87	3	219	OHX	1	0
87	3	220	OHX	1	0
87	3	222	OHX	2	0
87	3	225	OHX	1	0
87	4	224	OHX	2	0
87	4	226	OHX	1	0
87	4	227	OHX	1	0
87	4	229	OHX	1	0
87	4	233	OHX	3	0
87	5	3900	OHX	1	0
87	5	3906	OHX	1	0
87	5	3907	OHX	2	0
87	5	3910	OHX	1	0
87	5	3916	OHX	1	0
87	5	3917	OHX	1	0
87	5	3918	OHX	1	0
87	5	3923	OHX	1	0
87	5	3925	OHX	2	0
87	5	3933	OHX	1	0
87	5	3940	OHX	1	0
87	5	3943	OHX	7	0
87	5	3946	OHX	1	0
87	5	3949	OHX	1	0
87	5	3951	OHX	1	0
87	5	3954	OHX	1	0
87	5	3955	OHX	1	0
87	5	3957	OHX	1	0
87	5	3958	OHX	2	0
87	5	3960	OHX	1	0
87	5	3961	OHX	1	0
87	5	3963	OHX	5	0
87	5	3967	OHX	1	0
87	5	3970	OHX	1	0
87	5	3973	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	3974	OHX	5	0
87	5	3979	OHX	8	0
87	5	3984	OHX	1	0
87	5	3985	OHX	1	0
87	5	3987	OHX	1	0
87	5	3992	OHX	2	0
87	5	3996	OHX	1	0
87	5	3997	OHX	1	0
87	5	4001	OHX	4	0
87	5	4002	OHX	7	0
87	5	4003	OHX	3	0
87	5	4004	OHX	1	0
87	5	4012	OHX	6	0
87	5	4015	OHX	1	0
87	5	4018	OHX	1	0
87	5	4021	OHX	6	0
87	5	4023	OHX	1	0
87	5	4024	OHX	3	0
87	5	4025	OHX	2	0
87	5	4027	OHX	1	0
87	5	4030	OHX	1	0
87	5	4031	OHX	1	0
87	5	4032	OHX	1	0
87	5	4034	OHX	6	0
87	5	4035	OHX	5	0
87	5	4036	OHX	1	0
87	5	4040	OHX	1	0
87	5	4047	OHX	1	0
87	5	4050	OHX	1	0
87	5	4052	OHX	1	0
87	5	4053	OHX	1	0
87	5	4055	OHX	2	0
87	5	4056	OHX	6	0
87	5	4060	OHX	1	0
87	5	4063	OHX	1	0
87	5	4066	OHX	1	0
87	5	4067	OHX	7	0
87	5	4068	OHX	1	0
87	5	4069	OHX	2	0
87	5	4073	OHX	1	0
87	5	4075	OHX	1	0
87	5	4077	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	4080	OHX	1	0
87	5	4081	OHX	1	0
87	5	4082	OHX	6	0
87	5	4089	OHX	1	0
87	5	4090	OHX	8	0
87	5	4091	OHX	3	0
87	5	4092	OHX	1	0
87	5	4093	OHX	4	0
87	5	4094	OHX	1	0
87	5	4096	OHX	1	0
87	5	4097	OHX	2	0
87	5	4099	OHX	1	0
87	5	4102	OHX	2	0
87	5	4105	OHX	2	0
87	5	4106	OHX	1	0
87	5	4109	OHX	2	0
87	5	4110	OHX	1	0
87	5	4111	OHX	1	0
87	5	4113	OHX	1	0
87	5	4117	OHX	1	0
87	5	4118	OHX	4	0
87	5	4119	OHX	1	0
87	5	4120	OHX	2	0
87	5	4129	OHX	1	0
87	5	4130	OHX	1	0
87	5	4131	OHX	1	0
87	5	4132	OHX	1	0
87	5	4133	OHX	1	0
87	5	4137	OHX	2	0
87	5	4138	OHX	2	0
87	5	4142	OHX	1	0
87	5	4143	OHX	6	0
87	5	4144	OHX	2	0
87	5	4147	OHX	1	0
87	5	4153	OHX	1	0
87	5	4154	OHX	1	0
87	5	4159	OHX	2	0
87	5	4160	OHX	1	0
87	5	4162	OHX	2	0
87	5	4163	OHX	1	0
87	5	4168	OHX	1	0
87	5	4172	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	4178	OHX	2	0
87	5	4179	OHX	1	0
87	5	4180	OHX	1	0
87	5	4181	OHX	1	0
87	5	4184	OHX	1	0
87	5	4185	OHX	1	0
87	5	4187	OHX	1	0
87	5	4188	OHX	1	0
87	5	4189	OHX	3	0
87	5	4191	OHX	3	0
87	5	4192	OHX	7	0
87	5	4193	OHX	1	0
87	5	4194	OHX	1	0
87	5	4195	OHX	1	0
87	5	4197	OHX	1	0
87	5	4198	OHX	9	0
87	5	4199	OHX	7	0
87	5	4200	OHX	7	0
87	5	4201	OHX	2	0
87	5	4203	OHX	5	0
87	5	4205	OHX	1	0
87	5	4208	OHX	1	0
87	5	4213	OHX	2	0
87	5	4216	OHX	8	0
87	5	4222	OHX	1	0
87	5	4223	OHX	2	0
87	5	4225	OHX	2	0
87	5	4226	OHX	1	0
87	5	4227	OHX	1	0
87	5	4228	OHX	1	0
87	5	4231	OHX	2	0
87	5	4233	OHX	6	0
87	5	4235	OHX	2	0
87	5	4236	OHX	1	0
87	5	4239	OHX	1	0
87	5	4242	OHX	6	0
87	5	4243	OHX	1	0
87	5	4247	OHX	1	0
87	5	4248	OHX	2	0
89	5	4252	3HE	2	0
87	6	2055	OHX	1	0
87	6	2061	OHX	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	6	2062	OHX	1	0
87	6	2063	OHX	1	0
87	6	2064	OHX	1	0
87	6	2067	OHX	1	0
87	6	2068	OHX	1	0
87	6	2072	OHX	1	0
87	6	2075	OHX	3	0
87	6	2076	OHX	1	0
87	6	2079	OHX	1	0
87	6	2084	OHX	1	0
87	6	2085	OHX	1	0
87	6	2088	OHX	1	0
87	6	2094	OHX	1	0
87	6	2095	OHX	1	0
87	6	2097	OHX	1	0
87	6	2098	OHX	2	0
87	6	2100	OHX	1	0
87	6	2102	OHX	2	0
87	6	2104	OHX	1	0
87	6	2107	OHX	1	0
87	6	2109	OHX	1	0
87	6	2110	OHX	1	0
87	6	2111	OHX	1	0
87	6	2113	OHX	2	0
87	6	2114	OHX	1	0
87	6	2116	OHX	2	0
87	6	2119	OHX	1	0
87	6	2121	OHX	2	0
87	6	2122	OHX	8	0
87	6	2123	OHX	1	0
87	6	2125	OHX	1	0
87	6	2126	OHX	1	0
87	6	2127	OHX	4	0
87	6	2129	OHX	4	0
87	6	2131	OHX	2	0
87	6	2137	OHX	2	0
87	6	2139	OHX	1	0
87	6	2143	OHX	1	0
87	6	2145	OHX	1	0
87	6	2147	OHX	1	0
87	6	2148	OHX	7	0
87	6	2150	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	6	2151	OHX	1	0
87	6	2152	OHX	1	0
87	6	2155	OHX	3	0
87	6	2157	OHX	1	0
87	6	2158	OHX	1	0
87	6	2160	OHX	4	0
87	6	2161	OHX	1	0
87	6	2163	OHX	1	0
87	6	2164	OHX	1	0
87	6	2171	OHX	1	0
87	6	2172	OHX	9	0
87	6	2176	OHX	1	0
87	6	2177	OHX	1	0
87	6	2179	OHX	1	0
87	6	2181	OHX	1	0
87	6	2183	OHX	2	0
87	6	2184	OHX	1	0
87	6	2189	OHX	2	0
87	6	2190	OHX	3	0
87	6	2191	OHX	1	0
87	6	2197	OHX	1	0
87	6	2205	OHX	1	0
87	7	217	OHX	6	0
87	7	218	OHX	3	0
87	7	220	OHX	1	0
87	7	224	OHX	2	0
87	7	226	OHX	7	0
87	8	214	OHX	1	0
87	8	215	OHX	1	0
87	8	216	OHX	6	0
87	8	217	OHX	1	0
87	8	222	OHX	1	0
87	8	223	OHX	8	0
87	8	224	OHX	6	0
87	8	228	OHX	1	0
87	C5	201	OHX	6	0
87	C8	201	OHX	1	0
87	D9	102	OHX	4	0
87	L3	405	OHX	1	0
87	L4	402	OHX	2	0
87	M7	207	OHX	1	0
87	M7	208	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	M9	202	OHX	1	0
87	O3	202	OHX	1	0
87	O7	103	OHX	5	0
87	O7	104	OHX	1	0
87	O9	101	OHX	4	0
87	Q2	503	OHX	2	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	SR	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SR	161:LYS	C	162:ALA	N	0.76
1	SR	160:GLU	C	161:LYS	N	0.64

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

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

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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