



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 16, 2017 – 10:08 am GMT

PDB ID : 4U6F
Title : Crystal structure of T-2 toxin bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-28
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (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

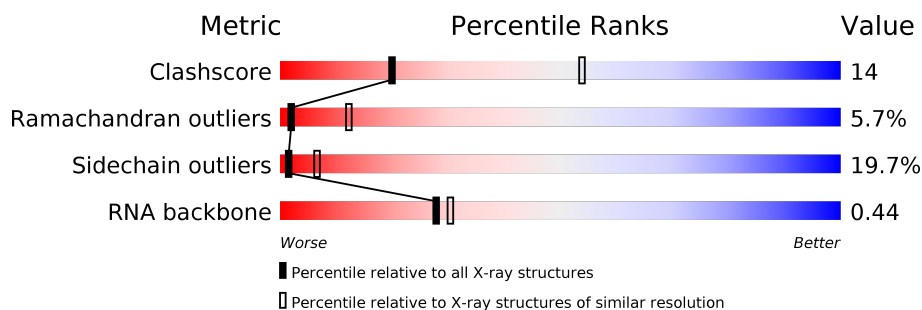
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RNA backbone	2435	1112 (3.50-2.70)

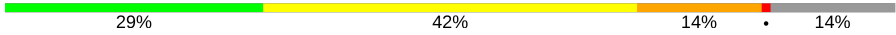

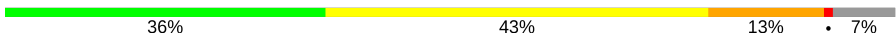



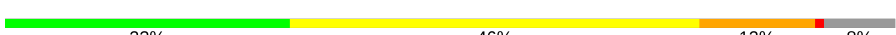




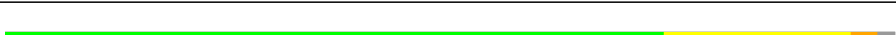


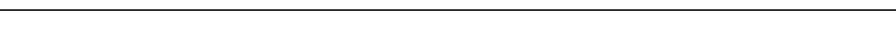
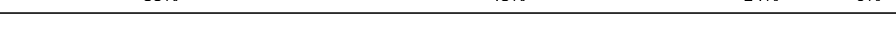

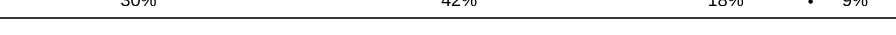



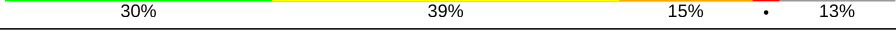



The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey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

Note EDS failed to run properly.

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


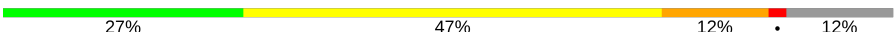



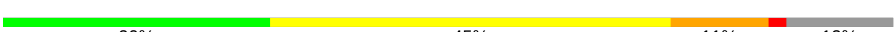








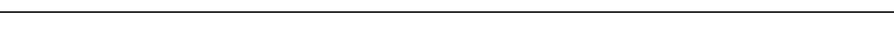

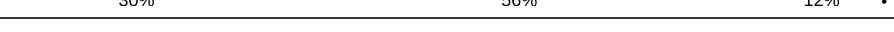

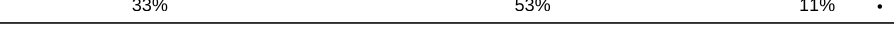





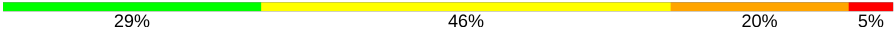
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Mol	Chain	Length	Quality of chain
4	S2	253	
4	s2	253	
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2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



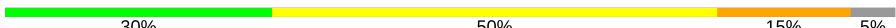

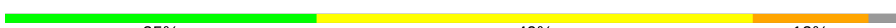




















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Mol	Chain	Length	Quality of chain
16	c4	136	
17	C5	141	
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134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



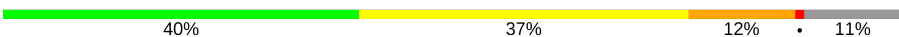



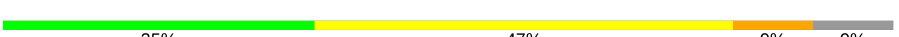

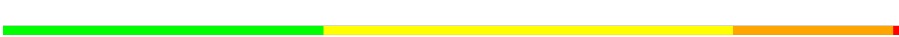

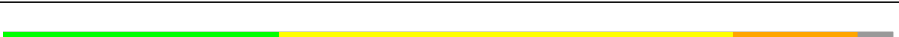


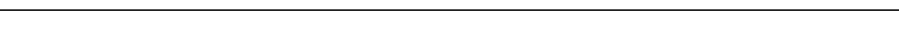











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Mol	Chain	Length	Quality of chain
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253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






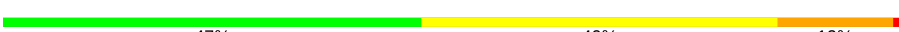








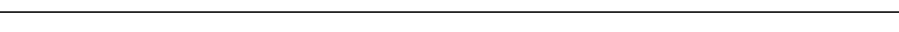

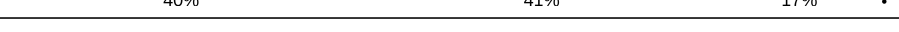

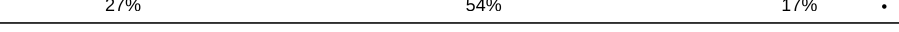





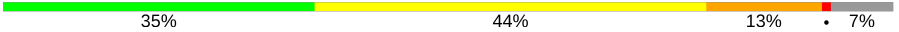
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Mol	Chain	Length	Quality of chain
42	L5	296	
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	
53	m7	183	
54	M8	185	



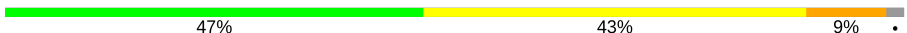



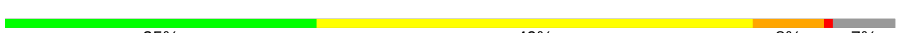







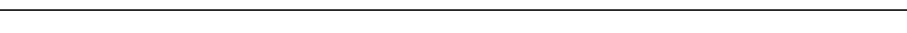




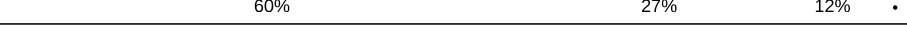

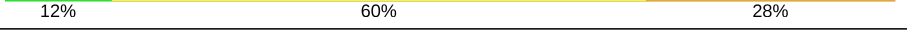



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Mol	Chain	Length	Quality of chain
54	m8	185	
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	104	
66	o0	104	






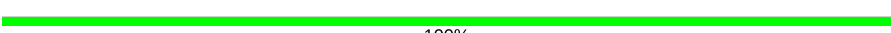
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Mol	Chain	Length	Quality of chain
67	O1	112	
67	o1	112	
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	120	
70	o4	120	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	

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Mol	Chain	Length	Quality of chain
79	q3	91	
80	e0	62	
81	p0	311	
82	m2	160	
83	p1	47	
84	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
86	OHX	1	3952	-	-	X	-
86	OHX	1	3966	-	-	X	-
86	OHX	1	3997	-	-	X	-
86	OHX	1	4026	-	-	X	-
86	OHX	1	4039	-	-	X	-
86	OHX	1	4050	-	-	X	-
86	OHX	1	4133	-	-	X	-
86	OHX	1	4151	-	-	X	-
86	OHX	1	4167	-	-	X	-
86	OHX	1	4176	-	-	X	-
86	OHX	1	4192	-	-	X	-
86	OHX	2	2034	-	-	X	-
86	OHX	2	2047	-	-	X	-
86	OHX	2	2093	-	-	X	-
86	OHX	2	2101	-	-	X	-
86	OHX	2	2134	-	-	X	-
86	OHX	2	2149	-	-	X	-
86	OHX	2	2160	-	-	X	-
86	OHX	5	3945	-	-	X	-
86	OHX	5	3964	-	-	X	-
86	OHX	5	3980	-	-	X	-
86	OHX	5	4004	-	-	X	-
86	OHX	5	4005	-	-	X	-
86	OHX	5	4014	-	-	X	-
86	OHX	5	4024	-	-	X	-
86	OHX	5	4059	-	-	X	-
86	OHX	5	4093	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	5	4201	-	-	X	-
86	OHX	5	4202	-	-	X	-
86	OHX	5	4203	-	-	X	-
86	OHX	5	4220	-	-	X	-
86	OHX	5	4237	-	-	X	-
86	OHX	5	4246	-	-	X	-
86	OHX	6	2060	-	-	X	-
86	OHX	6	2121	-	-	X	-
86	OHX	6	2149	-	-	X	-
86	OHX	6	2173	-	-	X	-
86	OHX	8	215	-	-	X	-
86	OHX	8	223	-	-	X	-
86	OHX	O1	201	-	-	X	-
86	OHX	O7	103	-	-	X	-
88	ZBA	1	4206	X	-	-	-

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411881 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	1781	Total	C	N	O	P	0	0	0
			37948	16965	6715	12487	1781			
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 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C0	89	ALA	GLY	conflict	UNP Q08745
C0	98	SER	THR	conflict	UNP Q08745
c0	89	ALA	GLY	conflict	UNP Q08745
c0	98	SER	THR	conflict	UNP Q08745

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O4	121	LYS	-	expression tag	UNP P87262
o4	121	LYS	-	expression tag	UNP P87262

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 81 is a protein called 60S acidic ribosomal protein P0.

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

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

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

- Molecule 83 is a protein called unknown protein chain p1.

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

- Molecule 84 is a protein called unknown protein chain p2.

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

- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L7	4	Total	Mg	0	0
			4	4		
85	n8	3	Total	Mg	0	0
			3	3		
85	o1	1	Total	Mg	0	0
			1	1		
85	N5	1	Total	Mg	0	0
			1	1		
85	6	147	Total	Mg	0	0
			147	147		
85	sM	2	Total	Mg	0	0
			2	2		
85	O4	1	Total	Mg	0	0
			1	1		
85	m5	5	Total	Mg	0	0
			5	5		
85	l3	3	Total	Mg	0	0
			3	3		
85	M1	1	Total	Mg	0	0
			1	1		
85	n0	1	Total	Mg	0	0
			1	1		
85	d6	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	2	126	Total 126	Mg 126	0	0
85	O3	1	Total 1	Mg 1	0	0
85	L4	2	Total 2	Mg 2	0	0
85	l7	1	Total 1	Mg 1	0	0
85	M5	2	Total 2	Mg 2	0	0
85	l4	1	Total 1	Mg 1	0	0
85	o0	1	Total 1	Mg 1	0	0
85	S2	1	Total 1	Mg 1	0	0
85	L8	1	Total 1	Mg 1	0	0
85	o4	1	Total 1	Mg 1	0	0
85	M9	1	Total 1	Mg 1	0	0
85	q0	1	Total 1	Mg 1	0	0
85	SM	1	Total 1	Mg 1	0	0
85	c8	2	Total 2	Mg 2	0	0
85	M0	2	Total 2	Mg 2	0	0
85	c1	2	Total 2	Mg 2	0	0
85	5	504	Total 504	Mg 504	0	0
85	L5	1	Total 1	Mg 1	0	0
85	O7	1	Total 1	Mg 1	0	0
85	Q2	1	Total 1	Mg 1	0	0
85	M4	1	Total 1	Mg 1	0	0

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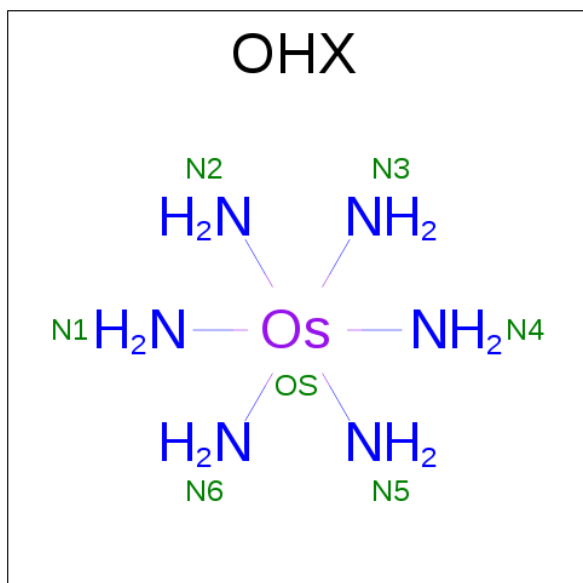
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	n9	1	Total 1	Mg 1	0	0
85	1	465	Total 465	Mg 465	0	0
85	n6	2	Total 2	Mg 2	0	0
85	S8	1	Total 1	Mg 1	0	0
85	l2	1	Total 1	Mg 1	0	0
85	d3	1	Total 1	Mg 1	0	0
85	q3	2	Total 2	Mg 2	0	0
85	o3	1	Total 1	Mg 1	0	0
85	M3	3	Total 3	Mg 3	0	0
85	N3	3	Total 3	Mg 3	0	0
85	N8	6	Total 6	Mg 6	0	0
85	4	22	Total 22	Mg 22	0	0
85	L2	2	Total 2	Mg 2	0	0
85	m1	2	Total 2	Mg 2	0	0
85	l5	2	Total 2	Mg 2	0	0
85	m7	4	Total 4	Mg 4	0	0
85	M7	5	Total 5	Mg 5	0	0
85	L6	2	Total 2	Mg 2	0	0
85	s1	1	Total 1	Mg 1	0	0
85	m6	2	Total 2	Mg 2	0	0
85	s8	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	c7	2	Total	Mg	0	0
			2	2		
85	7	17	Total	Mg	0	0
			17	17		
85	n3	2	Total	Mg	0	0
			2	2		
85	L3	3	Total	Mg	0	0
			3	3		
85	d4	1	Total	Mg	0	0
			1	1		
85	N6	1	Total	Mg	0	0
			1	1		
85	8	12	Total	Mg	0	0
			12	12		
85	M6	1	Total	Mg	0	0
			1	1		
85	N0	2	Total	Mg	0	0
			2	2		
85	3	14	Total	Mg	0	0
			14	14		

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	S8	1	Total 7	N 6	Os 1	0	0
86	S9	1	Total 7	N 6	Os 1	0	0
86	C1	1	Total 7	N 6	Os 1	0	0
86	C3	1	Total 7	N 6	Os 1	0	0
86	C5	1	Total 7	N 6	Os 1	0	0
86	C8	1	Total 7	N 6	Os 1	0	0
86	D9	1	Total 7	N 6	Os 1	0	0
86	SR	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
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86	1	1	Total	N	Os	0	0
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			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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			7	6	1		
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			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
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86	1	1	Total	N	Os	0	0
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			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	L3	1	Total 7	N 6	Os 1	0	0
86	L3	1	Total 7	N 6	Os 1	0	0
86	L3	1	Total 7	N 6	Os 1	0	0
86	L4	1	Total 7	N 6	Os 1	0	0
86	M0	1	Total 7	N 6	Os 1	0	0
86	M5	1	Total 7	N 6	Os 1	0	0
86	M6	1	Total 7	N 6	Os 1	0	0
86	M7	1	Total 7	N 6	Os 1	0	0
86	M7	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	M8	1	Total	N	Os	0	0
			7	6	1		
86	M9	1	Total	N	Os	0	0
			7	6	1		
86	N1	1	Total	N	Os	0	0
			7	6	1		
86	N9	1	Total	N	Os	0	0
			7	6	1		
86	O1	1	Total	N	Os	0	0
			7	6	1		
86	O2	1	Total	N	Os	0	0
			7	6	1		
86	O3	1	Total	N	Os	0	0
			7	6	1		
86	O7	1	Total	N	Os	0	0
			7	6	1		
86	O7	1	Total	N	Os	0	0
			7	6	1		
86	Q2	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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86	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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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	7	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	14	1	Total	N	Os	0	0
			7	6	1		
86	14	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l9	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m1	1	Total	N	Os	0	0
			7	6	1		
86	m4	1	Total	N	Os	0	0
			7	6	1		
86	m5	1	Total	N	Os	0	0
			7	6	1		
86	m7	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n5	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o2	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

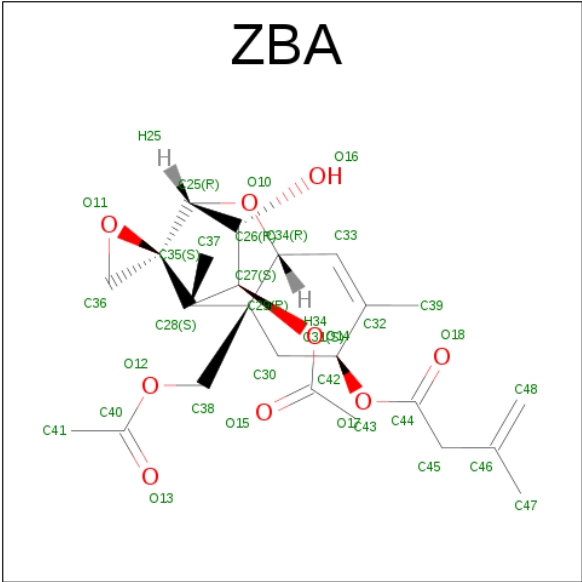
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	q0	1	Total	Zn	0	0
			1	1		
87	D6	1	Total	Zn	0	0
			1	1		

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

- Molecule 88 is 12,13-Epoxytrichothec-9-ene-3,4,8,15-tetrol-4,15-diacetate-8-isovalerate (three-letter code: ZBA) (formula: C₂₄H₃₂O₉).



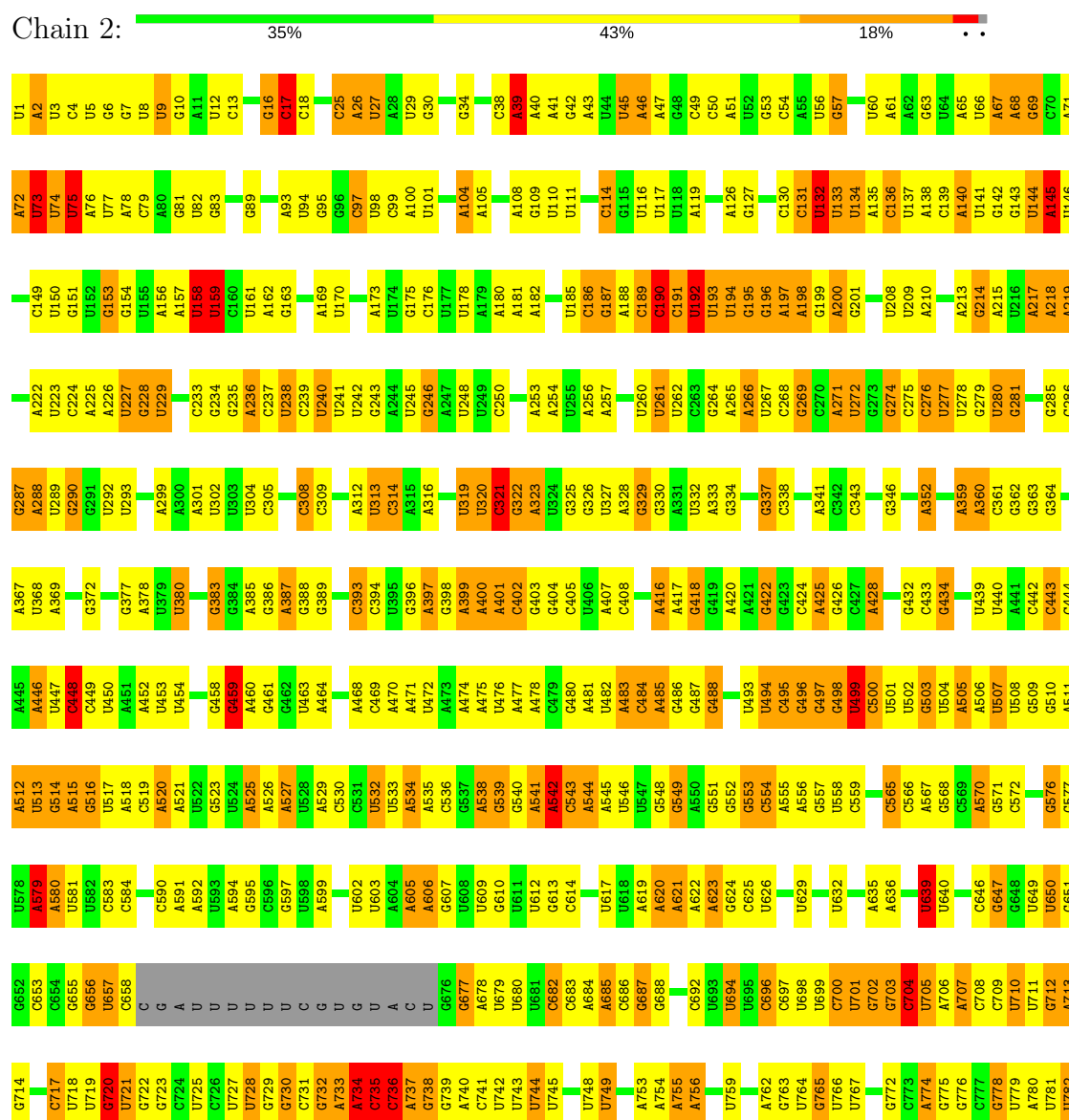
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	C	O	0	0
			33	24	9		
88	5	1	Total	C	O	0	0
			33	24	9		

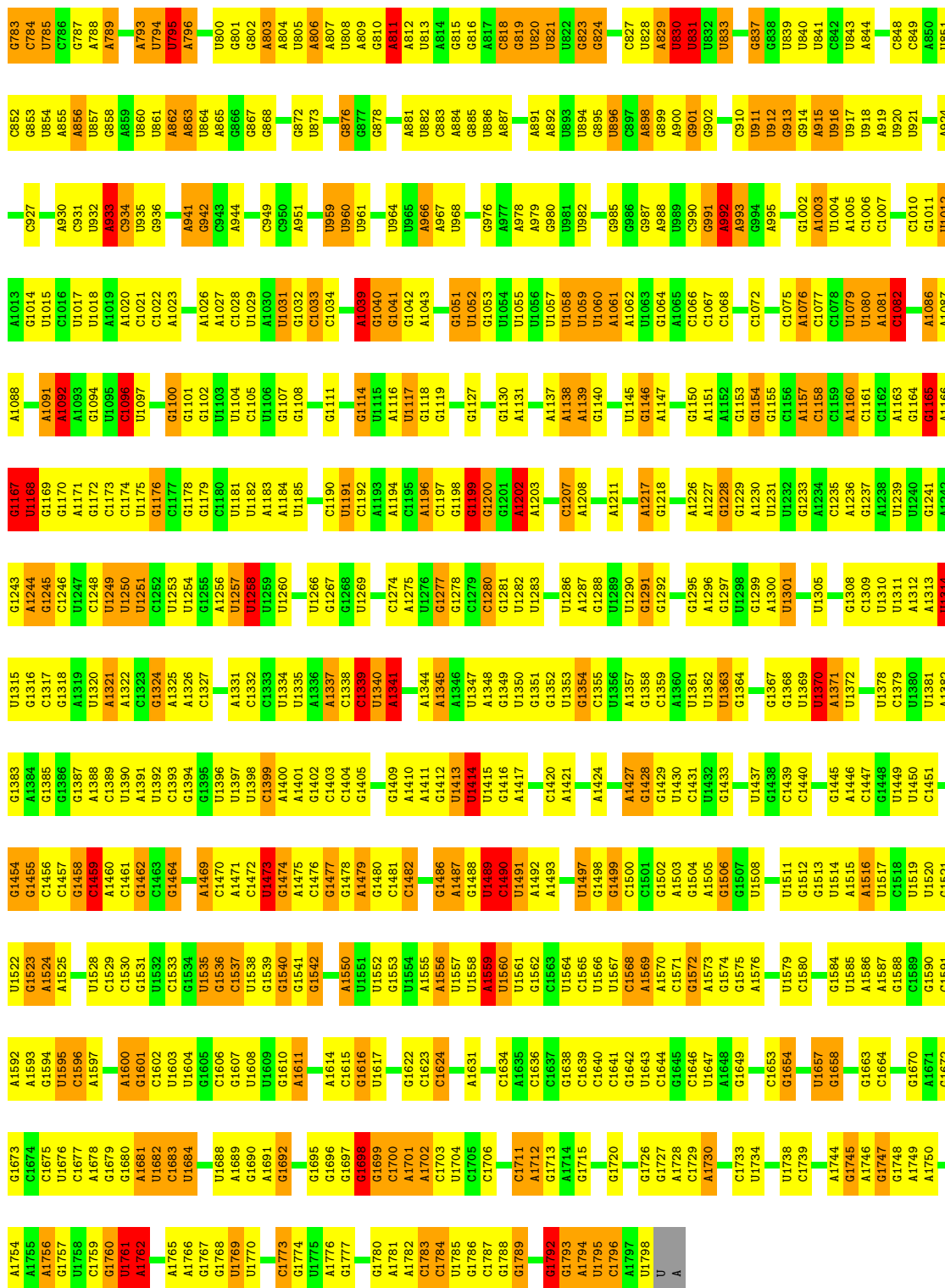
3 Residue-property plots

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.

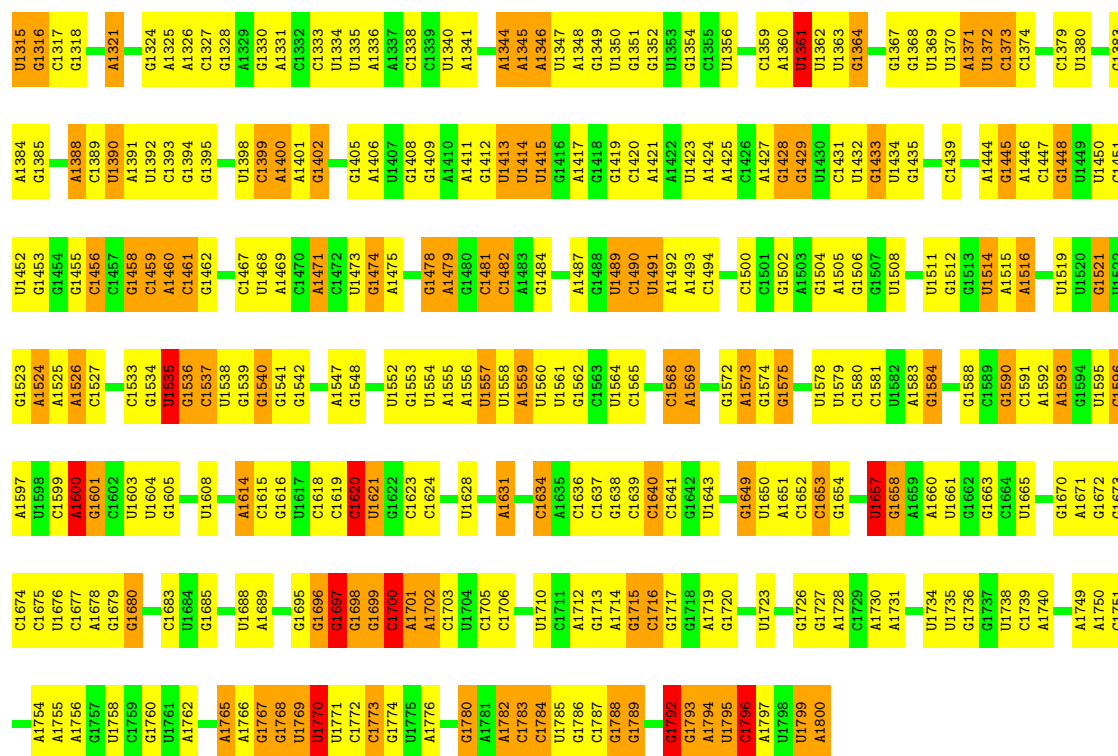
Note EDS failed to run properly.

• Molecule 1: 18S ribosomal RNA

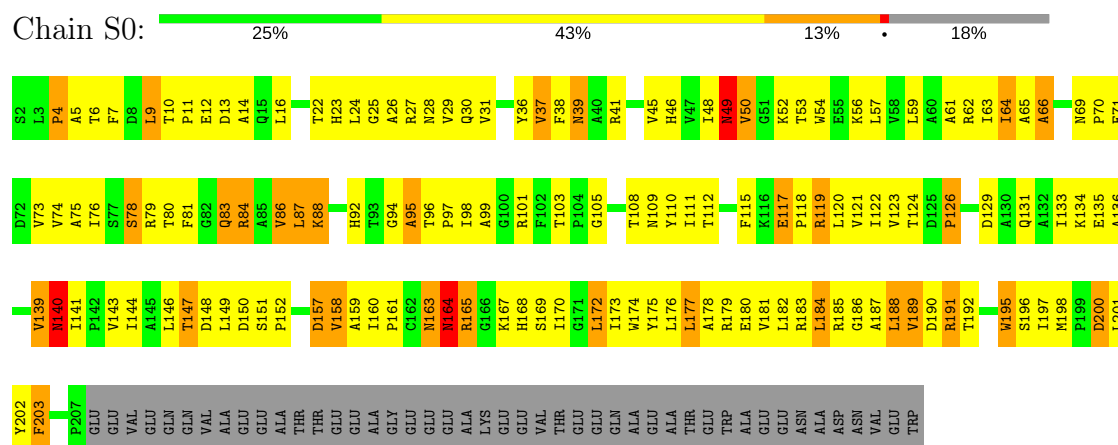




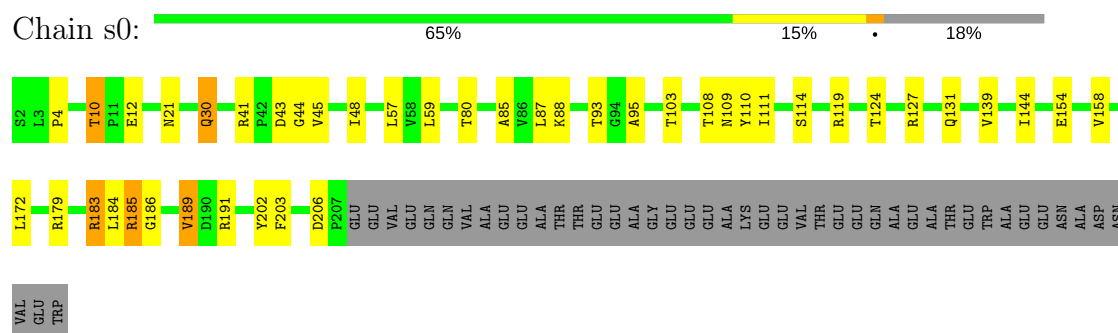




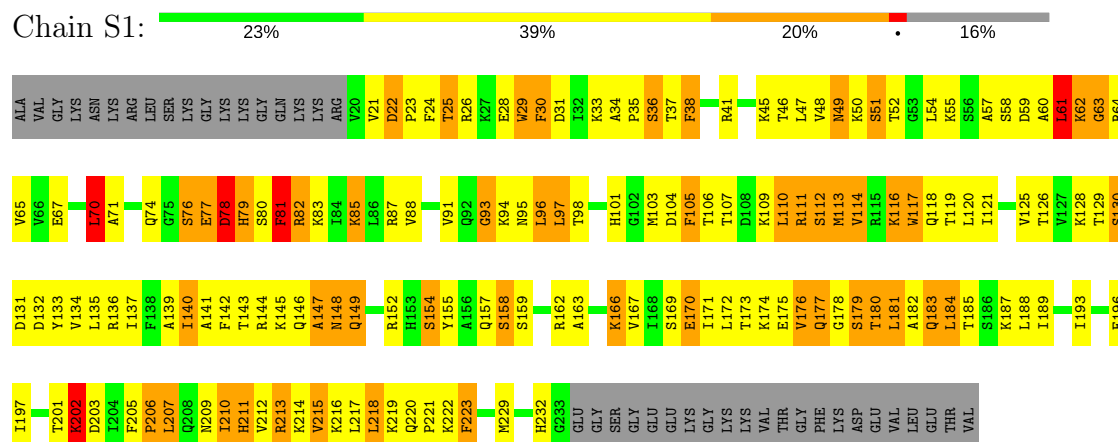
• Molecule 2: 40S ribosomal protein S0-A



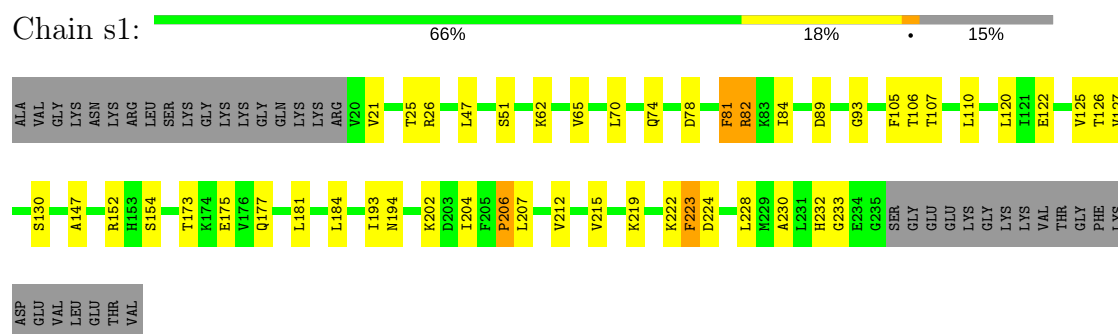
• Molecule 2: 40S ribosomal protein S0-A



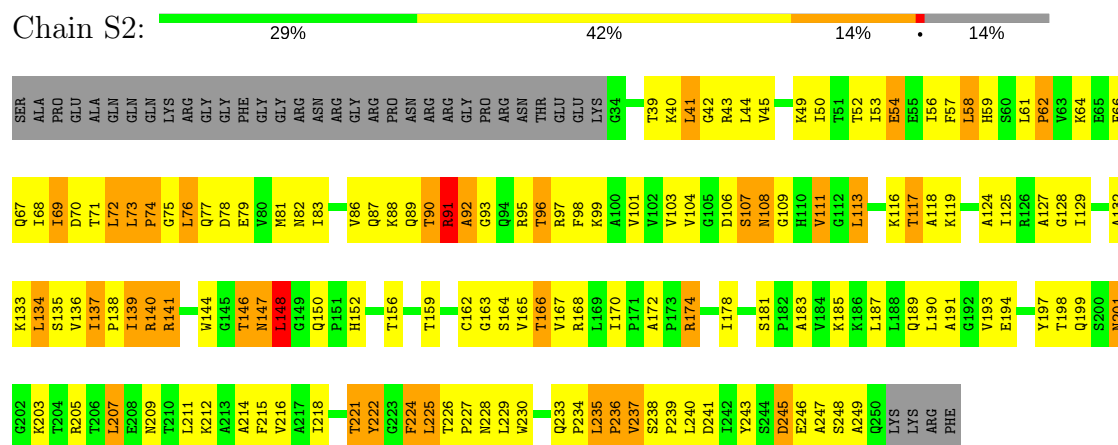
- Molecule 3: 40S ribosomal protein S1-A



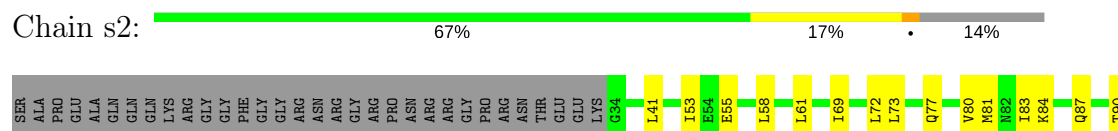
- Molecule 3: 40S ribosomal protein S1-A

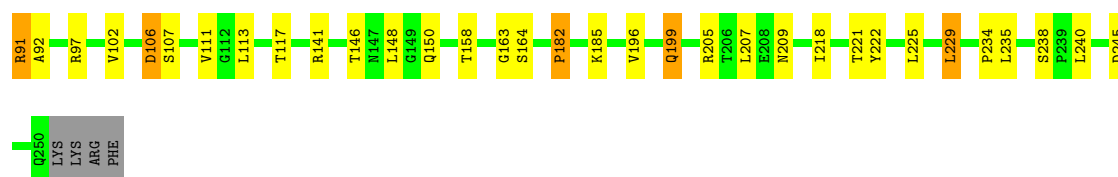


- Molecule 4: 40S ribosomal protein S2



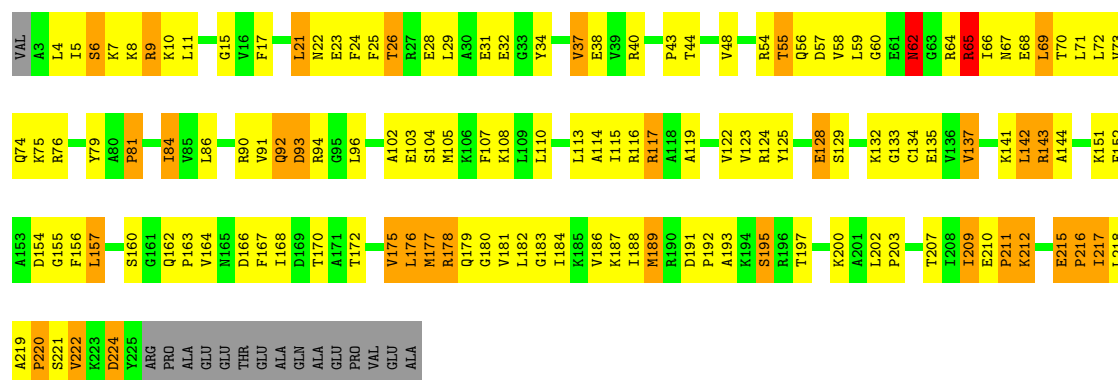
- Molecule 4: 40S ribosomal protein S2





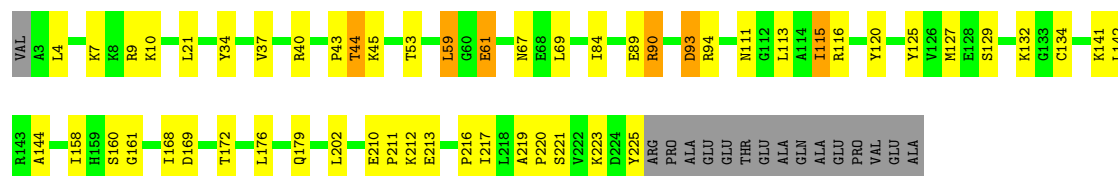
• Molecule 5: 40S ribosomal protein S3

Chain S3: 36% 43% 13% 7%



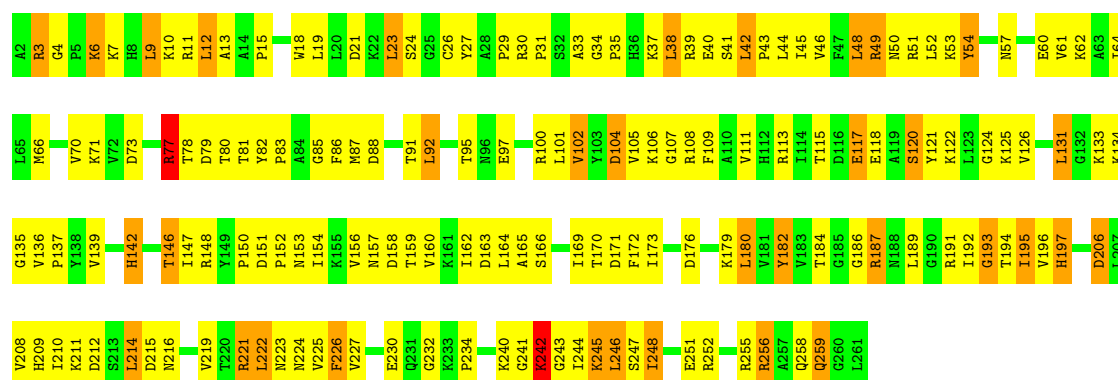
• Molecule 5: 40S ribosomal protein S3

Chain s3: 71% 20% 7%



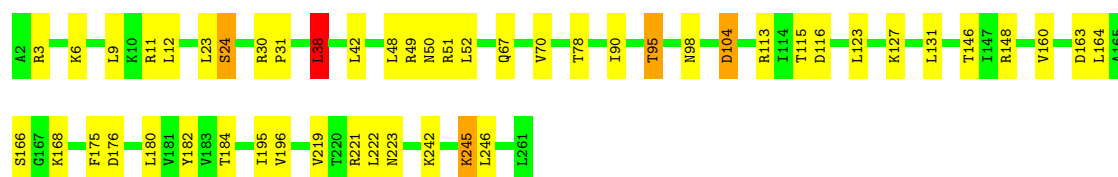
• Molecule 6: 40S ribosomal protein S4-A

Chain S4: 37% 50% 13%



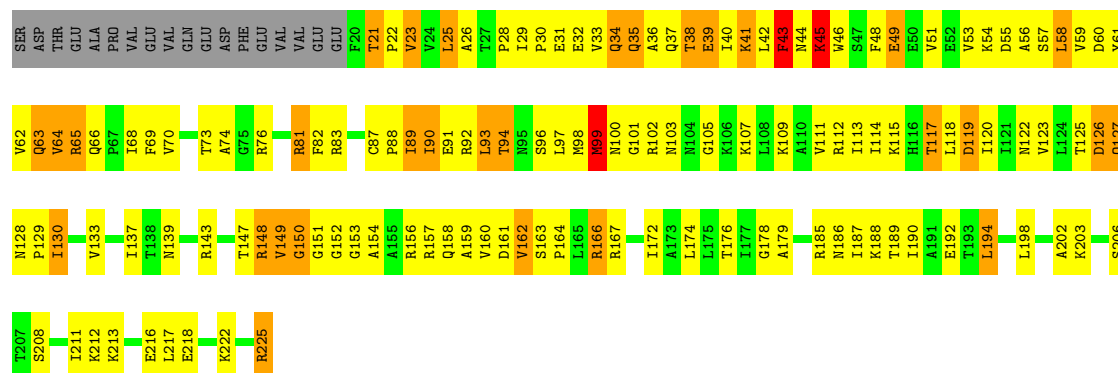
• Molecule 6: 40S ribosomal protein S4-A

Chain s4: 81% 17%



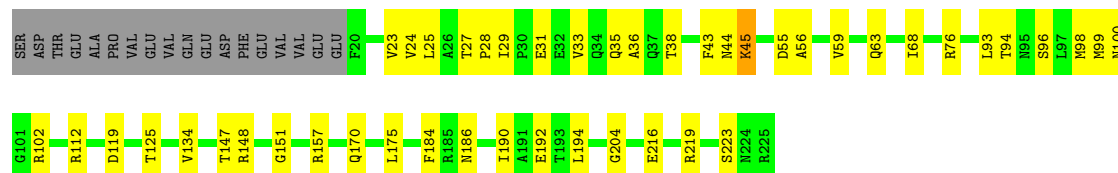
• Molecule 7: 40S ribosomal protein S5

Chain S5: 32% 46% 13% 8%



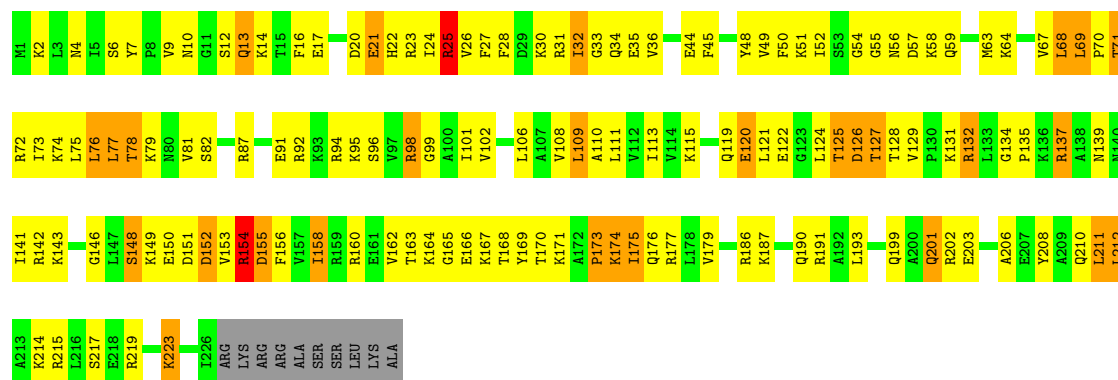
• Molecule 7: 40S ribosomal protein S5

Chain s5: 71% 20% 8%



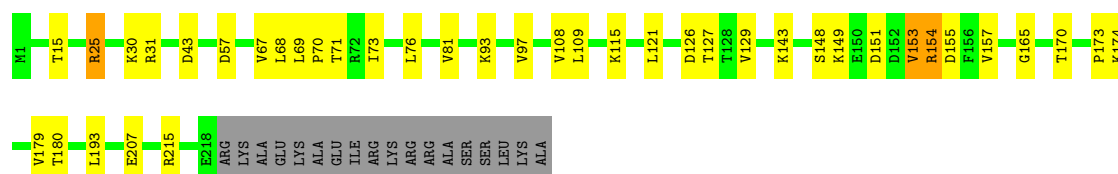
• Molecule 8: 40S ribosomal protein S6-A

Chain S6: 36% 47% 12%



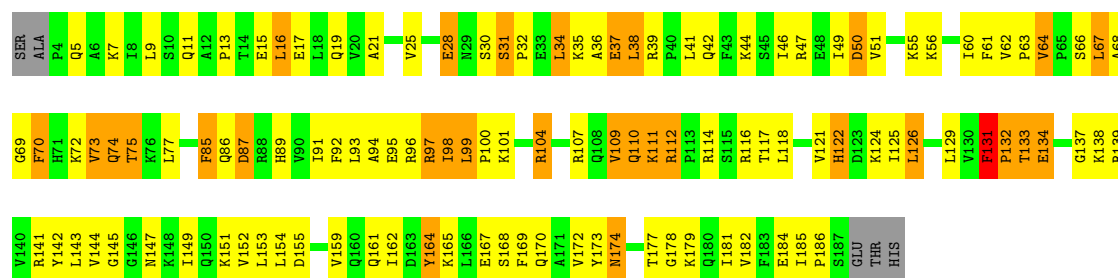
• Molecule 8: 40S ribosomal protein S6-A

Chain s6: 75% 16% 8%



• Molecule 9: 40S ribosomal protein S7-A

Chain S7: 36% 45% 16% ..



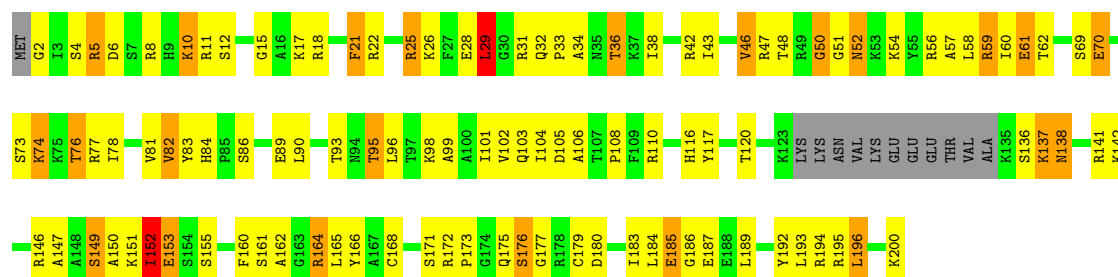
• Molecule 9: 40S ribosomal protein S7-A

Chain s7: 74% 21% ..



• Molecule 10: 40S ribosomal protein S8-A

Chain S8: 40% 42% 12% 6%

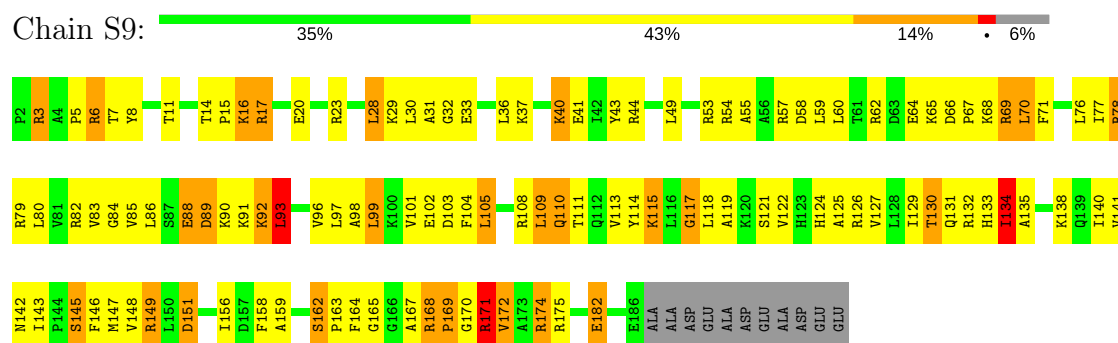


• Molecule 10: 40S ribosomal protein S8-A

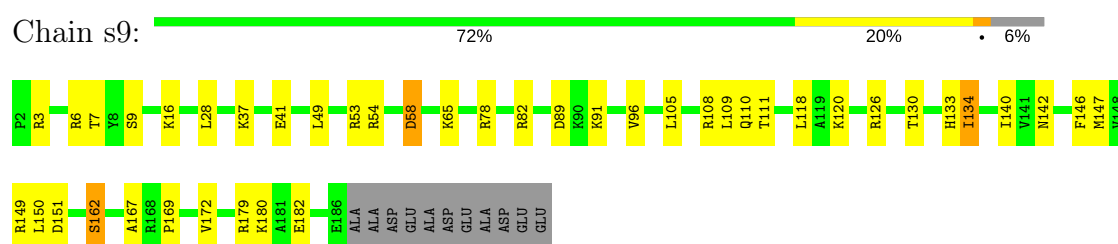
Chain s8: 80% 14% 6%



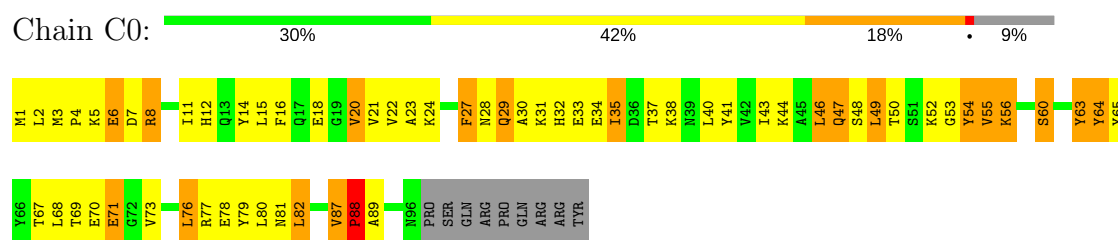
• Molecule 11: 40S ribosomal protein S9-A



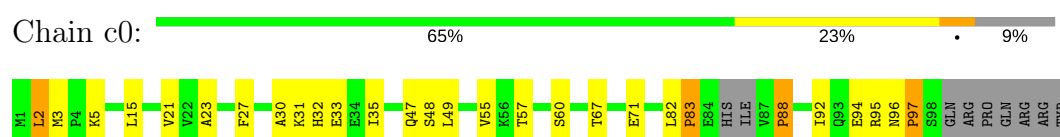
• Molecule 11: 40S ribosomal protein S9-A



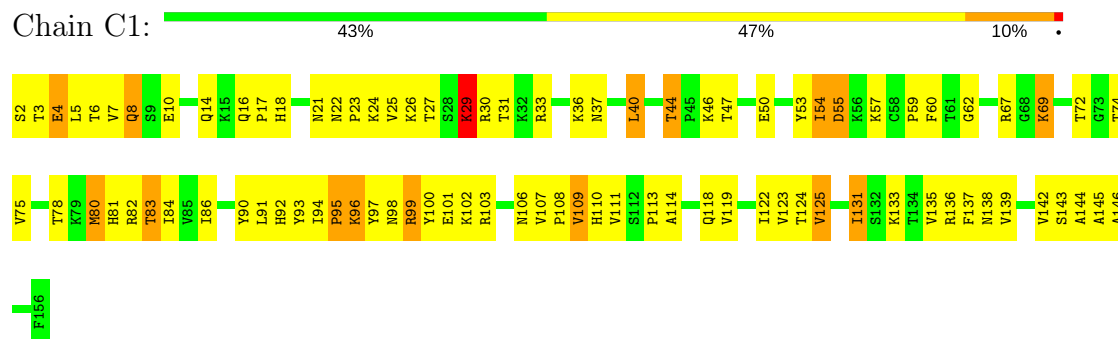
• Molecule 12: 40S ribosomal protein S10-A

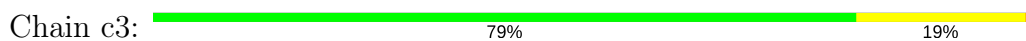


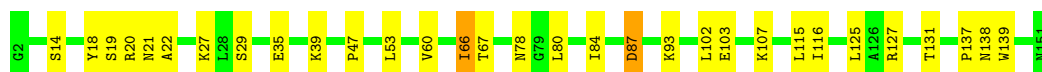
• Molecule 12: 40S ribosomal protein S10-A



• Molecule 13: 40S ribosomal protein S11-A

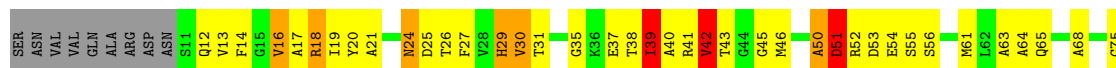






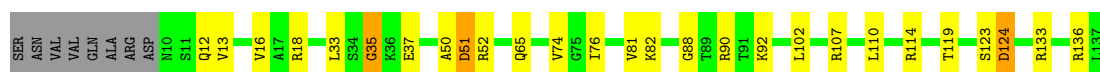
- Molecule 16: 40S ribosomal protein S14-A

Chain C4: 35% 45% 9% 5% 7%



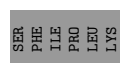
- Molecule 16: 40S ribosomal protein S14-A

Chain c4: 74% 18% 6%



- Molecule 17: 40S ribosomal protein S15

Chain C5: 27% 47% 12% 12%



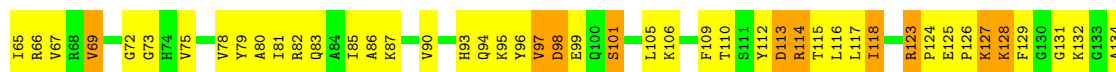
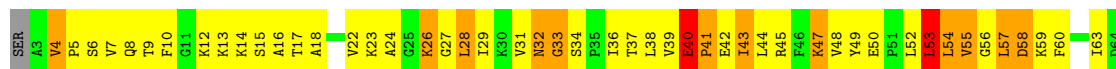
- Molecule 17: 40S ribosomal protein S15

Chain c5: 74% 17%



- Molecule 18: 40S ribosomal protein S16-A

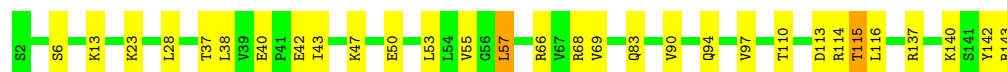
Chain C6: 27% 54% 16%





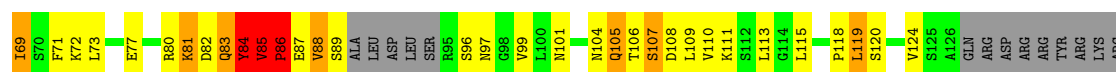
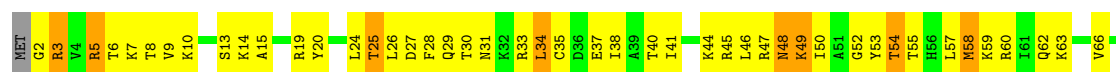
- Molecule 18: 40S ribosomal protein S16-A

Chain c6: 79% 20%



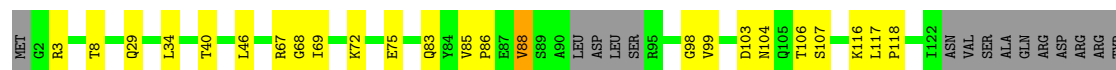
- Molecule 19: 40S ribosomal protein S17-A

Chain C7: 30% 45% 11% 12%



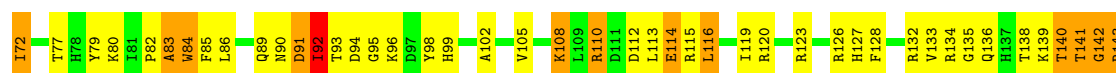
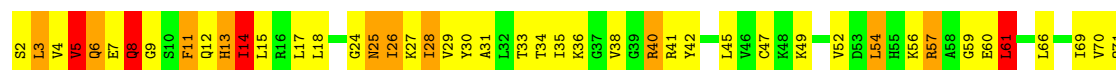
- Molecule 19: 40S ribosomal protein S17-A

Chain c7: 68% 17% 14%



- Molecule 20: 40S ribosomal protein S18-A

Chain C8: 37% 45% 15%



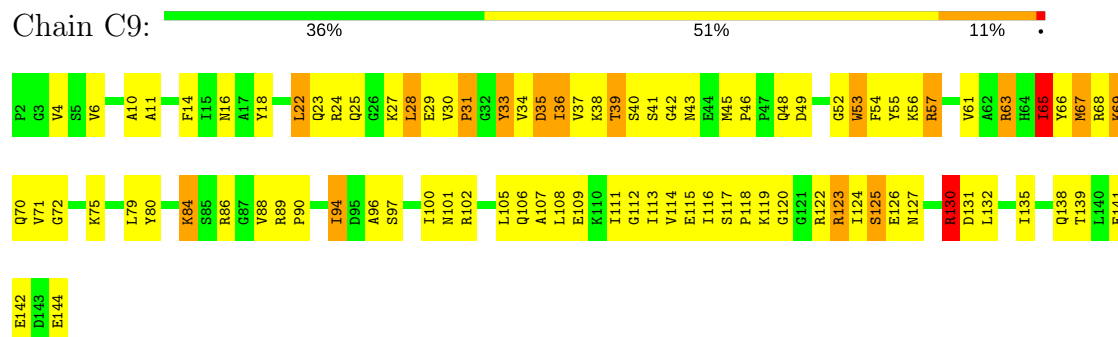
- Molecule 20: 40S ribosomal protein S18-A

Chain c8: 74% 23%

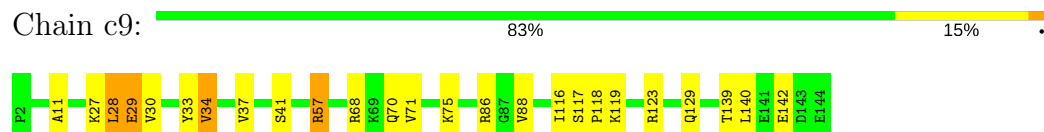


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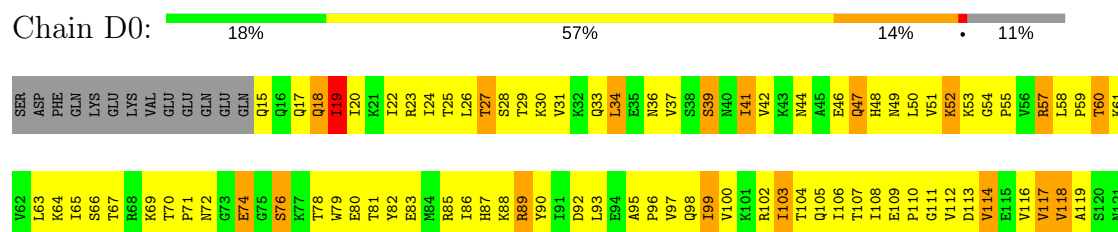
- Molecule 21: 40S ribosomal protein S19-A



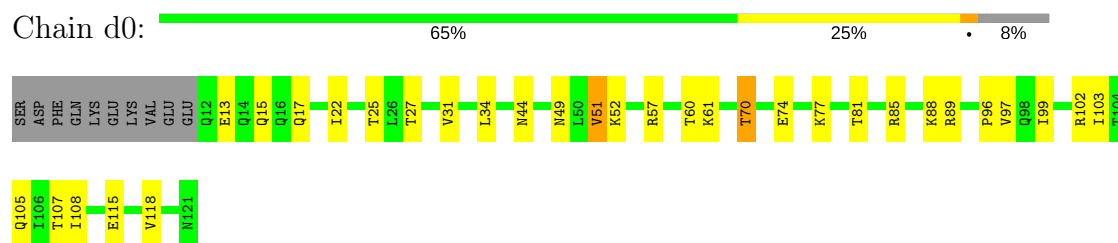
- Molecule 21: 40S ribosomal protein S19-A



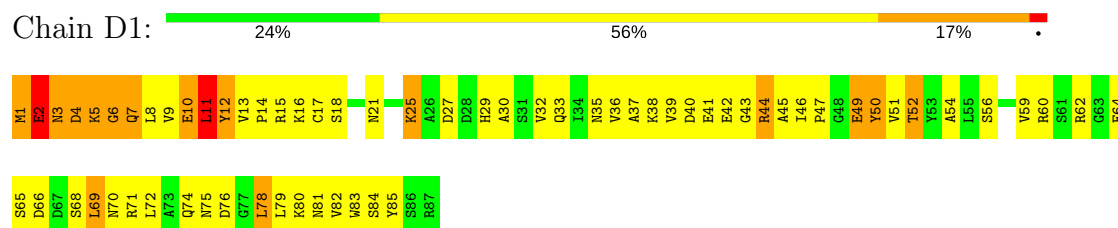
- Molecule 22: 40S ribosomal protein S20



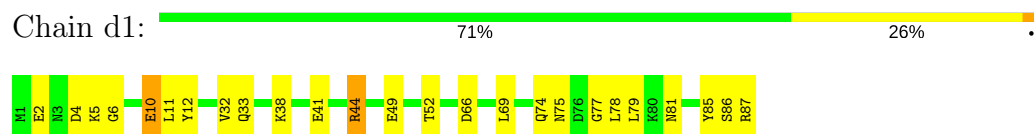
- Molecule 22: 40S ribosomal protein S20



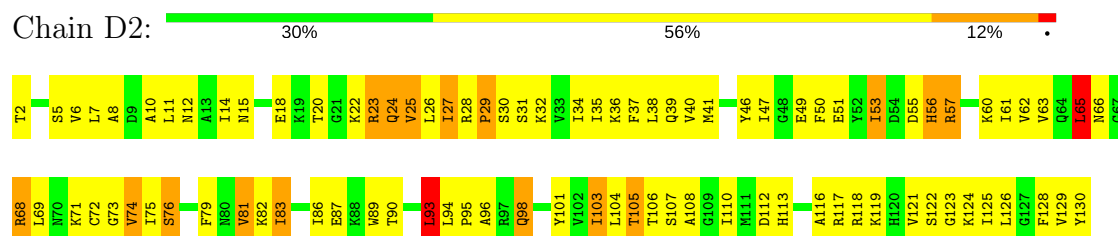
- Molecule 23: 40S ribosomal protein S21-A



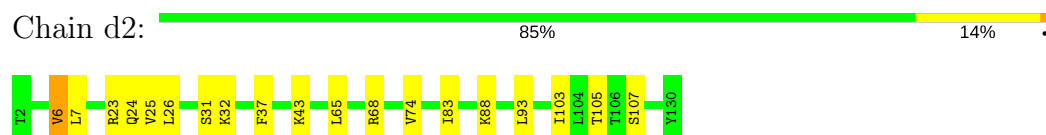
- Molecule 23: 40S ribosomal protein S21-A



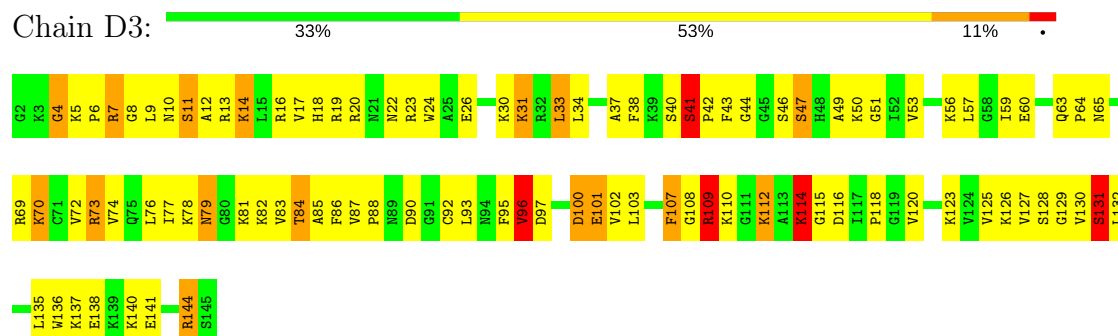
- Molecule 24: 40S ribosomal protein S22-A



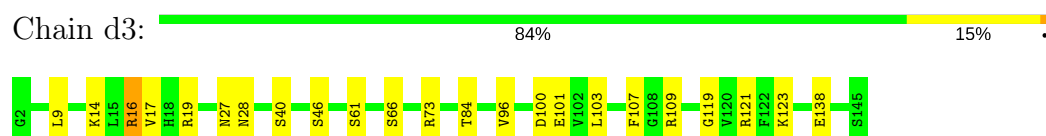
- Molecule 24: 40S ribosomal protein S22-A



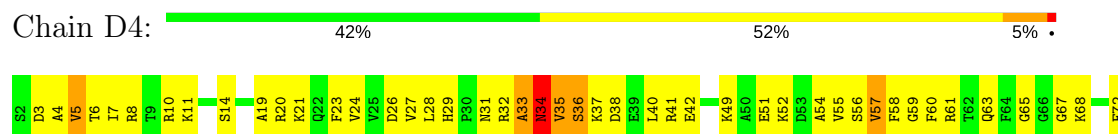
- Molecule 25: 40S ribosomal protein S23-A



- Molecule 25: 40S ribosomal protein S23-A



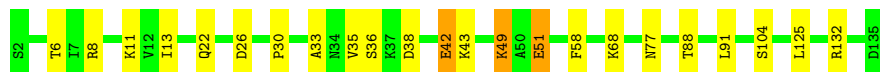
- Molecule 26: 40S ribosomal protein S24-A





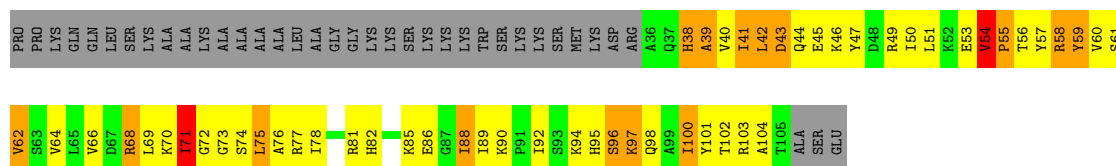
- Molecule 26: 40S ribosomal protein S24-A

Chain d4: 83% 15% .



- Molecule 27: 40S ribosomal protein S25-A

Chain D5: 15% 35% 14% . 35%



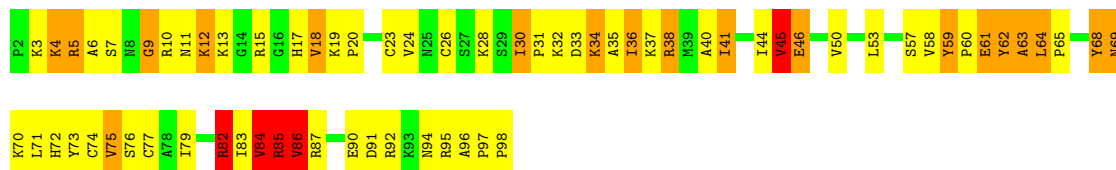
- Molecule 27: 40S ribosomal protein S25-A

Chain d5: 51% 13% 36%



- Molecule 28: 40S ribosomal protein S26-B

Chain D6: 29% 46% 20% 5%



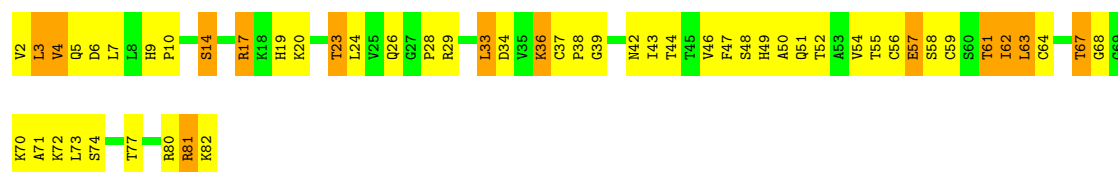
- Molecule 28: 40S ribosomal protein S26-B

Chain d6: 82% 16% .



- Molecule 29: 40S ribosomal protein S27-A

Chain D7: 33% 51% 16%



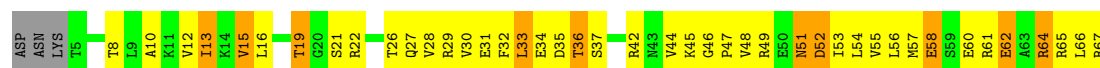
- Molecule 29: 40S ribosomal protein S27-A

Chain d7: 69% 28%



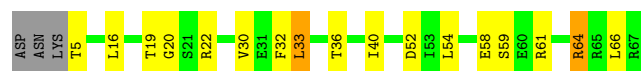
- Molecule 30: 40S ribosomal protein S28-A

Chain D8: 30% 50% 15% 5%



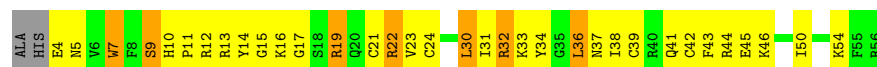
- Molecule 30: 40S ribosomal protein S28-A

Chain d8: 70% 23% 5%



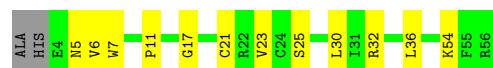
- Molecule 31: 40S ribosomal protein S29-A

Chain D9: 35% 49% 13%



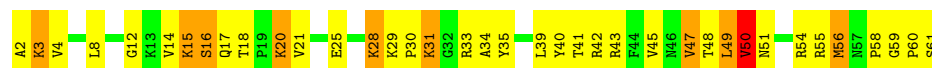
- Molecule 31: 40S ribosomal protein S29-A

Chain d9: 75% 22%



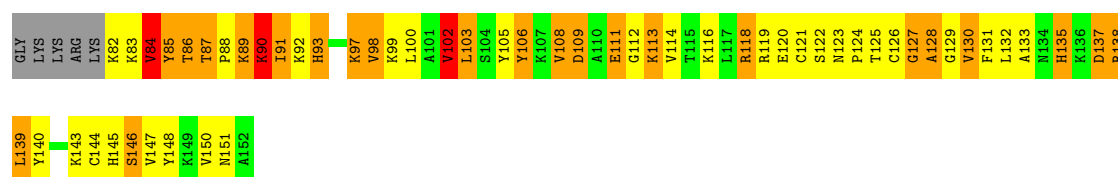
- Molecule 32: 40S ribosomal protein S30-A

Chain E0: 37% 47% 15%



- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1: 20% 39% 30% 7%



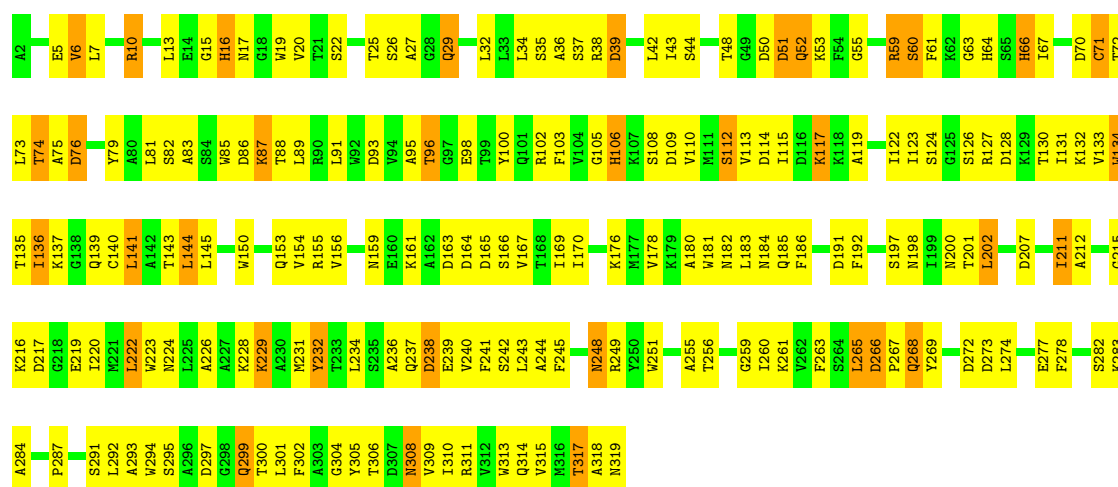
• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1: 55% 37% 8%



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

Chain SR: 38% 51% 11%



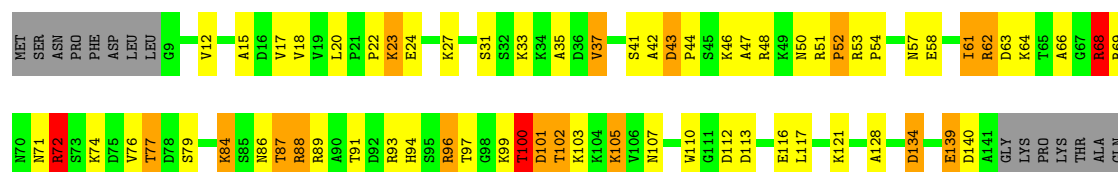
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

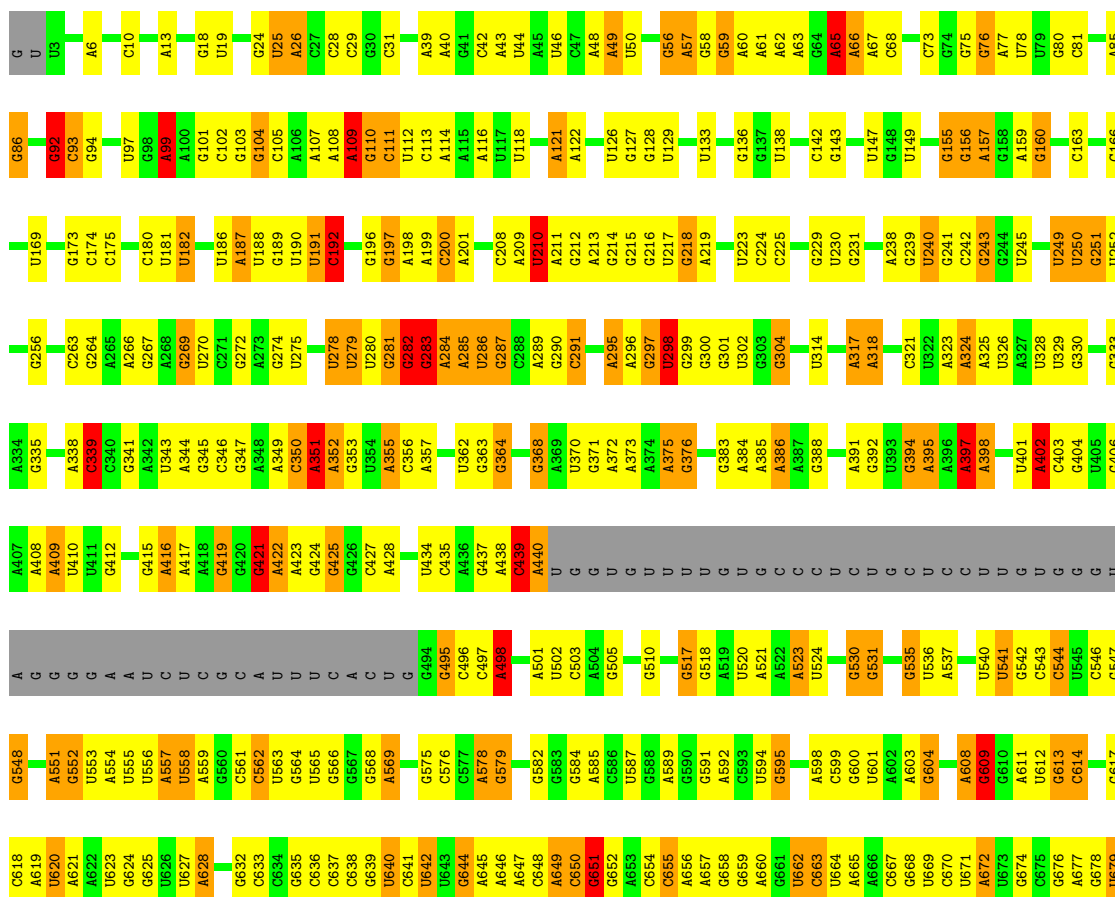
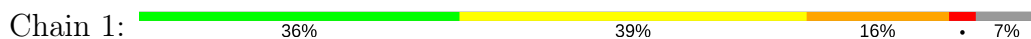
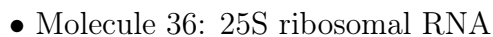
Chain sR: 87% 13%



• Molecule 35: Suppressor protein STM1

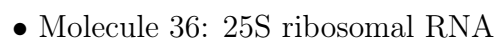
Chain SM: 29% 22% 6% 42%





G1766	G1688	G1689	G1695	G1701	G1702	G1709	G1785	G1786	G1787	G1788	G1789	G1790	G1791	G1792	G1793	G1794	G1795	G1802	A1806	G1807	G1808	A1809	A1810	A1814	A1815	G1816	G1817	G1818	G1819	G1820	G1821	G1822	G1825	G1826	G1827	A1831	A1832	G1833	A1834	A1835	A1836	G1837	G1838	A1839	G1840	A1841	A1842	C1843																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
G1681	G1682	A1683	G1684	G1685	G1686	G1687	G1688	G1689	G1690	G1691	G1692	G1693	G1694	G1695	G1696	G1697	G1698	G1699	G1700	G1701	G1702	G1703	G1704	A1705	G1706	G1707	G1708	A1709	G1710	G1711	G1712	G1713	G1714	G1715	A1716	G1717	G1718	G1719	G1720	G1721	G1725	G1726	G1727	G1728	G1729	G1730	G1731	G1732	G1733	G1734	A1735	A1736	G1739	A1743	A1744	G1745	A1746	A1747	G1748																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
C1749	G1750	A1751	G1752	G1753	C1754	C1755	C1756	C1757	C1758	C1759	C1760	C1761	C1762	C1763	C1764	C1765	C1766	C1767	C1768	C1769	C1770	C1771	C1772	C1773	C1774	C1775	C1776	C1777	C1778	C1779	C1780	C1781	C1782	C1783	C1784	C1785	C1786	C1787	C1788	C1789	C1790	C1791	C1792	C1793	C1794	C1795	C1796	C1797	C1798	C1799	C1800	C1801	C1802	C1803	C1804	C1805	C1806	C1807	C1808	C1809	C1810	C1811	C1812	C1813	C1814	C1815	C1816	C1817																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
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A2900	C2829	U2762	G2690	C2622	U2550	C	C2415	G2354	A2279	G2208	A1933	C1856
G2901	U2830	U2763	A2691	G2623	C2551	A	U2416	C2355	U2282	U2209	G2124	C1857
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C2903	U2832	U2765	U2693	G2625	U2553	C	U2418	A2357	C2284	G2211	G1939	G1863
U2904	G2833	G2766	A2694	A2626	A2554	G	A2419	C2357	C2285	A2213	G1940	A1864
C2905	U2834	U2767	U2695	C2627	C2555	A	C2420	C2358	C2286	G2212	C1941	A1865
U2906	C2835	U2768	A2696	U2628	U2556	C	U2421	C2359	G2287	A2214	U1942	C1866
A2907	U2836	U2769	U2697	U2629	A2557	U	G2422	C2360	G2288	U2215	U1943	U1871
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C2938	A2865	G2798	U2726	G2657	U2590	C	U2456	U2389	A2319	G2169	U1906	U1906
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C2940	A2867	G2800	U2728	G2659	C2592	C	U2458	U2391	A2321	G2171	A1911	A1911
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C2942	G2869	A2802	U2730	G2661	C2594	C	U2460	U2393	G2323	U2173	A1913	A1913
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C2944	A2871	U2804	U2732	G2663	U2596	C	U2462	A2385	U2325	U2175	U1915	U1915
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C2946	U2873	G2806	U2734	G2665	A2598	C	U2464	U2387	U2327	A2177	C1917	C1917
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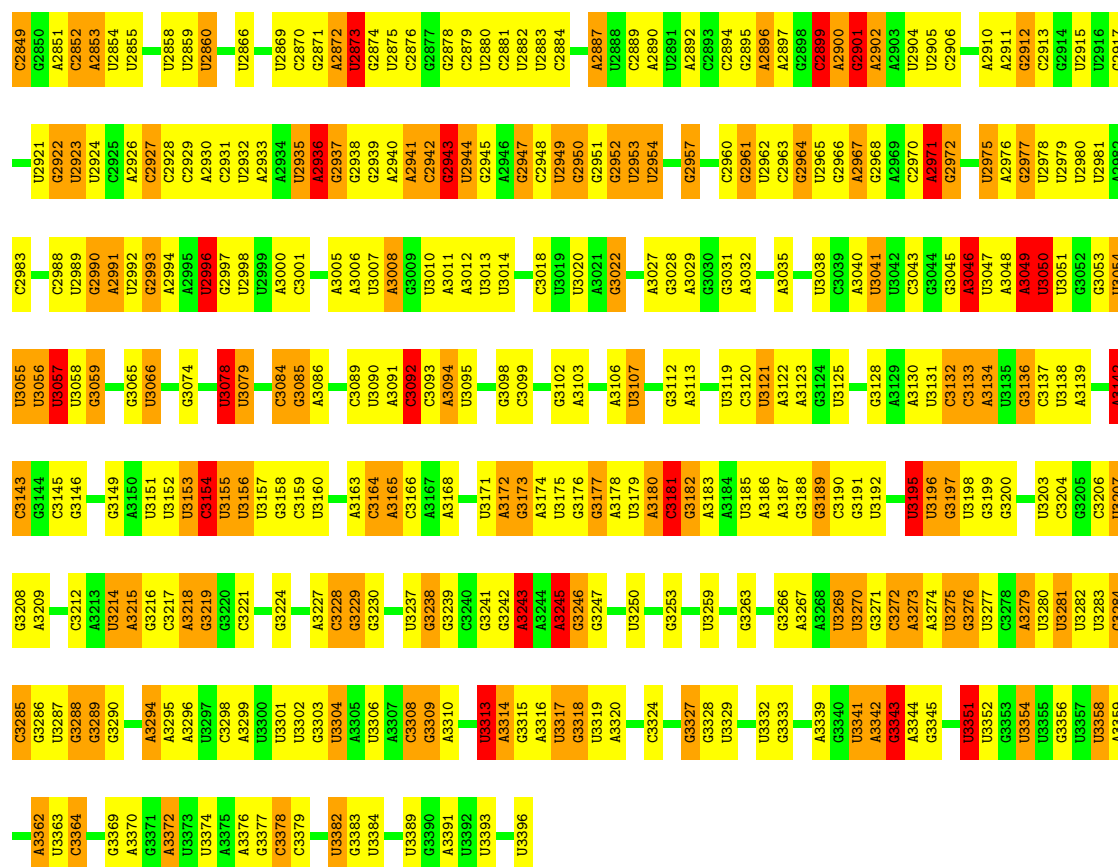


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Sometimes	17%
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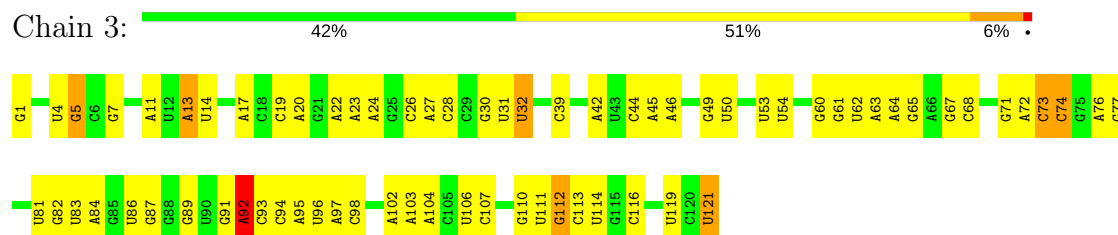


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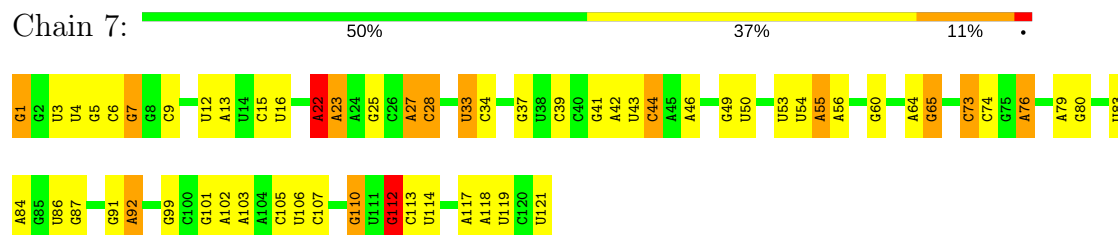
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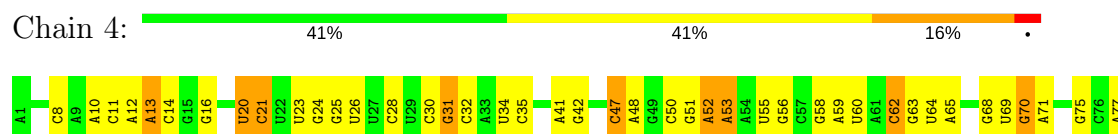
• Molecule 37: 5S ribosomal RNA

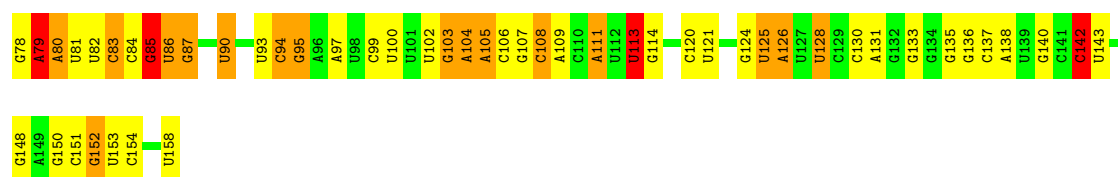


• Molecule 37: 5S ribosomal RNA

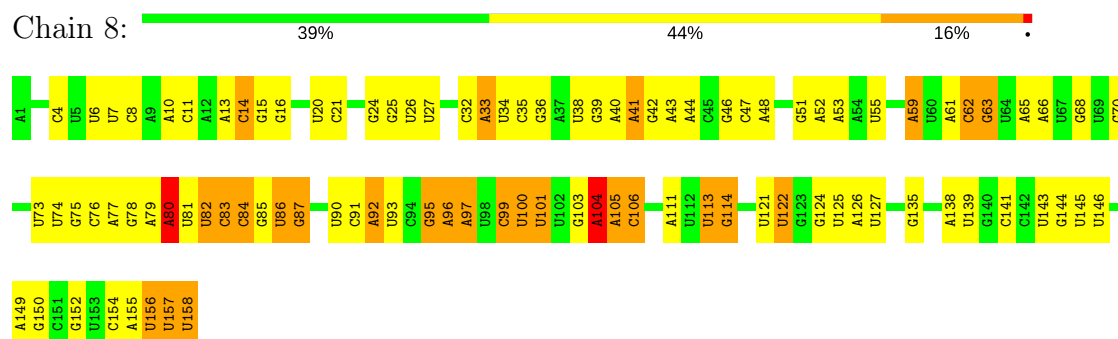


• Molecule 38: 5.8S ribosomal RNA

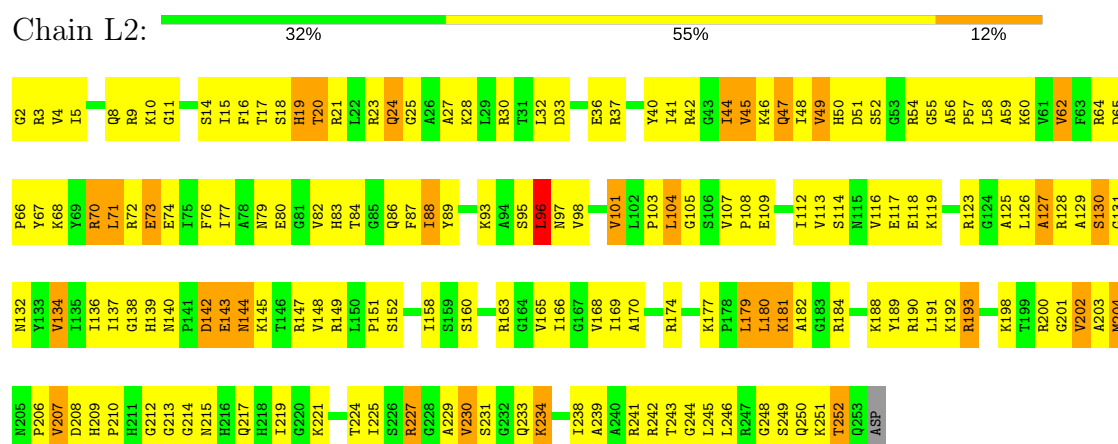




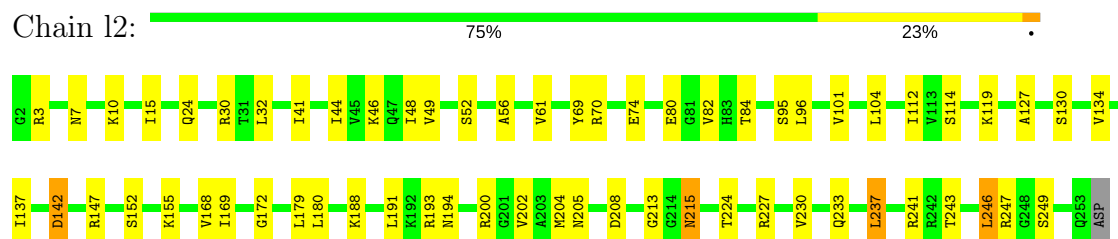
• Molecule 38: 5.8S ribosomal RNA



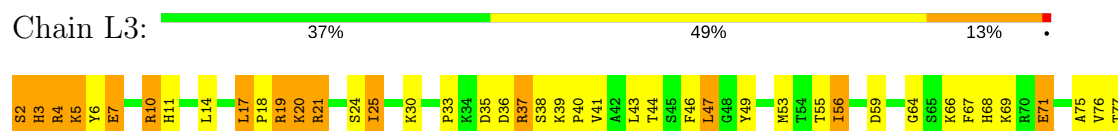
• Molecule 39: 60S ribosomal protein L2-A

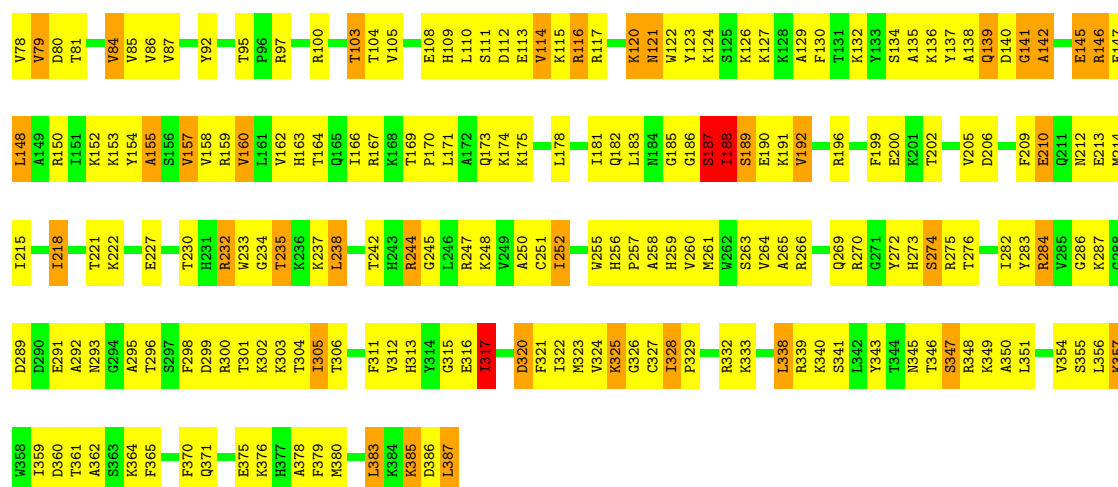


• Molecule 39: 60S ribosomal protein L2-A

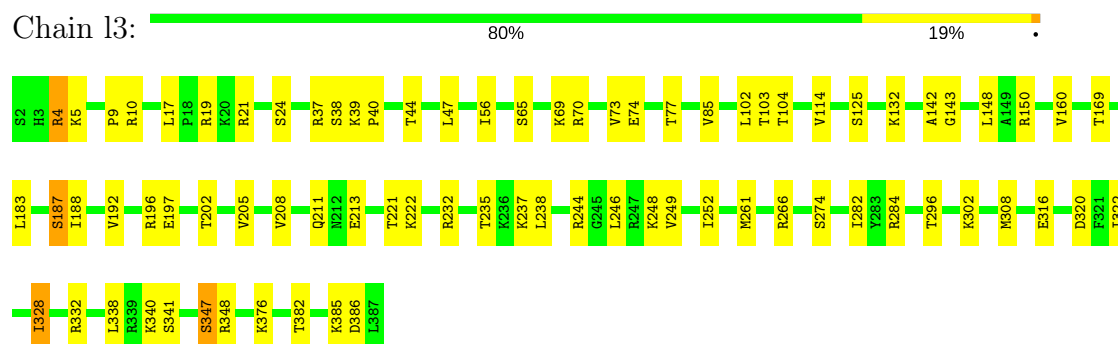


• Molecule 40: 60S ribosomal protein L3

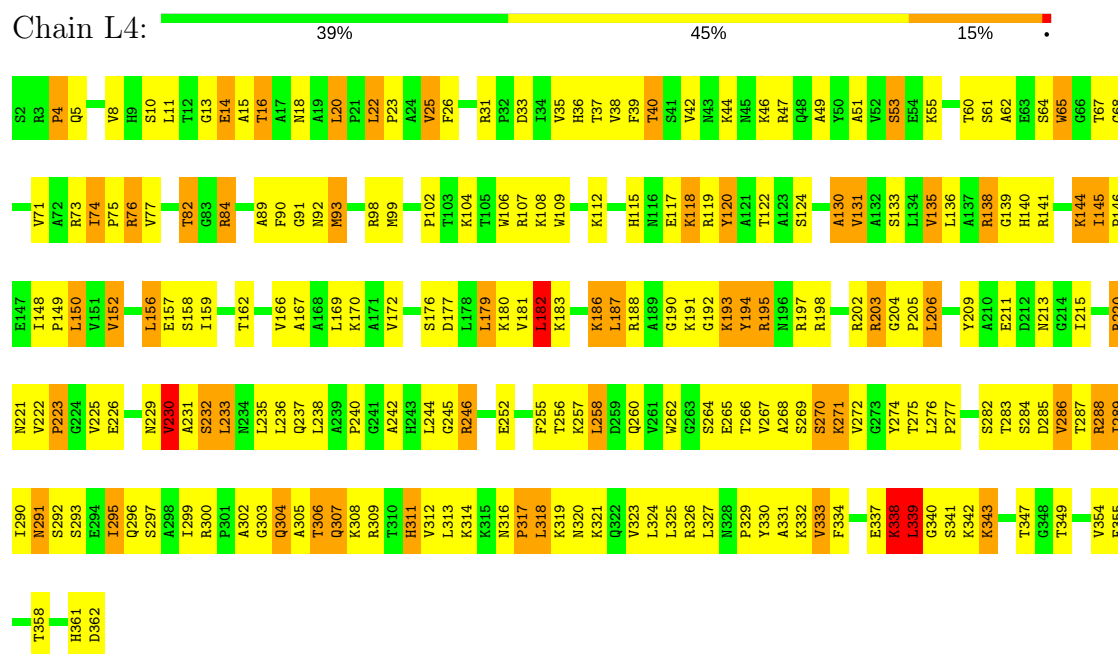




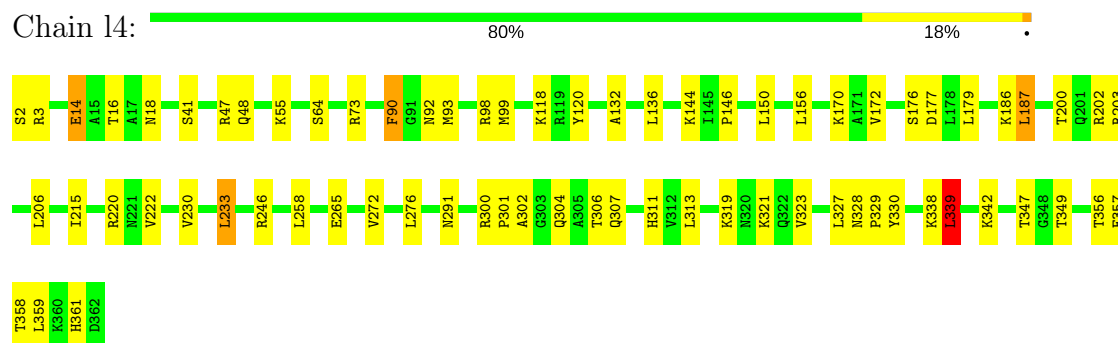
• Molecule 40: 60S ribosomal protein L3



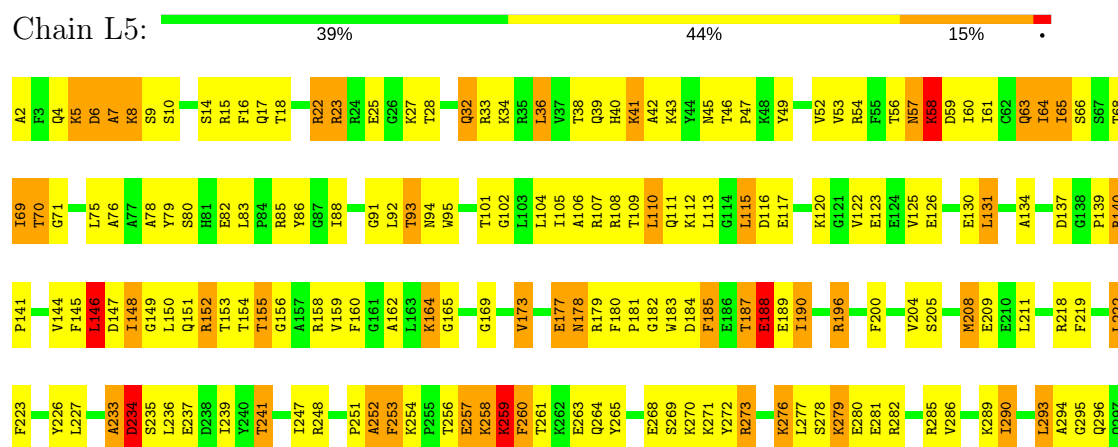
• Molecule 41: 60S ribosomal protein L4-A



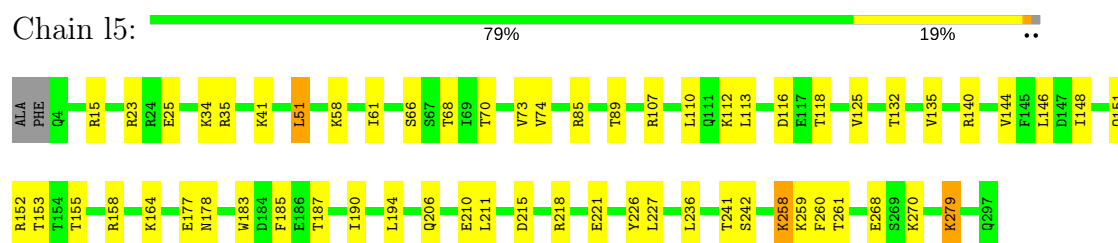
• Molecule 41: 60S ribosomal protein L4-A



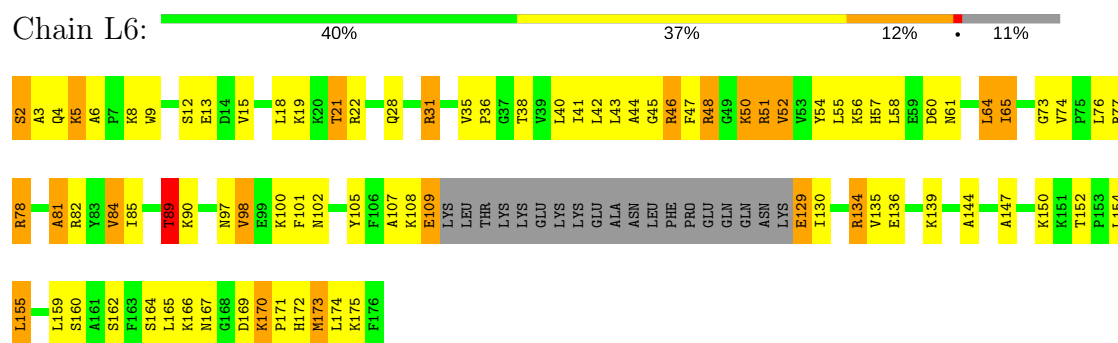
• Molecule 42: 60S ribosomal protein L5



• Molecule 42: 60S ribosomal protein L5

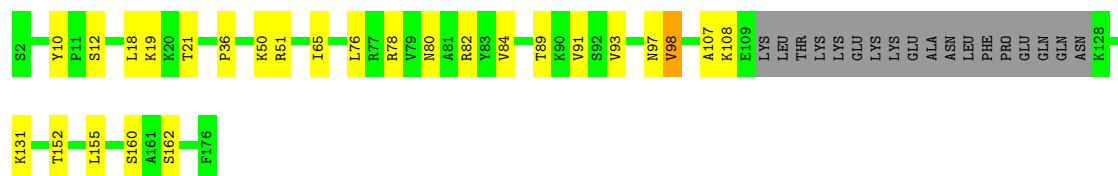


• Molecule 43: 60S ribosomal protein L6-A



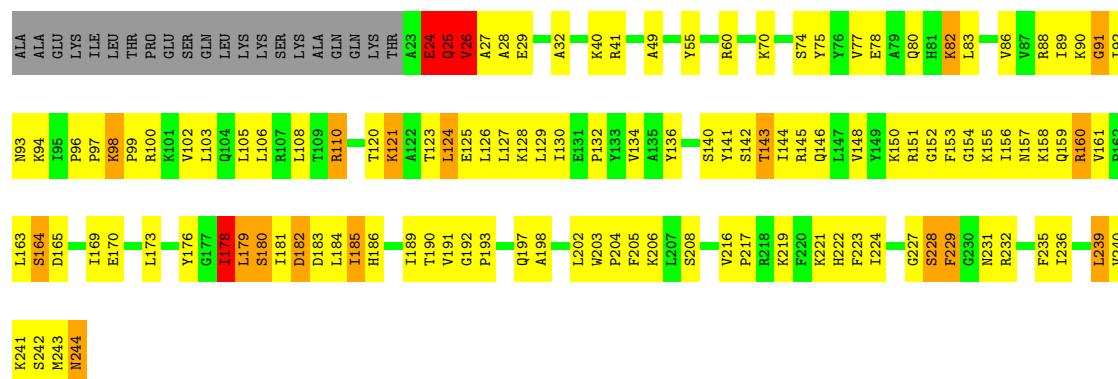
• Molecule 43: 60S ribosomal protein L6-A

Chain 16:



- Molecule 44: 60S ribosomal protein L7-A

Chain L7:



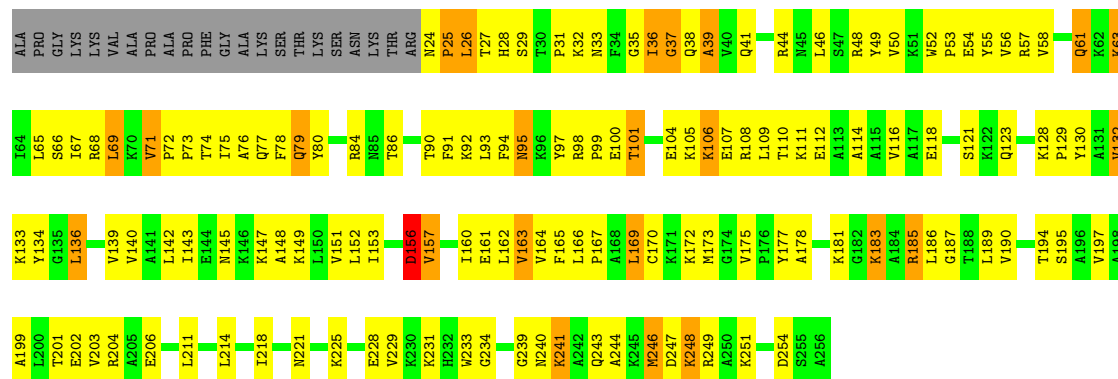
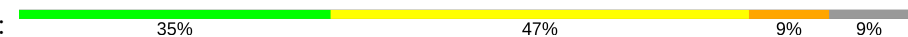
- Molecule 44: 60S ribosomal protein L7-A

Chain 17:

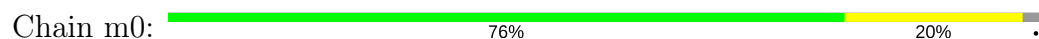


- Molecule 45: 60S ribosomal protein L8-A

Chain L8:



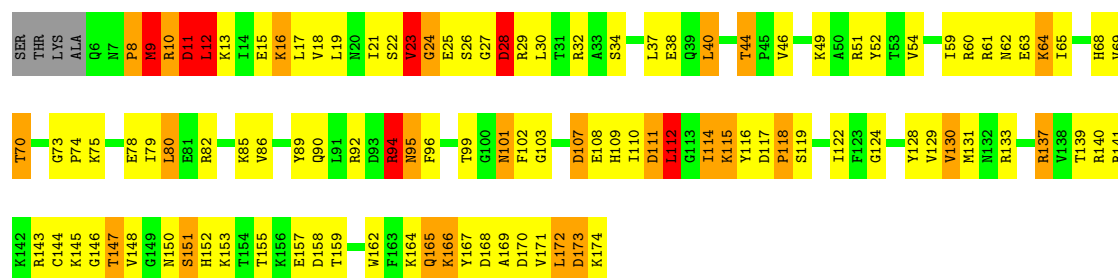
- Molecule 45: 60S ribosomal protein L8-A





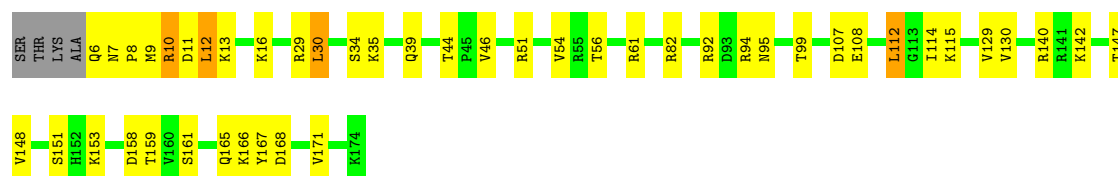
• Molecule 48: 60S ribosomal protein L11-B

Chain M1: 34% 46% 14%



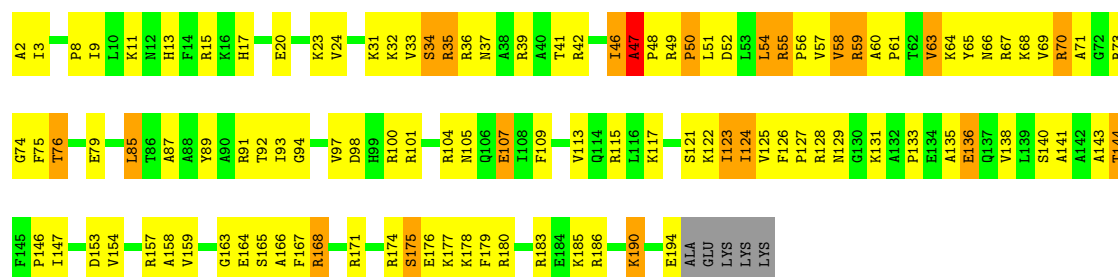
• Molecule 48: 60S ribosomal protein L11-B

Chain m1: 71% 24%



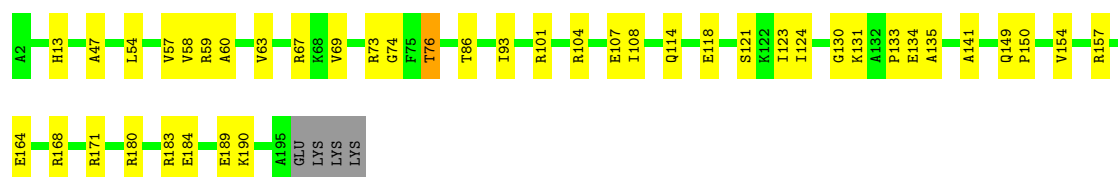
• Molecule 49: 60S ribosomal protein L13-A

Chain M3: 41% 46% 10%

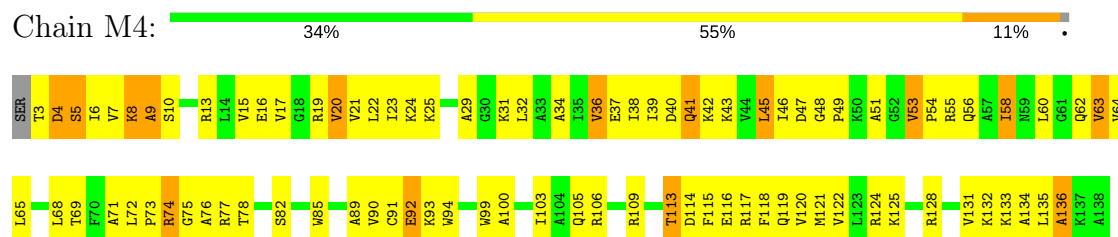


• Molecule 49: 60S ribosomal protein L13-A

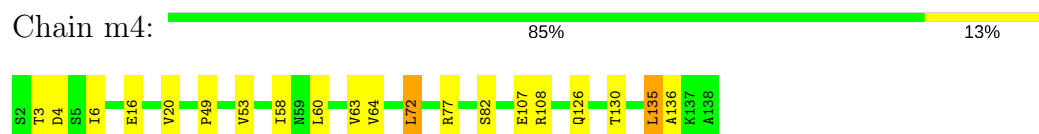
Chain m3: 77% 21%



- Molecule 50: 60S ribosomal protein L14-A



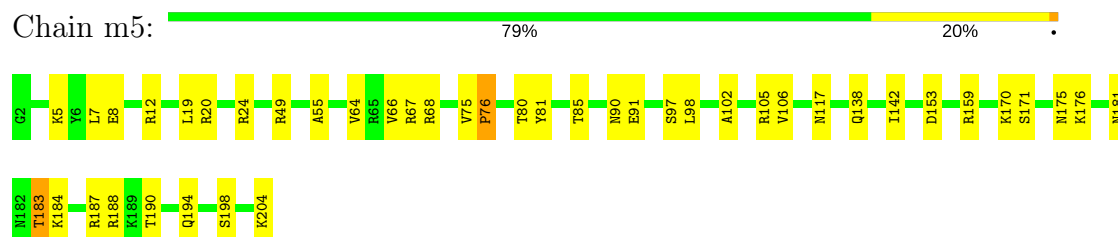
- Molecule 50: 60S ribosomal protein L14-A



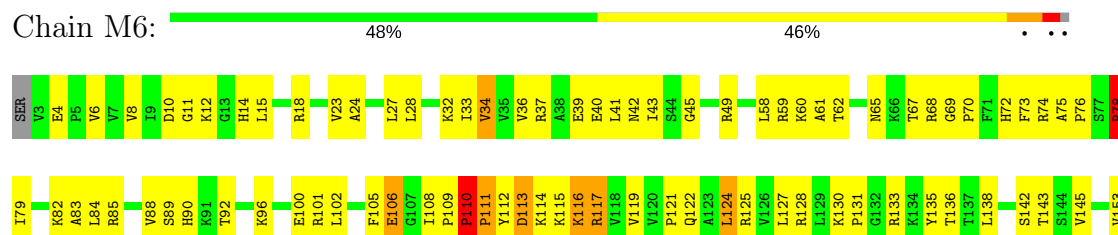
- Molecule 51: 60S ribosomal protein L15-A



- Molecule 51: 60S ribosomal protein L15-A



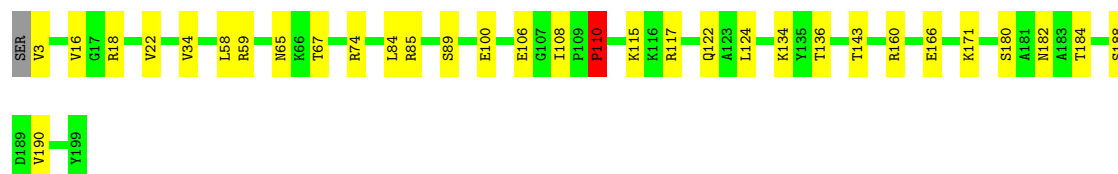
- Molecule 52: 60S ribosomal protein L16-A





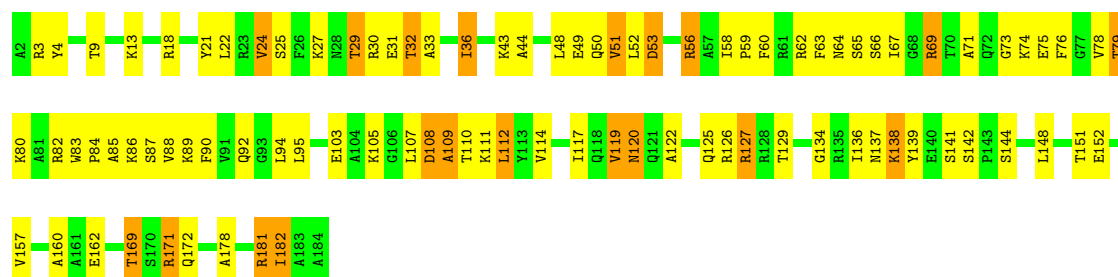
• Molecule 52: 60S ribosomal protein L16-A

Chain m6: 83% 16% ..



• Molecule 53: 60S ribosomal protein L17-A

Chain M7: 50% 39% 11%



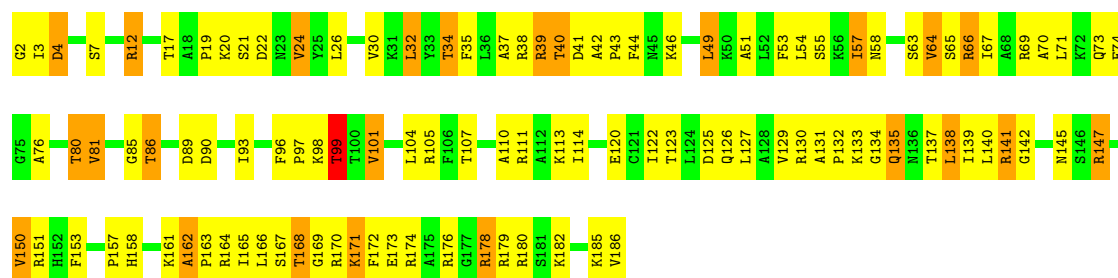
• Molecule 53: 60S ribosomal protein L17-A

Chain m7: 72% 13% 15%

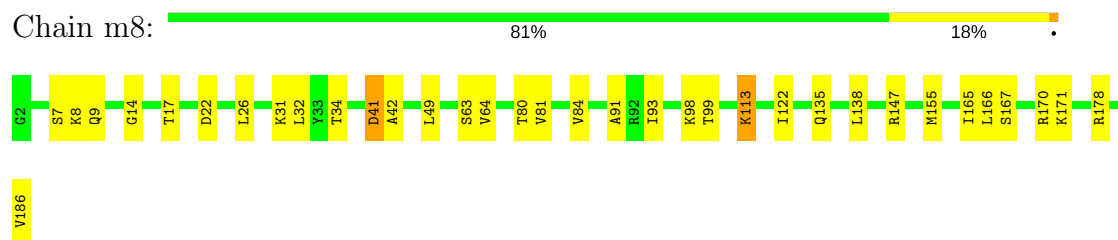


• Molecule 54: 60S ribosomal protein L18-A

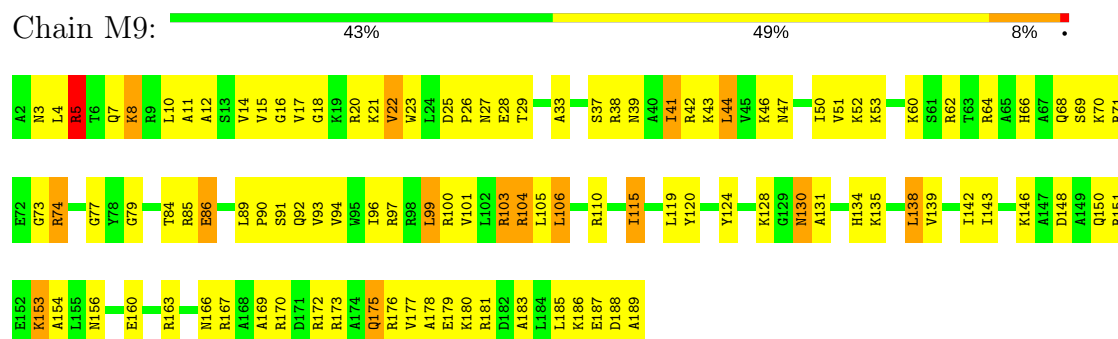
Chain M8: 41% 45% 13%



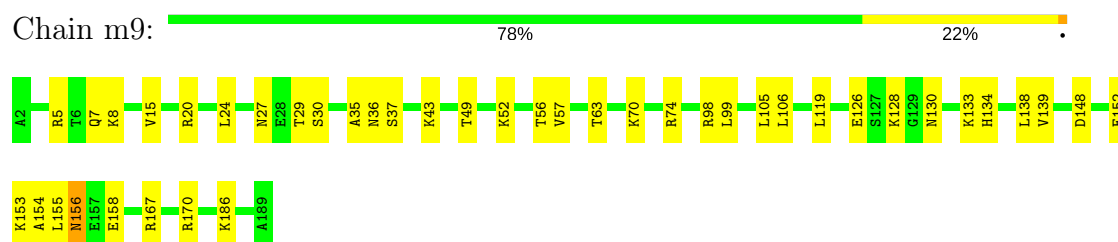
• Molecule 54: 60S ribosomal protein L18-A



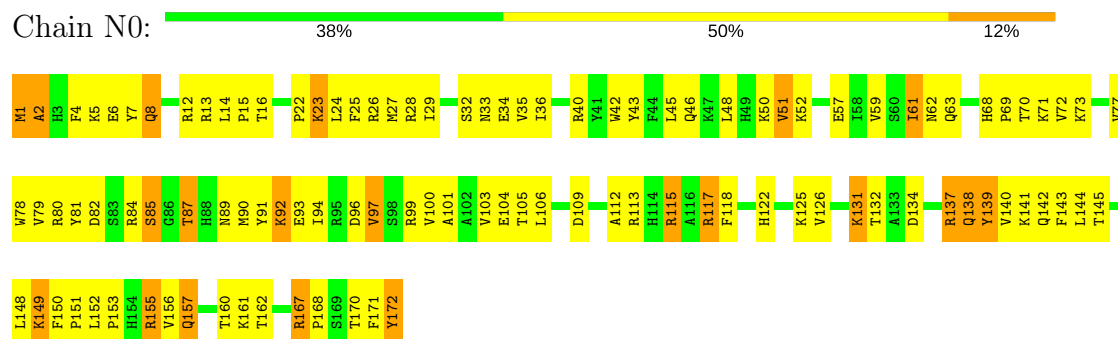
- Molecule 55: 60S ribosomal protein L19-A



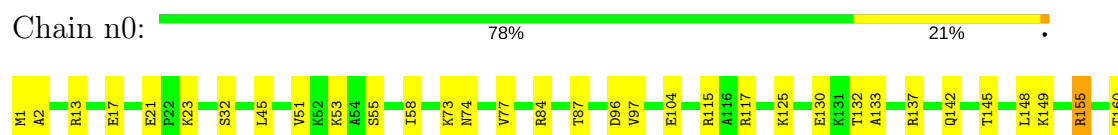
- Molecule 55: 60S ribosomal protein L19-A



- Molecule 56: 60S ribosomal protein L20-A



- Molecule 56: 60S ribosomal protein L20-A

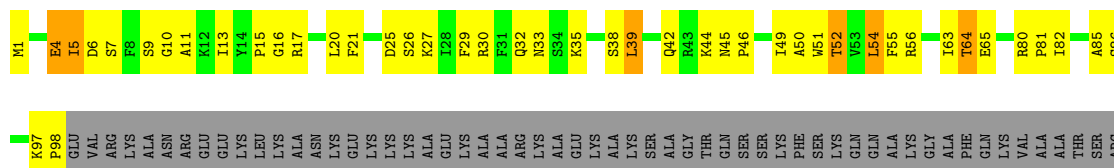


Chain n3:  93% 7%




- Molecule 60: 60S ribosomal protein L24-A

Chain N4:  34% 25% 37%



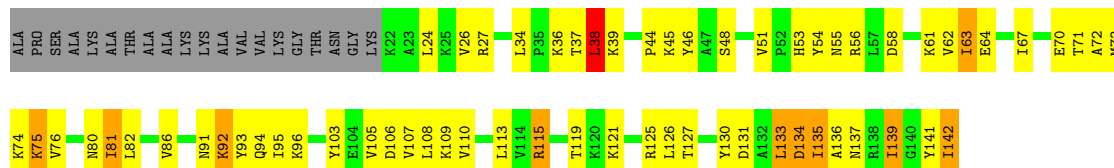
- Molecule 60: 60S ribosomal protein L24-A

Chain n4:  75% 12% 13%



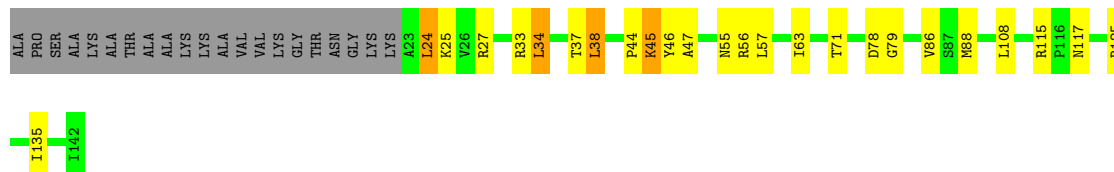
- Molecule 61: 60S ribosomal protein L25

Chain N5:  40% 38% 7% 14%



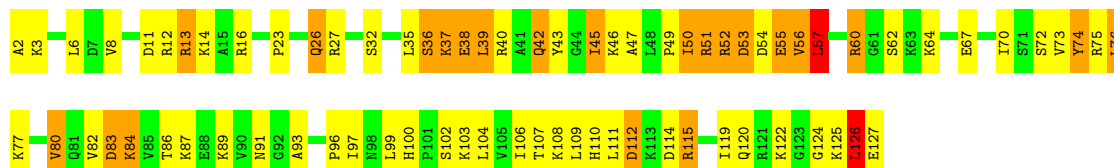
- Molecule 61: 60S ribosomal protein L25

Chain n5:  67% 15% 15%

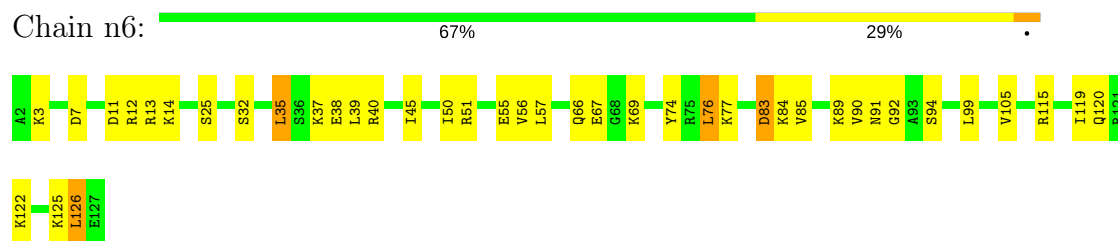


- Molecule 62: 60S ribosomal protein L26-A

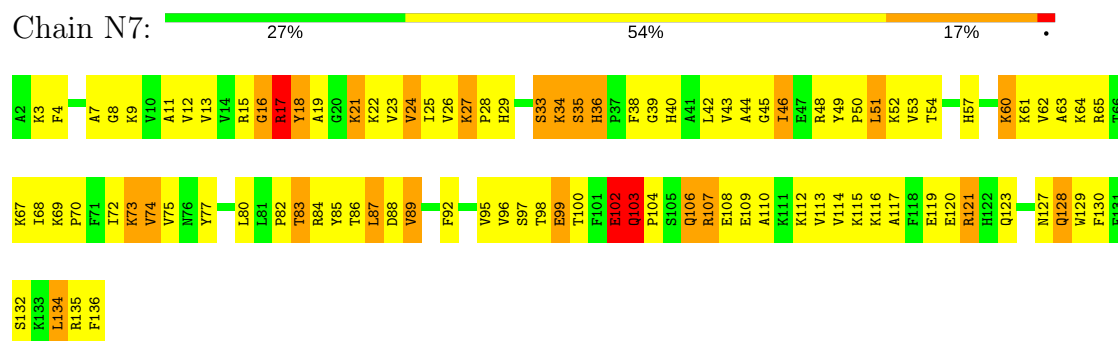
Chain N6:  40% 41% 17%



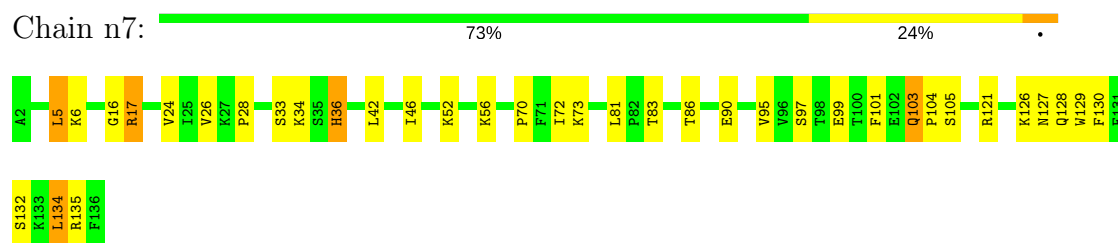
- Molecule 62: 60S ribosomal protein L26-A



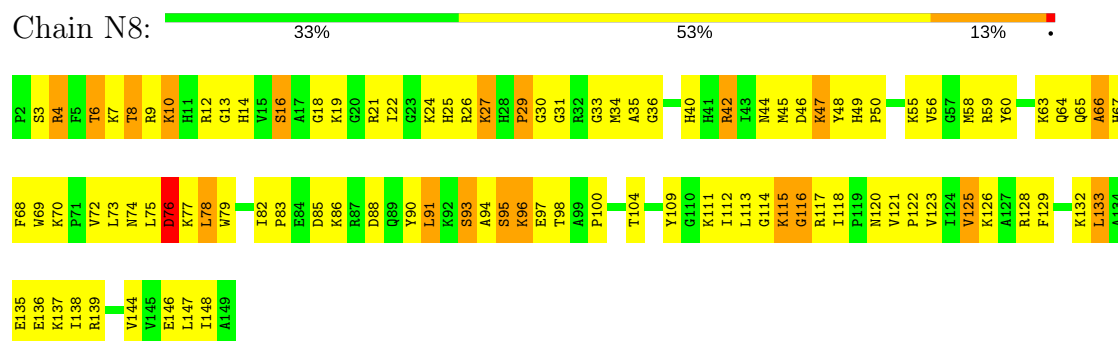
- Molecule 63: 60S ribosomal protein L27-A



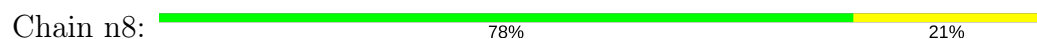
- Molecule 63: 60S ribosomal protein L27-A



- Molecule 64: 60S ribosomal protein L28



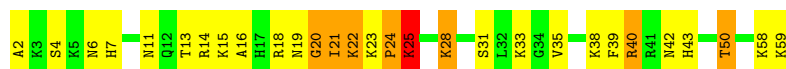
- Molecule 64: 60S ribosomal protein L28





- Molecule 65: 60S ribosomal protein L29

Chain N9: 50% 36% 12% .



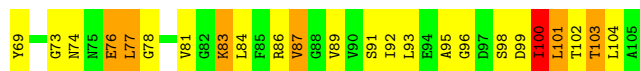
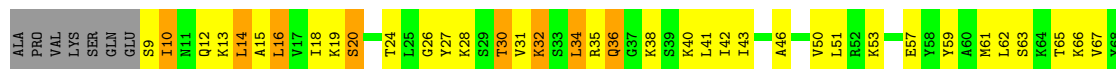
- Molecule 65: 60S ribosomal protein L29

Chain n9: 74% 22% . .



- Molecule 66: 60S ribosomal protein L30

Chain O0: 35% 44% 13% 7% . .



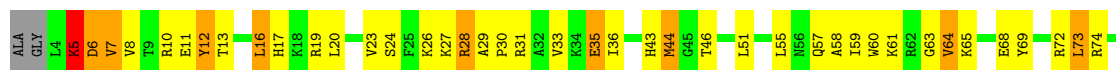
- Molecule 66: 60S ribosomal protein L30

Chain o0: 76% 20% .



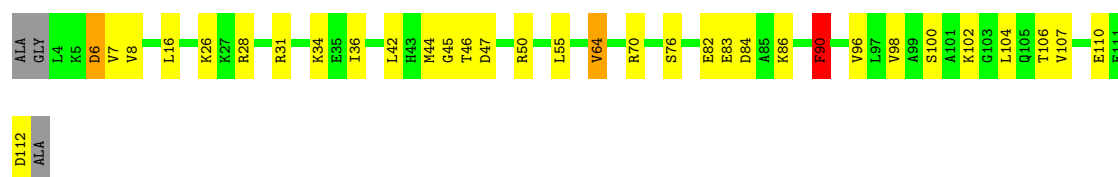
- Molecule 67: 60S ribosomal protein L31-A

Chain O1: 41% 44% 10% . . .



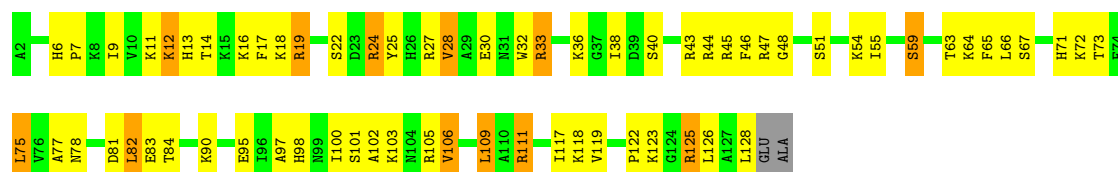
- Molecule 67: 60S ribosomal protein L31-A

Chain o1: 68% 27% . . .



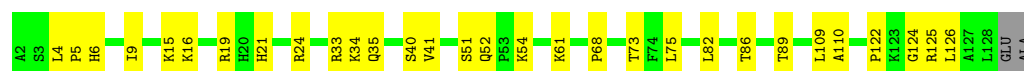
- Molecule 68: 60S ribosomal protein L32

Chain O2: 47% 43% 9%



- Molecule 68: 60S ribosomal protein L32

Chain o2: 75% 23%



- Molecule 69: 60S ribosomal protein L33-A

Chain O3: 44% 50% 6%



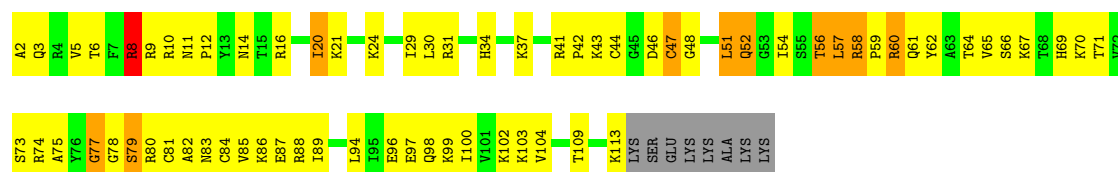
- Molecule 69: 60S ribosomal protein L33-A

Chain o3: 80% 18%




- Molecule 70: 60S ribosomal protein L34-A

Chain O4: 35% 49% 8% 7%



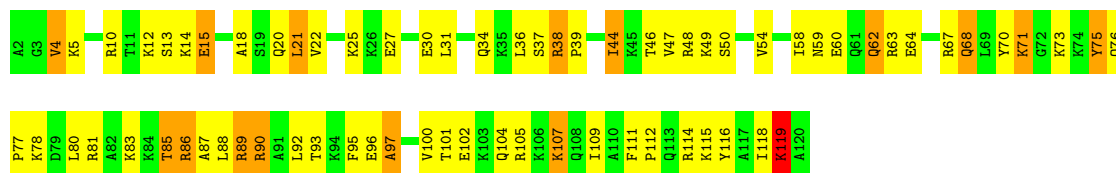
- Molecule 70: 60S ribosomal protein L34-A

Chain o4: 




- Molecule 71: 60S ribosomal protein L35-A

Chain O5: 



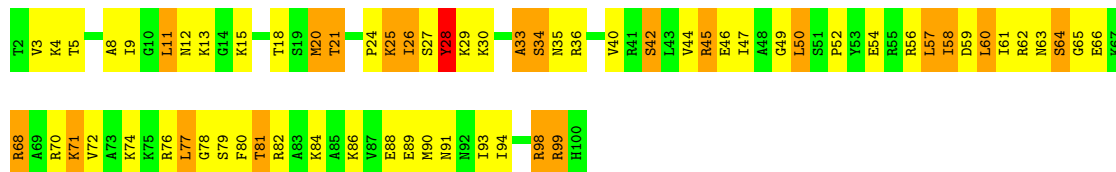
- Molecule 71: 60S ribosomal protein L35-A

Chain o5: 



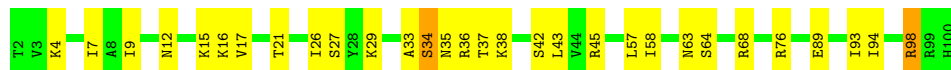
- Molecule 72: 60S ribosomal protein L36-A

Chain O6: 



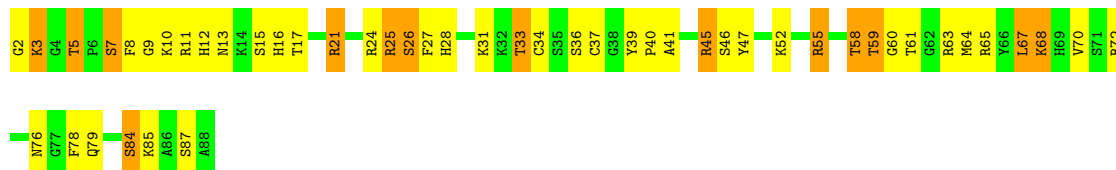
- Molecule 72: 60S ribosomal protein L36-A

Chain o6: 




- Molecule 73: 60S ribosomal protein L37-A

Chain O7: 



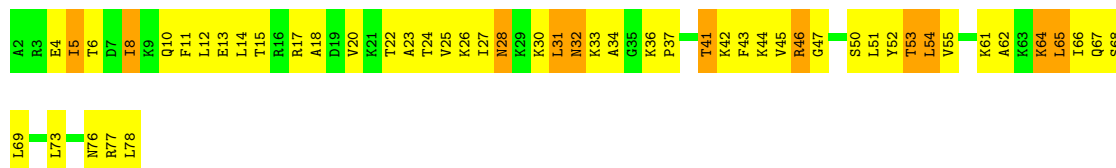
- Molecule 73: 60S ribosomal protein L37-A

Chain o7:  85% 14%



- Molecule 74: 60S ribosomal protein L38

Chain O8:  32% 53% 14%



- Molecule 74: 60S ribosomal protein L38

Chain o8:  70% 30%




- Molecule 75: 60S ribosomal protein L39

Chain O9:  40% 52% 8%



- Molecule 75: 60S ribosomal protein L39

Chain o9:  82% 18%




- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:  60% 27% 12%

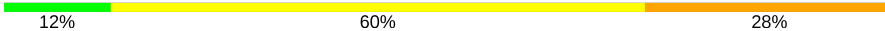


- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:  83% 15%



- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:  12% 60% 28%



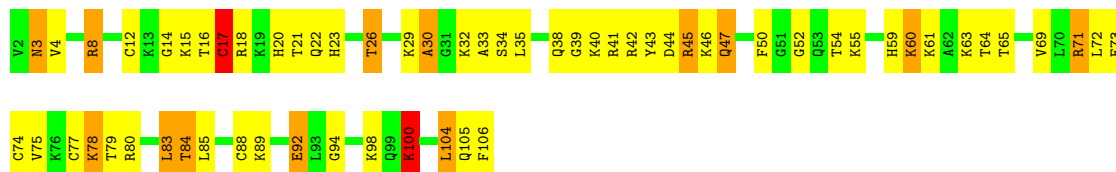
- Molecule 77: 60S ribosomal protein L41-A

Chain q1:  68% 32%




- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:  41% 45% 12%



- Molecule 78: 60S ribosomal protein L42-A

Chain q2:  80% 18%




- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:  46% 46% 8%



- Molecule 79: 60S ribosomal protein L43-A

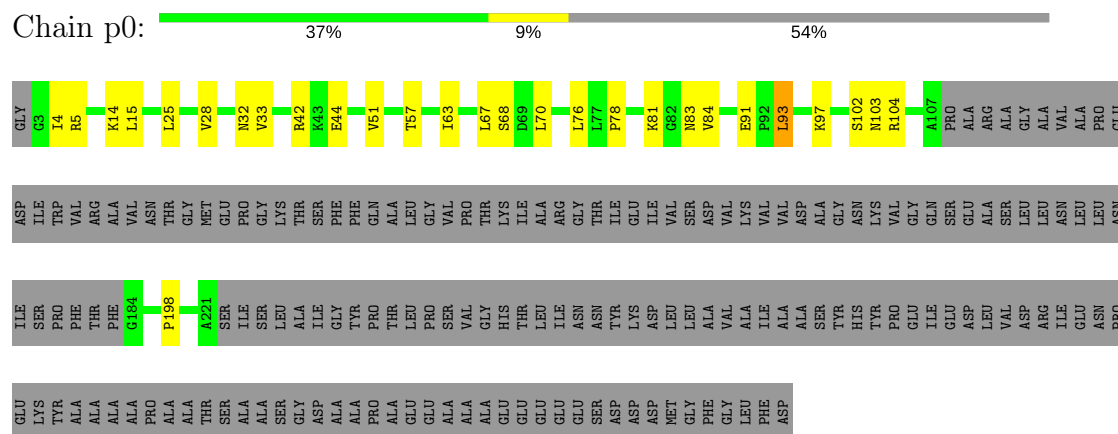
Chain q3:  80% 20%



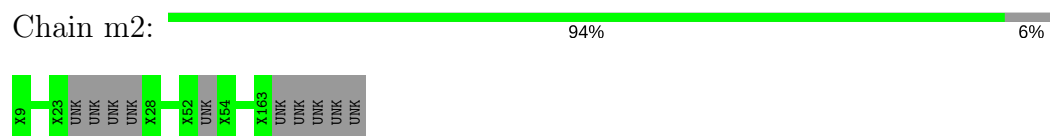
- Molecule 80: 40S ribosomal protein S30-A

Chain e0:  71% 27%

- Molecule 81: 60S acidic ribosomal protein P0



- Molecule 82: unknown protein chain m2



- Molecule 83: unknown protein chain p1



There are no outlier residues recorded for this chain.

- Molecule 84: unknown protein chain 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, α , β , γ	436.64Å 287.69Å 304.39Å 90.00° 98.98° 90.00°	Depositor
Resolution (Å)	300.66 – 3.10	Depositor
% Data completeness (in resolution range)	98.7 (300.66-3.10)	Depositor
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.198 , 0.247	Depositor
Wilson B-factor (Å ²)	71.8	Xtriage
Anisotropy	0.204	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411881	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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, ZBA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2	0.68	3/42442 (0.0%)	1.27	308/66130 (0.5%)
1	6	0.78	10/42765 (0.0%)	1.34	367/66634 (0.6%)
2	S0	0.43	0/1617	0.65	0/2215
2	s0	0.49	0/1623	0.71	0/2222
3	S1	0.38	0/1735	0.65	1/2335 (0.0%)
3	s1	0.49	0/1748	0.69	0/2352
4	S2	0.48	0/1665	0.68	0/2263
4	s2	0.51	0/1665	0.73	1/2263 (0.0%)
5	S3	0.45	0/1759	0.64	0/2368
5	s3	0.47	0/1759	0.62	0/2368
6	S4	0.47	0/2109	0.69	1/2839 (0.0%)
6	s4	0.50	0/2109	0.71	1/2839 (0.0%)
7	S5	0.40	0/1629	0.61	0/2202
7	s5	0.45	0/1629	0.65	0/2202
8	S6	0.45	0/1823	0.64	1/2439 (0.0%)
8	s6	0.49	0/1779	0.68	0/2379
9	S7	0.39	0/1506	0.64	0/2028
9	s7	0.45	0/1516	0.71	2/2043 (0.1%)
10	S8	0.52	0/1514	0.70	1/2021 (0.0%)
10	s8	0.56	0/1514	0.76	2/2021 (0.1%)
11	S9	0.44	0/1519	0.64	0/2035
11	s9	0.53	0/1519	0.74	0/2035
12	C0	0.45	0/790	0.73	3/1069 (0.3%)
12	c0	0.39	0/777	0.65	3/1049 (0.3%)
13	C1	0.52	0/1240	0.68	0/1675
13	c1	0.57	0/1194	0.75	2/1610 (0.1%)
14	C2	0.37	0/900	0.66	1/1224 (0.1%)
14	c2	0.30	0/900	0.61	1/1224 (0.1%)
15	C3	0.48	0/1215	0.68	2/1638 (0.1%)
15	c3	0.57	0/1215	0.73	0/1638
16	C4	0.37	0/901	0.66	0/1217
16	c4	0.47	0/960	0.73	1/1290 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.47	0/998	0.69	0/1341
17	c5	0.45	0/1060	0.68	1/1426 (0.1%)
18	C6	0.46	0/1125	0.72	3/1510 (0.2%)
18	c6	0.49	0/1131	0.70	0/1518
19	C7	0.45	0/935	0.66	0/1254
19	c7	0.47	0/914	0.67	0/1224
20	C8	0.47	0/1211	0.64	0/1628
20	c8	0.51	0/1211	0.69	1/1628 (0.1%)
21	C9	0.45	0/1130	0.62	0/1517
21	c9	0.49	0/1130	0.67	1/1517 (0.1%)
22	D0	0.41	0/865	0.67	0/1169
22	d0	0.44	0/892	0.66	0/1205
23	D1	0.45	0/693	0.65	0/935
23	d1	0.53	0/693	0.73	0/935
24	D2	0.49	0/1038	0.72	2/1395 (0.1%)
24	d2	0.58	0/1038	0.74	0/1395
25	D3	0.61	0/1139	0.77	1/1518 (0.1%)
25	d3	0.63	0/1139	0.77	1/1518 (0.1%)
26	D4	0.43	0/1087	0.61	0/1449
26	d4	0.47	0/1087	0.68	0/1449
27	D5	0.40	0/571	0.72	0/768
27	d5	0.40	0/566	0.65	0/761
28	D6	0.44	0/782	0.66	0/1047
28	d6	0.56	0/782	0.69	0/1047
29	D7	0.43	0/620	0.65	0/838
29	d7	0.49	0/620	0.70	0/838
30	D8	0.37	0/499	0.58	0/670
30	d8	0.42	0/499	0.65	0/670
31	D9	0.55	0/452	0.69	1/600 (0.2%)
31	d9	0.54	0/452	0.75	0/600
32	E0	0.43	0/483	0.61	0/643
33	E1	0.43	0/577	0.78	0/770
33	e1	0.42	0/619	0.75	0/822
34	SR	0.39	0/2494	0.59	0/3393
34	sR	0.39	0/2495	0.58	0/3395
35	SM	0.47	0/1113	0.68	2/1502 (0.1%)
35	sM	0.47	0/683	0.66	1/923 (0.1%)
36	1	1.00	50/75394 (0.1%)	1.56	1409/117545 (1.2%)
36	5	1.02	57/75414 (0.1%)	1.57	1376/117575 (1.2%)
37	3	0.82	0/2883	1.31	19/4491 (0.4%)
37	7	0.99	2/2883 (0.1%)	1.51	45/4491 (1.0%)
38	4	0.94	1/3746 (0.0%)	1.48	50/5832 (0.9%)
38	8	0.90	0/3746	1.44	40/5832 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.64	0/1948	0.85	1/2617 (0.0%)
39	l2	0.70	0/1946	0.88	4/2614 (0.2%)
40	L3	0.69	0/3146	0.81	0/4228
40	l3	0.76	0/3146	0.83	2/4228 (0.0%)
41	L4	0.73	1/2800 (0.0%)	0.88	8/3790 (0.2%)
41	l4	0.68	0/2800	0.81	2/3790 (0.1%)
42	L5	0.53	0/2425	0.66	1/3271 (0.0%)
42	l5	0.67	0/2408	0.75	1/3248 (0.0%)
43	L6	0.68	0/1260	0.79	0/1694
43	l6	0.70	0/1269	0.80	0/1705
44	L7	0.73	0/1821	0.84	0/2451
44	l7	0.77	0/1828	0.84	3/2461 (0.1%)
45	L8	0.51	0/1836	0.65	0/2481
45	l8	0.52	0/1795	0.67	2/2429 (0.1%)
46	L9	0.61	1/1539 (0.1%)	0.75	0/2073
46	l9	0.66	0/1539	0.77	0/2073
47	M0	0.63	0/1741	0.75	0/2335
47	m0	0.67	1/1758 (0.1%)	0.75	0/2358
48	M1	0.51	0/1374	0.72	1/1842 (0.1%)
48	m1	0.62	0/1374	0.80	3/1842 (0.2%)
49	M3	0.71	0/1568	0.81	2/2106 (0.1%)
49	m3	0.60	0/1573	0.82	0/2113
50	M4	0.68	0/1068	0.78	0/1438
50	m4	0.71	0/1074	0.79	2/1446 (0.1%)
51	M5	0.71	1/1757 (0.1%)	0.76	1/2354 (0.0%)
51	m5	0.63	0/1757	0.76	0/2354
52	M6	0.43	0/1585	0.60	1/2128 (0.0%)
52	m6	0.50	0/1585	0.64	0/2128
53	M7	0.72	0/1443	0.82	0/1944
53	m7	0.85	0/1250	0.86	1/1683 (0.1%)
54	M8	0.69	0/1465	0.86	2/1965 (0.1%)
54	m8	0.66	0/1465	0.86	0/1965
55	M9	0.58	0/1538	0.69	0/2050
55	m9	0.60	0/1538	0.71	0/2050
56	N0	0.69	0/1481	0.79	0/1990
56	n0	0.75	0/1481	0.85	1/1990 (0.1%)
57	N1	0.66	0/1300	0.75	0/1743
57	n1	0.78	2/1300 (0.2%)	0.80	0/1743
58	N2	0.43	0/812	0.61	0/1099
58	n2	0.46	0/794	0.65	0/1076
59	N3	0.68	0/1018	0.77	0/1369
59	n3	0.77	0/1018	0.82	0/1369
60	N4	0.51	0/712	0.67	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.61	0/1052	0.73	0/1398
61	N5	0.57	0/979	0.72	1/1321 (0.1%)
61	n5	0.57	0/974	0.74	1/1314 (0.1%)
62	N6	0.64	0/1004	0.83	2/1341 (0.1%)
62	n6	0.60	0/1004	0.80	2/1341 (0.1%)
63	N7	0.49	0/1118	0.68	0/1497
63	n7	0.47	0/1118	0.65	0/1497
64	N8	0.68	0/1204	0.81	1/1612 (0.1%)
64	n8	0.72	0/1204	0.85	1/1612 (0.1%)
65	N9	0.63	0/473	0.75	0/629
65	n9	0.70	0/473	0.90	2/629 (0.3%)
66	O0	0.50	0/751	0.65	0/1008
66	o0	0.52	0/775	0.68	0/1040
67	O1	0.61	0/890	0.75	0/1196
67	o1	0.65	0/897	0.84	2/1205 (0.2%)
68	O2	0.78	0/1041	0.85	0/1394
68	o2	0.75	0/1041	0.84	0/1394
69	O3	0.86	0/868	0.84	0/1168
69	o3	0.85	0/868	0.82	0/1168
70	O4	0.58	1/890 (0.1%)	0.81	3/1189 (0.3%)
70	o4	0.55	0/890	0.74	0/1189
71	O5	0.63	0/978	0.76	0/1301
71	o5	0.52	0/974	0.67	0/1297
72	O6	0.60	0/778	0.75	0/1034
72	o6	0.55	0/777	0.73	0/1033
73	O7	0.70	0/696	0.91	3/923 (0.3%)
73	o7	0.70	0/696	0.85	1/923 (0.1%)
74	O8	0.49	0/618	0.59	0/826
74	o8	0.44	0/614	0.63	0/822
75	O9	0.70	0/443	0.82	0/588
75	o9	0.61	0/443	0.81	0/588
76	Q0	0.61	0/423	0.79	2/562 (0.4%)
76	q0	0.75	0/423	0.83	0/562
77	Q1	0.60	0/234	0.98	1/300 (0.3%)
77	q1	0.63	0/234	0.87	0/300
78	Q2	0.79	1/860 (0.1%)	0.86	2/1136 (0.2%)
78	q2	0.73	1/860 (0.1%)	0.81	2/1136 (0.2%)
79	Q3	0.65	0/701	0.80	1/934 (0.1%)
79	q3	0.68	0/701	0.83	1/934 (0.1%)
80	e0	0.43	0/499	0.72	0/665
81	p0	0.44	0/1091	0.57	0/1472
All	All	0.80	132/430817 (0.0%)	1.24	3717/632520 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	S5	0	1
7	s5	0	2
9	S7	0	1
16	C4	0	2
16	c4	0	1
17	C5	0	1
17	c5	0	1
19	C7	0	1
20	c8	0	1
22	d0	0	1
27	D5	0	3
33	E1	0	2
33	e1	0	1
39	L2	0	1
39	l2	0	1
42	L5	0	1
42	l5	0	1
43	L6	0	2
43	l6	0	1
44	l7	0	2
49	m3	0	1
52	M6	0	1
52	m6	0	1
54	m8	0	1
56	n0	0	2
57	N1	0	1
63	n7	0	1
64	n8	0	2
65	N9	0	2
65	n9	0	2
67	O1	0	1
67	o1	0	2
68	o2	0	1
All	All	0	45

The worst 5 of 132 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	11.18	2.01	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1152	G	N9-C8	9.45	1.44	1.37
36	5	1152	G	N9-C4	-9.34	1.30	1.38
78	q2	17	CYS	CB-SG	9.32	1.98	1.82
36	1	2714	G	N9-C4	-7.82	1.31	1.38

The worst 5 of 3717 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-C5	22.88	140.04	128.60
36	5	1152	G	N3-C4-N9	-22.22	112.67	126.00
36	5	1152	G	C2-N3-C4	-17.60	103.10	111.90
1	6	1537	C	C6-N1-C2	-15.90	113.94	120.30
36	1	2714	G	N3-C4-C5	14.64	135.92	128.60

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
16	C4	124	ASP	Peptide
17	C5	99	GLY	Peptide
7	S5	99	MET	Peptide
9	S7	131	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37948	0	19093	903	0
1	6	38238	0	19240	868	0
2	S0	1577	0	1567	161	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	170	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	123	0
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	131	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	147	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	146	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	139	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	108	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	125	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	132	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	63	0
12	c0	762	0	699	0	0
13	C1	1214	0	1259	84	0
13	c1	1168	0	1231	0	0
14	C2	892	0	891	61	0
14	c2	892	0	891	0	0
15	C3	1192	0	1255	98	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	89	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	97	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	112	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	76	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	107	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	94	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	88	0
22	d0	882	0	939	0	0
23	D1	684	0	672	76	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	97	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	90	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	d4	1073	0	1132	0	0
27	D5	563	0	603	57	0
27	d5	558	0	598	0	0
28	D6	769	0	814	86	0
28	d6	769	0	814	0	0
29	D7	610	0	630	48	0
29	d7	610	0	631	0	0
30	D8	497	0	535	50	0
30	d8	497	0	535	0	0
31	D9	442	0	428	38	0
31	d9	442	0	428	0	0
32	E0	475	0	525	36	0
33	E1	566	0	601	64	0
33	e1	608	0	656	0	0
34	SR	2441	0	2397	164	0
34	sR	2442	0	2392	0	0
35	SM	1104	0	996	61	0
35	sM	680	0	607	0	0
36	1	67355	0	33845	1175	0
36	5	67376	0	33857	1235	0
37	3	2579	0	1304	53	0
37	7	2579	0	1303	40	0
38	4	3353	0	1695	52	0
38	8	3353	0	1695	63	0
39	L2	1914	0	1981	165	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	255	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	192	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	203	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	87	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	125	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	121	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	132	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1736	135	0
47	m0	1722	0	1755	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	M1	1353	0	1383	102	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	127	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	82	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	128	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	104	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	104	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	106	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	105	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	96	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	44	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	63	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	32	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	52	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	76	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	98	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	113	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	32	0
65	n9	462	0	491	0	0
66	O0	743	0	797	64	0
66	o0	767	0	816	0	0
67	O1	876	0	912	53	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	61	0
68	o2	1020	0	1090	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	O3	850	0	880	57	0
69	o3	850	0	879	0	0
70	O4	880	0	945	81	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	68	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	58	0
72	o6	770	0	846	0	0
73	O7	681	0	683	46	0
73	o7	681	0	683	0	0
74	O8	612	0	682	41	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	21	0
76	q0	417	0	455	0	0
77	Q1	233	0	284	38	0
77	q1	233	0	284	0	0
78	Q2	847	0	914	53	0
78	q2	847	0	914	0	0
79	Q3	694	0	734	52	0
79	q3	694	0	734	0	0
80	e0	491	0	542	0	0
81	p0	1076	0	1040	0	0
82	m2	750	0	175	0	0
83	p1	235	0	51	0	0
84	p2	230	0	51	0	0
85	1	465	0	0	0	0
85	2	126	0	0	0	0
85	3	14	0	0	0	0
85	4	22	0	0	0	0
85	5	504	0	0	0	0
85	6	147	0	0	0	0
85	7	17	0	0	0	0
85	8	12	0	0	0	0
85	L2	2	0	0	0	0
85	L3	3	0	0	0	0
85	L4	2	0	0	0	0
85	L5	1	0	0	0	0
85	L6	2	0	0	0	0
85	L7	4	0	0	0	0
85	L8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	M0	2	0	0	0	0
85	M1	1	0	0	0	0
85	M3	3	0	0	0	0
85	M4	1	0	0	0	0
85	M5	2	0	0	0	0
85	M6	1	0	0	0	0
85	M7	5	0	0	0	0
85	M9	1	0	0	0	0
85	N0	2	0	0	0	0
85	N3	3	0	0	0	0
85	N5	1	0	0	0	0
85	N6	1	0	0	0	0
85	N8	6	0	0	0	0
85	O3	1	0	0	0	0
85	O4	1	0	0	0	0
85	O7	1	0	0	0	0
85	Q2	1	0	0	0	0
85	S2	1	0	0	0	0
85	S8	1	0	0	0	0
85	SM	1	0	0	0	0
85	c1	2	0	0	0	0
85	c7	2	0	0	0	0
85	c8	2	0	0	0	0
85	d3	1	0	0	0	0
85	d4	1	0	0	0	0
85	d6	1	0	0	0	0
85	l2	1	0	0	0	0
85	l3	3	0	0	0	0
85	l4	1	0	0	0	0
85	l5	2	0	0	0	0
85	l7	1	0	0	0	0
85	m1	2	0	0	0	0
85	m5	5	0	0	0	0
85	m6	2	0	0	0	0
85	m7	4	0	0	0	0
85	n0	1	0	0	0	0
85	n3	2	0	0	0	0
85	n6	2	0	0	0	0
85	n8	3	0	0	0	0
85	n9	1	0	0	0	0
85	o0	1	0	0	0	0
85	o1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	o3	1	0	0	0	0
85	o4	1	0	0	0	0
85	q0	1	0	0	0	0
85	q3	2	0	0	0	0
85	s1	1	0	0	0	0
85	s8	2	0	0	0	0
85	sM	2	0	0	0	0
86	1	2422	0	0	167	0
86	2	1099	0	0	92	0
86	3	84	0	0	2	0
86	4	105	0	0	7	0
86	5	2478	0	0	207	0
86	6	1134	0	0	91	0
86	7	91	0	0	3	0
86	8	112	0	0	16	0
86	C1	7	0	0	1	0
86	C3	7	0	0	0	0
86	C5	7	0	0	2	0
86	C8	7	0	0	1	0
86	D9	7	0	0	0	0
86	L3	21	0	0	4	0
86	L4	7	0	0	1	0
86	M0	7	0	0	0	0
86	M5	7	0	0	1	0
86	M6	7	0	0	0	0
86	M7	14	0	0	2	0
86	M8	7	0	0	0	0
86	M9	7	0	0	1	0
86	N1	7	0	0	1	0
86	N9	7	0	0	0	0
86	O1	7	0	0	6	0
86	O2	7	0	0	1	0
86	O3	7	0	0	2	0
86	O7	14	0	0	4	0
86	Q2	7	0	0	1	0
86	S8	7	0	0	0	0
86	S9	7	0	0	1	0
86	SR	7	0	0	0	0
86	c3	7	0	0	0	0
86	c5	7	0	0	0	0
86	c8	7	0	0	0	0
86	d9	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	l3	14	0	0	0	0
86	l4	14	0	0	0	0
86	l5	21	0	0	0	0
86	l9	7	0	0	0	0
86	m0	14	0	0	0	0
86	m1	7	0	0	0	0
86	m4	7	0	0	0	0
86	m5	7	0	0	0	0
86	m7	7	0	0	0	0
86	n3	7	0	0	0	0
86	n5	7	0	0	0	0
86	n9	7	0	0	0	0
86	o2	7	0	0	0	0
86	o3	7	0	0	0	0
86	o7	7	0	0	0	0
86	q2	7	0	0	0	0
86	s1	7	0	0	0	0
86	s4	7	0	0	0	0
86	s8	7	0	0	0	0
86	sR	7	0	0	0	0
87	D6	1	0	0	0	0
87	D7	1	0	0	0	0
87	D9	1	0	0	0	0
87	E1	1	0	0	0	0
87	O7	1	0	0	0	0
87	Q0	1	0	0	0	0
87	Q2	1	0	0	0	0
87	Q3	1	0	0	0	0
87	d6	1	0	0	0	0
87	d7	1	0	0	0	0
87	d9	1	0	0	0	0
87	e1	1	0	0	0	0
87	o7	1	0	0	0	0
87	q0	1	0	0	0	0
87	q2	1	0	0	0	0
87	q3	1	0	0	0	0
88	1	33	0	32	2	0
88	5	33	0	32	3	0
All	All	411881	0	297678	9763	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 9763 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L3:41:VAL:HA	40:L3:185:GLY:HA3	1.40	1.01
36:5:3274:A:H3'	36:5:3275:U:H5''	1.43	0.99
79:Q3:46:THR:HB	79:Q3:58:SER:HB2	1.45	0.99
50:M4:55:ARG:NH2	50:M4:76:ALA:O	2.31	0.98
40:L3:25:ILE:H	40:L3:25:ILE:HD13	1.29	0.96

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	151 (74%)	32 (16%)	21 (10%)	0	3
2	s0	204/251 (81%)	152 (74%)	34 (17%)	18 (9%)	1	5
3	S1	212/254 (84%)	140 (66%)	34 (16%)	38 (18%)	0	0
3	s1	214/254 (84%)	168 (78%)	31 (14%)	15 (7%)	1	8
4	S2	215/253 (85%)	169 (79%)	31 (14%)	15 (7%)	1	8
4	s2	215/253 (85%)	173 (80%)	30 (14%)	12 (6%)	2	12
5	S3	221/239 (92%)	181 (82%)	25 (11%)	15 (7%)	1	8
5	s3	221/239 (92%)	178 (80%)	24 (11%)	19 (9%)	1	5
6	S4	258/260 (99%)	224 (87%)	23 (9%)	11 (4%)	3	18
6	s4	258/260 (99%)	220 (85%)	21 (8%)	17 (7%)	1	9
7	S5	204/224 (91%)	162 (79%)	25 (12%)	17 (8%)	1	6
7	s5	204/224 (91%)	152 (74%)	38 (19%)	14 (7%)	1	8
8	S6	224/236 (95%)	189 (84%)	23 (10%)	12 (5%)	2	14
8	s6	216/236 (92%)	179 (83%)	28 (13%)	9 (4%)	3	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	S7	182/189 (96%)	135 (74%)	30 (16%)	17 (9%)	1	4
9	s7	184/189 (97%)	148 (80%)	21 (11%)	15 (8%)	1	6
10	S8	184/200 (92%)	155 (84%)	19 (10%)	10 (5%)	2	14
10	s8	184/200 (92%)	155 (84%)	20 (11%)	9 (5%)	2	16
11	S9	183/196 (93%)	145 (79%)	28 (15%)	10 (6%)	2	13
11	s9	183/196 (93%)	142 (78%)	32 (18%)	9 (5%)	2	16
12	C0	94/105 (90%)	71 (76%)	16 (17%)	7 (7%)	1	7
12	c0	92/105 (88%)	63 (68%)	13 (14%)	16 (17%)	0	0
13	C1	153/155 (99%)	126 (82%)	18 (12%)	9 (6%)	2	12
13	c1	144/155 (93%)	122 (85%)	14 (10%)	8 (6%)	2	12
14	C2	122/142 (86%)	69 (57%)	34 (28%)	19 (16%)	0	0
14	c2	122/142 (86%)	66 (54%)	34 (28%)	22 (18%)	0	0
15	C3	148/150 (99%)	122 (82%)	15 (10%)	11 (7%)	1	7
15	c3	148/150 (99%)	121 (82%)	17 (12%)	10 (7%)	1	8
16	C4	125/136 (92%)	86 (69%)	26 (21%)	13 (10%)	0	3
16	c4	126/136 (93%)	99 (79%)	18 (14%)	9 (7%)	1	8
17	C5	122/141 (86%)	88 (72%)	22 (18%)	12 (10%)	1	4
17	c5	133/141 (94%)	94 (71%)	23 (17%)	16 (12%)	0	2
18	C6	139/142 (98%)	115 (83%)	13 (9%)	11 (8%)	1	6
18	c6	140/142 (99%)	116 (83%)	16 (11%)	8 (6%)	2	12
19	C7	116/136 (85%)	89 (77%)	20 (17%)	7 (6%)	2	11
19	c7	113/136 (83%)	87 (77%)	16 (14%)	10 (9%)	1	5
20	C8	143/145 (99%)	117 (82%)	13 (9%)	13 (9%)	1	4
20	c8	143/145 (99%)	117 (82%)	17 (12%)	9 (6%)	1	10
21	C9	141/143 (99%)	116 (82%)	19 (14%)	6 (4%)	3	18
21	c9	141/143 (99%)	115 (82%)	19 (14%)	7 (5%)	2	16
22	D0	105/120 (88%)	83 (79%)	16 (15%)	6 (6%)	2	12
22	d0	108/120 (90%)	89 (82%)	11 (10%)	8 (7%)	1	7
23	D1	85/87 (98%)	60 (71%)	18 (21%)	7 (8%)	1	6
23	d1	85/87 (98%)	73 (86%)	7 (8%)	5 (6%)	2	12
24	D2	127/129 (98%)	109 (86%)	15 (12%)	3 (2%)	7	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	d2	127/129 (98%)	108 (85%)	15 (12%)	4 (3%)	5	26
25	D3	142/144 (99%)	109 (77%)	23 (16%)	10 (7%)	1	8
25	d3	142/144 (99%)	118 (83%)	17 (12%)	7 (5%)	2	16
26	D4	132/134 (98%)	107 (81%)	16 (12%)	9 (7%)	1	8
26	d4	132/134 (98%)	106 (80%)	14 (11%)	12 (9%)	1	4
27	D5	68/107 (64%)	46 (68%)	11 (16%)	11 (16%)	0	0
27	d5	67/107 (63%)	51 (76%)	12 (18%)	4 (6%)	2	11
28	D6	95/97 (98%)	65 (68%)	15 (16%)	15 (16%)	0	0
28	d6	95/97 (98%)	73 (77%)	16 (17%)	6 (6%)	1	10
29	D7	79/81 (98%)	62 (78%)	13 (16%)	4 (5%)	2	15
29	d7	79/81 (98%)	61 (77%)	9 (11%)	9 (11%)	0	2
30	D8	61/66 (92%)	47 (77%)	11 (18%)	3 (5%)	2	16
30	d8	61/66 (92%)	42 (69%)	13 (21%)	6 (10%)	1	4
31	D9	51/55 (93%)	44 (86%)	7 (14%)	0	100	100
31	d9	51/55 (93%)	43 (84%)	3 (6%)	5 (10%)	1	4
32	E0	58/60 (97%)	47 (81%)	7 (12%)	4 (7%)	1	8
33	E1	69/76 (91%)	37 (54%)	17 (25%)	15 (22%)	0	0
33	e1	74/76 (97%)	38 (51%)	16 (22%)	20 (27%)	0	0
34	SR	316/318 (99%)	267 (84%)	42 (13%)	7 (2%)	8	35
34	sR	316/318 (99%)	264 (84%)	41 (13%)	11 (4%)	4	23
35	SM	155/273 (57%)	106 (68%)	21 (14%)	28 (18%)	0	0
35	sM	98/273 (36%)	60 (61%)	27 (28%)	11 (11%)	0	2
39	L2	250/253 (99%)	211 (84%)	26 (10%)	13 (5%)	2	14
39	l2	250/253 (99%)	210 (84%)	26 (10%)	14 (6%)	2	12
40	L3	384/386 (100%)	328 (85%)	41 (11%)	15 (4%)	3	21
40	l3	384/386 (100%)	338 (88%)	37 (10%)	9 (2%)	7	33
41	L4	359/361 (99%)	289 (80%)	49 (14%)	21 (6%)	2	12
41	l4	359/361 (99%)	298 (83%)	43 (12%)	18 (5%)	2	16
42	L5	294/296 (99%)	241 (82%)	35 (12%)	18 (6%)	2	11
42	l5	292/296 (99%)	257 (88%)	26 (9%)	9 (3%)	5	26
43	L6	152/175 (87%)	135 (89%)	10 (7%)	7 (5%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	l6	153/175 (87%)	133 (87%)	16 (10%)	4 (3%)	6	31
44	L7	220/243 (90%)	196 (89%)	17 (8%)	7 (3%)	5	25
44	l7	221/243 (91%)	194 (88%)	20 (9%)	7 (3%)	5	25
45	L8	231/255 (91%)	190 (82%)	33 (14%)	8 (4%)	4	23
45	l8	229/255 (90%)	179 (78%)	36 (16%)	14 (6%)	2	11
46	L9	189/191 (99%)	164 (87%)	20 (11%)	5 (3%)	6	31
46	l9	189/191 (99%)	164 (87%)	18 (10%)	7 (4%)	4	22
47	M0	207/220 (94%)	169 (82%)	32 (16%)	6 (3%)	5	28
47	m0	209/220 (95%)	164 (78%)	34 (16%)	11 (5%)	2	14
48	M1	167/173 (96%)	125 (75%)	19 (11%)	23 (14%)	0	1
48	m1	167/173 (96%)	137 (82%)	18 (11%)	12 (7%)	1	7
49	M3	191/198 (96%)	155 (81%)	29 (15%)	7 (4%)	4	22
49	m3	192/198 (97%)	159 (83%)	22 (12%)	11 (6%)	2	12
50	M4	134/137 (98%)	114 (85%)	12 (9%)	8 (6%)	2	11
50	m4	135/137 (98%)	120 (89%)	12 (9%)	3 (2%)	8	35
51	M5	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	5	27
51	m5	201/203 (99%)	177 (88%)	15 (8%)	9 (4%)	3	17
52	M6	195/198 (98%)	172 (88%)	19 (10%)	4 (2%)	8	36
52	m6	195/198 (98%)	176 (90%)	15 (8%)	4 (2%)	8	36
53	M7	181/183 (99%)	154 (85%)	18 (10%)	9 (5%)	2	16
53	m7	153/183 (84%)	139 (91%)	11 (7%)	3 (2%)	9	37
54	M8	183/185 (99%)	158 (86%)	20 (11%)	5 (3%)	6	30
54	m8	183/185 (99%)	151 (82%)	24 (13%)	8 (4%)	3	18
55	M9	186/188 (99%)	165 (89%)	18 (10%)	3 (2%)	11	43
55	m9	186/188 (99%)	164 (88%)	17 (9%)	5 (3%)	6	30
56	N0	170/172 (99%)	155 (91%)	14 (8%)	1 (1%)	28	67
56	n0	170/172 (99%)	159 (94%)	9 (5%)	2 (1%)	15	51
57	N1	157/159 (99%)	135 (86%)	17 (11%)	5 (3%)	5	25
57	n1	157/159 (99%)	137 (87%)	16 (10%)	4 (2%)	6	31
58	N2	98/120 (82%)	77 (79%)	13 (13%)	8 (8%)	1	6
58	n2	96/120 (80%)	82 (85%)	11 (12%)	3 (3%)	5	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	N3	134/136 (98%)	121 (90%)	10 (8%)	3 (2%)	8	35
59	n3	134/136 (98%)	121 (90%)	12 (9%)	1 (1%)	25	64
60	N4	96/155 (62%)	75 (78%)	15 (16%)	6 (6%)	1	10
60	n4	133/155 (86%)	109 (82%)	15 (11%)	9 (7%)	1	8
61	N5	119/141 (84%)	107 (90%)	12 (10%)	0	100	100
61	n5	118/141 (84%)	96 (81%)	13 (11%)	9 (8%)	1	6
62	N6	124/126 (98%)	114 (92%)	6 (5%)	4 (3%)	5	25
62	n6	124/126 (98%)	105 (85%)	12 (10%)	7 (6%)	2	12
63	N7	133/135 (98%)	98 (74%)	24 (18%)	11 (8%)	1	6
63	n7	133/135 (98%)	98 (74%)	22 (16%)	13 (10%)	1	4
64	N8	146/148 (99%)	121 (83%)	14 (10%)	11 (8%)	1	7
64	n8	146/148 (99%)	123 (84%)	18 (12%)	5 (3%)	4	24
65	N9	56/58 (97%)	46 (82%)	8 (14%)	2 (4%)	4	23
65	n9	56/58 (97%)	44 (79%)	9 (16%)	3 (5%)	2	14
66	O0	95/104 (91%)	81 (85%)	11 (12%)	3 (3%)	5	25
66	o0	98/104 (94%)	82 (84%)	14 (14%)	2 (2%)	9	37
67	O1	107/112 (96%)	94 (88%)	7 (6%)	6 (6%)	2	12
67	o1	107/112 (96%)	88 (82%)	12 (11%)	7 (6%)	1	9
68	O2	125/129 (97%)	109 (87%)	15 (12%)	1 (1%)	22	62
68	o2	125/129 (97%)	106 (85%)	11 (9%)	8 (6%)	1	9
69	O3	104/106 (98%)	96 (92%)	6 (6%)	2 (2%)	9	39
69	o3	104/106 (98%)	90 (86%)	10 (10%)	4 (4%)	4	22
70	O4	110/120 (92%)	100 (91%)	9 (8%)	1 (1%)	20	60
70	o4	110/120 (92%)	99 (90%)	9 (8%)	2 (2%)	10	40
71	O5	117/119 (98%)	100 (86%)	13 (11%)	4 (3%)	4	24
71	o5	117/119 (98%)	101 (86%)	14 (12%)	2 (2%)	11	42
72	O6	97/99 (98%)	74 (76%)	13 (13%)	10 (10%)	0	3
72	o6	97/99 (98%)	81 (84%)	10 (10%)	6 (6%)	2	10
73	O7	85/87 (98%)	74 (87%)	7 (8%)	4 (5%)	3	17
73	o7	85/87 (98%)	73 (86%)	10 (12%)	2 (2%)	7	32
74	O8	75/77 (97%)	66 (88%)	8 (11%)	1 (1%)	14	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	o8	75/77 (97%)	60 (80%)	11 (15%)	4 (5%)	2	14
75	O9	48/50 (96%)	40 (83%)	8 (17%)	0	100	100
75	o9	48/50 (96%)	45 (94%)	2 (4%)	1 (2%)	8	36
76	Q0	50/52 (96%)	44 (88%)	4 (8%)	2 (4%)	3	20
76	q0	50/52 (96%)	45 (90%)	3 (6%)	2 (4%)	3	20
77	Q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	3	18
77	q1	23/25 (92%)	19 (83%)	4 (17%)	0	100	100
78	Q2	103/105 (98%)	77 (75%)	18 (18%)	8 (8%)	1	6
78	q2	103/105 (98%)	93 (90%)	9 (9%)	1 (1%)	18	57
79	Q3	89/91 (98%)	76 (85%)	11 (12%)	2 (2%)	8	35
79	q3	89/91 (98%)	81 (91%)	6 (7%)	2 (2%)	8	35
80	e0	60/62 (97%)	44 (73%)	9 (15%)	7 (12%)	0	2
81	p0	139/311 (45%)	114 (82%)	20 (14%)	5 (4%)	4	23
All	All	22333/24143 (92%)	18335 (82%)	2722 (12%)	1276 (6%)	2	12

5 of 1276 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	39	ASN
2	S0	49	ASN
2	S0	66	ALA
2	S0	95	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/209 (78%)	134 (82%)	30 (18%)	2	9
2	s0	165/209 (79%)	135 (82%)	30 (18%)	2	9
3	S1	191/223 (86%)	156 (82%)	35 (18%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	s1	192/223 (86%)	154 (80%)	38 (20%)	1	6
4	S2	176/204 (86%)	132 (75%)	44 (25%)	1	2
4	s2	176/204 (86%)	136 (77%)	40 (23%)	1	4
5	S3	182/194 (94%)	149 (82%)	33 (18%)	2	9
5	s3	182/194 (94%)	141 (78%)	41 (22%)	1	4
6	S4	221/221 (100%)	178 (80%)	43 (20%)	1	7
6	s4	221/221 (100%)	183 (83%)	38 (17%)	2	11
7	S5	173/190 (91%)	136 (79%)	37 (21%)	1	5
7	s5	173/190 (91%)	142 (82%)	31 (18%)	2	9
8	S6	188/201 (94%)	151 (80%)	37 (20%)	1	6
8	s6	187/201 (93%)	153 (82%)	34 (18%)	2	9
9	S7	165/169 (98%)	138 (84%)	27 (16%)	2	12
9	s7	165/169 (98%)	130 (79%)	35 (21%)	1	5
10	S8	150/161 (93%)	126 (84%)	24 (16%)	3	12
10	s8	150/161 (93%)	129 (86%)	21 (14%)	4	18
11	S9	158/165 (96%)	124 (78%)	34 (22%)	1	5
11	s9	158/165 (96%)	121 (77%)	37 (23%)	1	3
12	C0	77/98 (79%)	61 (79%)	16 (21%)	1	6
12	c0	73/98 (74%)	60 (82%)	13 (18%)	2	9
13	C1	129/136 (95%)	108 (84%)	21 (16%)	3	12
13	c1	129/136 (95%)	102 (79%)	27 (21%)	1	6
14	C2	88/118 (75%)	63 (72%)	25 (28%)	0	1
14	c2	88/118 (75%)	59 (67%)	29 (33%)	0	0
15	C3	127/127 (100%)	102 (80%)	25 (20%)	1	6
15	c3	127/127 (100%)	104 (82%)	23 (18%)	2	9
16	C4	81/104 (78%)	57 (70%)	24 (30%)	0	1
16	c4	97/104 (93%)	78 (80%)	19 (20%)	1	7
17	C5	101/117 (86%)	81 (80%)	20 (20%)	1	6
17	c5	103/117 (88%)	85 (82%)	18 (18%)	2	10
18	C6	117/118 (99%)	94 (80%)	23 (20%)	1	6
18	c6	118/118 (100%)	94 (80%)	24 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	C7	94/124 (76%)	75 (80%)	19 (20%)	1	6
19	c7	92/124 (74%)	77 (84%)	15 (16%)	3	12
20	C8	128/128 (100%)	96 (75%)	32 (25%)	1	2
20	c8	128/128 (100%)	99 (77%)	29 (23%)	1	4
21	C9	115/115 (100%)	91 (79%)	24 (21%)	1	6
21	c9	115/115 (100%)	94 (82%)	21 (18%)	2	9
22	D0	100/113 (88%)	76 (76%)	24 (24%)	1	3
22	d0	103/113 (91%)	78 (76%)	25 (24%)	1	3
23	D1	74/74 (100%)	54 (73%)	20 (27%)	0	1
23	d1	74/74 (100%)	52 (70%)	22 (30%)	0	1
24	D2	110/110 (100%)	89 (81%)	21 (19%)	2	7
24	d2	110/110 (100%)	94 (86%)	16 (14%)	4	16
25	D3	119/119 (100%)	91 (76%)	28 (24%)	1	3
25	d3	119/119 (100%)	103 (87%)	16 (13%)	4	19
26	D4	112/112 (100%)	102 (91%)	10 (9%)	11	41
26	d4	112/112 (100%)	98 (88%)	14 (12%)	5	22
27	D5	61/88 (69%)	51 (84%)	10 (16%)	2	12
27	d5	61/88 (69%)	51 (84%)	10 (16%)	2	12
28	D6	83/83 (100%)	62 (75%)	21 (25%)	0	2
28	d6	83/83 (100%)	71 (86%)	12 (14%)	4	16
29	D7	70/70 (100%)	56 (80%)	14 (20%)	1	6
29	d7	70/70 (100%)	52 (74%)	18 (26%)	0	2
30	D8	56/59 (95%)	46 (82%)	10 (18%)	2	9
30	d8	56/59 (95%)	43 (77%)	13 (23%)	1	4
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2	11
31	d9	47/48 (98%)	40 (85%)	7 (15%)	3	15
32	E0	51/51 (100%)	39 (76%)	12 (24%)	1	3
33	E1	62/66 (94%)	42 (68%)	20 (32%)	0	0
33	e1	66/66 (100%)	47 (71%)	19 (29%)	0	1
34	SR	260/261 (100%)	219 (84%)	41 (16%)	3	13
34	sR	260/261 (100%)	231 (89%)	29 (11%)	7	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	SM	97/228 (42%)	78 (80%)	19 (20%)	1	7
35	sM	54/228 (24%)	44 (82%)	10 (18%)	2	8
39	L2	193/195 (99%)	156 (81%)	37 (19%)	1	7
39	l2	192/195 (98%)	145 (76%)	47 (24%)	1	3
40	L3	320/322 (99%)	250 (78%)	70 (22%)	1	5
40	l3	319/322 (99%)	248 (78%)	71 (22%)	1	4
41	L4	288/288 (100%)	224 (78%)	64 (22%)	1	4
41	l4	288/288 (100%)	231 (80%)	57 (20%)	1	6
42	L5	244/244 (100%)	197 (81%)	47 (19%)	1	7
42	l5	243/244 (100%)	191 (79%)	52 (21%)	1	5
43	L6	134/152 (88%)	106 (79%)	28 (21%)	1	6
43	l6	135/152 (89%)	113 (84%)	22 (16%)	3	12
44	L7	186/204 (91%)	162 (87%)	24 (13%)	5	21
44	l7	187/204 (92%)	161 (86%)	26 (14%)	4	18
45	L8	187/207 (90%)	152 (81%)	35 (19%)	2	8
45	l8	177/207 (86%)	148 (84%)	29 (16%)	2	12
46	L9	171/171 (100%)	132 (77%)	39 (23%)	1	4
46	l9	171/171 (100%)	134 (78%)	37 (22%)	1	5
47	M0	177/186 (95%)	139 (78%)	38 (22%)	1	5
47	m0	179/186 (96%)	144 (80%)	35 (20%)	1	7
48	M1	147/150 (98%)	119 (81%)	28 (19%)	2	7
48	m1	147/150 (98%)	112 (76%)	35 (24%)	1	3
49	M3	154/158 (98%)	127 (82%)	27 (18%)	2	10
49	m3	154/158 (98%)	123 (80%)	31 (20%)	1	6
50	M4	107/108 (99%)	89 (83%)	18 (17%)	2	11
50	m4	108/108 (100%)	91 (84%)	17 (16%)	3	13
51	M5	175/175 (100%)	146 (83%)	29 (17%)	2	11
51	m5	175/175 (100%)	139 (79%)	36 (21%)	1	6
52	M6	160/161 (99%)	142 (89%)	18 (11%)	7	28
52	m6	160/161 (99%)	131 (82%)	29 (18%)	2	9
53	M7	140/145 (97%)	115 (82%)	25 (18%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	m7	125/145 (86%)	106 (85%)	19 (15%)	3	14
54	M8	150/150 (100%)	119 (79%)	31 (21%)	1	6
54	m8	150/150 (100%)	122 (81%)	28 (19%)	2	8
55	M9	153/153 (100%)	134 (88%)	19 (12%)	5	23
55	m9	153/153 (100%)	115 (75%)	38 (25%)	1	2
56	N0	156/156 (100%)	123 (79%)	33 (21%)	1	5
56	n0	156/156 (100%)	123 (79%)	33 (21%)	1	5
57	N1	136/136 (100%)	111 (82%)	25 (18%)	2	9
57	n1	136/136 (100%)	112 (82%)	24 (18%)	2	10
58	N2	87/106 (82%)	73 (84%)	14 (16%)	3	12
58	n2	85/106 (80%)	67 (79%)	18 (21%)	1	5
59	N3	104/104 (100%)	90 (86%)	14 (14%)	4	19
59	n3	104/104 (100%)	95 (91%)	9 (9%)	12	43
60	N4	57/129 (44%)	49 (86%)	8 (14%)	4	18
60	n4	100/129 (78%)	89 (89%)	11 (11%)	7	30
61	N5	104/117 (89%)	81 (78%)	23 (22%)	1	4
61	n5	104/117 (89%)	85 (82%)	19 (18%)	2	9
62	N6	109/109 (100%)	86 (79%)	23 (21%)	1	5
62	n6	109/109 (100%)	73 (67%)	36 (33%)	0	0
63	N7	115/115 (100%)	91 (79%)	24 (21%)	1	6
63	n7	115/115 (100%)	87 (76%)	28 (24%)	1	3
64	N8	118/118 (100%)	101 (86%)	17 (14%)	4	16
64	n8	118/118 (100%)	91 (77%)	27 (23%)	1	4
65	N9	46/46 (100%)	37 (80%)	9 (20%)	1	7
65	n9	46/46 (100%)	34 (74%)	12 (26%)	0	2
66	O0	81/87 (93%)	65 (80%)	16 (20%)	1	6
66	o0	84/87 (97%)	65 (77%)	19 (23%)	1	4
67	O1	92/96 (96%)	71 (77%)	21 (23%)	1	4
67	o1	94/96 (98%)	67 (71%)	27 (29%)	0	1
68	O2	109/110 (99%)	91 (84%)	18 (16%)	2	12
68	o2	109/110 (99%)	88 (81%)	21 (19%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	O3	90/90 (100%)	82 (91%)	8 (9%)	11	41
69	o3	90/90 (100%)	71 (79%)	19 (21%)	1	5
70	O4	95/102 (93%)	80 (84%)	15 (16%)	3	13
70	o4	95/102 (93%)	76 (80%)	19 (20%)	1	6
71	O5	104/104 (100%)	80 (77%)	24 (23%)	1	4
71	o5	103/104 (99%)	80 (78%)	23 (22%)	1	4
72	O6	81/81 (100%)	57 (70%)	24 (30%)	0	1
72	o6	80/81 (99%)	54 (68%)	26 (32%)	0	0
73	O7	70/70 (100%)	58 (83%)	12 (17%)	2	11
73	o7	70/70 (100%)	59 (84%)	11 (16%)	3	13
74	O8	68/68 (100%)	50 (74%)	18 (26%)	0	1
74	o8	67/68 (98%)	48 (72%)	19 (28%)	0	1
75	O9	45/45 (100%)	39 (87%)	6 (13%)	4	20
75	o9	45/45 (100%)	37 (82%)	8 (18%)	2	9
76	Q0	47/47 (100%)	41 (87%)	6 (13%)	5	21
76	q0	47/47 (100%)	39 (83%)	8 (17%)	2	11
77	Q1	23/23 (100%)	16 (70%)	7 (30%)	0	1
77	q1	23/23 (100%)	15 (65%)	8 (35%)	0	0
78	Q2	90/90 (100%)	71 (79%)	19 (21%)	1	5
78	q2	90/90 (100%)	70 (78%)	20 (22%)	1	4
79	Q3	71/71 (100%)	61 (86%)	10 (14%)	4	18
79	q3	71/71 (100%)	56 (79%)	15 (21%)	1	5
80	e0	53/53 (100%)	41 (77%)	12 (23%)	1	4
81	p0	105/253 (42%)	81 (77%)	24 (23%)	1	4
All	All	18727/20241 (92%)	15046 (80%)	3681 (20%)	1	6

5 of 3681 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
70	O4	29	ILE
9	s7	35	LYS
65	n9	10	HIS
72	O6	60	LEU
3	s1	232	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
54	M8	145	ASN
65	N9	6	ASN
61	n5	111	ASN
56	N0	154	HIS
59	N3	98	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1777/1800 (98%)	496 (27%)	0
1	6	1792/1800 (99%)	470 (26%)	0
36	1	3145/3396 (92%)	697 (22%)	0
36	5	3145/3396 (92%)	693 (22%)	0
37	3	120/121 (99%)	17 (14%)	0
37	7	120/121 (99%)	18 (15%)	0
38	4	157/158 (99%)	38 (24%)	0
38	8	157/158 (99%)	35 (22%)	0
All	All	10413/10950 (95%)	2464 (23%)	0

5 of 2464 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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2558 ligands modelled in this entry, 1425 are monoatomic - leaving 1133 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	$\# Z > 2$
86	OHX	1	3860	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3861	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3862	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3863	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3864	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3865	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3866	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3867	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3868	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3869	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3870	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3871	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3872	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3880	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3888	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3889	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3890	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3891	-	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
86	OHX	1	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3934	-	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	$\# Z > 2$
86	OHX	1	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3977	-	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
86	OHX	1	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4020	-	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
86	OHX	1	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4063	-	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
86	OHX	1	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4106	-	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
86	OHX	1	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4149	-	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	$\# Z > 2$
86	OHX	1	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4192	-	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
86	OHX	1	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
88	ZBA	1	4206	85	34,36,36	1.20	1 (2%)	46,58,58	1.75	3 (6%)
86	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2054	-	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
86	OHX	2	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2097	-	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
86	OHX	2	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2140	-	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
86	OHX	2	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	214	-	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
86	OHX	3	215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	232	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	233	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	234	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	235	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	236	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	237	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3918	-	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
86	OHX	5	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3961	-	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	$\# Z > 2$
86	OHX	5	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4004	-	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
86	OHX	5	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4047	-	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
86	OHX	5	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4090	-	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
86	OHX	5	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4133	-	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
86	OHX	5	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4176	-	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
86	OHX	5	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4219	-	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
86	OHX	5	4220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4232	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4233	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4234	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4235	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4236	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4237	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4238	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4239	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4240	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4241	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4242	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4243	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4244	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4245	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4246	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4247	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4248	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4249	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4250	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4251	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4252	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4253	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4254	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4255	-	0,6,6	0.00	-	0,15,15	0.00	-
88	ZBA	5	4256	85	34,36,36	1.19	1 (2%)	46,58,58	1.74	5 (10%)
86	OHX	6	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2051	-	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
86	OHX	6	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2094	-	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
86	OHX	6	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2137	-	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
86	OHX	6	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2180	-	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
86	OHX	6	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2189	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	213	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	215	-	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
86	OHX	8	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	D9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	405	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	406	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	N1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	N9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	Q2	503	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	S8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	S9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c8	203	-	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
86	OHX	d9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	405	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	305	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l9	600	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m1	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m5	306	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m7	205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o7	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s1	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s4	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s8	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	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
86	OHX	1	3860	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3861	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3862	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3863	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3864	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3865	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3866	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3867	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3868	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3869	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3870	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3871	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3872	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3873	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3874	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3875	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3876	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3877	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3878	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3879	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3880	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3881	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3882	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3883	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3884	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3885	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3886	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3887	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3888	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3889	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3890	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3891	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3892	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3893	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3894	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3895	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3896	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3897	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3898	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3899	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3900	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3901	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3902	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3903	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3904	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3905	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3906	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3907	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3908	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3909	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3910	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3911	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3912	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3913	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3914	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3915	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3916	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3917	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3918	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3919	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3920	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3921	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3922	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3923	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3924	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3925	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3926	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3927	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3928	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3929	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3930	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3931	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3932	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3933	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3934	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3935	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3936	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3937	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3938	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3939	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3940	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3941	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3942	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3943	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3944	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3945	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3946	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3947	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3948	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3949	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3950	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3951	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3952	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3953	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3954	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3955	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3956	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3957	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3958	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3959	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3960	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3961	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3962	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3963	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3964	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3965	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3966	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3967	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3968	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3969	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3970	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3971	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3972	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3973	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3974	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3975	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3976	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3977	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3978	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3979	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3980	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3981	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3982	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3983	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3984	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3985	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3986	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3987	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3988	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3989	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3990	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3991	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3992	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3993	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3994	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3995	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3996	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3997	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3998	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3999	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4000	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4001	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4002	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4003	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4004	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4005	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4006	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4007	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4008	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4009	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4010	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4011	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4012	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4013	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4014	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4015	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4016	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4017	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4018	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4019	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4020	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4021	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4022	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4023	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4024	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4025	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4026	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4027	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4028	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4029	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4030	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4031	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4032	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4033	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4034	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4035	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4036	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4037	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4038	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4039	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4040	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4041	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4042	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4043	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4044	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4045	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4046	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4047	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4048	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4049	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4050	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4051	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4052	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4053	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4054	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4055	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4056	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4057	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4058	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4059	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4060	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4061	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4062	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4063	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4064	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4065	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4066	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4067	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4068	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4069	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4070	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4071	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4072	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4073	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4074	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4075	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4076	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4077	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4078	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4079	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4080	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4081	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4082	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4083	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4084	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4085	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4086	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4087	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4088	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4089	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4090	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4091	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4092	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4093	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4094	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4095	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4096	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4097	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4098	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4099	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4100	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4101	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4102	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4103	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4104	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4105	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4106	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4107	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4108	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4109	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4110	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4111	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4112	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4113	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4114	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4115	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4116	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4117	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4118	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4119	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4120	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4121	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4122	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4123	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4124	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4125	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4126	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4127	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4128	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4129	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4130	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4131	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4132	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4133	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4134	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4135	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4136	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4137	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4138	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4139	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4140	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4141	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4142	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4143	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4144	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4145	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4146	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4147	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4148	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4149	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4150	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4151	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4152	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4153	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4154	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4155	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4156	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4157	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4158	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4159	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4160	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4161	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4162	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4163	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4164	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4165	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4166	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4167	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4168	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4169	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4170	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4171	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4172	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4173	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4174	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4175	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4176	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4177	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4178	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4179	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4180	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4181	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4182	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4183	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4184	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4185	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4186	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4187	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4188	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4189	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4190	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4191	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4192	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4193	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4194	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4195	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4196	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4197	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4198	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4199	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4200	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4201	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4202	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4203	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4204	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4205	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	ZBA	1	4206	85	1/1/13/14	0/18/83/83	0/1/4/4
86	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2029	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2030	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2031	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2032	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2033	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2034	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2035	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2036	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2037	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2038	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2039	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2040	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2041	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2042	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2043	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2044	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2045	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2046	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2047	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2048	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2049	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2050	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2051	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2052	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2053	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2054	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2055	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2056	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2057	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2058	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2059	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2060	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2061	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2062	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2063	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2064	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2065	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2066	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2067	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2068	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2069	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2070	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2071	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2072	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2073	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2074	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2075	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2076	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2077	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2078	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2079	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2080	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2081	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2082	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2083	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2084	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2085	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2086	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2087	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2088	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2089	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2090	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2091	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2092	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2093	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2094	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2095	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2096	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2097	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2098	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2099	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2100	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2101	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2102	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2103	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2104	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2105	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2106	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2107	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2108	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2109	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2110	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2111	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2112	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2113	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2114	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2115	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2116	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2117	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2118	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2119	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2120	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2121	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2122	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2123	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2124	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2125	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2126	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2127	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2128	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2129	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2130	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2131	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2132	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2133	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2134	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2135	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2136	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2137	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2138	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2139	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2140	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2141	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2142	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2143	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2144	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2145	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2146	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2147	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2148	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2149	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2150	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2151	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2152	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2153	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2154	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2155	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2156	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2157	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2158	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2159	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2160	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2161	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2162	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2163	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2164	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2165	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2166	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2167	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2168	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2169	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2170	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2171	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2172	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2173	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2174	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2175	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2176	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2177	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2178	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2179	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2180	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2181	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2182	-	-	0/0/0/0	0/0/0/0
86	OHX	3	214	-	-	0/0/0/0	0/0/0/0
86	OHX	3	215	-	-	0/0/0/0	0/0/0/0
86	OHX	3	216	-	-	0/0/0/0	0/0/0/0
86	OHX	3	217	-	-	0/0/0/0	0/0/0/0
86	OHX	3	218	-	-	0/0/0/0	0/0/0/0
86	OHX	3	219	-	-	0/0/0/0	0/0/0/0
86	OHX	3	220	-	-	0/0/0/0	0/0/0/0
86	OHX	3	221	-	-	0/0/0/0	0/0/0/0
86	OHX	3	222	-	-	0/0/0/0	0/0/0/0
86	OHX	3	223	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	3	224	-	-	0/0/0/0	0/0/0/0
86	OHX	3	225	-	-	0/0/0/0	0/0/0/0
86	OHX	4	223	-	-	0/0/0/0	0/0/0/0
86	OHX	4	224	-	-	0/0/0/0	0/0/0/0
86	OHX	4	225	-	-	0/0/0/0	0/0/0/0
86	OHX	4	226	-	-	0/0/0/0	0/0/0/0
86	OHX	4	227	-	-	0/0/0/0	0/0/0/0
86	OHX	4	228	-	-	0/0/0/0	0/0/0/0
86	OHX	4	229	-	-	0/0/0/0	0/0/0/0
86	OHX	4	230	-	-	0/0/0/0	0/0/0/0
86	OHX	4	231	-	-	0/0/0/0	0/0/0/0
86	OHX	4	232	-	-	0/0/0/0	0/0/0/0
86	OHX	4	233	-	-	0/0/0/0	0/0/0/0
86	OHX	4	234	-	-	0/0/0/0	0/0/0/0
86	OHX	4	235	-	-	0/0/0/0	0/0/0/0
86	OHX	4	236	-	-	0/0/0/0	0/0/0/0
86	OHX	4	237	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3902	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3903	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3904	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3905	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3906	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3907	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3908	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3909	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3910	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3911	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3912	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3913	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3914	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3915	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3916	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3917	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3918	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3919	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3920	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3921	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3922	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3923	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3924	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3925	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3926	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3927	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3928	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3929	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3930	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3931	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3932	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3933	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3934	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3935	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3936	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3937	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3938	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3939	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3940	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3941	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3942	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3943	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3944	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3945	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3946	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3947	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3948	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3949	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3950	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3951	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3952	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3953	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3954	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3955	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3956	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3957	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3958	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3959	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3960	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3961	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3962	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3963	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3964	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3965	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3966	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3967	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3968	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3969	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3970	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3971	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3972	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3973	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3974	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3975	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3976	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3977	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3978	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3979	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3980	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3981	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3982	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3983	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3984	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3985	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3986	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3987	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3988	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3989	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3990	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3991	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3992	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3993	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3994	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3995	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3996	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3997	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3998	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3999	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4000	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4001	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4002	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4003	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4004	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4005	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4006	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4007	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4008	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4009	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4010	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4011	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4012	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4013	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4014	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4015	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4016	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4017	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4018	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4019	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4020	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4021	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4022	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4023	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4024	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4025	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4026	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4027	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4028	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4029	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4030	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4031	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4032	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4033	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4034	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4035	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4036	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4037	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4038	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4039	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4040	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4041	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4042	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4043	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4044	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4045	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4046	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4047	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4048	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4049	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4050	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4051	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4052	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4053	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4054	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4055	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4056	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4057	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4058	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4059	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4060	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4061	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4062	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4063	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4064	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4065	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4066	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4067	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4068	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4069	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4070	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4071	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4072	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4073	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4074	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4075	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4076	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4077	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4078	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4079	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4080	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4081	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4082	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4083	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4084	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4085	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4086	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4087	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4088	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4089	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4090	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4091	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4092	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4093	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4094	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4095	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4096	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4097	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4098	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4099	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4100	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4101	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4102	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4103	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4104	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4105	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4106	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4107	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4108	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4109	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4110	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4111	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4112	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4113	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4114	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4115	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4116	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4117	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4118	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4119	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4120	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4121	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4122	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4123	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4124	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4125	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4126	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4127	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4128	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4129	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4130	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4131	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4132	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4133	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4134	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4135	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4136	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4137	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4138	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4139	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4140	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4141	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4142	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4143	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4144	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4145	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4146	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4147	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4148	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4149	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4150	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4151	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4152	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4153	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4154	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4155	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4156	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4157	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4158	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4159	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4160	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4161	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4162	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4163	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4164	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4165	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4166	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4167	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4168	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4169	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4170	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4171	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4172	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4173	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4174	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4175	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4176	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4177	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4178	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4179	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4180	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4181	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4182	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4183	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4184	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4185	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4186	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4187	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4188	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4189	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4190	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4191	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4192	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4193	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4194	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4195	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4196	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4197	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4198	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4199	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4200	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4201	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4202	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4203	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4204	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4205	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4206	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4207	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4208	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4209	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4210	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4211	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4212	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4213	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4214	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4215	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4216	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4217	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4218	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4219	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4220	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4221	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4222	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4223	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4224	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4225	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4226	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4227	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4228	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4229	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4230	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4231	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4232	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4233	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4234	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4235	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4236	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4237	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4238	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4239	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4240	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4241	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4242	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4243	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4244	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4245	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4246	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4247	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4248	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4249	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4250	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4251	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4252	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4253	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4254	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4255	-	-	0/0/0/0	0/0/0/0
88	ZBA	5	4256	85	-	0/18/83/83	0/1/4/4
86	OHX	6	2046	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2047	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2049	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2050	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2051	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2052	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2053	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2054	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2055	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2056	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2057	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2058	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2059	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2060	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2061	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2062	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2063	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2064	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2065	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2066	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2067	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2068	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2069	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2070	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2071	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2072	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2073	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2074	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2075	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2076	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2077	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2078	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2079	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2080	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2081	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2082	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2083	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2084	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2085	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2086	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2087	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2088	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2089	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2090	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2091	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2092	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2093	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2094	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2095	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2096	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2097	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2098	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2099	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2100	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2101	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2102	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2103	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2104	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2105	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2106	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2107	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2108	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2109	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2110	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2111	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2112	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2113	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2114	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2115	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2116	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2117	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2118	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2119	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2120	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2121	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2122	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2123	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2124	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2125	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2126	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2127	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2128	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2129	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2130	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2131	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2132	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2133	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2134	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2135	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2136	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2137	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2138	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2139	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2140	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2141	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2142	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2143	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2144	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2145	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2146	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2147	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2148	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2149	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2150	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2151	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2152	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2153	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2154	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2155	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2156	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2157	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2158	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2159	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2160	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2161	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2162	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2163	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2164	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2165	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2166	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2167	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2168	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2169	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2170	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2171	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2172	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2173	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2174	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2175	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2176	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2177	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2178	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2179	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2180	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2181	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2182	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2183	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2184	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2185	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2186	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2187	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2188	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2189	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2190	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2191	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2192	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2193	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2194	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2195	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2196	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2197	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2198	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2199	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2200	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2201	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2202	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2203	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2204	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2205	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2206	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2207	-	-	0/0/0/0	0/0/0/0
86	OHX	7	217	-	-	0/0/0/0	0/0/0/0
86	OHX	7	218	-	-	0/0/0/0	0/0/0/0
86	OHX	7	219	-	-	0/0/0/0	0/0/0/0
86	OHX	7	220	-	-	0/0/0/0	0/0/0/0
86	OHX	7	221	-	-	0/0/0/0	0/0/0/0
86	OHX	7	222	-	-	0/0/0/0	0/0/0/0
86	OHX	7	223	-	-	0/0/0/0	0/0/0/0
86	OHX	7	224	-	-	0/0/0/0	0/0/0/0
86	OHX	7	225	-	-	0/0/0/0	0/0/0/0
86	OHX	7	226	-	-	0/0/0/0	0/0/0/0
86	OHX	7	227	-	-	0/0/0/0	0/0/0/0
86	OHX	7	228	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	7	229	-	-	0/0/0/0	0/0/0/0
86	OHX	8	213	-	-	0/0/0/0	0/0/0/0
86	OHX	8	214	-	-	0/0/0/0	0/0/0/0
86	OHX	8	215	-	-	0/0/0/0	0/0/0/0
86	OHX	8	216	-	-	0/0/0/0	0/0/0/0
86	OHX	8	217	-	-	0/0/0/0	0/0/0/0
86	OHX	8	218	-	-	0/0/0/0	0/0/0/0
86	OHX	8	219	-	-	0/0/0/0	0/0/0/0
86	OHX	8	220	-	-	0/0/0/0	0/0/0/0
86	OHX	8	221	-	-	0/0/0/0	0/0/0/0
86	OHX	8	222	-	-	0/0/0/0	0/0/0/0
86	OHX	8	223	-	-	0/0/0/0	0/0/0/0
86	OHX	8	224	-	-	0/0/0/0	0/0/0/0
86	OHX	8	225	-	-	0/0/0/0	0/0/0/0
86	OHX	8	226	-	-	0/0/0/0	0/0/0/0
86	OHX	8	227	-	-	0/0/0/0	0/0/0/0
86	OHX	8	228	-	-	0/0/0/0	0/0/0/0
86	OHX	C1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	D9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	404	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	405	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	406	-	-	0/0/0/0	0/0/0/0
86	OHX	L4	403	-	-	0/0/0/0	0/0/0/0
86	OHX	M0	303	-	-	0/0/0/0	0/0/0/0
86	OHX	M5	303	-	-	0/0/0/0	0/0/0/0
86	OHX	M6	202	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	206	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	207	-	-	0/0/0/0	0/0/0/0
86	OHX	M8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	M9	202	-	-	0/0/0/0	0/0/0/0
86	OHX	N1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	N9	101	-	-	0/0/0/0	0/0/0/0
86	OHX	O1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	O2	201	-	-	0/0/0/0	0/0/0/0
86	OHX	O3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	103	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	104	-	-	0/0/0/0	0/0/0/0
86	OHX	Q2	503	-	-	0/0/0/0	0/0/0/0
86	OHX	S8	302	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	S9	201	-	-	0/0/0/0	0/0/0/0
86	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
86	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c8	203	-	-	0/0/0/0	0/0/0/0
86	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	404	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	405	-	-	0/0/0/0	0/0/0/0
86	OHX	l4	402	-	-	0/0/0/0	0/0/0/0
86	OHX	l4	403	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	303	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	304	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	305	-	-	0/0/0/0	0/0/0/0
86	OHX	l9	600	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	301	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
86	OHX	m1	203	-	-	0/0/0/0	0/0/0/0
86	OHX	m4	201	-	-	0/0/0/0	0/0/0/0
86	OHX	m5	306	-	-	0/0/0/0	0/0/0/0
86	OHX	m7	205	-	-	0/0/0/0	0/0/0/0
86	OHX	n3	203	-	-	0/0/0/0	0/0/0/0
86	OHX	n5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	n9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	o2	201	-	-	0/0/0/0	0/0/0/0
86	OHX	o3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	o7	502	-	-	0/0/0/0	0/0/0/0
86	OHX	q2	502	-	-	0/0/0/0	0/0/0/0
86	OHX	s1	302	-	-	0/0/0/0	0/0/0/0
86	OHX	s4	301	-	-	0/0/0/0	0/0/0/0
86	OHX	s8	303	-	-	0/0/0/0	0/0/0/0
86	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4206	ZBA	C48-C46	6.36	1.51	1.33
88	5	4256	ZBA	C48-C46	6.42	1.51	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4206	ZBA	C45-C46-C48	-9.05	108.62	121.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	5	4256	ZBA	C45-C46-C48	-8.45	109.48	121.65
88	1	4206	ZBA	C47-C46-C48	-4.79	110.81	121.88
88	5	4256	ZBA	C47-C46-C48	-4.36	111.81	121.88
88	5	4256	ZBA	C47-C46-C45	-3.44	110.30	116.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
88	1	4206	ZBA	C35

There are no torsion outliers.

There are no ring outliers.

417 monomers are involved in 613 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3861	OHX	1	0
86	1	3862	OHX	1	0
86	1	3864	OHX	1	0
86	1	3865	OHX	2	0
86	1	3867	OHX	1	0
86	1	3869	OHX	1	0
86	1	3873	OHX	1	0
86	1	3876	OHX	1	0
86	1	3878	OHX	1	0
86	1	3879	OHX	2	0
86	1	3880	OHX	1	0
86	1	3884	OHX	1	0
86	1	3887	OHX	1	0
86	1	3891	OHX	1	0
86	1	3893	OHX	1	0
86	1	3895	OHX	1	0
86	1	3900	OHX	1	0
86	1	3906	OHX	2	0
86	1	3908	OHX	1	0
86	1	3909	OHX	2	0
86	1	3912	OHX	1	0
86	1	3921	OHX	2	0
86	1	3925	OHX	2	0
86	1	3927	OHX	2	0
86	1	3928	OHX	1	0
86	1	3934	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3940	OHX	1	0
86	1	3941	OHX	1	0
86	1	3945	OHX	1	0
86	1	3948	OHX	1	0
86	1	3951	OHX	1	0
86	1	3952	OHX	5	0
86	1	3953	OHX	1	0
86	1	3957	OHX	2	0
86	1	3958	OHX	1	0
86	1	3960	OHX	1	0
86	1	3962	OHX	1	0
86	1	3963	OHX	1	0
86	1	3966	OHX	6	0
86	1	3967	OHX	1	0
86	1	3970	OHX	3	0
86	1	3971	OHX	1	0
86	1	3974	OHX	1	0
86	1	3975	OHX	1	0
86	1	3976	OHX	2	0
86	1	3978	OHX	1	0
86	1	3981	OHX	1	0
86	1	3991	OHX	1	0
86	1	3995	OHX	1	0
86	1	3997	OHX	4	0
86	1	4002	OHX	1	0
86	1	4004	OHX	1	0
86	1	4007	OHX	1	0
86	1	4011	OHX	1	0
86	1	4013	OHX	1	0
86	1	4024	OHX	1	0
86	1	4026	OHX	5	0
86	1	4027	OHX	1	0
86	1	4028	OHX	1	0
86	1	4033	OHX	2	0
86	1	4035	OHX	1	0
86	1	4037	OHX	1	0
86	1	4038	OHX	2	0
86	1	4039	OHX	6	0
86	1	4041	OHX	2	0
86	1	4050	OHX	4	0
86	1	4051	OHX	2	0
86	1	4054	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	4056	OHX	1	0
86	1	4057	OHX	1	0
86	1	4060	OHX	1	0
86	1	4067	OHX	1	0
86	1	4068	OHX	1	0
86	1	4069	OHX	1	0
86	1	4073	OHX	1	0
86	1	4074	OHX	2	0
86	1	4078	OHX	1	0
86	1	4079	OHX	2	0
86	1	4081	OHX	1	0
86	1	4082	OHX	1	0
86	1	4089	OHX	1	0
86	1	4090	OHX	1	0
86	1	4092	OHX	1	0
86	1	4098	OHX	1	0
86	1	4103	OHX	2	0
86	1	4112	OHX	2	0
86	1	4114	OHX	1	0
86	1	4116	OHX	2	0
86	1	4119	OHX	1	0
86	1	4125	OHX	1	0
86	1	4126	OHX	2	0
86	1	4127	OHX	1	0
86	1	4129	OHX	1	0
86	1	4133	OHX	4	0
86	1	4136	OHX	1	0
86	1	4138	OHX	2	0
86	1	4141	OHX	1	0
86	1	4142	OHX	1	0
86	1	4145	OHX	1	0
86	1	4149	OHX	1	0
86	1	4150	OHX	3	0
86	1	4151	OHX	7	0
86	1	4154	OHX	1	0
86	1	4159	OHX	1	0
86	1	4160	OHX	1	0
86	1	4163	OHX	2	0
86	1	4167	OHX	4	0
86	1	4174	OHX	1	0
86	1	4176	OHX	5	0
86	1	4178	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	4190	OHX	1	0
86	1	4192	OHX	7	0
86	1	4193	OHX	1	0
86	1	4196	OHX	1	0
86	1	4200	OHX	1	0
88	1	4206	ZBA	2	0
86	2	2027	OHX	1	0
86	2	2029	OHX	2	0
86	2	2034	OHX	5	0
86	2	2035	OHX	1	0
86	2	2037	OHX	1	0
86	2	2039	OHX	1	0
86	2	2041	OHX	1	0
86	2	2042	OHX	2	0
86	2	2044	OHX	1	0
86	2	2045	OHX	1	0
86	2	2047	OHX	6	0
86	2	2048	OHX	2	0
86	2	2050	OHX	1	0
86	2	2053	OHX	1	0
86	2	2054	OHX	1	0
86	2	2056	OHX	1	0
86	2	2060	OHX	2	0
86	2	2061	OHX	1	0
86	2	2062	OHX	1	0
86	2	2067	OHX	1	0
86	2	2073	OHX	1	0
86	2	2074	OHX	1	0
86	2	2075	OHX	1	0
86	2	2076	OHX	1	0
86	2	2077	OHX	2	0
86	2	2079	OHX	1	0
86	2	2081	OHX	1	0
86	2	2085	OHX	1	0
86	2	2087	OHX	2	0
86	2	2089	OHX	1	0
86	2	2092	OHX	2	0
86	2	2093	OHX	5	0
86	2	2095	OHX	1	0
86	2	2096	OHX	1	0
86	2	2097	OHX	1	0
86	2	2098	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	2	2099	OHX	2	0
86	2	2101	OHX	7	0
86	2	2106	OHX	1	0
86	2	2107	OHX	1	0
86	2	2110	OHX	1	0
86	2	2111	OHX	1	0
86	2	2112	OHX	1	0
86	2	2113	OHX	2	0
86	2	2118	OHX	1	0
86	2	2119	OHX	1	0
86	2	2123	OHX	1	0
86	2	2125	OHX	1	0
86	2	2129	OHX	1	0
86	2	2132	OHX	1	0
86	2	2133	OHX	1	0
86	2	2134	OHX	6	0
86	2	2135	OHX	1	0
86	2	2138	OHX	1	0
86	2	2144	OHX	1	0
86	2	2148	OHX	2	0
86	2	2149	OHX	5	0
86	2	2151	OHX	1	0
86	2	2152	OHX	1	0
86	2	2157	OHX	2	0
86	2	2158	OHX	1	0
86	2	2160	OHX	4	0
86	2	2169	OHX	1	0
86	2	2175	OHX	1	0
86	3	217	OHX	1	0
86	3	220	OHX	1	0
86	4	224	OHX	1	0
86	4	225	OHX	1	0
86	4	226	OHX	1	0
86	4	228	OHX	1	0
86	4	229	OHX	1	0
86	4	233	OHX	2	0
86	5	3902	OHX	2	0
86	5	3904	OHX	1	0
86	5	3907	OHX	1	0
86	5	3908	OHX	1	0
86	5	3909	OHX	3	0
86	5	3911	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	3912	OHX	1	0
86	5	3913	OHX	2	0
86	5	3915	OHX	1	0
86	5	3918	OHX	1	0
86	5	3919	OHX	2	0
86	5	3920	OHX	1	0
86	5	3922	OHX	1	0
86	5	3924	OHX	1	0
86	5	3925	OHX	1	0
86	5	3926	OHX	1	0
86	5	3927	OHX	2	0
86	5	3933	OHX	1	0
86	5	3934	OHX	1	0
86	5	3935	OHX	1	0
86	5	3939	OHX	1	0
86	5	3942	OHX	1	0
86	5	3945	OHX	7	0
86	5	3948	OHX	1	0
86	5	3951	OHX	1	0
86	5	3956	OHX	3	0
86	5	3959	OHX	3	0
86	5	3960	OHX	1	0
86	5	3962	OHX	1	0
86	5	3964	OHX	5	0
86	5	3966	OHX	1	0
86	5	3968	OHX	1	0
86	5	3971	OHX	1	0
86	5	3974	OHX	2	0
86	5	3975	OHX	3	0
86	5	3976	OHX	1	0
86	5	3978	OHX	1	0
86	5	3980	OHX	9	0
86	5	3985	OHX	1	0
86	5	3986	OHX	2	0
86	5	3990	OHX	1	0
86	5	3992	OHX	1	0
86	5	3994	OHX	2	0
86	5	3999	OHX	1	0
86	5	4002	OHX	1	0
86	5	4004	OHX	7	0
86	5	4005	OHX	5	0
86	5	4006	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	4012	OHX	1	0
86	5	4014	OHX	6	0
86	5	4016	OHX	1	0
86	5	4017	OHX	1	0
86	5	4018	OHX	1	0
86	5	4024	OHX	6	0
86	5	4027	OHX	1	0
86	5	4028	OHX	1	0
86	5	4030	OHX	1	0
86	5	4031	OHX	1	0
86	5	4032	OHX	1	0
86	5	4035	OHX	1	0
86	5	4037	OHX	2	0
86	5	4038	OHX	1	0
86	5	4048	OHX	1	0
86	5	4049	OHX	1	0
86	5	4050	OHX	1	0
86	5	4054	OHX	1	0
86	5	4055	OHX	1	0
86	5	4059	OHX	6	0
86	5	4069	OHX	1	0
86	5	4070	OHX	2	0
86	5	4072	OHX	1	0
86	5	4076	OHX	1	0
86	5	4078	OHX	1	0
86	5	4080	OHX	1	0
86	5	4081	OHX	1	0
86	5	4083	OHX	1	0
86	5	4084	OHX	1	0
86	5	4085	OHX	3	0
86	5	4092	OHX	1	0
86	5	4093	OHX	7	0
86	5	4094	OHX	1	0
86	5	4095	OHX	2	0
86	5	4098	OHX	1	0
86	5	4101	OHX	1	0
86	5	4104	OHX	2	0
86	5	4107	OHX	2	0
86	5	4108	OHX	1	0
86	5	4112	OHX	1	0
86	5	4113	OHX	1	0
86	5	4121	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	4122	OHX	1	0
86	5	4132	OHX	1	0
86	5	4133	OHX	1	0
86	5	4140	OHX	2	0
86	5	4142	OHX	1	0
86	5	4143	OHX	1	0
86	5	4144	OHX	1	0
86	5	4145	OHX	1	0
86	5	4146	OHX	1	0
86	5	4149	OHX	1	0
86	5	4154	OHX	1	0
86	5	4155	OHX	1	0
86	5	4161	OHX	1	0
86	5	4162	OHX	1	0
86	5	4170	OHX	1	0
86	5	4175	OHX	2	0
86	5	4179	OHX	1	0
86	5	4180	OHX	1	0
86	5	4181	OHX	1	0
86	5	4182	OHX	1	0
86	5	4183	OHX	1	0
86	5	4185	OHX	1	0
86	5	4187	OHX	1	0
86	5	4188	OHX	2	0
86	5	4192	OHX	2	0
86	5	4194	OHX	2	0
86	5	4197	OHX	1	0
86	5	4200	OHX	1	0
86	5	4201	OHX	11	0
86	5	4202	OHX	7	0
86	5	4203	OHX	7	0
86	5	4204	OHX	2	0
86	5	4211	OHX	1	0
86	5	4220	OHX	6	0
86	5	4222	OHX	1	0
86	5	4227	OHX	1	0
86	5	4229	OHX	1	0
86	5	4231	OHX	1	0
86	5	4237	OHX	6	0
86	5	4239	OHX	2	0
86	5	4241	OHX	1	0
86	5	4243	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	4246	OHX	4	0
86	5	4250	OHX	1	0
86	5	4252	OHX	1	0
86	5	4253	OHX	1	0
88	5	4256	ZBA	3	0
86	6	2049	OHX	1	0
86	6	2054	OHX	1	0
86	6	2055	OHX	1	0
86	6	2056	OHX	1	0
86	6	2059	OHX	1	0
86	6	2060	OHX	5	0
86	6	2062	OHX	2	0
86	6	2066	OHX	1	0
86	6	2069	OHX	1	0
86	6	2071	OHX	1	0
86	6	2072	OHX	2	0
86	6	2074	OHX	2	0
86	6	2075	OHX	1	0
86	6	2080	OHX	1	0
86	6	2089	OHX	1	0
86	6	2090	OHX	1	0
86	6	2091	OHX	1	0
86	6	2093	OHX	1	0
86	6	2094	OHX	1	0
86	6	2096	OHX	1	0
86	6	2097	OHX	1	0
86	6	2101	OHX	3	0
86	6	2102	OHX	1	0
86	6	2103	OHX	2	0
86	6	2104	OHX	1	0
86	6	2106	OHX	1	0
86	6	2108	OHX	3	0
86	6	2109	OHX	2	0
86	6	2110	OHX	1	0
86	6	2112	OHX	1	0
86	6	2113	OHX	1	0
86	6	2115	OHX	2	0
86	6	2120	OHX	1	0
86	6	2121	OHX	7	0
86	6	2122	OHX	1	0
86	6	2124	OHX	2	0
86	6	2125	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	6	2127	OHX	3	0
86	6	2129	OHX	1	0
86	6	2131	OHX	3	0
86	6	2138	OHX	1	0
86	6	2139	OHX	1	0
86	6	2145	OHX	1	0
86	6	2148	OHX	1	0
86	6	2149	OHX	6	0
86	6	2151	OHX	1	0
86	6	2152	OHX	1	0
86	6	2153	OHX	1	0
86	6	2156	OHX	2	0
86	6	2161	OHX	1	0
86	6	2164	OHX	1	0
86	6	2165	OHX	1	0
86	6	2173	OHX	7	0
86	6	2177	OHX	1	0
86	6	2180	OHX	2	0
86	6	2181	OHX	1	0
86	6	2185	OHX	1	0
86	6	2189	OHX	1	0
86	6	2192	OHX	3	0
86	6	2193	OHX	1	0
86	6	2205	OHX	1	0
86	7	220	OHX	1	0
86	7	222	OHX	1	0
86	7	228	OHX	1	0
86	8	213	OHX	1	0
86	8	214	OHX	1	0
86	8	215	OHX	5	0
86	8	216	OHX	2	0
86	8	218	OHX	1	0
86	8	219	OHX	1	0
86	8	222	OHX	1	0
86	8	223	OHX	6	0
86	8	224	OHX	1	0
86	8	225	OHX	1	0
86	8	227	OHX	1	0
86	C1	201	OHX	1	0
86	C5	201	OHX	2	0
86	C8	201	OHX	1	0
86	L3	404	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	L3	405	OHX	1	0
86	L4	403	OHX	1	0
86	M5	303	OHX	1	0
86	M7	206	OHX	1	0
86	M7	207	OHX	1	0
86	M9	202	OHX	1	0
86	N1	201	OHX	1	0
86	O1	201	OHX	6	0
86	O2	201	OHX	1	0
86	O3	202	OHX	2	0
86	O7	103	OHX	4	0
86	Q2	503	OHX	1	0
86	S9	201	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
1	2	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1716:C	O3'	1717:G	P	4.21
1	2	1685:G	O3'	1686:C	P	2.96

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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