



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 31, 2020 – 10:01 AM BST

PDB ID : 4U56
Title : Crystal structure of Blasticidin S bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 3.45 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

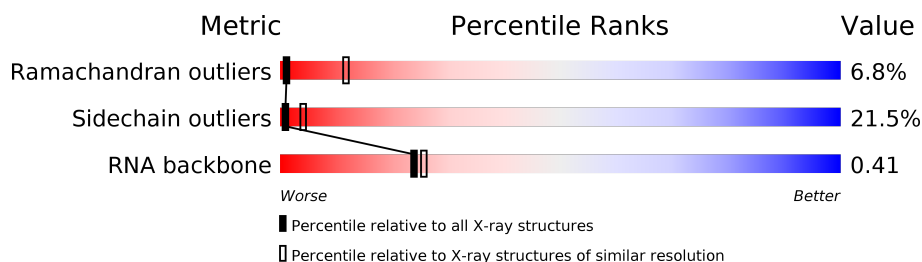
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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))
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RNA backbone	3102	1036 (3.96-2.96)





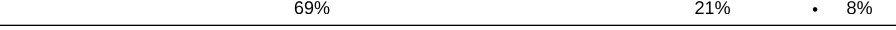
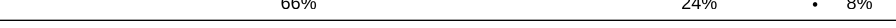

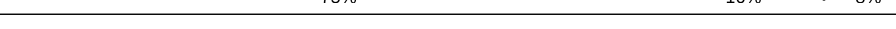
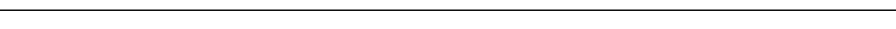
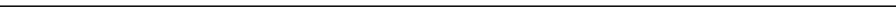















The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	2	1800	60% 32% 5% .
1	6	1800	62% 32% 6%
2	S0	251	59% 22% . 18%
2	s0	251	65% 15% . 18%
3	S1	254	58% 23% . 16%
3	s1	254	64% 20% . 15%
4	S2	253	65% 19% . 14%
4	s2	253	62% 22% . 14%




















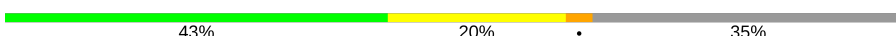





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Mol	Chain	Length	Quality of chain
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	
15	c3	150	
16	C4	136	
16	c4	136	
17	C5	141	

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Mol	Chain	Length	Quality of chain
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	
29	D7	81	
29	d7	81	


























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Mol	Chain	Length	Quality of chain
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	















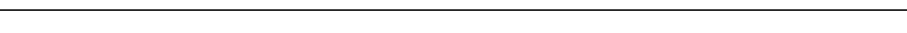




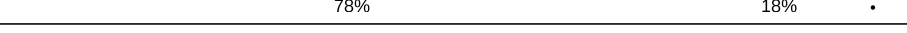





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Mol	Chain	Length	Quality of chain
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6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















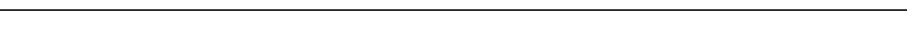




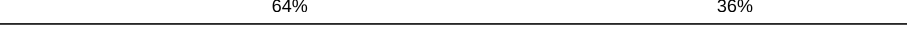





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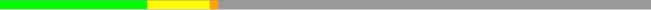

Mol	Chain	Length	Quality of chain
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	104	
66	o0	104	
67	O1	112	
67	o1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

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Mol	Chain	Length	Quality of chain
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	120	
70	o4	120	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	
79	q3	91	
80	e0	62	

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Mol	Chain	Length	Quality of chain
81	p0	311	
82	m2	160	
83	p1	47	
84	p2	46	

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411214 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	L4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
41	14	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	L5	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
42	15	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	L6	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
43	16	157	Total	C	N	O	S	0	0	0
			1248	806	224	217	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	L7	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
44	17	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L7	2	Total	Mg	0	0
			2	2		
85	m6	2	Total	Mg	0	0
			2	2		
85	n8	3	Total	Mg	0	0
			3	3		
85	N5	1	Total	Mg	0	0
			1	1		
85	6	147	Total	Mg	0	0
			147	147		
85	sM	1	Total	Mg	0	0
			1	1		
85	m5	5	Total	Mg	0	0
			5	5		
85	l3	3	Total	Mg	0	0
			3	3		
85	C1	1	Total	Mg	0	0
			1	1		
85	M1	1	Total	Mg	0	0
			1	1		
85	d6	1	Total	Mg	0	0
			1	1		
85	2	122	Total	Mg	0	0
			122	122		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	n0	1	Total 1	Mg 1	0	0
85	L4	3	Total 3	Mg 3	0	0
85	l7	1	Total 1	Mg 1	0	0
85	M5	2	Total 2	Mg 2	0	0
85	c9	1	Total 1	Mg 1	0	0
85	L8	1	Total 1	Mg 1	0	0
85	D3	1	Total 1	Mg 1	0	0
85	M9	1	Total 1	Mg 1	0	0
85	q0	2	Total 2	Mg 2	0	0
85	SM	1	Total 1	Mg 1	0	0
85	o4	3	Total 3	Mg 3	0	0
85	M0	3	Total 3	Mg 3	0	0
85	c1	1	Total 1	Mg 1	0	0
85	n6	2	Total 2	Mg 2	0	0
85	5	495	Total 495	Mg 495	0	0
85	c8	1	Total 1	Mg 1	0	0
85	O7	2	Total 2	Mg 2	0	0
85	Q2	1	Total 1	Mg 1	0	0
85	n9	2	Total 2	Mg 2	0	0
85	1	462	Total 462	Mg 462	0	0
85	c4	1	Total 1	Mg 1	0	0

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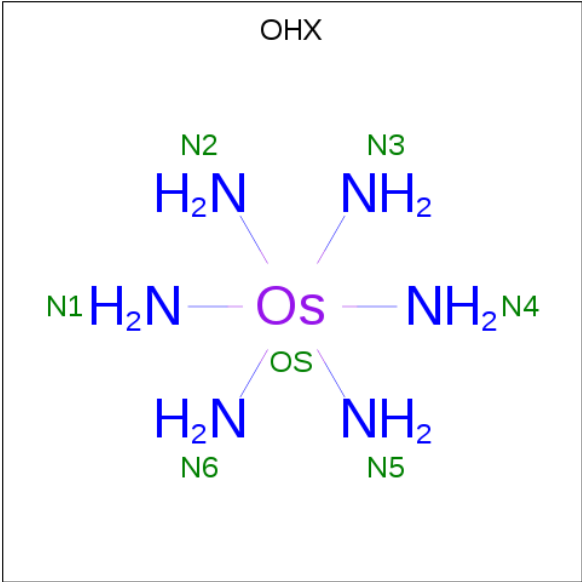
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	D0	1	Total 1	Mg 1	0	0
85	S8	1	Total 1	Mg 1	0	0
85	l2	3	Total 3	Mg 3	0	0
85	O2	2	Total 2	Mg 2	0	0
85	o7	1	Total 1	Mg 1	0	0
85	o3	2	Total 2	Mg 2	0	0
85	d3	3	Total 3	Mg 3	0	0
85	M3	2	Total 2	Mg 2	0	0
85	N3	3	Total 3	Mg 3	0	0
85	4	23	Total 23	Mg 23	0	0
85	D4	1	Total 1	Mg 1	0	0
85	S4	1	Total 1	Mg 1	0	0
85	L2	2	Total 2	Mg 2	0	0
85	m1	1	Total 1	Mg 1	0	0
85	l5	3	Total 3	Mg 3	0	0
85	d0	1	Total 1	Mg 1	0	0
85	M7	5	Total 5	Mg 5	0	0
85	m4	1	Total 1	Mg 1	0	0
85	N8	5	Total 5	Mg 5	0	0
85	s1	1	Total 1	Mg 1	0	0
85	l9	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	O1	1	Total 1	Mg 1	0	0
85	s8	1	Total 1	Mg 1	0	0
85	c7	1	Total 1	Mg 1	0	0
85	7	17	Total 17	Mg 17	0	0
85	n3	1	Total 1	Mg 1	0	0
85	q1	1	Total 1	Mg 1	0	0
85	L3	4	Total 4	Mg 4	0	0
85	O5	1	Total 1	Mg 1	0	0
85	N6	2	Total 2	Mg 2	0	0
85	8	14	Total 14	Mg 14	0	0
85	l4	1	Total 1	Mg 1	0	0
85	M6	1	Total 1	Mg 1	0	0
85	N0	1	Total 1	Mg 1	0	0
85	m0	1	Total 1	Mg 1	0	0
85	3	15	Total 15	Mg 15	0	0
85	m7	6	Total 6	Mg 6	0	0

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: H₁₂N₆Os).



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	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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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	C3	1	Total	N	Os	0	0
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86	C5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	D9	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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86	1	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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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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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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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	L4	1	Total	N	Os	0	0
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86	M5	1	Total	N	Os	0	0
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86	M7	1	Total	N	Os	0	0
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86	M9	1	Total	N	Os	0	0
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86	N9	1	Total	N	Os	0	0
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86	O3	1	Total	N	Os	0	0
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86	O7	1	Total	N	Os	0	0
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86	O7	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
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86	s1	1	Total 7	N 6	Os 1	0	0
86	s4	1	Total 7	N 6	Os 1	0	0
86	s8	1	Total 7	N 6	Os 1	0	0
86	s9	1	Total 7	N 6	Os 1	0	0
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86	c5	1	Total 7	N 6	Os 1	0	0
86	c8	1	Total 7	N 6	Os 1	0	0
86	d4	1	Total 7	N 6	Os 1	0	0
86	d9	1	Total 7	N 6	Os 1	0	0
86	sR	1	Total 7	N 6	Os 1	0	0

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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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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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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	13	1	Total 7	N 6	Os 1	0	0
86	13	1	Total 7	N 6	Os 1	0	0
86	14	1	Total 7	N 6	Os 1	0	0
86	14	1	Total 7	N 6	Os 1	0	0
86	15	1	Total 7	N 6	Os 1	0	0
86	15	1	Total 7	N 6	Os 1	0	0
86	15	1	Total 7	N 6	Os 1	0	0
86	19	1	Total 7	N 6	Os 1	0	0
86	m0	1	Total 7	N 6	Os 1	0	0
86	m0	1	Total 7	N 6	Os 1	0	0
86	m1	1	Total 7	N 6	Os 1	0	0
86	m4	1	Total 7	N 6	Os 1	0	0
86	m5	1	Total 7	N 6	Os 1	0	0
86	m6	1	Total 7	N 6	Os 1	0	0
86	m7	1	Total 7	N 6	Os 1	0	0
86	n1	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

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

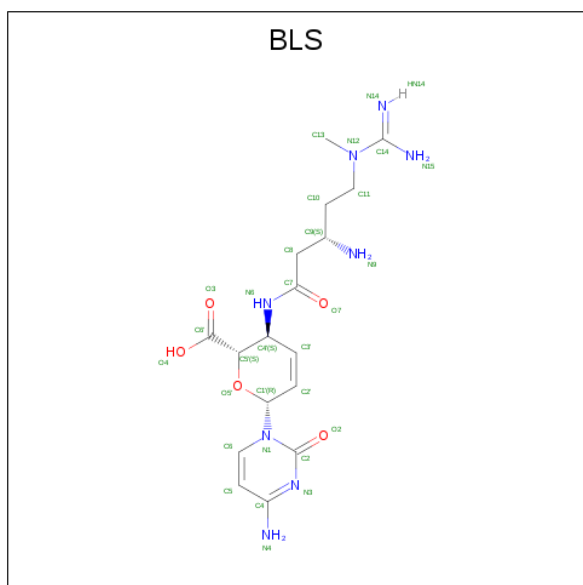
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	q0	1	Total	Zn	0	0
			1	1		
87	D6	1	Total	Zn	0	0
			1	1		
87	Q2	1	Total	Zn	0	0
			1	1		
87	e1	1	Total	Zn	0	0
			1	1		
87	Q3	1	Total	Zn	0	0
			1	1		
87	D9	1	Total	Zn	0	0
			1	1		
87	E1	1	Total	Zn	0	0
			1	1		
87	Q0	1	Total	Zn	0	0
			1	1		
87	d7	1	Total	Zn	0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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	O7	1	Total Zn 1 1	0	0
87	q2	1	Total Zn 1 1	0	0

- Molecule 88 is BLASTICIDIN S (three-letter code: BLS) (formula: $C_{17}H_{26}N_8O_5$).



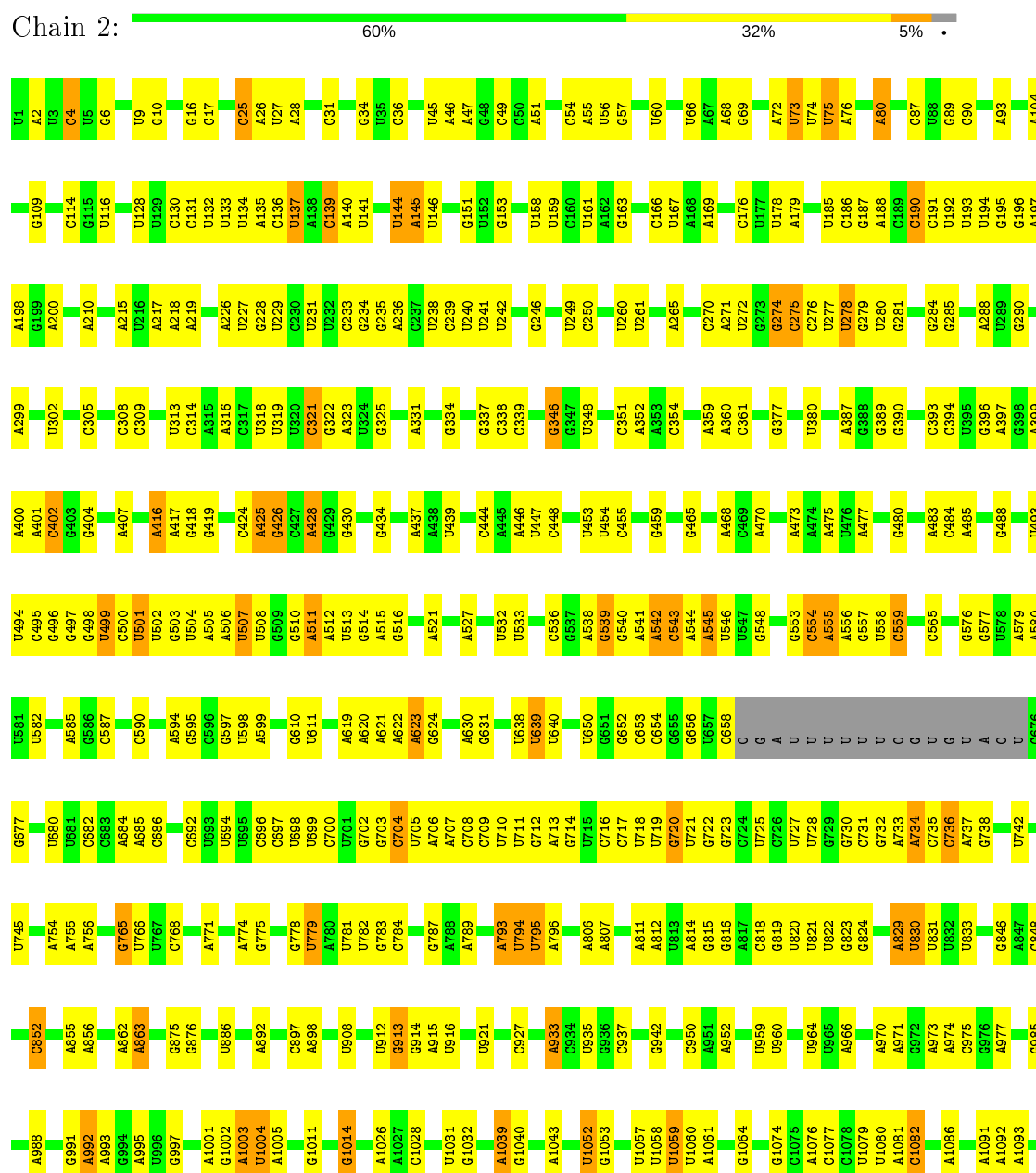
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
88	1	1	Total 30	C 17	N 8	O 5	0	0
88	5	1	Total 30	C 17	N 8	O 5	0	0

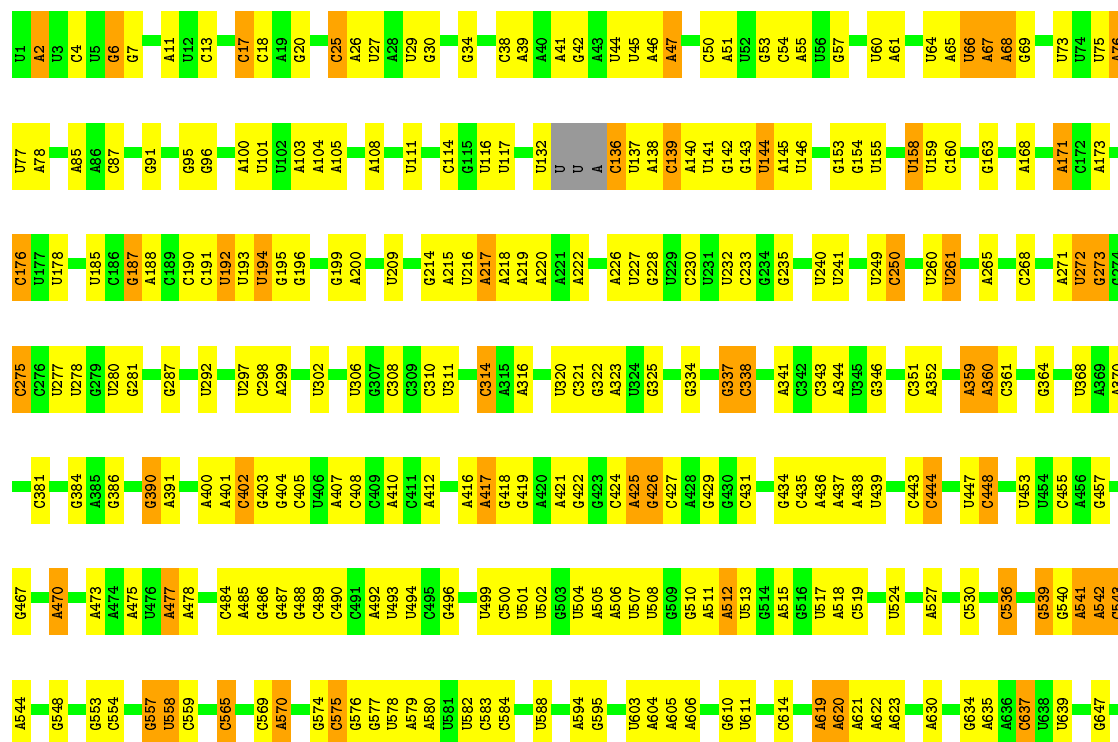
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

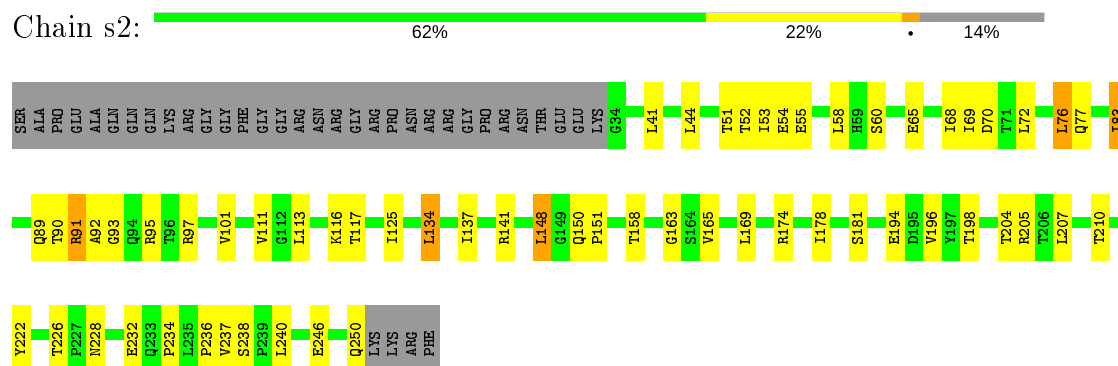
- Molecule 1: 18S ribosomal RNA



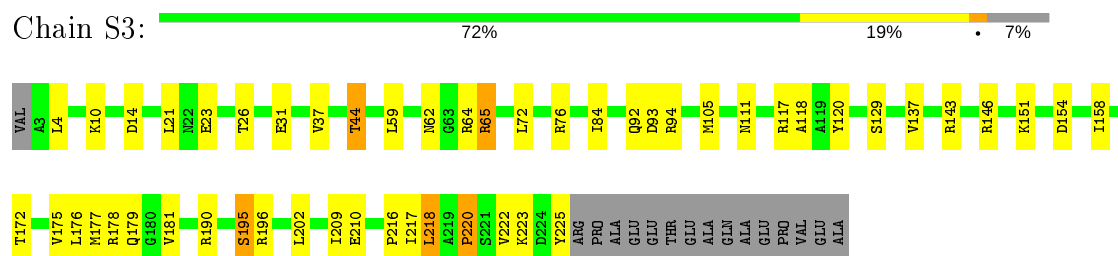


WORLDWIDE
PDB
PROTEIN DATA BANK

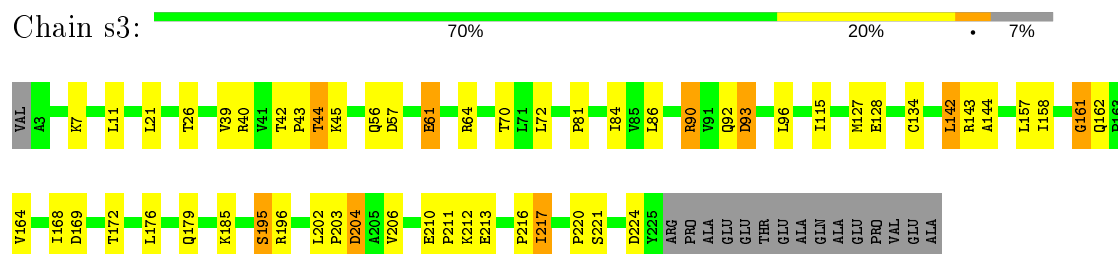
- Molecule 4: 40S ribosomal protein S2



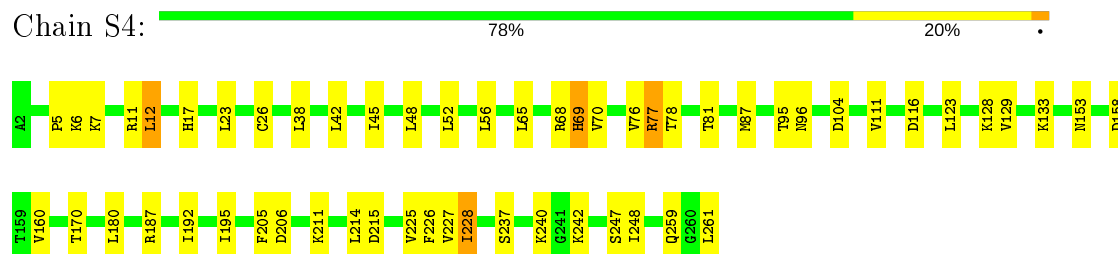
- Molecule 5: 40S ribosomal protein S3



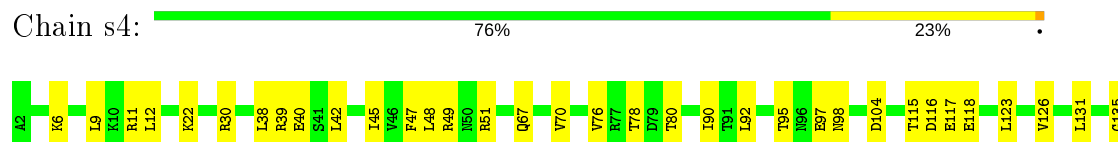
- Molecule 5: 40S ribosomal protein S3



- Molecule 6: 40S ribosomal protein S4-A



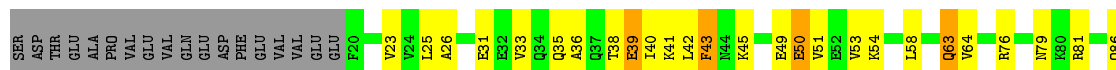
- Molecule 6: 40S ribosomal protein S4-A





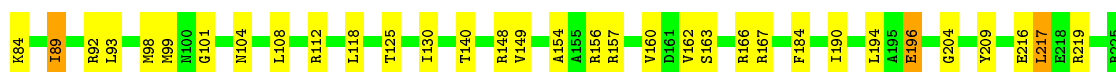
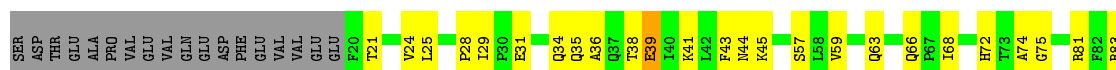
• Molecule 7: 40S ribosomal protein S5

Chain S5: 69% 21% 8%



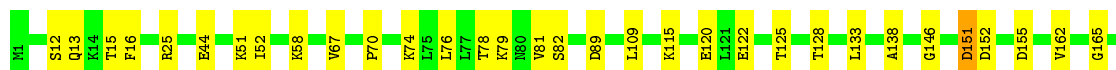
• Molecule 7: 40S ribosomal protein S5

Chain s5: 66% 24% 8%



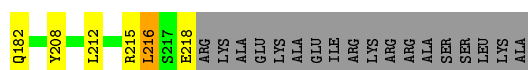
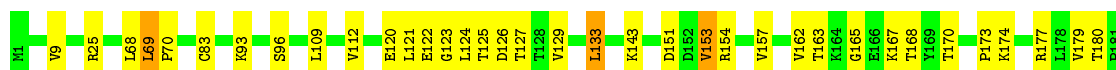
• Molecule 8: 40S ribosomal protein S6-A

Chain S6: 77% 18% 2%



• Molecule 8: 40S ribosomal protein S6-A

Chain s6: 75% 16% 8%



• Molecule 9: 40S ribosomal protein S7-A

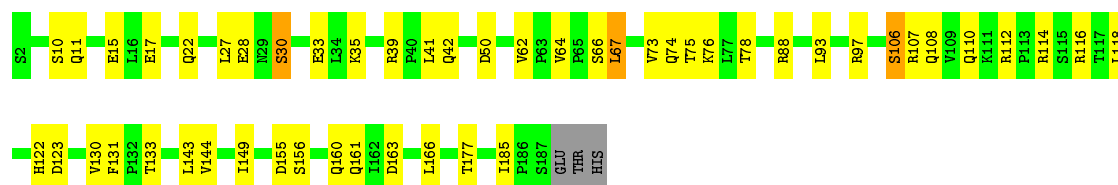
Chain S7: 72% 25% 2%





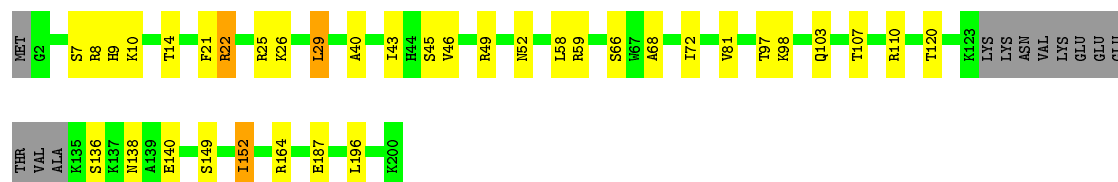
- Molecule 9: 40S ribosomal protein S7-A

Chain s7: 72% 25%



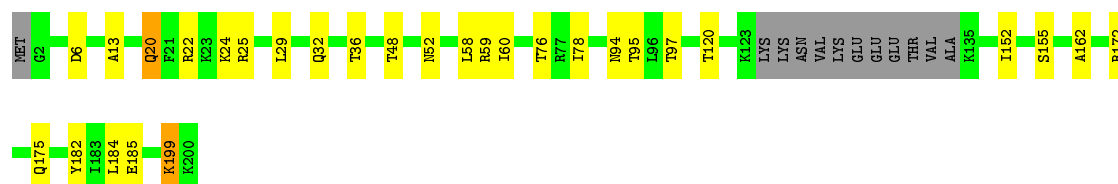
- Molecule 10: 40S ribosomal protein S8-A

Chain S8: 76% 17% 6%



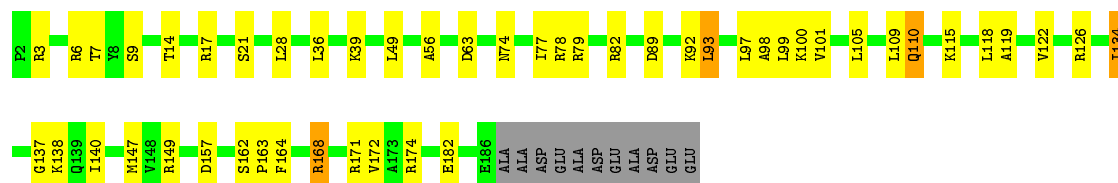
- Molecule 10: 40S ribosomal protein S8-A

Chain s8: 80% 14% 6%



- Molecule 11: 40S ribosomal protein S9-A

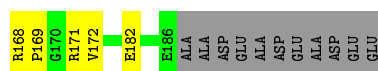
Chain S9: 69% 23% 6%



- Molecule 11: 40S ribosomal protein S9-A

Chain s9: 75% 18% 6%





- Molecule 12: 40S ribosomal protein S10-A

Chain C0: 70% 21% 9%



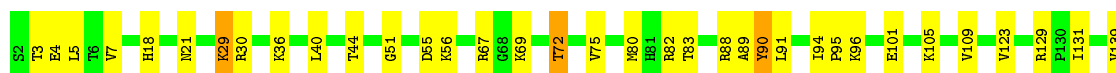
- Molecule 12: 40S ribosomal protein S10-A

Chain c0: 68% 20% 9%



- Molecule 13: 40S ribosomal protein S11-A

Chain C1: 74% 23% 3%



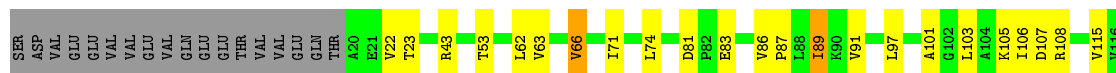
- Molecule 13: 40S ribosomal protein S11-A

Chain c1: 76% 18% 6%



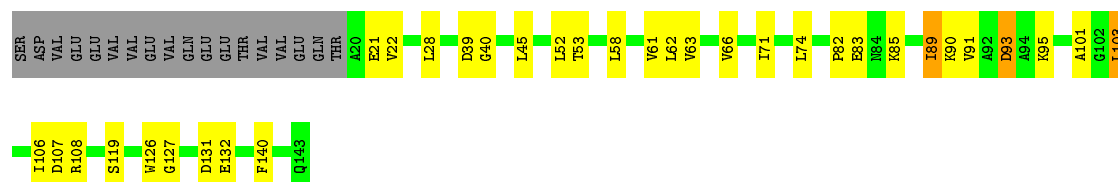
- Molecule 14: 40S ribosomal protein S12

Chain C2: 63% 21% 13%



- Molecule 14: 40S ribosomal protein S12

Chain c2: 63% 22% 13%



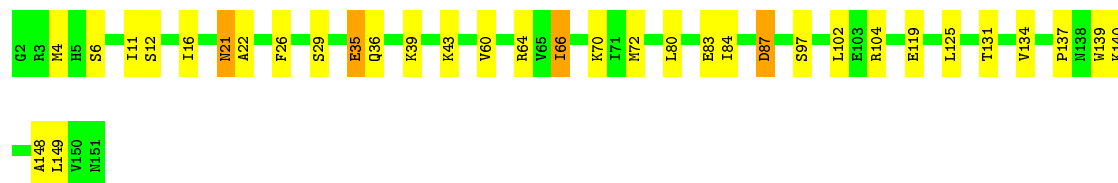
- Molecule 15: 40S ribosomal protein S13

Chain C3: 76% 22% •



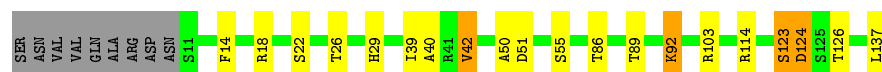
- Molecule 15: 40S ribosomal protein S13

Chain c3: 77% 20% •



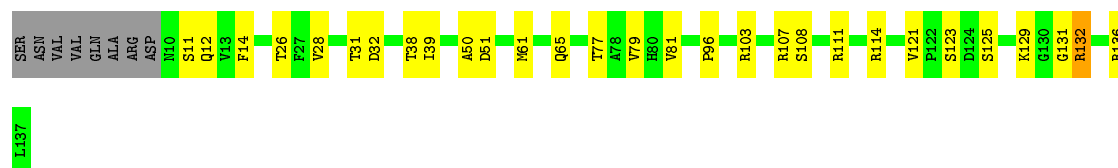
- Molecule 16: 40S ribosomal protein S14-A

Chain C4: 79% 12% 7% •



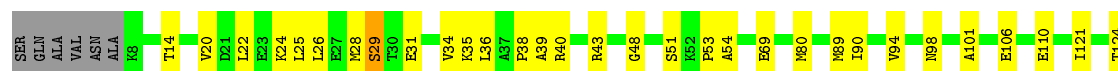
- Molecule 16: 40S ribosomal protein S14-A

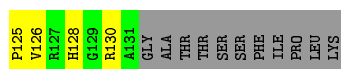
Chain c4: 73% 21% 6% •



- Molecule 17: 40S ribosomal protein S15

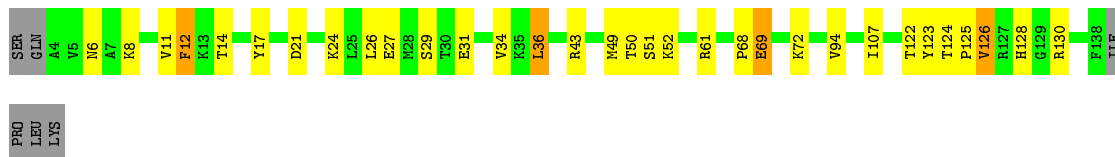
Chain C5: 63% 24% 12% •





- Molecule 17: 40S ribosomal protein S15

Chain c5: 73% 20%



- Molecule 18: 40S ribosomal protein S16-A

Chain C6: 81% 17%



- Molecule 18: 40S ribosomal protein S16-A

Chain c6: 77% 21%



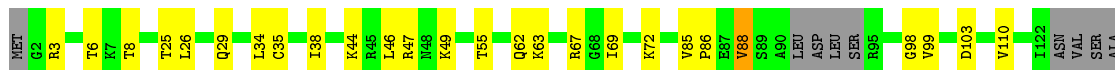
- Molecule 19: 40S ribosomal protein S17-A

Chain C7: 65% 18% 12%



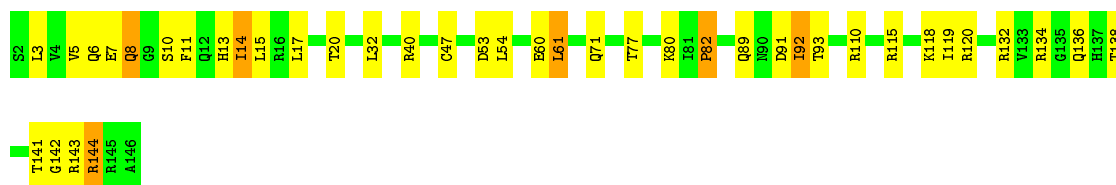
- Molecule 19: 40S ribosomal protein S17-A

Chain c7: 67% 18% 14%



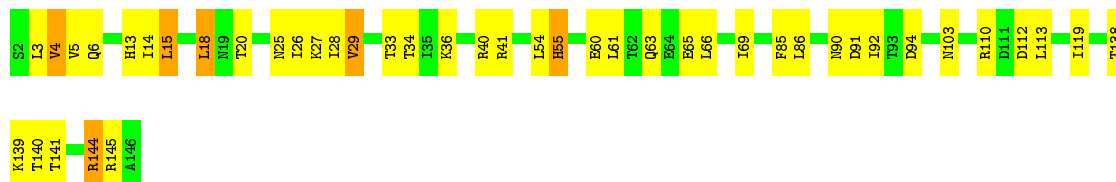
- Molecule 20: 40S ribosomal protein S18-A

Chain C8: 72% 23%



- Molecule 20: 40S ribosomal protein S18-A

Chain c8: 70% 26%



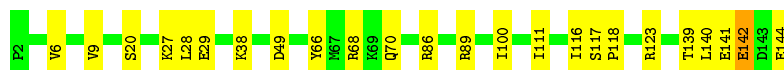
- Molecule 21: 40S ribosomal protein S19-A

Chain C9: 78% 20%



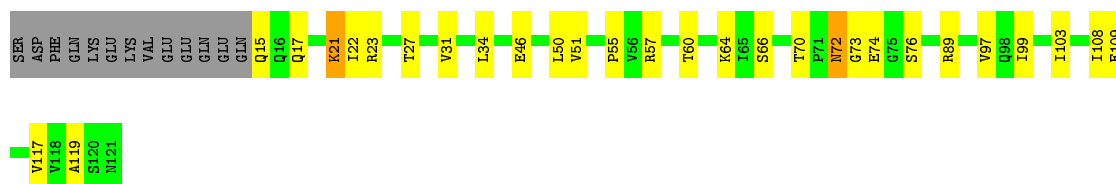
- Molecule 21: 40S ribosomal protein S19-A

Chain c9: 83% 16%



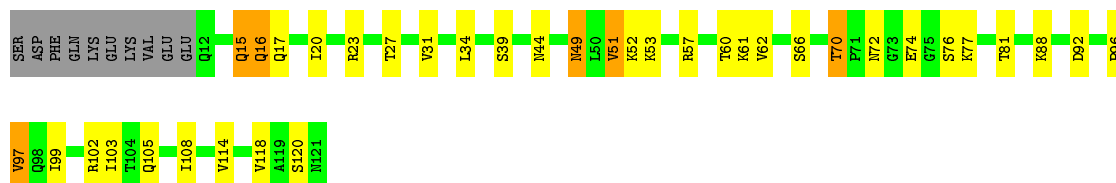
- Molecule 22: 40S ribosomal protein S20

Chain D0: 65% 23% 11%




- Molecule 22: 40S ribosomal protein S20

Chain d0: 61% 26% 5% 8%



- Molecule 23: 40S ribosomal protein S21-A

Chain D1:  77% 22%




- Molecule 23: 40S ribosomal protein S21-A

Chain d1:  76% 24%




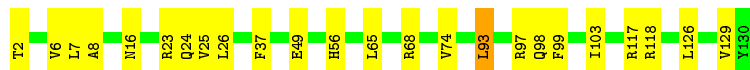
- Molecule 24: 40S ribosomal protein S22-A

Chain D2:  79% 21%




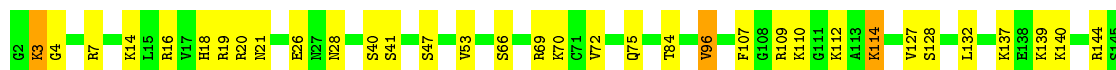
- Molecule 24: 40S ribosomal protein S22-A

Chain d2:  81% 18%




- Molecule 25: 40S ribosomal protein S23-A

Chain D3:  76% 22%




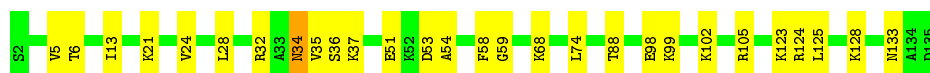
- Molecule 25: 40S ribosomal protein S23-A

Chain d3:  76% 22%

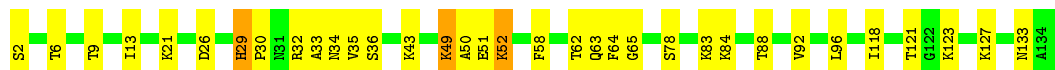


- Molecule 26: 40S ribosomal protein S24-A

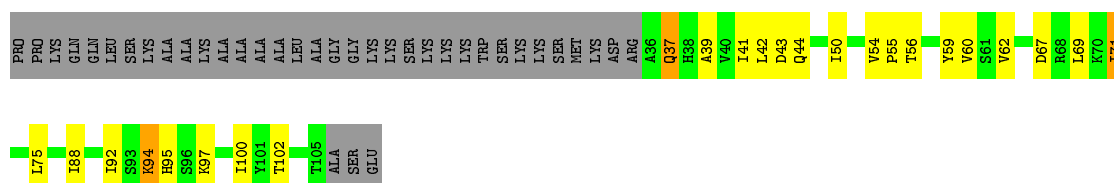
Chain D4:  79% 20%



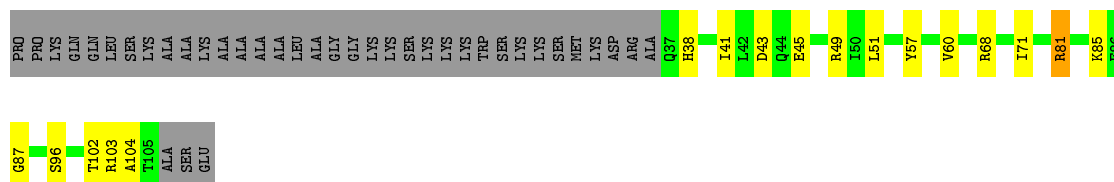
- Molecule 26: 40S ribosomal protein S24-A



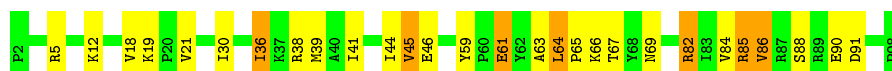
- Molecule 27: 40S ribosomal protein S25-A



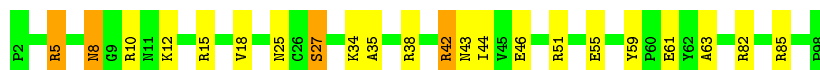
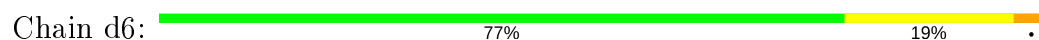
- Molecule 27: 40S ribosomal protein S25-A



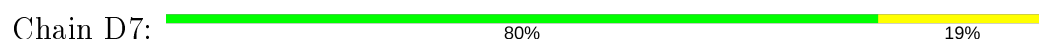
- Molecule 28: 40S ribosomal protein S26-B



- Molecule 28: 40S ribosomal protein S26-B

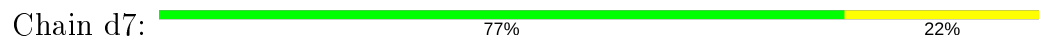


- Molecule 29: 40S ribosomal protein S27-A





- Molecule 29: 40S ribosomal protein S27-A



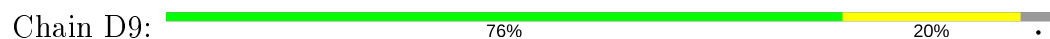
- Molecule 30: 40S ribosomal protein S28-A



- Molecule 30: 40S ribosomal protein S28-A



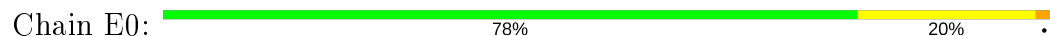
- Molecule 31: 40S ribosomal protein S29-A



- Molecule 31: 40S ribosomal protein S29-A



- Molecule 32: 40S ribosomal protein S30-A



- Molecule 33: Ubiquitin-40S ribosomal protein S31





G3377	U3260	U3192	G3110	G3000	U2920	G2850	C2773	A2679	G2608	U2513	A2445	A2367	G2288	A2198
C3378	U3281	U3195	U3111	C3001	U2921	A2851	C2774	A2680	A2609	U2514	U	A2368	A2295	G2199
C3379	G3286	U3196	G3112	G3002	G2922	C2852	G2777	U2681	G2610	U2515	G	G2370	A2296	U2200
U3382	G3287	G3197	A3113	G3003	U2923	A2853	G2778	C2689	U2611	A2516	A	G2371	U2297	G2201
U3389	G3288	U3198	G3113	G3004	U2924	U2854	A2779	U2684	U2612	A2519	G	U2372	U2298	U2205
G3390	G3289	G3199	G3118	A3005	C2927	G2856	G2787	G2687	G2614	G2522	G	A2373	A2299	U2206
U3396	G3290	G3200	U3119	A3006	G2928	C2857	C2788	U2688	G2615	G2523	G	G2374	A2207	A2207
U3293	G3202	A3011	U3121	G3012	A2930	U2858	G2796	A2690	G2616	A2524	U	G2376	A2208	G2210
A3294	U3203	A3012	A3122	A3013	A2933	U2859	G2797	G2691	U2617	G2525	U	G2377	A2303	G2210
A3295	G3204	G3015	G3128	G3015	U2935	U2861	C2797	A2691	G2619	G2530	A	U2378	G2306	A2213
U3302	G3206	G3206	A3129	G3206	A2936	U2862	G2800	A2694	G2620	C2531	A	U2379	G2307	A2213
G3303	U3207	U3207	A3130	A3021	A2937	A2864	A2801	A2696	G2621	C2532	A	U2380	C2308	C2308
U3304	G3208	U3131	U3131	G3022	G2938	U2865	A2802	G2697	G2622	G2533	U	G2381	A2309	A2309
A3305	A3209	C3132	C3133	G3028	C2942	U2866	A2803	G2698	U2624	G2534	U	C2382	U2294	A2294
U3306	A3210	C3211	A3134	A3029	C2942	C2867	A2804	G2699	G2625	U2537	A	C2383	G2311	U2295
G3309	C3212	C3212	A3138	G3030	G2945	U2868	A2805	G2704	A2626	U2538	G	U2388	A2312	A2298
A3310	A3213	U3214	A3139	U3041	A2946	U2869	G2806	A2704	G2627	C2539	U	A2387	A2313	A2298
C3311	U3214	U3214	A3140	U3041	G2947	C2870	U2807	A2705	U2629	C2540	G	U2388	A2314	A2299
U3312	U3214	U3214	A3140	U3041	C2948	A2872	A2808	G2708	U2631	U2543	G	U2388	A2315	A2299
U3313	A3217	C3217	A3141	A3046	U2949	U2873	C2809	G2714	U2632	U2544	G	U2388	A2315	A2299
A3316	A3218	A3218	A3142	A3049	U2953	U2874	C2810	G2714	U2633	C2545	U	U2388	A2315	A2299
U3317	G3219	G3219	C3143	U3050	U2954	U2875	A2811	G2714	U2633	C2545	U	U2388	A2315	A2299
U3318	G3224	G3224	C3144	U3050	U2954	C2877	A2812	G2714	U2633	C2545	U	U2388	A2315	A2299
U3319	G3224	G3224	C3144	U3050	U2954	C2877	A2812	G2714	U2633	C2545	U	U2388	A2315	A2299
A3320	G3224	G3224	C3144	U3050	U2954	C2877	A2812	G2714	U2633	C2545	U	U2388	A2315	A2299
A3335	G3224	G3224	C3144	U3050	U2954	C2877	A2812	G2714	U2633	C2545	U	U2388	A2315	A2299
U3341	G3242	G3242	C3154	U3057	G2968	U2883	A2817	G2727	U2643	U2553	G	A2401	C2329	G2248
A3342	A3243	A3243	U3155	U3058	A2969	U2884	A2818	G2728	U2644	U2554	G	A2402	C2330	G2249
A3343	A3244	A3244	U3156	G3059	C2970	U2885	A2819	U2729	U2645	C2555	C	A2403	C2331	G2250
A3344	A3245	A3245	U3157	A3063	A2971	U2886	A2820	G2730	U2646	C2556	C	A2404	C2332	G2251
G3246	G3246	G3246	G3158	C3063	G2972	U2887	C2821	U2731	U2647	U2557	A	C2405	U2334	A2252
G3247	G3247	G3247	G3159	G3074	C2973	U2888	U2822	G2732	U2648	A2561	G	C2406	G2335	A2253
C3248	C3248	C3248	C3164	G3074	U2974	C2889	C2823	G2732	U2649	A2562	U	C2407	U2336	A2254
C3249	C3249	C3249	C3165	U3078	U2975	A2890	G2824	A2739	U2650	C2568	G	U2408	A2256	A2256
G3253	G3253	G3253	C3166	U3079	A2976	C2893	U2827	C2741	U2651	A2569	A	U2409	A2257	A2257
U3259	U3259	U3259	A3167	G3080	U2977	C2894	U2828	G2741	U2652	U2570	A	U2410	U2342	G2261
U3263	U3263	U3263	U3169	G3085	U2979	A2896	U2829	A2746	C2653	C2572	U	G2412	U2344	A2262
G3266	G3266	G3266	A3170	A3086	A2982	A2897	G2830	A2747	A2656	G2573	A	G2414	C2350	U2266
U3269	U3269	U3269	U3171	G3087	C2983	G2898	G2831	A2748	A2657	U2581	C	G2415	U2351	U2267
U3270	U3270	U3270	A3172	A3088	C2984	C2899	C2832	U2752	G2658	C2582	C	U2416	A2352	G2272
A3273	A3273	A3273	G3173	G3089	C2985	U2903	C2836	G2753	G2659	C2583	A	U2417	G2353	G2273
A3274	A3274	A3274	A3174	A3090	C2986	U2904	A2837	G2754	G2660	C2584	C	U2418	C2354	G2274
U3275	U3275	U3275	U3175	U3091	A2987	U2905	A2838	C2755	G2661	C2585	U	A2419	G2355	G2275
U3276	U3276	U3276	G3176	A3092	C2988	U2906	G2839	C2756	G2662	C2586	C	C2422	A2356	G2276
U3277	U3277	U3277	U3177	C3093	C2989	A2911	G2840	A2758	G2663	A2593	U	U2423	A2357	C2277
A3278	A3278	A3278	A3178	G3094	U2990	C2912	U2842	U2759	C2664	C2594	U	U2424	A2358	C2278
A3279	A3279	A3279	U3179	A3180	C2991	C2913	C2843	C2760	G2672	C2595	U	U2425	A2359	A2279
U3280	U3280	U3280	G3181	G3099	U2992	G2914	C2844	G2761	A2673	A2596	U	U2426	A2360	A2280
U3281	U3281	U3281	G3182	U3100	U2993	U2915	C2845	A2762	A2674	A2597	A	U2427	A2361	U2281
U3282	U3282	U3282	G3183	U3101	U2994	U2916	C2846	A2763	A2675	G2602	U	U2428	A2362	U2282
U3283	U3283	U3283	A3187	U3102	A2995	U2917	U2847	C2764	G2676	C2603	U	U2429	A2363	G2283
U3284	U3284	U3284	U3103	U3103	U2996	G2918	G2848	A2677	A2677	C2604	U	U2430	A2364	C2284
A3279	A3279	A3279	A3106	U3106	G2997	A2919	C2849	C2772	A2678	C2607	U	U2431	A2365	C2285

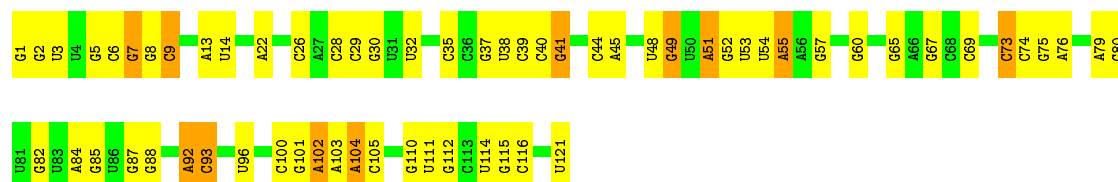
Chain 5: 47% 37% 8% 7%



U2434	G2362	G2288	C2197	A2100	A1891	G1796	G1666	C1562	G1466	C1391	A1318	G1232
G2435	A2363	U2289	A2198	C2101	G1892	A1797	A1667	C1563	A1467	C1393	G1319	U1235
U2436	C2364	C2290	G2199	U2102	U1893	A1810	A1683	G1564	A1468	G1392	C1320	G1236
A2437	C2365	A2291	C2204	U2102	U1894	A1810	A1683	G1565	C1321	G1393	G1321	G1237
A2438	A2368	A2295	U2205	G2111	A1895	A1814	G1685	U1566	G1473	A1394	U1324	A1394
A2439	G2369	U2297	C2205	U2112	G1896	U1815	U1686	U1567	A1474	G1395	U1325	C1238
G2440	G2370	U2298	U2209	A2113	G1897	U1815	U1686	U1568	A1475	U1398	A1326	C1239
A2441	G2371	G2210	G2210	C2114	G1898	A1816	U1687	U1569	G1476	U1400	U1329	A1240
A2443	A2372	U2211	U2211	G2115	G1899	G1817	U1688	U1570	A1477	A1399	U1241	G1243
G2442	G2373	G2300	G2211	G2116	A1900	U1818	U1695	U1571	G1480	G1400	A1330	G1244
C2444	U2301	U2301	A2223	G2116	C1901	U1821	U1695	U1572	A1481	G1404	A1331	A1244
A	G2302	G2302	A2224	G2121	U1902	U1821	U1695	G1573	A1482	U1405	A1332	A1245
U	A2303	A2303	U2225	G2122	G1903	G1830	A1704	A1574	G1483	A1406	A1332	G1246
A	C2304	C2304	U2225	G2123	U1904	U1831	C1710	A1575	U1484	A1407	C1335	
G	G2307	G2307	A2228	G2123	G1905	G1832	C1710	G1577	G1485	G1408	A1252	
G	U2307	U2307	C2128	C2128	U1906	U1832	U1710	G1577	U1485	G1409	U1258	
G	C2308	C2308	C2129	C2129	A1909	G1833	A1713	C1578	U1494	G1413	U1258	
U	A2309	A2309	G2130	G2130	U1910	U1839	A1714	C1579	U1495	U1405		
U	U2310	U2310	A2131	A2131	A1911	U1840	U1715	A1580	A1482	A1406		
G	C2312	C2312	C2132	C2132	U1912	U1841	U1716	C1581	G1483	A1407		
U	U2137	U2137	U2137	U2137	A1913	A1842	U1717	C1582	U1497	G1408		
U	A2138	A2138	U2141	U2141	G1914	A1842	U1724	A1583	C1502	U1409		
A	U2141	U2141	A2142	A2142	U1915	G1845	U1724	A1583	G1500	G1416		
A	A2142	A2142	U2142	U2142	U1916	C1846	A1729	A1588	U1501	A1417		
U	A2145	A2145	U2145	U2145	C1917	U1847	G1733	A1589	C1502	G1417		
U	U2152	U2152	U2152	U2152	G1918	G1848	G1733	A1590	G1507	A1428		
U	U2153	U2153	U2153	U2153	C1919	U1849	G1736	A1591	U1508	G1429		
U	U2154	U2154	U2154	U2154	U1920	A1850	G1736	G1592	A1509	U1430		
U	C2155	C2155	U2155	U2155	G1921	G1851	G1744	C1598	G1510	G1431		
U	C2156	C2156	U2156	U2156	A1922	U1852	G1744	G1599	U1511	A1355		
U	G2157	G2157	U2157	U2157	C1923	U1853	G1744	U1600	U1512	U1356		
U	U2158	U2158	U2158	U2158	G1927	C1854	A1750	U1600	U1513	C1432		
U	U2159	U2159	U2159	U2159	U1944	U1855	G1751	G1604	G1514	A1433		
U	U2160	U2160	U2160	U2160	U1944	C1856	A1752	G1604	U1435	G1434		
U	A2167	A2167	U2167	U2167	G1948	C1857	A1752	A1605	U1436	U1436		
U	A2168	A2168	U2168	U2168	U1953	U1866	A1760	U1606	U1517	G1437		
U	G2169	G2169	U2169	U2169	G1953	A1867	C1761	U1607	U1518	C1437		
U	U2176	U2176	U2176	U2176	U	G1868	C1762	C1608	U1519	U1438		
U	U2177	U2177	U2177	U2177	U	G1869	U1765	G1611	G1528	U1439		
U	U2178	U2178	U2178	U2178	U	C1870	U1766	A1619	U1533	G1441		
U	U2179	U2179	U2179	U2179	U	U1871	C1767	U1620	G1536	U1442		
U	U2180	U2180	U2180	U2180	U	U1872	U1768	U1628	A1301	G1443		
U	U2181	U2181	U2181	U2181	U	U1873	G1770	U1629	A1302	U1444		
U	U2182	U2182	U2182	U2182	U	U1874	G1770	U1629	A1303	A1445		
U	U2183	U2183	U2183	U2183	U	U1875	G1770	U1629	A1304	G1447		
U	U2184	U2184	U2184	U2184	U	U1876	G1770	U1629	C1372	U1448		
U	U2185	U2185	U2185	U2185	U	U1877	G1770	U1629	A1373	U1449		
U	U2186	U2186	U2186	U2186	U	U1878	G1770	U1629	G1374	G1306		
U	U2187	U2187	U2187	U2187	U	U1879	G1770	U1629	G1375	G1307		
U	U2188	U2188	U2188	U2188	U	U1880	G1770	U1629	C1376	A1308		
U	U2189	U2189	U2189	U2189	U	U1881	G1770	U1629	G1377	U1309		
U	U2190	U2190	U2190	U2190	U	U1882	G1770	U1629	U1378	U1310		
U	U2191	U2191	U2191	U2191	U	U1883	G1770	U1629	G1379	G1311		
U	U2192	U2192	U2192	U2192	U	U1884	G1770	U1629	U1457	U1312		
U	U2193	U2193	U2193	U2193	U	U1885	G1770	U1629	A1381	G1313		
U	U2194	U2194	U2194	U2194	U	U1886	G1770	U1629	U1384	G1314		
U	U2195	U2195	U2195	U2195	U	U1887	G1770	U1629	U1385	U1315		
U	U2196	U2196	U2196	U2196	U	U1888	G1770	U1629	A1386	G1316		
U	U2197	U2197	U2197	U2197	U	U1889	G1770	U1629				
U	U2198	U2198	U2198	U2198	U	U1890	G1770	U1629				
U	U2199	U2199	U2199	U2199	U	U1891	G1770	U1629				
U	U2200	U2200	U2200	U2200	U	U1892	G1770	U1629				
U	U2201	U2201	U2201	U2201	U	U1893	G1770	U1629				
U	U2202	U2202	U2202	U2202	U	U1894	G1770	U1629				
U	U2203	U2203	U2203	U2203	U	U1895	G1770	U1629				
U	U2204	U2204	U2204	U2204	U	U1896	G1770	U1629				
U	U2205	U2205	U2205	U2205	U	U1897	G1770	U1629				
U	U2206	U2206	U2206	U2206	U	U1898	G1770	U1629				
U	U2207	U2207	U2207	U2207	U	U1899	G1770	U1629				
U	U2208	U2208	U2208	U2208	U	U1900	G1770	U1629				
U	U2209	U2209	U2209	U2209	U	U1901	G1770	U1629				
U	U2210	U2210	U2210	U2210	U	U1902	G1770	U1629				
U	U2211	U2211	U2211	U2211	U	U1903	G1770	U1629				
U	U2212	U2212	U2212	U2212	U	U1904	G1770	U1629				
U	U2213	U2213	U2213	U2213	U	U1905	G1770	U1629				
U	U2214	U2214	U2214	U2214	U	U1906	G1770	U1629				
U	U2215	U2215	U2215	U2215	U	U1907	G1770	U1629				
U	U2216	U2216	U2216	U2216	U	U1908	G1770	U1629				
U	U2217	U2217	U2217	U2217	U	U1909	G1770	U1629				
U	U2218	U2218	U2218	U2218	U	U1910	G1770	U1629				
U	U2219	U2219	U2219	U2219	U	U1911	G1770	U1629				
U	U2220	U2220	U2220	U2220	U	U1912	G1770	U1629				
U	U2221	U2221	U2221	U2221	U	U1913	G1770	U1629				
U	U2222	U2222	U2222	U2222	U	U1914	G1770	U1629				
U	U2223	U2223	U2223	U2223	U	U1915	G1770	U1629				
U	U2224	U2224	U2224	U2224	U	U1916	G1770	U1629				
U	U2225	U2225	U2225	U2225	U	U1917	G1770	U1629				
U	U2226	U2226	U2226	U2226	U	U1918	G1770	U1629				
U	U2227	U2227	U2227	U2227	U	U1919	G1770	U1629				
U	U2228	U2228	U2228	U2228	U	U1920	G1770	U1629				
U	U2229	U2229	U2229	U2229	U	U1921	G1770	U1629				
U	U2230	U2230	U2230	U2230	U	U1922	G1770	U1629				
U	U2231	U2231	U2231	U2231	U	U1923	G1770	U1629				
U	U2232	U2232	U2232	U2232	U	U1924	G1770	U1629				
U	U2233	U2233	U2233	U2233	U	U1925	G1770	U1629				
U	U2234	U2234	U2234	U2234	U	U1926	G1770	U1629				
U	U2235	U2235	U2235	U2235	U	U1927	G1770	U1629				
U	U2236	U2236	U2236	U2236	U	U1928	G1770	U1629				
U	U2237	U2237	U2237	U2237	U	U1929	G1770	U1629				
U	U2238	U2238	U2238	U2238	U	U1930	G1770	U1629				
U	U2239	U2239	U2239	U2239	U	U1931	G1770	U1629				
U	U2240	U2240	U2240	U2240	U	U1932	G1770	U1629				
U	U2241	U2241	U2241	U2241	U	U1933	G1770	U1629				
U	U2242	U2242	U2242	U2242	U	U1934	G1770	U1629				
U	U2243	U2243	U2243	U2243	U	U1935	G1770	U1629				
U	U2244	U2244	U2244	U2244	U	U1936	G1770	U1629				
U	U2245	U2245	U2245	U2245	U	U1937	G1770	U1629				
U	U2246	U2246	U2246	U2246	U	U1938	G1770	U1629				
U	U2247	U2247	U2247	U2247	U	U1939	G1770	U1629				
U	U2248	U2248	U2248	U2248	U	U1940	G1770	U1629				
U	U2249	U2249	U2249	U2249	U	U1941	G1770	U1629				
U	U2250	U2250	U2250	U2250	U	U1942	G1770	U1629				
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U	U2252	U2252	U225									

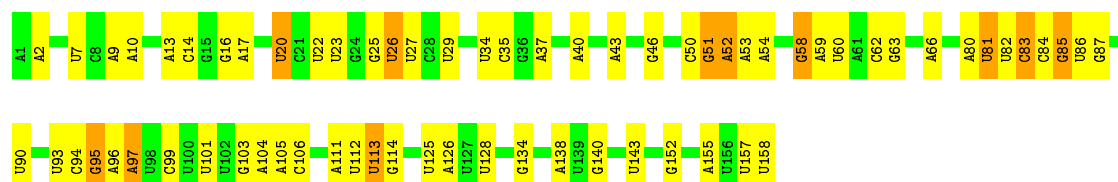
- Molecule 37: 5S ribosomal RNA

Chain 7: 



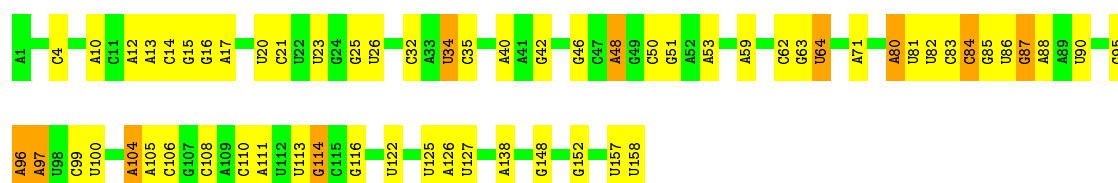
- Molecule 38: 5.8S ribosomal RNA

Chain 4: 




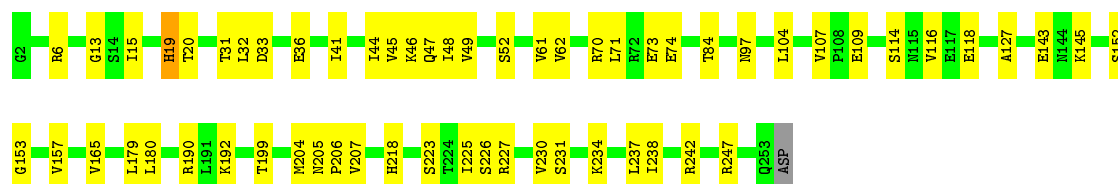
- Molecule 38: 5.8S ribosomal RNA

Chain 8: 



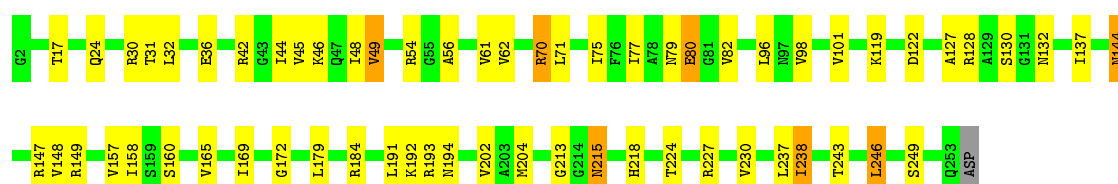
- Molecule 39: 60S ribosomal protein L2-A

Chain L2: 

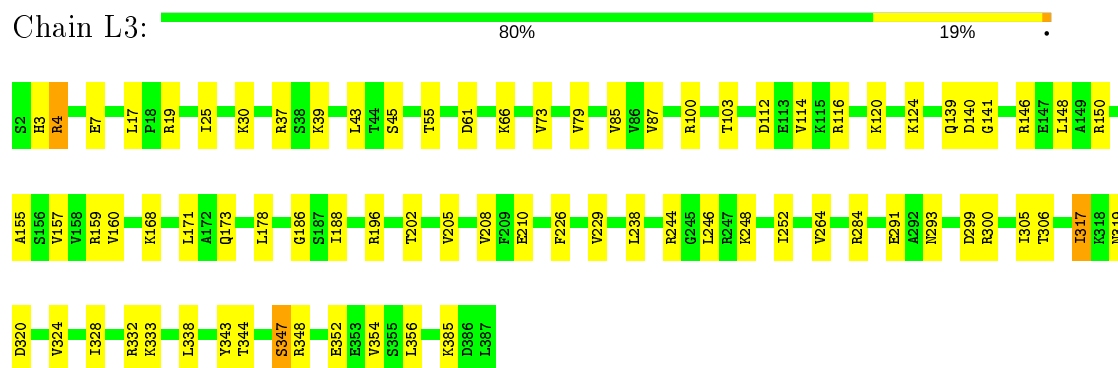


- Molecule 39: 60S ribosomal protein L2-A

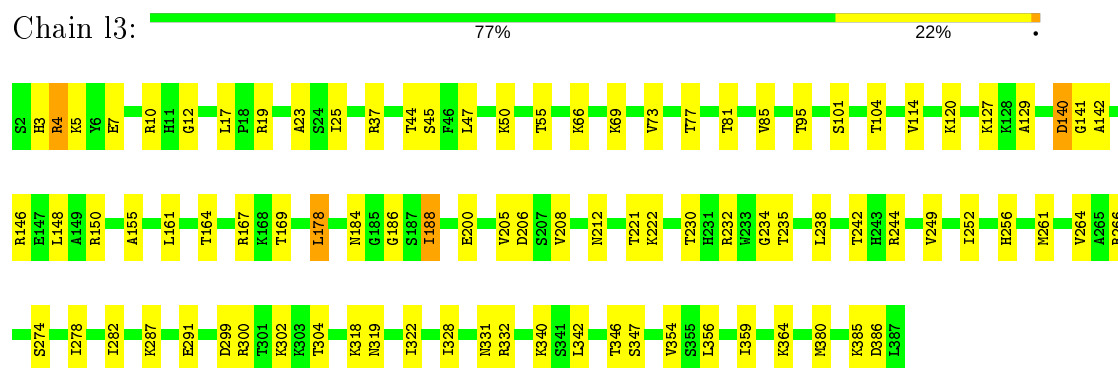
Chain l2: 



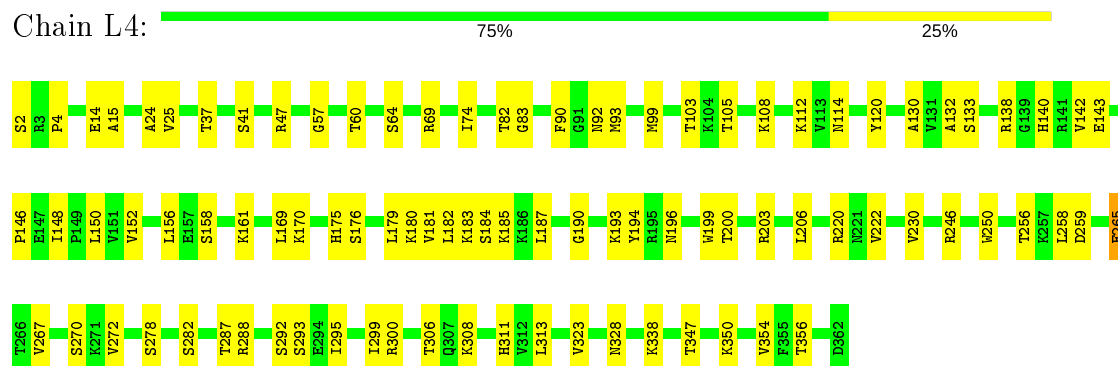
- Molecule 40: 60S ribosomal protein L3



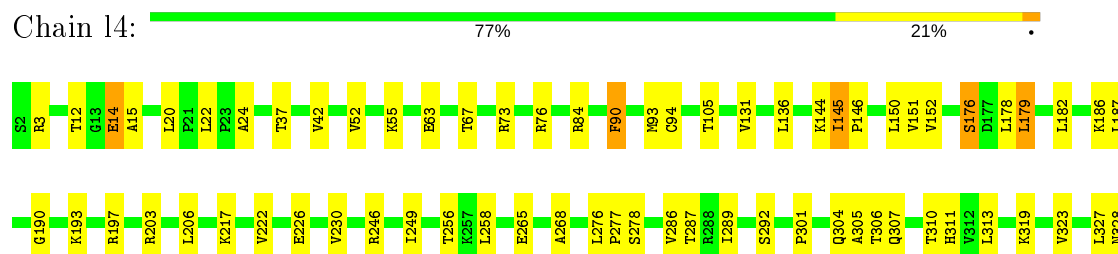
- Molecule 40: 60S ribosomal protein L3

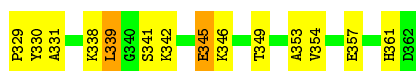


- Molecule 41: 60S ribosomal protein L4-A



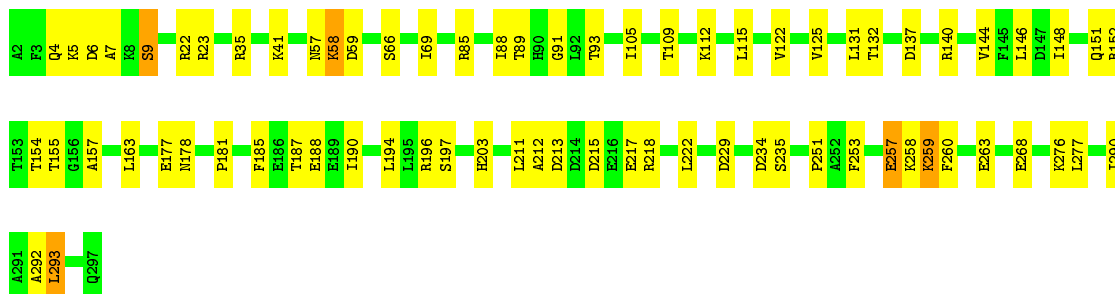
- Molecule 41: 60S ribosomal protein L4-A





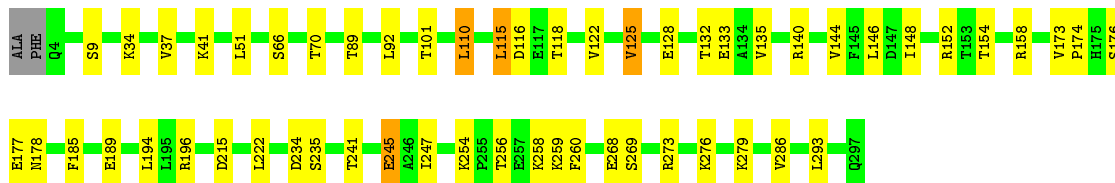
• Molecule 42: 60S ribosomal protein L5

Chain L5: 76% 23%



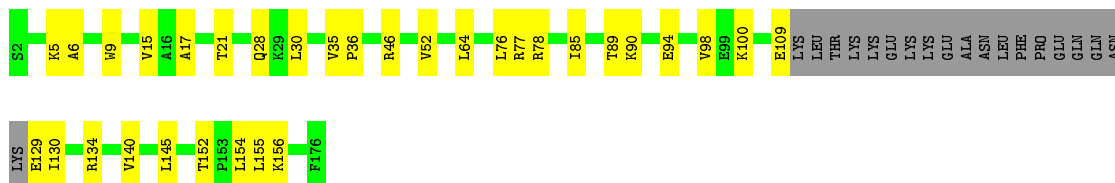
• Molecule 42: 60S ribosomal protein L5

Chain l5: 81% 17%



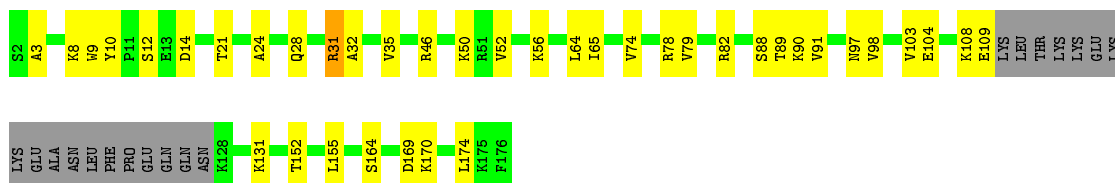
• Molecule 43: 60S ribosomal protein L6-A

Chain L6: 71% 18% 11%



• Molecule 43: 60S ribosomal protein L6-A

Chain l6: 67% 22% 10%



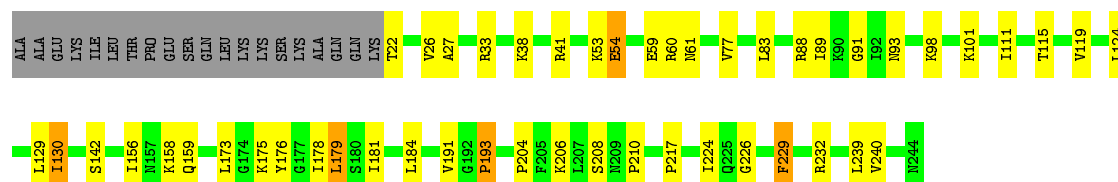
• Molecule 44: 60S ribosomal protein L7-A

Chain L7: 74% 15% 9%



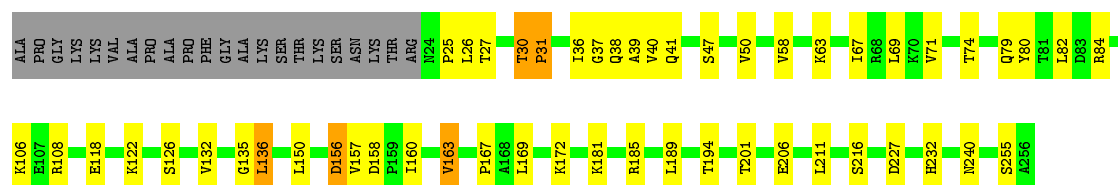
• Molecule 44: 60S ribosomal protein L7-A

Chain 17: 72% 18% 8%



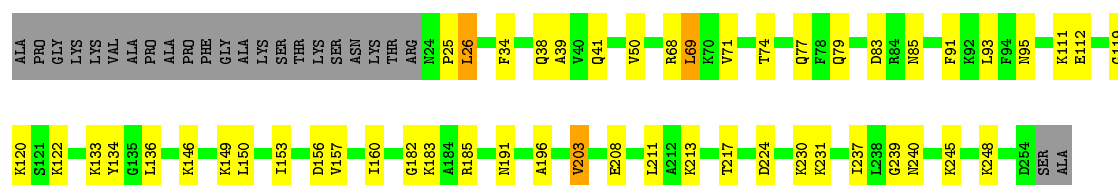
• Molecule 45: 60S ribosomal protein L8-A

Chain L8: 71% 18% 9%



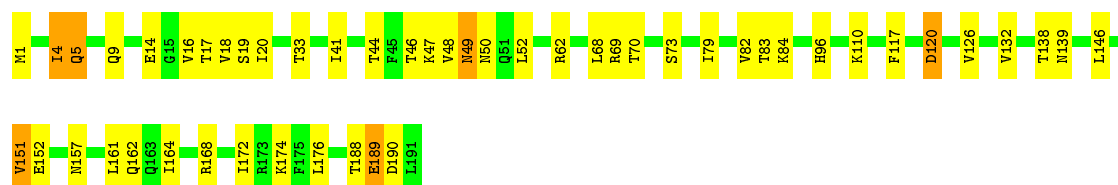
• Molecule 45: 60S ribosomal protein L8-A

Chain 18: 71% 19% 9%



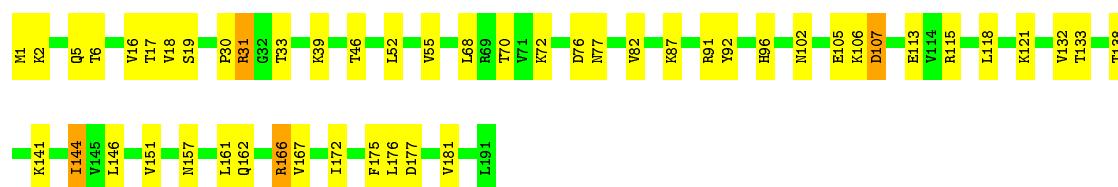
• Molecule 46: 60S ribosomal protein L9-A

Chain L9: 74% 23% 3%



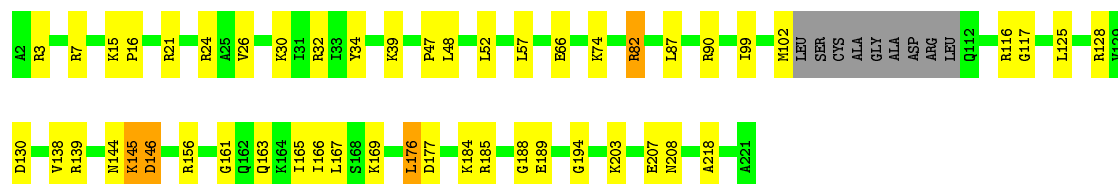
• Molecule 46: 60S ribosomal protein L9-A

Chain 19: 74% 24% 2%



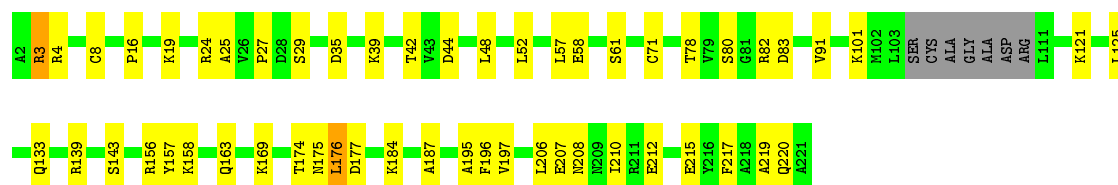
- Molecule 47: 60S ribosomal protein L10

Chain M0: 73% 21% . .



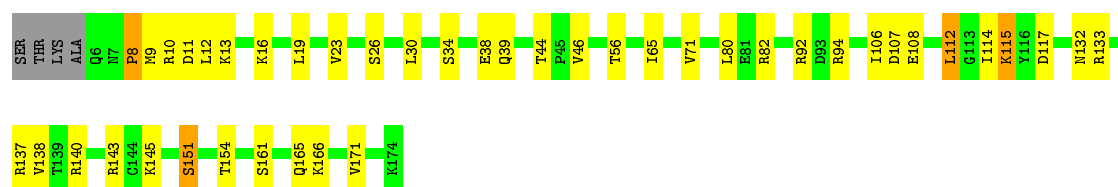
- Molecule 47: 60S ribosomal protein L10

Chain m0: 73% 23% . .



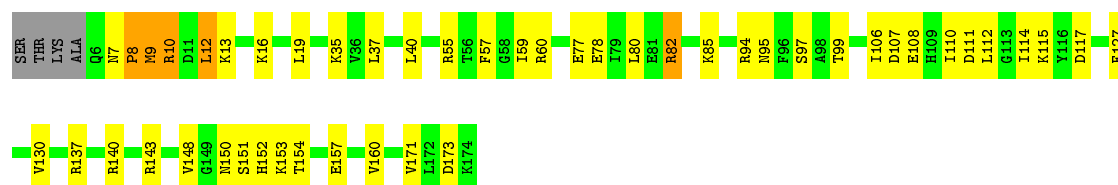
- Molecule 48: 60S ribosomal protein L11-B

Chain M1: 73% 23% . .



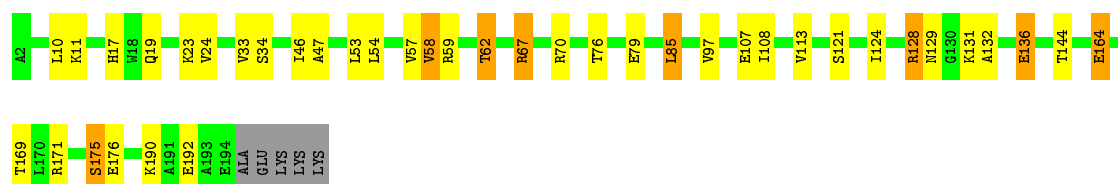
- Molecule 48: 60S ribosomal protein L11-B

Chain m1: 70% 25% . .



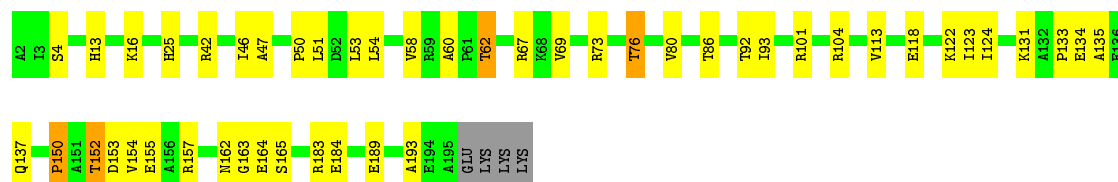
- Molecule 49: 60S ribosomal protein L13-A

Chain M3: 77% 16% . .



- Molecule 49: 60S ribosomal protein L13-A

Chain m3: 74% 22% ..



- Molecule 50: 60S ribosomal protein L14-A

Chain M4: 77% 21% ..



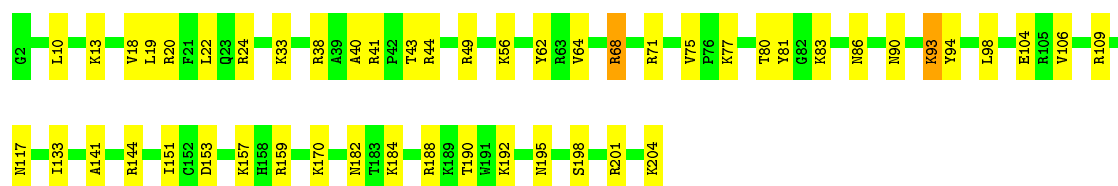
- Molecule 50: 60S ribosomal protein L14-A

Chain m4: 82% 16% .



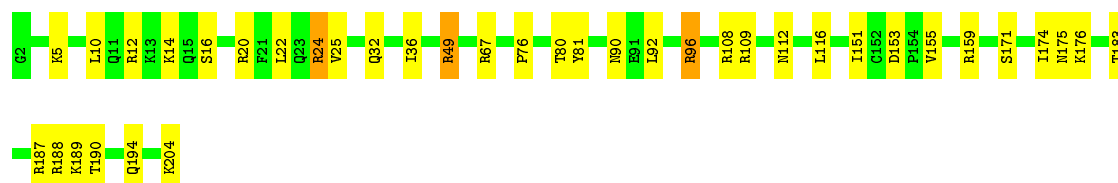
- Molecule 51: 60S ribosomal protein L15-A

Chain M5: 75% 24% .

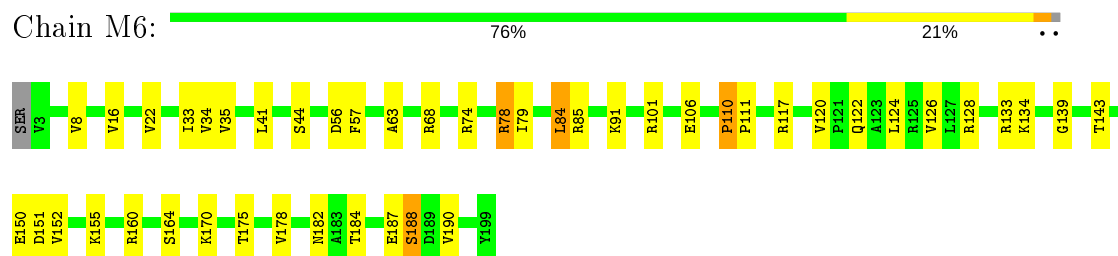


- Molecule 51: 60S ribosomal protein L15-A

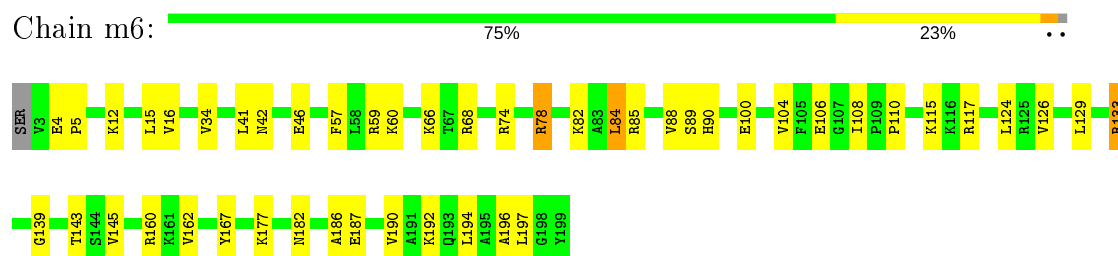
Chain m5: 81% 17% .



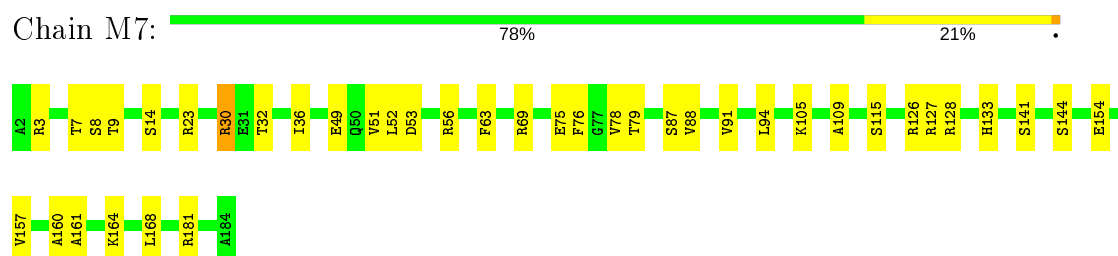
- Molecule 52: 60S ribosomal protein L16-A



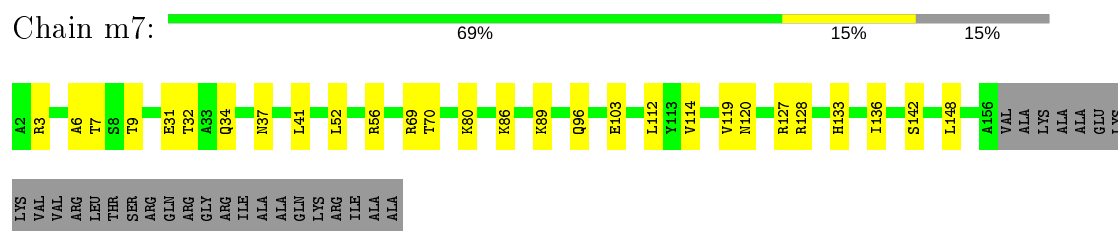
- Molecule 52: 60S ribosomal protein L16-A



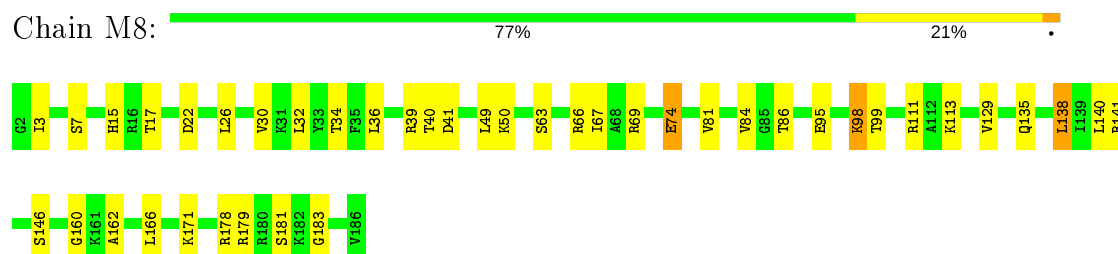
- Molecule 53: 60S ribosomal protein L17-A



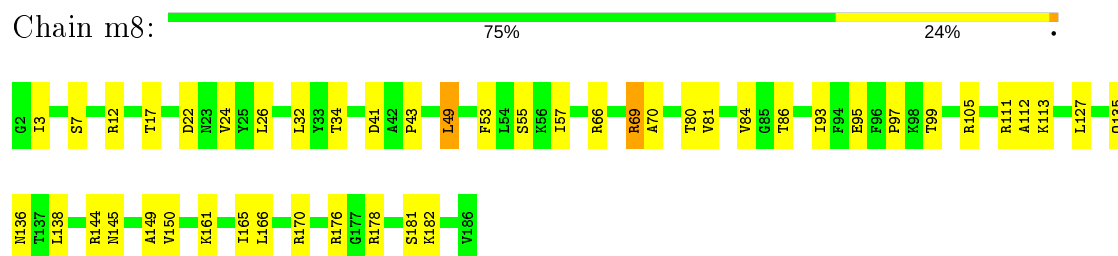
- Molecule 53: 60S ribosomal protein L17-A



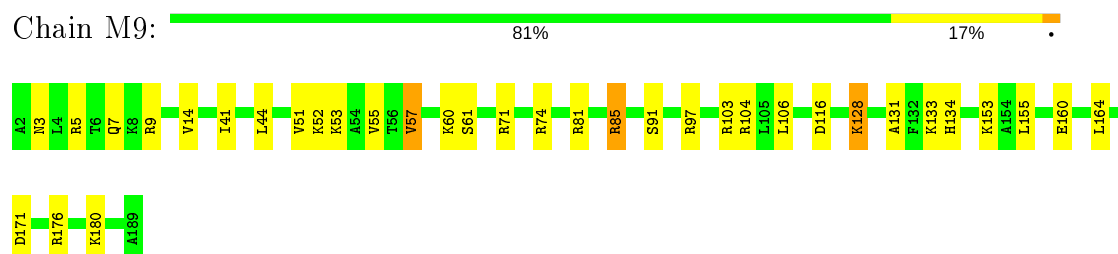
- Molecule 54: 60S ribosomal protein L18-A



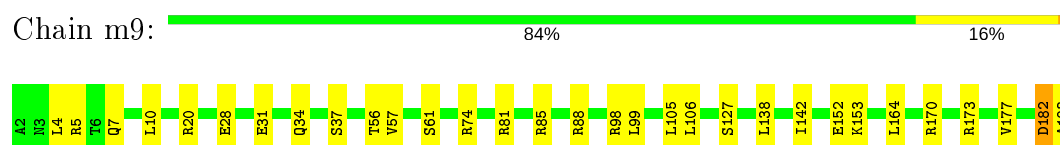
- Molecule 54: 60S ribosomal protein L18-A



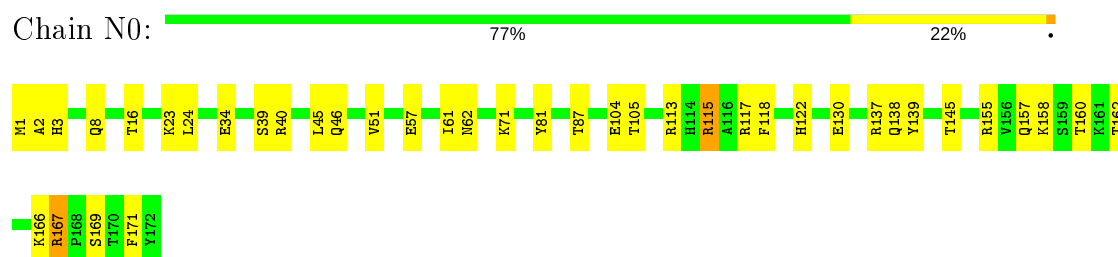
- Molecule 55: 60S ribosomal protein L19-A



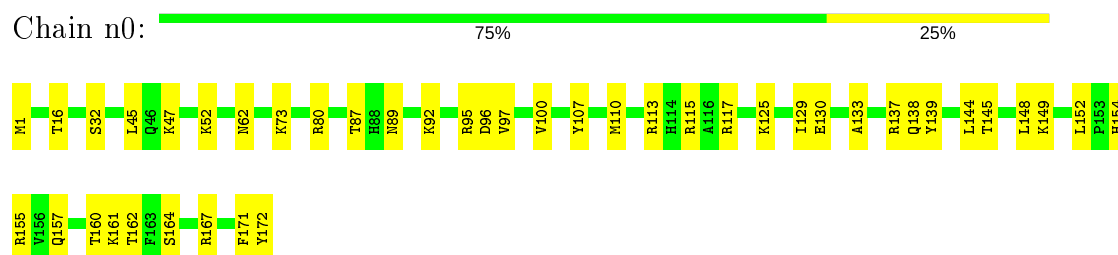
- Molecule 55: 60S ribosomal protein L19-A




- Molecule 56: 60S ribosomal protein L20-A

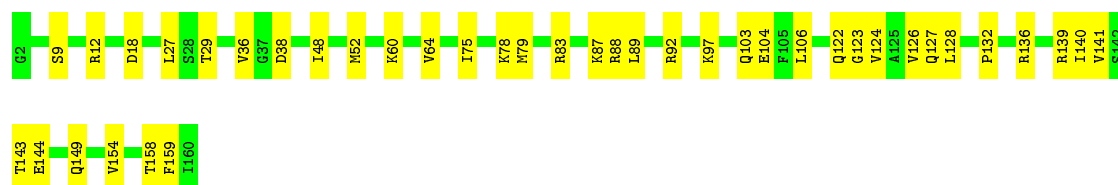


- Molecule 56: 60S ribosomal protein L20-A




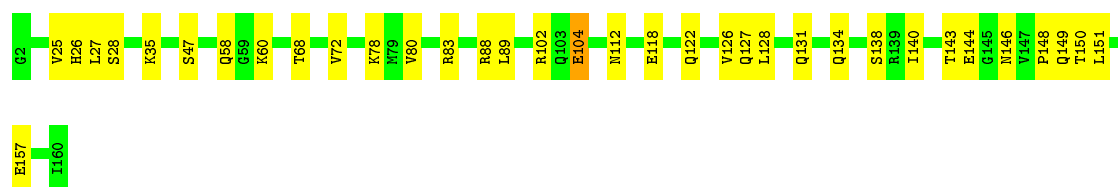
- Molecule 57: 60S ribosomal protein L21-A

Chain N1:  75% 25%



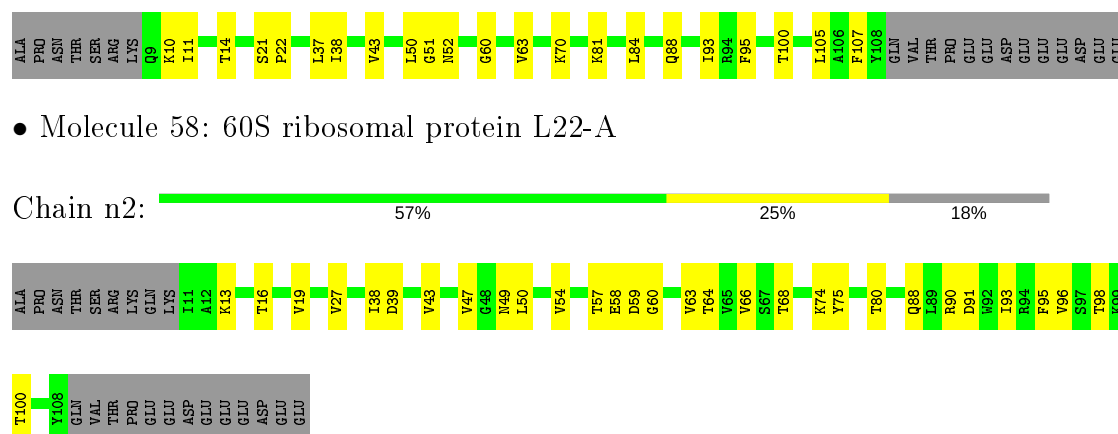
- Molecule 57: 60S ribosomal protein L21-A

Chain n1:  78% 21% .




- Molecule 58: 60S ribosomal protein L22-A

Chain N2:  65% 18% 17%




- Molecule 59: 60S ribosomal protein L23-A

Chain N3:  81% 19%

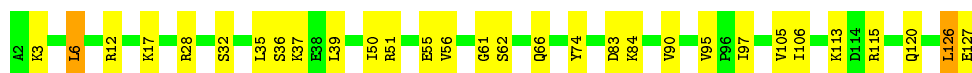


- Molecule 59: 60S ribosomal protein L23-A

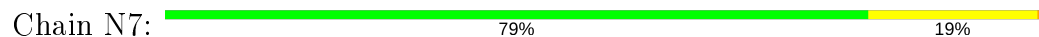
Chain n3:  81% 18% .



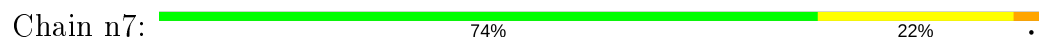
- Chain n6: 76% 22% .



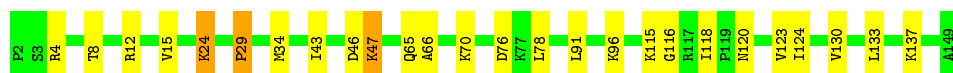
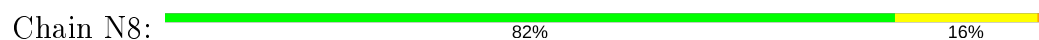
- Molecule 63: 60S ribosomal protein L27-A



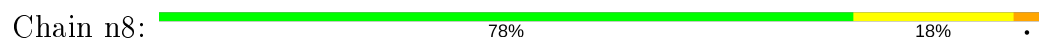
- Molecule 63: 60S ribosomal protein L27-A



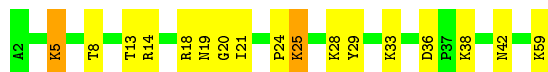
- Molecule 64: 60S ribosomal protein L28



- Molecule 64: 60S ribosomal protein L28



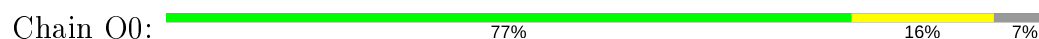
- Molecule 65: 60S ribosomal protein L29



- Molecule 65: 60S ribosomal protein L29

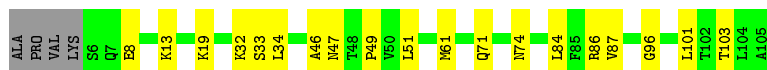
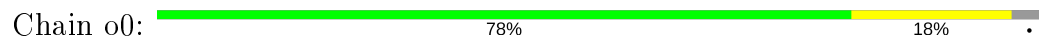


- Molecule 66: 60S ribosomal protein L30





- Molecule 66: 60S ribosomal protein L30



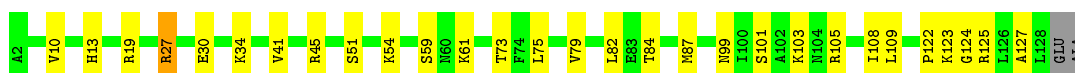
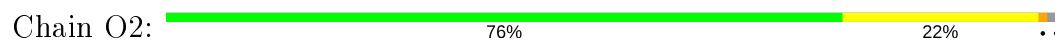
- Molecule 67: 60S ribosomal protein L31-A



- Molecule 67: 60S ribosomal protein L31-A



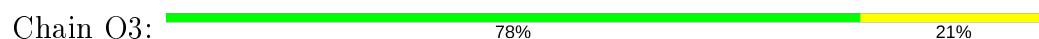
- Molecule 68: 60S ribosomal protein L32

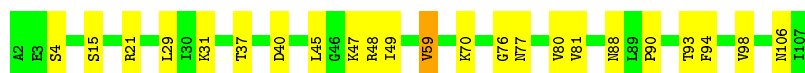


- Molecule 68: 60S ribosomal protein L32

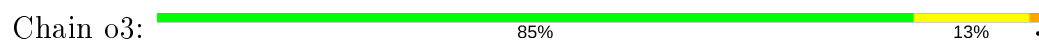


- Molecule 69: 60S ribosomal protein L33-A

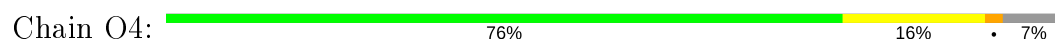




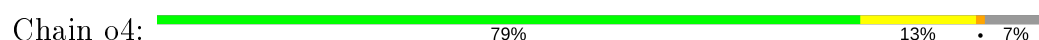
- Molecule 69: 60S ribosomal protein L33-A



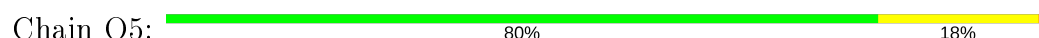
- Molecule 70: 60S ribosomal protein L34-A



- Molecule 70: 60S ribosomal protein L34-A



- Molecule 71: 60S ribosomal protein L35-A



- Molecule 71: 60S ribosomal protein L35-A

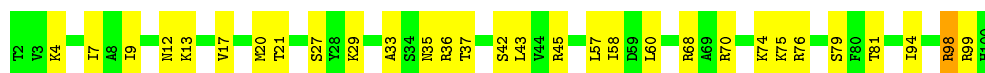


- Molecule 72: 60S ribosomal protein L36-A

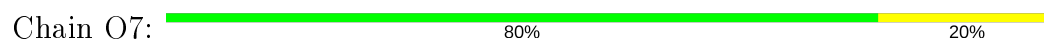


- Molecule 72: 60S ribosomal protein L36-A

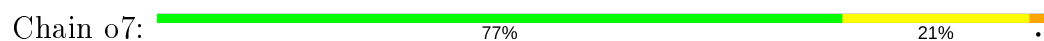




- Molecule 73: 60S ribosomal protein L37-A



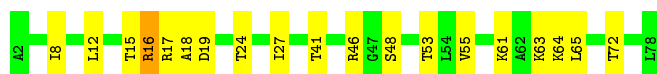
- Molecule 73: 60S ribosomal protein L37-A



- Molecule 74: 60S ribosomal protein L38



- Molecule 74: 60S ribosomal protein L38



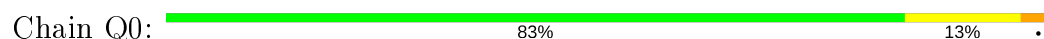
- Molecule 75: 60S ribosomal protein L39

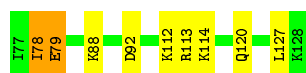


- Molecule 75: 60S ribosomal protein L39



- Molecule 76: Ubiquitin-60S ribosomal protein L40





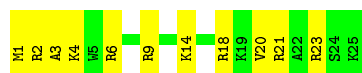
- Molecule 76: Ubiquitin-60S ribosomal protein L40



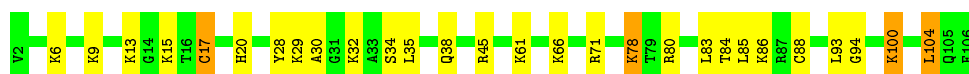
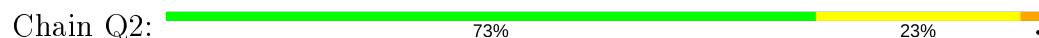
- Molecule 77: 60S ribosomal protein L41-A



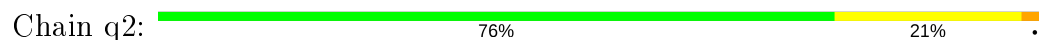
- Molecule 77: 60S ribosomal protein L41-A



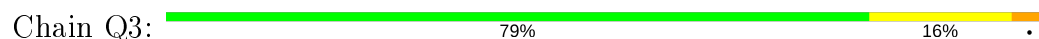
- Molecule 78: 60S ribosomal protein L42-A



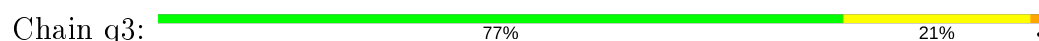
- Molecule 78: 60S ribosomal protein L42-A

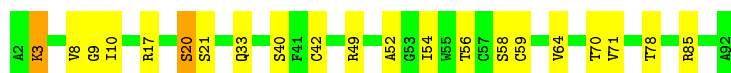


- Molecule 79: 60S ribosomal protein L43-A



- Molecule 79: 60S ribosomal protein L43-A





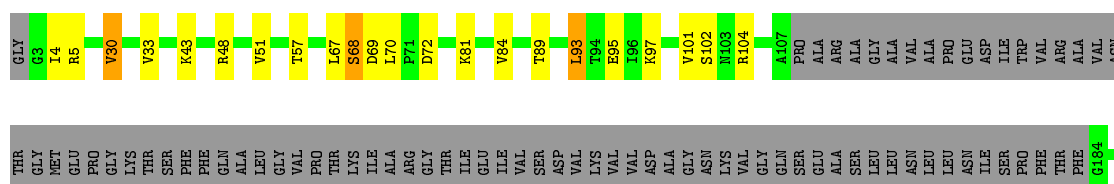
- Molecule 80: 40S ribosomal protein S30-A

Chain e0: 68% 29%



- Molecule 81: 60S acidic ribosomal protein P0

Chain p0: 38% 7% 54%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	435.64Å 286.76Å 303.26Å 90.00° 98.72° 90.00°	Depositor
Resolution (Å)	299.76 – 3.45	Depositor
% Data completeness (in resolution range)	100.0 (299.76-3.45)	Depositor
R_{merge}	0.45	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.196 , 0.260	Depositor
Wilson B-factor (Å ²)	93.1	Xtriage
Anisotropy	0.148	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411214	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.74	4/41698 (0.0%)	1.34	362/64972 (0.6%)
1	6	0.83	14/42765 (0.0%)	1.39	467/66634 (0.7%)
2	S0	0.45	0/1617	0.68	0/2215
2	s0	0.47	0/1623	0.67	0/2222
3	S1	0.39	0/1735	0.66	1/2335 (0.0%)
3	s1	0.49	0/1748	0.68	0/2352
4	S2	0.49	0/1665	0.66	0/2263
4	s2	0.55	0/1665	0.77	0/2263
5	S3	0.50	0/1759	0.66	0/2368
5	s3	0.46	0/1759	0.64	1/2368 (0.0%)
6	S4	0.52	0/2109	0.73	0/2839
6	s4	0.53	0/2109	0.72	0/2839
7	S5	0.42	0/1629	0.64	0/2202
7	s5	0.45	0/1629	0.69	0/2202
8	S6	0.49	0/1823	0.65	0/2439
8	s6	0.59	1/1779 (0.1%)	0.72	1/2379 (0.0%)
9	S7	0.44	0/1506	0.68	0/2028
9	s7	0.45	0/1516	0.69	0/2043
10	S8	0.56	0/1514	0.74	1/2021 (0.0%)
10	s8	0.55	0/1514	0.71	0/2021
11	S9	0.48	0/1519	0.68	1/2035 (0.0%)
11	s9	0.54	0/1519	0.71	0/2035
12	C0	0.46	0/790	0.68	1/1069 (0.1%)
12	c0	0.41	0/777	0.69	3/1049 (0.3%)
13	C1	0.59	0/1240	0.76	1/1675 (0.1%)
13	c1	0.59	0/1194	0.76	0/1610
14	C2	0.41	0/900	0.65	0/1224
14	c2	0.32	0/900	0.60	0/1224
15	C3	0.52	0/1215	0.70	2/1638 (0.1%)
15	c3	0.55	0/1215	0.69	0/1638
16	C4	0.40	0/901	0.64	0/1217
16	c4	0.50	0/960	0.70	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.52	0/998	0.72	0/1341
17	c5	0.49	0/1060	0.69	1/1426 (0.1%)
18	C6	0.48	0/1125	0.68	2/1510 (0.1%)
18	c6	0.49	0/1131	0.71	0/1518
19	C7	0.48	0/935	0.68	1/1254 (0.1%)
19	c7	0.48	0/914	0.69	0/1224
20	C8	0.47	0/1211	0.70	0/1628
20	c8	0.50	0/1211	0.72	2/1628 (0.1%)
21	C9	0.44	0/1130	0.62	0/1517
21	c9	0.51	0/1130	0.67	0/1517
22	D0	0.45	0/865	0.71	1/1169 (0.1%)
22	d0	0.46	0/892	0.68	0/1205
23	D1	0.47	0/693	0.64	0/935
23	d1	0.51	0/693	0.68	0/935
24	D2	0.49	0/1038	0.71	0/1395
24	d2	0.59	0/1038	0.76	1/1395 (0.1%)
25	D3	0.61	0/1139	0.75	0/1518
25	d3	0.70	0/1139	0.83	1/1518 (0.1%)
26	D4	0.46	0/1087	0.65	0/1449
26	d4	0.55	0/1087	0.73	0/1449
27	D5	0.44	0/571	0.75	0/768
27	d5	0.45	0/566	0.68	0/761
28	D6	0.47	0/782	0.66	0/1047
28	d6	0.54	0/782	0.79	1/1047 (0.1%)
29	D7	0.42	0/620	0.65	0/838
29	d7	0.47	0/620	0.71	0/838
30	D8	0.42	0/499	0.64	0/670
30	d8	0.43	0/499	0.62	0/670
31	D9	0.53	0/452	0.67	0/600
31	d9	0.64	0/452	0.69	0/600
32	E0	0.48	0/483	0.65	0/643
33	E1	0.49	0/577	0.80	0/770
33	e1	0.42	0/619	0.75	1/822 (0.1%)
34	SR	0.40	0/2494	0.63	0/3393
34	sR	0.39	0/2495	0.58	0/3395
35	SM	0.53	0/1113	0.71	2/1502 (0.1%)
35	sM	0.49	0/682	0.69	1/921 (0.1%)
36	1	1.12	138/75394 (0.2%)	1.68	1938/117545 (1.6%)
36	5	1.11	157/75414 (0.2%)	1.68	1917/117575 (1.6%)
37	3	0.99	2/2883 (0.1%)	1.47	39/4491 (0.9%)
37	7	1.11	3/2883 (0.1%)	1.76	76/4491 (1.7%)
38	4	1.02	1/3746 (0.0%)	1.59	63/5832 (1.1%)
38	8	0.90	2/3746 (0.1%)	1.47	43/5832 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.68	0/1948	0.81	1/2617 (0.0%)
39	l2	0.60	0/1946	0.82	2/2614 (0.1%)
40	L3	0.74	0/3146	0.83	0/4228
40	l3	0.78	0/3146	0.86	2/4228 (0.0%)
41	L4	0.78	1/2800 (0.0%)	0.90	1/3790 (0.0%)
41	l4	0.73	1/2800 (0.0%)	0.88	3/3790 (0.1%)
42	L5	0.61	0/2425	0.73	0/3271
42	l5	0.72	0/2408	0.83	1/3248 (0.0%)
43	L6	0.78	0/1260	0.85	0/1694
43	l6	0.81	0/1269	0.87	0/1705
44	L7	0.83	0/1821	0.91	3/2451 (0.1%)
44	l7	0.87	0/1828	0.97	5/2461 (0.2%)
45	L8	0.54	0/1836	0.71	2/2481 (0.1%)
45	l8	0.48	0/1795	0.68	1/2429 (0.0%)
46	L9	0.69	0/1539	0.81	1/2073 (0.0%)
46	l9	0.76	0/1539	0.84	2/2073 (0.1%)
47	M0	0.76	0/1741	0.84	3/2335 (0.1%)
47	m0	0.76	1/1758 (0.1%)	0.82	0/2358
48	M1	0.56	0/1374	0.74	1/1842 (0.1%)
48	m1	0.70	0/1374	0.80	1/1842 (0.1%)
49	M3	0.72	0/1568	0.86	2/2106 (0.1%)
49	m3	0.64	0/1573	0.78	0/2113
50	M4	0.81	0/1068	0.88	1/1438 (0.1%)
50	m4	0.82	0/1074	0.84	1/1446 (0.1%)
51	M5	0.75	0/1757	0.86	2/2354 (0.1%)
51	m5	0.61	0/1757	0.79	2/2354 (0.1%)
52	M6	0.85	0/1585	0.92	4/2128 (0.2%)
52	m6	0.96	0/1585	0.98	4/2128 (0.2%)
53	M7	0.76	0/1443	0.83	0/1944
53	m7	0.83	0/1250	0.87	1/1683 (0.1%)
54	M8	0.75	0/1465	0.90	4/1965 (0.2%)
54	m8	0.72	0/1465	0.86	1/1965 (0.1%)
55	M9	0.60	0/1538	0.75	0/2050
55	m9	0.58	0/1538	0.69	0/2050
56	N0	0.78	0/1481	0.85	1/1990 (0.1%)
56	n0	0.88	0/1481	0.90	2/1990 (0.1%)
57	N1	0.74	0/1300	0.82	1/1743 (0.1%)
57	n1	0.81	1/1300 (0.1%)	0.88	0/1743
58	N2	0.48	0/812	0.63	0/1099
58	n2	0.49	0/794	0.68	0/1076
59	N3	0.69	0/1018	0.81	0/1369
59	n3	0.80	0/1018	0.82	0/1369
60	N4	0.62	0/712	0.74	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.65	0/1052	0.75	0/1398
61	N5	0.64	0/979	0.79	1/1321 (0.1%)
61	n5	0.60	0/974	0.77	1/1314 (0.1%)
62	N6	0.72	0/1004	0.86	1/1341 (0.1%)
62	n6	0.62	0/1004	0.81	0/1341
63	N7	0.54	0/1118	0.68	0/1497
63	n7	0.48	0/1118	0.66	0/1497
64	N8	0.73	0/1204	0.85	0/1612
64	n8	0.73	0/1204	0.84	1/1612 (0.1%)
65	N9	0.69	0/473	0.83	1/629 (0.2%)
65	n9	0.71	0/473	0.88	0/629
66	O0	0.49	0/751	0.68	0/1008
66	o0	0.53	0/775	0.69	0/1040
67	O1	0.65	0/890	0.80	0/1196
67	o1	0.71	0/897	0.86	2/1205 (0.2%)
68	O2	0.79	0/1041	0.87	0/1394
68	o2	0.87	0/1041	0.89	0/1394
69	O3	0.86	0/868	0.94	0/1168
69	o3	0.87	0/868	0.90	0/1168
70	O4	0.59	0/890	0.77	1/1189 (0.1%)
70	o4	0.52	0/890	0.74	0/1189
71	O5	0.67	0/978	0.78	0/1301
71	o5	0.58	0/974	0.77	2/1297 (0.2%)
72	O6	0.61	0/778	0.77	0/1034
72	o6	0.58	0/777	0.68	0/1033
73	O7	0.74	0/696	0.87	1/923 (0.1%)
73	o7	0.64	0/696	0.79	0/923
74	O8	0.53	0/618	0.66	0/826
74	o8	0.45	0/614	0.66	0/822
75	O9	0.64	0/443	0.82	0/588
75	o9	0.62	0/443	0.78	0/588
76	Q0	0.79	0/423	0.93	0/562
76	q0	0.90	1/423 (0.2%)	0.98	0/562
77	Q1	0.67	0/234	0.87	0/300
77	q1	0.58	0/234	0.89	0/300
78	Q2	0.83	1/860 (0.1%)	0.84	0/1136
78	q2	0.73	1/860 (0.1%)	0.83	2/1136 (0.2%)
79	Q3	0.71	0/701	0.83	0/934
79	q3	0.68	0/701	0.78	0/934
80	e0	0.51	0/499	0.75	0/665
81	p0	0.48	0/1091	0.64	0/1472
All	All	0.87	329/430072 (0.1%)	1.32	4999/631360 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	S1	0	1
7	s5	0	2
9	S7	0	1
9	s7	0	1
10	S8	0	1
11	S9	0	1
16	C4	0	1
18	C6	0	1
18	c6	0	1
19	C7	0	1
20	c8	0	1
22	d0	0	1
26	d4	0	1
27	D5	0	2
33	E1	0	1
39	L2	0	1
39	l2	0	1
40	L3	0	1
40	l3	0	1
42	L5	0	1
43	L6	0	1
44	l7	0	1
45	L8	0	1
47	M0	0	1
48	M1	0	1
48	m1	0	1
50	M4	0	1
52	M6	0	1
56	n0	0	2
64	n8	0	1
65	N9	0	1
67	O1	0	1
69	o3	0	1
80	e0	0	1
All	All	0	37

The worst 5 of 329 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	12.22	2.03	1.82
36	5	1152	G	N9-C4	-12.11	1.28	1.38
36	5	2145	A	N7-C5	-9.34	1.33	1.39
78	q2	17	CYS	CB-SG	9.04	1.97	1.82
36	5	3040	A	N9-C4	-8.70	1.32	1.37

The worst 5 of 4999 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-19.38	114.37	126.00
36	5	1152	G	N3-C4-C5	17.87	137.53	128.60
36	5	1152	G	C2-N3-C4	-16.63	103.58	111.90
36	1	645	A	N1-C6-N6	-16.45	108.73	118.60
36	1	343	U	O5'-P-OP2	-14.33	92.80	105.70

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
3	S1	177	GLN	Peptide
9	S7	131	PHE	Peptide
10	S8	8	ARG	Peptide
11	S9	137	GLY	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	142 (70%)	37 (18%)	25 (12%)	0	4
2	s0	204/251 (81%)	150 (74%)	36 (18%)	18 (9%)	1	7
3	S1	212/254 (84%)	142 (67%)	42 (20%)	28 (13%)	0	3
3	s1	214/254 (84%)	165 (77%)	37 (17%)	12 (6%)	2	15
4	S2	215/253 (85%)	175 (81%)	23 (11%)	17 (8%)	1	9
4	s2	215/253 (85%)	169 (79%)	28 (13%)	18 (8%)	1	8
5	S3	221/239 (92%)	170 (77%)	37 (17%)	14 (6%)	1	13
5	s3	221/239 (92%)	174 (79%)	25 (11%)	22 (10%)	0	6
6	S4	258/260 (99%)	201 (78%)	43 (17%)	14 (5%)	2	16
6	s4	258/260 (99%)	206 (80%)	35 (14%)	17 (7%)	1	12
7	S5	204/224 (91%)	150 (74%)	33 (16%)	21 (10%)	0	6
7	s5	204/224 (91%)	140 (69%)	41 (20%)	23 (11%)	0	5
8	S6	224/236 (95%)	181 (81%)	33 (15%)	10 (4%)	2	20
8	s6	216/236 (92%)	172 (80%)	34 (16%)	10 (5%)	2	20
9	S7	182/189 (96%)	137 (75%)	27 (15%)	18 (10%)	0	6
9	s7	184/189 (97%)	133 (72%)	34 (18%)	17 (9%)	1	7
10	S8	184/200 (92%)	145 (79%)	29 (16%)	10 (5%)	2	16
10	s8	184/200 (92%)	149 (81%)	27 (15%)	8 (4%)	2	21
11	S9	183/196 (93%)	144 (79%)	27 (15%)	12 (7%)	1	12
11	s9	183/196 (93%)	133 (73%)	40 (22%)	10 (6%)	2	16
12	C0	94/105 (90%)	68 (72%)	19 (20%)	7 (7%)	1	10
12	c0	92/105 (88%)	68 (74%)	11 (12%)	13 (14%)	0	3
13	C1	153/155 (99%)	107 (70%)	27 (18%)	19 (12%)	0	4
13	c1	144/155 (93%)	114 (79%)	23 (16%)	7 (5%)	2	18
14	C2	122/142 (86%)	66 (54%)	39 (32%)	17 (14%)	0	3
14	c2	122/142 (86%)	72 (59%)	30 (25%)	20 (16%)	0	2
15	C3	148/150 (99%)	117 (79%)	24 (16%)	7 (5%)	2	19
15	c3	148/150 (99%)	107 (72%)	28 (19%)	13 (9%)	1	7
16	C4	125/136 (92%)	93 (74%)	23 (18%)	9 (7%)	1	10
16	c4	126/136 (93%)	99 (79%)	18 (14%)	9 (7%)	1	11
17	C5	122/141 (86%)	84 (69%)	24 (20%)	14 (12%)	0	5
17	c5	133/141 (94%)	92 (69%)	24 (18%)	17 (13%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	C6	139/142 (98%)	117 (84%)	16 (12%)	6 (4%)	2	21
18	c6	140/142 (99%)	106 (76%)	23 (16%)	11 (8%)	1	9
19	C7	116/136 (85%)	85 (73%)	18 (16%)	13 (11%)	0	5
19	c7	113/136 (83%)	84 (74%)	22 (20%)	7 (6%)	1	13
20	C8	143/145 (99%)	107 (75%)	23 (16%)	13 (9%)	1	7
20	c8	143/145 (99%)	105 (73%)	25 (18%)	13 (9%)	1	7
21	C9	141/143 (99%)	108 (77%)	27 (19%)	6 (4%)	2	21
21	c9	141/143 (99%)	114 (81%)	21 (15%)	6 (4%)	2	21
22	D0	105/120 (88%)	79 (75%)	20 (19%)	6 (6%)	1	15
22	d0	108/120 (90%)	83 (77%)	14 (13%)	11 (10%)	0	6
23	D1	85/87 (98%)	58 (68%)	19 (22%)	8 (9%)	0	7
23	d1	85/87 (98%)	68 (80%)	12 (14%)	5 (6%)	1	14
24	D2	127/129 (98%)	103 (81%)	17 (13%)	7 (6%)	2	16
24	d2	127/129 (98%)	101 (80%)	23 (18%)	3 (2%)	6	34
25	D3	142/144 (99%)	107 (75%)	22 (16%)	13 (9%)	1	7
25	d3	142/144 (99%)	115 (81%)	19 (13%)	8 (6%)	2	15
26	D4	132/134 (98%)	105 (80%)	17 (13%)	10 (8%)	1	9
26	d4	132/134 (98%)	100 (76%)	15 (11%)	17 (13%)	0	3
27	D5	68/107 (64%)	44 (65%)	14 (21%)	10 (15%)	0	2
27	d5	67/107 (63%)	47 (70%)	15 (22%)	5 (8%)	1	10
28	D6	95/97 (98%)	59 (62%)	23 (24%)	13 (14%)	0	3
28	d6	95/97 (98%)	70 (74%)	18 (19%)	7 (7%)	1	10
29	D7	79/81 (98%)	55 (70%)	18 (23%)	6 (8%)	1	9
29	d7	79/81 (98%)	53 (67%)	21 (27%)	5 (6%)	1	13
30	D8	61/66 (92%)	42 (69%)	14 (23%)	5 (8%)	1	8
30	d8	61/66 (92%)	43 (70%)	14 (23%)	4 (7%)	1	12
31	D9	51/55 (93%)	37 (72%)	10 (20%)	4 (8%)	1	9
31	d9	51/55 (93%)	39 (76%)	8 (16%)	4 (8%)	1	9
32	E0	58/60 (97%)	43 (74%)	10 (17%)	5 (9%)	1	8
33	E1	69/76 (91%)	32 (46%)	20 (29%)	17 (25%)	0	0
33	e1	74/76 (97%)	33 (45%)	21 (28%)	20 (27%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	SR	316/318 (99%)	231 (73%)	58 (18%)	27 (8%)	1	8
34	sR	316/318 (99%)	255 (81%)	49 (16%)	12 (4%)	3	24
35	SM	155/273 (57%)	99 (64%)	34 (22%)	22 (14%)	0	3
35	sM	98/273 (36%)	63 (64%)	23 (24%)	12 (12%)	0	4
39	L2	250/253 (99%)	214 (86%)	28 (11%)	8 (3%)	4	28
39	l2	250/253 (99%)	200 (80%)	32 (13%)	18 (7%)	1	10
40	L3	384/386 (100%)	324 (84%)	45 (12%)	15 (4%)	3	24
40	l3	384/386 (100%)	323 (84%)	42 (11%)	19 (5%)	2	18
41	L4	359/361 (99%)	279 (78%)	54 (15%)	26 (7%)	1	10
41	l4	359/361 (99%)	277 (77%)	56 (16%)	26 (7%)	1	10
42	L5	294/296 (99%)	237 (81%)	34 (12%)	23 (8%)	1	9
42	l5	292/296 (99%)	240 (82%)	39 (13%)	13 (4%)	2	20
43	L6	152/175 (87%)	121 (80%)	26 (17%)	5 (3%)	4	27
43	l6	153/175 (87%)	121 (79%)	25 (16%)	7 (5%)	2	20
44	L7	220/243 (90%)	183 (83%)	24 (11%)	13 (6%)	1	14
44	l7	221/243 (91%)	177 (80%)	30 (14%)	14 (6%)	1	13
45	L8	231/255 (91%)	179 (78%)	35 (15%)	17 (7%)	1	10
45	l8	229/255 (90%)	176 (77%)	36 (16%)	17 (7%)	1	10
46	L9	189/191 (99%)	150 (79%)	28 (15%)	11 (6%)	1	15
46	l9	189/191 (99%)	153 (81%)	27 (14%)	9 (5%)	2	19
47	M0	207/220 (94%)	167 (81%)	30 (14%)	10 (5%)	2	19
47	m0	209/220 (95%)	163 (78%)	27 (13%)	19 (9%)	1	7
48	M1	167/173 (96%)	126 (75%)	31 (19%)	10 (6%)	1	14
48	m1	167/173 (96%)	127 (76%)	25 (15%)	15 (9%)	1	7
49	M3	191/198 (96%)	140 (73%)	37 (19%)	14 (7%)	1	10
49	m3	192/198 (97%)	150 (78%)	24 (12%)	18 (9%)	0	7
50	M4	134/137 (98%)	106 (79%)	19 (14%)	9 (7%)	1	12
50	m4	135/137 (98%)	116 (86%)	16 (12%)	3 (2%)	6	35
51	M5	201/203 (99%)	170 (85%)	24 (12%)	7 (4%)	3	26
51	m5	201/203 (99%)	171 (85%)	25 (12%)	5 (2%)	5	32
52	M6	195/198 (98%)	167 (86%)	22 (11%)	6 (3%)	4	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	m6	195/198 (98%)	164 (84%)	23 (12%)	8 (4%)	3	23
53	M7	181/183 (99%)	142 (78%)	27 (15%)	12 (7%)	1	12
53	m7	153/183 (84%)	130 (85%)	20 (13%)	3 (2%)	7	37
54	M8	183/185 (99%)	148 (81%)	28 (15%)	7 (4%)	3	24
54	m8	183/185 (99%)	140 (76%)	30 (16%)	13 (7%)	1	11
55	M9	186/188 (99%)	160 (86%)	17 (9%)	9 (5%)	2	19
55	m9	186/188 (99%)	156 (84%)	26 (14%)	4 (2%)	6	35
56	N0	170/172 (99%)	149 (88%)	14 (8%)	7 (4%)	3	23
56	n0	170/172 (99%)	146 (86%)	19 (11%)	5 (3%)	4	30
57	N1	157/159 (99%)	136 (87%)	16 (10%)	5 (3%)	4	28
57	n1	157/159 (99%)	125 (80%)	26 (17%)	6 (4%)	3	24
58	N2	98/120 (82%)	74 (76%)	16 (16%)	8 (8%)	1	8
58	n2	96/120 (80%)	76 (79%)	17 (18%)	3 (3%)	4	29
59	N3	134/136 (98%)	114 (85%)	14 (10%)	6 (4%)	2	20
59	n3	134/136 (98%)	116 (87%)	9 (7%)	9 (7%)	1	12
60	N4	96/155 (62%)	68 (71%)	20 (21%)	8 (8%)	1	8
60	n4	133/155 (86%)	99 (74%)	21 (16%)	13 (10%)	0	6
61	N5	119/141 (84%)	98 (82%)	17 (14%)	4 (3%)	3	27
61	n5	118/141 (84%)	97 (82%)	16 (14%)	5 (4%)	3	22
62	N6	124/126 (98%)	99 (80%)	16 (13%)	9 (7%)	1	10
62	n6	124/126 (98%)	100 (81%)	16 (13%)	8 (6%)	1	12
63	N7	133/135 (98%)	104 (78%)	20 (15%)	9 (7%)	1	12
63	n7	133/135 (98%)	91 (68%)	30 (23%)	12 (9%)	1	7
64	N8	146/148 (99%)	114 (78%)	23 (16%)	9 (6%)	1	13
64	n8	146/148 (99%)	119 (82%)	19 (13%)	8 (6%)	2	16
65	N9	56/58 (97%)	39 (70%)	11 (20%)	6 (11%)	0	5
65	n9	56/58 (97%)	36 (64%)	11 (20%)	9 (16%)	0	2
66	O0	95/104 (91%)	76 (80%)	17 (18%)	2 (2%)	7	36
66	o0	98/104 (94%)	83 (85%)	11 (11%)	4 (4%)	3	23
67	O1	107/112 (96%)	87 (81%)	13 (12%)	7 (6%)	1	12
67	o1	107/112 (96%)	87 (81%)	12 (11%)	8 (8%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	O2	125/129 (97%)	99 (79%)	18 (14%)	8 (6%)	1	13
68	o2	125/129 (97%)	102 (82%)	14 (11%)	9 (7%)	1	10
69	O3	104/106 (98%)	86 (83%)	13 (12%)	5 (5%)	2	19
69	o3	104/106 (98%)	95 (91%)	7 (7%)	2 (2%)	8	38
70	O4	110/120 (92%)	92 (84%)	16 (14%)	2 (2%)	8	39
70	o4	110/120 (92%)	90 (82%)	15 (14%)	5 (4%)	2	20
71	O5	117/119 (98%)	99 (85%)	13 (11%)	5 (4%)	2	21
71	o5	117/119 (98%)	89 (76%)	22 (19%)	6 (5%)	2	17
72	O6	97/99 (98%)	70 (72%)	15 (16%)	12 (12%)	0	4
72	o6	97/99 (98%)	83 (86%)	10 (10%)	4 (4%)	3	23
73	O7	85/87 (98%)	66 (78%)	18 (21%)	1 (1%)	13	48
73	o7	85/87 (98%)	69 (81%)	12 (14%)	4 (5%)	2	19
74	O8	75/77 (97%)	61 (81%)	11 (15%)	3 (4%)	3	23
74	o8	75/77 (97%)	63 (84%)	10 (13%)	2 (3%)	5	31
75	O9	48/50 (96%)	41 (85%)	6 (12%)	1 (2%)	7	36
75	o9	48/50 (96%)	38 (79%)	6 (12%)	4 (8%)	1	8
76	Q0	50/52 (96%)	42 (84%)	3 (6%)	5 (10%)	0	6
76	q0	50/52 (96%)	40 (80%)	8 (16%)	2 (4%)	3	23
77	Q1	23/25 (92%)	16 (70%)	5 (22%)	2 (9%)	1	8
77	q1	23/25 (92%)	19 (83%)	2 (9%)	2 (9%)	1	8
78	Q2	103/105 (98%)	77 (75%)	18 (18%)	8 (8%)	1	9
78	q2	103/105 (98%)	87 (84%)	11 (11%)	5 (5%)	2	18
79	Q3	89/91 (98%)	74 (83%)	8 (9%)	7 (8%)	1	9
79	q3	89/91 (98%)	70 (79%)	13 (15%)	6 (7%)	1	12
80	e0	60/62 (97%)	39 (65%)	15 (25%)	6 (10%)	0	6
81	p0	139/311 (45%)	108 (78%)	24 (17%)	7 (5%)	2	18
All	All	22333/24143 (92%)	17400 (78%)	3410 (15%)	1523 (7%)	1	12

5 of 1523 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	39	ASN

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Mol	Chain	Res	Type
2	S0	68	PRO
2	S0	139	VAL
2	S0	158	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/209 (78%)	125 (76%)	39 (24%)	0	3
2	s0	165/209 (79%)	135 (82%)	30 (18%)	1	8
3	S1	191/223 (86%)	146 (76%)	45 (24%)	1	3
3	s1	192/223 (86%)	147 (77%)	45 (23%)	1	3
4	S2	176/204 (86%)	136 (77%)	40 (23%)	1	3
4	s2	176/204 (86%)	128 (73%)	48 (27%)	0	2
5	S3	182/194 (94%)	140 (77%)	42 (23%)	1	3
5	s3	182/194 (94%)	140 (77%)	42 (23%)	1	3
6	S4	221/221 (100%)	175 (79%)	46 (21%)	1	5
6	s4	221/221 (100%)	173 (78%)	48 (22%)	1	4
7	S5	173/190 (91%)	139 (80%)	34 (20%)	1	6
7	s5	173/190 (91%)	136 (79%)	37 (21%)	1	4
8	S6	188/201 (94%)	151 (80%)	37 (20%)	1	6
8	s6	187/201 (93%)	153 (82%)	34 (18%)	1	8
9	S7	165/169 (98%)	135 (82%)	30 (18%)	1	8
9	s7	165/169 (98%)	130 (79%)	35 (21%)	1	4
10	S8	150/161 (93%)	123 (82%)	27 (18%)	1	8
10	s8	150/161 (93%)	127 (85%)	23 (15%)	2	15
11	S9	158/165 (96%)	119 (75%)	39 (25%)	0	3
11	s9	158/165 (96%)	128 (81%)	30 (19%)	1	7
12	C0	77/98 (79%)	61 (79%)	16 (21%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	c0	73/98 (74%)	60 (82%)	13 (18%)	2	8
13	C1	129/136 (95%)	105 (81%)	24 (19%)	1	7
13	c1	129/136 (95%)	108 (84%)	21 (16%)	2	12
14	C2	88/118 (75%)	67 (76%)	21 (24%)	0	3
14	c2	88/118 (75%)	71 (81%)	17 (19%)	1	6
15	C3	127/127 (100%)	96 (76%)	31 (24%)	0	3
15	c3	127/127 (100%)	102 (80%)	25 (20%)	1	6
16	C4	81/104 (78%)	67 (83%)	14 (17%)	2	10
16	c4	97/104 (93%)	76 (78%)	21 (22%)	1	4
17	C5	101/117 (86%)	79 (78%)	22 (22%)	1	4
17	c5	103/117 (88%)	85 (82%)	18 (18%)	2	9
18	C6	117/118 (99%)	97 (83%)	20 (17%)	2	10
18	c6	118/118 (100%)	96 (81%)	22 (19%)	1	7
19	C7	94/124 (76%)	70 (74%)	24 (26%)	0	2
19	c7	92/124 (74%)	72 (78%)	20 (22%)	1	4
20	C8	128/128 (100%)	95 (74%)	33 (26%)	0	2
20	c8	128/128 (100%)	94 (73%)	34 (27%)	0	2
21	C9	115/115 (100%)	86 (75%)	29 (25%)	0	3
21	c9	115/115 (100%)	96 (84%)	19 (16%)	2	12
22	D0	100/113 (88%)	76 (76%)	24 (24%)	0	3
22	d0	103/113 (91%)	72 (70%)	31 (30%)	0	2
23	D1	74/74 (100%)	61 (82%)	13 (18%)	2	9
23	d1	74/74 (100%)	58 (78%)	16 (22%)	1	4
24	D2	110/110 (100%)	90 (82%)	20 (18%)	1	8
24	d2	110/110 (100%)	89 (81%)	21 (19%)	1	6
25	D3	119/119 (100%)	95 (80%)	24 (20%)	1	5
25	d3	119/119 (100%)	91 (76%)	28 (24%)	1	3
26	D4	112/112 (100%)	93 (83%)	19 (17%)	2	10
26	d4	112/112 (100%)	93 (83%)	19 (17%)	2	10
27	D5	61/88 (69%)	46 (75%)	15 (25%)	0	3
27	d5	61/88 (69%)	48 (79%)	13 (21%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	D6	83/83 (100%)	61 (74%)	22 (26%)	0	2
28	d6	83/83 (100%)	65 (78%)	18 (22%)	1	4
29	D7	70/70 (100%)	59 (84%)	11 (16%)	2	14
29	d7	70/70 (100%)	55 (79%)	15 (21%)	1	4
30	D8	56/59 (95%)	45 (80%)	11 (20%)	1	6
30	d8	56/59 (95%)	43 (77%)	13 (23%)	1	3
31	D9	47/48 (98%)	40 (85%)	7 (15%)	3	16
31	d9	47/48 (98%)	36 (77%)	11 (23%)	1	3
32	E0	51/51 (100%)	42 (82%)	9 (18%)	2	9
33	E1	62/66 (94%)	48 (77%)	14 (23%)	1	3
33	e1	66/66 (100%)	49 (74%)	17 (26%)	0	2
34	SR	260/261 (100%)	223 (86%)	37 (14%)	3	17
34	sR	260/261 (100%)	222 (85%)	38 (15%)	3	16
35	SM	97/228 (42%)	72 (74%)	25 (26%)	0	2
35	sM	54/228 (24%)	45 (83%)	9 (17%)	2	11
39	L2	193/195 (99%)	143 (74%)	50 (26%)	0	2
39	l2	192/195 (98%)	144 (75%)	48 (25%)	0	3
40	L3	320/322 (99%)	256 (80%)	64 (20%)	1	5
40	l3	320/322 (99%)	248 (78%)	72 (22%)	1	3
41	L4	288/288 (100%)	223 (77%)	65 (23%)	1	3
41	l4	288/288 (100%)	229 (80%)	59 (20%)	1	5
42	L5	244/244 (100%)	191 (78%)	53 (22%)	1	4
42	l5	243/244 (100%)	198 (82%)	45 (18%)	1	7
43	L6	134/152 (88%)	108 (81%)	26 (19%)	1	6
43	l6	135/152 (89%)	102 (76%)	33 (24%)	0	3
44	L7	186/204 (91%)	154 (83%)	32 (17%)	2	10
44	l7	187/204 (92%)	152 (81%)	35 (19%)	1	7
45	L8	187/207 (90%)	150 (80%)	37 (20%)	1	5
45	l8	177/207 (86%)	141 (80%)	36 (20%)	1	5
46	L9	171/171 (100%)	127 (74%)	44 (26%)	0	2
46	l9	171/171 (100%)	128 (75%)	43 (25%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	M0	177/186 (95%)	137 (77%)	40 (23%)	1	3
47	m0	179/186 (96%)	144 (80%)	35 (20%)	1	6
48	M1	147/150 (98%)	112 (76%)	35 (24%)	0	3
48	m1	147/150 (98%)	111 (76%)	36 (24%)	0	3
49	M3	154/158 (98%)	122 (79%)	32 (21%)	1	5
49	m3	154/158 (98%)	120 (78%)	34 (22%)	1	4
50	M4	107/108 (99%)	85 (79%)	22 (21%)	1	5
50	m4	108/108 (100%)	86 (80%)	22 (20%)	1	5
51	M5	175/175 (100%)	132 (75%)	43 (25%)	0	3
51	m5	175/175 (100%)	141 (81%)	34 (19%)	1	6
52	M6	160/161 (99%)	121 (76%)	39 (24%)	0	3
52	m6	160/161 (99%)	120 (75%)	40 (25%)	0	3
53	M7	140/145 (97%)	111 (79%)	29 (21%)	1	5
53	m7	125/145 (86%)	101 (81%)	24 (19%)	1	6
54	M8	150/150 (100%)	116 (77%)	34 (23%)	1	3
54	m8	150/150 (100%)	116 (77%)	34 (23%)	1	3
55	M9	153/153 (100%)	124 (81%)	29 (19%)	1	7
55	m9	153/153 (100%)	125 (82%)	28 (18%)	1	7
56	N0	156/156 (100%)	122 (78%)	34 (22%)	1	4
56	n0	156/156 (100%)	122 (78%)	34 (22%)	1	4
57	N1	136/136 (100%)	102 (75%)	34 (25%)	0	3
57	n1	136/136 (100%)	107 (79%)	29 (21%)	1	4
58	N2	87/106 (82%)	73 (84%)	14 (16%)	2	13
58	n2	85/106 (80%)	58 (68%)	27 (32%)	0	2
59	N3	104/104 (100%)	84 (81%)	20 (19%)	1	6
59	n3	104/104 (100%)	85 (82%)	19 (18%)	1	7
60	N4	57/129 (44%)	47 (82%)	10 (18%)	2	9
60	n4	100/129 (78%)	79 (79%)	21 (21%)	1	4
61	N5	104/117 (89%)	78 (75%)	26 (25%)	0	3
61	n5	104/117 (89%)	85 (82%)	19 (18%)	1	7
62	N6	109/109 (100%)	88 (81%)	21 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	n6	109/109 (100%)	85 (78%)	24 (22%)	1	4
63	N7	115/115 (100%)	94 (82%)	21 (18%)	1	7
63	n7	115/115 (100%)	87 (76%)	28 (24%)	0	3
64	N8	118/118 (100%)	98 (83%)	20 (17%)	2	11
64	n8	118/118 (100%)	91 (77%)	27 (23%)	1	3
65	N9	46/46 (100%)	35 (76%)	11 (24%)	0	3
65	n9	46/46 (100%)	30 (65%)	16 (35%)	0	1
66	O0	81/87 (93%)	66 (82%)	15 (18%)	1	7
66	o0	84/87 (97%)	69 (82%)	15 (18%)	2	8
67	O1	92/96 (96%)	69 (75%)	23 (25%)	0	3
67	o1	94/96 (98%)	63 (67%)	31 (33%)	0	1
68	O2	109/110 (99%)	87 (80%)	22 (20%)	1	5
68	o2	109/110 (99%)	81 (74%)	28 (26%)	0	2
69	O3	90/90 (100%)	71 (79%)	19 (21%)	1	4
69	o3	90/90 (100%)	75 (83%)	15 (17%)	2	11
70	O4	95/102 (93%)	75 (79%)	20 (21%)	1	4
70	o4	95/102 (93%)	82 (86%)	13 (14%)	3	18
71	O5	104/104 (100%)	83 (80%)	21 (20%)	1	5
71	o5	103/104 (99%)	76 (74%)	27 (26%)	0	2
72	O6	81/81 (100%)	56 (69%)	25 (31%)	0	2
72	o6	80/81 (99%)	53 (66%)	27 (34%)	0	1
73	O7	70/70 (100%)	55 (79%)	15 (21%)	1	4
73	o7	70/70 (100%)	52 (74%)	18 (26%)	0	2
74	O8	68/68 (100%)	50 (74%)	18 (26%)	0	2
74	o8	67/68 (98%)	49 (73%)	18 (27%)	0	2
75	O9	45/45 (100%)	40 (89%)	5 (11%)	6	26
75	o9	45/45 (100%)	33 (73%)	12 (27%)	0	2
76	Q0	47/47 (100%)	41 (87%)	6 (13%)	4	20
76	q0	47/47 (100%)	32 (68%)	15 (32%)	0	2
77	Q1	23/23 (100%)	16 (70%)	7 (30%)	0	2
77	q1	23/23 (100%)	14 (61%)	9 (39%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	Q2	90/90 (100%)	67 (74%)	23 (26%)	0	2
78	q2	90/90 (100%)	70 (78%)	20 (22%)	1	4
79	Q3	71/71 (100%)	55 (78%)	16 (22%)	1	3
79	q3	71/71 (100%)	54 (76%)	17 (24%)	0	3
80	e0	53/53 (100%)	38 (72%)	15 (28%)	0	2
81	p0	105/253 (42%)	84 (80%)	21 (20%)	1	5
All	All	18728/20241 (92%)	14710 (78%)	4018 (22%)	1	4

5 of 4018 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
69	O3	48	ARG
8	s6	133	LEU
64	n8	132	LYS
72	O6	20	MET
3	s1	154	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
58	N2	52	ASN
72	O6	91	ASN
62	n6	66	GLN
64	N8	74	ASN
2	s0	46	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	541 (30%)	51 (2%)
1	6	1793/1800 (99%)	494 (27%)	48 (2%)
36	1	3145/3396 (92%)	774 (24%)	86 (2%)
36	5	3145/3396 (92%)	801 (25%)	77 (2%)
37	3	120/121 (99%)	20 (16%)	0
37	7	120/121 (99%)	28 (23%)	2 (1%)
38	4	157/158 (99%)	42 (26%)	3 (1%)
38	8	157/158 (99%)	44 (28%)	2 (1%)
All	All	10384/10950 (94%)	2744 (26%)	269 (2%)

5 of 2744 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	10	G
1	2	25	C
1	2	26	A

5 of 269 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	3078	U
1	6	240	U
36	5	2887	A
36	1	3218	A
36	1	3382	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2557 ligands modelled in this entry, 1423 are monoatomic - leaving 1134 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	1	4156	-	0,6,6	0.00	-	-		
86	OHX	3	222	-	0,6,6	0.00	-	-		
86	OHX	1	4045	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4062	-	0,6,6	0.00	-	-		
86	OHX	2	2118	-	0,6,6	0.00	-	-		
86	OHX	6	2054	-	0,6,6	0.00	-	-		
86	OHX	5	4146	-	0,6,6	0.00	-	-		
86	OHX	6	2108	-	0,6,6	0.00	-	-		
86	OHX	2	2093	-	0,6,6	0.00	-	-		
86	OHX	6	2121	-	0,6,6	0.00	-	-		
86	OHX	1	4197	-	0,6,6	0.00	-	-		
86	OHX	2	2081	-	0,6,6	0.00	-	-		
86	OHX	1	4002	-	0,6,6	0.00	-	-		
86	OHX	2	2084	-	0,6,6	0.00	-	-		
86	OHX	2	2114	-	0,6,6	0.00	-	-		
86	OHX	6	2138	-	0,6,6	0.00	-	-		
86	OHX	1	4128	-	0,6,6	0.00	-	-		
86	OHX	5	4191	-	0,6,6	0.00	-	-		
86	OHX	6	2190	-	0,6,6	0.00	-	-		
86	OHX	O7	104	-	0,6,6	0.00	-	-		
86	OHX	6	2189	-	0,6,6	0.00	-	-		
86	OHX	2	2060	-	0,6,6	0.00	-	-		
86	OHX	2	2132	-	0,6,6	0.00	-	-		
86	OHX	6	2073	-	0,6,6	0.00	-	-		
86	OHX	6	2053	-	0,6,6	0.00	-	-		
86	OHX	5	4233	-	0,6,6	0.00	-	-		
86	OHX	N9	101	-	0,6,6	0.00	-	-		
86	OHX	2	2074	-	0,6,6	0.00	-	-		
86	OHX	1	3947	-	0,6,6	0.00	-	-		
86	OHX	5	4132	-	0,6,6	0.00	-	-		
86	OHX	6	2194	-	0,6,6	0.00	-	-		
86	OHX	1	4106	-	0,6,6	0.00	-	-		
86	OHX	5	4147	-	0,6,6	0.00	-	-		
86	OHX	1	4056	-	0,6,6	0.00	-	-		
86	OHX	1	4054	-	0,6,6	0.00	-	-		
86	OHX	5	4230	-	0,6,6	0.00	-	-		
86	OHX	5	4047	-	0,6,6	0.00	-	-		
86	OHX	5	4083	-	0,6,6	0.00	-	-		
86	OHX	14	403	-	0,6,6	0.00	-	-		
86	OHX	5	3989	-	0,6,6	0.00	-	-		
86	OHX	2	2103	-	0,6,6	0.00	-	-		
86	OHX	1	4182	-	0,6,6	0.00	-	-		
86	OHX	5	4099	-	0,6,6	0.00	-	-		
86	OHX	5	4231	-	0,6,6	0.00	-	-		
86	OHX	5	4153	-	0,6,6	0.00	-	-		
86	OHX	5	4024	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3941	-	0,6,6	0.00	-	-		
86	OHX	5	4246	-	0,6,6	0.00	-	-		
86	OHX	C5	201	-	0,6,6	0.00	-	-		
86	OHX	6	2185	-	0,6,6	0.00	-	-		
86	OHX	1	4031	-	0,6,6	0.00	-	-		
86	OHX	5	4039	-	0,6,6	0.00	-	-		
86	OHX	2	2099	-	0,6,6	0.00	-	-		
86	OHX	6	2061	-	0,6,6	0.00	-	-		
86	OHX	5	4050	-	0,6,6	0.00	-	-		
86	OHX	1	3881	-	0,6,6	0.00	-	-		
86	OHX	6	2154	-	0,6,6	0.00	-	-		
86	OHX	6	2173	-	0,6,6	0.00	-	-		
86	OHX	5	4211	-	0,6,6	0.00	-	-		
86	OHX	2	2037	-	0,6,6	0.00	-	-		
86	OHX	6	2133	-	0,6,6	0.00	-	-		
86	OHX	5	4130	-	0,6,6	0.00	-	-		
86	OHX	6	2149	-	0,6,6	0.00	-	-		
86	OHX	5	4017	-	0,6,6	0.00	-	-		
86	OHX	1	4102	-	0,6,6	0.00	-	-		
86	OHX	5	4074	-	0,6,6	0.00	-	-		
86	OHX	5	4101	-	0,6,6	0.00	-	-		
86	OHX	6	2203	-	0,6,6	0.00	-	-		
86	OHX	3	224	-	0,6,6	0.00	-	-		
86	OHX	5	4223	-	0,6,6	0.00	-	-		
86	OHX	1	4068	-	0,6,6	0.00	-	-		
86	OHX	5	4216	-	0,6,6	0.00	-	-		
86	OHX	5	3974	-	0,6,6	0.00	-	-		
86	OHX	1	4103	-	0,6,6	0.00	-	-		
86	OHX	O1	202	-	0,6,6	0.00	-	-		
86	OHX	1	4015	-	0,6,6	0.00	-	-		
86	OHX	5	3958	-	0,6,6	0.00	-	-		
86	OHX	1	3936	-	0,6,6	0.00	-	-		
86	OHX	5	4178	-	0,6,6	0.00	-	-		
86	OHX	5	4166	-	0,6,6	0.00	-	-		
86	OHX	4	224	-	0,6,6	0.00	-	-		
86	OHX	2	2157	-	0,6,6	0.00	-	-		
86	OHX	5	3911	-	0,6,6	0.00	-	-		
86	OHX	3	221	-	0,6,6	0.00	-	-		
86	OHX	1	3894	-	0,6,6	0.00	-	-		
86	OHX	2	2026	-	0,6,6	0.00	-	-		
86	OHX	5	3988	-	0,6,6	0.00	-	-		
86	OHX	5	4125	-	0,6,6	0.00	-	-		
86	OHX	1	4114	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4104	-	0,6,6	0.00	-	-		
86	OHX	1	3979	-	0,6,6	0.00	-	-		
86	OHX	1	3865	-	0,6,6	0.00	-	-		
86	OHX	2	2053	-	0,6,6	0.00	-	-		
86	OHX	1	4057	-	0,6,6	0.00	-	-		
86	OHX	1	4133	-	0,6,6	0.00	-	-		
86	OHX	5	3923	-	0,6,6	0.00	-	-		
86	OHX	5	4127	-	0,6,6	0.00	-	-		
86	OHX	1	3916	-	0,6,6	0.00	-	-		
86	OHX	5	4048	-	0,6,6	0.00	-	-		
86	OHX	1	4032	-	0,6,6	0.00	-	-		
86	OHX	5	4116	-	0,6,6	0.00	-	-		
86	OHX	1	4118	-	0,6,6	0.00	-	-		
86	OHX	5	4187	-	0,6,6	0.00	-	-		
86	OHX	1	3882	-	0,6,6	0.00	-	-		
86	OHX	2	2160	-	0,6,6	0.00	-	-		
86	OHX	m5	306	-	0,6,6	0.00	-	-		
86	OHX	5	3925	-	0,6,6	0.00	-	-		
86	OHX	5	3893	-	0,6,6	0.00	-	-		
86	OHX	1	4097	-	0,6,6	0.00	-	-		
86	OHX	2	2150	-	0,6,6	0.00	-	-		
86	OHX	1	4080	-	0,6,6	0.00	-	-		
86	OHX	6	2143	-	0,6,6	0.00	-	-		
86	OHX	7	223	-	0,6,6	0.00	-	-		
86	OHX	6	2200	-	0,6,6	0.00	-	-		
86	OHX	2	2122	-	0,6,6	0.00	-	-		
86	OHX	2	2062	-	0,6,6	0.00	-	-		
86	OHX	6	2050	-	0,6,6	0.00	-	-		
86	OHX	1	4055	-	0,6,6	0.00	-	-		
86	OHX	1	3907	-	0,6,6	0.00	-	-		
86	OHX	2	2124	-	0,6,6	0.00	-	-		
86	OHX	5	3930	-	0,6,6	0.00	-	-		
86	OHX	5	3975	-	0,6,6	0.00	-	-		
86	OHX	6	2164	-	0,6,6	0.00	-	-		
86	OHX	D3	202	-	0,6,6	0.00	-	-		
86	OHX	5	3948	-	0,6,6	0.00	-	-		
86	OHX	1	4190	-	0,6,6	0.00	-	-		
86	OHX	1	4063	-	0,6,6	0.00	-	-		
86	OHX	n3	202	-	0,6,6	0.00	-	-		
86	OHX	1	4003	-	0,6,6	0.00	-	-		
86	OHX	5	4092	-	0,6,6	0.00	-	-		
86	OHX	6	2144	-	0,6,6	0.00	-	-		
86	OHX	1	4082	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2163	-	0,6,6	0.00	-	-		
86	OHX	1	4209	-	0,6,6	0.00	-	-		
86	OHX	6	2106	-	0,6,6	0.00	-	-		
86	OHX	6	2109	-	0,6,6	0.00	-	-		
86	OHX	5	4077	-	0,6,6	0.00	-	-		
86	OHX	6	2046	-	0,6,6	0.00	-	-		
86	OHX	5	4005	-	0,6,6	0.00	-	-		
86	OHX	1	3966	-	0,6,6	0.00	-	-		
86	OHX	7	224	-	0,6,6	0.00	-	-		
86	OHX	5	3955	-	0,6,6	0.00	-	-		
86	OHX	2	2048	-	0,6,6	0.00	-	-		
86	OHX	1	4160	-	0,6,6	0.00	-	-		
86	OHX	5	4094	-	0,6,6	0.00	-	-		
86	OHX	1	4207	-	0,6,6	0.00	-	-		
86	OHX	2	2168	-	0,6,6	0.00	-	-		
86	OHX	1	4093	-	0,6,6	0.00	-	-		
86	OHX	5	4063	-	0,6,6	0.00	-	-		
86	OHX	5	4025	-	0,6,6	0.00	-	-		
86	OHX	7	228	-	0,6,6	0.00	-	-		
86	OHX	2	2171	-	0,6,6	0.00	-	-		
86	OHX	2	2059	-	0,6,6	0.00	-	-		
86	OHX	1	4060	-	0,6,6	0.00	-	-		
86	OHX	6	2049	-	0,6,6	0.00	-	-		
86	OHX	1	4201	-	0,6,6	0.00	-	-		
86	OHX	1	4142	-	0,6,6	0.00	-	-		
86	OHX	6	2077	-	0,6,6	0.00	-	-		
86	OHX	1	3897	-	0,6,6	0.00	-	-		
86	OHX	2	2091	-	0,6,6	0.00	-	-		
86	OHX	2	2134	-	0,6,6	0.00	-	-		
86	OHX	6	2091	-	0,6,6	0.00	-	-		
86	OHX	5	4081	-	0,6,6	0.00	-	-		
86	OHX	6	2157	-	0,6,6	0.00	-	-		
86	OHX	1	3879	-	0,6,6	0.00	-	-		
86	OHX	5	4031	-	0,6,6	0.00	-	-		
86	OHX	2	2061	-	0,6,6	0.00	-	-		
86	OHX	5	3995	-	0,6,6	0.00	-	-		
86	OHX	1	4050	-	0,6,6	0.00	-	-		
86	OHX	2	2106	-	0,6,6	0.00	-	-		
86	OHX	5	4131	-	0,6,6	0.00	-	-		
86	OHX	6	2056	-	0,6,6	0.00	-	-		
86	OHX	1	4151	-	0,6,6	0.00	-	-		
86	OHX	6	2179	-	0,6,6	0.00	-	-		
86	OHX	2	2176	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4194	-	0,6,6	0.00	-	-		
86	OHX	1	4189	-	0,6,6	0.00	-	-		
86	OHX	5	4072	-	0,6,6	0.00	-	-		
86	OHX	1	4017	-	0,6,6	0.00	-	-		
86	OHX	5	4103	-	0,6,6	0.00	-	-		
86	OHX	1	4175	-	0,6,6	0.00	-	-		
86	OHX	5	4205	-	0,6,6	0.00	-	-		
86	OHX	6	2097	-	0,6,6	0.00	-	-		
86	OHX	5	3971	-	0,6,6	0.00	-	-		
86	OHX	1	3969	-	0,6,6	0.00	-	-		
86	OHX	8	224	-	0,6,6	0.00	-	-		
86	OHX	1	3896	-	0,6,6	0.00	-	-		
86	OHX	6	2103	-	0,6,6	0.00	-	-		
86	OHX	5	4038	-	0,6,6	0.00	-	-		
86	OHX	5	4220	-	0,6,6	0.00	-	-		
86	OHX	6	2064	-	0,6,6	0.00	-	-		
86	OHX	1	3934	-	0,6,6	0.00	-	-		
86	OHX	1	3954	-	0,6,6	0.00	-	-		
86	OHX	4	238	-	0,6,6	0.00	-	-		
86	OHX	5	3913	-	0,6,6	0.00	-	-		
86	OHX	1	4147	-	0,6,6	0.00	-	-		
86	OHX	2	2075	-	0,6,6	0.00	-	-		
86	OHX	O3	201	-	0,6,6	0.00	-	-		
86	OHX	q2	502	-	0,6,6	0.00	-	-		
86	OHX	5	3964	-	0,6,6	0.00	-	-		
86	OHX	1	3940	-	0,6,6	0.00	-	-		
86	OHX	6	2086	-	0,6,6	0.00	-	-		
86	OHX	2	2082	-	0,6,6	0.00	-	-		
86	OHX	6	2082	-	0,6,6	0.00	-	-		
86	OHX	5	4126	-	0,6,6	0.00	-	-		
86	OHX	2	2046	-	0,6,6	0.00	-	-		
86	OHX	5	3933	-	0,6,6	0.00	-	-		
86	OHX	1	4065	-	0,6,6	0.00	-	-		
86	OHX	m0	302	-	0,6,6	0.00	-	-		
86	OHX	m0	303	-	0,6,6	0.00	-	-		
86	OHX	1	4117	-	0,6,6	0.00	-	-		
86	OHX	1	4064	-	0,6,6	0.00	-	-		
86	OHX	1	4071	-	0,6,6	0.00	-	-		
86	OHX	2	2024	-	0,6,6	0.00	-	-		
86	OHX	7	222	-	0,6,6	0.00	-	-		
86	OHX	2	2169	-	0,6,6	0.00	-	-		
86	OHX	5	3942	-	0,6,6	0.00	-	-		
86	OHX	8	216	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3873	-	0,6,6	0.00	-	-		
86	OHX	5	4096	-	0,6,6	0.00	-	-		
86	OHX	5	3957	-	0,6,6	0.00	-	-		
86	OHX	5	4238	-	0,6,6	0.00	-	-		
86	OHX	1	4022	-	0,6,6	0.00	-	-		
86	OHX	2	2055	-	0,6,6	0.00	-	-		
86	OHX	5	4235	-	0,6,6	0.00	-	-		
86	OHX	1	3933	-	0,6,6	0.00	-	-		
86	OHX	6	2080	-	0,6,6	0.00	-	-		
86	OHX	2	2126	-	0,6,6	0.00	-	-		
86	OHX	1	4094	-	0,6,6	0.00	-	-		
86	OHX	5	4046	-	0,6,6	0.00	-	-		
86	OHX	5	4229	-	0,6,6	0.00	-	-		
86	OHX	5	4043	-	0,6,6	0.00	-	-		
86	OHX	5	4093	-	0,6,6	0.00	-	-		
86	OHX	1	3978	-	0,6,6	0.00	-	-		
86	OHX	1	4152	-	0,6,6	0.00	-	-		
86	OHX	1	3928	-	0,6,6	0.00	-	-		
86	OHX	1	3880	-	0,6,6	0.00	-	-		
86	OHX	6	2171	-	0,6,6	0.00	-	-		
86	OHX	6	2153	-	0,6,6	0.00	-	-		
86	OHX	1	3875	-	0,6,6	0.00	-	-		
86	OHX	8	227	-	0,6,6	0.00	-	-		
86	OHX	5	4119	-	0,6,6	0.00	-	-		
86	OHX	1	4132	-	0,6,6	0.00	-	-		
86	OHX	1	4179	-	0,6,6	0.00	-	-		
86	OHX	1	4206	-	0,6,6	0.00	-	-		
86	OHX	6	2176	-	0,6,6	0.00	-	-		
86	OHX	1	3956	-	0,6,6	0.00	-	-		
86	OHX	1	3886	-	0,6,6	0.00	-	-		
86	OHX	5	3932	-	0,6,6	0.00	-	-		
86	OHX	6	2183	-	0,6,6	0.00	-	-		
86	OHX	5	3956	-	0,6,6	0.00	-	-		
86	OHX	6	2104	-	0,6,6	0.00	-	-		
86	OHX	1	3943	-	0,6,6	0.00	-	-		
86	OHX	5	4032	-	0,6,6	0.00	-	-		
86	OHX	c3	201	-	0,6,6	0.00	-	-		
86	OHX	4	232	-	0,6,6	0.00	-	-		
86	OHX	1	4150	-	0,6,6	0.00	-	-		
86	OHX	1	3888	-	0,6,6	0.00	-	-		
86	OHX	5	3935	-	0,6,6	0.00	-	-		
86	OHX	2	2043	-	0,6,6	0.00	-	-		
86	OHX	C8	201	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2168	-	0,6,6	0.00	-	-		
86	OHX	1	3924	-	0,6,6	0.00	-	-		
86	OHX	6	2161	-	0,6,6	0.00	-	-		
86	OHX	2	2136	-	0,6,6	0.00	-	-		
86	OHX	5	4080	-	0,6,6	0.00	-	-		
86	OHX	5	4002	-	0,6,6	0.00	-	-		
86	OHX	6	2187	-	0,6,6	0.00	-	-		
86	OHX	5	4214	-	0,6,6	0.00	-	-		
86	OHX	1	3944	-	0,6,6	0.00	-	-		
86	OHX	5	3972	-	0,6,6	0.00	-	-		
86	OHX	1	3923	-	0,6,6	0.00	-	-		
86	OHX	6	2170	-	0,6,6	0.00	-	-		
86	OHX	1	3955	-	0,6,6	0.00	-	-		
86	OHX	6	2065	-	0,6,6	0.00	-	-		
86	OHX	1	3909	-	0,6,6	0.00	-	-		
86	OHX	1	4029	-	0,6,6	0.00	-	-		
86	OHX	5	4217	-	0,6,6	0.00	-	-		
86	OHX	n1	201	-	0,6,6	0.00	-	-		
86	OHX	1	4202	-	0,6,6	0.00	-	-		
86	OHX	2	2110	-	0,6,6	0.00	-	-		
86	OHX	5	3985	-	0,6,6	0.00	-	-		
86	OHX	5	4174	-	0,6,6	0.00	-	-		
86	OHX	1	4058	-	0,6,6	0.00	-	-		
86	OHX	5	3928	-	0,6,6	0.00	-	-		
86	OHX	1	4203	-	0,6,6	0.00	-	-		
86	OHX	6	2117	-	0,6,6	0.00	-	-		
86	OHX	5	4204	-	0,6,6	0.00	-	-		
86	OHX	1	3938	-	0,6,6	0.00	-	-		
86	OHX	1	4004	-	0,6,6	0.00	-	-		
86	OHX	4	236	-	0,6,6	0.00	-	-		
86	OHX	s8	302	-	0,6,6	0.00	-	-		
86	OHX	7	221	-	0,6,6	0.00	-	-		
86	OHX	1	3972	-	0,6,6	0.00	-	-		
86	OHX	2	2152	-	0,6,6	0.00	-	-		
86	OHX	5	4184	-	0,6,6	0.00	-	-		
86	OHX	5	3983	-	0,6,6	0.00	-	-		
86	OHX	6	2177	-	0,6,6	0.00	-	-		
86	OHX	d9	102	-	0,6,6	0.00	-	-		
86	OHX	1	3997	-	0,6,6	0.00	-	-		
86	OHX	5	4236	-	0,6,6	0.00	-	-		
86	OHX	1	4174	-	0,6,6	0.00	-	-		
86	OHX	1	4052	-	0,6,6	0.00	-	-		
86	OHX	1	3957	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4181	-	0,6,6	0.00	-	-		
86	OHX	6	2058	-	0,6,6	0.00	-	-		
86	OHX	6	2175	-	0,6,6	0.00	-	-		
86	OHX	6	2115	-	0,6,6	0.00	-	-		
86	OHX	1	3994	-	0,6,6	0.00	-	-		
86	OHX	2	2146	-	0,6,6	0.00	-	-		
86	OHX	6	2122	-	0,6,6	0.00	-	-		
86	OHX	2	2064	-	0,6,6	0.00	-	-		
86	OHX	1	4154	-	0,6,6	0.00	-	-		
86	OHX	o7	103	-	0,6,6	0.00	-	-		
86	OHX	1	4198	-	0,6,6	0.00	-	-		
86	OHX	5	3977	-	0,6,6	0.00	-	-		
86	OHX	5	3978	-	0,6,6	0.00	-	-		
86	OHX	1	3939	-	0,6,6	0.00	-	-		
86	OHX	7	226	-	0,6,6	0.00	-	-		
86	OHX	2	2151	-	0,6,6	0.00	-	-		
86	OHX	2	2080	-	0,6,6	0.00	-	-		
86	OHX	1	3932	-	0,6,6	0.00	-	-		
86	OHX	5	4137	-	0,6,6	0.00	-	-		
86	OHX	1	3995	-	0,6,6	0.00	-	-		
86	OHX	6	2193	-	0,6,6	0.00	-	-		
86	OHX	2	2087	-	0,6,6	0.00	-	-		
86	OHX	1	3901	-	0,6,6	0.00	-	-		
86	OHX	1	4176	-	0,6,6	0.00	-	-		
86	OHX	1	4112	-	0,6,6	0.00	-	-		
86	OHX	L3	405	-	0,6,6	0.00	-	-		
86	OHX	5	4218	-	0,6,6	0.00	-	-		
86	OHX	1	3990	-	0,6,6	0.00	-	-		
86	OHX	1	3942	-	0,6,6	0.00	-	-		
86	OHX	5	3970	-	0,6,6	0.00	-	-		
86	OHX	2	2131	-	0,6,6	0.00	-	-		
86	OHX	6	2060	-	0,6,6	0.00	-	-		
86	OHX	1	4086	-	0,6,6	0.00	-	-		
86	OHX	2	2045	-	0,6,6	0.00	-	-		
86	OHX	4	233	-	0,6,6	0.00	-	-		
86	OHX	5	4108	-	0,6,6	0.00	-	-		
86	OHX	2	2162	-	0,6,6	0.00	-	-		
86	OHX	1	3876	-	0,6,6	0.00	-	-		
86	OHX	5	4221	-	0,6,6	0.00	-	-		
86	OHX	5	4190	-	0,6,6	0.00	-	-		
86	OHX	5	3991	-	0,6,6	0.00	-	-		
86	OHX	1	4081	-	0,6,6	0.00	-	-		
86	OHX	2	2096	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	3	217	-	0,6,6	0.00	-	-		
86	OHX	6	2160	-	0,6,6	0.00	-	-		
86	OHX	2	2049	-	0,6,6	0.00	-	-		
86	OHX	6	2139	-	0,6,6	0.00	-	-		
86	OHX	5	4029	-	0,6,6	0.00	-	-		
86	OHX	2	2063	-	0,6,6	0.00	-	-		
86	OHX	5	3915	-	0,6,6	0.00	-	-		
86	OHX	3	216	-	0,6,6	0.00	-	-		
86	OHX	5	4057	-	0,6,6	0.00	-	-		
86	OHX	5	3929	-	0,6,6	0.00	-	-		
86	OHX	5	4222	-	0,6,6	0.00	-	-		
86	OHX	2	2125	-	0,6,6	0.00	-	-		
86	OHX	5	4209	-	0,6,6	0.00	-	-		
86	OHX	1	3977	-	0,6,6	0.00	-	-		
86	OHX	2	2112	-	0,6,6	0.00	-	-		
86	OHX	3	220	-	0,6,6	0.00	-	-		
86	OHX	1	4105	-	0,6,6	0.00	-	-		
86	OHX	6	2078	-	0,6,6	0.00	-	-		
86	OHX	2	2109	-	0,6,6	0.00	-	-		
86	OHX	n9	103	-	0,6,6	0.00	-	-		
86	OHX	1	4194	-	0,6,6	0.00	-	-		
86	OHX	6	2110	-	0,6,6	0.00	-	-		
86	OHX	1	3911	-	0,6,6	0.00	-	-		
86	OHX	1	3914	-	0,6,6	0.00	-	-		
86	OHX	2	2117	-	0,6,6	0.00	-	-		
86	OHX	5	4138	-	0,6,6	0.00	-	-		
86	OHX	5	4011	-	0,6,6	0.00	-	-		
86	OHX	1	4139	-	0,6,6	0.00	-	-		
86	OHX	1	4014	-	0,6,6	0.00	-	-		
86	OHX	1	3931	-	0,6,6	0.00	-	-		
86	OHX	1	4092	-	0,6,6	0.00	-	-		
86	OHX	2	2180	-	0,6,6	0.00	-	-		
86	OHX	1	4119	-	0,6,6	0.00	-	-		
86	OHX	1	3993	-	0,6,6	0.00	-	-		
86	OHX	1	3941	-	0,6,6	0.00	-	-		
86	OHX	6	2066	-	0,6,6	0.00	-	-		
86	OHX	4	229	-	0,6,6	0.00	-	-		
86	OHX	2	2161	-	0,6,6	0.00	-	-		
86	OHX	6	2195	-	0,6,6	0.00	-	-		
86	OHX	6	2048	-	0,6,6	0.00	-	-		
86	OHX	5	4019	-	0,6,6	0.00	-	-		
86	OHX	5	4168	-	0,6,6	0.00	-	-		
86	OHX	5	4167	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2177	-	0,6,6	0.00	-	-		
86	OHX	5	3897	-	0,6,6	0.00	-	-		
86	OHX	5	4156	-	0,6,6	0.00	-	-		
86	OHX	1	3860	-	0,6,6	0.00	-	-		
86	OHX	1	4155	-	0,6,6	0.00	-	-		
86	OHX	5	4175	-	0,6,6	0.00	-	-		
86	OHX	1	3918	-	0,6,6	0.00	-	-		
86	OHX	sR	401	-	0,6,6	0.00	-	-		
86	OHX	5	3944	-	0,6,6	0.00	-	-		
86	OHX	6	2093	-	0,6,6	0.00	-	-		
86	OHX	5	3953	-	0,6,6	0.00	-	-		
86	OHX	5	4016	-	0,6,6	0.00	-	-		
86	OHX	5	4027	-	0,6,6	0.00	-	-		
86	OHX	5	4136	-	0,6,6	0.00	-	-		
86	OHX	5	4177	-	0,6,6	0.00	-	-		
86	OHX	5	3919	-	0,6,6	0.00	-	-		
86	OHX	5	4203	-	0,6,6	0.00	-	-		
86	OHX	2	2104	-	0,6,6	0.00	-	-		
86	OHX	6	2172	-	0,6,6	0.00	-	-		
86	OHX	1	3985	-	0,6,6	0.00	-	-		
86	OHX	5	3916	-	0,6,6	0.00	-	-		
86	OHX	1	3867	-	0,6,6	0.00	-	-		
86	OHX	2	2031	-	0,6,6	0.00	-	-		
86	OHX	1	3945	-	0,6,6	0.00	-	-		
86	OHX	5	3998	-	0,6,6	0.00	-	-		
86	OHX	l3	404	-	0,6,6	0.00	-	-		
86	OHX	5	4105	-	0,6,6	0.00	-	-		
86	OHX	2	2119	-	0,6,6	0.00	-	-		
86	OHX	4	234	-	0,6,6	0.00	-	-		
86	OHX	5	4158	-	0,6,6	0.00	-	-		
86	OHX	5	4090	-	0,6,6	0.00	-	-		
86	OHX	1	4161	-	0,6,6	0.00	-	-		
86	OHX	5	3952	-	0,6,6	0.00	-	-		
86	OHX	5	3980	-	0,6,6	0.00	-	-		
86	OHX	5	3910	-	0,6,6	0.00	-	-		
86	OHX	1	4146	-	0,6,6	0.00	-	-		
86	OHX	1	3926	-	0,6,6	0.00	-	-		
86	OHX	2	2143	-	0,6,6	0.00	-	-		
86	OHX	5	4163	-	0,6,6	0.00	-	-		
86	OHX	6	2150	-	0,6,6	0.00	-	-		
86	OHX	6	2180	-	0,6,6	0.00	-	-		
86	OHX	2	2086	-	0,6,6	0.00	-	-		
86	OHX	6	2181	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3895	-	0,6,6	0.00	-	-		
86	OHX	2	2054	-	0,6,6	0.00	-	-		
86	OHX	1	4101	-	0,6,6	0.00	-	-		
86	OHX	5	3999	-	0,6,6	0.00	-	-		
86	OHX	5	4143	-	0,6,6	0.00	-	-		
86	OHX	6	2072	-	0,6,6	0.00	-	-		
86	OHX	c8	202	-	0,6,6	0.00	-	-		
86	OHX	6	2128	-	0,6,6	0.00	-	-		
86	OHX	6	2147	-	0,6,6	0.00	-	-		
86	OHX	1	3905	-	0,6,6	0.00	-	-		
86	OHX	5	3926	-	0,6,6	0.00	-	-		
86	OHX	1	4010	-	0,6,6	0.00	-	-		
86	OHX	6	2124	-	0,6,6	0.00	-	-		
86	OHX	5	3905	-	0,6,6	0.00	-	-		
86	OHX	8	226	-	0,6,6	0.00	-	-		
86	OHX	5	3973	-	0,6,6	0.00	-	-		
86	OHX	5	4067	-	0,6,6	0.00	-	-		
86	OHX	5	4164	-	0,6,6	0.00	-	-		
86	OHX	5	3976	-	0,6,6	0.00	-	-		
86	OHX	1	3915	-	0,6,6	0.00	-	-		
86	OHX	6	2156	-	0,6,6	0.00	-	-		
86	OHX	2	2139	-	0,6,6	0.00	-	-		
86	OHX	5	3992	-	0,6,6	0.00	-	-		
86	OHX	5	3946	-	0,6,6	0.00	-	-		
86	OHX	1	4078	-	0,6,6	0.00	-	-		
86	OHX	3	218	-	0,6,6	0.00	-	-		
86	OHX	2	2028	-	0,6,6	0.00	-	-		
86	OHX	6	2199	-	0,6,6	0.00	-	-		
86	OHX	1	4184	-	0,6,6	0.00	-	-		
86	OHX	5	4087	-	0,6,6	0.00	-	-		
86	OHX	6	2202	-	0,6,6	0.00	-	-		
86	OHX	1	4125	-	0,6,6	0.00	-	-		
86	OHX	6	2057	-	0,6,6	0.00	-	-		
86	OHX	1	3890	-	0,6,6	0.00	-	-		
86	OHX	5	4056	-	0,6,6	0.00	-	-		
86	OHX	5	4088	-	0,6,6	0.00	-	-		
86	OHX	5	4115	-	0,6,6	0.00	-	-		
86	OHX	1	3884	-	0,6,6	0.00	-	-		
86	OHX	1	4016	-	0,6,6	0.00	-	-		
86	OHX	1	3982	-	0,6,6	0.00	-	-		
86	OHX	5	4140	-	0,6,6	0.00	-	-		
86	OHX	2	2094	-	0,6,6	0.00	-	-		
86	OHX	1	3998	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	BLS	5	4248	-	25,31,31	1.46	2 (8%)	23,43,43	1.75	3 (13%)
86	OHX	5	4055	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4083	-	0,6,6	0.00	-	-	-	-
86	OHX	5	4225	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4191	-	0,6,6	0.00	-	-	-	-
86	OHX	7	219	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2172	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3894	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2068	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2144	-	0,6,6	0.00	-	-	-	-
86	OHX	M7	206	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4025	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3920	-	0,6,6	0.00	-	-	-	-
86	OHX	5	4026	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2174	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4019	-	0,6,6	0.00	-	-	-	-
86	OHX	5	4151	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4138	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4109	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2073	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2123	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3900	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2074	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2047	-	0,6,6	0.00	-	-	-	-
86	OHX	5	4045	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2149	-	0,6,6	0.00	-	-	-	-
86	OHX	5	4036	-	0,6,6	0.00	-	-	-	-
86	OHX	5	4198	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3858	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3909	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2151	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4023	-	0,6,6	0.00	-	-	-	-
86	OHX	L3	406	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4116	-	0,6,6	0.00	-	-	-	-
86	OHX	5	4023	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4145	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3917	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4013	-	0,6,6	0.00	-	-	-	-
86	OHX	s1	302	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4183	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3982	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2163	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3874	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3935	-	0,6,6	0.00	-	-		
86	OHX	5	3898	-	0,6,6	0.00	-	-		
86	OHX	6	2116	-	0,6,6	0.00	-	-		
86	OHX	5	4240	-	0,6,6	0.00	-	-		
86	OHX	5	4244	-	0,6,6	0.00	-	-		
86	OHX	6	2076	-	0,6,6	0.00	-	-		
86	OHX	2	2101	-	0,6,6	0.00	-	-		
86	OHX	2	2097	-	0,6,6	0.00	-	-		
86	OHX	5	4035	-	0,6,6	0.00	-	-		
86	OHX	6	2159	-	0,6,6	0.00	-	-		
86	OHX	5	4030	-	0,6,6	0.00	-	-		
86	OHX	5	3921	-	0,6,6	0.00	-	-		
86	OHX	5	4001	-	0,6,6	0.00	-	-		
86	OHX	6	2131	-	0,6,6	0.00	-	-		
86	OHX	2	2165	-	0,6,6	0.00	-	-		
86	OHX	5	4142	-	0,6,6	0.00	-	-		
86	OHX	5	4195	-	0,6,6	0.00	-	-		
86	OHX	2	2032	-	0,6,6	0.00	-	-		
86	OHX	6	2130	-	0,6,6	0.00	-	-		
86	OHX	1	3948	-	0,6,6	0.00	-	-		
86	OHX	5	4058	-	0,6,6	0.00	-	-		
86	OHX	2	2036	-	0,6,6	0.00	-	-		
86	OHX	1	4178	-	0,6,6	0.00	-	-		
86	OHX	O7	105	-	0,6,6	0.00	-	-		
86	OHX	5	4208	-	0,6,6	0.00	-	-		
86	OHX	5	4009	-	0,6,6	0.00	-	-		
86	OHX	6	2092	-	0,6,6	0.00	-	-		
86	OHX	1	3965	-	0,6,6	0.00	-	-		
86	OHX	5	4086	-	0,6,6	0.00	-	-		
86	OHX	5	4201	-	0,6,6	0.00	-	-		
86	OHX	2	2079	-	0,6,6	0.00	-	-		
86	OHX	1	3925	-	0,6,6	0.00	-	-		
86	OHX	5	4113	-	0,6,6	0.00	-	-		
86	OHX	2	2067	-	0,6,6	0.00	-	-		
86	OHX	2	2070	-	0,6,6	0.00	-	-		
86	OHX	2	2025	-	0,6,6	0.00	-	-		
86	OHX	M9	202	-	0,6,6	0.00	-	-		
86	OHX	5	4134	-	0,6,6	0.00	-	-		
86	OHX	1	3919	-	0,6,6	0.00	-	-		
86	OHX	1	3869	-	0,6,6	0.00	-	-		
86	OHX	1	3866	-	0,6,6	0.00	-	-		
86	OHX	6	2120	-	0,6,6	0.00	-	-		
86	OHX	5	4228	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4171	-	0,6,6	0.00	-	-		
86	OHX	8	220	-	0,6,6	0.00	-	-		
86	OHX	1	4043	-	0,6,6	0.00	-	-		
86	OHX	5	3959	-	0,6,6	0.00	-	-		
86	OHX	5	3954	-	0,6,6	0.00	-	-		
86	OHX	5	3943	-	0,6,6	0.00	-	-		
86	OHX	1	3863	-	0,6,6	0.00	-	-		
86	OHX	5	4124	-	0,6,6	0.00	-	-		
86	OHX	1	3961	-	0,6,6	0.00	-	-		
86	OHX	1	4041	-	0,6,6	0.00	-	-		
86	OHX	5	4234	-	0,6,6	0.00	-	-		
86	OHX	5	3945	-	0,6,6	0.00	-	-		
86	OHX	6	2085	-	0,6,6	0.00	-	-		
86	OHX	6	2148	-	0,6,6	0.00	-	-		
86	OHX	1	3872	-	0,6,6	0.00	-	-		
86	OHX	6	2069	-	0,6,6	0.00	-	-		
86	OHX	5	4061	-	0,6,6	0.00	-	-		
86	OHX	2	2135	-	0,6,6	0.00	-	-		
86	OHX	1	3950	-	0,6,6	0.00	-	-		
86	OHX	5	4239	-	0,6,6	0.00	-	-		
86	OHX	1	3992	-	0,6,6	0.00	-	-		
86	OHX	1	4066	-	0,6,6	0.00	-	-		
86	OHX	6	2158	-	0,6,6	0.00	-	-		
86	OHX	1	3893	-	0,6,6	0.00	-	-		
86	OHX	1	3885	-	0,6,6	0.00	-	-		
86	OHX	M5	303	-	0,6,6	0.00	-	-		
86	OHX	5	3968	-	0,6,6	0.00	-	-		
86	OHX	5	3949	-	0,6,6	0.00	-	-		
86	OHX	1	4192	-	0,6,6	0.00	-	-		
86	OHX	1	4110	-	0,6,6	0.00	-	-		
86	OHX	5	4148	-	0,6,6	0.00	-	-		
86	OHX	1	3870	-	0,6,6	0.00	-	-		
86	OHX	1	4115	-	0,6,6	0.00	-	-		
86	OHX	1	3959	-	0,6,6	0.00	-	-		
86	OHX	5	4122	-	0,6,6	0.00	-	-		
86	OHX	1	3971	-	0,6,6	0.00	-	-		
86	OHX	1	3906	-	0,6,6	0.00	-	-		
86	OHX	6	2090	-	0,6,6	0.00	-	-		
86	OHX	4	227	-	0,6,6	0.00	-	-		
86	OHX	5	4170	-	0,6,6	0.00	-	-		
86	OHX	14	402	-	0,6,6	0.00	-	-		
86	OHX	5	4082	-	0,6,6	0.00	-	-		
86	OHX	6	2145	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4008	-	0,6,6	0.00	-	-		
86	OHX	M7	207	-	0,6,6	0.00	-	-		
86	OHX	d4	201	-	0,6,6	0.00	-	-		
86	OHX	2	2137	-	0,6,6	0.00	-	-		
86	OHX	6	2062	-	0,6,6	0.00	-	-		
86	OHX	4	225	-	0,6,6	0.00	-	-		
86	OHX	1	3887	-	0,6,6	0.00	-	-		
86	OHX	6	2192	-	0,6,6	0.00	-	-		
86	OHX	5	4227	-	0,6,6	0.00	-	-		
86	OHX	1	4122	-	0,6,6	0.00	-	-		
86	OHX	5	4059	-	0,6,6	0.00	-	-		
86	OHX	1	4087	-	0,6,6	0.00	-	-		
86	OHX	5	4150	-	0,6,6	0.00	-	-		
86	OHX	6	2107	-	0,6,6	0.00	-	-		
86	OHX	1	3964	-	0,6,6	0.00	-	-		
86	OHX	2	2040	-	0,6,6	0.00	-	-		
86	OHX	5	4003	-	0,6,6	0.00	-	-		
86	OHX	5	4068	-	0,6,6	0.00	-	-		
86	OHX	2	2113	-	0,6,6	0.00	-	-		
86	OHX	5	3899	-	0,6,6	0.00	-	-		
86	OHX	6	2083	-	0,6,6	0.00	-	-		
86	OHX	5	4157	-	0,6,6	0.00	-	-		
86	OHX	6	2140	-	0,6,6	0.00	-	-		
86	OHX	2	2090	-	0,6,6	0.00	-	-		
86	OHX	4	235	-	0,6,6	0.00	-	-		
86	OHX	5	3987	-	0,6,6	0.00	-	-		
86	OHX	2	2121	-	0,6,6	0.00	-	-		
86	OHX	2	2173	-	0,6,6	0.00	-	-		
86	OHX	1	3989	-	0,6,6	0.00	-	-		
86	OHX	6	2135	-	0,6,6	0.00	-	-		
86	OHX	5	4247	-	0,6,6	0.00	-	-		
86	OHX	6	2126	-	0,6,6	0.00	-	-		
86	OHX	1	4042	-	0,6,6	0.00	-	-		
86	OHX	3	219	-	0,6,6	0.00	-	-		
86	OHX	2	2142	-	0,6,6	0.00	-	-		
86	OHX	1	4030	-	0,6,6	0.00	-	-		
86	OHX	5	4149	-	0,6,6	0.00	-	-		
86	OHX	5	4028	-	0,6,6	0.00	-	-		
86	OHX	1	3912	-	0,6,6	0.00	-	-		
86	OHX	2	2175	-	0,6,6	0.00	-	-		
86	OHX	1	4000	-	0,6,6	0.00	-	-		
86	OHX	1	3899	-	0,6,6	0.00	-	-		
86	OHX	1	4165	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4199	-	0,6,6	0.00	-	-		
86	OHX	5	3966	-	0,6,6	0.00	-	-		
86	OHX	2	2156	-	0,6,6	0.00	-	-		
86	OHX	6	2067	-	0,6,6	0.00	-	-		
86	OHX	5	4241	-	0,6,6	0.00	-	-		
86	OHX	1	4104	-	0,6,6	0.00	-	-		
86	OHX	5	4109	-	0,6,6	0.00	-	-		
86	OHX	5	4128	-	0,6,6	0.00	-	-		
86	OHX	1	4095	-	0,6,6	0.00	-	-		
86	OHX	4	230	-	0,6,6	0.00	-	-		
86	OHX	1	4090	-	0,6,6	0.00	-	-		
86	OHX	1	3973	-	0,6,6	0.00	-	-		
86	OHX	2	2034	-	0,6,6	0.00	-	-		
86	OHX	6	2188	-	0,6,6	0.00	-	-		
86	OHX	5	4133	-	0,6,6	0.00	-	-		
86	OHX	2	2148	-	0,6,6	0.00	-	-		
86	OHX	S8	302	-	0,6,6	0.00	-	-		
86	OHX	2	2100	-	0,6,6	0.00	-	-		
86	OHX	s1	303	-	0,6,6	0.00	-	-		
86	OHX	1	4196	-	0,6,6	0.00	-	-		
86	OHX	5	4162	-	0,6,6	0.00	-	-		
86	OHX	1	4136	-	0,6,6	0.00	-	-		
86	OHX	1	3930	-	0,6,6	0.00	-	-		
86	OHX	6	2051	-	0,6,6	0.00	-	-		
86	OHX	6	2201	-	0,6,6	0.00	-	-		
86	OHX	1	3902	-	0,6,6	0.00	-	-		
86	OHX	5	4006	-	0,6,6	0.00	-	-		
86	OHX	D9	102	-	0,6,6	0.00	-	-		
86	OHX	1	4172	-	0,6,6	0.00	-	-		
86	OHX	5	4144	-	0,6,6	0.00	-	-		
86	OHX	1	4007	-	0,6,6	0.00	-	-		
86	OHX	5	4076	-	0,6,6	0.00	-	-		
86	OHX	8	225	-	0,6,6	0.00	-	-		
86	OHX	1	4134	-	0,6,6	0.00	-	-		
86	OHX	3	225	-	0,6,6	0.00	-	-		
86	OHX	1	4153	-	0,6,6	0.00	-	-		
86	OHX	2	2108	-	0,6,6	0.00	-	-		
86	OHX	8	219	-	0,6,6	0.00	-	-		
86	OHX	2	2102	-	0,6,6	0.00	-	-		
86	OHX	1	3868	-	0,6,6	0.00	-	-		
86	OHX	1	4035	-	0,6,6	0.00	-	-		
86	OHX	1	3983	-	0,6,6	0.00	-	-		
86	OHX	5	4226	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3895	-	0,6,6	0.00	-	-		
86	OHX	1	4159	-	0,6,6	0.00	-	-		
86	OHX	5	4012	-	0,6,6	0.00	-	-		
86	OHX	5	4176	-	0,6,6	0.00	-	-		
86	OHX	5	4033	-	0,6,6	0.00	-	-		
86	OHX	5	3947	-	0,6,6	0.00	-	-		
86	OHX	1	3877	-	0,6,6	0.00	-	-		
86	OHX	1	4044	-	0,6,6	0.00	-	-		
86	OHX	7	229	-	0,6,6	0.00	-	-		
86	OHX	1	4077	-	0,6,6	0.00	-	-		
86	OHX	6	2118	-	0,6,6	0.00	-	-		
86	OHX	5	4013	-	0,6,6	0.00	-	-		
86	OHX	6	2059	-	0,6,6	0.00	-	-		
86	OHX	5	4078	-	0,6,6	0.00	-	-		
86	OHX	1	4089	-	0,6,6	0.00	-	-		
86	OHX	5	4051	-	0,6,6	0.00	-	-		
86	OHX	2	2178	-	0,6,6	0.00	-	-		
86	OHX	6	2047	-	0,6,6	0.00	-	-		
86	OHX	6	2152	-	0,6,6	0.00	-	-		
86	OHX	6	2186	-	0,6,6	0.00	-	-		
86	OHX	1	3963	-	0,6,6	0.00	-	-		
86	OHX	5	3914	-	0,6,6	0.00	-	-		
86	OHX	5	4091	-	0,6,6	0.00	-	-		
86	OHX	8	221	-	0,6,6	0.00	-	-		
86	OHX	m1	202	-	0,6,6	0.00	-	-		
86	OHX	6	2095	-	0,6,6	0.00	-	-		
86	OHX	1	4073	-	0,6,6	0.00	-	-		
86	OHX	1	4100	-	0,6,6	0.00	-	-		
86	OHX	1	4098	-	0,6,6	0.00	-	-		
86	OHX	6	2071	-	0,6,6	0.00	-	-		
86	OHX	5	4196	-	0,6,6	0.00	-	-		
86	OHX	2	2072	-	0,6,6	0.00	-	-		
86	OHX	5	4197	-	0,6,6	0.00	-	-		
86	OHX	5	4075	-	0,6,6	0.00	-	-		
86	OHX	1	4074	-	0,6,6	0.00	-	-		
86	OHX	5	3962	-	0,6,6	0.00	-	-		
86	OHX	5	4202	-	0,6,6	0.00	-	-		
86	OHX	1	4170	-	0,6,6	0.00	-	-		
86	OHX	5	3993	-	0,6,6	0.00	-	-		
86	OHX	5	4065	-	0,6,6	0.00	-	-		
86	OHX	1	4149	-	0,6,6	0.00	-	-		
86	OHX	1	3864	-	0,6,6	0.00	-	-		
86	OHX	6	2105	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4168	-	0,6,6	0.00	-	-		
86	OHX	5	4000	-	0,6,6	0.00	-	-		
86	OHX	6	2129	-	0,6,6	0.00	-	-		
86	OHX	7	225	-	0,6,6	0.00	-	-		
86	OHX	1	4091	-	0,6,6	0.00	-	-		
86	OHX	6	2136	-	0,6,6	0.00	-	-		
86	OHX	5	4112	-	0,6,6	0.00	-	-		
86	OHX	2	2107	-	0,6,6	0.00	-	-		
86	OHX	1	4051	-	0,6,6	0.00	-	-		
86	OHX	5	3903	-	0,6,6	0.00	-	-		
86	OHX	5	4014	-	0,6,6	0.00	-	-		
86	OHX	5	4062	-	0,6,6	0.00	-	-		
86	OHX	6	2162	-	0,6,6	0.00	-	-		
86	OHX	6	2169	-	0,6,6	0.00	-	-		
86	OHX	2	2140	-	0,6,6	0.00	-	-		
86	OHX	4	237	-	0,6,6	0.00	-	-		
86	OHX	2	2167	-	0,6,6	0.00	-	-		
86	OHX	5	4089	-	0,6,6	0.00	-	-		
86	OHX	2	2042	-	0,6,6	0.00	-	-		
86	OHX	6	2204	-	0,6,6	0.00	-	-		
86	OHX	6	2142	-	0,6,6	0.00	-	-		
86	OHX	5	4054	-	0,6,6	0.00	-	-		
86	OHX	2	2089	-	0,6,6	0.00	-	-		
86	OHX	5	4155	-	0,6,6	0.00	-	-		
86	OHX	5	4020	-	0,6,6	0.00	-	-		
86	OHX	3	223	-	0,6,6	0.00	-	-		
86	OHX	5	3901	-	0,6,6	0.00	-	-		
86	OHX	1	4008	-	0,6,6	0.00	-	-		
88	BLS	1	4211	-	25,31,31	1.98	7 (28%)	23,43,43	2.77	8 (34%)
86	OHX	1	4067	-	0,6,6	0.00	-	-		
86	OHX	1	3949	-	0,6,6	0.00	-	-		
86	OHX	1	4009	-	0,6,6	0.00	-	-		
86	OHX	5	4021	-	0,6,6	0.00	-	-		
86	OHX	2	2085	-	0,6,6	0.00	-	-		
86	OHX	1	4204	-	0,6,6	0.00	-	-		
86	OHX	1	3871	-	0,6,6	0.00	-	-		
86	OHX	2	2077	-	0,6,6	0.00	-	-		
86	OHX	2	2076	-	0,6,6	0.00	-	-		
86	OHX	1	4135	-	0,6,6	0.00	-	-		
86	OHX	1	4120	-	0,6,6	0.00	-	-		
86	OHX	6	2087	-	0,6,6	0.00	-	-		
86	OHX	1	4084	-	0,6,6	0.00	-	-		
86	OHX	1	4072	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2191	-	0,6,6	0.00	-	-		
86	OHX	1	4108	-	0,6,6	0.00	-	-		
86	OHX	1	3878	-	0,6,6	0.00	-	-		
86	OHX	8	229	-	0,6,6	0.00	-	-		
86	OHX	2	2030	-	0,6,6	0.00	-	-		
86	OHX	2	2105	-	0,6,6	0.00	-	-		
86	OHX	6	2184	-	0,6,6	0.00	-	-		
86	OHX	1	4129	-	0,6,6	0.00	-	-		
86	OHX	5	4123	-	0,6,6	0.00	-	-		
86	OHX	2	2133	-	0,6,6	0.00	-	-		
86	OHX	7	220	-	0,6,6	0.00	-	-		
86	OHX	6	2125	-	0,6,6	0.00	-	-		
86	OHX	1	4099	-	0,6,6	0.00	-	-		
86	OHX	5	3965	-	0,6,6	0.00	-	-		
86	OHX	5	4224	-	0,6,6	0.00	-	-		
86	OHX	6	2111	-	0,6,6	0.00	-	-		
86	OHX	6	2088	-	0,6,6	0.00	-	-		
86	OHX	1	4040	-	0,6,6	0.00	-	-		
86	OHX	6	2114	-	0,6,6	0.00	-	-		
86	OHX	5	4110	-	0,6,6	0.00	-	-		
86	OHX	6	2063	-	0,6,6	0.00	-	-		
86	OHX	5	3900	-	0,6,6	0.00	-	-		
86	OHX	2	2027	-	0,6,6	0.00	-	-		
86	OHX	Q2	503	-	0,6,6	0.00	-	-		
86	OHX	5	3936	-	0,6,6	0.00	-	-		
86	OHX	5	4004	-	0,6,6	0.00	-	-		
86	OHX	1	4059	-	0,6,6	0.00	-	-		
86	OHX	4	226	-	0,6,6	0.00	-	-		
86	OHX	c5	201	-	0,6,6	0.00	-	-		
86	OHX	6	2141	-	0,6,6	0.00	-	-		
86	OHX	2	2138	-	0,6,6	0.00	-	-		
86	OHX	5	4066	-	0,6,6	0.00	-	-		
86	OHX	5	3920	-	0,6,6	0.00	-	-		
86	OHX	6	2084	-	0,6,6	0.00	-	-		
86	OHX	1	4039	-	0,6,6	0.00	-	-		
86	OHX	1	4033	-	0,6,6	0.00	-	-		
86	OHX	6	2134	-	0,6,6	0.00	-	-		
86	OHX	6	2113	-	0,6,6	0.00	-	-		
86	OHX	5	3950	-	0,6,6	0.00	-	-		
86	OHX	1	4038	-	0,6,6	0.00	-	-		
86	OHX	5	4053	-	0,6,6	0.00	-	-		
86	OHX	5	4118	-	0,6,6	0.00	-	-		
86	OHX	1	3889	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4210	-	0,6,6	0.00	-	-		
86	OHX	5	4242	-	0,6,6	0.00	-	-		
86	OHX	5	4106	-	0,6,6	0.00	-	-		
86	OHX	5	3902	-	0,6,6	0.00	-	-		
86	OHX	1	3968	-	0,6,6	0.00	-	-		
86	OHX	1	4180	-	0,6,6	0.00	-	-		
86	OHX	8	217	-	0,6,6	0.00	-	-		
86	OHX	6	2132	-	0,6,6	0.00	-	-		
86	OHX	5	4073	-	0,6,6	0.00	-	-		
86	OHX	1	4034	-	0,6,6	0.00	-	-		
86	OHX	2	2083	-	0,6,6	0.00	-	-		
86	OHX	5	4173	-	0,6,6	0.00	-	-		
86	OHX	2	2066	-	0,6,6	0.00	-	-		
86	OHX	5	4049	-	0,6,6	0.00	-	-		
86	OHX	6	2178	-	0,6,6	0.00	-	-		
86	OHX	6	2155	-	0,6,6	0.00	-	-		
86	OHX	5	4207	-	0,6,6	0.00	-	-		
86	OHX	2	2069	-	0,6,6	0.00	-	-		
86	OHX	2	2116	-	0,6,6	0.00	-	-		
86	OHX	5	4192	-	0,6,6	0.00	-	-		
86	OHX	5	4060	-	0,6,6	0.00	-	-		
86	OHX	6	2119	-	0,6,6	0.00	-	-		
86	OHX	5	4154	-	0,6,6	0.00	-	-		
86	OHX	8	223	-	0,6,6	0.00	-	-		
86	OHX	1	3988	-	0,6,6	0.00	-	-		
86	OHX	6	2089	-	0,6,6	0.00	-	-		
86	OHX	1	4028	-	0,6,6	0.00	-	-		
86	OHX	1	3952	-	0,6,6	0.00	-	-		
86	OHX	5	4022	-	0,6,6	0.00	-	-		
86	OHX	1	4046	-	0,6,6	0.00	-	-		
86	OHX	5	3907	-	0,6,6	0.00	-	-		
86	OHX	6	2052	-	0,6,6	0.00	-	-		
86	OHX	5	3939	-	0,6,6	0.00	-	-		
86	OHX	2	2115	-	0,6,6	0.00	-	-		
86	OHX	1	4140	-	0,6,6	0.00	-	-		
86	OHX	5	4212	-	0,6,6	0.00	-	-		
86	OHX	5	4135	-	0,6,6	0.00	-	-		
86	OHX	2	2154	-	0,6,6	0.00	-	-		
86	OHX	6	2166	-	0,6,6	0.00	-	-		
86	OHX	o3	203	-	0,6,6	0.00	-	-		
86	OHX	5	4040	-	0,6,6	0.00	-	-		
86	OHX	1	4195	-	0,6,6	0.00	-	-		
86	OHX	5	3904	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2153	-	0,6,6	0.00	-	-		
86	OHX	5	4102	-	0,6,6	0.00	-	-		
86	OHX	1	3999	-	0,6,6	0.00	-	-		
86	OHX	1	3991	-	0,6,6	0.00	-	-		
86	OHX	1	4005	-	0,6,6	0.00	-	-		
86	OHX	8	222	-	0,6,6	0.00	-	-		
86	OHX	2	2145	-	0,6,6	0.00	-	-		
86	OHX	1	4026	-	0,6,6	0.00	-	-		
86	OHX	SR	401	-	0,6,6	0.00	-	-		
86	OHX	1	3980	-	0,6,6	0.00	-	-		
86	OHX	2	2179	-	0,6,6	0.00	-	-		
86	OHX	5	4037	-	0,6,6	0.00	-	-		
86	OHX	2	2130	-	0,6,6	0.00	-	-		
86	OHX	5	3918	-	0,6,6	0.00	-	-		
86	OHX	5	4171	-	0,6,6	0.00	-	-		
86	OHX	2	2166	-	0,6,6	0.00	-	-		
86	OHX	2	2071	-	0,6,6	0.00	-	-		
86	OHX	2	2033	-	0,6,6	0.00	-	-		
86	OHX	15	306	-	0,6,6	0.00	-	-		
86	OHX	1	4137	-	0,6,6	0.00	-	-		
86	OHX	1	4169	-	0,6,6	0.00	-	-		
86	OHX	5	4042	-	0,6,6	0.00	-	-		
86	OHX	1	4193	-	0,6,6	0.00	-	-		
86	OHX	5	4179	-	0,6,6	0.00	-	-		
86	OHX	5	4079	-	0,6,6	0.00	-	-		
86	OHX	1	4158	-	0,6,6	0.00	-	-		
86	OHX	1	3974	-	0,6,6	0.00	-	-		
86	OHX	1	3922	-	0,6,6	0.00	-	-		
86	OHX	2	2065	-	0,6,6	0.00	-	-		
86	OHX	1	3929	-	0,6,6	0.00	-	-		
86	OHX	1	4006	-	0,6,6	0.00	-	-		
86	OHX	1	4085	-	0,6,6	0.00	-	-		
86	OHX	5	3940	-	0,6,6	0.00	-	-		
86	OHX	1	3976	-	0,6,6	0.00	-	-		
86	OHX	5	3927	-	0,6,6	0.00	-	-		
86	OHX	5	4185	-	0,6,6	0.00	-	-		
86	OHX	2	2164	-	0,6,6	0.00	-	-		
86	OHX	2	2023	-	0,6,6	0.00	-	-		
86	OHX	5	4200	-	0,6,6	0.00	-	-		
86	OHX	1	4144	-	0,6,6	0.00	-	-		
86	OHX	6	2070	-	0,6,6	0.00	-	-		
86	OHX	5	4237	-	0,6,6	0.00	-	-		
86	OHX	5	4018	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3937	-	0,6,6	0.00	-	-		
86	OHX	1	3857	-	0,6,6	0.00	-	-		
86	OHX	7	218	-	0,6,6	0.00	-	-		
86	OHX	1	3908	-	0,6,6	0.00	-	-		
86	OHX	1	4079	-	0,6,6	0.00	-	-		
86	OHX	2	2088	-	0,6,6	0.00	-	-		
86	OHX	5	4243	-	0,6,6	0.00	-	-		
86	OHX	1	4148	-	0,6,6	0.00	-	-		
86	OHX	1	4075	-	0,6,6	0.00	-	-		
86	OHX	15	305	-	0,6,6	0.00	-	-		
86	OHX	1	4088	-	0,6,6	0.00	-	-		
86	OHX	5	4172	-	0,6,6	0.00	-	-		
86	OHX	1	3962	-	0,6,6	0.00	-	-		
86	OHX	5	4182	-	0,6,6	0.00	-	-		
86	OHX	5	3986	-	0,6,6	0.00	-	-		
86	OHX	2	2158	-	0,6,6	0.00	-	-		
86	OHX	5	3997	-	0,6,6	0.00	-	-		
86	OHX	5	4084	-	0,6,6	0.00	-	-		
86	OHX	5	4186	-	0,6,6	0.00	-	-		
86	OHX	19	202	-	0,6,6	0.00	-	-		
86	OHX	1	4188	-	0,6,6	0.00	-	-		
86	OHX	6	2100	-	0,6,6	0.00	-	-		
86	OHX	6	2094	-	0,6,6	0.00	-	-		
86	OHX	6	2127	-	0,6,6	0.00	-	-		
86	OHX	2	2120	-	0,6,6	0.00	-	-		
86	OHX	1	4096	-	0,6,6	0.00	-	-		
86	OHX	5	4210	-	0,6,6	0.00	-	-		
86	OHX	5	4095	-	0,6,6	0.00	-	-		
86	OHX	2	2174	-	0,6,6	0.00	-	-		
86	OHX	5	4193	-	0,6,6	0.00	-	-		
86	OHX	5	3969	-	0,6,6	0.00	-	-		
86	OHX	1	4018	-	0,6,6	0.00	-	-		
86	OHX	5	3967	-	0,6,6	0.00	-	-		
86	OHX	2	2041	-	0,6,6	0.00	-	-		
86	OHX	1	4199	-	0,6,6	0.00	-	-		
86	OHX	5	4165	-	0,6,6	0.00	-	-		
86	OHX	1	3967	-	0,6,6	0.00	-	-		
86	OHX	5	4160	-	0,6,6	0.00	-	-		
86	OHX	5	4215	-	0,6,6	0.00	-	-		
86	OHX	6	2146	-	0,6,6	0.00	-	-		
86	OHX	5	3951	-	0,6,6	0.00	-	-		
86	OHX	1	4200	-	0,6,6	0.00	-	-		
86	OHX	1	4037	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	M0	304	-	0,6,6	0.00	-	-		
86	OHX	1	3953	-	0,6,6	0.00	-	-		
86	OHX	5	4183	-	0,6,6	0.00	-	-		
86	OHX	5	4189	-	0,6,6	0.00	-	-		
86	OHX	8	218	-	0,6,6	0.00	-	-		
86	OHX	s4	301	-	0,6,6	0.00	-	-		
86	OHX	1	3903	-	0,6,6	0.00	-	-		
86	OHX	5	3984	-	0,6,6	0.00	-	-		
86	OHX	1	4173	-	0,6,6	0.00	-	-		
86	OHX	1	3883	-	0,6,6	0.00	-	-		
86	OHX	5	3963	-	0,6,6	0.00	-	-		
86	OHX	5	3896	-	0,6,6	0.00	-	-		
86	OHX	2	2098	-	0,6,6	0.00	-	-		
86	OHX	1	3913	-	0,6,6	0.00	-	-		
86	OHX	5	4098	-	0,6,6	0.00	-	-		
86	OHX	5	4034	-	0,6,6	0.00	-	-		
86	OHX	1	3904	-	0,6,6	0.00	-	-		
86	OHX	2	2095	-	0,6,6	0.00	-	-		
86	OHX	4	228	-	0,6,6	0.00	-	-		
86	OHX	6	2167	-	0,6,6	0.00	-	-		
86	OHX	1	4167	-	0,6,6	0.00	-	-		
86	OHX	5	4085	-	0,6,6	0.00	-	-		
86	OHX	6	2197	-	0,6,6	0.00	-	-		
86	OHX	2	2129	-	0,6,6	0.00	-	-		
86	OHX	5	4120	-	0,6,6	0.00	-	-		
86	OHX	1	4048	-	0,6,6	0.00	-	-		
86	OHX	5	4213	-	0,6,6	0.00	-	-		
86	OHX	1	3859	-	0,6,6	0.00	-	-		
86	OHX	6	2165	-	0,6,6	0.00	-	-		
86	OHX	1	3970	-	0,6,6	0.00	-	-		
86	OHX	5	4206	-	0,6,6	0.00	-	-		
86	OHX	1	3921	-	0,6,6	0.00	-	-		
86	OHX	2	2051	-	0,6,6	0.00	-	-		
86	OHX	1	4053	-	0,6,6	0.00	-	-		
86	OHX	5	4069	-	0,6,6	0.00	-	-		
86	OHX	5	4121	-	0,6,6	0.00	-	-		
86	OHX	5	3938	-	0,6,6	0.00	-	-		
86	OHX	1	4162	-	0,6,6	0.00	-	-		
86	OHX	2	2092	-	0,6,6	0.00	-	-		
86	OHX	1	4111	-	0,6,6	0.00	-	-		
86	OHX	5	4071	-	0,6,6	0.00	-	-		
86	OHX	l3	405	-	0,6,6	0.00	-	-		
86	OHX	2	2123	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	4	231	-	0,6,6	0.00	-	-		
86	OHX	1	3987	-	0,6,6	0.00	-	-		
86	OHX	1	4121	-	0,6,6	0.00	-	-		
86	OHX	5	4100	-	0,6,6	0.00	-	-		
86	OHX	1	4011	-	0,6,6	0.00	-	-		
86	OHX	2	2159	-	0,6,6	0.00	-	-		
86	OHX	1	4049	-	0,6,6	0.00	-	-		
86	OHX	5	3908	-	0,6,6	0.00	-	-		
86	OHX	1	4164	-	0,6,6	0.00	-	-		
86	OHX	1	4208	-	0,6,6	0.00	-	-		
86	OHX	1	3951	-	0,6,6	0.00	-	-		
86	OHX	5	4245	-	0,6,6	0.00	-	-		
86	OHX	5	3981	-	0,6,6	0.00	-	-		
86	OHX	1	3917	-	0,6,6	0.00	-	-		
86	OHX	5	4007	-	0,6,6	0.00	-	-		
86	OHX	1	3986	-	0,6,6	0.00	-	-		
86	OHX	1	4127	-	0,6,6	0.00	-	-		
86	OHX	2	2039	-	0,6,6	0.00	-	-		
86	OHX	2	2035	-	0,6,6	0.00	-	-		
86	OHX	5	4111	-	0,6,6	0.00	-	-		
86	OHX	s9	201	-	0,6,6	0.00	-	-		
86	OHX	1	4126	-	0,6,6	0.00	-	-		
86	OHX	1	4131	-	0,6,6	0.00	-	-		
86	OHX	8	228	-	0,6,6	0.00	-	-		
86	OHX	m4	202	-	0,6,6	0.00	-	-		
86	OHX	2	2155	-	0,6,6	0.00	-	-		
86	OHX	1	3892	-	0,6,6	0.00	-	-		
86	OHX	1	4020	-	0,6,6	0.00	-	-		
86	OHX	1	3898	-	0,6,6	0.00	-	-		
86	OHX	5	4159	-	0,6,6	0.00	-	-		
86	OHX	1	4187	-	0,6,6	0.00	-	-		
86	OHX	1	3996	-	0,6,6	0.00	-	-		
86	OHX	2	2147	-	0,6,6	0.00	-	-		
86	OHX	1	4024	-	0,6,6	0.00	-	-		
86	OHX	1	4157	-	0,6,6	0.00	-	-		
86	OHX	l5	304	-	0,6,6	0.00	-	-		
86	OHX	6	2075	-	0,6,6	0.00	-	-		
86	OHX	5	4141	-	0,6,6	0.00	-	-		
86	OHX	1	4143	-	0,6,6	0.00	-	-		
86	OHX	5	4161	-	0,6,6	0.00	-	-		
86	OHX	5	3961	-	0,6,6	0.00	-	-		
86	OHX	5	3994	-	0,6,6	0.00	-	-		
86	OHX	6	2137	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	m6	203	-	0,6,6	0.00	-	-		
86	OHX	1	3891	-	0,6,6	0.00	-	-		
86	OHX	2	2068	-	0,6,6	0.00	-	-		
86	OHX	5	4117	-	0,6,6	0.00	-	-		
86	OHX	6	2198	-	0,6,6	0.00	-	-		
86	OHX	2	2029	-	0,6,6	0.00	-	-		
86	OHX	1	4047	-	0,6,6	0.00	-	-		
86	OHX	6	2099	-	0,6,6	0.00	-	-		
86	OHX	8	215	-	0,6,6	0.00	-	-		
86	OHX	6	2182	-	0,6,6	0.00	-	-		
86	OHX	C3	201	-	0,6,6	0.00	-	-		
86	OHX	6	2101	-	0,6,6	0.00	-	-		
86	OHX	6	2096	-	0,6,6	0.00	-	-		
86	OHX	1	3960	-	0,6,6	0.00	-	-		
86	OHX	1	3927	-	0,6,6	0.00	-	-		
86	OHX	1	4130	-	0,6,6	0.00	-	-		
86	OHX	5	3912	-	0,6,6	0.00	-	-		
86	OHX	5	3924	-	0,6,6	0.00	-	-		
86	OHX	2	2141	-	0,6,6	0.00	-	-		
86	OHX	5	4181	-	0,6,6	0.00	-	-		
86	OHX	1	4001	-	0,6,6	0.00	-	-		
86	OHX	6	2055	-	0,6,6	0.00	-	-		
86	OHX	1	3861	-	0,6,6	0.00	-	-		
86	OHX	1	4113	-	0,6,6	0.00	-	-		
86	OHX	6	2102	-	0,6,6	0.00	-	-		
86	OHX	5	4107	-	0,6,6	0.00	-	-		
86	OHX	2	2128	-	0,6,6	0.00	-	-		
86	OHX	2	2127	-	0,6,6	0.00	-	-		
86	OHX	5	3922	-	0,6,6	0.00	-	-		
86	OHX	2	2038	-	0,6,6	0.00	-	-		
86	OHX	2	2044	-	0,6,6	0.00	-	-		
86	OHX	5	4097	-	0,6,6	0.00	-	-		
86	OHX	1	4069	-	0,6,6	0.00	-	-		
86	OHX	1	4185	-	0,6,6	0.00	-	-		
86	OHX	1	4036	-	0,6,6	0.00	-	-		
86	OHX	1	4107	-	0,6,6	0.00	-	-		
86	OHX	5	4052	-	0,6,6	0.00	-	-		
86	OHX	5	4145	-	0,6,6	0.00	-	-		
86	OHX	1	4205	-	0,6,6	0.00	-	-		
86	OHX	5	4232	-	0,6,6	0.00	-	-		
86	OHX	5	3892	-	0,6,6	0.00	-	-		
86	OHX	5	4180	-	0,6,6	0.00	-	-		
86	OHX	1	4061	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4010	-	0,6,6	0.00	-	-		
86	OHX	5	4152	-	0,6,6	0.00	-	-		
86	OHX	1	4141	-	0,6,6	0.00	-	-		
86	OHX	5	3979	-	0,6,6	0.00	-	-		
86	OHX	5	4015	-	0,6,6	0.00	-	-		
86	OHX	6	2112	-	0,6,6	0.00	-	-		
86	OHX	5	4114	-	0,6,6	0.00	-	-		
86	OHX	1	4166	-	0,6,6	0.00	-	-		
86	OHX	5	4219	-	0,6,6	0.00	-	-		
86	OHX	2	2111	-	0,6,6	0.00	-	-		
86	OHX	5	3934	-	0,6,6	0.00	-	-		
86	OHX	6	2081	-	0,6,6	0.00	-	-		
86	OHX	5	4070	-	0,6,6	0.00	-	-		
86	OHX	2	2170	-	0,6,6	0.00	-	-		
86	OHX	5	3960	-	0,6,6	0.00	-	-		
86	OHX	5	4169	-	0,6,6	0.00	-	-		
86	OHX	2	2078	-	0,6,6	0.00	-	-		
86	OHX	7	227	-	0,6,6	0.00	-	-		
86	OHX	1	3910	-	0,6,6	0.00	-	-		
86	OHX	5	4129	-	0,6,6	0.00	-	-		
86	OHX	1	4123	-	0,6,6	0.00	-	-		
86	OHX	2	2052	-	0,6,6	0.00	-	-		
86	OHX	1	3958	-	0,6,6	0.00	-	-		
86	OHX	2	2058	-	0,6,6	0.00	-	-		
86	OHX	2	2057	-	0,6,6	0.00	-	-		
86	OHX	1	4163	-	0,6,6	0.00	-	-		
86	OHX	1	4186	-	0,6,6	0.00	-	-		
86	OHX	1	3946	-	0,6,6	0.00	-	-		
86	OHX	L4	404	-	0,6,6	0.00	-	-		
86	OHX	5	3906	-	0,6,6	0.00	-	-		
86	OHX	1	4076	-	0,6,6	0.00	-	-		
86	OHX	5	4188	-	0,6,6	0.00	-	-		
86	OHX	5	4041	-	0,6,6	0.00	-	-		
86	OHX	5	4064	-	0,6,6	0.00	-	-		
86	OHX	6	2079	-	0,6,6	0.00	-	-		
86	OHX	1	3975	-	0,6,6	0.00	-	-		
86	OHX	1	3862	-	0,6,6	0.00	-	-		
86	OHX	1	4124	-	0,6,6	0.00	-	-		
86	OHX	1	4027	-	0,6,6	0.00	-	-		
86	OHX	1	4021	-	0,6,6	0.00	-	-		
86	OHX	1	4177	-	0,6,6	0.00	-	-		
86	OHX	1	3937	-	0,6,6	0.00	-	-		
86	OHX	5	3996	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2196	-	0,6,6	0.00	-	-		
86	OHX	2	2050	-	0,6,6	0.00	-	-		
86	OHX	5	4139	-	0,6,6	0.00	-	-		
86	OHX	1	4012	-	0,6,6	0.00	-	-		
86	OHX	6	2098	-	0,6,6	0.00	-	-		
86	OHX	1	4070	-	0,6,6	0.00	-	-		
86	OHX	m7	207	-	0,6,6	0.00	-	-		
86	OHX	5	3990	-	0,6,6	0.00	-	-		
86	OHX	2	2056	-	0,6,6	0.00	-	-		
86	OHX	1	3981	-	0,6,6	0.00	-	-		
86	OHX	1	3984	-	0,6,6	0.00	-	-		
86	OHX	5	4044	-	0,6,6	0.00	-	-		
86	OHX	5	3931	-	0,6,6	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
88	BLS	5	4248	-	-	7/17/38/38	0/2/2/2
88	BLS	1	4211	-	-	3/17/38/38	0/2/2/2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	5	4248	BLS	C11-N12	-5.35	1.36	1.47
88	1	4211	BLS	C6-N1	4.43	1.41	1.35
88	1	4211	BLS	C2-N3	-4.20	1.29	1.38
88	1	4211	BLS	C5-C4	3.59	1.49	1.41
88	1	4211	BLS	C11-N12	3.19	1.53	1.47

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4211	BLS	C2-N3-C4	10.01	126.48	116.34
88	5	4248	BLS	O5'-C1'-C2'	-5.93	109.92	113.13
88	5	4248	BLS	C2-N3-C4	4.27	120.66	116.34
88	1	4211	BLS	N4-C4-N3	3.65	122.25	116.49
88	1	4211	BLS	C4'-N6-C7	3.44	126.81	123.13

There are no chirality outliers.

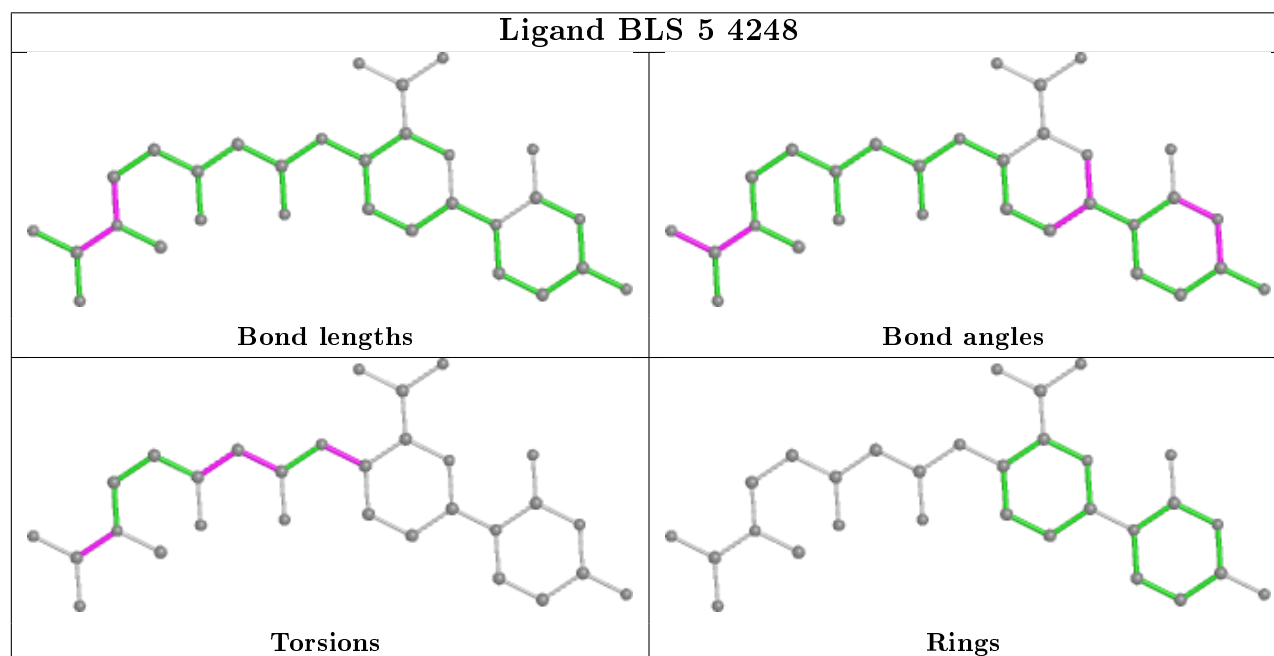
5 of 10 torsion outliers are listed below:

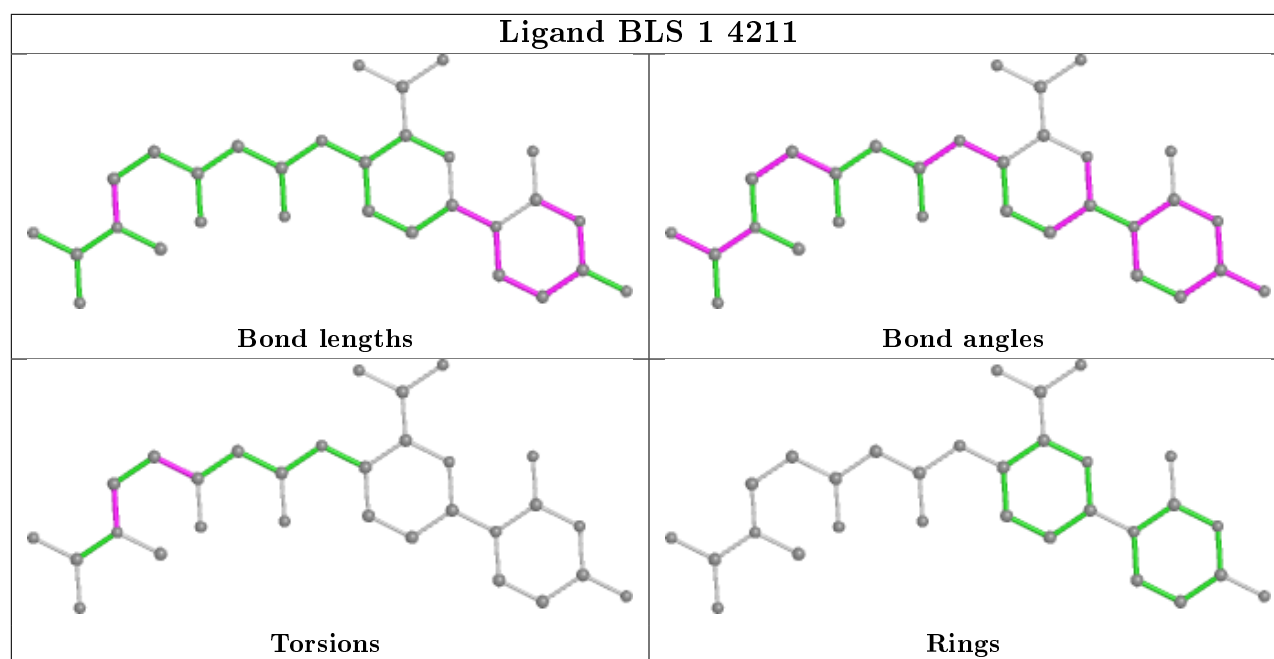
Mol	Chain	Res	Type	Atoms
88	5	4248	BLS	C3'-C4'-N6-C7
88	5	4248	BLS	C7-C8-C9-N9
88	5	4248	BLS	N14-C14-N12-C11
88	5	4248	BLS	N15-C14-N12-C11
88	1	4211	BLS	C11-C10-C9-C8

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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 is therefore empty.

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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