



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:59 PM GMT

PDB ID : 4U3M  
Title : Crystal structure of Anisomycin bound to the yeast 80S ribosome  
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.  
Deposited on : 2014-07-22  
Resolution : 3.00 Å(reported)

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

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

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

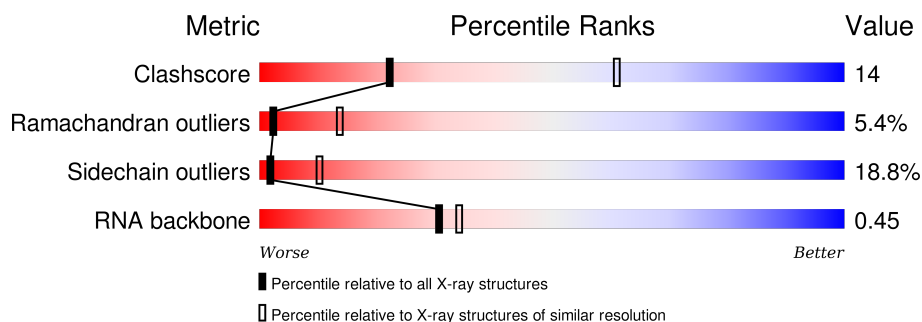
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

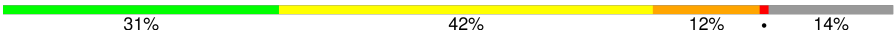





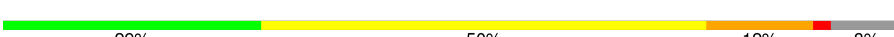

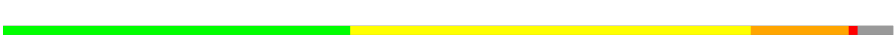

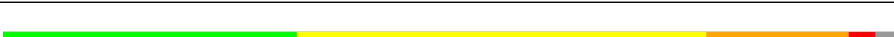


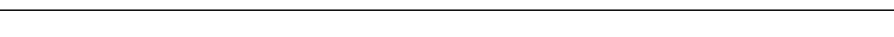
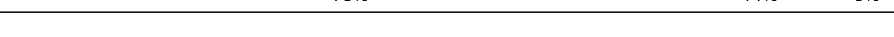
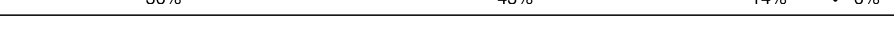



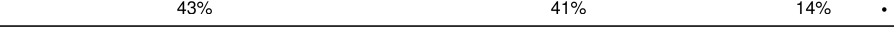

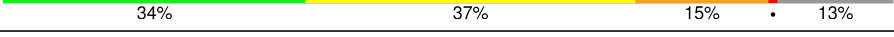



The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria.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

Note EDS failed to run properly.

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


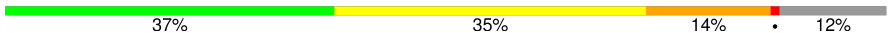



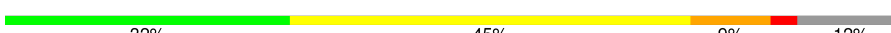





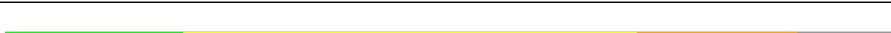













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Mol	Chain	Length	Quality of chain
4	S2	253	
4	s2	253	
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2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

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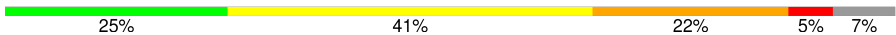
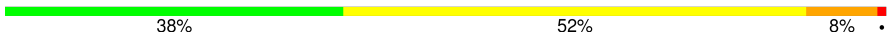



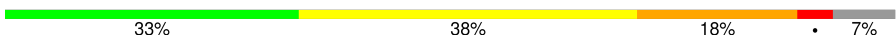
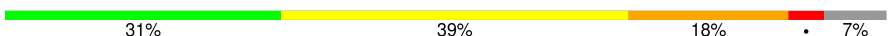











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Mol	Chain	Length	Quality of chain
16	c4	136	
17	C5	141	
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134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

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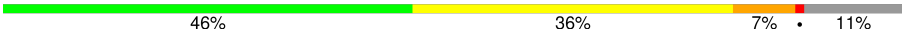



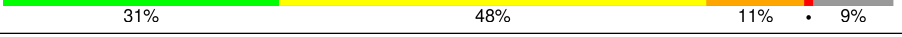


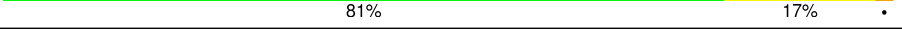

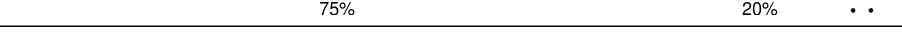
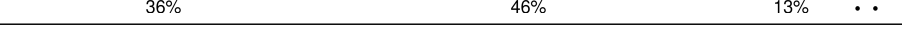

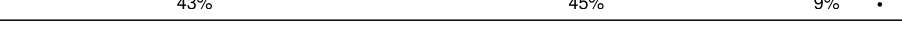


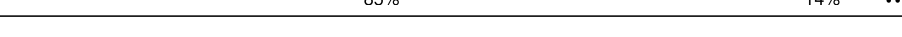

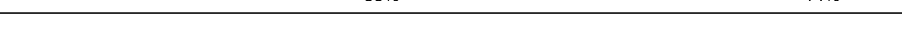








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Mol	Chain	Length	Quality of chain
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3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





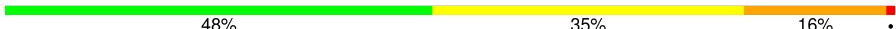

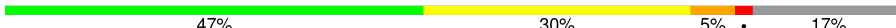



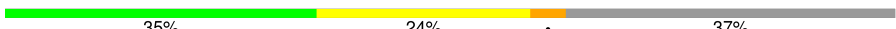

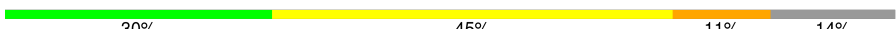



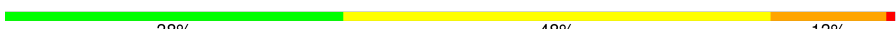





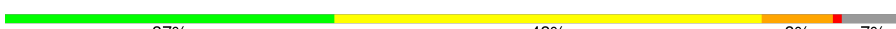


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Mol	Chain	Length	Quality of chain
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6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


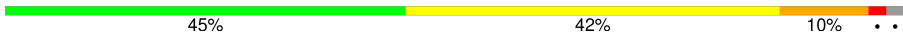









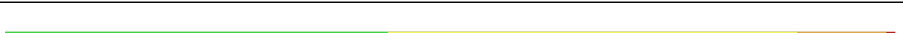








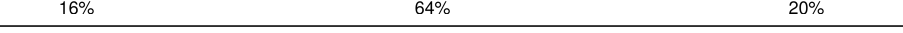




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Mol	Chain	Length	Quality of chain
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8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

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	OHX	1	3961	-	-	X	-
87	OHX	1	3963	-	-	X	-
87	OHX	1	3975	-	-	X	-
87	OHX	1	4007	-	-	X	-
87	OHX	1	4023	-	-	X	-
87	OHX	1	4032	-	-	X	-
87	OHX	1	4036	-	-	X	-
87	OHX	1	4047	-	-	X	-
87	OHX	1	4048	-	-	X	-
87	OHX	1	4059	-	-	X	-
87	OHX	1	4060	-	-	X	-
87	OHX	1	4061	-	-	X	-
87	OHX	1	4084	-	-	X	-
87	OHX	1	4088	-	-	X	-
87	OHX	1	4144	-	-	X	-
87	OHX	1	4151	-	-	X	-
87	OHX	1	4159	-	-	X	-
87	OHX	1	4161	-	-	X	-
87	OHX	1	4168	-	-	X	-
87	OHX	1	4177	-	-	X	-
87	OHX	1	4186	-	-	X	-
87	OHX	1	4203	-	-	X	-
87	OHX	2	2031	-	-	X	-
87	OHX	2	2044	-	-	X	-
87	OHX	2	2075	-	-	X	-
87	OHX	2	2089	-	-	X	-
87	OHX	2	2090	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	OHX	2	2095	-	-	X	-
87	OHX	2	2096	-	-	X	-
87	OHX	2	2099	-	-	X	-
87	OHX	2	2109	-	-	X	-
87	OHX	2	2116	-	-	X	-
87	OHX	2	2132	-	-	X	-
87	OHX	2	2147	-	-	X	-
87	OHX	2	2163	-	-	X	-
87	OHX	5	3947	-	-	X	-
87	OHX	5	3967	-	-	X	-
87	OHX	5	3978	-	-	X	-
87	OHX	5	3983	-	-	X	-
87	OHX	5	4005	-	-	X	-
87	OHX	5	4006	-	-	X	-
87	OHX	5	4016	-	-	X	-
87	OHX	5	4026	-	-	X	-
87	OHX	5	4041	-	-	X	-
87	OHX	5	4061	-	-	X	-
87	OHX	5	4072	-	-	X	-
87	OHX	5	4096	-	-	X	-
87	OHX	5	4101	-	-	X	-
87	OHX	5	4150	-	-	X	-
87	OHX	5	4200	-	-	X	-
87	OHX	5	4206	-	-	X	-
87	OHX	5	4207	-	-	X	-
87	OHX	5	4208	-	-	X	-
87	OHX	5	4211	-	-	X	-
87	OHX	5	4221	-	-	X	-
87	OHX	5	4224	-	-	X	-
87	OHX	5	4231	-	-	X	-
87	OHX	5	4241	-	-	X	-
87	OHX	5	4243	-	-	X	-
87	OHX	5	4245	-	-	X	-
87	OHX	5	4250	-	-	X	-
87	OHX	6	2057	-	-	X	-
87	OHX	6	2118	-	-	X	-
87	OHX	6	2123	-	-	X	-
87	OHX	6	2145	-	-	X	-
87	OHX	6	2169	-	-	X	-
87	OHX	7	217	-	-	X	-
87	OHX	7	224	-	-	X	-
87	OHX	8	214	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	OHX	8	221	-	-	X	-
87	OHX	8	222	-	-	X	-
87	OHX	L4	402	-	-	X	-
87	OHX	O1	202	-	-	X	-
87	OHX	O7	104	-	-	X	-
88	ZN	Q2	501	-	-	X	-

## 2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 411204 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 rRNA.

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C0	6	GLU	GLN	conflict	UNP P46784
C0	7	ASP	GLU	conflict	UNP P46784
C0	89	ALA	GLY	conflict	UNP P46784
c0	6	GLU	GLN	conflict	UNP P46784
c0	7	ASP	GLU	conflict	UNP P46784
c0	89	ALA	GLY	conflict	UNP P46784

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

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

- Molecule 36 is a RNA chain called 25s rRNA.

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 5.8s rRNA.

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 rRNA.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	12	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

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

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

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

- 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	S	0	0	0
			1420	882	281	257				
53	m7	155	Total	C	N	O	S	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	S	0	0	0
			1521	935	326	260				
55	m9	188	Total	C	N	O	S	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	n5	120	Total	C	N	O	S	0	0	0
			959	617	168	172	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 82 is a protein called UNKNOWN PROTEIN m2.

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

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

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

- Molecule 84 is a protein called UNKNOWN PROTEIN p1.

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

- Molecule 85 is a protein called UNKNOWN PROTEIN p2.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	L7	2	Total	Mg	0	0
			2	2		
86	n8	4	Total	Mg	0	0
			4	4		
86	o1	2	Total	Mg	0	0
			2	2		
86	N5	1	Total	Mg	0	0
			1	1		
86	6	145	Total	Mg	0	0
			145	145		
86	sM	2	Total	Mg	0	0
			2	2		
86	O4	1	Total	Mg	0	0
			1	1		
86	m5	4	Total	Mg	0	0
			4	4		
86	l3	2	Total	Mg	0	0
			2	2		
86	M1	1	Total	Mg	0	0
			1	1		
86	d6	1	Total	Mg	0	0
			1	1		
86	2	124	Total	Mg	0	0
			124	124		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	n0	2	Total 2	Mg 2	0	0
86	L4	1	Total 1	Mg 1	0	0
86	l7	1	Total 1	Mg 1	0	0
86	M5	2	Total 2	Mg 2	0	0
86	c9	1	Total 1	Mg 1	0	0
86	S2	2	Total 2	Mg 2	0	0
86	L8	1	Total 1	Mg 1	0	0
86	D3	1	Total 1	Mg 1	0	0
86	o4	1	Total 1	Mg 1	0	0
86	M9	1	Total 1	Mg 1	0	0
86	q0	1	Total 1	Mg 1	0	0
86	SM	1	Total 1	Mg 1	0	0
86	c8	1	Total 1	Mg 1	0	0
86	M0	2	Total 2	Mg 2	0	0
86	c1	2	Total 2	Mg 2	0	0
86	5	507	Total 507	Mg 507	0	0
86	L5	1	Total 1	Mg 1	0	0
86	O7	2	Total 2	Mg 2	0	0
86	Q2	1	Total 1	Mg 1	0	0
86	n9	1	Total 1	Mg 1	0	0
86	1	474	Total 474	Mg 474	0	0

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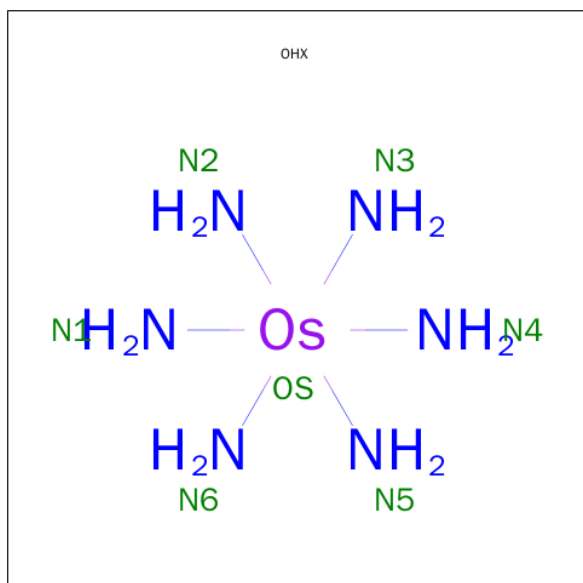
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	n6	2	Total 2	Mg 2	0	0
86	S8	1	Total 1	Mg 1	0	0
86	l2	2	Total 2	Mg 2	0	0
86	d3	2	Total 2	Mg 2	0	0
86	q3	1	Total 1	Mg 1	0	0
86	o3	1	Total 1	Mg 1	0	0
86	M3	3	Total 3	Mg 3	0	0
86	N3	3	Total 3	Mg 3	0	0
86	4	23	Total 23	Mg 23	0	0
86	L2	1	Total 1	Mg 1	0	0
86	m1	1	Total 1	Mg 1	0	0
86	l5	3	Total 3	Mg 3	0	0
86	m7	5	Total 5	Mg 5	0	0
86	M7	5	Total 5	Mg 5	0	0
86	N8	4	Total 4	Mg 4	0	0
86	s1	1	Total 1	Mg 1	0	0
86	m6	1	Total 1	Mg 1	0	0
86	O1	1	Total 1	Mg 1	0	0
86	s8	2	Total 2	Mg 2	0	0
86	c7	2	Total 2	Mg 2	0	0
86	7	15	Total 15	Mg 15	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	n3	2	Total 2	Mg 2	0	0
86	q1	1	Total 1	Mg 1	0	0
86	L3	2	Total 2	Mg 2	0	0
86	d4	1	Total 1	Mg 1	0	0
86	N6	1	Total 1	Mg 1	0	0
86	8	12	Total 12	Mg 12	0	0
86	14	1	Total 1	Mg 1	0	0
86	M6	1	Total 1	Mg 1	0	0
86	N0	1	Total 1	Mg 1	0	0
86	3	14	Total 14	Mg 14	0	0

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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			7	6	1		
87	4	1	Total	N	Os	0	0
			7	6	1		
87	4	1	Total	N	Os	0	0
			7	6	1		
87	L3	1	Total	N	Os	0	0
			7	6	1		
87	L3	1	Total	N	Os	0	0
			7	6	1		
87	L4	1	Total	N	Os	0	0
			7	6	1		
87	M0	1	Total	N	Os	0	0
			7	6	1		
87	M5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	M7	1	Total	N	Os	0	0
			7	6	1		
87	M7	1	Total	N	Os	0	0
			7	6	1		
87	M8	1	Total	N	Os	0	0
			7	6	1		
87	M9	1	Total	N	Os	0	0
			7	6	1		
87	N9	1	Total	N	Os	0	0
			7	6	1		
87	O1	1	Total	N	Os	0	0
			7	6	1		
87	O2	1	Total	N	Os	0	0
			7	6	1		
87	O3	1	Total	N	Os	0	0
			7	6	1		
87	O7	1	Total	N	Os	0	0
			7	6	1		
87	Q2	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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

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

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

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

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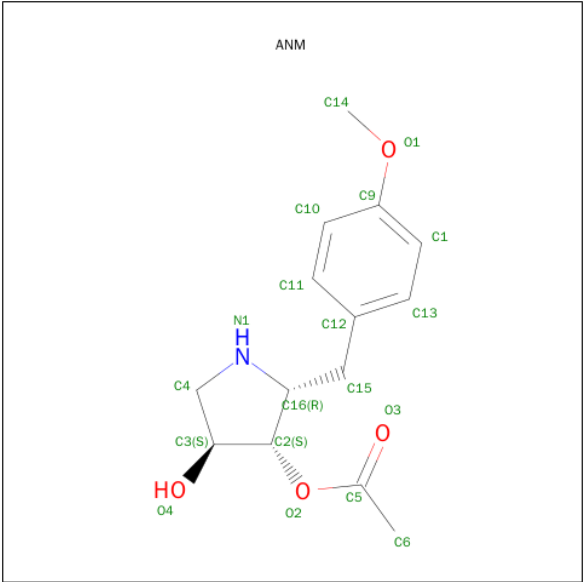
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	l5	1	Total	N	Os	0	0
			7	6	1		
87	l5	1	Total	N	Os	0	0
			7	6	1		
87	l5	1	Total	N	Os	0	0
			7	6	1		
87	l9	1	Total	N	Os	0	0
			7	6	1		
87	m0	1	Total	N	Os	0	0
			7	6	1		
87	m0	1	Total	N	Os	0	0
			7	6	1		
87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

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

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

- Molecule 89 is ANISOMYCIN (three-letter code: ANM) (formula: C<sub>14</sub>H<sub>19</sub>NO<sub>4</sub>).



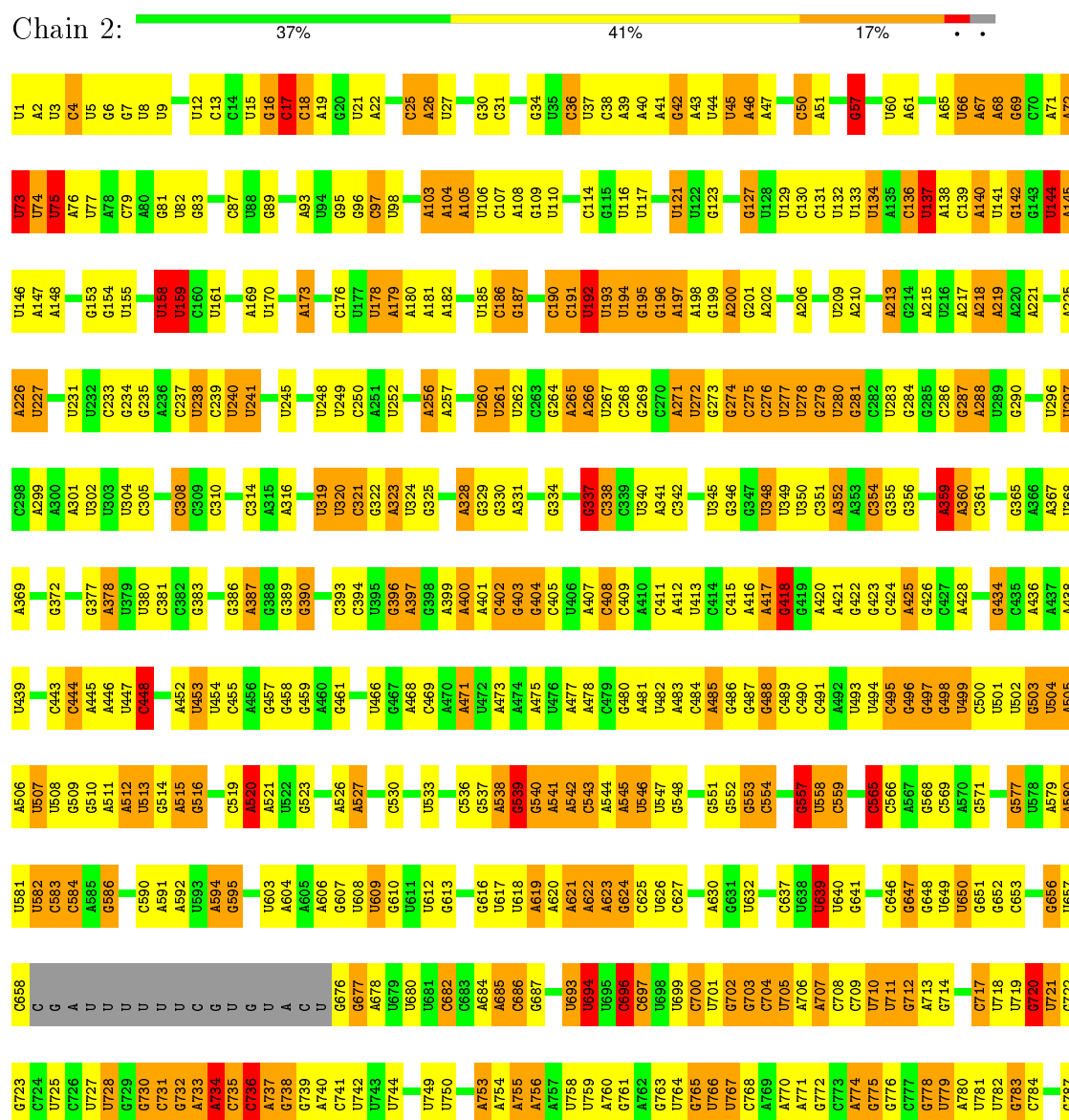
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
89	1	1	Total	C	N	O	0	0
			19	14	1	4		
89	5	1	Total	C	N	O	0	0
			19	14	1	4		

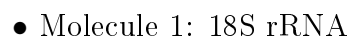
### 3 Residue-property plots

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

Note EDS failed to run properly.

#### • Molecule 1: 18S rRNA

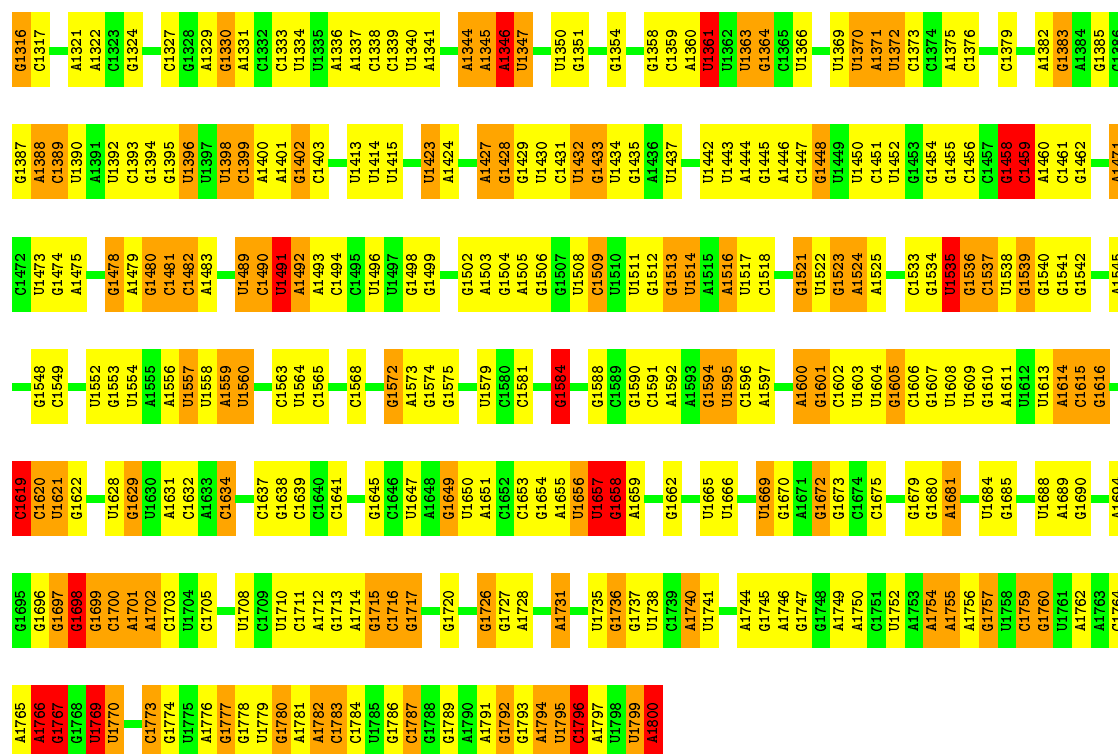




Response	Percentage
Yes, more action is needed	38%
No, the U.S. is doing enough	41%
Don't know	18%
Other	3%

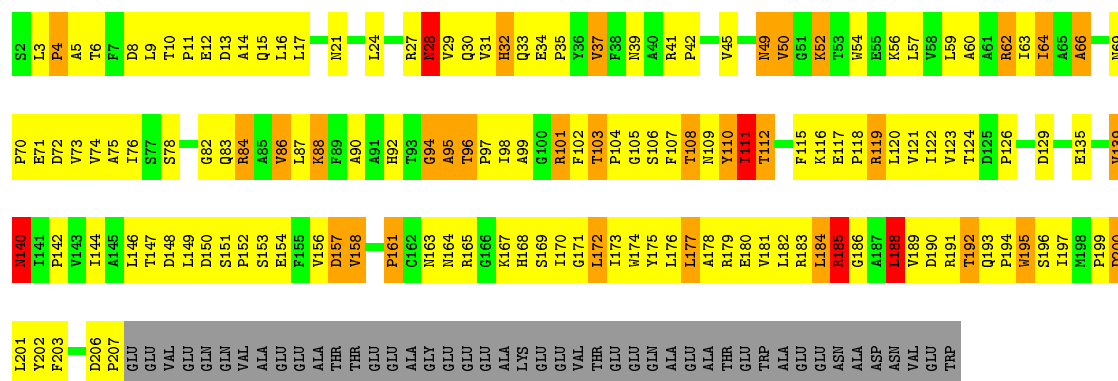


G1237	G1156	G1075	G1010	U935	G858	U792	C724	G655	U581	A512	C648	C381	U304	U227	U150	U82
A1238	A1157	A1076	G1011	G936	A859	A793	U727	G656	U582	U513	A451	C382	C305	U228	U151	G83
U1239	C1158	C1077	G1014	G937	G857	U794	U728	G657	C583	G514	A452	C383	C308	U229	U152	A84
U1240	C1159	C1078	G1015	G938	G858	U795	G729	G658	A585	G515	U453	C384	C309	U230	U153	A85
G1241	A1160	U1079	U1016	A941	A863	U800	G730	G659	G586	U516	U454	C385	C310	U231	G154	A86
A1242	C1161	U1080	C1016	G942	U864	G801	G731	G660	C587	U517	U455	C386	C311	U232	G155	C87
G1243	G1162	A1081	U1017	U943	G865	G802	A733	G661	U588	U518	U456	C387	U313	U233	U156	C90
A1244	A1163	C1082	U1018	U946	G866	A803	A734	G662	C589	A520	U457	C388	C314	U234	U157	G91
G1245	G1164	G1083	A1019	U947	G867	A804	C735	U663	C590	A521	U458	C389	A316	G235	U158	A92
A1246	G1165	G1084	C1021	U948	G868	U805	C736	U664	U589	U522	U459	C390	A317	A236	U159	A93
U1247	A1087	A1087	C1022	A952	G871	U806	G737	U665	A594	G523	U460	C391	C318	U240	G160	U94
G1248	A1091	A1091	U1023	G953	U873	A807	A738	U666	G595	U524	U461	C392	U319	U241	G161	G95
U1249	A1092	A1092	A1025	G954	C874	U808	U749	U667	C596	U525	U462	C393	U320	U242	G162	G96
U1250	C1173	A1093	A1026	A955	C875	A809	U750	U668	C597	A527	U463	C394	U321	U243	G163	G97
U1251	G1172	G1094	A1027	A956	G876	G810	G751	U669	U600	U533	U464	C395	G322	U244	G164	U98
U1253	U1095	U1095	G1028	G957	G877	A811	A752	U670	U601	U534	U465	C396	A323	G245	G165	G99
U1254	C1096	U1096	U1029	U958	G878	A812	A753	U671	A604	A535	U466	C397	U324	U246	U170	U101
U1255	G1175	U1097	A1030	U959	G879	U813	U748	A673	U603	A536	U467	C398	U325	U247	U171	U102
A1256	G1176	U1098	U1031	U960	C874	A814	U749	C874	A604	A537	U468	C399	G326	U248	U172	A103
U1257	C1177	U1099	U1032	U961	G875	G815	U750	U675	G607	U538	U469	C400	G327	U249	U173	A104
U1258	G1178	U1100	C1033	C962	G876	G816	A751	G676	U608	A539	U470	C401	A330	U255	U174	A105
U1259	U1181	G1101	G1034	A963	G677	A817	A752	G677	U609	G540	U471	C402	U332	A256	U175	A106
U1260	U1182	U1106	G1035	A966	A754	G818	A753	A678	U610	G541	U472	C403	U333	A257	U176	U107
G1261	A1183	U1107	A1036	A967	U755	G819	A754	U679	G611	G542	U473	C404	U334	A258	U177	A108
U1262	A1184	U1108	C1037	A968	A756	U820	A755	U680	U611	A543	U474	C405	U335	A259	U178	A109
G1263	U1185	G1109	U1038	U970	U757	U821	A756	U681	U612	A544	U475	C406	U336	U261	U179	
G1264	C1190	U1110	A1039	A971	A758	U822	A757	C682	U613	A545	U476	C407	U337	U262	U180	
G1268	U1111	A1112	G1040	A972	U759	G823	U758	C683	U614	A546	U477	C408	U338	U263	U181	
U1269	G1114	G1114	G1041	A973	U759	G824	U759	C684	U615	A547	U478	C409	U339	U264	U182	
U1270	U1115	U1115	A1043	A974	A760	U825	A760	C685	A621	U547	U479	C410	U340	U265	U183	
U1271	A1116	A1116	A1044	G976	A761	U826	A761	C686	A622	U548	U480	C411	U341	U266	U184	
U1272	U1117	G901	C1045	A977	A762	C827	A762	G687	A623	G549	U481	C412	U342	U267	U185	
C1279	G1197	U1120	G1046	A978	U763	U828	U763	C691	A624	A550	U482	C413	U343	A271	U186	
G1280	U1198	A906	U1048	A979	U764	A829	U764	U694	U626	A551	U483	C414	U344	U272	U187	
G1281	G1199	A907	U1049	G980	U765	U830	U765	U695	C627	A552	U484	C415	U345	U273	U188	
U1282	G1201	U908	G1050	U981	U766	U831	U766	U696	G628	A553	U485	C416	U346	U274	U189	
U1285	A1202	U909	U1051	U982	C768	U832	C768	C696	U629	U554	U486	C417	U347	U275	U190	
U1286	A1203	C910	U1052	A983	U769	U833	A769	C697	A630	U555	U487	C418	U348	U276	U191	
U1287	C1207	U911	G1053	G986	A770	U834	A770	U698	G631	U556	U488	C419	U349	U277	U192	
G1288	U1130	U912	U1054	G987	C773	U835	C773	U699	G632	G561	U489	C420	U350	U278	U193	
U1291	A1131	G913	U1055	A988	U774	U836	U774	C700	G633	A562	U490	C421	U351	U279	U194	
G1292	A1132	C914	U1056	A989	G775	G837	G775	U701	A634	A563	U491	C422	U352	U280	U195	
U1293	A1133	A915	U1057	U989	U776	U838	U776	C708	A635	C665	U492	C423	U353	U281	U196	
U1294	C1134	U916	U1058	C990	G777	U839	G777	C709	C637	C666	U493	C424	U354	U282	U197	
U1295	U1135	U917	U1059	G991	U778	U840	U778	C710	U638	A567	U494	C425	U355	U283	U198	
U1296	U1136	U918	U1060	A992	U779	U841	U779	C711	U639	C667	U495	C426	U356	U284	U199	
G1299	A1137	A919	A1061	A993	U780	U842	U780	U711	U640	C668	U496	C427	U357	U285	U200	
A1300	A1138	G922	A1062	G997	U781	G843	A780	G714	U641	A570	U497	C428	U358	U286	A200	
G1304	A1139	A923	U1063	U997	U782	G844	U781	U715	C645	C669	U498	C429	U359	U287	U201	
U1305	G1140	A924	C1066	C1000	U783	A845	U782	C716	C646	C670	U499	C430	U360	U288	U202	
C1306	U1144	A926	U1067	A1001	C784	C948	C784	C717	G647	C671	U500	C431	U361	U289	A210	
U1307	U1145	C927	C1068	U1002	U785	U846	U785	C718	G648	C672	U501	C432	U362	U290	A211	
U1312	U1231	U851	U851	A1003	G787	U847	G787	U719	U650	C673	U502	C433	U363	U291	A212	
A1313	U1234	G1150	U1071	U1004	A788	C852	A788	C720	G651	C674	U503	C434	U364	U292	A213	
U1314	C1235	A1151	C1072	A1005	A789	C853	A789	C721	G652	C675	U504	C435	U365	U293	A214	
U1315	A1236	G1155	G1074	C1006	U791	A856	A791	C722	G653	C676	U505	C436	U366	U294	A215	
						U857		C723	C654	A580	A511	U447	A378		U223	



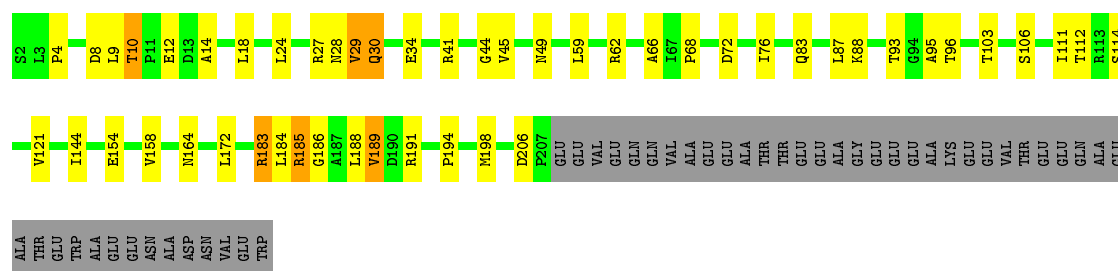
• Molecule 2: 40S ribosomal protein S0-A

Chain S0: 24% 44% 12% 18%

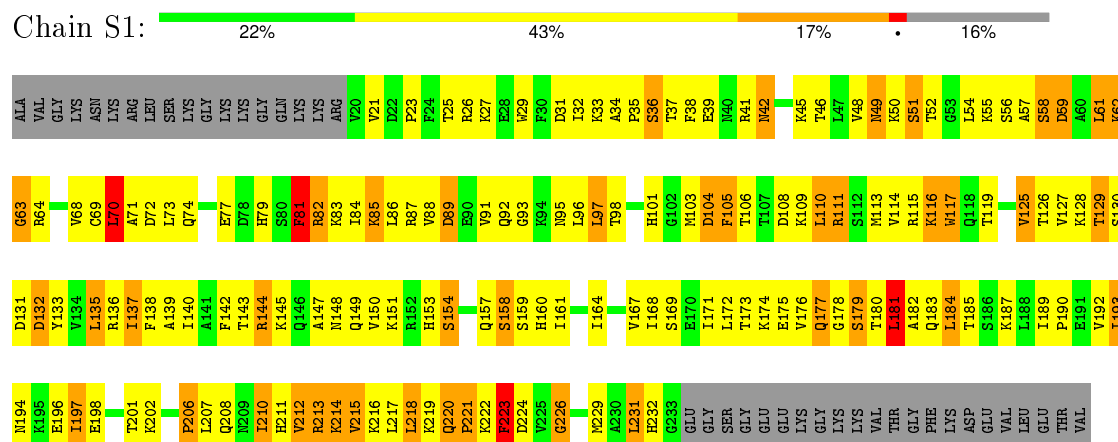


• Molecule 2: 40S ribosomal protein S0-A

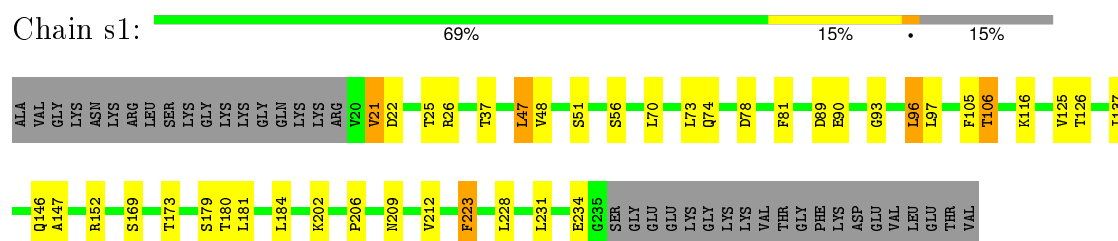
Chain s0: 62% 18% 18%



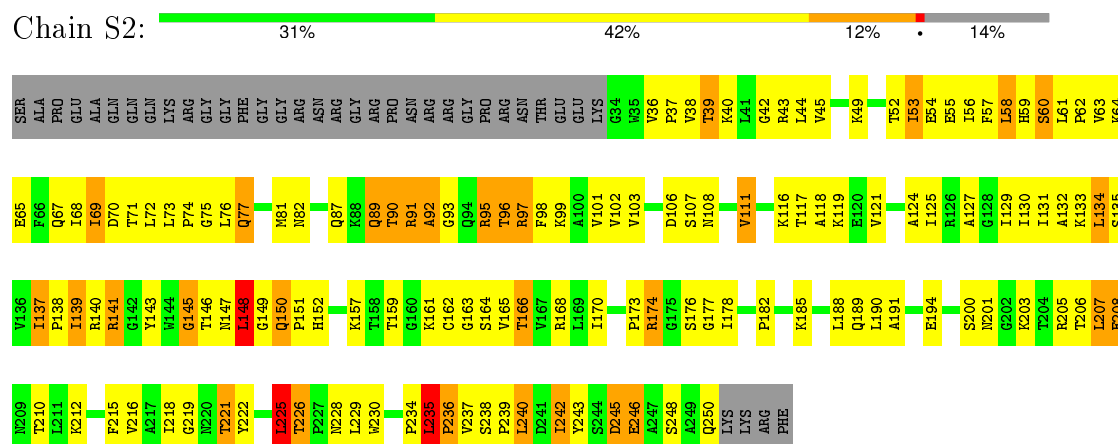
- Molecule 3: 40S ribosomal protein S1-A



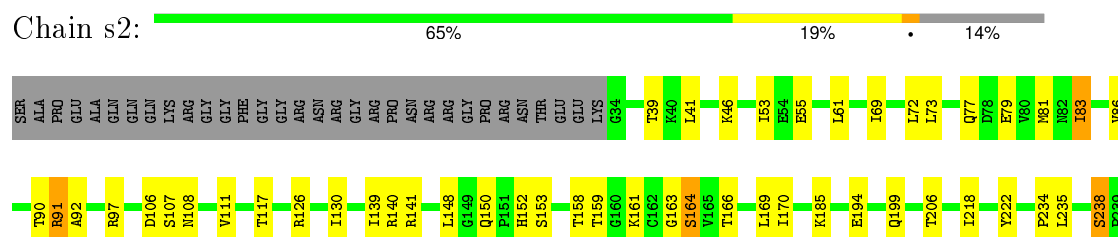
- Molecule 3: 40S ribosomal protein S1-A



- Molecule 4: 40S ribosomal protein S2



- Molecule 4: 40S ribosomal protein S2

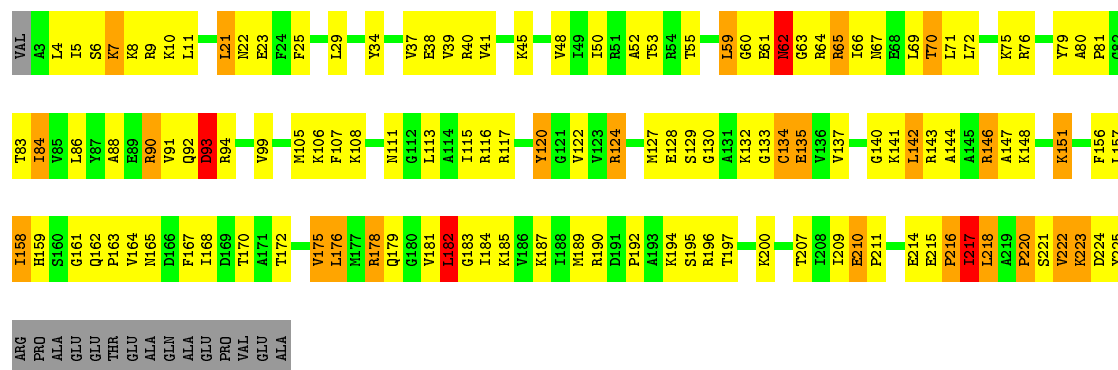






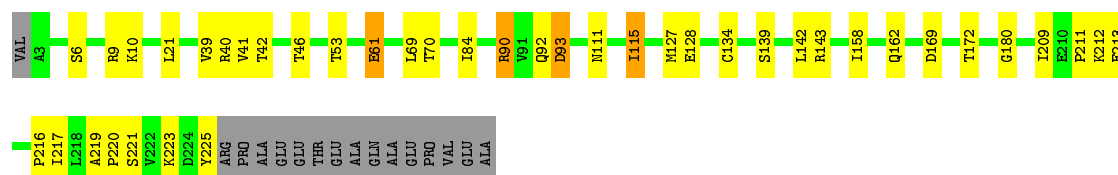
• Molecule 5: 40S ribosomal protein S3

Chain S3: 39% 42% 10% 7%



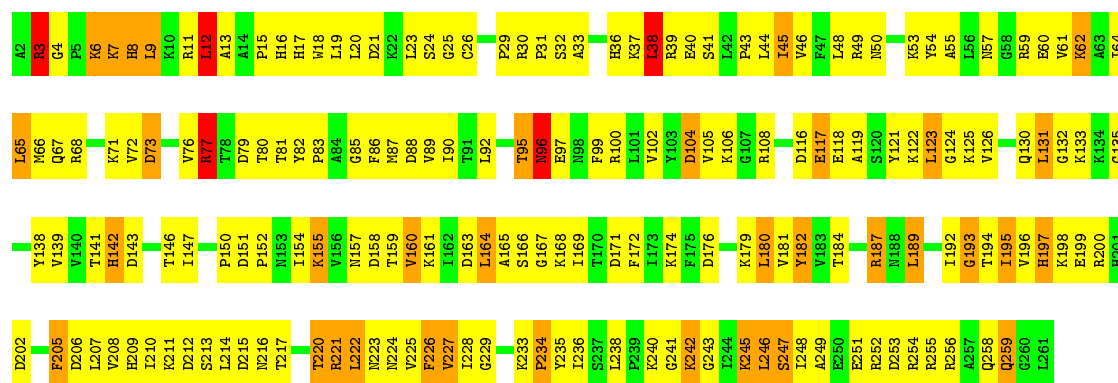
• Molecule 5: 40S ribosomal protein S3

Chain s3: 76% 15% 7%



• Molecule 6: 40S ribosomal protein S4-A

Chain S4: 30% 55% 14%



• Molecule 6: 40S ribosomal protein S4-A

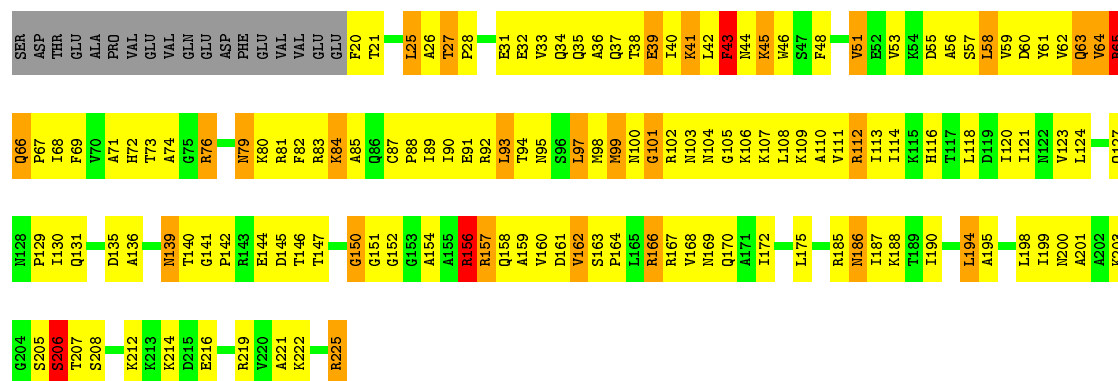
Chain s4: 81% 17%





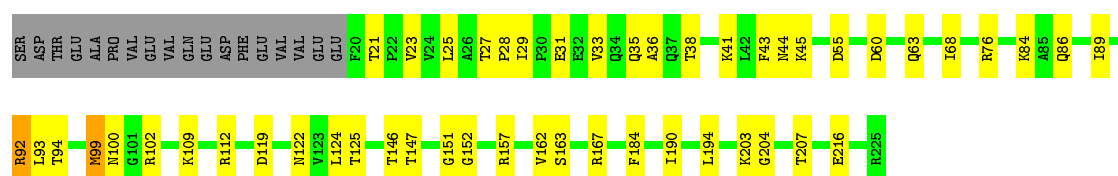
• Molecule 7: 40S ribosomal protein S5

Chain S5: 29% 50% 12% 8%



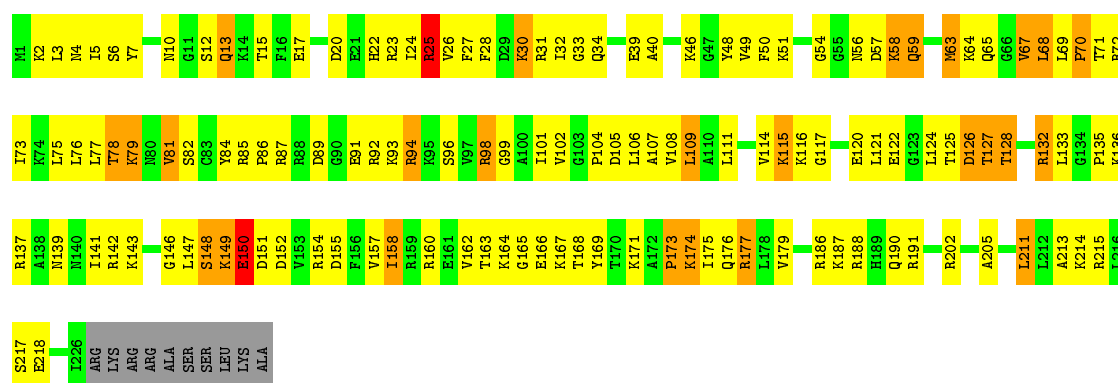
• Molecule 7: 40S ribosomal protein S5

Chain s5: 70% 21% 8%



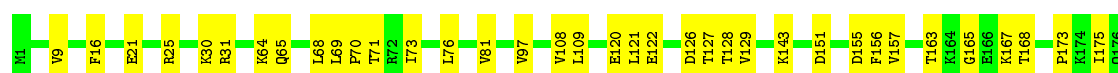
• Molecule 8: 40S ribosomal protein S6-A

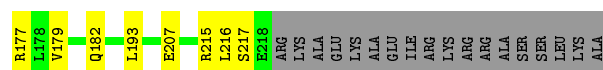
Chain S6: 39% 45% 11%



• Molecule 8: 40S ribosomal protein S6-A

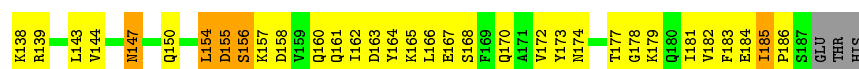
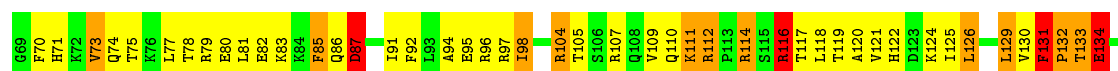
Chain s6: 74% 19% 8%





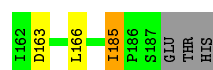
- Molecule 9: 40S ribosomal protein S7-A

Chain S7: 33% 46% 16% . .



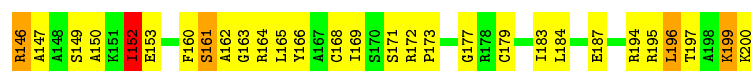
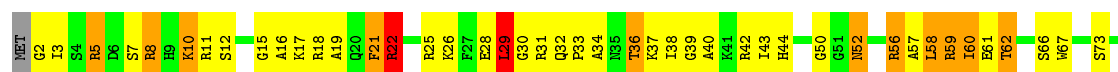
- Molecule 9: 40S ribosomal protein S7-A

Chain s7: 79% 17% . .



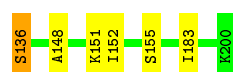
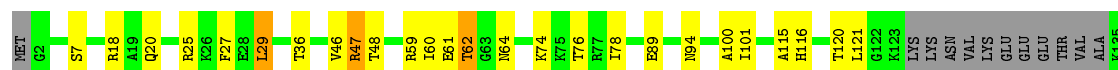
- Molecule 10: 40S ribosomal protein S8-A

Chain S8: 40% 42% 10% 6%



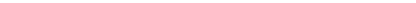
- Molecule 10: 40S ribosomal protein S8-A

Chain s8: 78% 14% 6%



- Molecule 11: 40S ribosomal protein S9-A

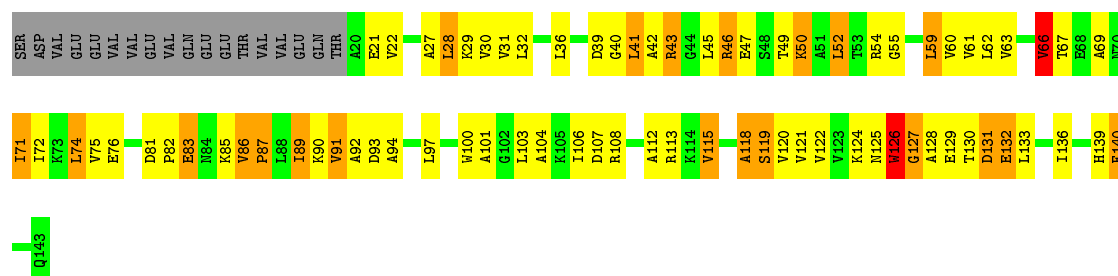


Chain c1:  78% 15% • 6%



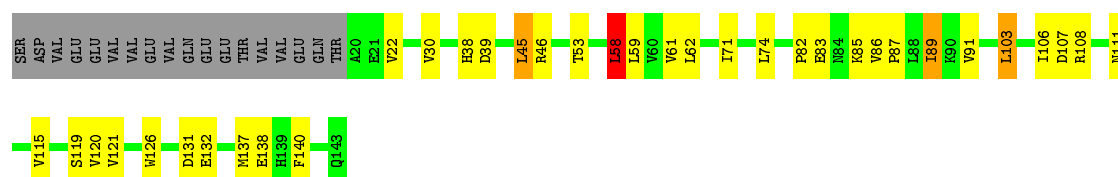
- Molecule 14: 40S ribosomal protein S12

Chain C2: 



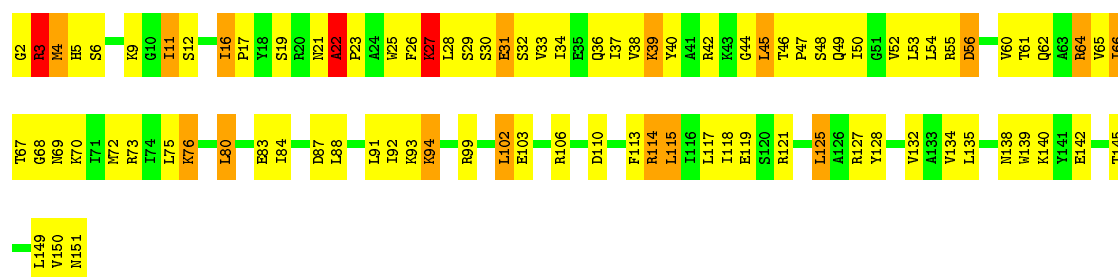
- Molecule 14: 40S ribosomal protein S12

Chain c2:  63% 22% .. 13%



- Molecule 15: 40S ribosomal protein S13

Chain C3: 



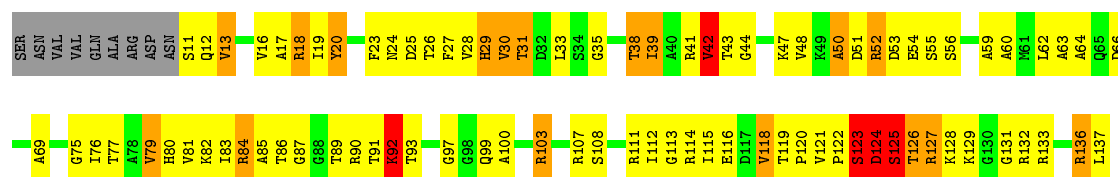
- Molecule 15: 40S ribosomal protein S13

Chain c3:  80% 19%

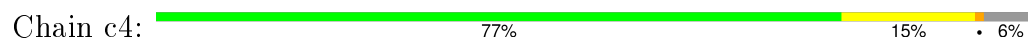


- Molecule 16: 40S ribosomal protein S14-A

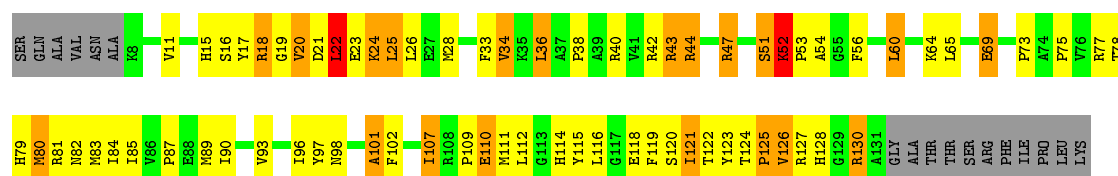
Chain C4: 



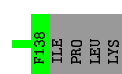
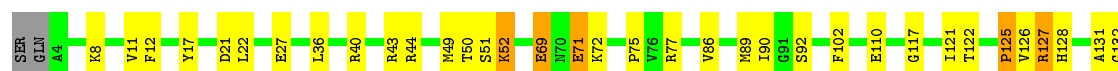
- Molecule 16: 40S ribosomal protein S14-A



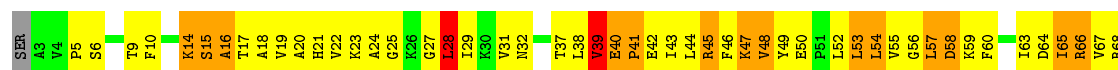
- Molecule 17: 40S ribosomal protein S15



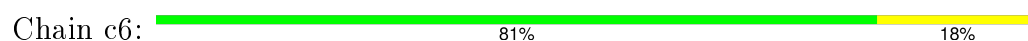
- Molecule 17: 40S ribosomal protein S15



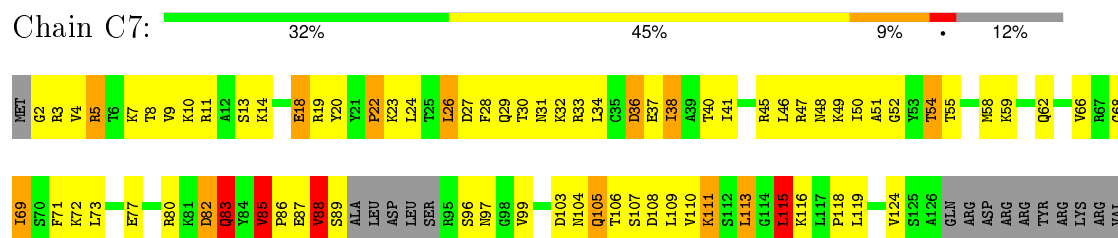
- Molecule 18: 40S ribosomal protein S16-A



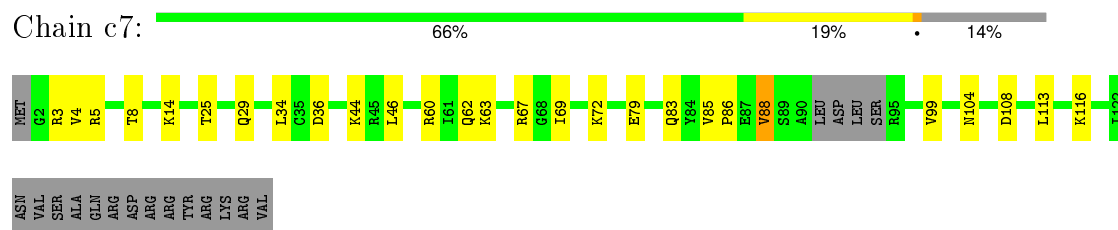
- Molecule 18: 40S ribosomal protein S16-A



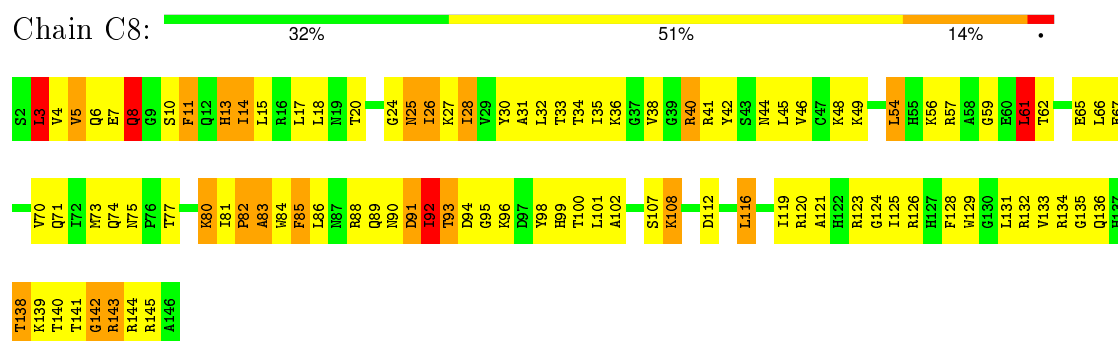
- Molecule 19: 40S ribosomal protein S17-A



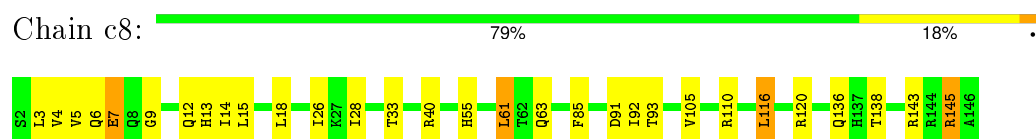
- Molecule 19: 40S ribosomal protein S17-A



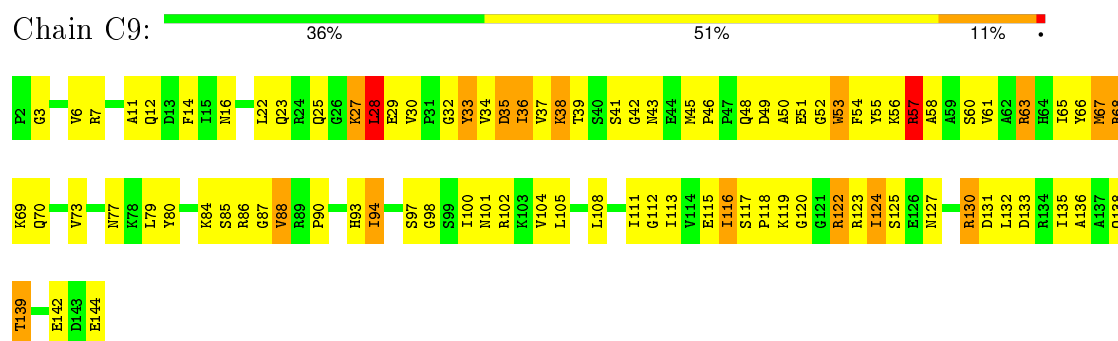
- Molecule 20: 40S ribosomal protein S18-A



- Molecule 20: 40S ribosomal protein S18-A



- Molecule 21: 40S ribosomal protein S19-A



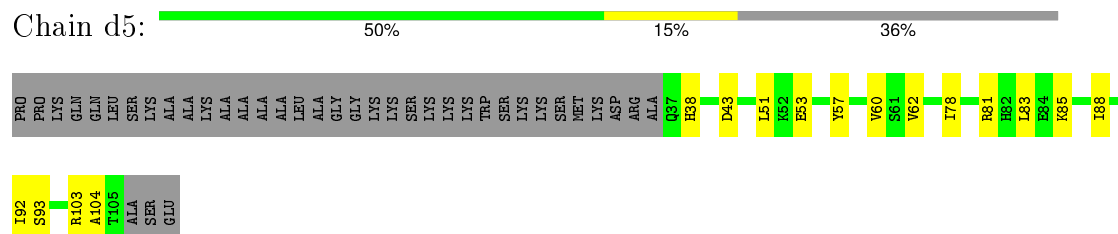
- Molecule 21: 40S ribosomal protein S19-A



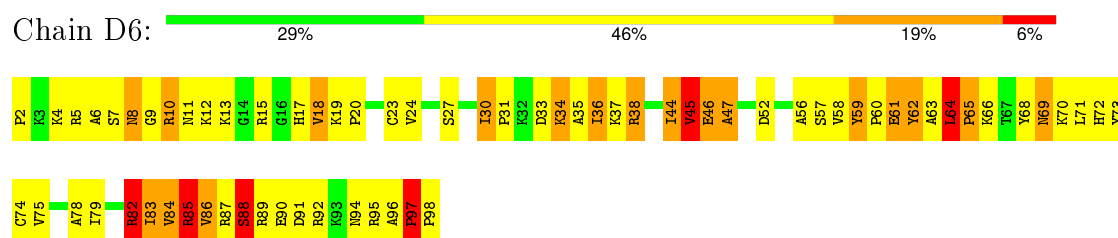


- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| PRO | PRO | LVS | GLN | GLN | SER | LVS | ALA | ALA | LVS | ALA | ALA | ALA | ALA | LYS | LEU | LYS | GLY | GLY | LVS | LVS | LVS | SER | SER | LVS | LVS | SER | SER | MET | LVS | LVS | ASP | ARG | ARG | A36 | Q37 | H38 | A39 | V40 | I41 | L42 | D43 | Q44 | E45 | K46 | Y47 | D48 | R49 | F50 | L51 | K52 | E53 | V54 | P55 | T56 | F57 | R58 | Y59 | V60 | F61 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

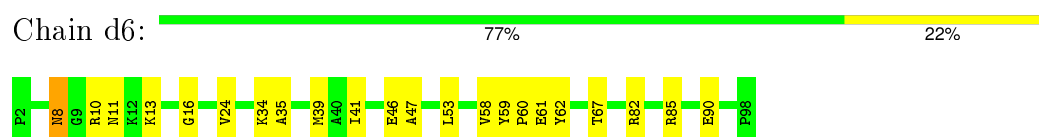
- Molecule 27: 40S ribosomal protein S25-A



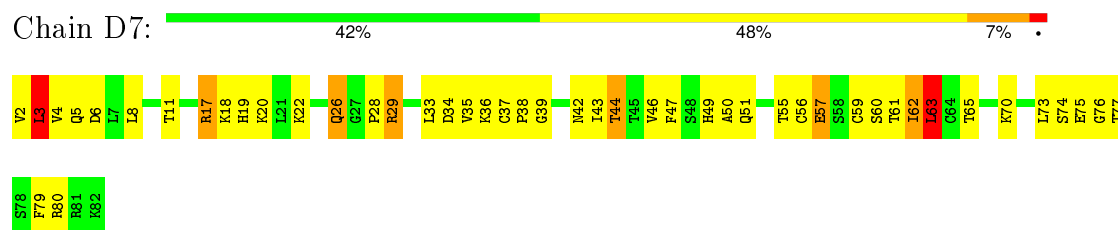
- Molecule 28: 40S ribosomal protein S26-B



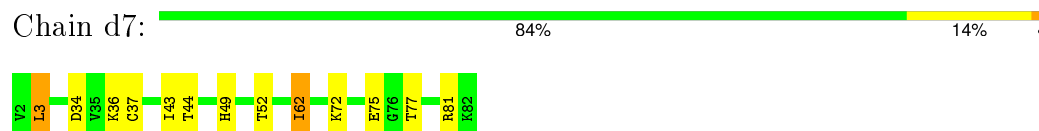
- Molecule 28: 40S ribosomal protein S26-B



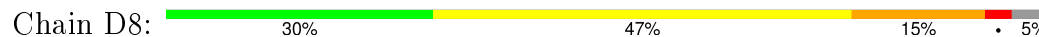
- Molecule 29: 40S ribosomal protein S27-A

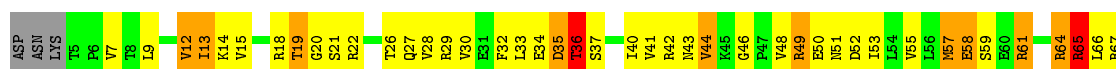


- Molecule 29: 40S ribosomal protein S27-A



- Molecule 30: 40S ribosomal protein S28-A

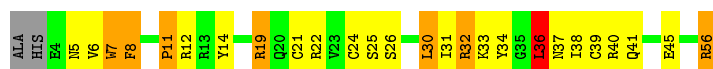




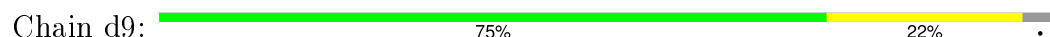
- Molecule 30: 40S ribosomal protein S28-A



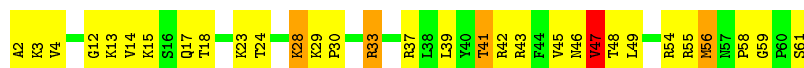
- Molecule 31: 40S ribosomal protein S29-A



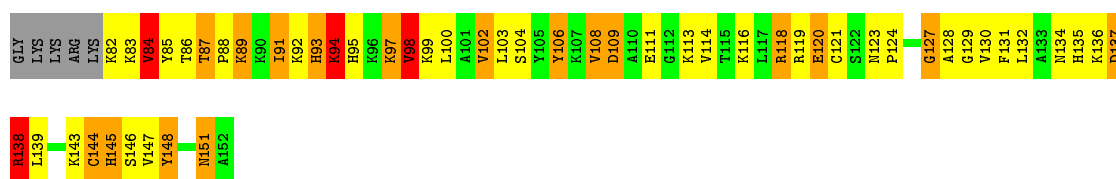
- Molecule 31: 40S ribosomal protein S29-A



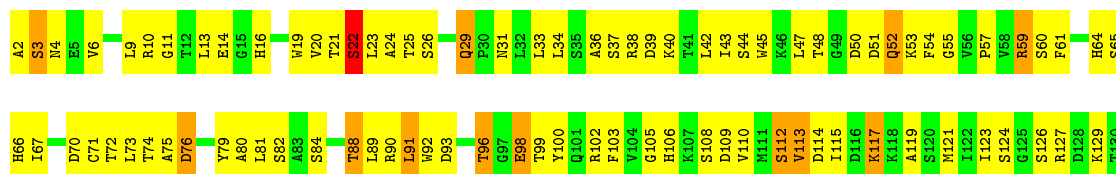
- Molecule 32: 40S ribosomal protein S30-A

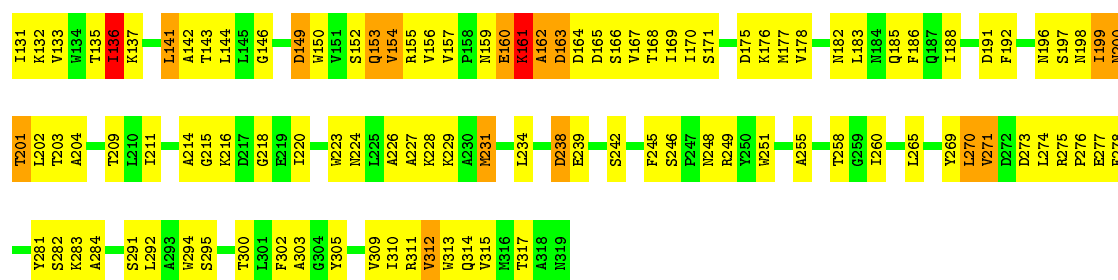


- Molecule 33: Ubiquitin-40S ribosomal protein S31



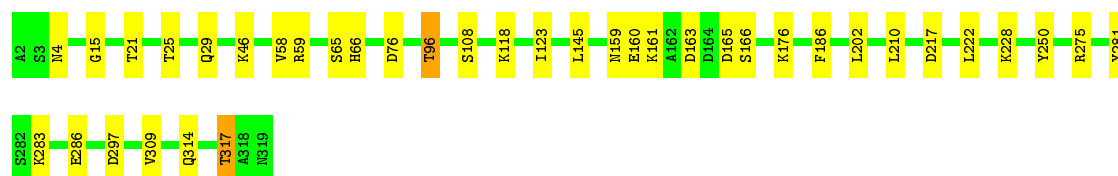
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein





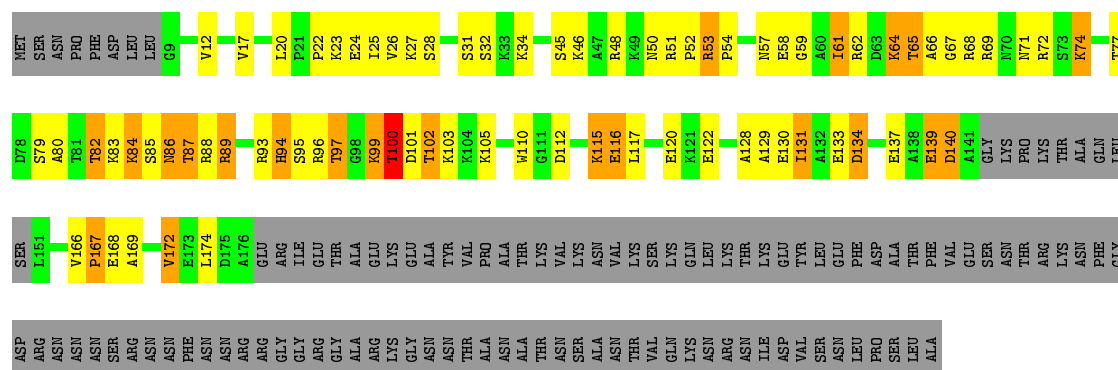
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR: 88% 11%



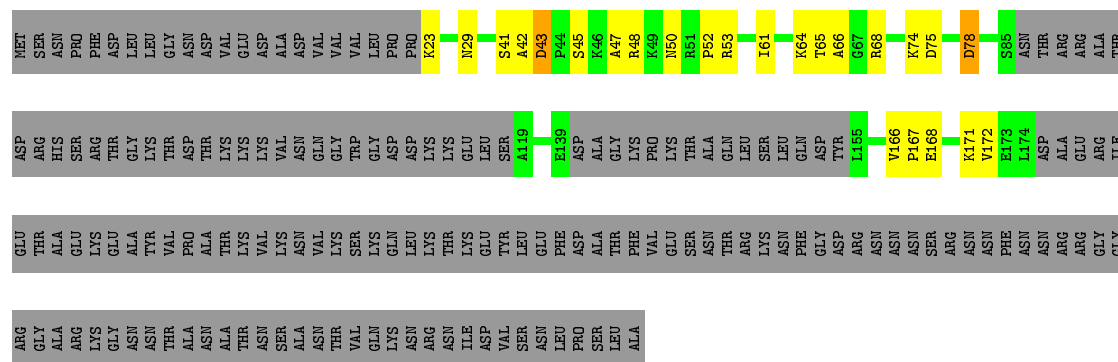
- Molecule 35: Suppressor protein STM1

Chain SM: 29% 21% 8% 42%



- Molecule 35: Suppressor protein STM1

Chain sM: 29% 8% 62%



- Molecule 36: 25s rRNA

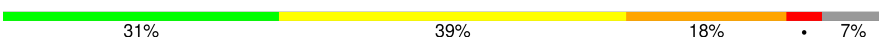






G3390  
A3391  
U3392  
U3393  
U3394  
G3395  
U3396

• Molecule 36: 25s rRNA

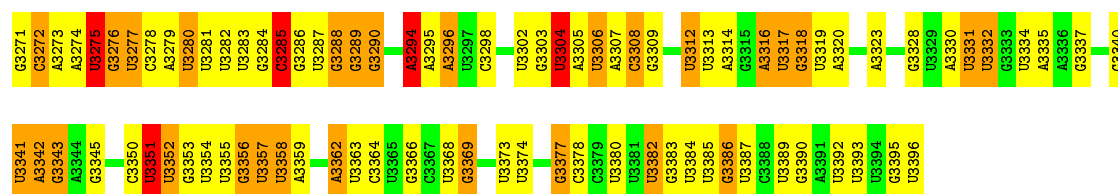
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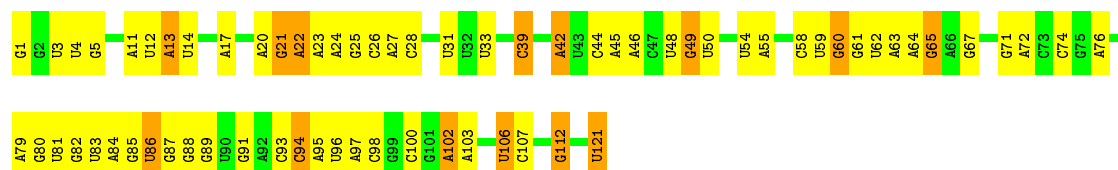


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				A2969		G2839	C2777	G2714	A2635		A2372	
				U2970		U2840	G2778	U2715	A2636		A2373	G2239
				G2971		C2841	G2779	U2716	A2637		C2374	
				U2972		U2842	U2780	U2717	C2638		G2375	A2243
				A2973		C2843	A2781	U2718	G2639		G2376	A2244
				U2974		U2844	U2782	U2719	C2640		G2377	A2245
				G2975		C2845	U2783	G2720	U2641		C2378	G2246
				U2976		A2846	G2784	A2721			U2379	G2247
				G2977		U2847	A2785	U2722	C2644		U2380	C2248
				U2978		G2848	G2786	U2723	G2645		G2381	G2249
				G2979		U2849	G2787	U2724	C2646		U2382	G2250
				U2980		G2850		U2725			C2383	G2251
				U2981		U2851	A2790	C2726	A2649		A2384	A2252
				A2982		C2852	G2791	A2727	U2650		G2385	G2253
				U2983		U2853	A2792	U2728	G2651		A2386	U2254
				C2984		U2854	G2793	U2729	U2652		U2387	A2255
				U2985		G2855	G2794	U2730	G2653		A2388	A2256
				C2986		U2856	U2795	U2731	C2654		C2389	C2257
				A2987		G2856						



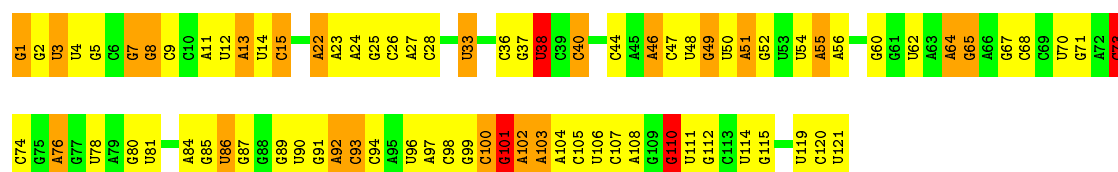
• Molecule 37: 5.8s rRNA

Chain 3: 44% 45% 12%



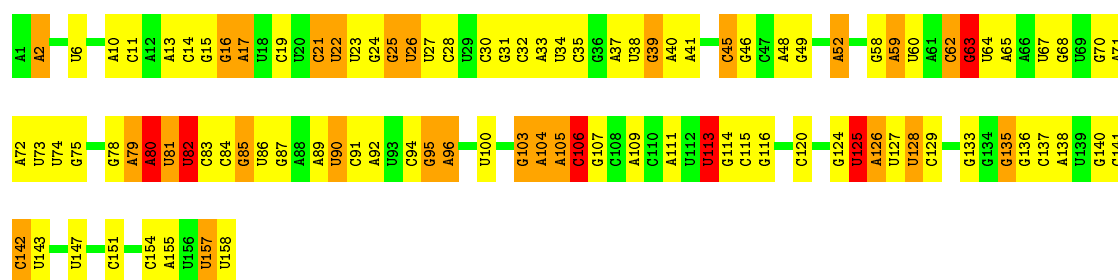
• Molecule 37: 5.8s rRNA

Chain 7: 33% 45% 18%



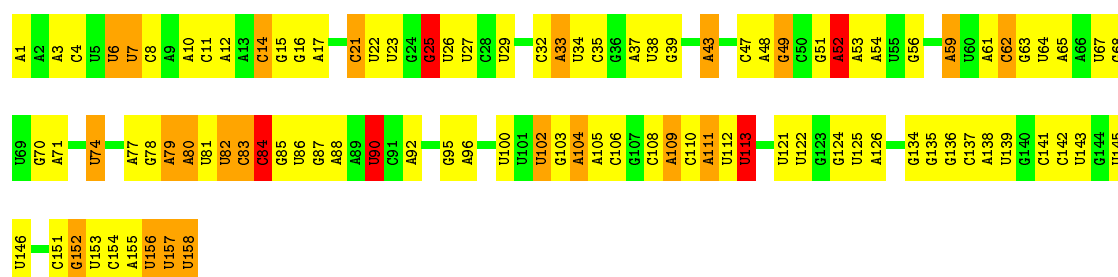
• Molecule 38: 5.8s rRNA

Chain 4: 37% 43% 16%

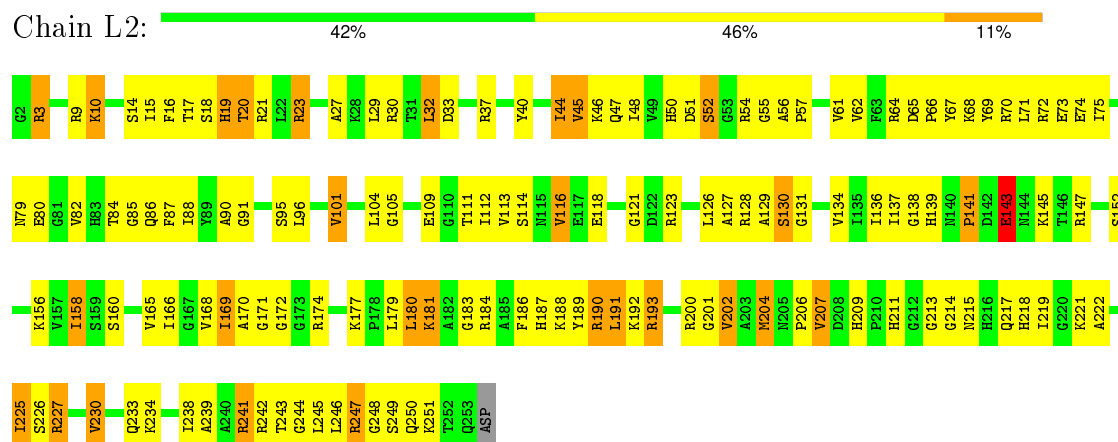


• Molecule 38: 5.8s rRNA

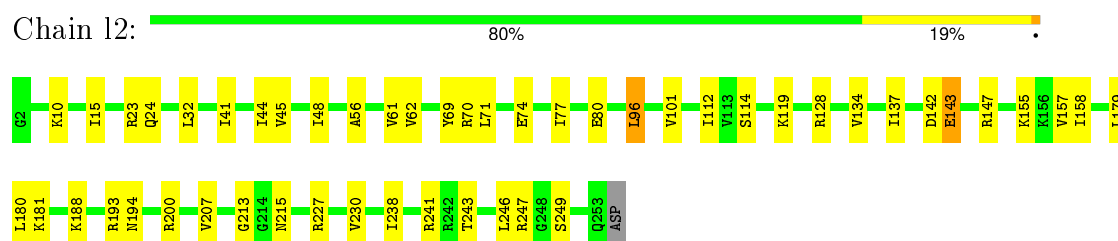
Chain 8: 37% 46% 14%



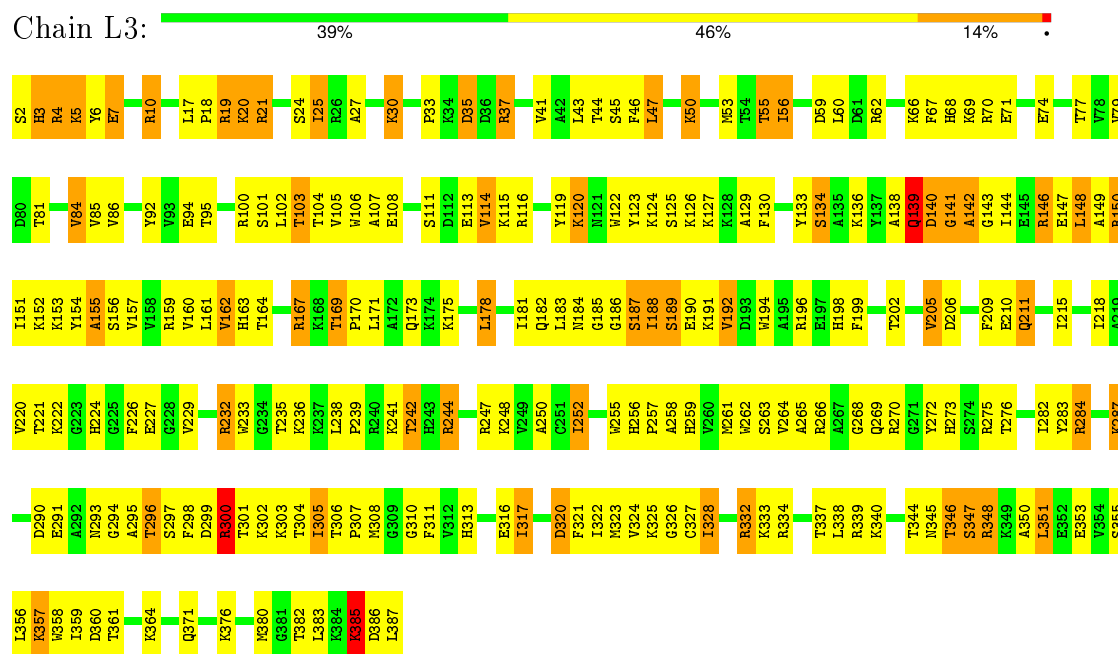
- Molecule 39: 60S ribosomal protein L2-A



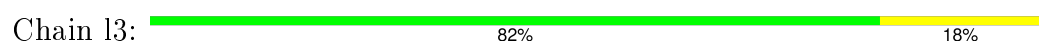
- Molecule 39: 60S ribosomal protein L2-A

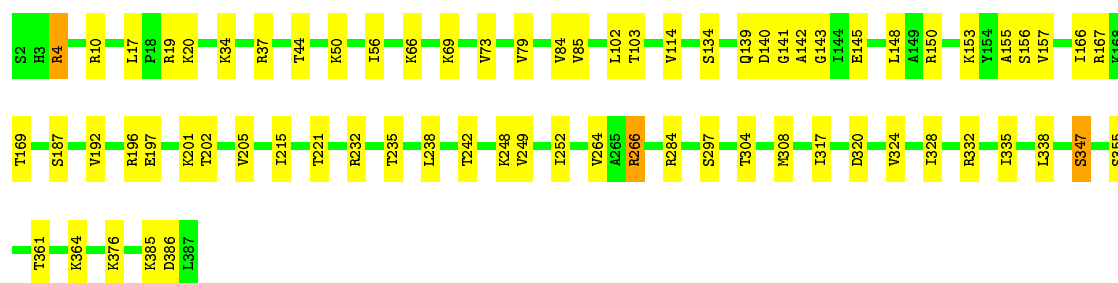


- Molecule 40: 60S ribosomal protein L3



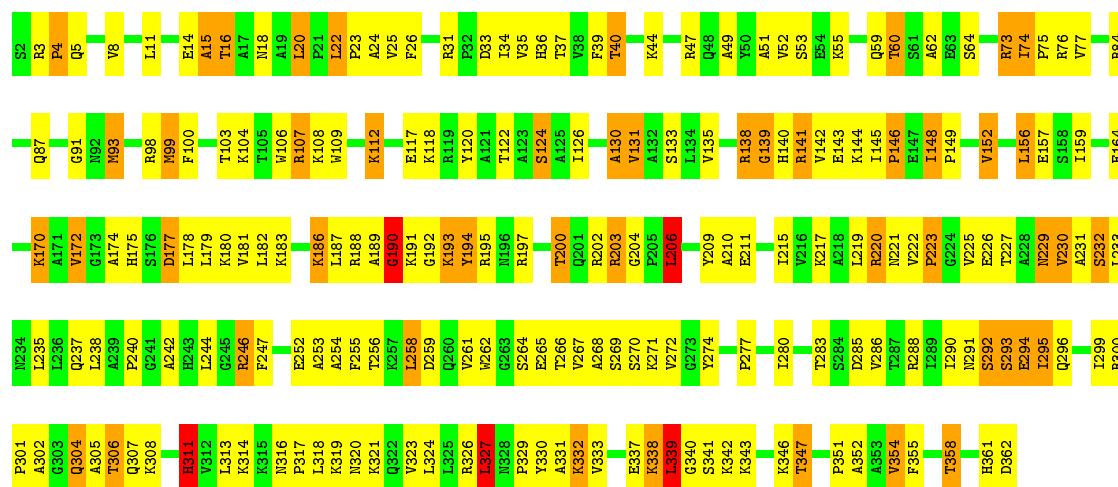
- Molecule 40: 60S ribosomal protein L3





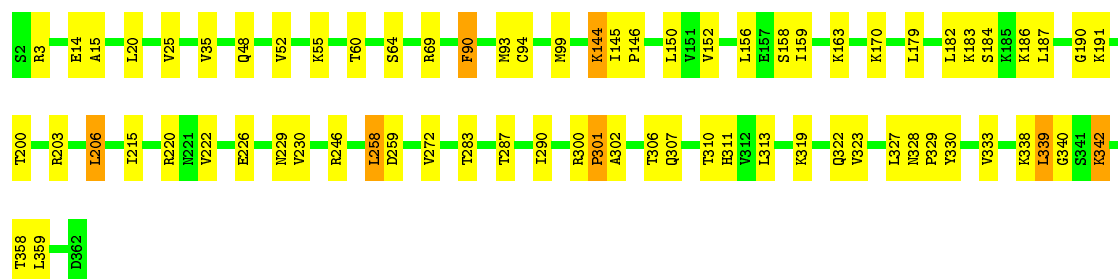
• Molecule 41: 60S ribosomal protein L4-A

Chain L4: 43% 42% 14%



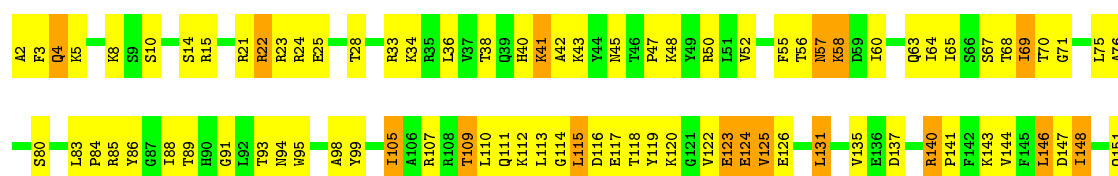
• Molecule 41: 60S ribosomal protein L4-A

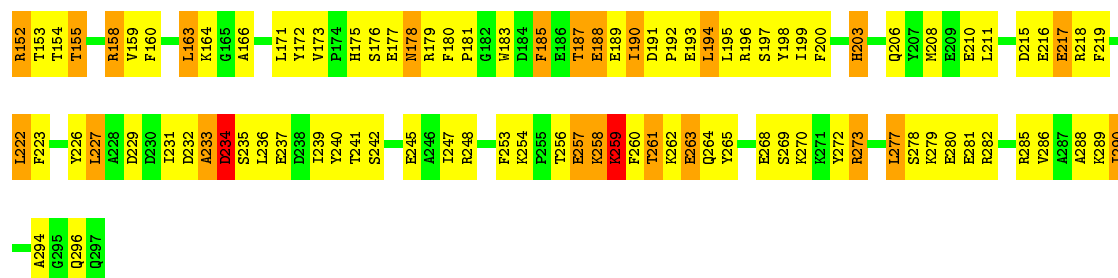
Chain L4: 80% 18%



• Molecule 42: 60S ribosomal protein L5

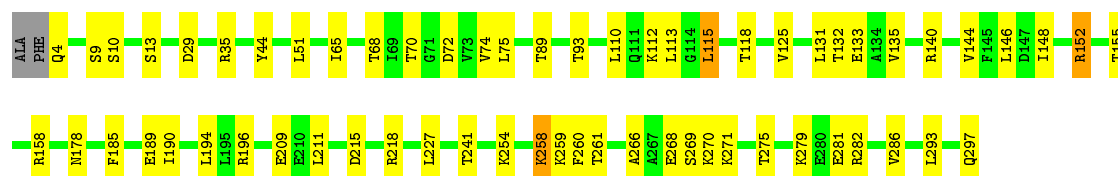
Chain L5: 39% 47% 13%





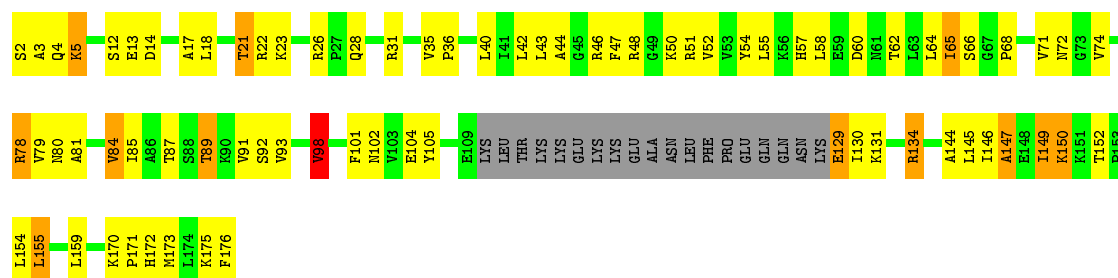
• Molecule 42: 60S ribosomal protein L5

Chain 15: 78% 20% ..



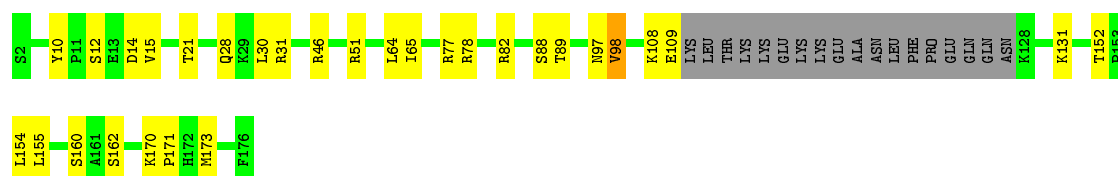
• Molecule 43: 60S ribosomal protein L6-A

Chain L6: 46% 36% 7% 11%



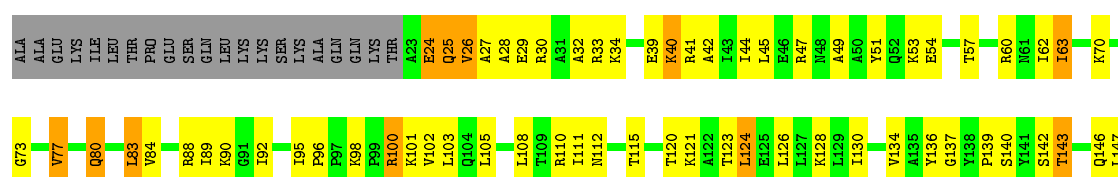
• Molecule 43: 60S ribosomal protein L6-A

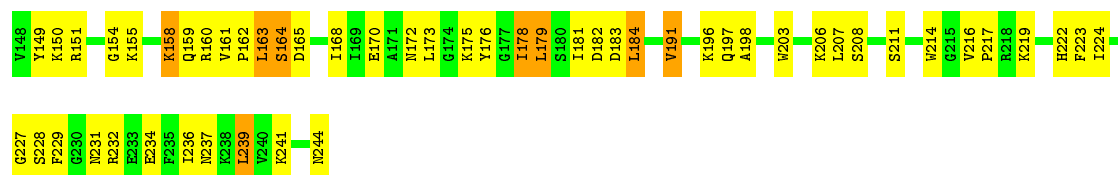
Chain l6: 73% 17% 10%



• Molecule 44: 60S ribosomal protein L7-A

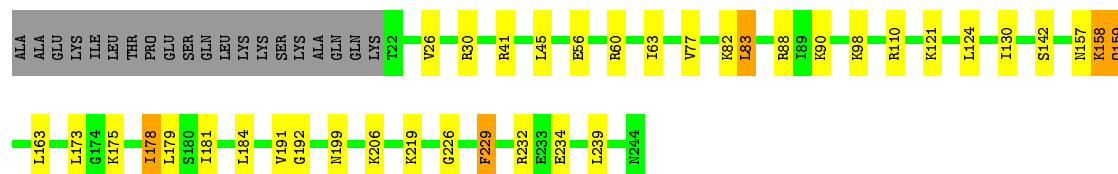
Chain L7: 44% 40% 8% 9%





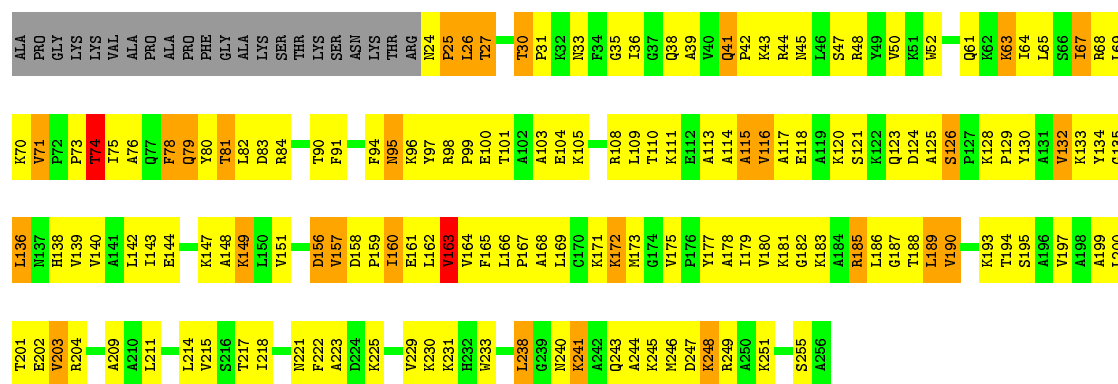
- Molecule 44: 60S ribosomal protein L7-A

Chain 17: 76% 14% 8%



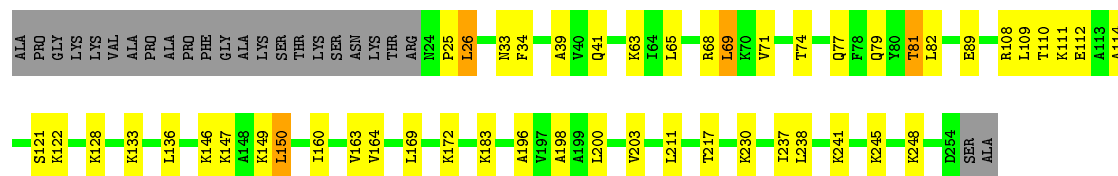
- Molecule 45: 60S ribosomal protein L8-A

Chain L8: 31% 48% 11% 9%



- Molecule 45: 60S ribosomal protein L8-A

Chain l8: 71% 18% 9%



- Molecule 46: 60S ribosomal protein L9-A

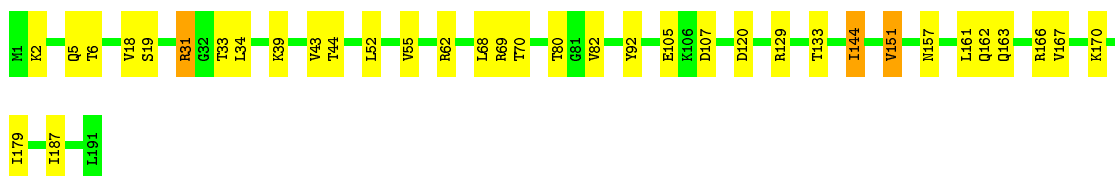
Chain L9: 36% 52% 11%





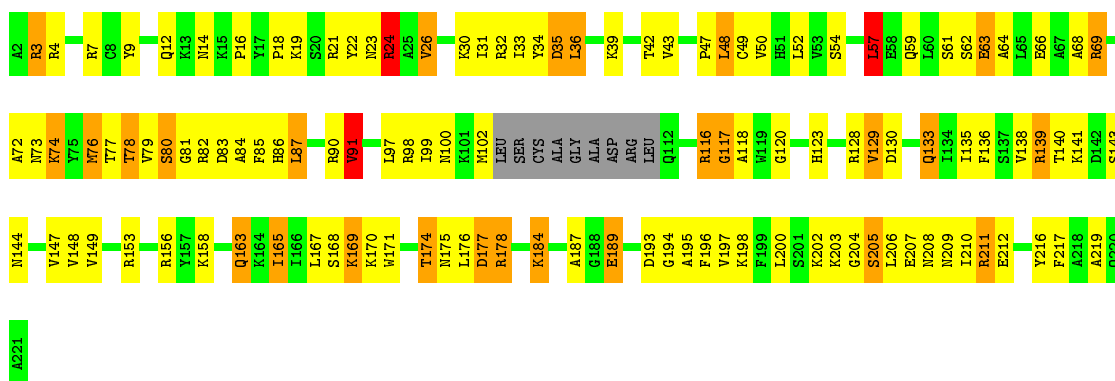
• Molecule 46: 60S ribosomal protein L9-A

Chain 19: 81% 17%



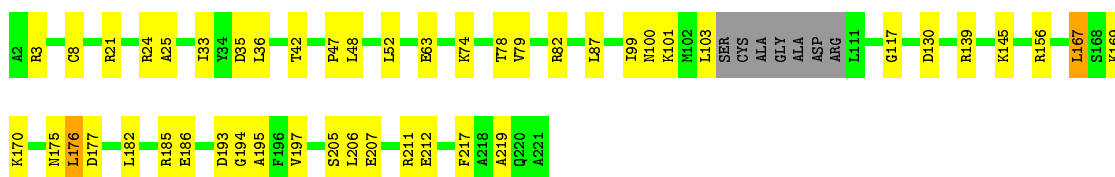
• Molecule 47: 60S ribosomal protein L10

Chain M0: 41% 41% 12%



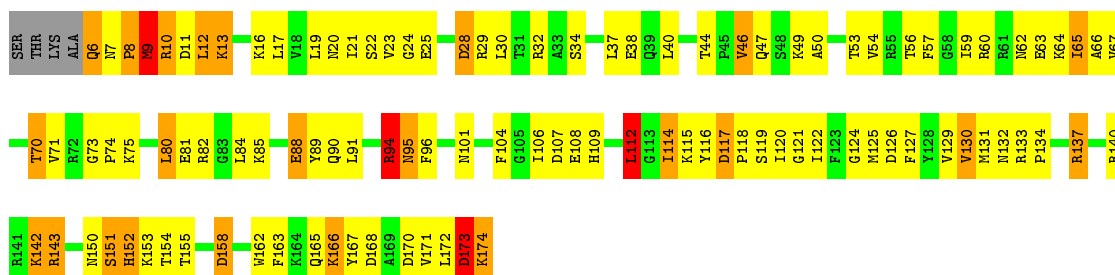
• Molecule 47: 60S ribosomal protein L10

Chain m0: 75% 20%



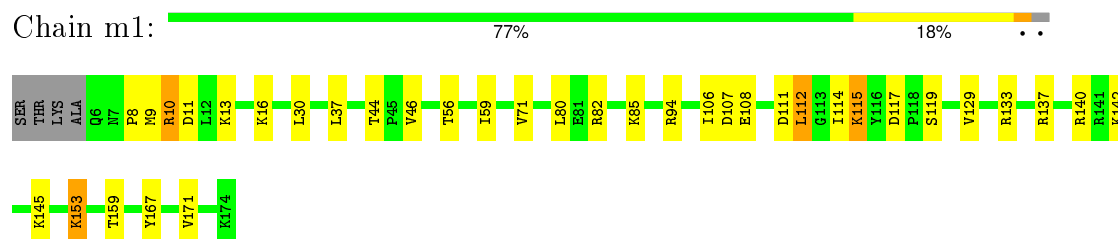
• Molecule 48: 60S ribosomal protein L11-B

Chain M1: 36% 46% 13%

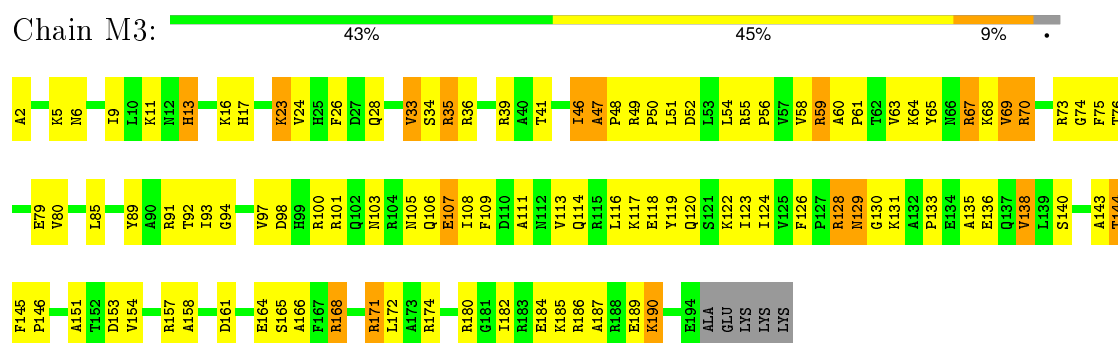




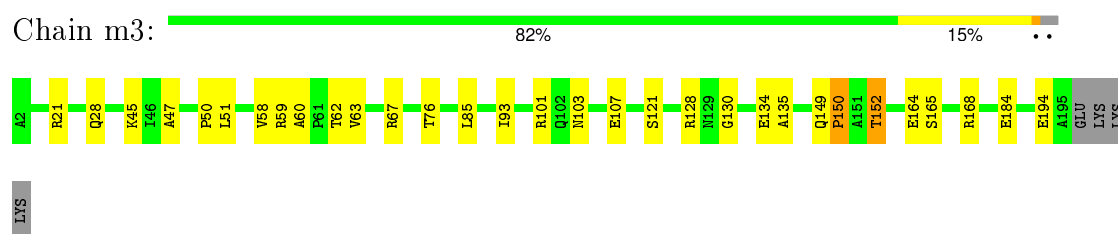
- Molecule 48: 60S ribosomal protein L11-B



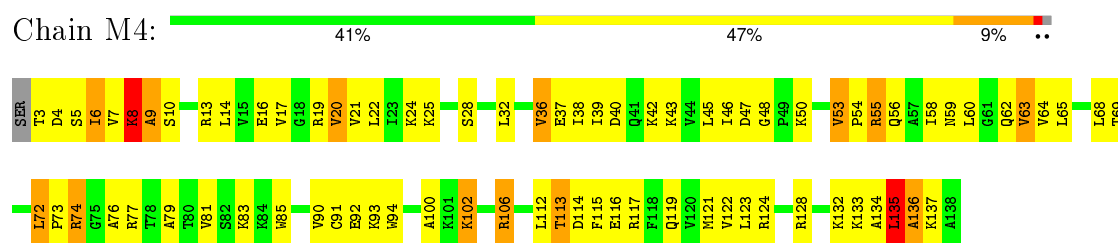
- Molecule 49: 60S ribosomal protein L13-A



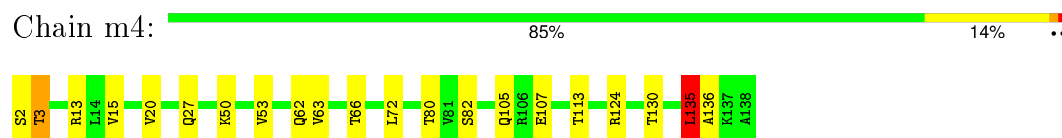
- Molecule 49: 60S ribosomal protein L13-A



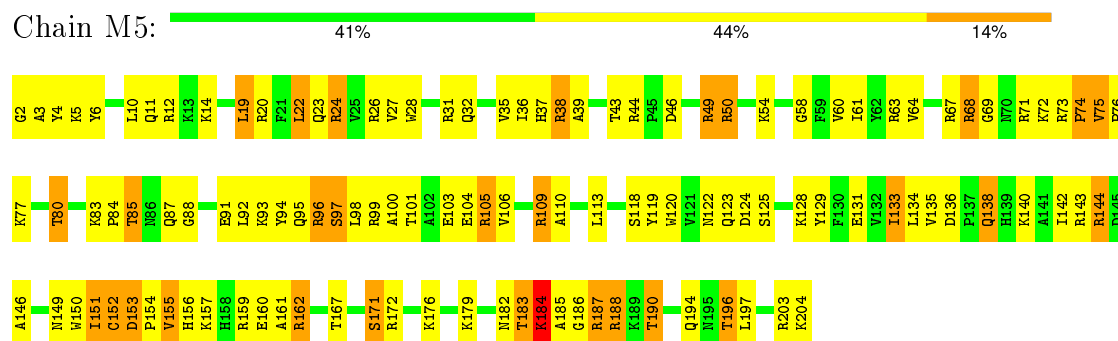
- Molecule 50: 60S ribosomal protein L14-A



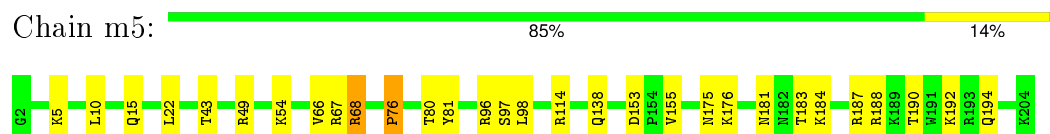
- Molecule 50: 60S ribosomal protein L14-A



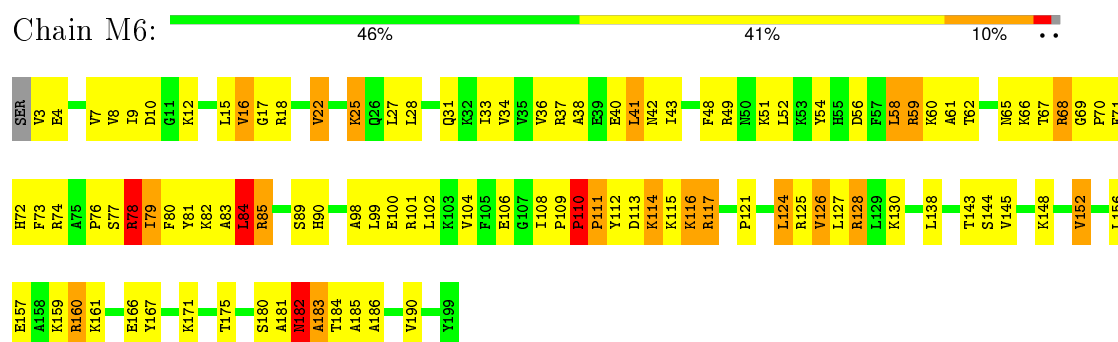
- Molecule 51: 60S ribosomal protein L15-A



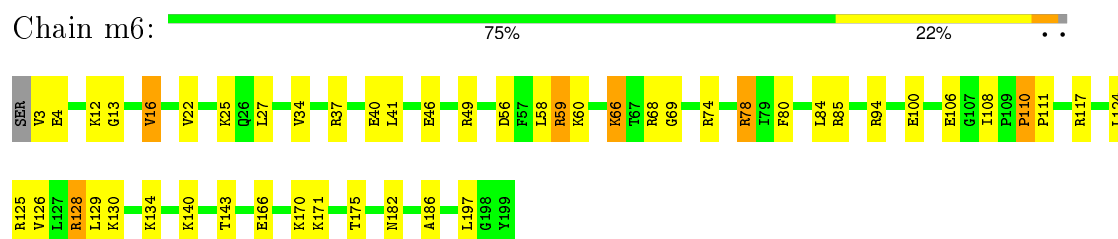
- Molecule 51: 60S ribosomal protein L15-A



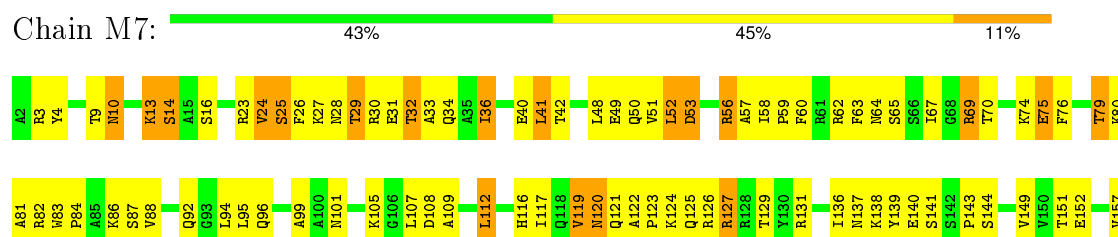
- Molecule 52: 60S ribosomal protein L16-A



- Molecule 52: 60S ribosomal protein L16-A



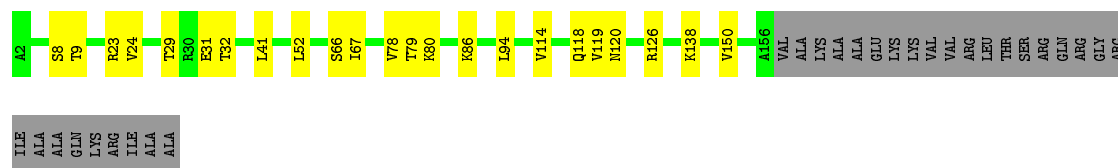
- Molecule 53: 60S ribosomal protein L17-A





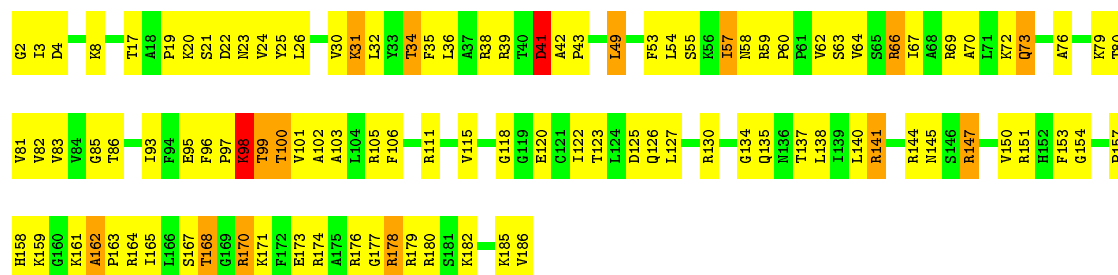
• Molecule 53: 60S ribosomal protein L17-A

Chain m7: 72% 13% 15%



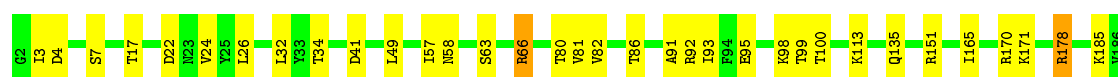
• Molecule 54: 60S ribosomal protein L18-A

Chain M8: 43% 49% 8%



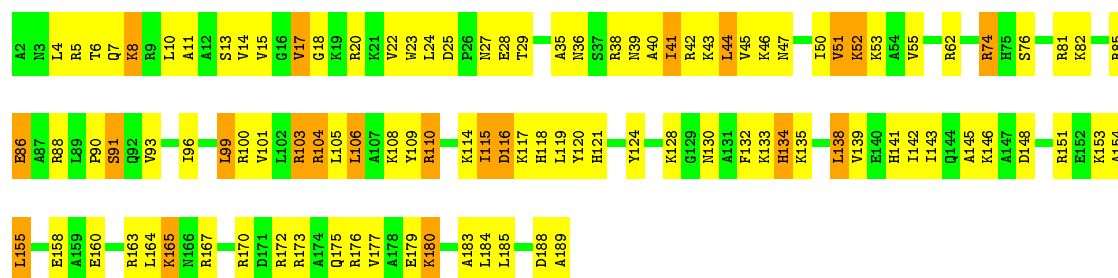
• Molecule 54: 60S ribosomal protein L18-A

Chain m8: 82% 17%



• Molecule 55: 60S ribosomal protein L19-A

Chain M9: 44% 45% 11%



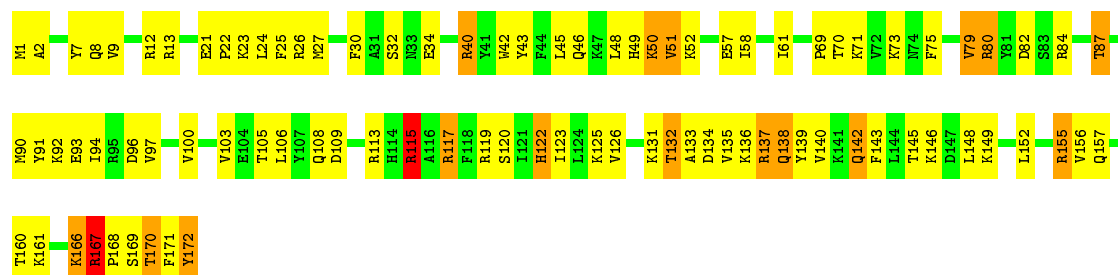
• Molecule 55: 60S ribosomal protein L19-A

Chain m9: 85% 14%



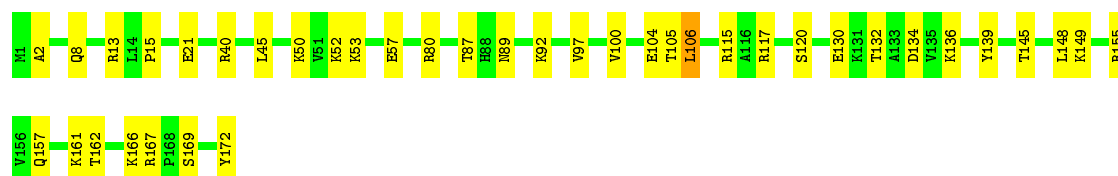
- Molecule 56: 60S ribosomal protein L20-A

Chain N0: 47% 42% 9%



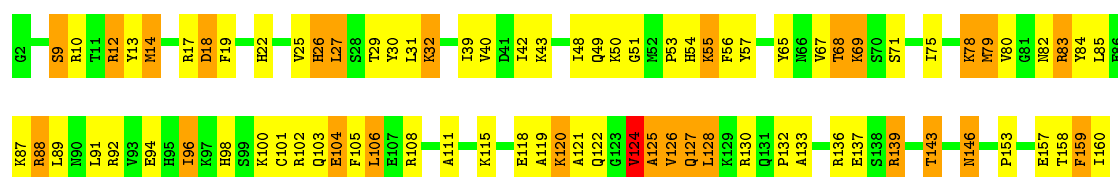
- Molecule 56: 60S ribosomal protein L20-A

Chain n0: 77% 22%



- Molecule 57: 60S ribosomal protein L21-A

Chain N1: 48% 35% 16%



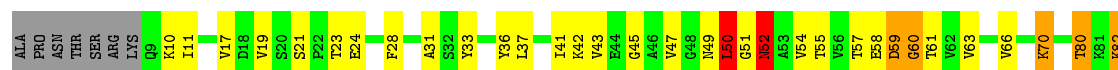
- Molecule 57: 60S ribosomal protein L21-A

Chain n1: 80% 18%



- Molecule 58: 60S ribosomal protein L22-A

Chain N2: 47% 30% 5% 17%



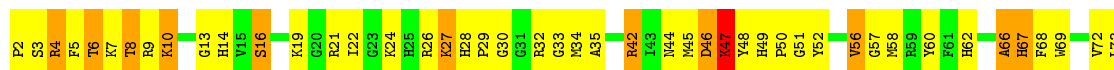






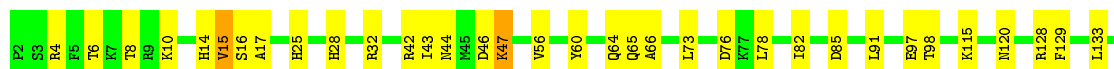
• Molecule 64: 60S ribosomal protein L28

Chain N8: 34% 53% 11%



• Molecule 64: 60S ribosomal protein L28

Chain n8: 76% 22%



• Molecule 65: 60S ribosomal protein L29

Chain N9: 50% 38% 7% 5%



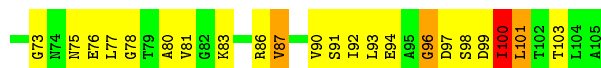
• Molecule 65: 60S ribosomal protein L29

Chain n9: 74% 22%




• Molecule 66: 60S ribosomal protein L30

Chain O0: 37% 48% 8% 7%



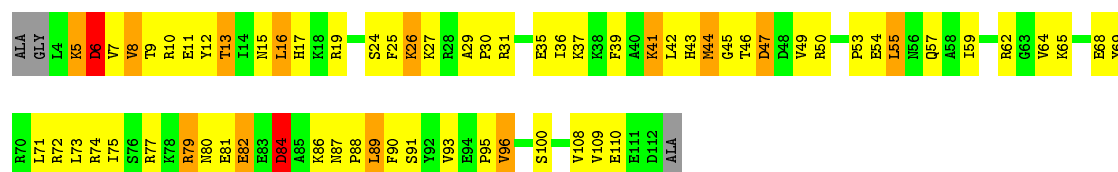
• Molecule 66: 60S ribosomal protein L30

Chain o0:  78% 17% • •




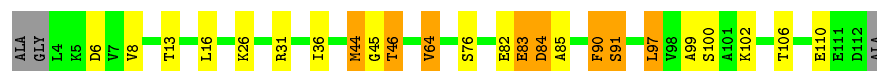
- Molecule 67: 60S ribosomal protein L31-A

Chain O1:  38% 46% 12% • •



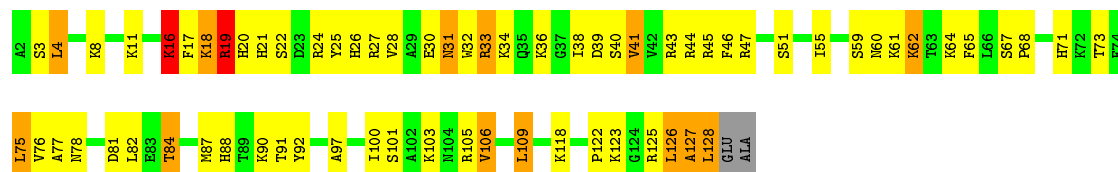
- Molecule 67: 60S ribosomal protein L31-A

Chain o1:  76% 14% 7% •




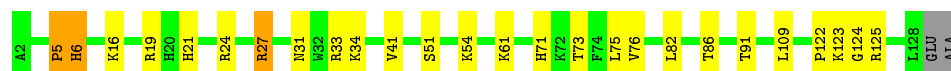
- Molecule 68: 60S ribosomal protein L32

Chain O2:  45% 42% 10% • •



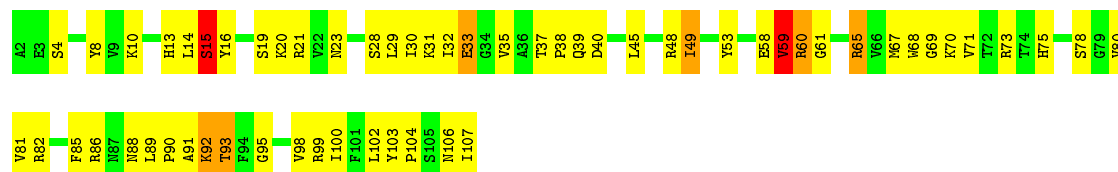
- Molecule 68: 60S ribosomal protein L32

Chain o2:  78% 18% • •




- Molecule 69: 60S ribosomal protein L33-A

Chain O3:  44% 48% 6% •



- Molecule 69: 60S ribosomal protein L33-A

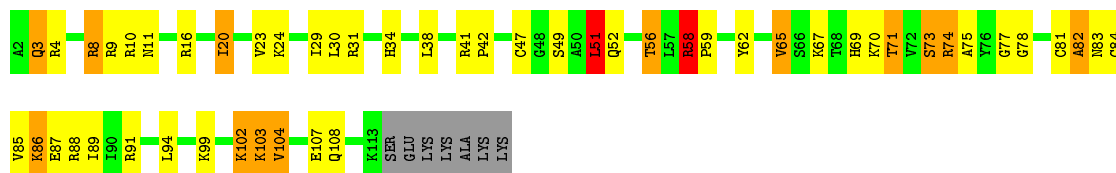


Chain o3:  84% 16%




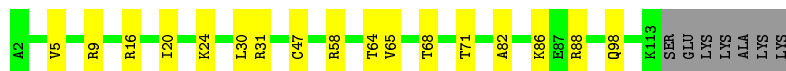
- Molecule 70: 60S ribosomal protein L34-A

Chain O4:  50% 31% 11% 6%



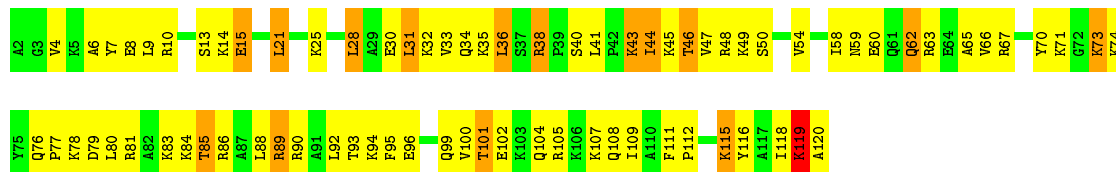
- Molecule 70: 60S ribosomal protein L34-A

Chain o4:  80% 14% 6%




- Molecule 71: 60S ribosomal protein L35-A

Chain O5:  35% 51% 13%



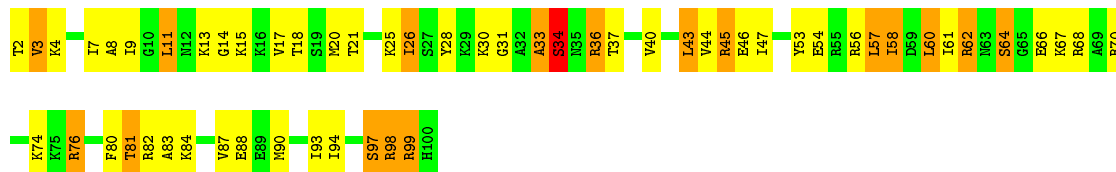
- Molecule 71: 60S ribosomal protein L35-A

Chain o5:  78% 20%



- Molecule 72: 60S ribosomal protein L36-A

Chain O6:  42% 39% 17%



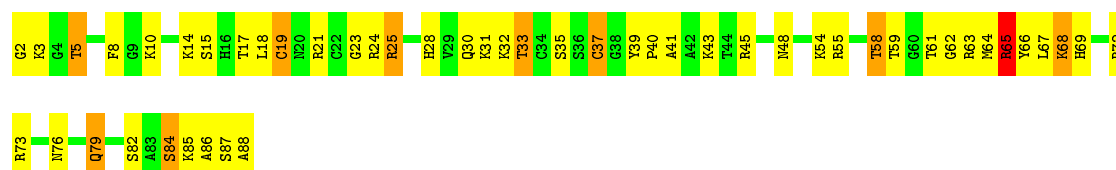
- Molecule 72: 60S ribosomal protein L36-A

Chain o6:  74% 23%



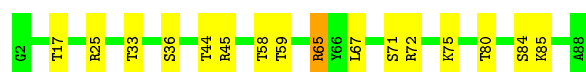
- Molecule 73: 60S ribosomal protein L37-A

Chain O7:  43% 46% 10%



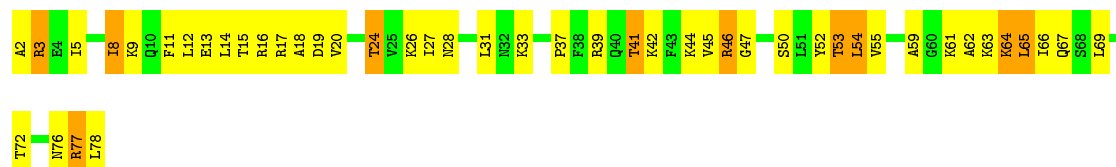
- Molecule 73: 60S ribosomal protein L37-A

Chain o7:  82% 17%




- Molecule 74: 60S ribosomal protein L38

Chain O8:  39% 48% 13%



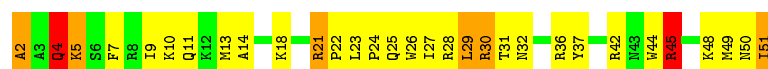
- Molecule 74: 60S ribosomal protein L38

Chain o8:  79% 19%




- Molecule 75: 60S ribosomal protein L39

Chain O9:  38% 46% 12%

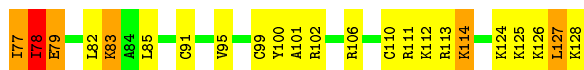


- Molecule 75: 60S ribosomal protein L39

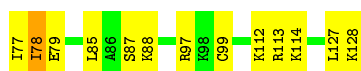
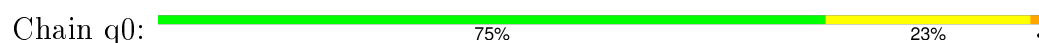
Chain o9:  76% 24%



- Molecule 76: Ubiquitin-60S ribosomal protein L40



- Molecule 76: Ubiquitin-60S ribosomal protein L40



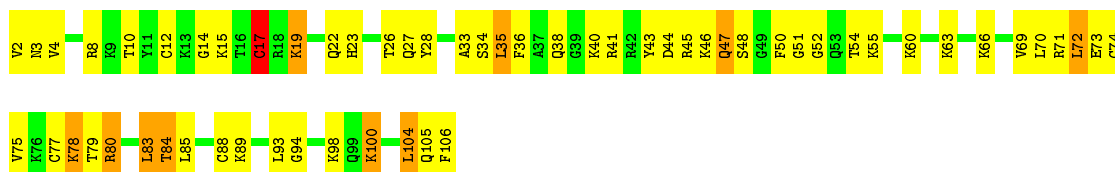
- Molecule 77: 60S ribosomal protein L41-A



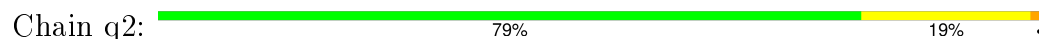
- Molecule 77: 60S ribosomal protein L41-A



- Molecule 78: 60S ribosomal protein L42-A



- Molecule 78: 60S ribosomal protein L42-A



- Molecule 79: 60S ribosomal protein L43-A



- Molecule 84: UNKNOWN PROTEIN p1

Chain p1:  100%

There are no outlier residues recorded for this chain.

- Molecule 85: UNKNOWN PROTEIN p2

Chain p2:  100%

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	436.68Å 287.99Å 304.76Å 90.00° 99.01° 90.00°	Depositor
Resolution (Å)	99.80 – 3.00	Depositor
% Data completeness (in resolution range)	100.0 (99.80-3.00)	Depositor
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, $R_{free}$	0.199 , 0.245	Depositor
Wilson B-factor (Å <sup>2</sup> )	74.8	Xtriage
Anisotropy	0.176	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 1479408 reflections	Xtriage
Total number of atoms	411204	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	2	0.79	4/41698 (0.0%)	1.35	389/64972 (0.6%)
1	6	0.93	38/42765 (0.1%)	1.43	556/66634 (0.8%)
2	S0	0.48	0/1617	0.67	0/2215
2	s0	0.52	0/1623	0.70	0/2222
3	S1	0.39	0/1735	0.66	3/2335 (0.1%)
3	s1	0.55	0/1748	0.73	3/2352 (0.1%)
4	S2	0.53	0/1665	0.70	1/2263 (0.0%)
4	s2	0.63	0/1665	0.77	0/2263
5	S3	0.52	0/1759	0.67	1/2368 (0.0%)
5	s3	0.48	0/1759	0.61	0/2368
6	S4	0.51	0/2109	0.77	4/2839 (0.1%)
6	s4	0.58	0/2109	0.81	1/2839 (0.0%)
7	S5	0.44	0/1629	0.62	0/2202
7	s5	0.49	0/1629	0.69	1/2202 (0.0%)
8	S6	0.51	0/1823	0.69	0/2439
8	s6	0.61	1/1779 (0.1%)	0.72	0/2379
9	S7	0.45	0/1506	0.66	0/2028
9	s7	0.50	0/1516	0.70	1/2043 (0.0%)
10	S8	0.58	0/1514	0.78	1/2021 (0.0%)
10	s8	0.67	0/1514	0.81	2/2021 (0.1%)
11	S9	0.53	0/1519	0.68	0/2035
11	s9	0.58	0/1519	0.78	1/2035 (0.0%)
12	C0	0.45	0/790	0.74	2/1069 (0.2%)
12	c0	0.40	0/777	0.65	3/1049 (0.3%)
13	C1	0.63	0/1240	0.78	1/1675 (0.1%)
13	c1	0.68	1/1194 (0.1%)	0.78	1/1610 (0.1%)
14	C2	0.39	0/900	0.62	0/1224
14	c2	0.32	0/900	0.59	1/1224 (0.1%)
15	C3	0.52	0/1215	0.69	2/1638 (0.1%)
15	c3	0.62	0/1215	0.77	0/1638
16	C4	0.41	0/901	0.66	0/1217
16	c4	0.56	0/960	0.80	1/1290 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	C5	0.50	0/998	0.69	0/1341
17	c5	0.53	0/1060	0.72	0/1426
18	C6	0.48	0/1125	0.70	2/1510 (0.1%)
18	c6	0.52	0/1131	0.73	0/1518
19	C7	0.47	0/935	0.67	0/1254
19	c7	0.56	0/914	0.73	0/1224
20	C8	0.48	0/1211	0.67	1/1628 (0.1%)
20	c8	0.52	0/1211	0.71	1/1628 (0.1%)
21	C9	0.46	0/1130	0.66	1/1517 (0.1%)
21	c9	0.52	0/1130	0.69	0/1517
22	D0	0.51	0/865	0.64	0/1169
22	d0	0.54	0/892	0.71	0/1205
23	D1	0.50	0/693	0.67	0/935
23	d1	0.57	0/693	0.76	0/935
24	D2	0.53	0/1038	0.73	1/1395 (0.1%)
24	d2	0.66	0/1038	0.81	1/1395 (0.1%)
25	D3	0.65	0/1139	0.84	2/1518 (0.1%)
25	d3	0.74	0/1139	0.90	3/1518 (0.2%)
26	D4	0.48	0/1087	0.64	1/1449 (0.1%)
26	d4	0.57	0/1087	0.72	0/1449
27	D5	0.39	0/571	0.69	0/768
27	d5	0.45	0/566	0.68	0/761
28	D6	0.48	0/782	0.70	0/1047
28	d6	0.59	0/782	0.70	0/1047
29	D7	0.48	0/620	0.67	0/838
29	d7	0.49	0/620	0.73	0/838
30	D8	0.38	0/499	0.58	0/670
30	d8	0.47	0/499	0.71	0/670
31	D9	0.58	0/452	0.77	1/600 (0.2%)
31	d9	0.61	0/452	0.68	0/600
32	E0	0.49	0/483	0.68	0/643
33	E1	0.49	0/577	0.78	0/770
34	SR	0.42	0/2494	0.65	1/3393 (0.0%)
34	sR	0.41	0/2495	0.56	0/3395
35	SM	0.54	0/1113	0.74	2/1502 (0.1%)
35	sM	0.56	0/683	0.70	1/923 (0.1%)
36	1	1.22	218/75394 (0.3%)	1.73	2216/117545 (1.9%)
36	5	1.28	278/75414 (0.4%)	1.76	2268/117575 (1.9%)
37	3	1.01	2/2883 (0.1%)	1.53	48/4491 (1.1%)
37	7	1.25	7/2883 (0.2%)	1.72	82/4491 (1.8%)
38	4	1.15	2/3746 (0.1%)	1.66	87/5832 (1.5%)
38	8	1.11	6/3746 (0.2%)	1.57	46/5832 (0.8%)
39	L2	0.73	0/1948	0.88	1/2617 (0.0%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	l2	0.81	1/1946 (0.1%)	0.89	0/2614
40	L3	0.77	0/3146	0.86	2/4228 (0.0%)
40	l3	0.90	1/3146 (0.0%)	0.94	5/4228 (0.1%)
41	L4	0.88	0/2800	0.98	8/3790 (0.2%)
41	l4	0.80	1/2800 (0.0%)	0.95	4/3790 (0.1%)
42	L5	0.59	0/2425	0.70	0/3271
42	l5	0.77	0/2408	0.86	3/3248 (0.1%)
43	L6	0.83	0/1260	0.85	0/1694
43	l6	0.83	0/1269	0.90	3/1705 (0.2%)
44	L7	0.81	1/1821 (0.1%)	0.90	2/2451 (0.1%)
44	l7	0.90	1/1828 (0.1%)	0.95	4/2461 (0.2%)
45	L8	0.61	0/1836	0.72	0/2481
45	l8	0.58	0/1795	0.70	2/2429 (0.1%)
46	L9	0.71	0/1539	0.78	0/2073
46	l9	0.85	0/1539	0.86	1/2073 (0.0%)
47	M0	0.80	0/1741	0.90	4/2335 (0.2%)
47	m0	0.80	1/1758 (0.1%)	0.84	1/2358 (0.0%)
48	M1	0.56	0/1374	0.74	1/1842 (0.1%)
48	m1	0.69	0/1374	0.83	1/1842 (0.1%)
49	M3	0.80	0/1568	0.85	0/2106
49	m3	0.73	0/1573	0.85	1/2113 (0.0%)
50	M4	0.77	0/1068	0.82	1/1438 (0.1%)
50	m4	0.86	0/1074	0.85	1/1446 (0.1%)
51	M5	0.81	1/1757 (0.1%)	0.91	3/2354 (0.1%)
51	m5	0.73	0/1757	0.83	1/2354 (0.0%)
52	M6	0.93	1/1585 (0.1%)	0.94	3/2128 (0.1%)
52	m6	1.11	5/1585 (0.3%)	1.08	10/2128 (0.5%)
53	M7	0.84	0/1443	0.87	0/1944
53	m7	0.95	0/1250	0.90	0/1683
54	M8	0.83	0/1465	0.93	3/1965 (0.2%)
54	m8	0.81	0/1465	0.97	4/1965 (0.2%)
55	M9	0.61	0/1538	0.71	0/2050
55	m9	0.68	0/1538	0.75	1/2050 (0.0%)
56	N0	0.81	0/1481	0.89	3/1990 (0.2%)
56	n0	0.92	0/1481	0.93	3/1990 (0.2%)
57	N1	0.84	1/1300 (0.1%)	0.84	0/1743
57	n1	0.90	2/1300 (0.2%)	0.86	0/1743
58	N2	0.45	0/812	0.64	0/1099
58	n2	0.54	0/794	0.69	0/1076
59	N3	0.75	0/1018	0.87	1/1369 (0.1%)
59	n3	0.89	0/1018	0.93	2/1369 (0.1%)
60	N4	0.62	0/712	0.72	0/958
60	n4	0.75	0/1052	0.82	0/1398

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
61	N5	0.65	0/979	0.78	2/1321 (0.2%)
61	n5	0.69	0/974	0.82	0/1314
62	N6	0.75	0/1004	0.95	2/1341 (0.1%)
62	n6	0.71	0/1004	0.88	0/1341
63	N7	0.56	0/1118	0.69	0/1497
63	n7	0.51	0/1118	0.72	3/1497 (0.2%)
64	N8	0.83	0/1204	0.96	3/1612 (0.2%)
64	n8	0.84	1/1204 (0.1%)	0.95	2/1612 (0.1%)
65	N9	0.81	0/473	0.84	0/629
65	n9	0.88	0/473	0.98	1/629 (0.2%)
66	O0	0.52	0/751	0.69	0/1008
66	o0	0.56	0/775	0.70	0/1040
67	O1	0.67	0/890	0.77	1/1196 (0.1%)
67	o1	0.85	0/897	0.91	0/1205
68	O2	0.91	0/1041	0.95	2/1394 (0.1%)
68	o2	0.93	0/1041	0.98	1/1394 (0.1%)
69	O3	0.98	1/868 (0.1%)	0.88	1/1168 (0.1%)
69	o3	0.94	0/868	0.89	1/1168 (0.1%)
70	O4	0.69	0/890	0.84	2/1189 (0.2%)
70	o4	0.65	0/890	0.82	0/1189
71	O5	0.78	0/978	0.81	1/1301 (0.1%)
71	o5	0.62	0/974	0.73	0/1297
72	O6	0.69	0/778	0.82	0/1034
72	o6	0.63	0/777	0.71	0/1033
73	O7	0.89	1/696 (0.1%)	0.98	1/923 (0.1%)
73	o7	0.77	0/696	0.90	2/923 (0.2%)
74	O8	0.58	0/618	0.67	0/826
74	o8	0.46	0/614	0.65	0/822
75	O9	0.88	1/443 (0.2%)	0.91	1/588 (0.2%)
75	o9	0.74	0/443	0.88	0/588
76	Q0	0.76	0/423	0.88	0/562
76	q0	1.00	1/423 (0.2%)	0.96	0/562
77	Q1	0.67	0/234	0.84	0/300
77	q1	0.90	0/234	1.10	3/300 (1.0%)
78	Q2	0.98	1/860 (0.1%)	0.90	0/1136
78	q2	0.86	1/860 (0.1%)	0.86	0/1136
79	Q3	0.77	0/701	0.85	1/934 (0.1%)
79	q3	0.78	0/701	0.87	1/934 (0.1%)
80	e0	0.59	0/499	0.81	0/665
81	e1	0.42	0/619	0.66	0/822
83	p0	0.49	0/1092	0.63	0/1474
All	All	0.96	580/430074 (0.1%)	1.37	5850/631364 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	s5	0	2
9	S7	0	1
9	s7	0	1
16	C4	0	1
16	c4	0	1
17	c5	0	1
18	c6	0	1
19	C7	0	2
22	d0	0	1
26	d4	0	1
27	D5	0	1
28	D6	0	2
33	E1	0	1
39	L2	0	1
39	l2	0	1
40	L3	0	1
41	L4	0	1
43	l6	0	1
44	l7	0	3
45	L8	0	2
48	m1	0	1
49	M3	0	1
50	M4	0	1
52	M6	0	2
52	m6	0	1
53	m7	0	1
59	n3	0	1
60	n4	0	1
64	N8	0	1
64	n8	0	1
65	N9	0	1
65	n9	0	1
67	O1	0	1
75	o9	0	1
79	q3	0	1
81	e1	0	1
All	All	0	43

The worst 5 of 580 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2872	A	N9-C4	-14.78	1.28	1.37
78	Q2	17	CYS	CB-SG	14.00	2.06	1.82
36	5	1152	G	N9-C4	-11.81	1.28	1.38
78	q2	17	CYS	CB-SG	10.92	2.00	1.82
36	1	2404	A	N9-C4	-10.49	1.31	1.37

The worst 5 of 5850 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-C5	28.07	142.64	128.60
36	5	1152	G	N3-C4-N9	-28.03	109.18	126.00
36	1	2945	G	O5'-P-OP2	-22.30	83.93	110.70
36	5	1152	G	C2-N3-C4	-19.70	102.05	111.90
36	1	1308	A	O5'-P-OP2	-19.57	87.22	110.70

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	124	ASP	Peptide
19	C7	22	PRO	Peptide
19	C7	85	VAL	Peptide
27	D5	94	LYS	Peptide
9	S7	131	PHE	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37283	0	18757	844	0
1	6	38238	0	19240	808	0
2	S0	1577	0	1567	156	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	163	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	131	0
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	110	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	163	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	159	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	139	0
8	s6	1755	0	1845	0	0
9	S7	1481	0	1572	114	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	113	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	128	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	50	0
12	c0	762	0	699	0	0
13	C1	1214	0	1259	79	0
13	c1	1168	0	1231	0	0
14	C2	892	0	891	58	0
14	c2	892	0	891	0	0
15	C3	1192	0	1255	92	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	101	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	89	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	99	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	74	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	119	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	83	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	86	0
22	d0	882	0	939	0	0
23	D1	684	0	672	57	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	78	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	82	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	84	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	48	0
27	d5	558	0	598	0	0
28	D6	769	0	814	99	0
28	d6	769	0	814	0	0
29	D7	610	0	631	34	0
29	d7	610	0	632	0	0
30	D8	497	0	535	45	0
30	d8	497	0	535	0	0
31	D9	442	0	428	31	0
31	d9	442	0	428	0	0
32	E0	475	0	525	39	0
33	E1	566	0	602	56	0
34	SR	2441	0	2397	178	0
34	sR	2442	0	2392	0	1
35	SM	1104	0	996	88	0
35	sM	680	0	607	0	0
36	1	67355	0	33846	1138	1
36	5	67376	0	33854	1158	0
37	3	2579	0	1304	49	0
37	7	2579	0	1303	45	0
38	4	3353	0	1695	64	0
38	8	3353	0	1695	67	0
39	L2	1914	0	1981	137	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	232	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	201	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	191	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	72	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	112	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1875	143	0
45	l8	1763	0	1817	0	0
46	L9	1518	0	1587	100	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1736	128	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	118	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	73	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	135	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	98	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	102	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	108	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	84	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	100	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	27	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	67	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	28	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	63	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	76	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	77	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	96	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	34	0
65	n9	462	0	491	0	0
66	O0	743	0	797	55	0
66	o0	767	0	816	0	0
67	O1	876	0	912	56	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	67	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	o3	850	0	880	0	0
70	O4	880	0	945	56	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	75	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	59	0
72	o6	770	0	846	0	0
73	O7	681	0	683	42	0
73	o7	681	0	683	0	0
74	O8	612	0	682	40	0
74	o8	608	0	671	0	0
75	O9	436	0	475	44	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	18	0
76	q0	417	0	455	0	0
77	Q1	233	0	284	28	0
77	q1	233	0	284	0	0
78	Q2	847	0	916	57	0
78	q2	847	0	915	0	0
79	Q3	694	0	734	54	0
79	q3	694	0	734	0	0
80	e0	491	0	542	0	0
81	e1	608	0	655	0	0
82	m2	750	0	175	0	0
83	p0	1077	0	1041	0	0
84	p1	235	0	51	0	0
85	p2	230	0	54	0	0
86	1	474	0	0	0	0
86	2	124	0	0	0	0
86	3	14	0	0	0	0
86	4	23	0	0	0	0
86	5	507	0	0	0	0
86	6	145	0	0	0	0
86	7	15	0	0	0	0
86	8	12	0	0	0	0
86	D3	1	0	0	0	0
86	L2	1	0	0	0	0
86	L3	2	0	0	0	0
86	L4	1	0	0	0	0
86	L5	1	0	0	0	0
86	L7	2	0	0	0	0
86	L8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	M0	2	0	0	0	0
86	M1	1	0	0	0	0
86	M3	3	0	0	0	0
86	M5	2	0	0	0	0
86	M6	1	0	0	0	0
86	M7	5	0	0	0	0
86	M9	1	0	0	0	0
86	N0	1	0	0	0	0
86	N3	3	0	0	0	0
86	N5	1	0	0	0	0
86	N6	1	0	0	0	0
86	N8	4	0	0	0	0
86	O1	1	0	0	0	0
86	O4	1	0	0	0	0
86	O7	2	0	0	0	0
86	Q2	1	0	0	0	0
86	S2	2	0	0	0	0
86	S8	1	0	0	0	0
86	SM	1	0	0	0	0
86	c1	2	0	0	0	0
86	c7	2	0	0	0	0
86	c8	1	0	0	0	0
86	c9	1	0	0	0	0
86	d3	2	0	0	0	0
86	d4	1	0	0	0	0
86	d6	1	0	0	0	0
86	l2	2	0	0	0	0
86	l3	2	0	0	0	0
86	l4	1	0	0	0	0
86	l5	3	0	0	0	0
86	l7	1	0	0	0	0
86	m1	1	0	0	0	0
86	m5	4	0	0	0	0
86	m6	1	0	0	0	0
86	m7	5	0	0	0	0
86	n0	2	0	0	0	0
86	n3	2	0	0	0	0
86	n6	2	0	0	0	0
86	n8	4	0	0	0	0
86	n9	1	0	0	0	0
86	o1	2	0	0	0	0
86	o3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	o4	1	0	0	0	0
86	q0	1	0	0	0	0
86	q1	1	0	0	0	0
86	q3	1	0	0	0	0
86	s1	1	0	0	0	0
86	s8	2	0	0	0	0
86	sM	2	0	0	0	0
87	1	2450	0	0	243	0
87	2	1113	0	0	125	0
87	3	84	0	0	4	0
87	4	105	0	0	7	0
87	5	2499	0	0	244	0
87	6	1120	0	0	107	0
87	7	77	0	0	9	0
87	8	98	0	0	21	0
87	C3	7	0	0	0	0
87	C5	7	0	0	3	0
87	C8	7	0	0	0	0
87	D9	7	0	0	0	0
87	L3	14	0	0	1	0
87	L4	7	0	0	4	0
87	M0	7	0	0	0	0
87	M5	7	0	0	1	0
87	M6	7	0	0	0	0
87	M7	14	0	0	2	0
87	M8	7	0	0	0	0
87	M9	7	0	0	1	0
87	N9	7	0	0	0	0
87	O1	7	0	0	6	0
87	O2	7	0	0	0	0
87	O3	7	0	0	1	0
87	O7	7	0	0	6	0
87	Q2	7	0	0	1	0
87	S8	7	0	0	0	0
87	SR	7	0	0	0	0
87	c3	7	0	0	0	0
87	c5	7	0	0	0	0
87	c8	7	0	0	0	0
87	d4	7	0	0	0	0
87	d9	7	0	0	0	0
87	l3	14	0	0	0	0
87	l4	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	l5	21	0	0	0	0
87	l9	7	0	0	0	0
87	m0	14	0	0	0	0
87	m1	7	0	0	0	0
87	m4	7	0	0	0	0
87	m5	7	0	0	0	0
87	m6	7	0	0	0	0
87	m7	7	0	0	0	0
87	m8	7	0	0	0	0
87	n3	7	0	0	0	0
87	n9	7	0	0	0	0
87	o2	7	0	0	0	0
87	o3	7	0	0	0	0
87	o7	7	0	0	0	0
87	o9	7	0	0	0	0
87	q2	7	0	0	0	0
87	s1	14	0	0	0	0
87	s4	7	0	0	0	0
87	s8	7	0	0	0	0
87	sR	7	0	0	0	0
88	D6	1	0	0	0	0
88	D7	1	0	0	0	0
88	D9	1	0	0	0	0
88	E1	1	0	0	0	0
88	O7	1	0	0	0	0
88	Q0	1	0	0	0	0
88	Q2	1	0	0	2	0
88	Q3	1	0	0	0	0
88	d6	1	0	0	0	0
88	d7	1	0	0	0	0
88	d9	1	0	0	0	0
88	e1	1	0	0	0	0
88	o7	1	0	0	0	0
88	q0	1	0	0	0	0
88	q2	1	0	0	0	0
88	q3	1	0	0	0	0
89	1	19	0	19	0	0
89	5	19	0	19	0	0
All	All	411204	0	297319	9494	1

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 9494 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:Q2:17:CYS:CB	78:Q2:17:CYS:SG	2.06	1.44
78:Q2:17:CYS:CB	88:Q2:501:ZN:ZN	1.06	1.30
78:Q2:17:CYS:SG	78:Q2:77:CYS:HB3	2.09	1.21
78:Q2:17:CYS:SG	88:Q2:501:ZN:ZN	1.35	1.16
36:5:2273:G:O6	87:5:4206:OHX:N5	1.88	1.06

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1:3156:U:O4	34:sR:46:LYS:NZ[2_656]	2.17	0.03

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	141 (69%)	40 (20%)	23 (11%)	0	2
2	s0	204/251 (81%)	156 (76%)	27 (13%)	21 (10%)	1	3
3	S1	212/254 (84%)	147 (69%)	38 (18%)	27 (13%)	0	1
3	s1	214/254 (84%)	179 (84%)	27 (13%)	8 (4%)	4	23
4	S2	215/253 (85%)	179 (83%)	22 (10%)	14 (6%)	1	8
4	s2	215/253 (85%)	178 (83%)	26 (12%)	11 (5%)	2	15
5	S3	221/239 (92%)	181 (82%)	32 (14%)	8 (4%)	4	24
5	s3	221/239 (92%)	185 (84%)	24 (11%)	12 (5%)	2	14
6	S4	258/260 (99%)	206 (80%)	33 (13%)	19 (7%)	1	6
6	s4	258/260 (99%)	209 (81%)	34 (13%)	15 (6%)	2	12
7	S5	204/224 (91%)	159 (78%)	27 (13%)	18 (9%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	s5	204/224 (91%)	159 (78%)	32 (16%)	13 (6%)	2	9
8	S6	224/236 (95%)	198 (88%)	13 (6%)	13 (6%)	2	12
8	s6	216/236 (92%)	188 (87%)	21 (10%)	7 (3%)	5	27
9	S7	182/189 (96%)	134 (74%)	25 (14%)	23 (13%)	0	1
9	s7	184/189 (97%)	145 (79%)	27 (15%)	12 (6%)	1	8
10	S8	184/200 (92%)	149 (81%)	24 (13%)	11 (6%)	2	11
10	s8	184/200 (92%)	152 (83%)	22 (12%)	10 (5%)	2	14
11	S9	183/196 (93%)	152 (83%)	20 (11%)	11 (6%)	2	11
11	s9	183/196 (93%)	150 (82%)	27 (15%)	6 (3%)	5	26
12	C0	94/105 (90%)	74 (79%)	11 (12%)	9 (10%)	1	3
12	c0	92/105 (88%)	61 (66%)	12 (13%)	19 (21%)	0	0
13	C1	153/155 (99%)	120 (78%)	18 (12%)	15 (10%)	1	3
13	c1	144/155 (93%)	126 (88%)	14 (10%)	4 (3%)	6	30
14	C2	122/142 (86%)	69 (57%)	33 (27%)	20 (16%)	0	1
14	c2	122/142 (86%)	72 (59%)	35 (29%)	15 (12%)	0	2
15	C3	148/150 (99%)	123 (83%)	19 (13%)	6 (4%)	3	20
15	c3	148/150 (99%)	120 (81%)	17 (12%)	11 (7%)	1	6
16	C4	125/136 (92%)	96 (77%)	17 (14%)	12 (10%)	1	3
16	c4	126/136 (93%)	102 (81%)	17 (14%)	7 (6%)	2	13
17	C5	122/141 (86%)	96 (79%)	15 (12%)	11 (9%)	1	4
17	c5	133/141 (94%)	96 (72%)	20 (15%)	17 (13%)	0	1
18	C6	139/142 (98%)	115 (83%)	17 (12%)	7 (5%)	3	15
18	c6	140/142 (99%)	123 (88%)	9 (6%)	8 (6%)	2	12
19	C7	116/136 (85%)	88 (76%)	20 (17%)	8 (7%)	1	7
19	c7	113/136 (83%)	89 (79%)	19 (17%)	5 (4%)	3	18
20	C8	143/145 (99%)	114 (80%)	19 (13%)	10 (7%)	1	7
20	c8	143/145 (99%)	116 (81%)	18 (13%)	9 (6%)	2	9
21	C9	141/143 (99%)	114 (81%)	22 (16%)	5 (4%)	4	24
21	c9	141/143 (99%)	120 (85%)	16 (11%)	5 (4%)	4	24
22	D0	105/120 (88%)	83 (79%)	14 (13%)	8 (8%)	1	6
22	d0	108/120 (90%)	84 (78%)	13 (12%)	11 (10%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	D1	85/87 (98%)	62 (73%)	18 (21%)	5 (6%)	2	11
23	d1	85/87 (98%)	71 (84%)	12 (14%)	2 (2%)	7	35
24	D2	127/129 (98%)	108 (85%)	17 (13%)	2 (2%)	12	48
24	d2	127/129 (98%)	111 (87%)	14 (11%)	2 (2%)	12	48
25	D3	142/144 (99%)	110 (78%)	17 (12%)	15 (11%)	0	3
25	d3	142/144 (99%)	120 (84%)	18 (13%)	4 (3%)	6	30
26	D4	132/134 (98%)	114 (86%)	8 (6%)	10 (8%)	1	6
26	d4	132/134 (98%)	104 (79%)	20 (15%)	8 (6%)	2	11
27	D5	68/107 (64%)	48 (71%)	13 (19%)	7 (10%)	1	3
27	d5	67/107 (63%)	46 (69%)	16 (24%)	5 (8%)	1	6
28	D6	95/97 (98%)	62 (65%)	14 (15%)	19 (20%)	0	0
28	d6	95/97 (98%)	73 (77%)	10 (10%)	12 (13%)	0	1
29	D7	79/81 (98%)	54 (68%)	17 (22%)	8 (10%)	1	3
29	d7	79/81 (98%)	61 (77%)	15 (19%)	3 (4%)	4	22
30	D8	61/66 (92%)	49 (80%)	7 (12%)	5 (8%)	1	5
30	d8	61/66 (92%)	43 (70%)	12 (20%)	6 (10%)	1	3
31	D9	51/55 (93%)	42 (82%)	6 (12%)	3 (6%)	2	11
31	d9	51/55 (93%)	41 (80%)	6 (12%)	4 (8%)	1	6
32	E0	58/60 (97%)	46 (79%)	10 (17%)	2 (3%)	5	25
33	E1	69/76 (91%)	36 (52%)	14 (20%)	19 (28%)	0	0
34	SR	316/318 (99%)	248 (78%)	51 (16%)	17 (5%)	2	14
34	sR	316/318 (99%)	274 (87%)	30 (10%)	12 (4%)	4	22
35	SM	155/273 (57%)	111 (72%)	24 (16%)	20 (13%)	0	1
35	sM	98/273 (36%)	64 (65%)	20 (20%)	14 (14%)	0	1
39	L2	250/253 (99%)	224 (90%)	17 (7%)	9 (4%)	4	24
39	l2	250/253 (99%)	218 (87%)	21 (8%)	11 (4%)	3	18
40	L3	384/386 (100%)	346 (90%)	22 (6%)	16 (4%)	3	20
40	l3	384/386 (100%)	345 (90%)	30 (8%)	9 (2%)	8	36
41	L4	359/361 (99%)	312 (87%)	28 (8%)	19 (5%)	2	14
41	l4	359/361 (99%)	298 (83%)	44 (12%)	17 (5%)	3	17
42	L5	294/296 (99%)	252 (86%)	29 (10%)	13 (4%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	l5	292/296 (99%)	254 (87%)	26 (9%)	12 (4%)	3	20
43	L6	152/175 (87%)	132 (87%)	16 (10%)	4 (3%)	7	33
43	l6	153/175 (87%)	132 (86%)	16 (10%)	5 (3%)	5	26
44	L7	220/243 (90%)	196 (89%)	19 (9%)	5 (2%)	8	36
44	l7	221/243 (91%)	194 (88%)	22 (10%)	5 (2%)	8	36
45	L8	231/255 (91%)	188 (81%)	31 (13%)	12 (5%)	2	15
45	l8	229/255 (90%)	182 (80%)	31 (14%)	16 (7%)	1	7
46	L9	189/191 (99%)	162 (86%)	21 (11%)	6 (3%)	5	27
46	l9	189/191 (99%)	165 (87%)	19 (10%)	5 (3%)	7	33
47	M0	207/220 (94%)	179 (86%)	21 (10%)	7 (3%)	5	25
47	m0	209/220 (95%)	170 (81%)	22 (10%)	17 (8%)	1	5
48	M1	167/173 (96%)	133 (80%)	17 (10%)	17 (10%)	1	3
48	m1	167/173 (96%)	141 (84%)	17 (10%)	9 (5%)	2	14
49	M3	191/198 (96%)	160 (84%)	26 (14%)	5 (3%)	7	33
49	m3	192/198 (97%)	160 (83%)	20 (10%)	12 (6%)	2	9
50	M4	134/137 (98%)	113 (84%)	12 (9%)	9 (7%)	1	8
50	m4	135/137 (98%)	126 (93%)	6 (4%)	3 (2%)	8	38
51	M5	201/203 (99%)	183 (91%)	12 (6%)	6 (3%)	5	29
51	m5	201/203 (99%)	185 (92%)	10 (5%)	6 (3%)	5	29
52	M6	195/198 (98%)	175 (90%)	15 (8%)	5 (3%)	7	33
52	m6	195/198 (98%)	179 (92%)	9 (5%)	7 (4%)	4	24
53	M7	181/183 (99%)	156 (86%)	20 (11%)	5 (3%)	6	30
53	m7	153/183 (84%)	142 (93%)	10 (6%)	1 (1%)	26	70
54	M8	183/185 (99%)	161 (88%)	18 (10%)	4 (2%)	8	38
54	m8	183/185 (99%)	155 (85%)	21 (12%)	7 (4%)	4	22
55	M9	186/188 (99%)	166 (89%)	19 (10%)	1 (0%)	34	76
55	m9	186/188 (99%)	170 (91%)	13 (7%)	3 (2%)	12	48
56	N0	170/172 (99%)	157 (92%)	11 (6%)	2 (1%)	16	56
56	n0	170/172 (99%)	158 (93%)	10 (6%)	2 (1%)	16	56
57	N1	157/159 (99%)	139 (88%)	11 (7%)	7 (4%)	3	18
57	n1	157/159 (99%)	140 (89%)	11 (7%)	6 (4%)	4	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	N2	98/120 (82%)	72 (74%)	19 (19%)	7 (7%)	1	7
58	n2	96/120 (80%)	81 (84%)	11 (12%)	4 (4%)	3	20
59	N3	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	13	50
59	n3	134/136 (98%)	125 (93%)	9 (7%)	0	100	100
60	N4	96/155 (62%)	75 (78%)	12 (12%)	9 (9%)	1	4
60	n4	133/155 (86%)	105 (79%)	16 (12%)	12 (9%)	1	4
61	N5	119/141 (84%)	106 (89%)	12 (10%)	1 (1%)	24	66
61	n5	118/141 (84%)	101 (86%)	12 (10%)	5 (4%)	3	20
62	N6	124/126 (98%)	112 (90%)	6 (5%)	6 (5%)	3	17
62	n6	124/126 (98%)	113 (91%)	6 (5%)	5 (4%)	4	21
63	N7	133/135 (98%)	112 (84%)	12 (9%)	9 (7%)	1	7
63	n7	133/135 (98%)	106 (80%)	19 (14%)	8 (6%)	2	11
64	N8	146/148 (99%)	119 (82%)	19 (13%)	8 (6%)	2	13
64	n8	146/148 (99%)	124 (85%)	15 (10%)	7 (5%)	3	17
65	N9	56/58 (97%)	48 (86%)	4 (7%)	4 (7%)	1	7
65	n9	56/58 (97%)	43 (77%)	6 (11%)	7 (12%)	0	1
66	O0	95/104 (91%)	86 (90%)	6 (6%)	3 (3%)	5	27
66	o0	98/104 (94%)	84 (86%)	11 (11%)	3 (3%)	5	28
67	O1	107/112 (96%)	96 (90%)	7 (6%)	4 (4%)	4	23
67	o1	107/112 (96%)	88 (82%)	7 (6%)	12 (11%)	0	2
68	O2	125/129 (97%)	110 (88%)	14 (11%)	1 (1%)	24	66
68	o2	125/129 (97%)	108 (86%)	12 (10%)	5 (4%)	4	21
69	O3	104/106 (98%)	96 (92%)	6 (6%)	2 (2%)	10	43
69	o3	104/106 (98%)	95 (91%)	7 (7%)	2 (2%)	10	43
70	O4	110/119 (92%)	95 (86%)	13 (12%)	2 (2%)	11	45
70	o4	110/119 (92%)	99 (90%)	10 (9%)	1 (1%)	21	64
71	O5	117/119 (98%)	106 (91%)	10 (8%)	1 (1%)	21	64
71	o5	117/119 (98%)	97 (83%)	11 (9%)	9 (8%)	1	6
72	O6	97/99 (98%)	80 (82%)	11 (11%)	6 (6%)	2	10
72	o6	97/99 (98%)	84 (87%)	9 (9%)	4 (4%)	3	20
73	O7	85/87 (98%)	73 (86%)	8 (9%)	4 (5%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
73	o7	85/87 (98%)	72 (85%)	12 (14%)	1 (1%)	16	56
74	O8	75/77 (97%)	66 (88%)	8 (11%)	1 (1%)	15	53
74	o8	75/77 (97%)	66 (88%)	6 (8%)	3 (4%)	4	21
75	O9	48/50 (96%)	43 (90%)	4 (8%)	1 (2%)	9	40
75	o9	48/50 (96%)	40 (83%)	7 (15%)	1 (2%)	9	40
76	Q0	50/52 (96%)	47 (94%)	1 (2%)	2 (4%)	4	21
76	q0	50/52 (96%)	45 (90%)	4 (8%)	1 (2%)	9	41
77	Q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	3	19
77	q1	23/25 (92%)	19 (83%)	4 (17%)	0	100	100
78	Q2	103/105 (98%)	82 (80%)	18 (18%)	3 (3%)	6	29
78	q2	103/105 (98%)	93 (90%)	8 (8%)	2 (2%)	10	43
79	Q3	89/91 (98%)	77 (86%)	10 (11%)	2 (2%)	8	38
79	q3	89/91 (98%)	80 (90%)	8 (9%)	1 (1%)	17	58
80	e0	60/62 (97%)	45 (75%)	8 (13%)	7 (12%)	0	2
81	e1	74/76 (97%)	36 (49%)	19 (26%)	19 (26%)	0	0
83	p0	139/311 (45%)	119 (86%)	16 (12%)	4 (3%)	6	29
All	All	22333/24141 (92%)	18606 (83%)	2512 (11%)	1215 (5%)	2	14

5 of 1215 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	39	ASN
2	S0	66	ALA
2	S0	139	VAL
2	S0	140	ASN

### 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%)	138 (84%)	26 (16%)	3	15
2	s0	165/209 (79%)	130 (79%)	35 (21%)	1	6
3	S1	191/223 (86%)	152 (80%)	39 (20%)	1	7
3	s1	192/223 (86%)	156 (81%)	36 (19%)	2	10
4	S2	176/204 (86%)	143 (81%)	33 (19%)	2	10
4	s2	176/204 (86%)	131 (74%)	45 (26%)	0	3
5	S3	182/194 (94%)	138 (76%)	44 (24%)	1	4
5	s3	182/194 (94%)	149 (82%)	33 (18%)	2	11
6	S4	221/221 (100%)	181 (82%)	40 (18%)	2	11
6	s4	221/221 (100%)	184 (83%)	37 (17%)	3	13
7	S5	173/190 (91%)	145 (84%)	28 (16%)	3	14
7	s5	173/190 (91%)	137 (79%)	36 (21%)	1	7
8	S6	188/201 (94%)	156 (83%)	32 (17%)	2	13
8	s6	187/201 (93%)	151 (81%)	36 (19%)	2	9
9	S7	165/169 (98%)	137 (83%)	28 (17%)	2	13
9	s7	165/169 (98%)	139 (84%)	26 (16%)	3	15
10	S8	150/161 (93%)	127 (85%)	23 (15%)	3	16
10	s8	150/161 (93%)	126 (84%)	24 (16%)	3	15
11	S9	158/165 (96%)	125 (79%)	33 (21%)	1	7
11	s9	158/165 (96%)	128 (81%)	30 (19%)	2	10
12	C0	77/98 (79%)	65 (84%)	12 (16%)	3	16
12	c0	73/98 (74%)	61 (84%)	12 (16%)	3	14
13	C1	129/136 (95%)	105 (81%)	24 (19%)	2	10
13	c1	129/136 (95%)	109 (84%)	20 (16%)	3	16
14	C2	88/118 (75%)	68 (77%)	20 (23%)	1	5
14	c2	88/118 (75%)	64 (73%)	24 (27%)	0	2
15	C3	127/127 (100%)	106 (84%)	21 (16%)	3	13
15	c3	127/127 (100%)	106 (84%)	21 (16%)	3	13
16	C4	81/104 (78%)	57 (70%)	24 (30%)	0	2
16	c4	97/104 (93%)	81 (84%)	16 (16%)	3	13
17	C5	101/117 (86%)	84 (83%)	17 (17%)	2	13
17	c5	103/117 (88%)	81 (79%)	22 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	C6	117/118 (99%)	90 (77%)	27 (23%)	1	5
18	c6	118/118 (100%)	99 (84%)	19 (16%)	3	14
19	C7	94/124 (76%)	73 (78%)	21 (22%)	1	5
19	c7	92/124 (74%)	69 (75%)	23 (25%)	1	3
20	C8	128/128 (100%)	101 (79%)	27 (21%)	1	6
20	c8	128/128 (100%)	104 (81%)	24 (19%)	2	10
21	C9	115/115 (100%)	89 (77%)	26 (23%)	1	5
21	c9	115/115 (100%)	94 (82%)	21 (18%)	2	11
22	D0	100/113 (88%)	76 (76%)	24 (24%)	1	4
22	d0	103/113 (91%)	81 (79%)	22 (21%)	1	6
23	D1	74/74 (100%)	54 (73%)	20 (27%)	0	3
23	d1	74/74 (100%)	59 (80%)	15 (20%)	1	7
24	D2	110/110 (100%)	85 (77%)	25 (23%)	1	5
24	d2	110/110 (100%)	98 (89%)	12 (11%)	8	30
25	D3	119/119 (100%)	97 (82%)	22 (18%)	2	10
25	d3	119/119 (100%)	96 (81%)	23 (19%)	2	9
26	D4	112/112 (100%)	95 (85%)	17 (15%)	3	16
26	d4	112/112 (100%)	97 (87%)	15 (13%)	5	21
27	D5	61/88 (69%)	47 (77%)	14 (23%)	1	5
27	d5	61/88 (69%)	50 (82%)	11 (18%)	2	11
28	D6	83/83 (100%)	70 (84%)	13 (16%)	3	15
28	d6	83/83 (100%)	72 (87%)	11 (13%)	5	21
29	D7	70/70 (100%)	56 (80%)	14 (20%)	1	8
29	d7	70/70 (100%)	58 (83%)	12 (17%)	2	12
30	D8	56/59 (95%)	42 (75%)	14 (25%)	1	3
30	d8	56/59 (95%)	44 (79%)	12 (21%)	1	6
31	D9	47/48 (98%)	40 (85%)	7 (15%)	4	17
31	d9	47/48 (98%)	39 (83%)	8 (17%)	2	13
32	E0	51/51 (100%)	44 (86%)	7 (14%)	4	20
33	E1	62/66 (94%)	47 (76%)	15 (24%)	1	4
34	SR	260/261 (100%)	230 (88%)	30 (12%)	7	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	sR	260/261 (100%)	233 (90%)	27 (10%)	9	32
35	SM	97/228 (42%)	78 (80%)	19 (20%)	1	9
35	sM	54/228 (24%)	43 (80%)	11 (20%)	1	7
39	L2	193/195 (99%)	152 (79%)	41 (21%)	1	6
39	l2	192/195 (98%)	153 (80%)	39 (20%)	1	7
40	L3	321/322 (100%)	248 (77%)	73 (23%)	1	5
40	l3	320/322 (99%)	259 (81%)	61 (19%)	2	10
41	L4	288/288 (100%)	242 (84%)	46 (16%)	3	15
41	l4	288/288 (100%)	231 (80%)	57 (20%)	1	8
42	L5	244/244 (100%)	196 (80%)	48 (20%)	1	9
42	l5	243/244 (100%)	192 (79%)	51 (21%)	1	7
43	L6	134/152 (88%)	116 (87%)	18 (13%)	5	21
43	l6	135/152 (89%)	113 (84%)	22 (16%)	3	14
44	L7	186/204 (91%)	163 (88%)	23 (12%)	6	24
44	l7	187/204 (92%)	157 (84%)	30 (16%)	3	15
45	L8	187/207 (90%)	153 (82%)	34 (18%)	2	11
45	l8	177/207 (86%)	141 (80%)	36 (20%)	1	7
46	L9	171/171 (100%)	137 (80%)	34 (20%)	1	8
46	l9	171/171 (100%)	138 (81%)	33 (19%)	2	9
47	M0	177/186 (95%)	139 (78%)	38 (22%)	1	6
47	m0	179/186 (96%)	149 (83%)	30 (17%)	2	13
48	M1	147/150 (98%)	122 (83%)	25 (17%)	2	13
48	m1	147/150 (98%)	118 (80%)	29 (20%)	1	9
49	M3	154/158 (98%)	129 (84%)	25 (16%)	3	14
49	m3	154/158 (98%)	134 (87%)	20 (13%)	5	22
50	M4	107/108 (99%)	89 (83%)	18 (17%)	2	13
50	m4	108/108 (100%)	88 (82%)	20 (18%)	2	10
51	M5	175/175 (100%)	147 (84%)	28 (16%)	3	15
51	m5	175/175 (100%)	150 (86%)	25 (14%)	4	19
52	M6	160/161 (99%)	133 (83%)	27 (17%)	2	13
52	m6	160/161 (99%)	125 (78%)	35 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	M7	140/145 (97%)	112 (80%)	28 (20%)	1	8
53	m7	125/145 (86%)	104 (83%)	21 (17%)	2	13
54	M8	150/150 (100%)	124 (83%)	26 (17%)	2	12
54	m8	150/150 (100%)	125 (83%)	25 (17%)	3	13
55	M9	153/153 (100%)	128 (84%)	25 (16%)	3	14
55	m9	153/153 (100%)	128 (84%)	25 (16%)	3	14
56	N0	156/156 (100%)	125 (80%)	31 (20%)	1	8
56	n0	156/156 (100%)	120 (77%)	36 (23%)	1	5
57	N1	136/136 (100%)	109 (80%)	27 (20%)	1	8
57	n1	136/136 (100%)	107 (79%)	29 (21%)	1	6
58	N2	87/106 (82%)	76 (87%)	11 (13%)	5	24
58	n2	85/106 (80%)	72 (85%)	13 (15%)	3	16
59	N3	104/104 (100%)	84 (81%)	20 (19%)	2	10
59	n3	104/104 (100%)	89 (86%)	15 (14%)	4	18
60	N4	57/129 (44%)	50 (88%)	7 (12%)	6	25
60	n4	100/129 (78%)	84 (84%)	16 (16%)	3	15
61	N5	104/117 (89%)	81 (78%)	23 (22%)	1	5
61	n5	104/117 (89%)	81 (78%)	23 (22%)	1	5
62	N6	109/109 (100%)	86 (79%)	23 (21%)	1	6
62	n6	109/109 (100%)	80 (73%)	29 (27%)	0	3
63	N7	115/115 (100%)	93 (81%)	22 (19%)	2	10
63	n7	115/115 (100%)	88 (76%)	27 (24%)	1	4
64	N8	118/118 (100%)	98 (83%)	20 (17%)	2	13
64	n8	118/118 (100%)	92 (78%)	26 (22%)	1	6
65	N9	46/46 (100%)	37 (80%)	9 (20%)	1	9
65	n9	46/46 (100%)	37 (80%)	9 (20%)	1	9
66	O0	81/87 (93%)	69 (85%)	12 (15%)	4	17
66	o0	84/87 (97%)	67 (80%)	17 (20%)	1	8
67	O1	92/96 (96%)	74 (80%)	18 (20%)	1	9
67	o1	94/96 (98%)	74 (79%)	20 (21%)	1	6
68	O2	109/110 (99%)	87 (80%)	22 (20%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	o2	109/110 (99%)	86 (79%)	23 (21%)	1	6
69	O3	90/90 (100%)	77 (86%)	13 (14%)	4	18
69	o3	90/90 (100%)	76 (84%)	14 (16%)	3	16
70	O4	95/101 (94%)	79 (83%)	16 (17%)	2	13
70	o4	95/101 (94%)	79 (83%)	16 (17%)	2	13
71	O5	104/104 (100%)	78 (75%)	26 (25%)	1	3
71	o5	103/104 (99%)	84 (82%)	19 (18%)	2	10
72	O6	81/81 (100%)	64 (79%)	17 (21%)	1	7
72	o6	80/81 (99%)	55 (69%)	25 (31%)	0	2
73	O7	70/70 (100%)	57 (81%)	13 (19%)	2	10
73	o7	70/70 (100%)	56 (80%)	14 (20%)	1	8
74	O8	68/68 (100%)	53 (78%)	15 (22%)	1	5
74	o8	67/68 (98%)	53 (79%)	14 (21%)	1	7
75	O9	45/45 (100%)	36 (80%)	9 (20%)	1	8
75	o9	45/45 (100%)	35 (78%)	10 (22%)	1	5
76	Q0	47/47 (100%)	39 (83%)	8 (17%)	2	13
76	q0	47/47 (100%)	35 (74%)	12 (26%)	1	3
77	Q1	23/23 (100%)	16 (70%)	7 (30%)	0	2
77	q1	23/23 (100%)	15 (65%)	8 (35%)	0	1
78	Q2	90/90 (100%)	71 (79%)	19 (21%)	1	6
78	q2	90/90 (100%)	69 (77%)	21 (23%)	1	4
79	Q3	71/71 (100%)	57 (80%)	14 (20%)	1	9
79	q3	71/71 (100%)	61 (86%)	10 (14%)	4	19
80	e0	53/53 (100%)	40 (76%)	13 (24%)	1	4
81	e1	66/66 (100%)	52 (79%)	14 (21%)	1	6
83	p0	105/253 (42%)	88 (84%)	17 (16%)	3	14
All	All	18729/20239 (92%)	15216 (81%)	3513 (19%)	2	10

5 of 3513 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
69	O3	15	SER
7	s5	216	GLU

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Mol	Chain	Res	Type
64	n8	42	ARG
71	O5	89	ARG
3	s1	48	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
58	N2	49	ASN
9	s7	71	HIS
62	n6	120	GLN
59	N3	98	ASN
63	N7	57	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	451 (25%)	52 (2%)
1	6	1792/1800 (99%)	445 (24%)	46 (2%)
36	1	3145/3396 (92%)	661 (21%)	86 (2%)
36	5	3145/3396 (92%)	639 (20%)	90 (2%)
37	3	120/121 (99%)	14 (11%)	2 (1%)
37	7	120/121 (99%)	21 (17%)	1 (0%)
38	4	157/158 (99%)	34 (21%)	5 (3%)
38	8	157/158 (99%)	35 (22%)	2 (1%)
All	All	10383/10950 (94%)	2300 (22%)	284 (2%)

5 of 2300 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

5 of 284 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	3218	A
1	6	468	A

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Mol	Chain	Res	Type
36	5	2818	U
36	1	3275	U
38	4	126	A

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2561 ligands modelled in this entry, 1426 are monoatomic - leaving 1135 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
87	OHX	1	3868	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3869	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3870	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3871	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3872	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3880	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3882	-	0,6,6	0.00	-	0,15,15	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3888	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3889	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3890	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3891	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3925	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3968	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4011	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4054	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4097	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4140	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4183	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
89	ANM	1	4218	-	19,20,20	0.83	0	22,27,27	1.39	3 (13%)
87	OHX	2	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2030	-	0,6,6	0.00	-	0,15,15	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2073	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	2	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2116	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	2	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2159	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	2	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	227	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	228	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	229	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	230	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	231	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	232	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	4	233	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	234	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	235	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	236	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	237	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	238	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3939	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3947	87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3982	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4025	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4068	-	0,6,6	0.00	-	0,15,15	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4111	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4154	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4197	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4227	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4228	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4229	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4230	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4231	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4232	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4233	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4234	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4235	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4236	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4237	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4238	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4239	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4240	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	4241	87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4242	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4243	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4244	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4245	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4246	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4247	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4248	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4249	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4250	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4251	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4252	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4253	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4254	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4255	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4256	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4257	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4258	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4259	-	0,6,6	0.00	-	0,15,15	0.00	-
89	ANM	5	4260	-	19,20,20	1.31	3 (15%)	22,27,27	1.73	5 (22%)
87	OHX	6	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2066	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	6	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2109	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	6	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2152	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	6	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2182	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2183	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2184	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2185	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2186	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2187	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2188	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2189	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2190	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2191	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2192	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2193	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2194	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2195	-	0,6,6	0.00	-	0,15,15	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	6	2196	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2197	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2198	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2199	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2200	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	213	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	214	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	C3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	C5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	C8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	D9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M6	202	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	M7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M7	207	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	N9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O1	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O7	104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Q2	503	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	S8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c8	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	d4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	d9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	305	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	306	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l9	600	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m0	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m1	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m5	305	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	n3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	n9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o7	502	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	s1	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	s1	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	s4	301	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	s8	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	sR	401	-	0,6,6	0.00	-	0,15,15	0.00	-

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	3902	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3903	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3904	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3905	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3906	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3907	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3908	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3909	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3910	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3911	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3912	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3913	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3914	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3915	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3916	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3917	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3918	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3919	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3920	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3921	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3922	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3923	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3924	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3925	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3926	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3927	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3928	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3929	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3930	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3931	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3932	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3933	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3934	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3935	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3936	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3937	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3938	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3939	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3940	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3941	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3942	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3943	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	3944	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3945	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3946	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3947	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3948	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3949	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3950	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3951	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3952	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3953	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3954	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3955	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3956	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3957	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3958	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3959	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3960	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3961	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3962	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3963	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3964	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3965	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3966	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3967	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3968	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3969	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3970	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3971	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3972	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3973	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3974	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3975	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3976	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3977	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3978	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3979	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3980	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3981	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3982	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3983	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3984	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3985	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	3986	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3987	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3988	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3989	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3990	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3991	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3992	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3993	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3994	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3995	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3996	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3997	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3998	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3999	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4000	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4001	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4002	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4003	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4004	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4005	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4006	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4007	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4008	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4009	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4010	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4011	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4012	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4013	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4014	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4015	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4016	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4017	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4018	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4019	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4020	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4021	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4022	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4023	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4024	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4025	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4026	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4027	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4028	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4029	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4030	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4031	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4032	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4033	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4034	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4035	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4036	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4037	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4038	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4039	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4040	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4041	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4042	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4043	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4044	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4045	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4046	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4047	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4048	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4049	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4050	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4051	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4052	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4053	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4054	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4055	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4056	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4057	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4058	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4059	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4060	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4061	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4062	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4063	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4064	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4065	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4066	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4067	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4068	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4069	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4070	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4071	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4072	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4073	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4074	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4075	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4076	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4077	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4078	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4079	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4080	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4081	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4082	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4083	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4084	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4085	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4086	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4087	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4088	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4089	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4090	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4091	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4092	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4093	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4094	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4095	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4096	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4097	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4098	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4099	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4100	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4101	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4102	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4103	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4104	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4105	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4106	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4107	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4108	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4109	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4110	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4111	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4112	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4113	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4114	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4115	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4116	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4117	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4118	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4119	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4120	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4121	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4122	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4123	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4124	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4125	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4126	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4127	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4128	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4129	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4130	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4131	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4132	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4133	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4134	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4135	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4136	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4137	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4138	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4139	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4140	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4141	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4142	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4143	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4144	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4145	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4146	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4147	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4148	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4149	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4150	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4151	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4152	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4153	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4154	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4155	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4156	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4157	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4158	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4159	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4160	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4161	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4162	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4163	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4164	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4165	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4166	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4167	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4168	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4169	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4170	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4171	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4172	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4173	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4174	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4175	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4176	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4177	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4178	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4179	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4180	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4181	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4182	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4183	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4184	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4185	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4186	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4187	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4188	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4189	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4190	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4191	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4192	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4193	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4194	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4195	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4196	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4197	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4198	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4199	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4200	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4201	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4202	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4203	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4204	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4205	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4206	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4207	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4208	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4209	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4210	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4211	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4212	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4213	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4214	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4215	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4216	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4217	-	-	0/0/0/0	0/0/0/0
89	ANM	1	4218	-	-	0/10/23/23	0/2/2/2
87	OHX	2	2023	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2024	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2025	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2029	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2030	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2031	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2032	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2033	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2034	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2035	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2036	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2037	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2038	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2039	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2040	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2041	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2042	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2043	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2044	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2045	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2046	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2047	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2048	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2049	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2050	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2051	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2052	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2053	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2054	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2055	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2056	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2057	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2058	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2059	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2060	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2061	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2062	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2063	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2064	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2065	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2066	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2067	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2068	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2069	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2070	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2071	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2072	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2073	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2074	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2075	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2076	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2077	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2078	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2079	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2080	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2081	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2082	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2083	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2084	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2085	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2086	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2087	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2088	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2089	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2090	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2091	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2092	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2093	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2094	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2095	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2096	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2097	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2098	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2099	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2100	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2101	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2102	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2103	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2104	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2105	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2106	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2107	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2108	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2109	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2110	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2111	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2112	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2113	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2114	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2115	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2116	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2117	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2118	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2119	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2120	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2121	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2122	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2123	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2124	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2125	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2126	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2127	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2128	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2129	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2130	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2131	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2132	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2133	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2134	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2135	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2136	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2137	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2138	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2139	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2140	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2141	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2142	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2143	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2144	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2145	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2146	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2147	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2148	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2149	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2150	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2151	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2152	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2153	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2154	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2155	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2156	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2157	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2158	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2159	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2160	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2161	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2162	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2163	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2164	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2165	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2166	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2167	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2168	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2169	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2170	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2171	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2172	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2173	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2174	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2175	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2176	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2177	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2178	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2179	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2180	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2181	-	-	0/0/0/0	0/0/0/0
87	OHX	3	215	-	-	0/0/0/0	0/0/0/0
87	OHX	3	216	-	-	0/0/0/0	0/0/0/0
87	OHX	3	217	-	-	0/0/0/0	0/0/0/0
87	OHX	3	218	-	-	0/0/0/0	0/0/0/0
87	OHX	3	219	-	-	0/0/0/0	0/0/0/0
87	OHX	3	220	-	-	0/0/0/0	0/0/0/0
87	OHX	3	221	-	-	0/0/0/0	0/0/0/0
87	OHX	3	222	-	-	0/0/0/0	0/0/0/0
87	OHX	3	223	-	-	0/0/0/0	0/0/0/0
87	OHX	3	224	-	-	0/0/0/0	0/0/0/0
87	OHX	3	225	-	-	0/0/0/0	0/0/0/0
87	OHX	3	226	-	-	0/0/0/0	0/0/0/0
87	OHX	4	224	-	-	0/0/0/0	0/0/0/0
87	OHX	4	225	-	-	0/0/0/0	0/0/0/0
87	OHX	4	226	-	-	0/0/0/0	0/0/0/0
87	OHX	4	227	-	-	0/0/0/0	0/0/0/0
87	OHX	4	228	-	-	0/0/0/0	0/0/0/0
87	OHX	4	229	-	-	0/0/0/0	0/0/0/0
87	OHX	4	230	-	-	0/0/0/0	0/0/0/0
87	OHX	4	231	-	-	0/0/0/0	0/0/0/0
87	OHX	4	232	-	-	0/0/0/0	0/0/0/0
87	OHX	4	233	-	-	0/0/0/0	0/0/0/0
87	OHX	4	234	-	-	0/0/0/0	0/0/0/0
87	OHX	4	235	-	-	0/0/0/0	0/0/0/0
87	OHX	4	236	-	-	0/0/0/0	0/0/0/0
87	OHX	4	237	-	-	0/0/0/0	0/0/0/0
87	OHX	4	238	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3903	-	-	0/0/0/0	0/0/0/0

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

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

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

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

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

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4240	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4241	87	-	0/0/0/0	0/0/0/0
87	OHX	5	4242	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4243	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4244	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4245	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4246	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4247	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4248	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4249	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4250	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4251	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4252	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4253	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4254	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4255	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4256	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4257	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4258	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4259	-	-	0/0/0/0	0/0/0/0
89	ANM	5	4260	-	-	0/10/23/23	0/2/2/2
87	OHX	6	2044	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2045	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2046	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2047	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2049	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2050	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2051	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2052	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2053	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2054	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2055	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2056	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2057	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2058	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2059	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2060	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2061	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2062	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2063	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2064	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2065	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2066	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2067	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2068	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2069	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2070	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2071	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2072	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2073	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2074	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2075	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2076	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2077	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2078	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2079	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2080	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2081	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2082	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2083	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2084	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2085	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2086	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2087	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2088	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2089	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2090	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2091	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2092	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2093	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2094	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2095	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2096	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2097	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2098	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2099	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2100	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2101	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2102	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2103	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2104	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2105	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2106	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2107	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2108	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2109	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2110	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2111	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2112	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2113	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2114	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2115	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2116	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2117	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2118	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2119	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2120	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2121	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2122	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2123	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2124	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2125	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2126	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2127	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2128	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2129	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2130	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2131	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2132	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2133	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2134	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2135	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2136	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2137	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2138	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2139	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2140	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2141	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2142	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2143	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2144	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2145	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2146	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2147	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2148	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2149	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2150	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2151	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2152	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2153	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2154	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2155	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2156	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2157	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2158	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2159	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2160	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2161	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2162	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2163	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2164	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2165	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2166	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2167	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2168	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2169	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2170	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2171	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2172	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2173	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2174	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2175	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2176	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2177	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2178	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2179	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2180	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2181	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2182	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2183	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2184	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2185	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2186	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2187	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2188	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2189	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2190	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2191	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2192	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2193	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2194	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2195	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2196	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2197	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2198	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2199	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2200	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2201	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2202	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2203	-	-	0/0/0/0	0/0/0/0
87	OHX	7	215	-	-	0/0/0/0	0/0/0/0
87	OHX	7	216	-	-	0/0/0/0	0/0/0/0
87	OHX	7	217	-	-	0/0/0/0	0/0/0/0
87	OHX	7	218	-	-	0/0/0/0	0/0/0/0
87	OHX	7	219	-	-	0/0/0/0	0/0/0/0
87	OHX	7	220	-	-	0/0/0/0	0/0/0/0
87	OHX	7	221	-	-	0/0/0/0	0/0/0/0
87	OHX	7	222	-	-	0/0/0/0	0/0/0/0
87	OHX	7	223	-	-	0/0/0/0	0/0/0/0
87	OHX	7	224	-	-	0/0/0/0	0/0/0/0
87	OHX	7	225	-	-	0/0/0/0	0/0/0/0
87	OHX	8	213	-	-	0/0/0/0	0/0/0/0
87	OHX	8	214	-	-	0/0/0/0	0/0/0/0
87	OHX	8	215	-	-	0/0/0/0	0/0/0/0
87	OHX	8	216	-	-	0/0/0/0	0/0/0/0
87	OHX	8	217	-	-	0/0/0/0	0/0/0/0
87	OHX	8	218	-	-	0/0/0/0	0/0/0/0
87	OHX	8	219	-	-	0/0/0/0	0/0/0/0
87	OHX	8	220	-	-	0/0/0/0	0/0/0/0
87	OHX	8	221	-	-	0/0/0/0	0/0/0/0
87	OHX	8	222	-	-	0/0/0/0	0/0/0/0
87	OHX	8	223	-	-	0/0/0/0	0/0/0/0
87	OHX	8	224	-	-	0/0/0/0	0/0/0/0
87	OHX	8	225	-	-	0/0/0/0	0/0/0/0
87	OHX	8	226	-	-	0/0/0/0	0/0/0/0
87	OHX	C3	201	-	-	0/0/0/0	0/0/0/0
87	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
87	OHX	C8	201	-	-	0/0/0/0	0/0/0/0
87	OHX	D9	102	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	L3	403	-	-	0/0/0/0	0/0/0/0
87	OHX	L3	404	-	-	0/0/0/0	0/0/0/0
87	OHX	L4	402	-	-	0/0/0/0	0/0/0/0
87	OHX	M0	303	-	-	0/0/0/0	0/0/0/0
87	OHX	M5	303	-	-	0/0/0/0	0/0/0/0
87	OHX	M6	202	-	-	0/0/0/0	0/0/0/0
87	OHX	M7	206	-	-	0/0/0/0	0/0/0/0
87	OHX	M7	207	-	-	0/0/0/0	0/0/0/0
87	OHX	M8	201	-	-	0/0/0/0	0/0/0/0
87	OHX	M9	202	-	-	0/0/0/0	0/0/0/0
87	OHX	N9	101	-	-	0/0/0/0	0/0/0/0
87	OHX	O1	202	-	-	0/0/0/0	0/0/0/0
87	OHX	O2	201	-	-	0/0/0/0	0/0/0/0
87	OHX	O3	201	-	-	0/0/0/0	0/0/0/0
87	OHX	O7	104	-	-	0/0/0/0	0/0/0/0
87	OHX	Q2	503	-	-	0/0/0/0	0/0/0/0
87	OHX	S8	302	-	-	0/0/0/0	0/0/0/0
87	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
87	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
87	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
87	OHX	c8	202	-	-	0/0/0/0	0/0/0/0
87	OHX	d4	202	-	-	0/0/0/0	0/0/0/0
87	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
87	OHX	l3	403	-	-	0/0/0/0	0/0/0/0
87	OHX	l3	404	-	-	0/0/0/0	0/0/0/0
87	OHX	l4	402	-	-	0/0/0/0	0/0/0/0
87	OHX	l4	403	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	304	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	305	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	306	-	-	0/0/0/0	0/0/0/0
87	OHX	l9	600	-	-	0/0/0/0	0/0/0/0
87	OHX	m0	301	-	-	0/0/0/0	0/0/0/0
87	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
87	OHX	m1	202	-	-	0/0/0/0	0/0/0/0
87	OHX	m4	201	-	-	0/0/0/0	0/0/0/0
87	OHX	m5	305	-	-	0/0/0/0	0/0/0/0
87	OHX	m6	202	-	-	0/0/0/0	0/0/0/0
87	OHX	m7	206	-	-	0/0/0/0	0/0/0/0
87	OHX	m8	201	-	-	0/0/0/0	0/0/0/0
87	OHX	n3	203	-	-	0/0/0/0	0/0/0/0
87	OHX	n9	102	-	-	0/0/0/0	0/0/0/0
87	OHX	o2	201	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	o3	202	-	-	0/0/0/0	0/0/0/0
87	OHX	o7	502	-	-	0/0/0/0	0/0/0/0
87	OHX	o9	101	-	-	0/0/0/0	0/0/0/0
87	OHX	q2	502	-	-	0/0/0/0	0/0/0/0
87	OHX	s1	302	-	-	0/0/0/0	0/0/0/0
87	OHX	s1	303	-	-	0/0/0/0	0/0/0/0
87	OHX	s4	301	-	-	0/0/0/0	0/0/0/0
87	OHX	s8	303	-	-	0/0/0/0	0/0/0/0
87	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	5	4260	ANM	O1-C9	2.29	1.42	1.37
89	5	4260	ANM	C13-C1	2.80	1.43	1.38
89	5	4260	ANM	C11-C10	2.82	1.43	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	5	4260	ANM	O2-C2-C16	-3.40	102.23	110.42
89	5	4260	ANM	O2-C2-C3	-3.31	101.21	109.56
89	1	4218	ANM	O2-C2-C3	-3.28	101.28	109.56
89	5	4260	ANM	C13-C1-C9	-3.06	115.89	119.74
89	5	4260	ANM	C11-C10-C9	-3.04	115.91	119.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

475 monomers are involved in 773 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	3868	OHX	1	0
87	1	3873	OHX	1	0
87	1	3875	OHX	1	0
87	1	3876	OHX	1	0
87	1	3878	OHX	1	0
87	1	3880	OHX	1	0
87	1	3882	OHX	1	0
87	1	3884	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	3885	OHX	1	0
87	1	3886	OHX	1	0
87	1	3887	OHX	2	0
87	1	3888	OHX	2	0
87	1	3890	OHX	2	0
87	1	3892	OHX	1	0
87	1	3893	OHX	1	0
87	1	3896	OHX	1	0
87	1	3897	OHX	1	0
87	1	3903	OHX	1	0
87	1	3904	OHX	1	0
87	1	3905	OHX	2	0
87	1	3910	OHX	1	0
87	1	3911	OHX	1	0
87	1	3916	OHX	1	0
87	1	3919	OHX	2	0
87	1	3920	OHX	1	0
87	1	3924	OHX	1	0
87	1	3925	OHX	1	0
87	1	3931	OHX	2	0
87	1	3935	OHX	2	0
87	1	3937	OHX	3	0
87	1	3938	OHX	1	0
87	1	3941	OHX	1	0
87	1	3945	OHX	1	0
87	1	3951	OHX	1	0
87	1	3954	OHX	2	0
87	1	3957	OHX	1	0
87	1	3960	OHX	2	0
87	1	3961	OHX	6	0
87	1	3962	OHX	1	0
87	1	3963	OHX	6	0
87	1	3967	OHX	2	0
87	1	3969	OHX	1	0
87	1	3972	OHX	1	0
87	1	3975	OHX	6	0
87	1	3976	OHX	1	0
87	1	3978	OHX	1	0
87	1	3979	OHX	1	0
87	1	3980	OHX	1	0
87	1	3984	OHX	1	0
87	1	3985	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	3986	OHX	1	0
87	1	3987	OHX	1	0
87	1	3989	OHX	1	0
87	1	3992	OHX	1	0
87	1	3994	OHX	1	0
87	1	4000	OHX	1	0
87	1	4005	OHX	2	0
87	1	4006	OHX	2	0
87	1	4007	OHX	7	0
87	1	4010	OHX	2	0
87	1	4012	OHX	1	0
87	1	4017	OHX	1	0
87	1	4019	OHX	1	0
87	1	4021	OHX	1	0
87	1	4023	OHX	5	0
87	1	4031	OHX	2	0
87	1	4032	OHX	5	0
87	1	4034	OHX	2	0
87	1	4036	OHX	6	0
87	1	4037	OHX	2	0
87	1	4038	OHX	1	0
87	1	4039	OHX	1	0
87	1	4041	OHX	3	0
87	1	4042	OHX	2	0
87	1	4043	OHX	1	0
87	1	4044	OHX	1	0
87	1	4046	OHX	1	0
87	1	4047	OHX	4	0
87	1	4048	OHX	7	0
87	1	4049	OHX	1	0
87	1	4051	OHX	2	0
87	1	4052	OHX	1	0
87	1	4054	OHX	1	0
87	1	4056	OHX	2	0
87	1	4059	OHX	6	0
87	1	4060	OHX	4	0
87	1	4061	OHX	5	0
87	1	4064	OHX	1	0
87	1	4065	OHX	3	0
87	1	4066	OHX	1	0
87	1	4067	OHX	1	0
87	1	4070	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	4076	OHX	1	0
87	1	4079	OHX	1	0
87	1	4080	OHX	1	0
87	1	4082	OHX	1	0
87	1	4084	OHX	4	0
87	1	4086	OHX	1	0
87	1	4088	OHX	6	0
87	1	4089	OHX	2	0
87	1	4091	OHX	1	0
87	1	4092	OHX	1	0
87	1	4094	OHX	1	0
87	1	4098	OHX	1	0
87	1	4099	OHX	1	0
87	1	4102	OHX	1	0
87	1	4111	OHX	1	0
87	1	4113	OHX	1	0
87	1	4122	OHX	1	0
87	1	4123	OHX	1	0
87	1	4126	OHX	1	0
87	1	4132	OHX	1	0
87	1	4135	OHX	1	0
87	1	4136	OHX	2	0
87	1	4137	OHX	1	0
87	1	4139	OHX	1	0
87	1	4142	OHX	2	0
87	1	4143	OHX	3	0
87	1	4144	OHX	5	0
87	1	4145	OHX	2	0
87	1	4146	OHX	1	0
87	1	4147	OHX	1	0
87	1	4148	OHX	2	0
87	1	4149	OHX	1	0
87	1	4151	OHX	6	0
87	1	4152	OHX	1	0
87	1	4155	OHX	3	0
87	1	4159	OHX	4	0
87	1	4160	OHX	2	0
87	1	4161	OHX	7	0
87	1	4165	OHX	1	0
87	1	4168	OHX	6	0
87	1	4169	OHX	2	0
87	1	4170	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	4172	OHX	3	0
87	1	4173	OHX	2	0
87	1	4174	OHX	2	0
87	1	4177	OHX	9	0
87	1	4179	OHX	2	0
87	1	4184	OHX	1	0
87	1	4185	OHX	1	0
87	1	4186	OHX	4	0
87	1	4188	OHX	1	0
87	1	4189	OHX	1	0
87	1	4198	OHX	1	0
87	1	4200	OHX	1	0
87	1	4201	OHX	1	0
87	1	4203	OHX	7	0
87	1	4204	OHX	1	0
87	1	4206	OHX	1	0
87	1	4208	OHX	2	0
87	1	4211	OHX	1	0
87	1	4213	OHX	1	0
87	2	2023	OHX	1	0
87	2	2026	OHX	1	0
87	2	2031	OHX	7	0
87	2	2033	OHX	1	0
87	2	2034	OHX	1	0
87	2	2035	OHX	1	0
87	2	2036	OHX	3	0
87	2	2038	OHX	1	0
87	2	2039	OHX	2	0
87	2	2044	OHX	7	0
87	2	2045	OHX	1	0
87	2	2047	OHX	2	0
87	2	2048	OHX	1	0
87	2	2053	OHX	1	0
87	2	2054	OHX	1	0
87	2	2057	OHX	1	0
87	2	2062	OHX	1	0
87	2	2064	OHX	1	0
87	2	2071	OHX	1	0
87	2	2072	OHX	1	0
87	2	2073	OHX	1	0
87	2	2075	OHX	6	0
87	2	2076	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	2	2078	OHX	1	0
87	2	2082	OHX	1	0
87	2	2083	OHX	2	0
87	2	2084	OHX	1	0
87	2	2085	OHX	2	0
87	2	2086	OHX	1	0
87	2	2089	OHX	4	0
87	2	2090	OHX	6	0
87	2	2092	OHX	1	0
87	2	2093	OHX	1	0
87	2	2095	OHX	6	0
87	2	2096	OHX	4	0
87	2	2097	OHX	2	0
87	2	2099	OHX	7	0
87	2	2104	OHX	1	0
87	2	2105	OHX	1	0
87	2	2106	OHX	1	0
87	2	2108	OHX	1	0
87	2	2109	OHX	8	0
87	2	2110	OHX	1	0
87	2	2111	OHX	2	0
87	2	2115	OHX	2	0
87	2	2116	OHX	4	0
87	2	2117	OHX	1	0
87	2	2119	OHX	1	0
87	2	2121	OHX	3	0
87	2	2123	OHX	1	0
87	2	2126	OHX	1	0
87	2	2127	OHX	1	0
87	2	2128	OHX	1	0
87	2	2130	OHX	2	0
87	2	2131	OHX	1	0
87	2	2132	OHX	8	0
87	2	2133	OHX	1	0
87	2	2137	OHX	2	0
87	2	2139	OHX	1	0
87	2	2141	OHX	1	0
87	2	2142	OHX	1	0
87	2	2145	OHX	1	0
87	2	2146	OHX	2	0
87	2	2147	OHX	7	0
87	2	2149	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	2	2150	OHX	1	0
87	2	2153	OHX	1	0
87	2	2155	OHX	2	0
87	2	2156	OHX	1	0
87	2	2158	OHX	2	0
87	2	2161	OHX	2	0
87	2	2163	OHX	6	0
87	2	2166	OHX	1	0
87	2	2167	OHX	2	0
87	2	2168	OHX	1	0
87	2	2170	OHX	1	0
87	3	218	OHX	2	0
87	3	221	OHX	1	0
87	3	226	OHX	1	0
87	4	224	OHX	1	0
87	4	226	OHX	1	0
87	4	230	OHX	1	0
87	4	234	OHX	3	0
87	4	238	OHX	1	0
87	5	3909	OHX	2	0
87	5	3911	OHX	2	0
87	5	3917	OHX	1	0
87	5	3920	OHX	1	0
87	5	3921	OHX	2	0
87	5	3922	OHX	2	0
87	5	3924	OHX	1	0
87	5	3927	OHX	1	0
87	5	3929	OHX	1	0
87	5	3935	OHX	1	0
87	5	3937	OHX	1	0
87	5	3941	OHX	1	0
87	5	3943	OHX	1	0
87	5	3944	OHX	1	0
87	5	3946	OHX	1	0
87	5	3947	OHX	7	0
87	5	3953	OHX	1	0
87	5	3954	OHX	1	0
87	5	3958	OHX	2	0
87	5	3959	OHX	1	0
87	5	3961	OHX	1	0
87	5	3962	OHX	3	0
87	5	3967	OHX	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	3969	OHX	1	0
87	5	3971	OHX	1	0
87	5	3974	OHX	1	0
87	5	3977	OHX	2	0
87	5	3978	OHX	6	0
87	5	3979	OHX	1	0
87	5	3981	OHX	1	0
87	5	3983	OHX	9	0
87	5	3988	OHX	1	0
87	5	3991	OHX	1	0
87	5	3992	OHX	1	0
87	5	3996	OHX	3	0
87	5	4000	OHX	1	0
87	5	4004	OHX	1	0
87	5	4005	OHX	6	0
87	5	4006	OHX	7	0
87	5	4007	OHX	2	0
87	5	4008	OHX	1	0
87	5	4012	OHX	2	0
87	5	4016	OHX	6	0
87	5	4018	OHX	2	0
87	5	4019	OHX	1	0
87	5	4024	OHX	2	0
87	5	4025	OHX	1	0
87	5	4026	OHX	7	0
87	5	4029	OHX	3	0
87	5	4030	OHX	1	0
87	5	4034	OHX	1	0
87	5	4035	OHX	1	0
87	5	4036	OHX	1	0
87	5	4037	OHX	1	0
87	5	4039	OHX	1	0
87	5	4040	OHX	1	0
87	5	4041	OHX	5	0
87	5	4045	OHX	1	0
87	5	4052	OHX	1	0
87	5	4055	OHX	1	0
87	5	4056	OHX	1	0
87	5	4057	OHX	1	0
87	5	4058	OHX	1	0
87	5	4059	OHX	1	0
87	5	4061	OHX	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	4062	OHX	1	0
87	5	4065	OHX	1	0
87	5	4071	OHX	2	0
87	5	4072	OHX	7	0
87	5	4074	OHX	1	0
87	5	4078	OHX	1	0
87	5	4080	OHX	2	0
87	5	4086	OHX	1	0
87	5	4087	OHX	1	0
87	5	4094	OHX	1	0
87	5	4095	OHX	1	0
87	5	4096	OHX	7	0
87	5	4098	OHX	1	0
87	5	4099	OHX	2	0
87	5	4100	OHX	3	0
87	5	4101	OHX	6	0
87	5	4103	OHX	1	0
87	5	4104	OHX	1	0
87	5	4106	OHX	1	0
87	5	4109	OHX	1	0
87	5	4112	OHX	2	0
87	5	4113	OHX	1	0
87	5	4114	OHX	1	0
87	5	4117	OHX	1	0
87	5	4118	OHX	1	0
87	5	4121	OHX	1	0
87	5	4124	OHX	1	0
87	5	4126	OHX	1	0
87	5	4137	OHX	1	0
87	5	4138	OHX	2	0
87	5	4140	OHX	1	0
87	5	4144	OHX	1	0
87	5	4145	OHX	1	0
87	5	4149	OHX	1	0
87	5	4150	OHX	6	0
87	5	4151	OHX	1	0
87	5	4154	OHX	1	0
87	5	4156	OHX	1	0
87	5	4160	OHX	1	0
87	5	4161	OHX	1	0
87	5	4166	OHX	2	0
87	5	4169	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	4170	OHX	1	0
87	5	4173	OHX	1	0
87	5	4175	OHX	1	0
87	5	4177	OHX	1	0
87	5	4181	OHX	1	0
87	5	4187	OHX	3	0
87	5	4188	OHX	1	0
87	5	4192	OHX	1	0
87	5	4193	OHX	1	0
87	5	4197	OHX	3	0
87	5	4199	OHX	3	0
87	5	4200	OHX	6	0
87	5	4201	OHX	1	0
87	5	4202	OHX	1	0
87	5	4203	OHX	2	0
87	5	4205	OHX	1	0
87	5	4206	OHX	11	0
87	5	4207	OHX	7	0
87	5	4208	OHX	7	0
87	5	4209	OHX	1	0
87	5	4211	OHX	5	0
87	5	4216	OHX	1	0
87	5	4221	OHX	4	0
87	5	4224	OHX	8	0
87	5	4228	OHX	1	0
87	5	4230	OHX	1	0
87	5	4231	OHX	4	0
87	5	4233	OHX	1	0
87	5	4234	OHX	1	0
87	5	4235	OHX	1	0
87	5	4236	OHX	1	0
87	5	4239	OHX	1	0
87	5	4241	OHX	6	0
87	5	4243	OHX	7	0
87	5	4244	OHX	1	0
87	5	4245	OHX	5	0
87	5	4247	OHX	2	0
87	5	4250	OHX	7	0
87	5	4251	OHX	1	0
87	5	4256	OHX	1	0
87	6	2047	OHX	2	0
87	6	2052	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	6	2055	OHX	1	0
87	6	2057	OHX	6	0
87	6	2058	OHX	1	0
87	6	2059	OHX	1	0
87	6	2063	OHX	1	0
87	6	2066	OHX	1	0
87	6	2068	OHX	1	0
87	6	2069	OHX	1	0
87	6	2071	OHX	2	0
87	6	2072	OHX	1	0
87	6	2073	OHX	1	0
87	6	2074	OHX	1	0
87	6	2077	OHX	1	0
87	6	2081	OHX	2	0
87	6	2086	OHX	1	0
87	6	2090	OHX	1	0
87	6	2091	OHX	1	0
87	6	2093	OHX	1	0
87	6	2094	OHX	2	0
87	6	2098	OHX	3	0
87	6	2100	OHX	2	0
87	6	2101	OHX	1	0
87	6	2103	OHX	1	0
87	6	2104	OHX	1	0
87	6	2105	OHX	2	0
87	6	2106	OHX	1	0
87	6	2107	OHX	1	0
87	6	2109	OHX	1	0
87	6	2110	OHX	1	0
87	6	2112	OHX	2	0
87	6	2117	OHX	2	0
87	6	2118	OHX	8	0
87	6	2119	OHX	1	0
87	6	2121	OHX	2	0
87	6	2122	OHX	1	0
87	6	2123	OHX	5	0
87	6	2124	OHX	3	0
87	6	2126	OHX	1	0
87	6	2128	OHX	1	0
87	6	2135	OHX	2	0
87	6	2136	OHX	1	0
87	6	2140	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	6	2141	OHX	1	0
87	6	2142	OHX	1	0
87	6	2144	OHX	1	0
87	6	2145	OHX	7	0
87	6	2147	OHX	1	0
87	6	2148	OHX	3	0
87	6	2149	OHX	1	0
87	6	2152	OHX	2	0
87	6	2153	OHX	1	0
87	6	2155	OHX	1	0
87	6	2157	OHX	3	0
87	6	2159	OHX	1	0
87	6	2160	OHX	1	0
87	6	2168	OHX	1	0
87	6	2169	OHX	8	0
87	6	2173	OHX	1	0
87	6	2176	OHX	2	0
87	6	2177	OHX	1	0
87	6	2181	OHX	1	0
87	6	2182	OHX	1	0
87	6	2187	OHX	2	0
87	6	2188	OHX	2	0
87	6	2189	OHX	2	0
87	6	2194	OHX	1	0
87	6	2201	OHX	1	0
87	7	217	OHX	6	0
87	7	218	OHX	3	0
87	7	224	OHX	6	0
87	8	213	OHX	1	0
87	8	214	OHX	6	0
87	8	215	OHX	1	0
87	8	217	OHX	1	0
87	8	218	OHX	2	0
87	8	221	OHX	7	0
87	8	222	OHX	6	0
87	8	223	OHX	2	0
87	8	225	OHX	1	0
87	C5	201	OHX	3	0
87	L3	403	OHX	1	0
87	L4	402	OHX	4	0
87	M5	303	OHX	1	0
87	M7	206	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	M9	202	OHX	1	0
87	O1	202	OHX	6	0
87	O3	201	OHX	1	0
87	O7	104	OHX	6	0
87	Q2	503	OHX	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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