



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 1, 2020 – 02:54 pm BST

PDB ID : 5FCJ
Title : Structure of the anisomycin-containing uL3 W255C mutant 80S yeast ribosome
Authors : Mailliot, J.; Garreau de Loubresse, N.; Yusupova, G.; Dinman, J.D.; Yusupov, M.
Deposited on : 2015-12-15
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

<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 : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

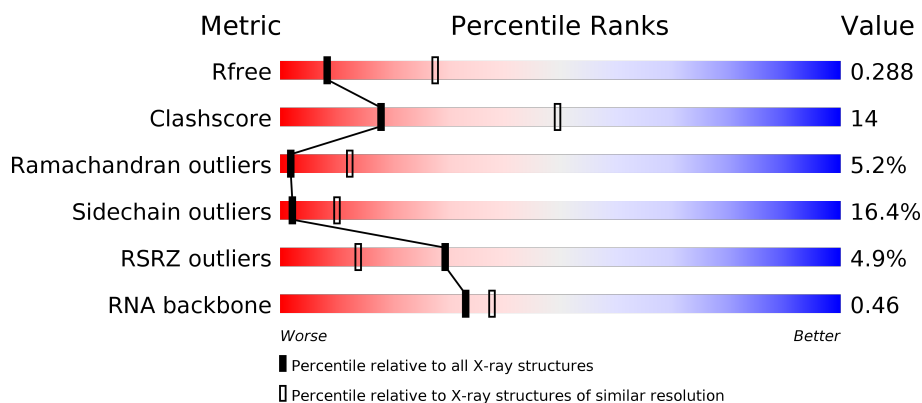
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



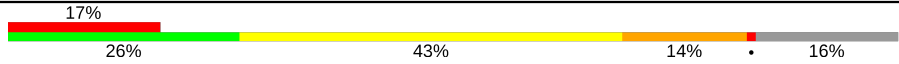

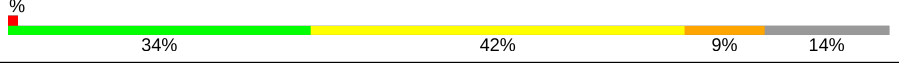

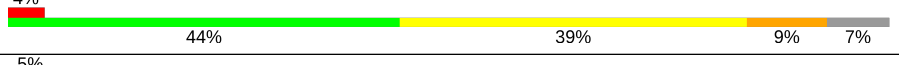
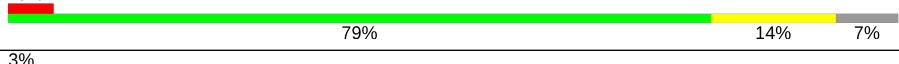
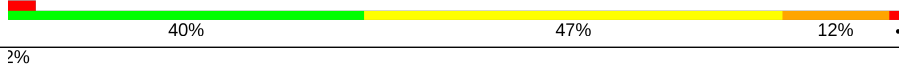

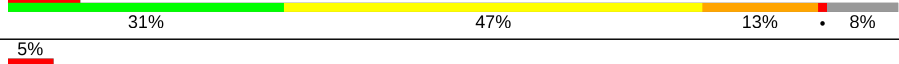


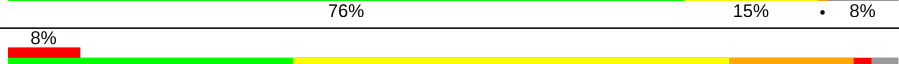

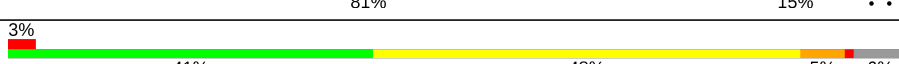

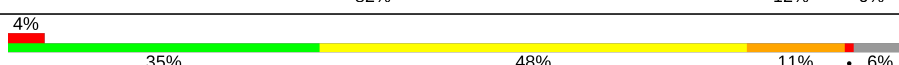
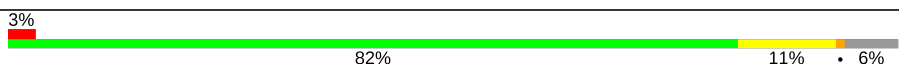
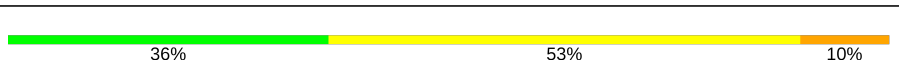
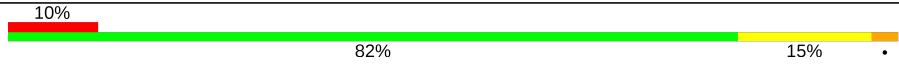


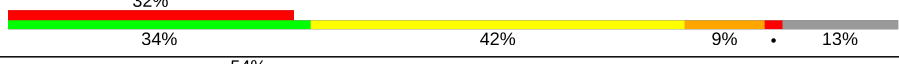
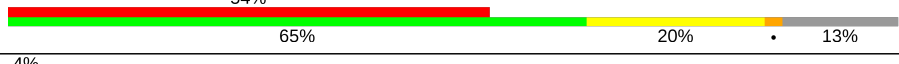
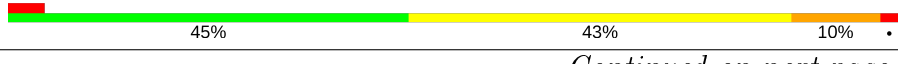

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1800	<div> <div>8%</div> <div> <div>39%</div> <div>43%</div> <div>16%</div> <div>..</div> </div> </div>
1	6	1800	<div> <div>7%</div> <div> <div>43%</div> <div>40%</div> <div>15%</div> <div>.</div> </div> </div>
2	S0	251	<div> <div>6%</div> <div> <div>27%</div> <div>43%</div> <div>12%</div> <div>18%</div> </div> </div>
2	s0	251	<div> <div>2%</div> <div> <div>66%</div> <div>16%</div> <div>18%</div> </div> </div>




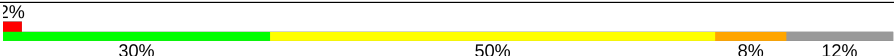
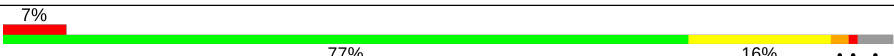
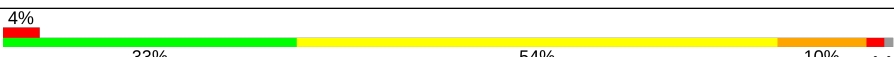
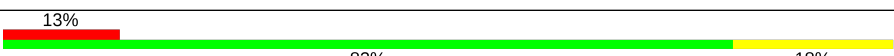
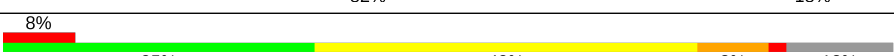
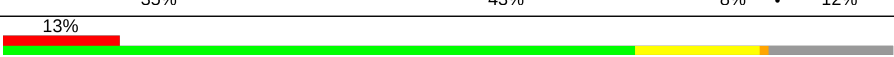
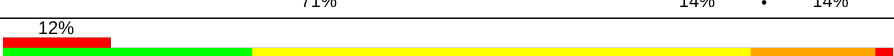
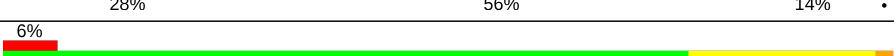
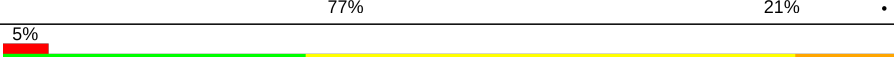

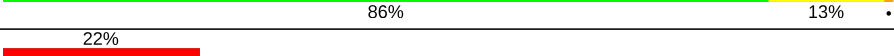
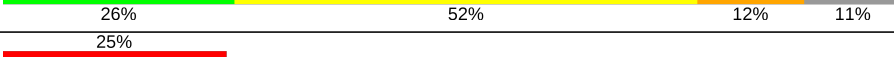

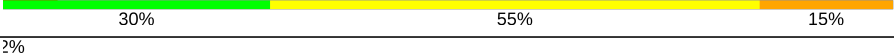


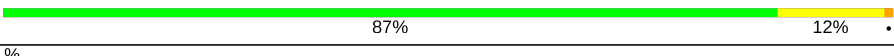
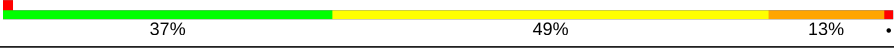
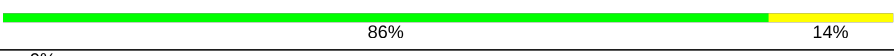



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Mol	Chain	Length	Quality of chain
3	S1	254	
3	s1	254	
4	S2	253	
4	s2	253	
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	96	
12	c0	96	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	

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Mol	Chain	Length	Quality of chain
15	c3	150	
16	C4	136	
16	c4	136	
17	C5	141	
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107	
27	d5	107	




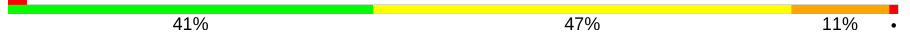



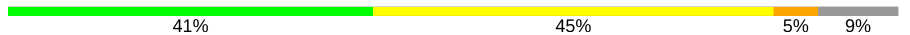

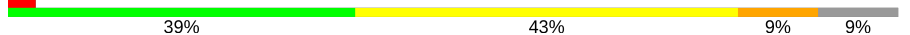

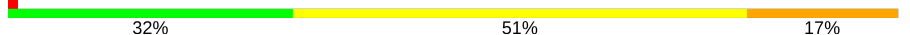













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Mol	Chain	Length	Quality of chain
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	62	
32	e0	62	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	182	
35	sM	182	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	

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Mol	Chain	Length	Quality of chain
40	l3	386	
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	



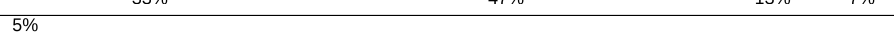

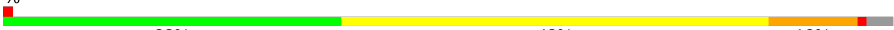
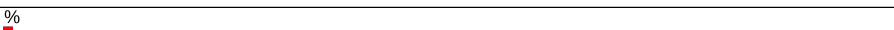
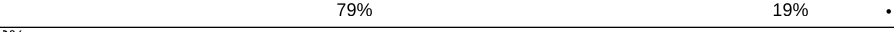
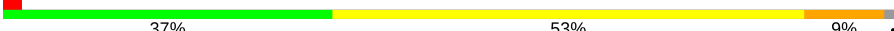

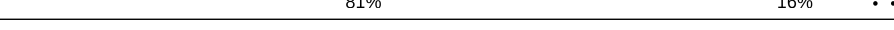











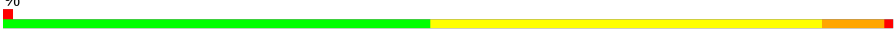



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Mol	Chain	Length	Quality of chain
53	M7	183	
53	m7	183	
54	M8	185	
54	m8	185	
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	

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Mol	Chain	Length	Quality of chain
65	n9	58	
66	O0	104	
66	o0	104	
67	O1	112	
67	o1	112	
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	120	
70	o4	120	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	

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Mol	Chain	Length	Quality of chain
78	Q2	105	
78	q2	105	
79	Q3	91	
79	q3	91	
80	m2	150	
81	p0	311	
82	p1	47	
83	p2	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	MG	1	3414	-	-	-	X
84	MG	1	3435	-	-	-	X
84	MG	1	3487	-	-	-	X
84	MG	1	3496	-	-	-	X
84	MG	1	3568	-	-	-	X
84	MG	1	3570	-	-	-	X
84	MG	1	3599	-	-	-	X
84	MG	1	3630	-	-	-	X
84	MG	1	3639	-	-	-	X
84	MG	1	3667	-	-	-	X
84	MG	1	3673	-	-	-	X
84	MG	1	3694	-	-	-	X
84	MG	1	3709	-	-	-	X
84	MG	1	3715	-	-	-	X
84	MG	1	4043	-	-	-	X
84	MG	2	1904	-	-	-	X
84	MG	2	1909	-	-	-	X
84	MG	2	1911	-	-	-	X
84	MG	2	1912	-	-	-	X
84	MG	2	1915	-	-	-	X
84	MG	2	1923	-	-	-	X
84	MG	2	1941	-	-	-	X
84	MG	2	1946	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	MG	2	1956	-	-	-	X
84	MG	2	1962	-	-	-	X
84	MG	2	1969	-	-	-	X
84	MG	2	1970	-	-	-	X
84	MG	2	1972	-	-	-	X
84	MG	2	1978	-	-	-	X
84	MG	4	202	-	-	-	X
84	MG	5	3457	-	-	-	X
84	MG	5	3476	-	-	-	X
84	MG	5	3542	-	-	-	X
84	MG	5	3617	-	-	-	X
84	MG	5	3632	-	-	-	X
84	MG	5	3636	-	-	-	X
84	MG	5	3641	-	-	-	X
84	MG	5	3643	-	-	-	X
84	MG	5	3655	-	-	-	X
84	MG	5	3709	-	-	-	X
84	MG	5	3731	-	-	-	X
84	MG	6	1917	-	-	-	X
84	MG	6	1930	-	-	-	X
84	MG	6	1938	-	-	-	X
84	MG	6	1961	-	-	-	X
84	MG	6	1965	-	-	-	X
84	MG	6	1969	-	-	-	X
84	MG	6	1971	-	-	-	X
84	MG	6	1984	-	-	-	X
84	MG	6	2001	-	-	-	X
84	MG	6	2002	-	-	-	X
84	MG	6	2008	-	-	-	X
84	MG	8	207	-	-	-	X
84	MG	O7	103	-	-	-	X
84	MG	SM	201	-	-	-	X
84	MG	l6	201	-	-	-	X
85	OHX	1	3818	-	-	X	-
85	OHX	1	3832	-	-	X	-
85	OHX	1	3836	-	-	X	-
85	OHX	1	3880	-	-	X	-
85	OHX	1	3904	-	-	X	-
85	OHX	1	3912	-	-	X	-
85	OHX	1	3916	-	-	X	-
85	OHX	1	3927	-	-	X	-
85	OHX	1	3940	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	OHX	1	3944	-	-	X	-
85	OHX	1	3975	-	-	X	-
85	OHX	1	4004	-	-	X	-
85	OHX	1	4008	-	-	X	-
85	OHX	1	4009	-	-	X	-
85	OHX	1	4017	-	-	X	-
85	OHX	2	2048	-	-	X	-
85	OHX	2	2054	-	-	X	-
85	OHX	2	2068	-	-	X	-
85	OHX	2	2079	-	-	X	-
85	OHX	5	3806	-	-	X	-
85	OHX	5	3822	-	-	X	-
85	OHX	5	3844	-	-	X	-
85	OHX	5	3846	-	-	X	-
85	OHX	5	3854	-	-	X	-
85	OHX	5	3877	-	-	X	-
85	OHX	5	3898	-	-	X	-
85	OHX	5	3923	-	-	X	-
85	OHX	5	3934	-	-	X	-
85	OHX	5	4007	-	-	X	-
85	OHX	5	4025	-	-	X	-
85	OHX	5	4027	-	-	X	-
85	OHX	5	4035	-	-	X	-
85	OHX	5	4036	-	-	X	-
85	OHX	5	4037	-	-	X	-
85	OHX	5	4038	-	-	X	-
85	OHX	5	4049	-	-	X	-
85	OHX	5	4054	-	-	X	-
85	OHX	6	2023	-	-	X	-
85	OHX	6	2109	-	-	X	-
85	OHX	6	2116	-	-	X	-
85	OHX	6	2121	-	-	X	-
85	OHX	6	2152	-	-	X	-
85	OHX	7	219	-	-	X	-
85	OHX	L4	401	-	-	X	-
87	ANM	1	3401	X	-	X	X

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 410912 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	1781	Total	C	N	O	P	0	1	0
			37970	16975	6720	12493	1782			
1	6	1795	Total	C	N	O	P	0	1	0
			38260	17105	6763	12596	1796			

- 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
			1612	1034	285	291	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	S7	184	Total	C	N	O	S	0	0	0
			1481	951	265	265				
9	s7	186	Total	C	N	O	S	0	0	0
			1492	957	267	268				

- 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,40S ribosomal protein S10-A,40S ribosomal protein S10-A,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			

- Molecule 13 is a protein called 40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A (uS17).

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
			1169	748	221	197	3			

- 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
			890	560	156	172	2			
14	c2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

- 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			

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	C7	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			
19	c7	117	Total	C	N	O	S	0	0	0
			944	591	179	172	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	d9	53	Total	C	N	O	S	0	0	0
			443	275	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			
32	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	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
			2437	1541	418	470	8			
34	sR	318	Total	C	N	O	S	0	0	0
			2445	1546	419	472	8			

- Molecule 35 is a protein called Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	5	3150	Total	C	N	O	P	0	0	0
			67377	30095	12145	21987	3150			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	l2	252	Total	C	N	O	S	0	0	0
			1918	1193	389	335	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
			3067	1942	583	533	9			
40	l3	386	Total	C	N	O	S	0	0	0
			3073	1948	583	533	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L3	255	CYS	TRP	engineered mutation	UNP P14126
l3	255	CYS	TRP	engineered mutation	UNP P14126

- 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
			2749	1730	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	18	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	19	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
			1733	1101	327	299	6			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	N4	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			
60	n4	135	Total	C	N	O	S	0	0	0
			1089	682	219	187	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	S	0	0	0
			993	625	192	176				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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
			890	565	168	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
			881	546	179	152	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
71	O5	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			
71	o5	119	Total	C	N	O	S	0	0	0
			969	615	186	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
			771	481	156	132	2			

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 60S ribosomal protein L12-A (uL11).

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

- 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
			1077	687	192	195	3			

- Molecule 82 is a protein called 60S ribosomal protein P1 alpha.

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

- Molecule 83 is a protein called 60S ribosomal protein P2 beta.

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

- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	L7	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	l6	1	Total 1	Mg 1	0	0
84	o1	1	Total 1	Mg 1	0	0
84	6	110	Total 110	Mg 110	0	0
84	sM	2	Total 2	Mg 2	0	0
84	O4	2	Total 2	Mg 2	0	0
84	m5	3	Total 3	Mg 3	0	0
84	l3	5	Total 5	Mg 5	0	0
84	d6	1	Total 1	Mg 1	0	0
84	2	82	Total 82	Mg 82	0	0
84	n0	2	Total 2	Mg 2	0	0
84	m6	1	Total 1	Mg 1	0	0
84	l7	1	Total 1	Mg 1	0	0
84	M5	1	Total 1	Mg 1	0	0
84	O3	1	Total 1	Mg 1	0	0
84	q0	1	Total 1	Mg 1	0	0
84	SM	1	Total 1	Mg 1	0	0
84	o4	1	Total 1	Mg 1	0	0
84	M0	1	Total 1	Mg 1	0	0
84	c1	1	Total 1	Mg 1	0	0
84	5	349	Total 349	Mg 349	0	0
84	O7	2	Total 2	Mg 2	0	0

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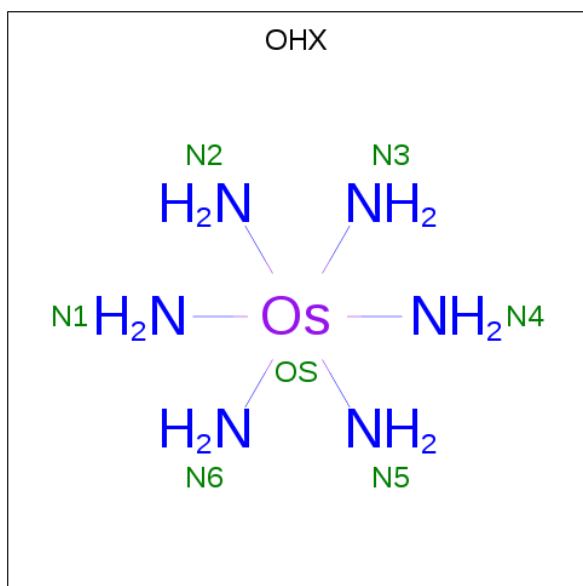
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	n9	1	Total 1	Mg 1	0	0
84	1	330	Total 330	Mg 330	0	0
84	l8	1	Total 1	Mg 1	0	0
84	Q2	1	Total 1	Mg 1	0	0
84	m1	1	Total 1	Mg 1	0	0
84	O2	1	Total 1	Mg 1	0	0
84	D9	1	Total 1	Mg 1	0	0
84	o3	1	Total 1	Mg 1	0	0
84	M3	1	Total 1	Mg 1	0	0
84	N3	1	Total 1	Mg 1	0	0
84	N8	2	Total 2	Mg 2	0	0
84	4	14	Total 14	Mg 14	0	0
84	S4	1	Total 1	Mg 1	0	0
84	L2	2	Total 2	Mg 2	0	0
84	n6	2	Total 2	Mg 2	0	0
84	M7	4	Total 4	Mg 4	0	0
84	L6	1	Total 1	Mg 1	0	0
84	l9	1	Total 1	Mg 1	0	0
84	s8	1	Total 1	Mg 1	0	0
84	m7	3	Total 3	Mg 3	0	0
84	n8	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	7	10	Total	Mg	0	0
			10	10		
84	n3	1	Total	Mg	0	0
			1	1		
84	q1	1	Total	Mg	0	0
			1	1		
84	L3	1	Total	Mg	0	0
			1	1		
84	l2	3	Total	Mg	0	0
			3	3		
84	8	10	Total	Mg	0	0
			10	10		
84	M6	1	Total	Mg	0	0
			1	1		
84	3	10	Total	Mg	0	0
			10	10		

- Molecule 85 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
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			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
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85	2	1	Total	N	Os	0	0
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85	2	1	Total	N	Os	0	0
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85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
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85	2	1	Total	N	Os	0	0
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85	2	1	Total	N	Os	0	0
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			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	S6	1	Total	N	Os	0	0
			7	6	1		
85	S8	1	Total	N	Os	0	0
			7	6	1		
85	C3	1	Total	N	Os	0	0
			7	6	1		
85	C5	1	Total	N	Os	0	0
			7	6	1		
85	C8	1	Total	N	Os	0	0
			7	6	1		
85	D9	1	Total	N	Os	0	0
			7	6	1		
85	SR	1	Total	N	Os	0	0
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			7	6	1		
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			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
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85	1	1	Total	N	Os	0	0
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85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
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85	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	1	1	Total	N	Os	0	0
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85	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	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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85	1	1	Total	N	Os	0	0
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85	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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85	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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85	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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85	3	1	Total	N	Os	0	0
			7	6	1		
85	3	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	4	1	Total	N	Os	0	0
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85	L3	1	Total	N	Os	0	0
			7	6	1		
85	L3	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	M0	1	Total	N	Os	0	0
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85	M5	1	Total	N	Os	0	0
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85	M6	1	Total	N	Os	0	0
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85	M7	1	Total	N	Os	0	0
			7	6	1		
85	M9	1	Total	N	Os	0	0
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85	N1	1	Total	N	Os	0	0
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85	N8	1	Total	N	Os	0	0
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85	N9	1	Total	N	Os	0	0
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85	O7	1	Total	N	Os	0	0
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85	O7	1	Total	N	Os	0	0
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85	O9	1	Total	N	Os	0	0
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85	Q2	1	Total	N	Os	0	0
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85	6	1	Total	N	Os	0	0
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85	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	6	1	Total	N	Os	0	0
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85	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	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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85	6	1	Total 7	N 6	Os 1	0	0
85	6	1	Total 7	N 6	Os 1	0	0
85	6	1	Total 7	N 6	Os 1	0	0
85	6	1	Total 7	N 6	Os 1	0	0
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85	6	1	Total 7	N 6	Os 1	0	0
85	6	1	Total 7	N 6	Os 1	0	0
85	6	1	Total 7	N 6	Os 1	0	0
85	6	1	Total 7	N 6	Os 1	0	0
85	6	1	Total 7	N 6	Os 1	0	0
85	6	1	Total 7	N 6	Os 1	0	0
85	6	1	Total 7	N 6	Os 1	0	0
85	6	1	Total 7	N 6	Os 1	0	0
85	6	1	Total 7	N 6	Os 1	0	0
85	6	1	Total 7	N 6	Os 1	0	0
85	6	1	Total 7	N 6	Os 1	0	0
85	s4	1	Total 7	N 6	Os 1	0	0
85	s8	1	Total 7	N 6	Os 1	0	0
85	s9	1	Total 7	N 6	Os 1	0	0
85	c3	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	c8	1	Total	N	Os	0	0
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85	d4	1	Total	N	Os	0	0
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85	sR	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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85	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
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85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
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85	7	1	Total	N	Os	0	0
			7	6	1		
85	7	1	Total	N	Os	0	0
			7	6	1		
85	7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	7	1	Total	N	Os	0	0
			7	6	1		
85	7	1	Total	N	Os	0	0
			7	6	1		
85	7	1	Total	N	Os	0	0
			7	6	1		
85	7	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
85	7	1	Total	N	Os	0	0
			7	6	1		
85	7	1	Total	N	Os	0	0
			7	6	1		
85	8	1	Total	N	Os	0	0
			7	6	1		
85	8	1	Total	N	Os	0	0
			7	6	1		
85	8	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
85	8	1	Total	N	Os	0	0
			7	6	1		
85	8	1	Total	N	Os	0	0
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85	8	1	Total	N	Os	0	0
			7	6	1		
85	8	1	Total	N	Os	0	0
			7	6	1		
85	8	1	Total	N	Os	0	0
			7	6	1		
85	8	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	8	1	Total	N	Os	0	0
			7	6	1		
85	8	1	Total	N	Os	0	0
			7	6	1		
85	l3	1	Total	N	Os	0	0
			7	6	1		
85	l3	1	Total	N	Os	0	0
			7	6	1		
85	l3	1	Total	N	Os	0	0
			7	6	1		
85	l4	1	Total	N	Os	0	0
			7	6	1		
85	l4	1	Total	N	Os	0	0
			7	6	1		
85	l5	1	Total	N	Os	0	0
			7	6	1		
85	l5	1	Total	N	Os	0	0
			7	6	1		
85	l9	1	Total	N	Os	0	0
			7	6	1		
85	m0	1	Total	N	Os	0	0
			7	6	1		
85	m0	1	Total	N	Os	0	0
			7	6	1		
85	m1	1	Total	N	Os	0	0
			7	6	1		
85	m5	1	Total	N	Os	0	0
			7	6	1		
85	m5	1	Total	N	Os	0	0
			7	6	1		
85	m7	1	Total	N	Os	0	0
			7	6	1		
85	n3	1	Total	N	Os	0	0
			7	6	1		
85	n3	1	Total	N	Os	0	0
			7	6	1		
85	n9	1	Total	N	Os	0	0
			7	6	1		
85	o3	1	Total	N	Os	0	0
			7	6	1		
85	o7	1	Total	N	Os	0	0
			7	6	1		

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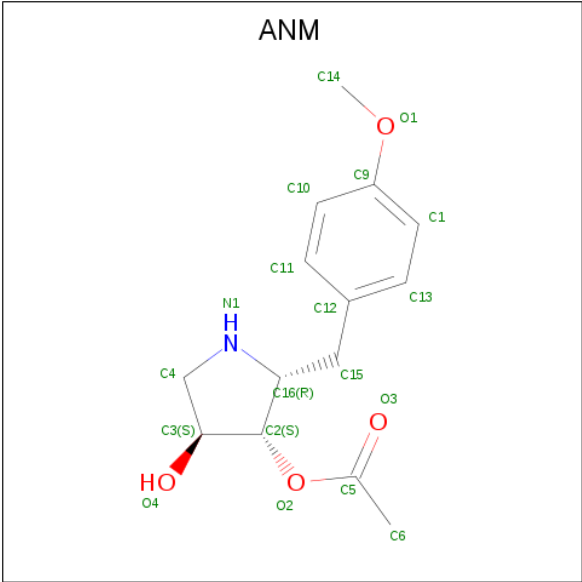
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	o9	1	Total	N	Os	0	0
			7	6	1		
85	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 87 is ANISOMYCIN (three-letter code: ANM) (formula: C₁₄H₁₉NO₄).

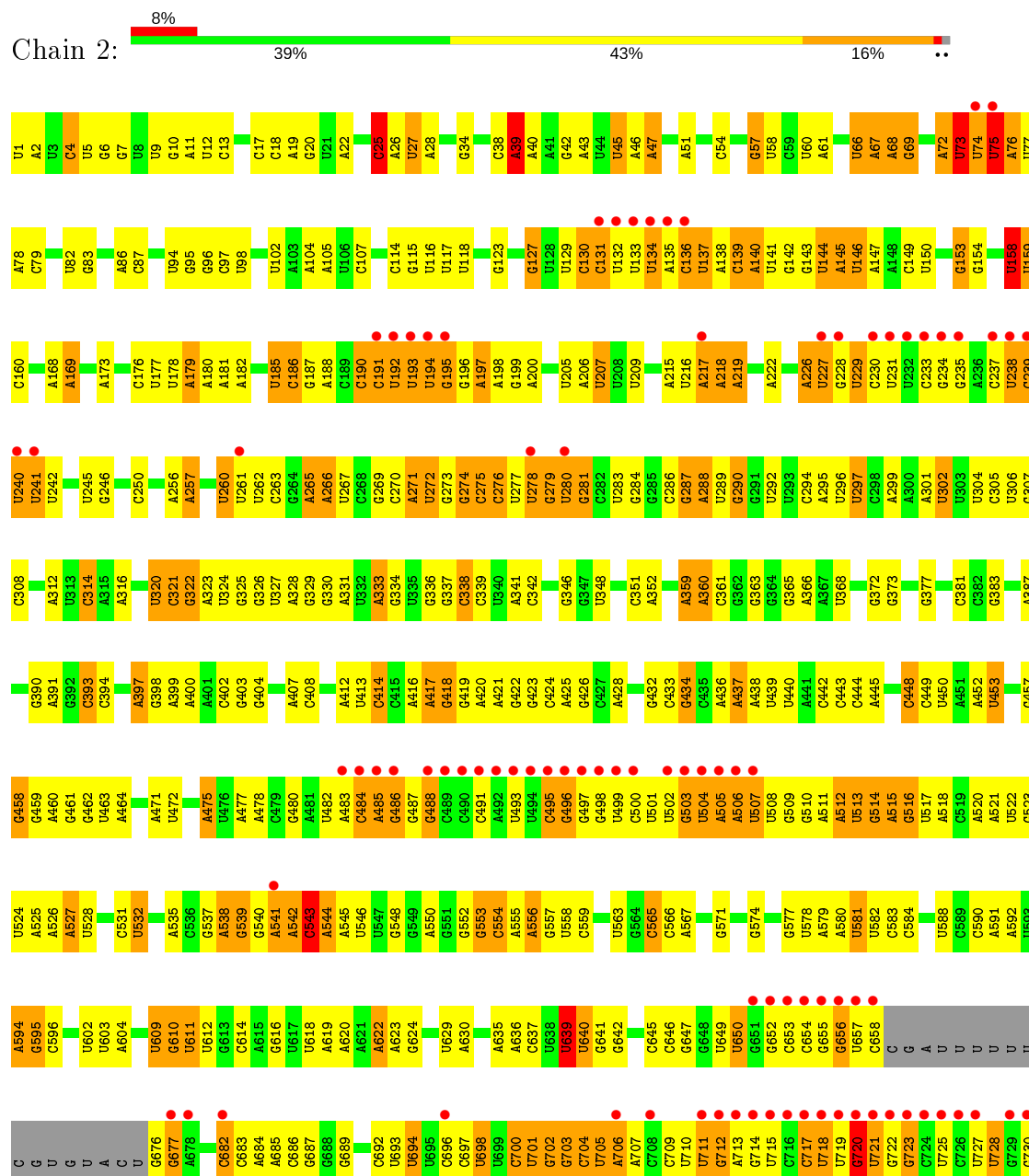


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
87	1	1	Total	C	N	O	0	0
			19	14	1	4		

3 Residue-property plots

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

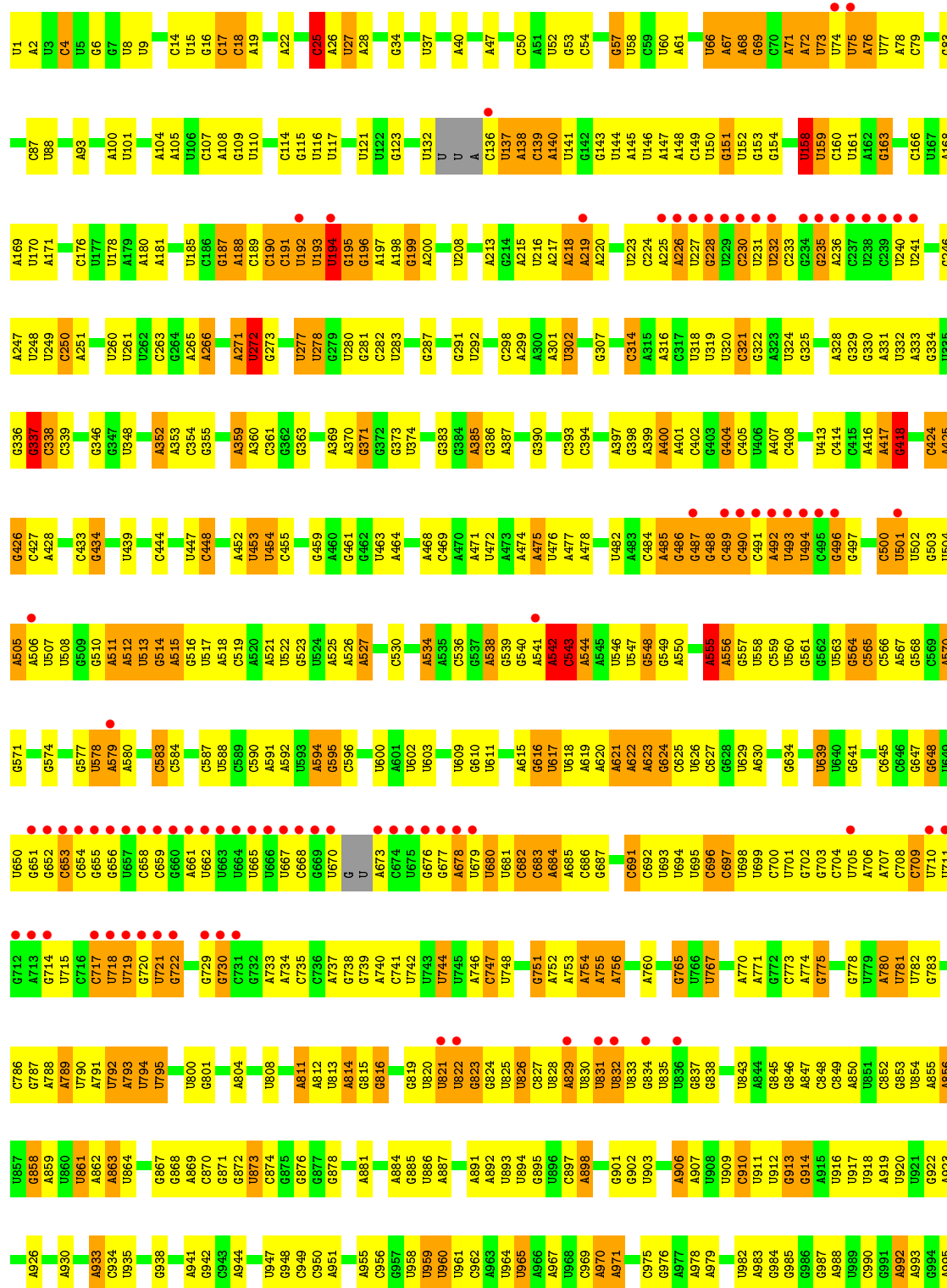
- Molecule 1: 18S ribosomal RNA

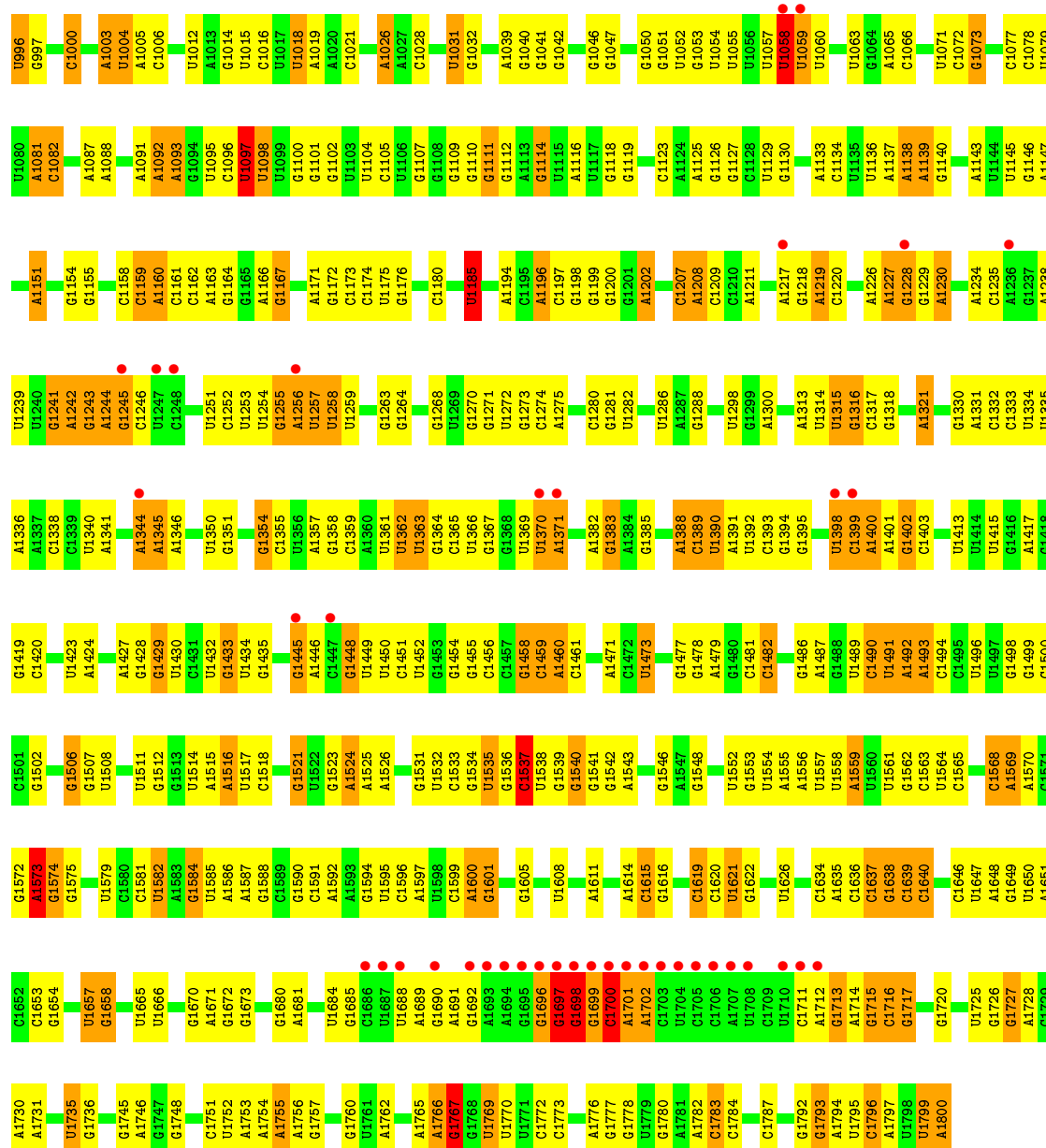


A1712	A1713	A1714	A1715	A1716	A1727	A1730	A1731	A1732	A1735	U1738	U1739	G1745	G1748	U1752	A1756	G1759	G1760	A1761	A1762	A1765	A1766	A1767	G1768	U1769	U1770	G1773	U1776	G1777	A1780	A1781	A1782	G1783	G1784	U1785	G1788	G1792	G1793	A1794	U1795	G1796	A1797	U1798	U	A																																																																																																																																																																																																																																																																																																																																					
U1627	U1628	G1629	G1714	A1631	A1635	G1642	G1645	A1731	A1732	U1735	U1738	U1739	G1654	U1657	G1658	U1665	U1667	A1646	G1649	G1654	U1657	G1658	U1665	G1672	G1673	A1678	G1679	A1680	A1681	G1682	G1683	U1684	G1685	U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1702	U1703	U1704	U1705	U1706	U1707	U1708	U1709	U1710	U1711																																																																																																																																																																																																																																																																																																																						
U1564	C1565	U1566	U1567	C1568	A1569	A1570	C1571	G1572	A1573	G1574	G1575	U1578	U1579	C1580	U1581	U1582	A1583	G1584	U1585	A1586	A1587	G1588	G1589	G1590	C1591	A1592	A1593	G1594	U1595	C1596	G1597	A1600	C1601	C1602	U1603	U1604	G1605	G1606	G1607	U1608	U1609	G1610	U1611	U1612	U1613	A1614	C1615	G1616	C1619	G1620	U1621	U1622	U1623	C1624	U1625	U1626																																																																																																																																																																																																																																																																																																																									
C1494	C1495	U1496	U1497	U1498	G1499	C1500	G1504	A1505	U1508	G1512	U1513	U1514	C1515	A1516	U1517	C1518	U1519	U1520	A1521	U1522	G1523	A1524	A1525	A1526	C1527	U1528	G1529	C1530	U1531	U1532	U1533	U1534	U1535	U1536	C1537	A1538	U1539	G1540	G1541	G1542	G1546	A1555	A1556	U1557	U1558	A1559	U1560	U1561	A1562	C1563																																																																																																																																																																																																																																																																																																																															
A1417	A1424	U1425	U1426	G1427	G1428	G1429	U1430	G1431	U1432	U1433	U1434	G1435	G1438	C1439	C1440	A1446	C1447	G1448	U1449	C1450	C1451	U1452	G1455	C1456	C1457	U1458	C1459	A1460	C1461	C1467	U1468	A1469	C1470	A1471	U1472	G1473	G1474	A1475	C1476	G1480	C1481	C1482	A1483	G1484	C1485	A1486	U1487	G1488	U1489	C1490	U1491	A1492	A1493																																																																																																																																																																																																																																																																																																																												
A1345	A1346	U1347	A1348	G1349	U1350	G1351	C1352	U1353	G1354	C1355	U1356	A1357	G1358	C1359	A1360	U1361	U1362	U1363	G1364	C1365	U1366	G1367	U1370	A1371	U1372	A1375	C1376	U1380	U1381	G1385	U1386	G1387	A1388	C1389	U1390	A1391	U1392	U1393	G1394	U1397	U1398	C1399	A1400	A1401	G1402	C1403	G1409	A1410	U1411	U1412	U1413	U1414	U1415	G1416																																																																																																																																																																																																																																																																																																																											
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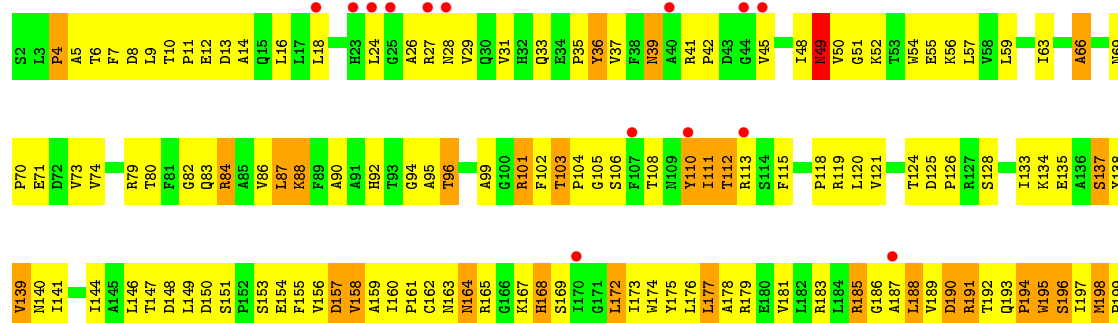
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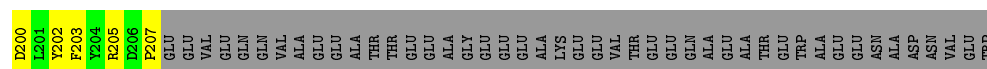
Chain 6: 



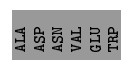
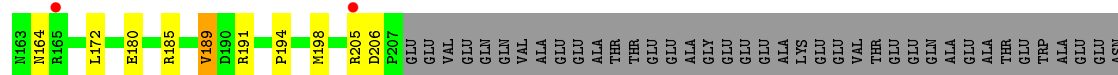


• Molecule 2: 40S ribosomal protein S0-A

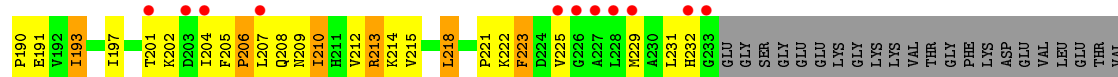
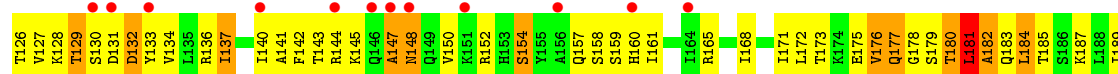
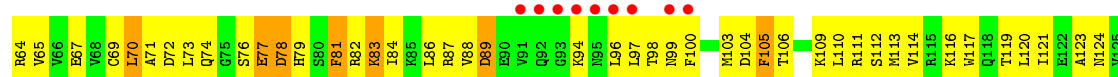
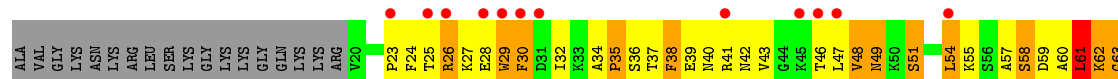




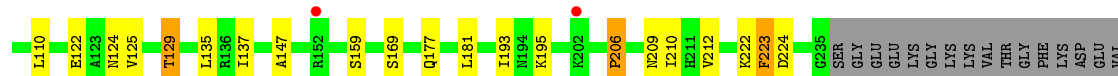
• Molecule 2: 40S ribosomal protein S0-A



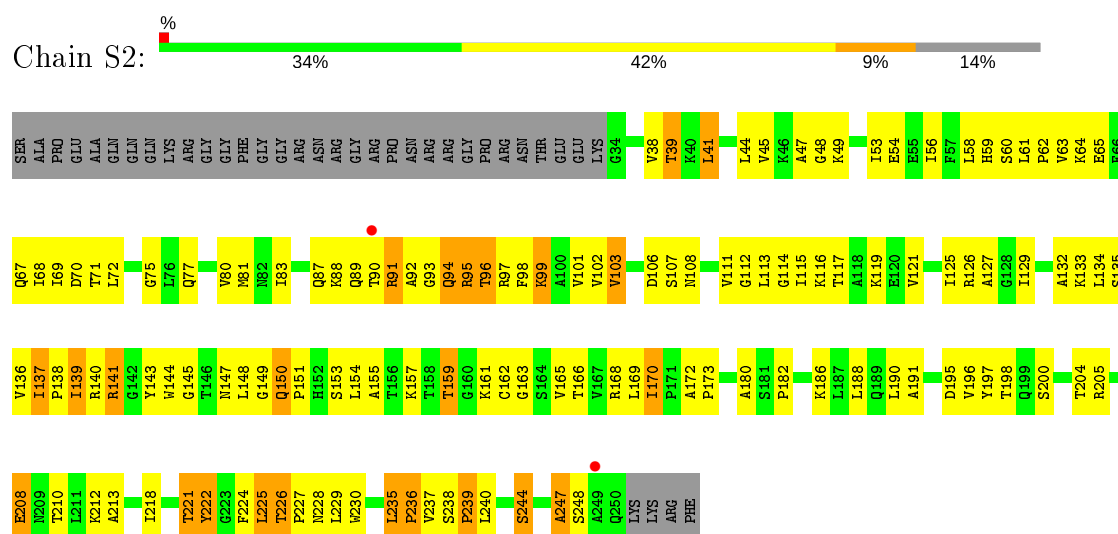
• Molecule 3: 40S ribosomal protein S1-A



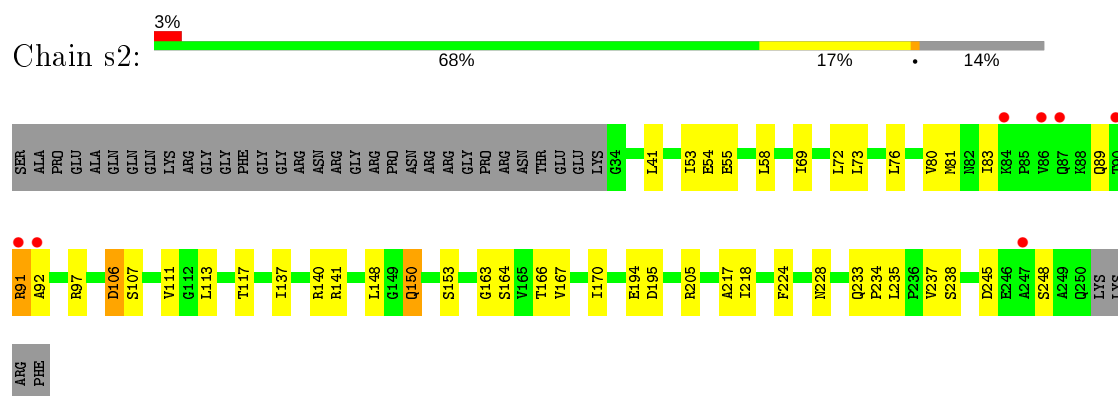
• Molecule 3: 40S ribosomal protein S1-A



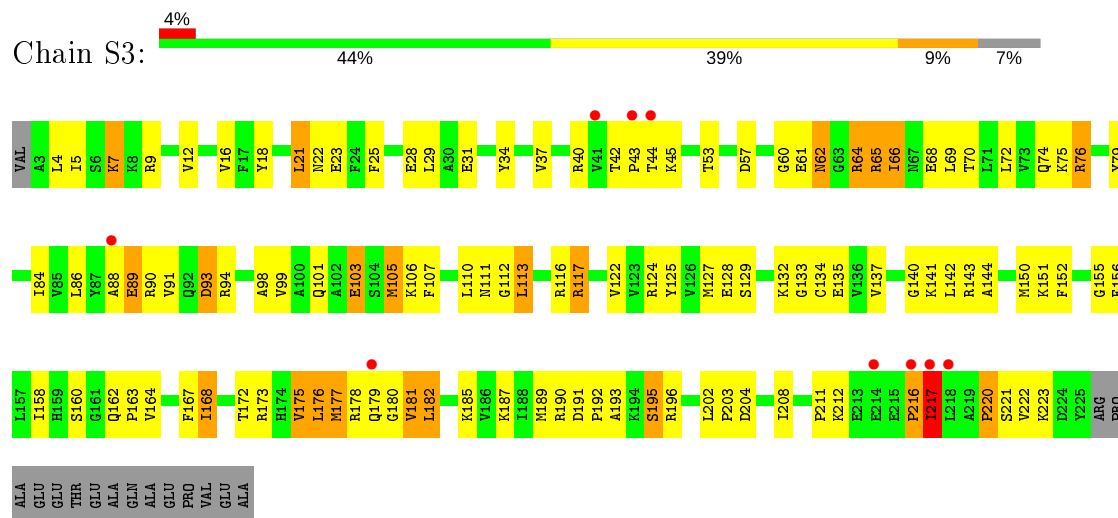
• Molecule 4: 40S ribosomal protein S2



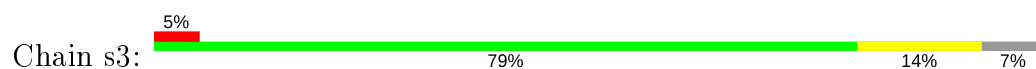
- Molecule 4: 40S ribosomal protein S2

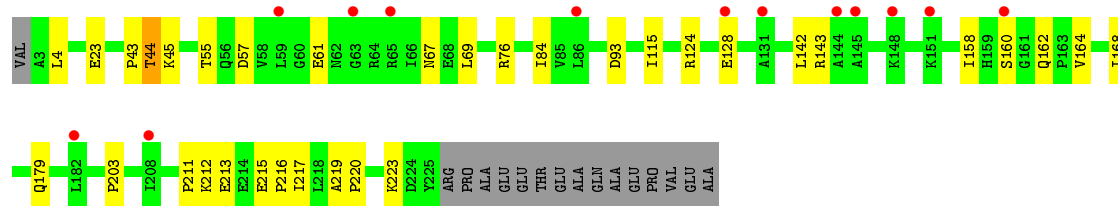


- Molecule 5: 40S ribosomal protein S3

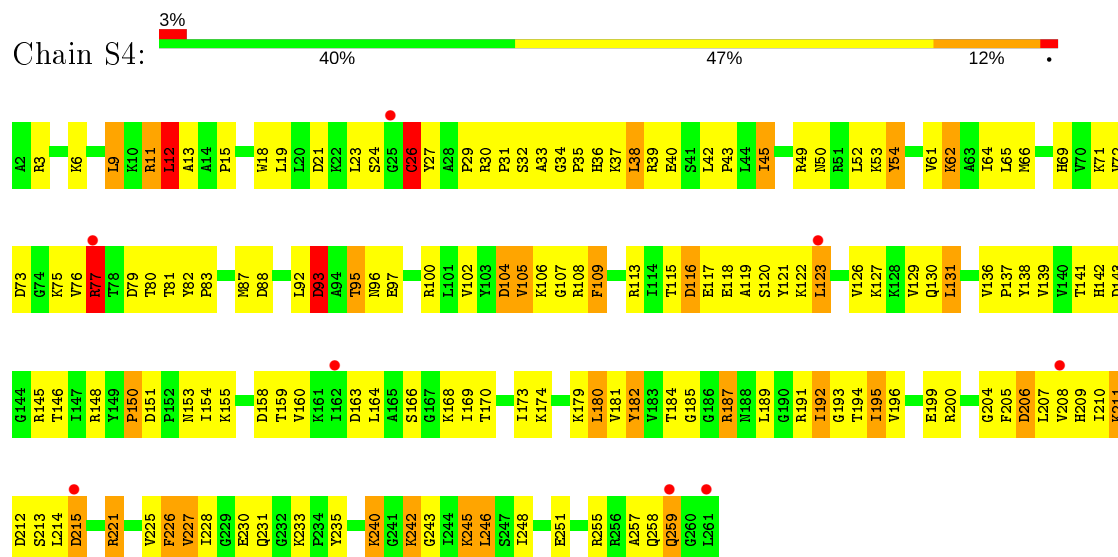


- Molecule 5: 40S ribosomal protein S3

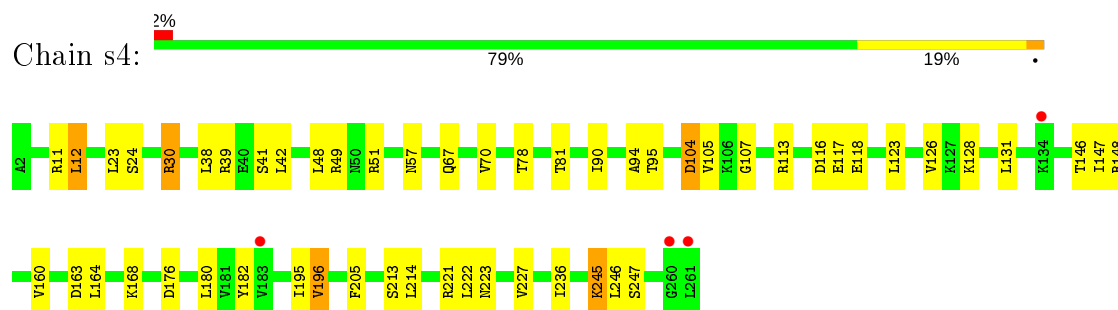




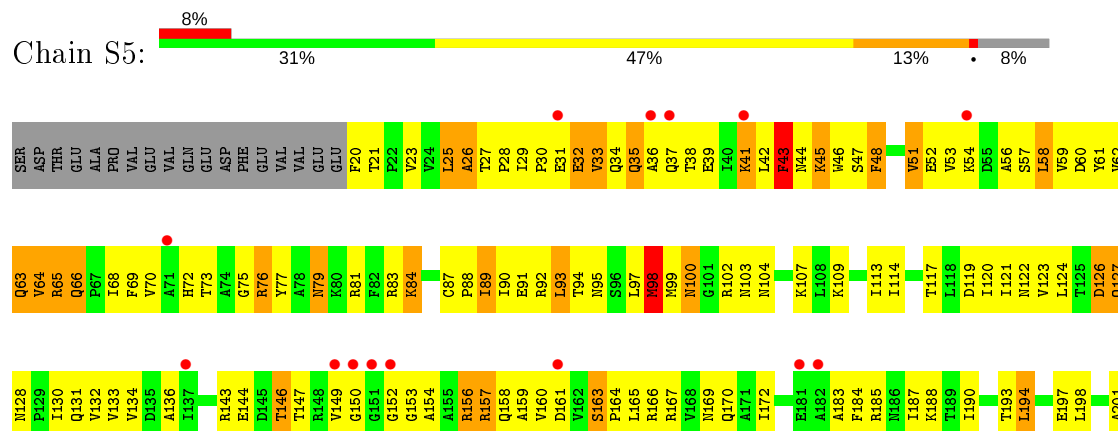
• Molecule 6: 40S ribosomal protein S4-A

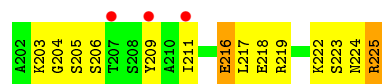


• Molecule 6: 40S ribosomal protein S4-A

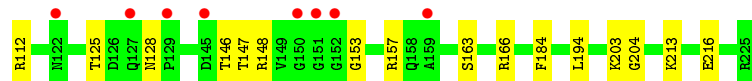
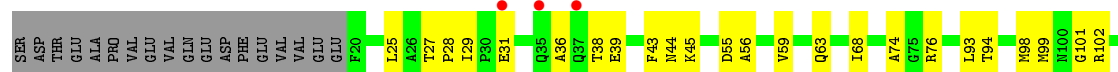
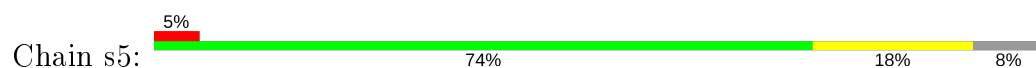


• Molecule 7: 40S ribosomal protein S5

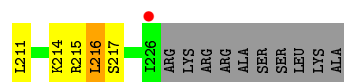
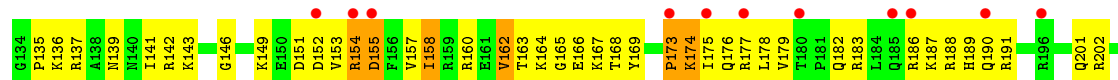
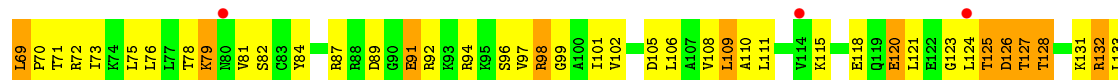




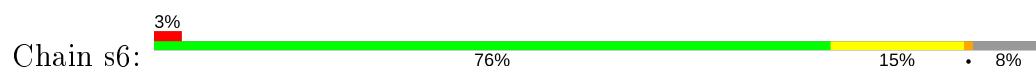
- Molecule 7: 40S ribosomal protein S5



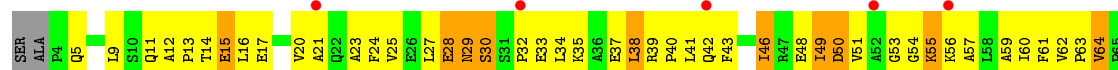
- Molecule 8: 40S ribosomal protein S6-A

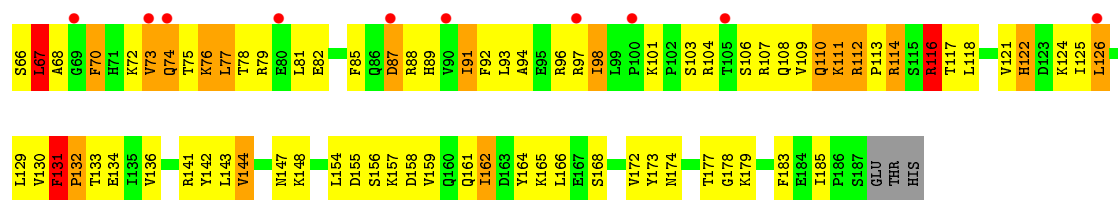


- Molecule 8: 40S ribosomal protein S6-A

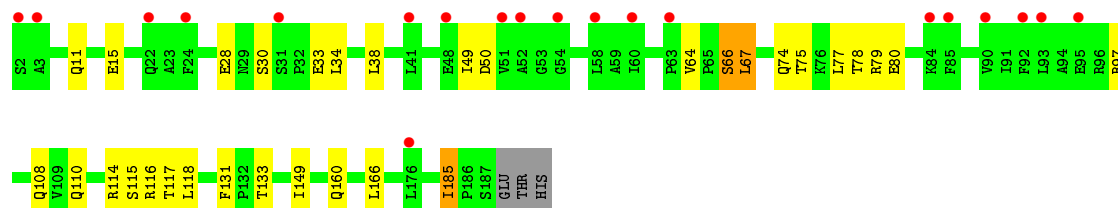
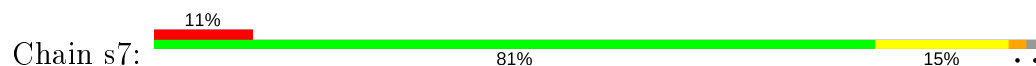


- Molecule 9: 40S ribosomal protein S7-A

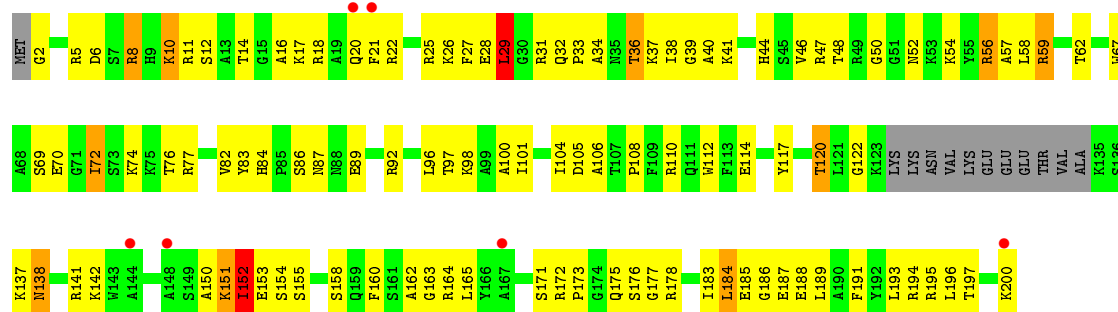
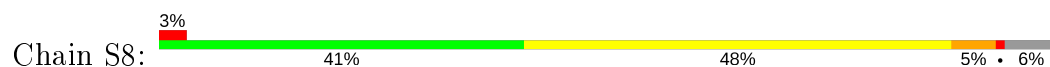




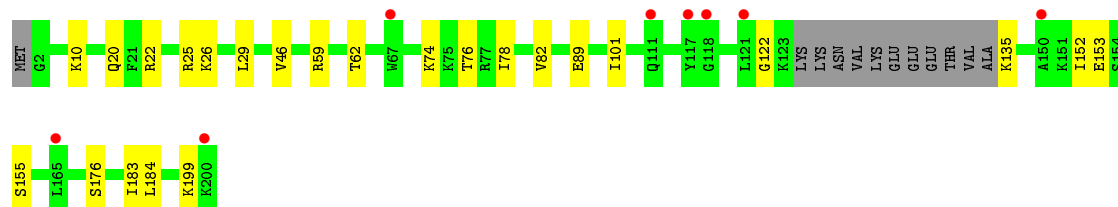
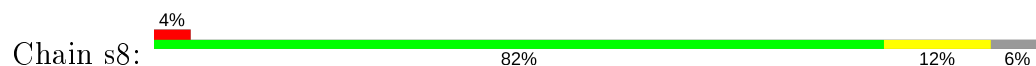
• Molecule 9: 40S ribosomal protein S7-A



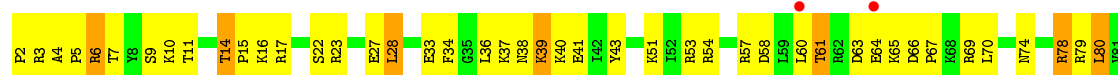
• Molecule 10: 40S ribosomal protein S8-A

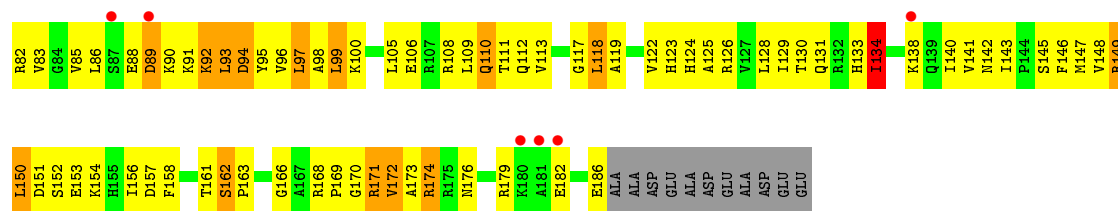


• Molecule 10: 40S ribosomal protein S8-A

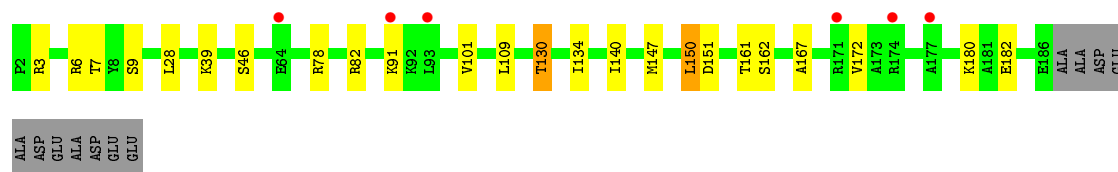
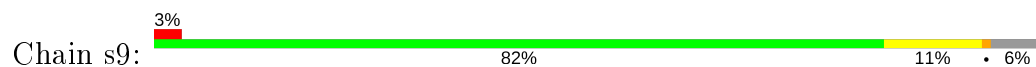


• Molecule 11: 40S ribosomal protein S9-A

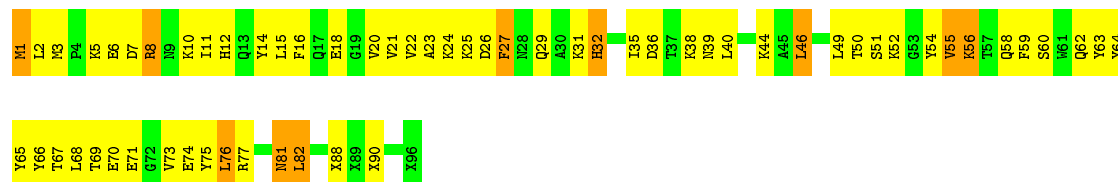




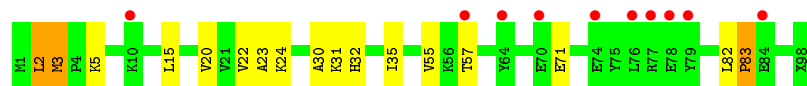
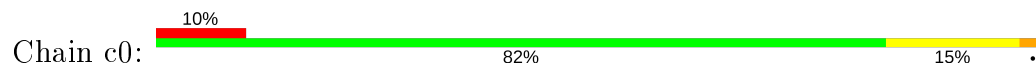
• Molecule 11: 40S ribosomal protein S9-A



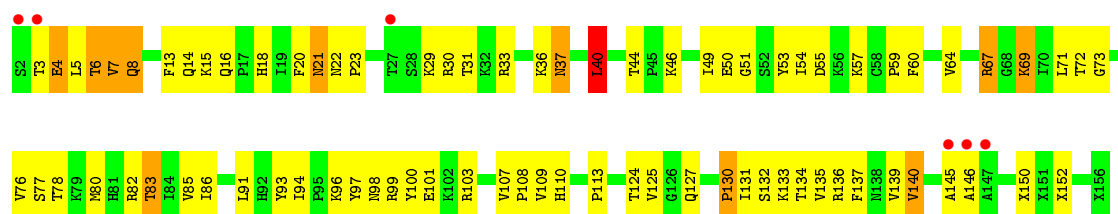
• Molecule 12: 40S ribosomal protein S10-A,40S ribosomal protein S10-A,40S ribosomal protein S10-A,40S ribosomal protein S10-A



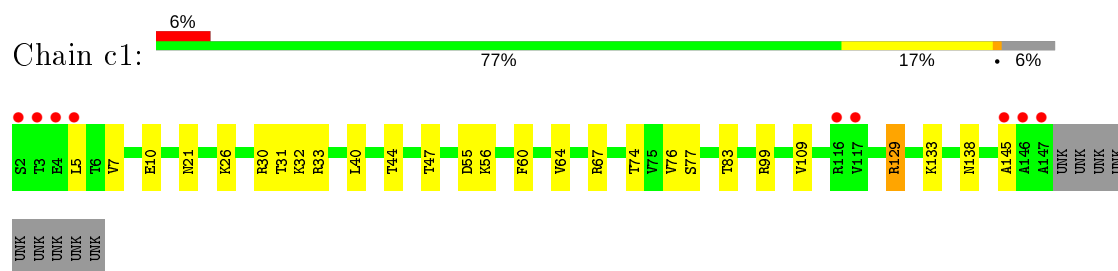
• Molecule 12: 40S ribosomal protein S10-A,40S ribosomal protein S10-A,40S ribosomal protein S10-A,40S ribosomal protein S10-A



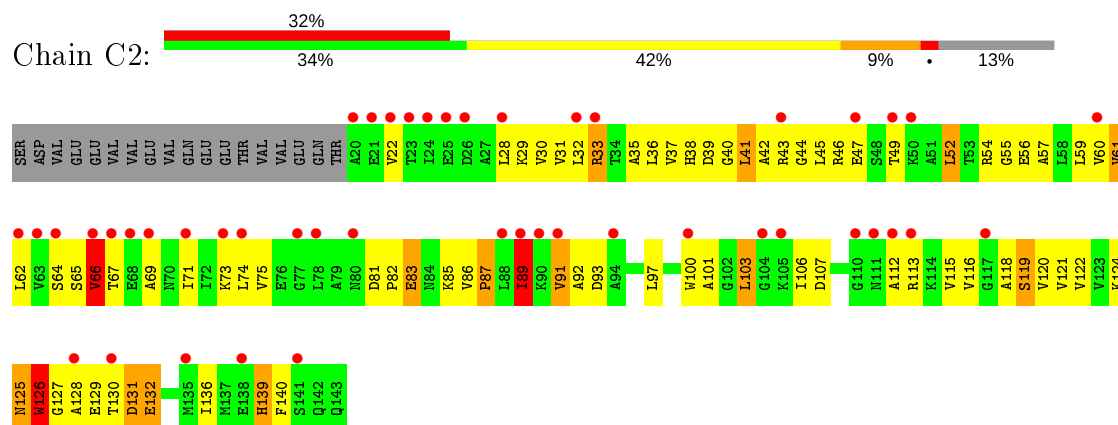
• Molecule 13: 40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A (uS17)



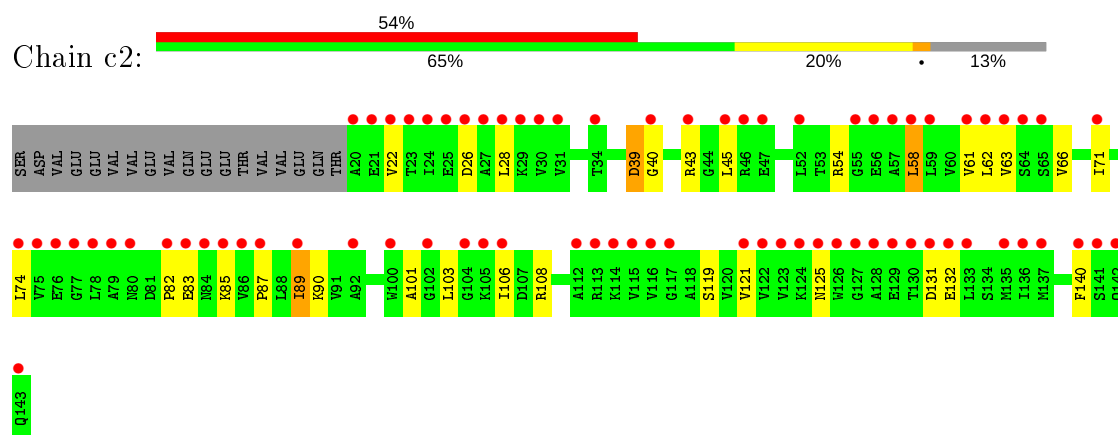
- Molecule 13: 40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A (uS17)



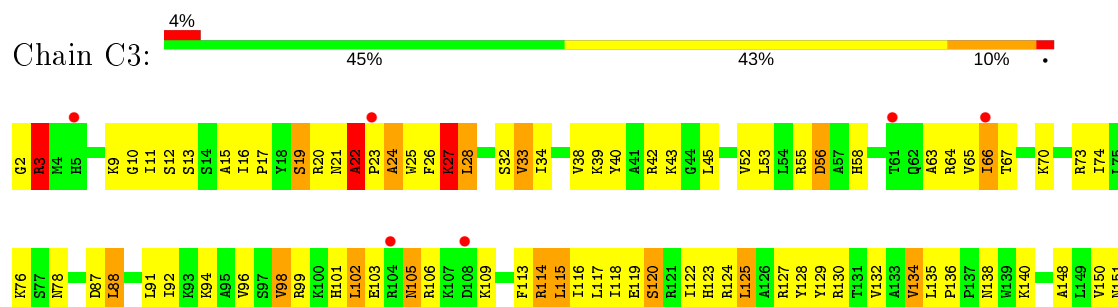
- Molecule 14: 40S ribosomal protein S12




- Molecule 14: 40S ribosomal protein S12



- Molecule 15: 40S ribosomal protein S13



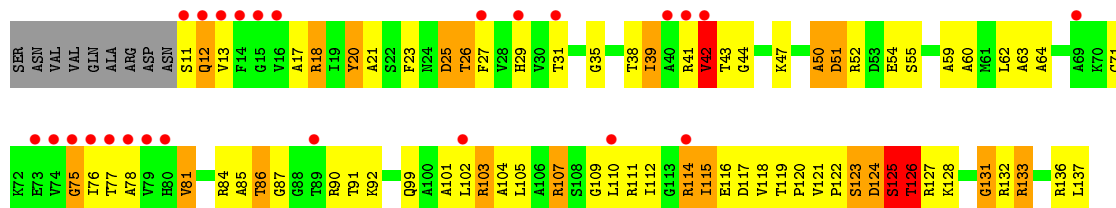
- Molecule 15: 40S ribosomal protein S13

Chain c3: 




- Molecule 16: 40S ribosomal protein S14-A

Chain C4: 



- Molecule 16: 40S ribosomal protein S14-A

Chain c4: 




- Molecule 17: 40S ribosomal protein S15

Chain C5: 



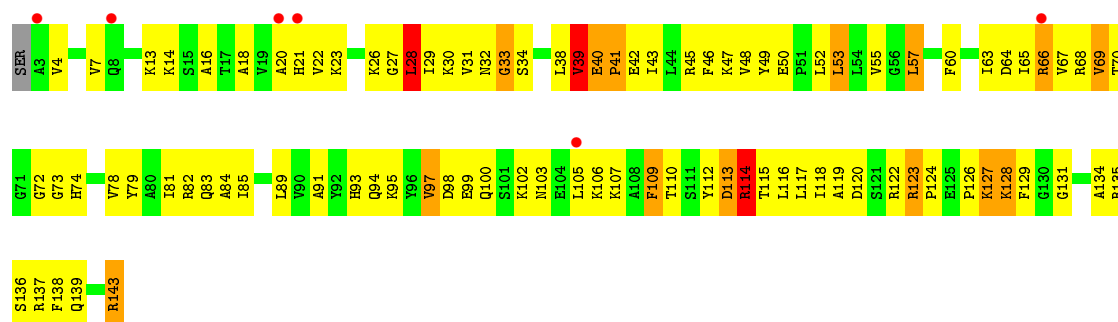
- Molecule 17: 40S ribosomal protein S15

Chain c5: 

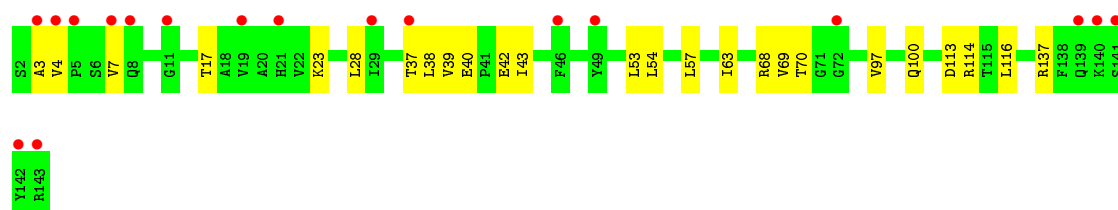
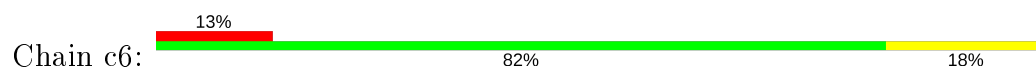


- Molecule 18: 40S ribosomal protein S16-A

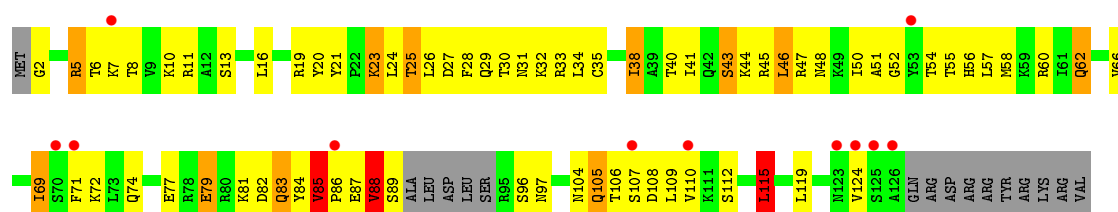
Chain C6: 



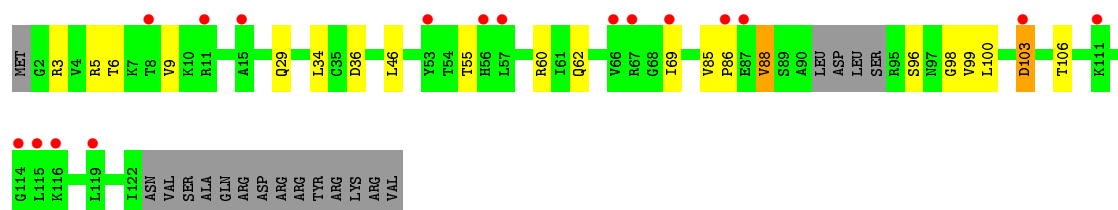
• Molecule 18: 40S ribosomal protein S16-A



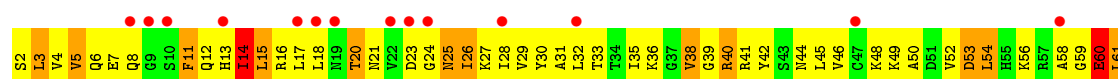
• Molecule 19: 40S ribosomal protein S17-A

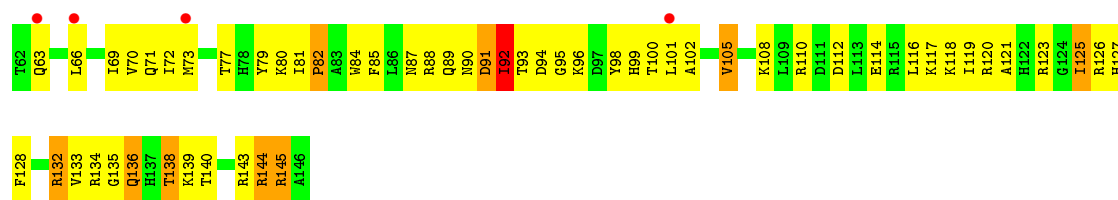


• Molecule 19: 40S ribosomal protein S17-A

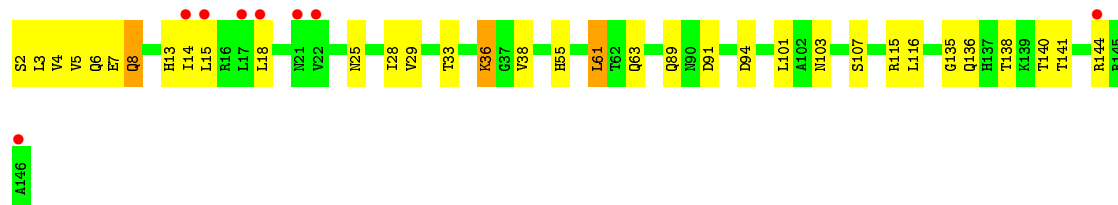
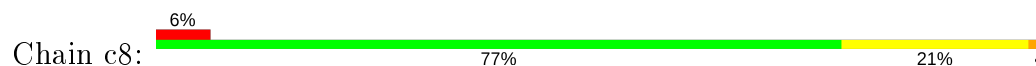


• Molecule 20: 40S ribosomal protein S18-A

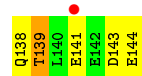
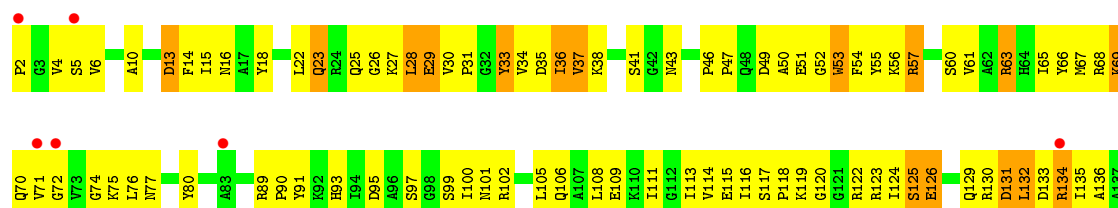




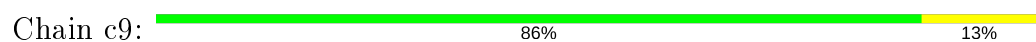
- Molecule 20: 40S ribosomal protein S18-A



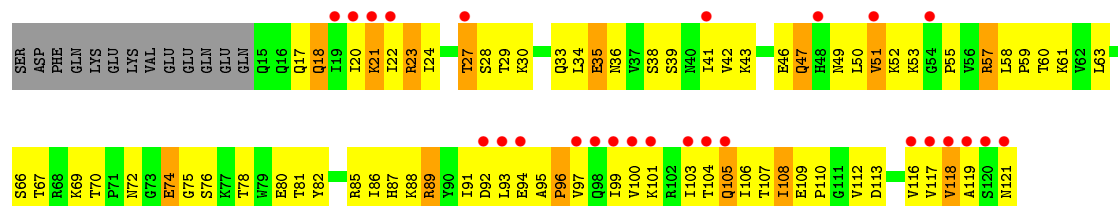
- Molecule 21: 40S ribosomal protein S19-A



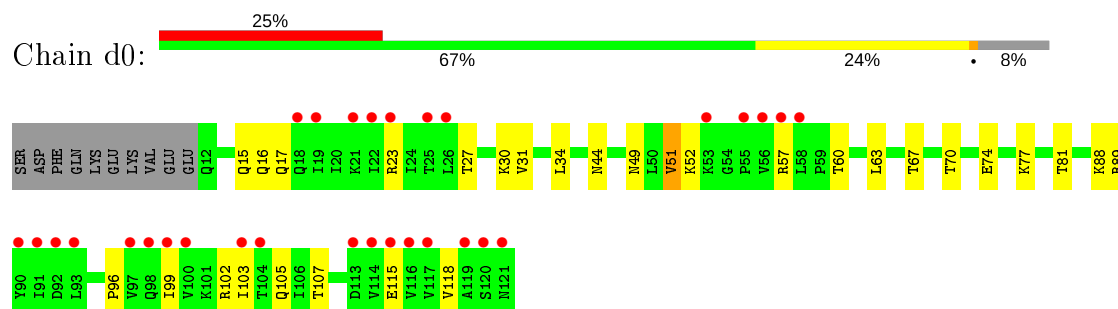
- Molecule 21: 40S ribosomal protein S19-A



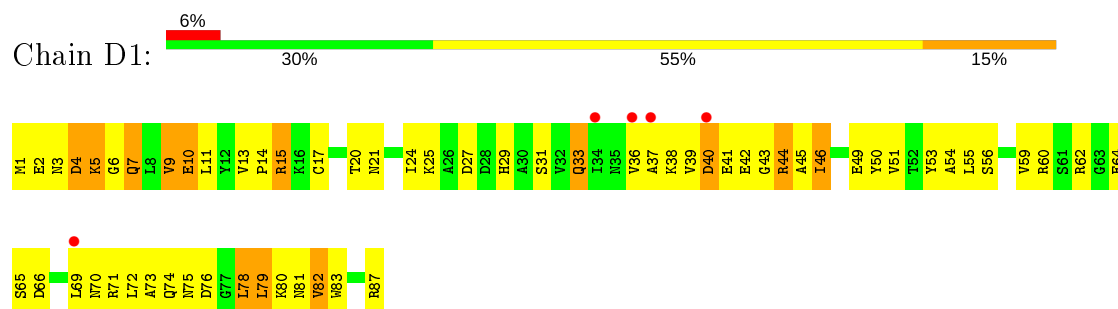
- Molecule 22: 40S ribosomal protein S20



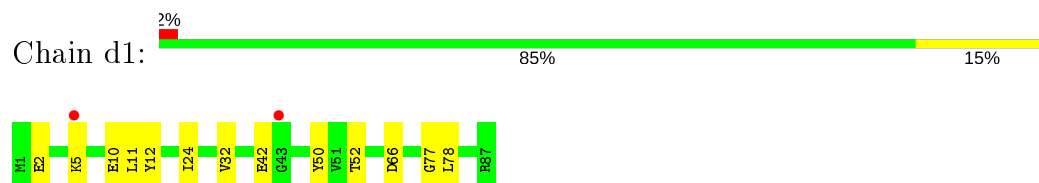
- Molecule 22: 40S ribosomal protein S20



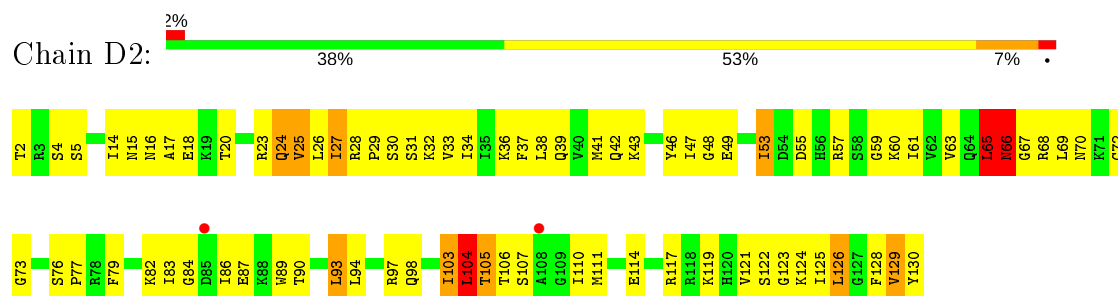
- Molecule 23: 40S ribosomal protein S21-A



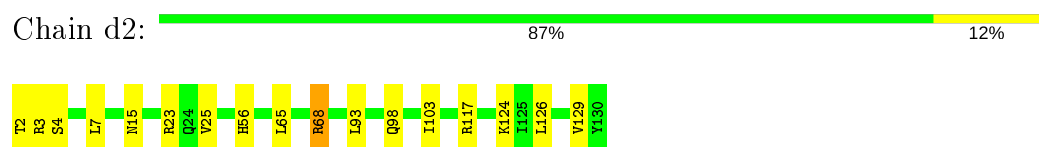
- Molecule 23: 40S ribosomal protein S21-A



- Molecule 24: 40S ribosomal protein S22-A

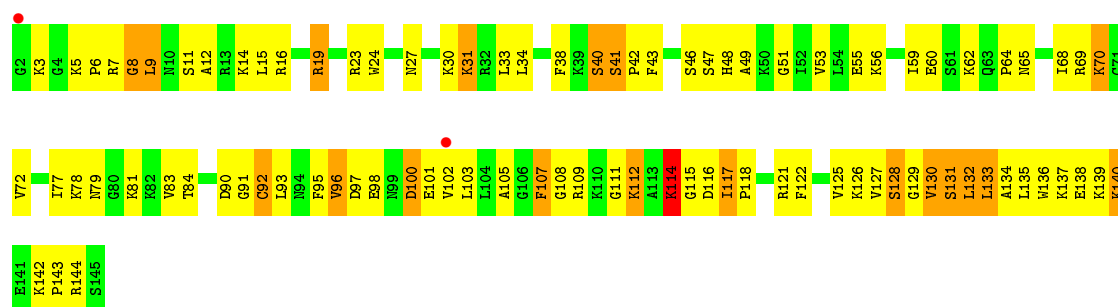


- Molecule 24: 40S ribosomal protein S22-A

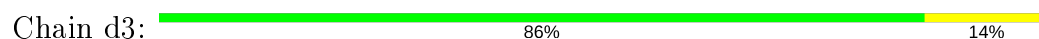


- Molecule 25: 40S ribosomal protein S23-A

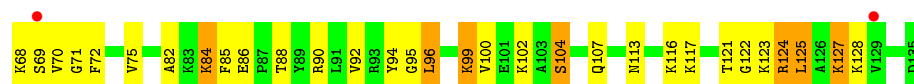
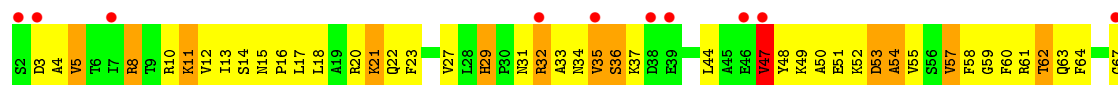
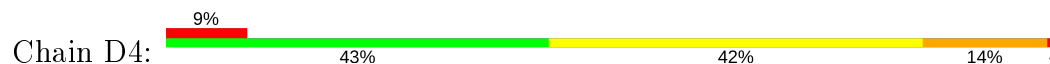




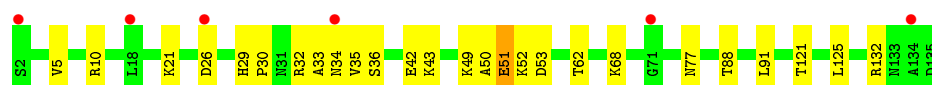
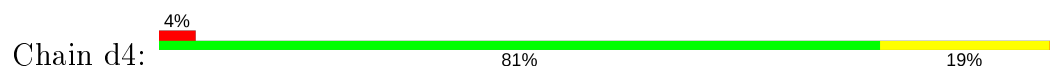
- Molecule 25: 40S ribosomal protein S23-A



- Molecule 26: 40S ribosomal protein S24-A



- Molecule 26: 40S ribosomal protein S24-A

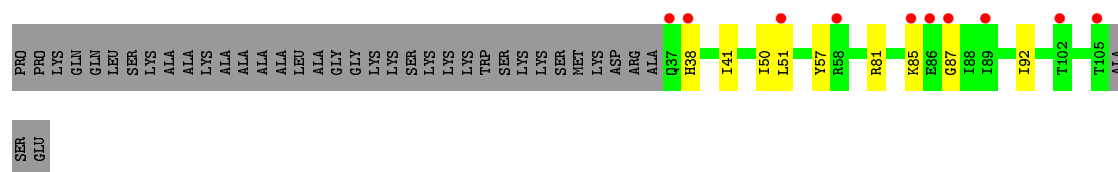


- Molecule 27: 40S ribosomal protein S25-A

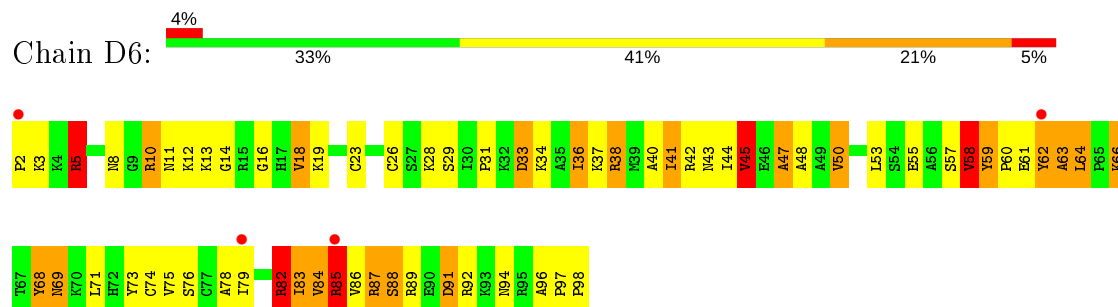


- Molecule 27: 40S ribosomal protein S25-A

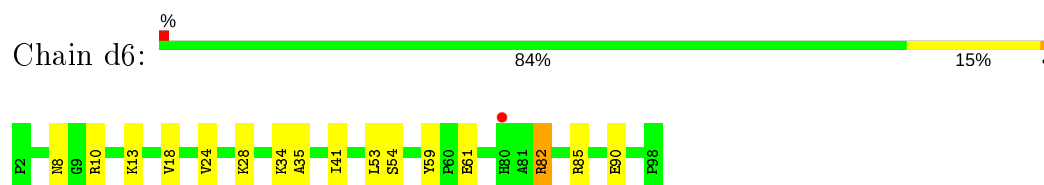




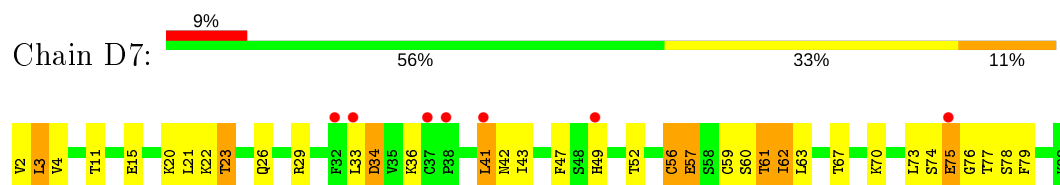
- Molecule 28: 40S ribosomal protein S26-B



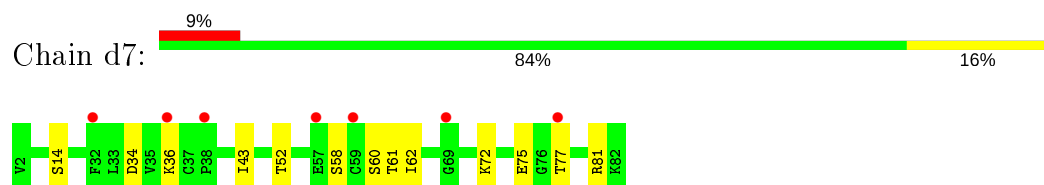
- Molecule 28: 40S ribosomal protein S26-B



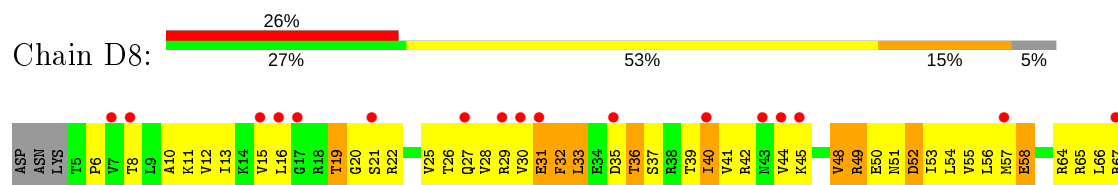
- Molecule 29: 40S ribosomal protein S27-A



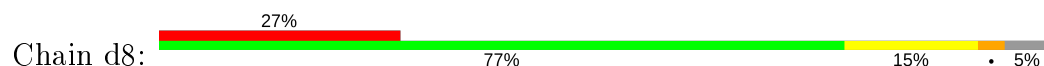
- Molecule 29: 40S ribosomal protein S27-A



- Molecule 30: 40S ribosomal protein S28-A



- Molecule 30: 40S ribosomal protein S28-A

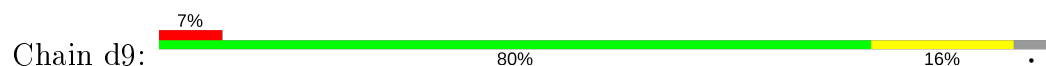




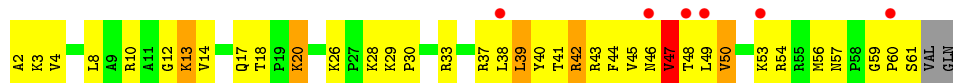
- Molecule 31: 40S ribosomal protein S29-A



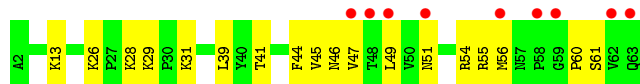
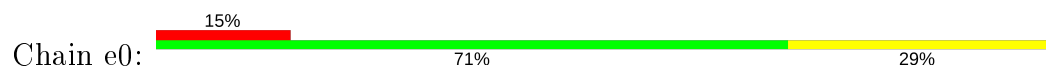
- Molecule 31: 40S ribosomal protein S29-A



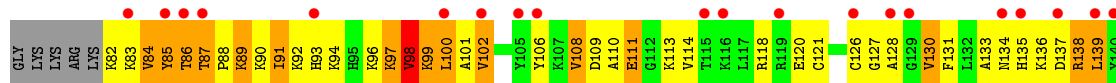
- Molecule 32: 40S ribosomal protein S30-A



- Molecule 32: 40S ribosomal protein S30-A



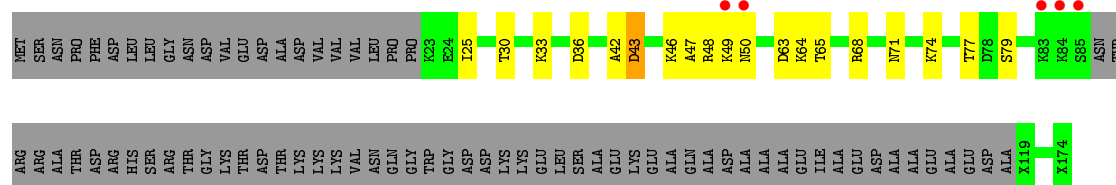
- Molecule 33: Ubiquitin-40S ribosomal protein S31

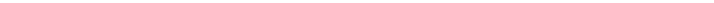


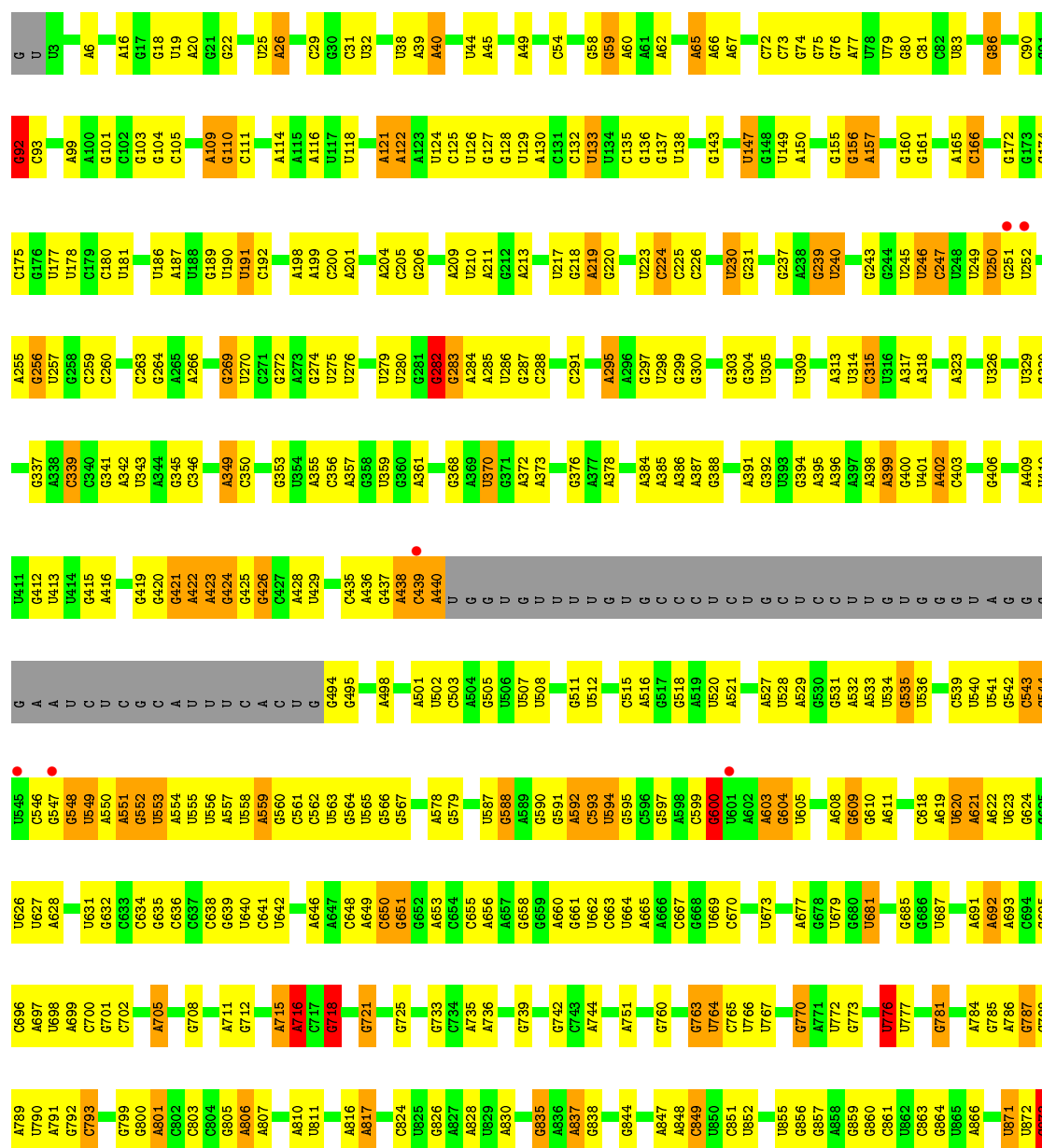
- Molecule 33: Ubiquitin-40S ribosomal protein S31



- Chain sM: 

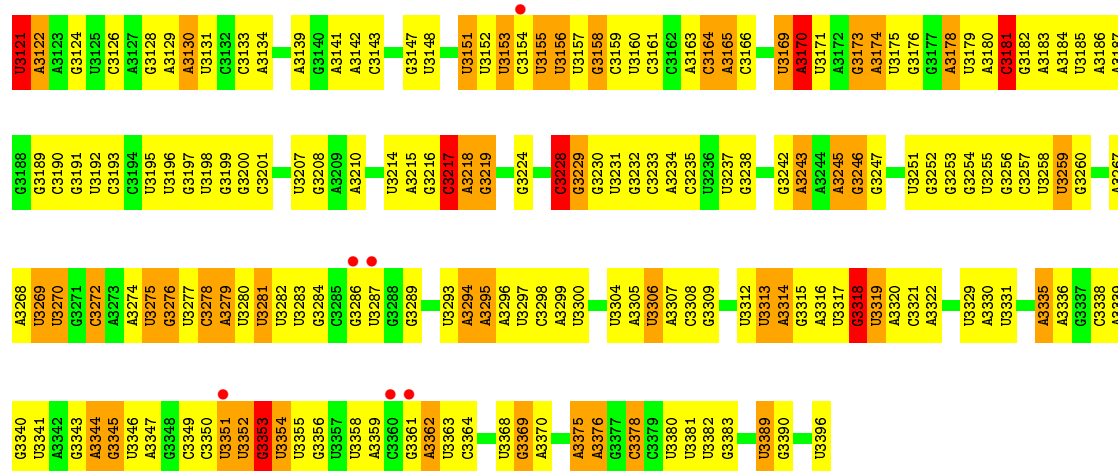


- Chain 1: 

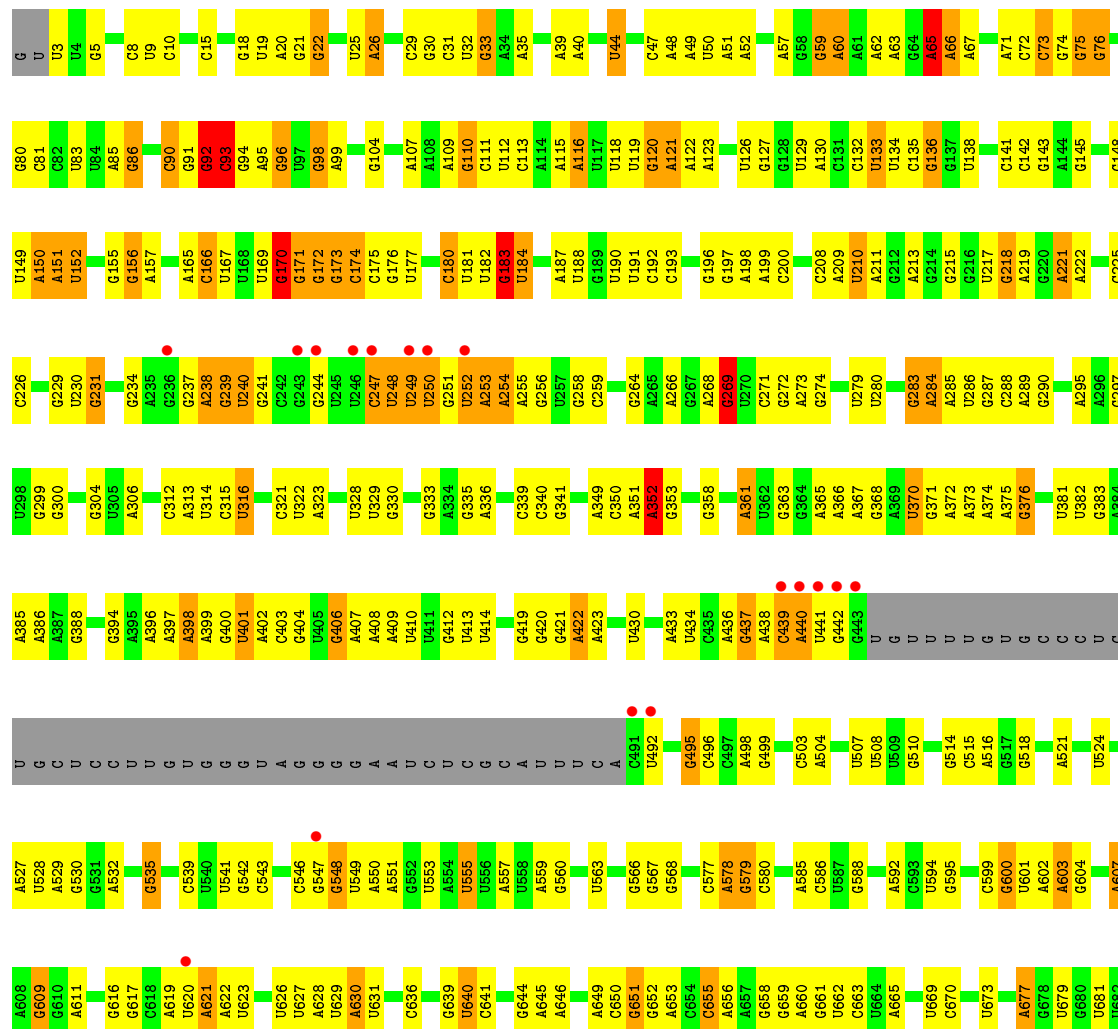


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A1887	A1799	C1725	A1642	U1570	G1485	G1412	A1332	G1261	G1115	U1033	G964	G875
A1888	C1803	A1729	A1643	A1571	G1486	G1414	C1333	A1262	G1116	U1033	A965	A876
A1889	G1730	A1731	U1645	G1573	G1488	U1415	U1334	A1263	G1117	A1034	A966	U879
G1898	G1808	A1732	U1646	C1574	A1489	C1416	G1340	U1265	C1119	A1035	U966	C800
G1899	A1809	U1733	A1647	A1575	A1490	G1417	U1341	G1266	U1120	C1037	G968	
A1900	A1810	G1734	U1651	G1576	A1491	A1418	G1345	U1269	U1121	C1038		A895
G1902	A1814	G1735	A1654	C1577	G1492	A1419	G1346	A1270	U1122	U1039	G971	A972
C1904	U1815	G1736		U1495	U1495	C1421	U1347	A1271	G1127	A1040	A973	U897
G1905	A1816		C1657	A1580	C1496	U1425	U1348	G1272	U1128	A1047	G974	U898
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	U1818		G1659	A1583	A1498	U1427	A1351	A1274	A1130	G1049	C977	
U1912	U1819	G1743	C1660	U1587	G1500	A1428	U1353	U1275	C1132	U1060	U979	G908
A1913	U1820	G1744	G1661	A1588	U1501	G1429	G1277	U1210	A1133	A1062	U980	C911
G1914	U1821	C1745	G1662	A1589	C1502	U1430	G1354	A1278	G1134	G1063	C982	G912
A1915	C1822	U1746		A1593	A1503	G1431	A1355	C1279	A1135	A1064	C983	A914
U1916	A1823	G1747	G1673	G1596	A1504	C1432	U1356	G1280	U1138	G1065	U985	A915
C1917	U1824	G1748	G1674	G1597	C1505	A1433	G1357	G1281	C1141	C1068	U986	G916
C1918	G1825	A1749	G1675	C1598	A1506	G1434	A1364	G1282	G1145	C1069	U987	A917
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U1938	A1839	G1758	G1680	U1599	G1521	G1443	U1369	G1289	G1149	U1073	G994	U922
G1939	U1840	A1760	U1681	U1601	A1524	U1445	A1369	C1227	A1150	U1074		C923
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G1948	C1854	U1768	A1896		A1535	U1455	U1384	C1296	G1161	A1006	G937	G937
G1949	U1855	G1769	C1701	A1613	G1543	U1456	G1385	C1297	U1162	A1093	C938	C938
U1950	C1856	U1770	U1702	C1614	A1544	U1457	A1386	G1307	A1094	U1094	U939	U939
C1951	C1857	C1771	U1703	U1615	A1546	U1458	G1387	U1241	U1095	G1010	G940	G940
G1952	C1857		U1703	U1616	G1547	U1459	U1388	G1242	U1096	G1013	U943	U943
G1953	A1858	G1775	U1705	G1617	C1548	A1462	U1389	G1243	G1097	U1014	C944	C944
C1954	G1861	U1776	C1706	A1619	U1554	G1464	A1390	G1244	G1101	G1016	U945	U945
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G	C1872	G1786	G1712		A1559	U1470	A1401	G1249	G1172	G1021	U954	U954
G	U1873	A1787	U1716	U1629	G1560	U1471	G1399		C1176	G1024	U955	U955
G	C1874	G1788	U1717	C1633	G1561	U1472	G1405	A1282	G1177	A1025	C957	C957
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U	A1879	G1794	G1720	G1635	G1565	A1475	A1408	G1256	A1180	U1110	G1029	G1029
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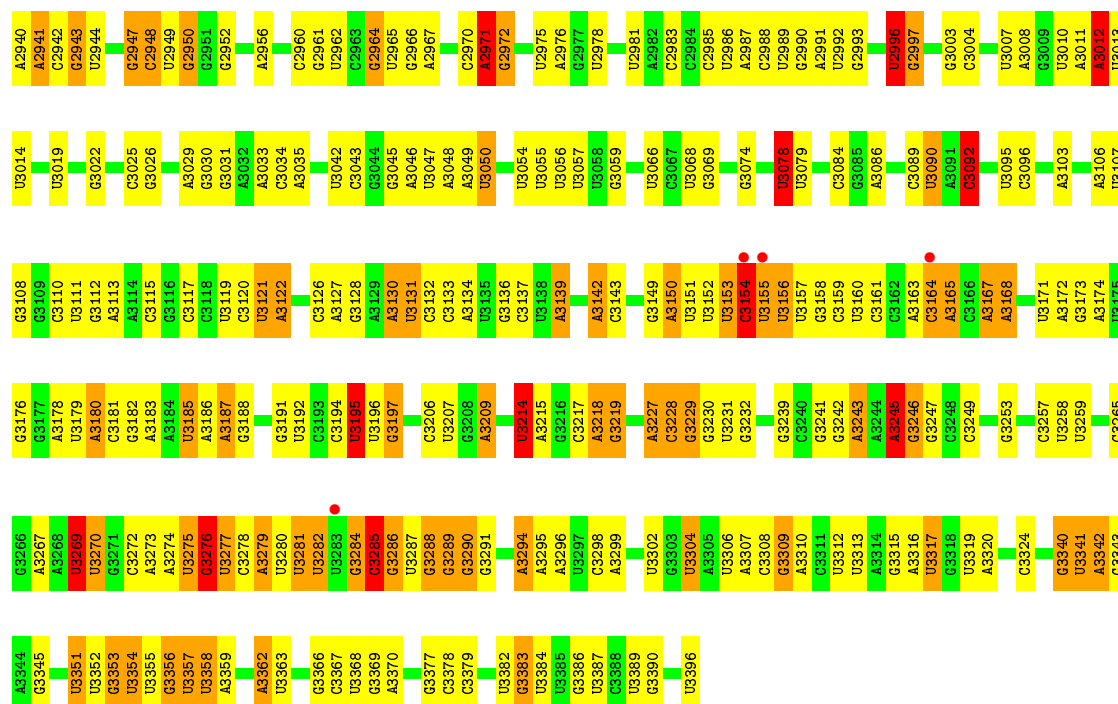


• Molecule 36: 25S ribosomal RNA

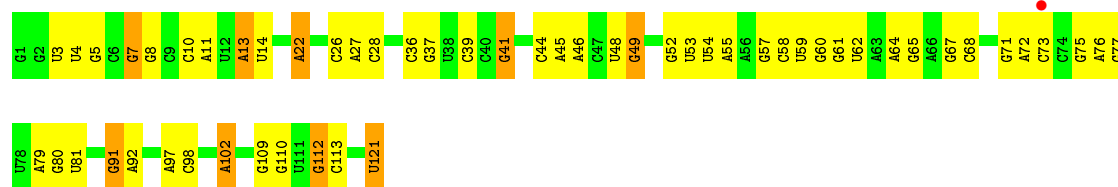




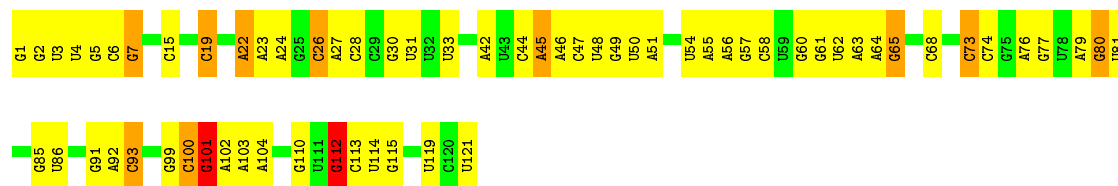




• Molecule 37: 5S ribosomal RNA



• Molecule 37: 5S ribosomal RNA



• Molecule 38: 5.8S ribosomal RNA

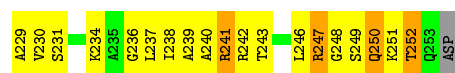
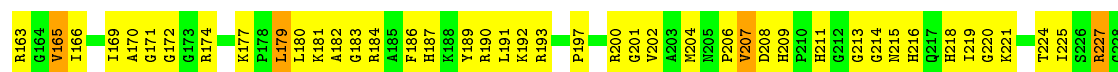
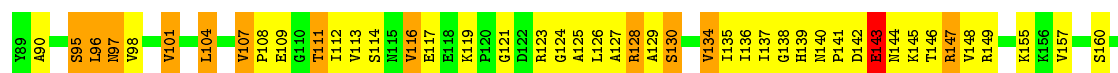




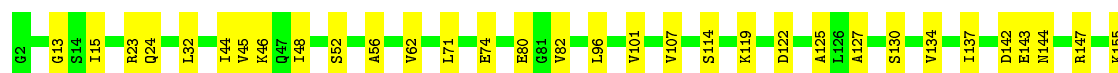
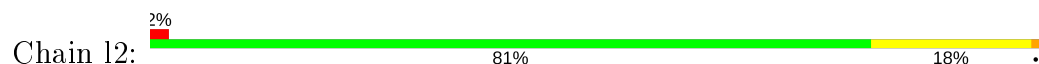
- Molecule 38: 5.8S ribosomal RNA



- Molecule 39: 60S ribosomal protein L2-A

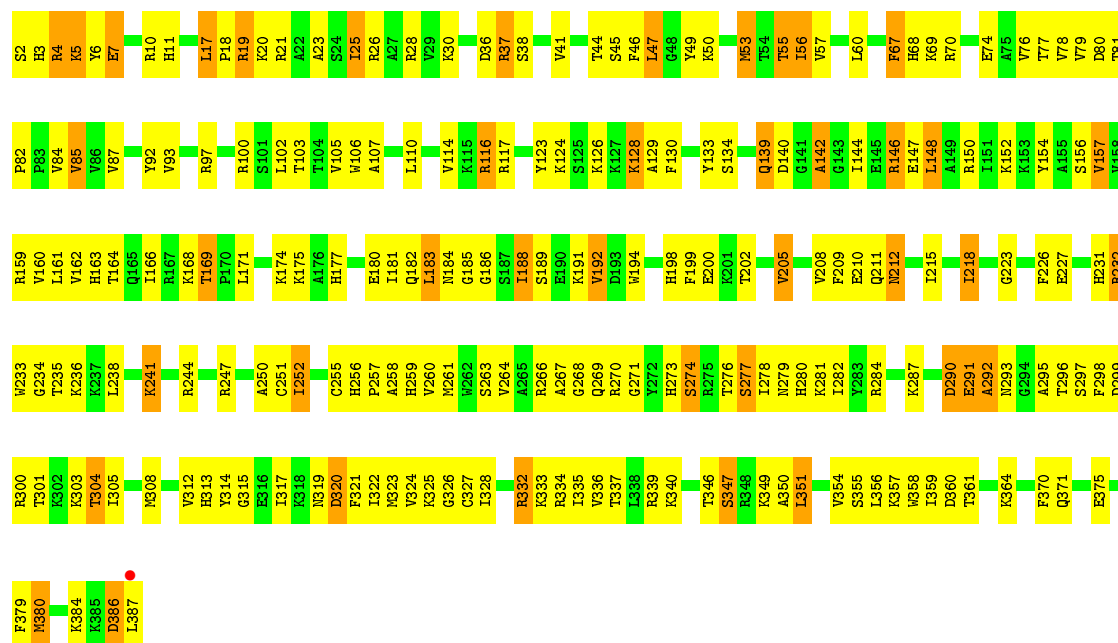


- Molecule 39: 60S ribosomal protein L2-A



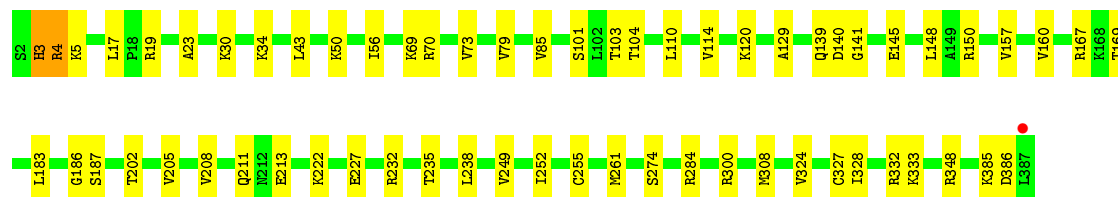
- Molecule 40: 60S ribosomal protein L3





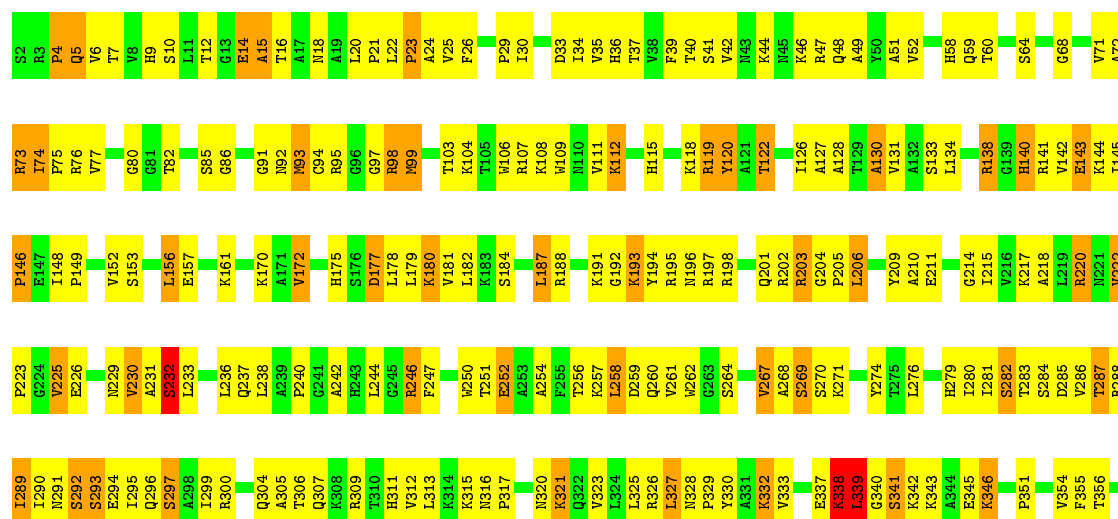
- Molecule 40: 60S ribosomal protein L3

Chain L3: 84% 16%



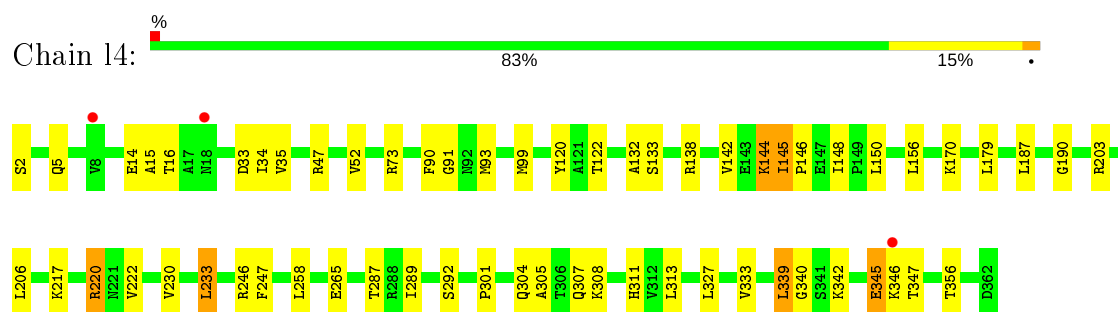
- Molecule 41: 60S ribosomal protein L4-A

Chain L4: 39% 47% 13%

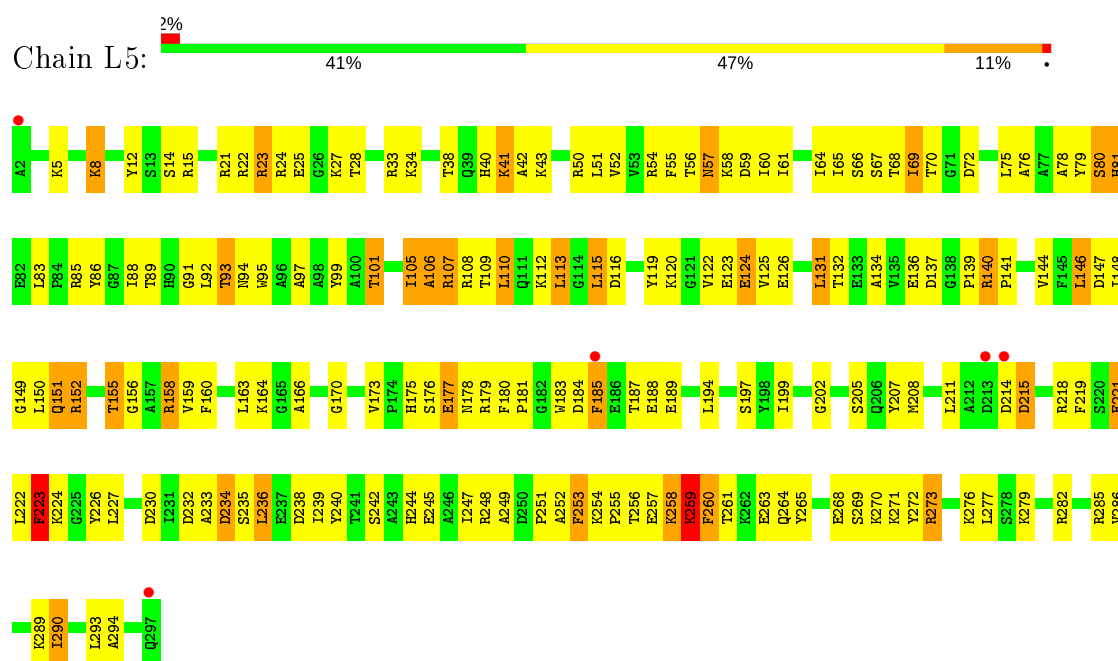


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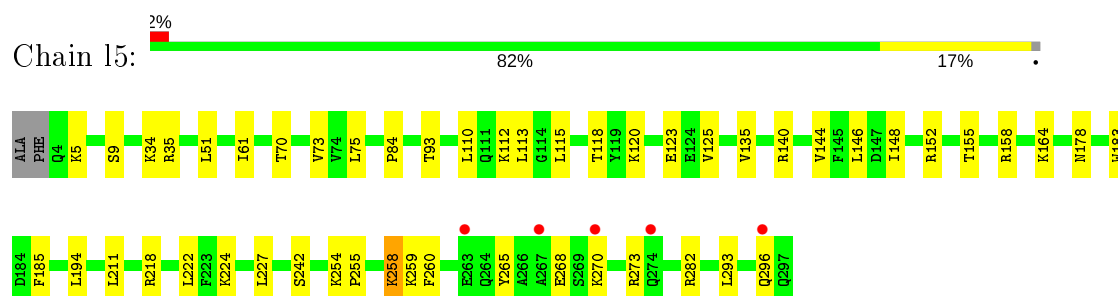
- Molecule 41: 60S ribosomal protein L4-A



- Molecule 42: 60S ribosomal protein L5

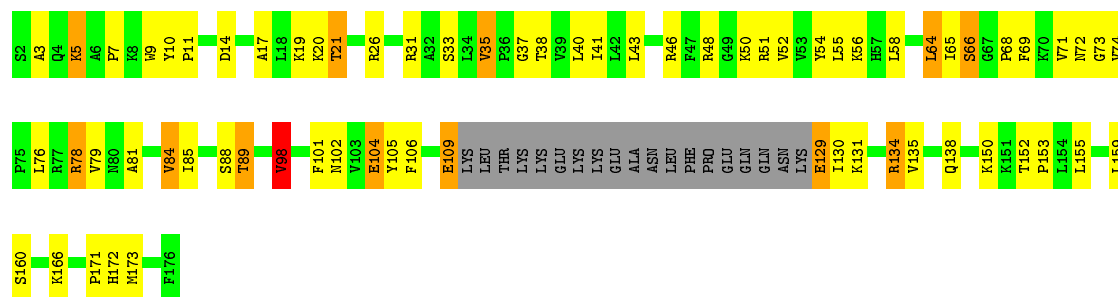


- Molecule 42: 60S ribosomal protein L5

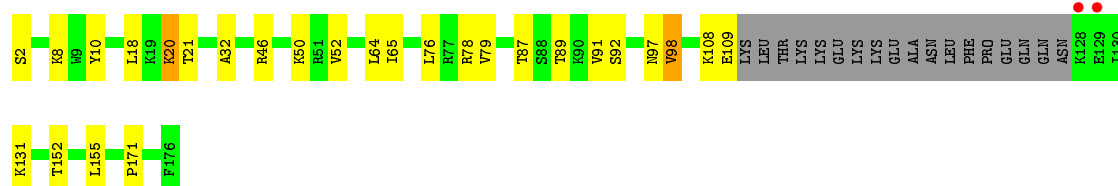


- Molecule 43: 60S ribosomal protein L6-A

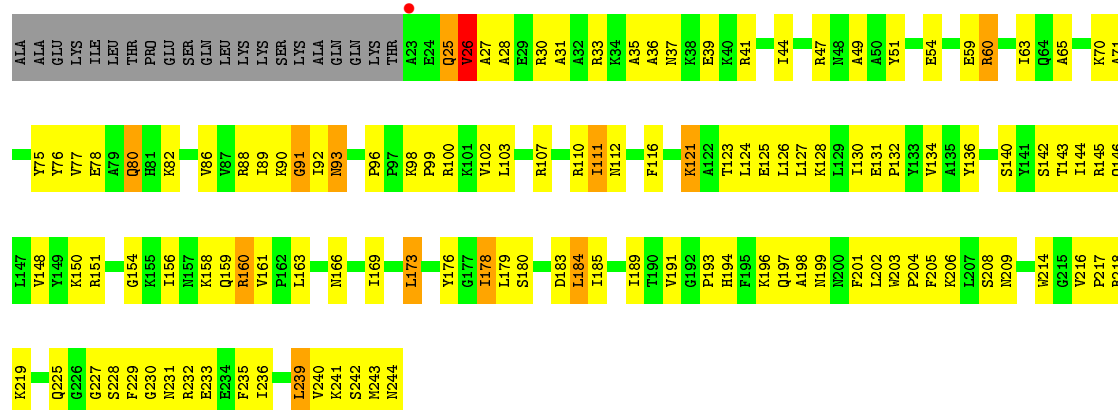




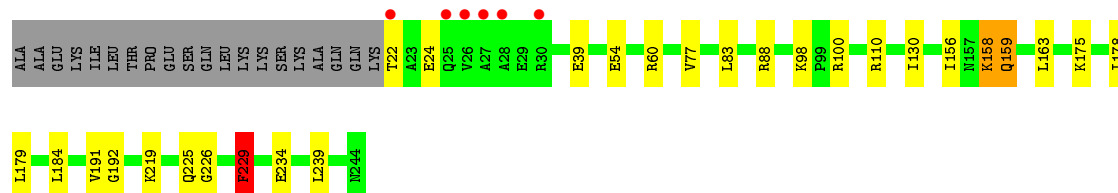
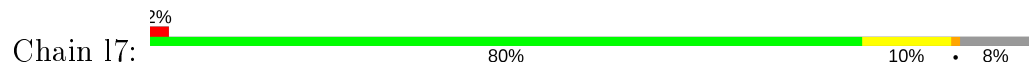
- Molecule 43: 60S ribosomal protein L6-A



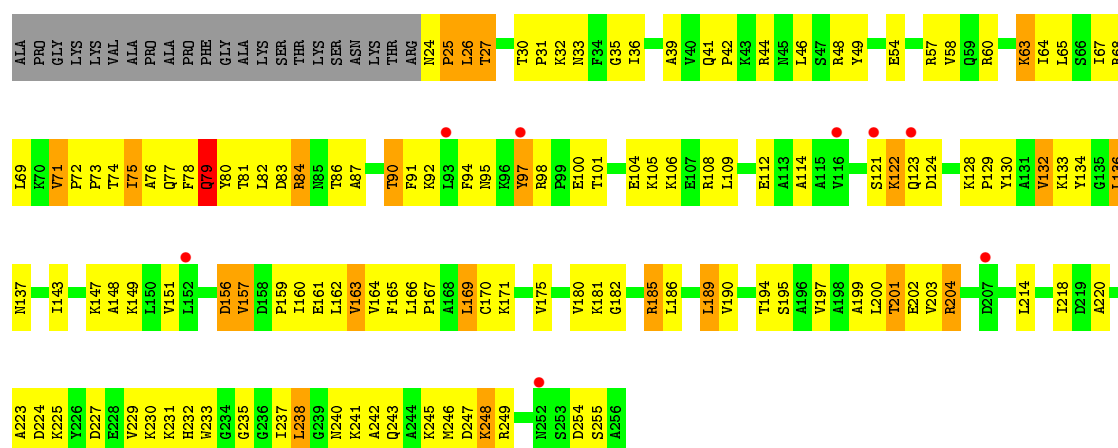
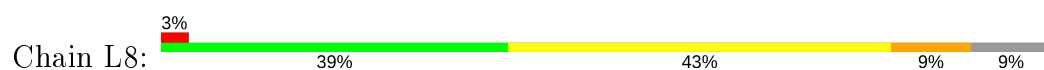
- Molecule 44: 60S ribosomal protein L7-A



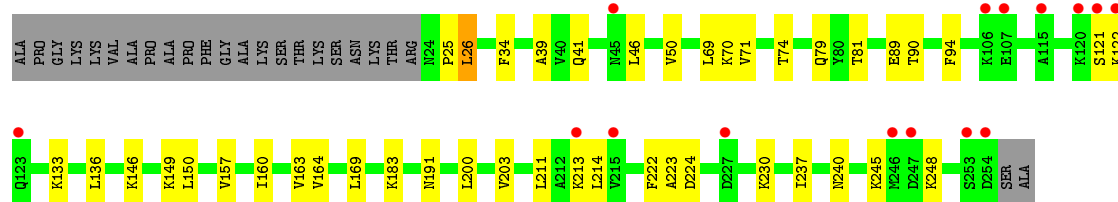
- Molecule 44: 60S ribosomal protein L7-A



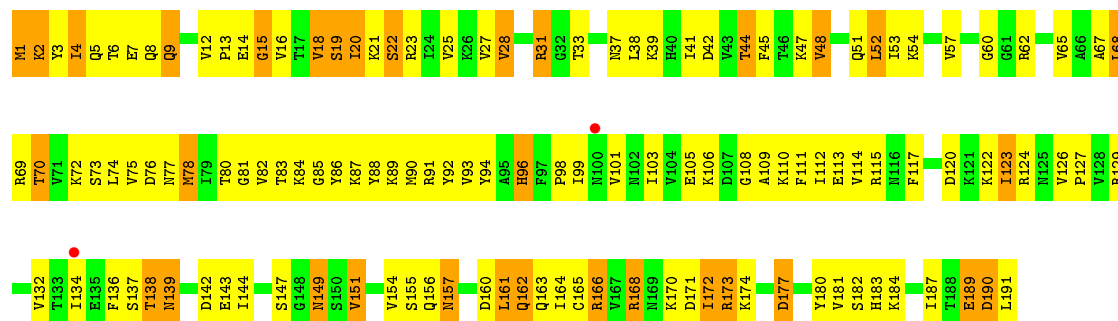
- Molecule 45: 60S ribosomal protein L8-A



• Molecule 45: 60S ribosomal protein L8-A

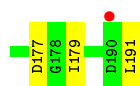


• Molecule 46: 60S ribosomal protein L9-A

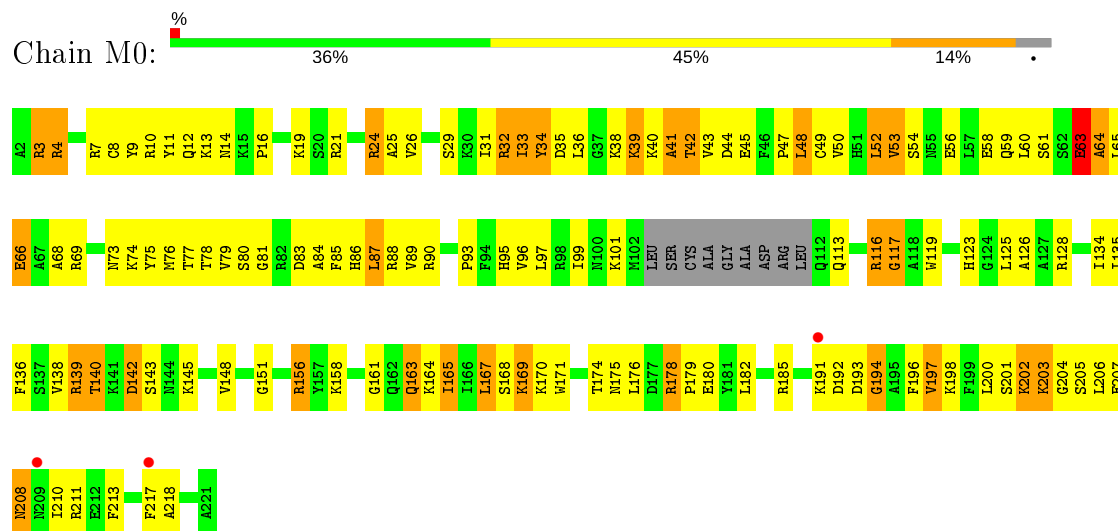


• Molecule 46: 60S ribosomal protein L9-A

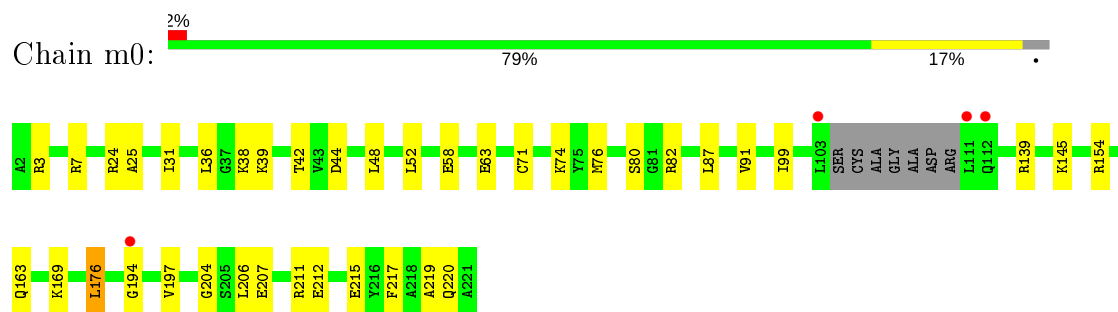




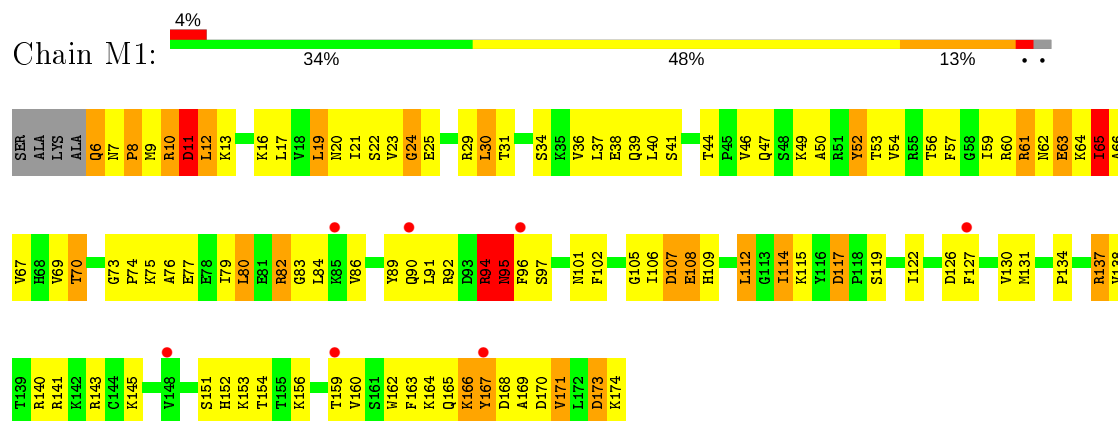
- Molecule 47: 60S ribosomal protein L10



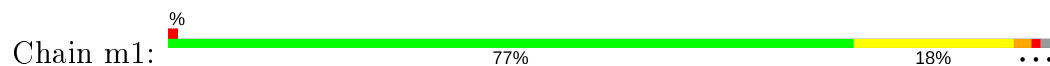
- Molecule 47: 60S ribosomal protein L10

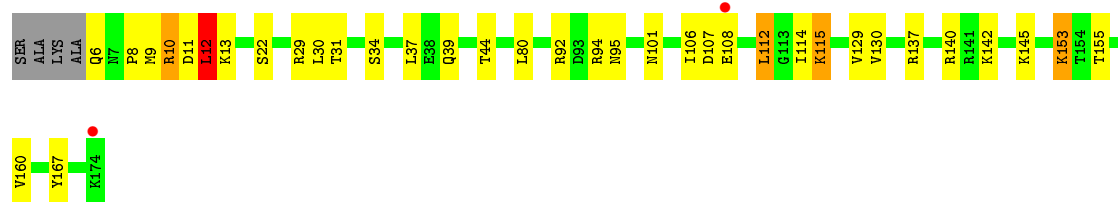


- Molecule 48: 60S ribosomal protein L11-A

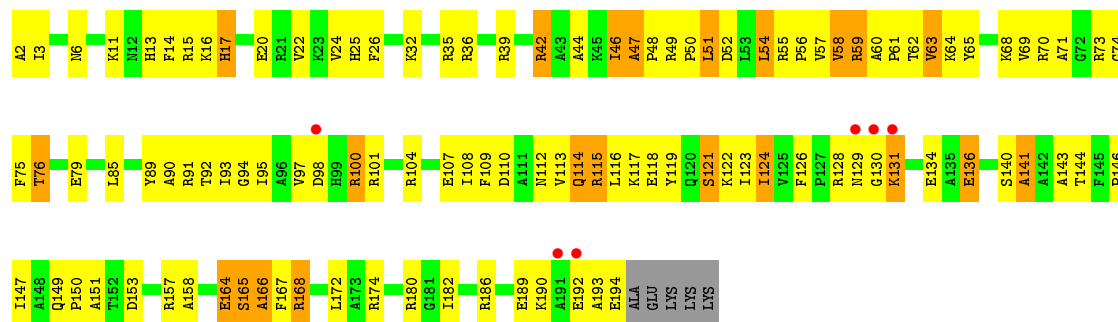
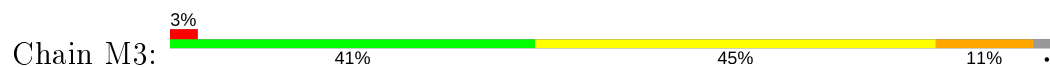


- Molecule 48: 60S ribosomal protein L11-A

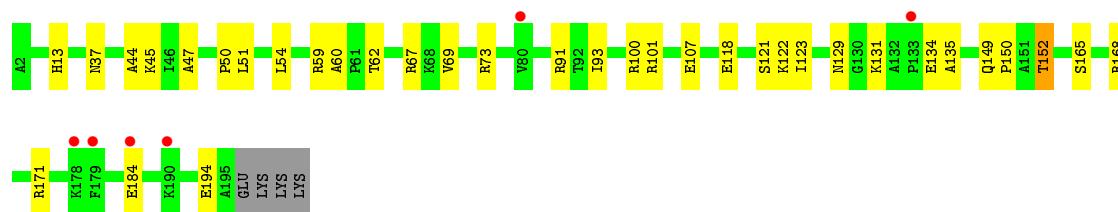
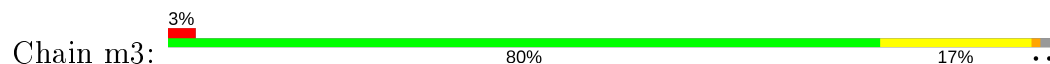




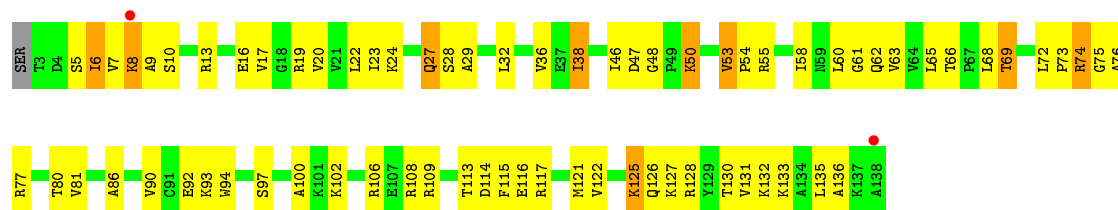
• Molecule 49: 60S ribosomal protein L13-A



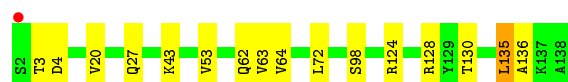
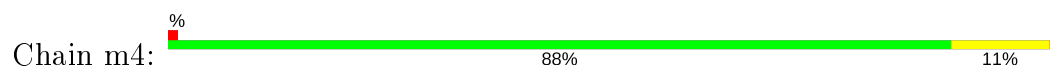
• Molecule 49: 60S ribosomal protein L13-A



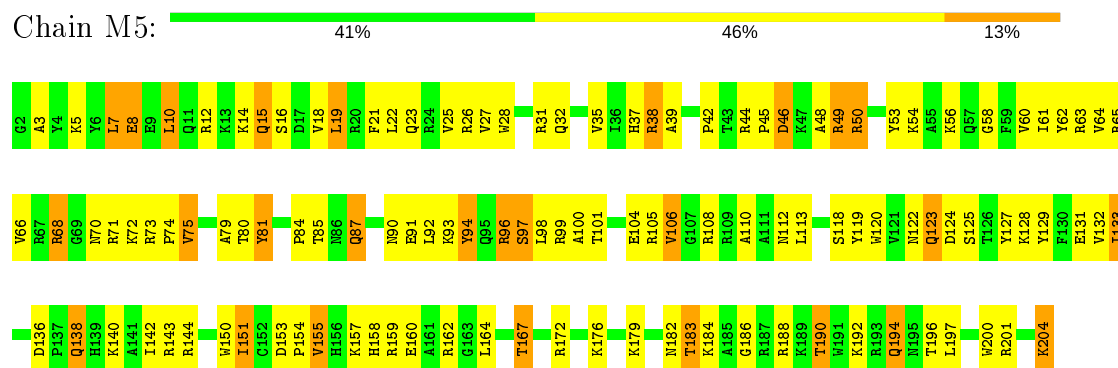
• Molecule 50: 60S ribosomal protein L14-A



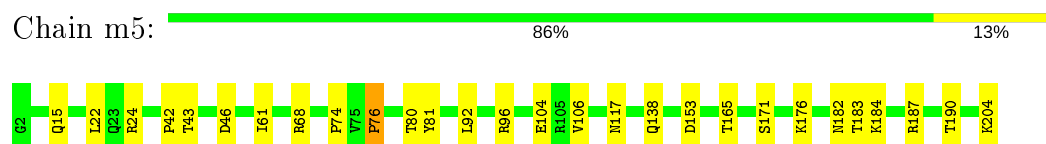
• Molecule 50: 60S ribosomal protein L14-A



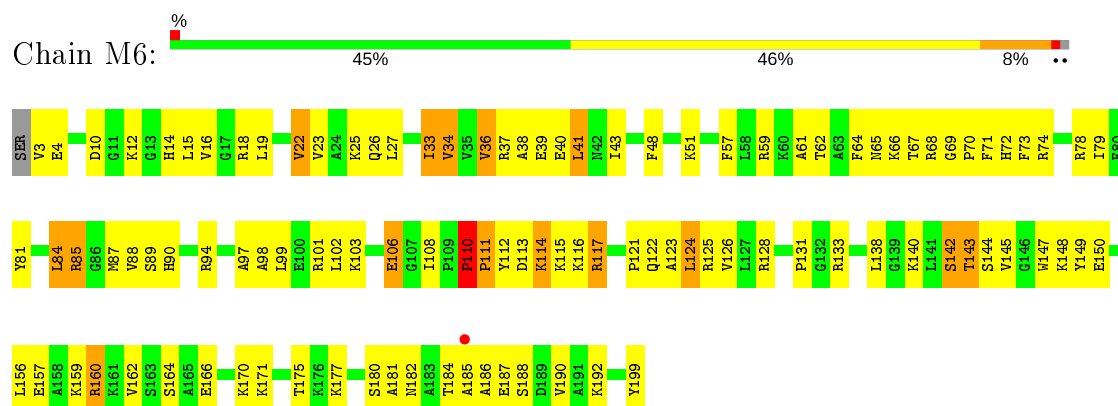
- Molecule 51: 60S ribosomal protein L15-A



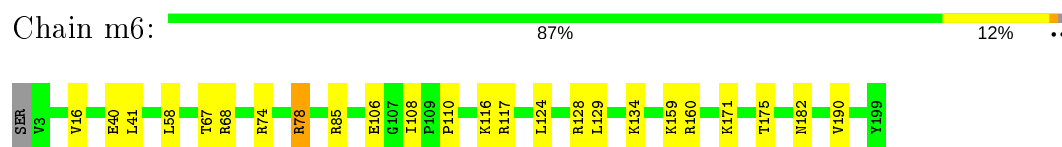
- Molecule 51: 60S ribosomal protein L15-A



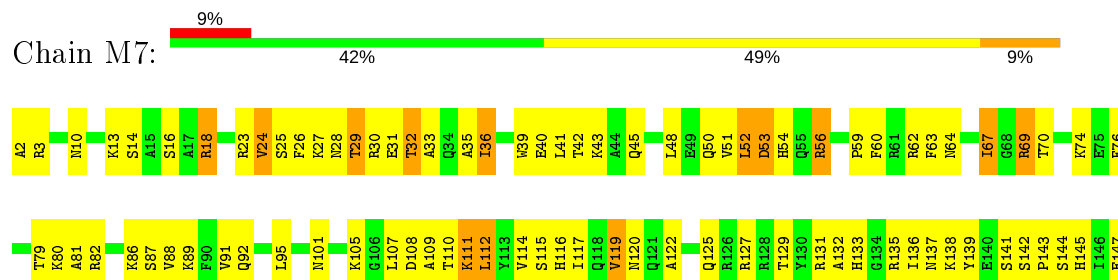
- Molecule 52: 60S ribosomal protein L16-A

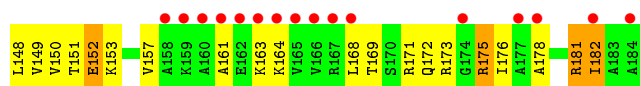


- Molecule 52: 60S ribosomal protein L16-A

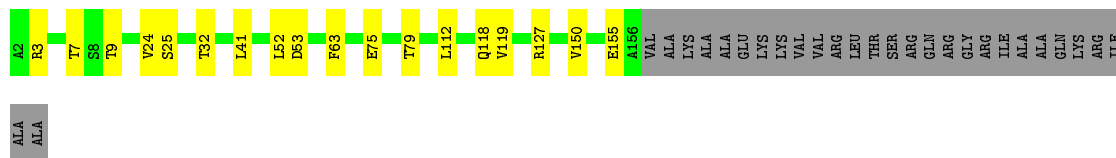


- Molecule 53: 60S ribosomal protein L17-A

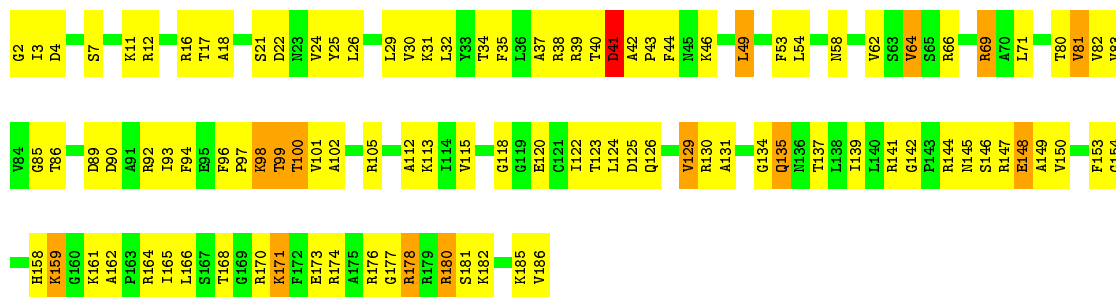




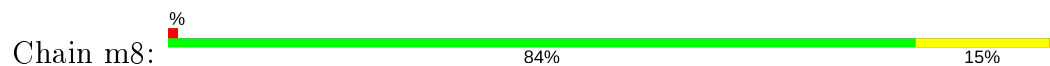
- Molecule 53: 60S ribosomal protein L17-A



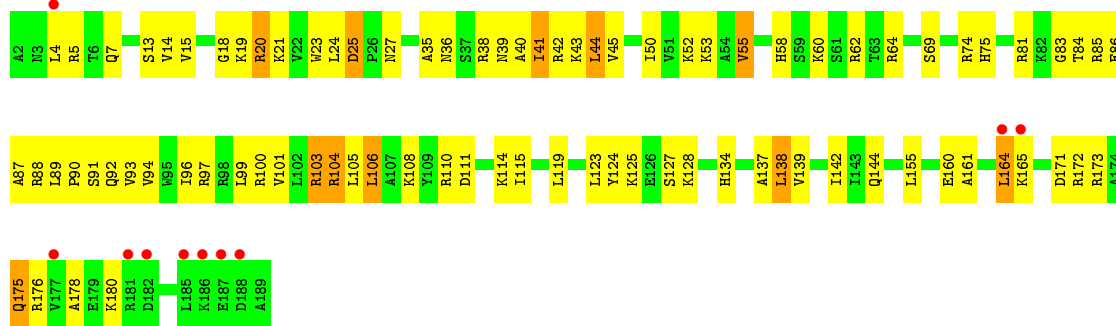
- Molecule 54: 60S ribosomal protein L18-A



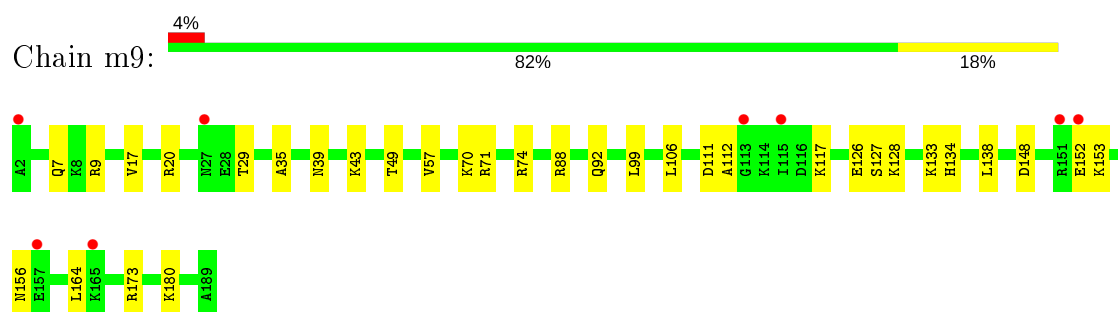
- Molecule 54: 60S ribosomal protein L18-A



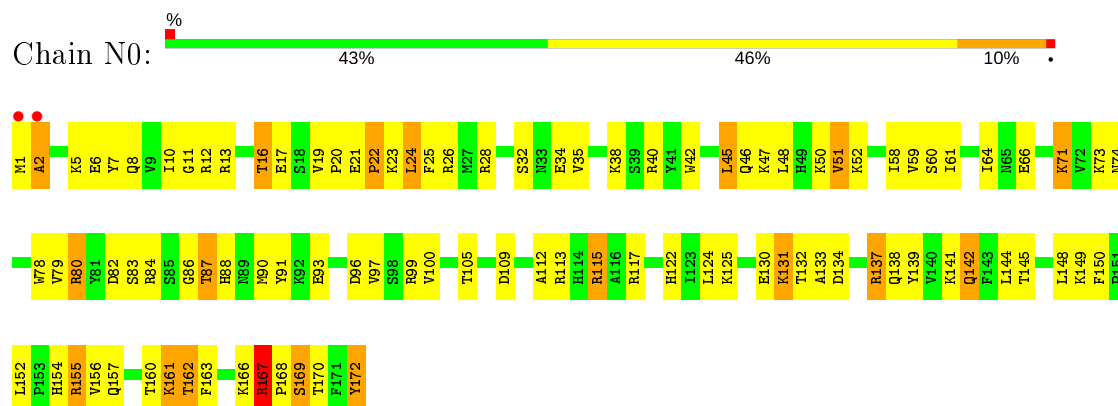
- Molecule 55: 60S ribosomal protein L19-A



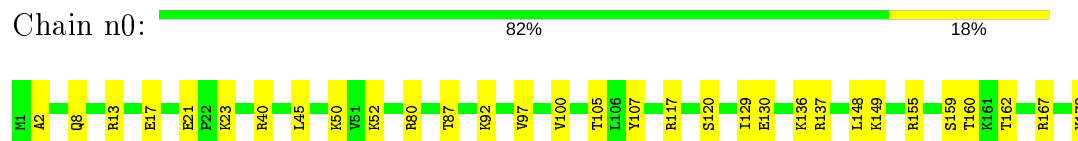
- Molecule 55: 60S ribosomal protein L19-A



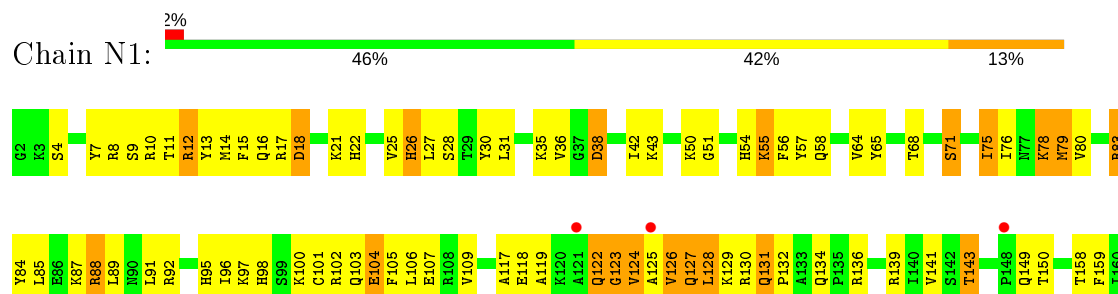
- Molecule 56: 60S ribosomal protein L20-A



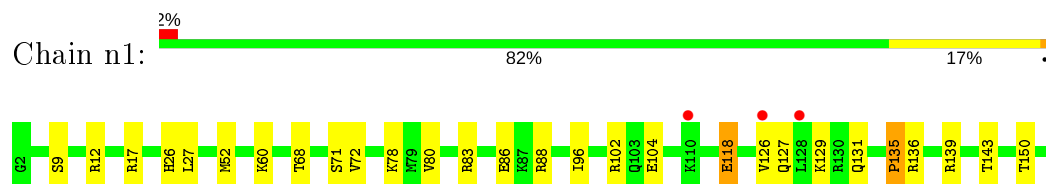
- Molecule 56: 60S ribosomal protein L20-A



- Molecule 57: 60S ribosomal protein L21-A

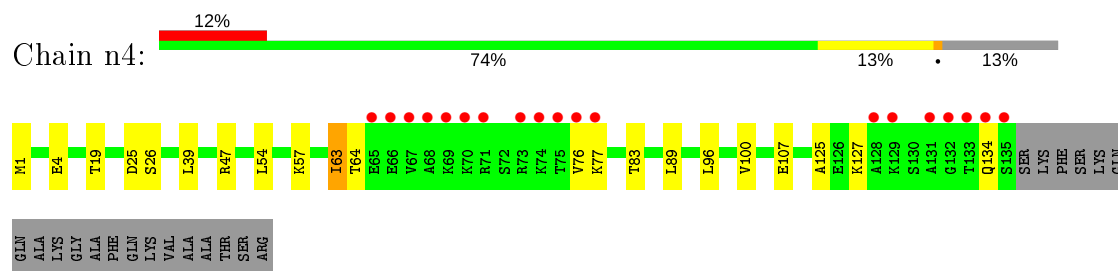


- Molecule 57: 60S ribosomal protein L21-A

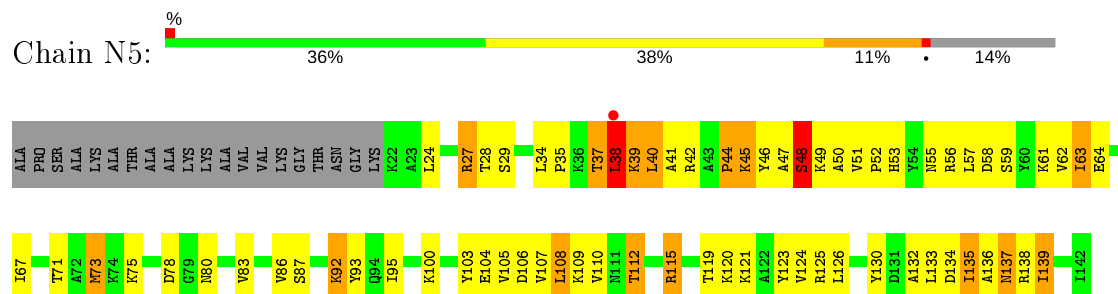


- Molecule 58: 60S ribosomal protein L22-A

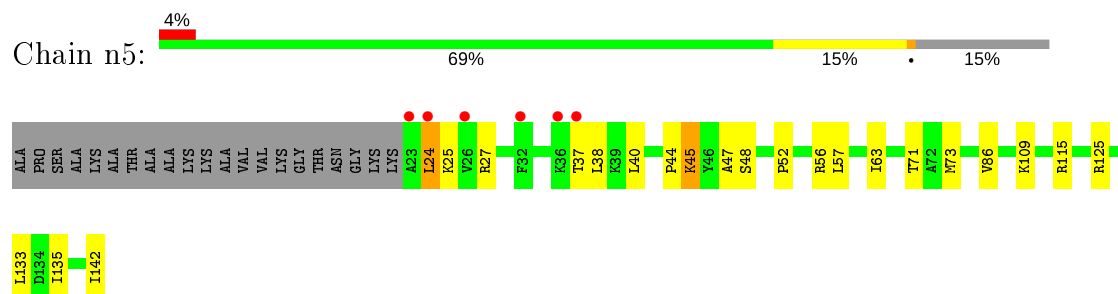
- Molecule 60: 60S ribosomal protein L24-A



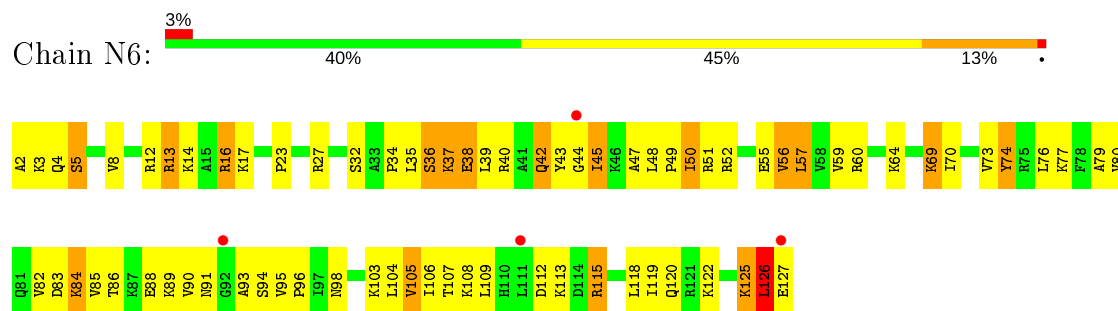
- Molecule 61: 60S ribosomal protein L25



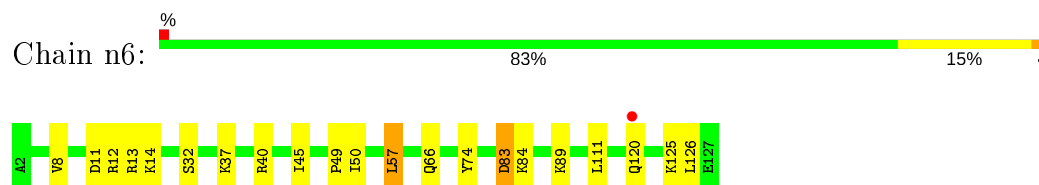
- Molecule 61: 60S ribosomal protein L25



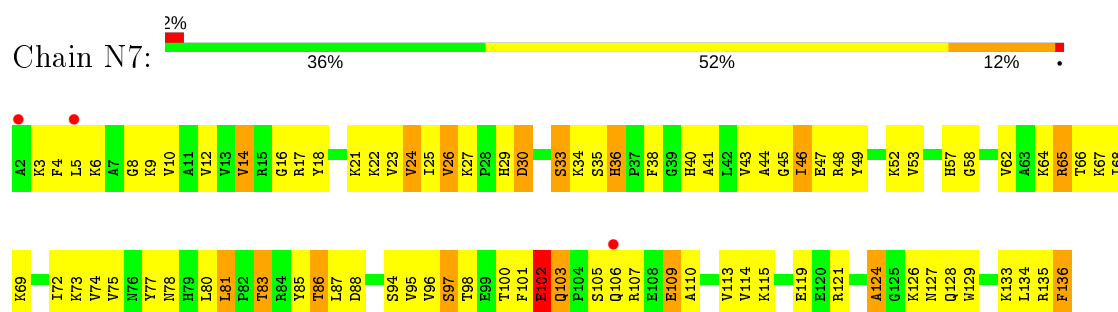
- Molecule 62: 60S ribosomal protein L26-A



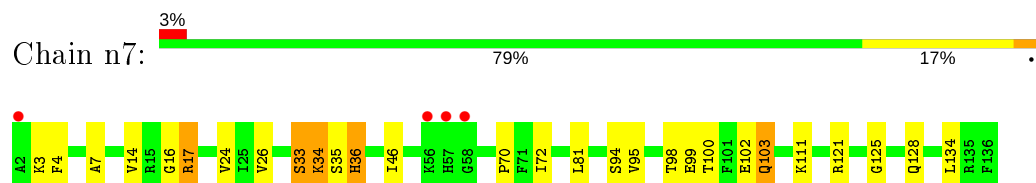
- Molecule 62: 60S ribosomal protein L26-A



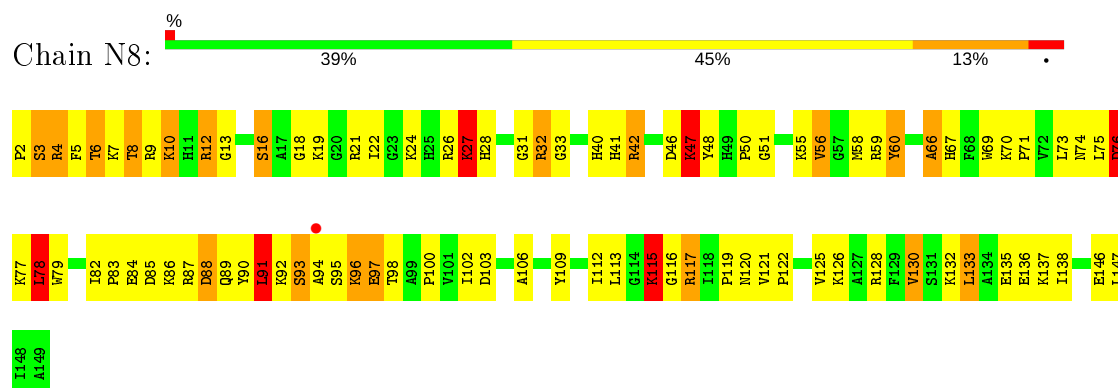
- Molecule 63: 60S ribosomal protein L27-A



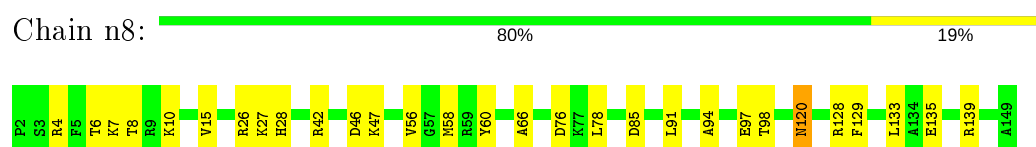
- Molecule 63: 60S ribosomal protein L27-A



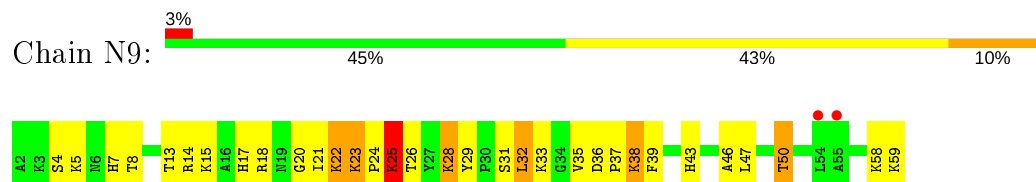
- Molecule 64: 60S ribosomal protein L28



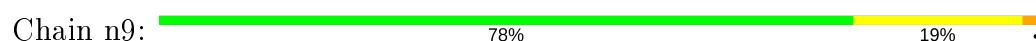
- Molecule 64: 60S ribosomal protein L28



- Molecule 65: 60S ribosomal protein L29

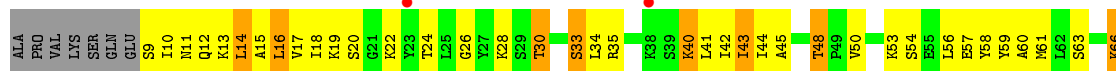


- Molecule 65: 60S ribosomal protein L29

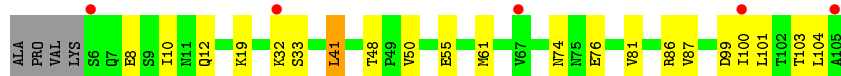




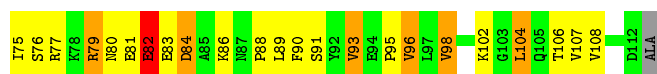
- Molecule 66: 60S ribosomal protein L30



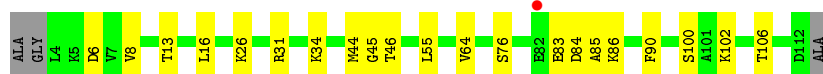
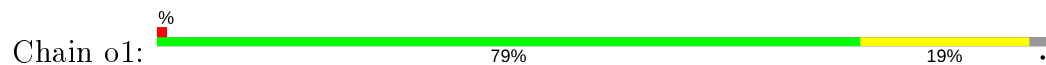
- Molecule 66: 60S ribosomal protein L30



- Molecule 67: 60S ribosomal protein L31-A



- Molecule 67: 60S ribosomal protein L31-A



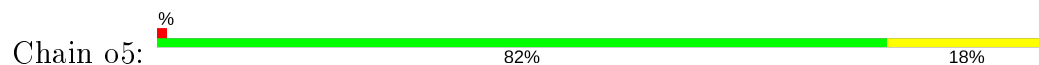
- Molecule 68: 60S ribosomal protein L32



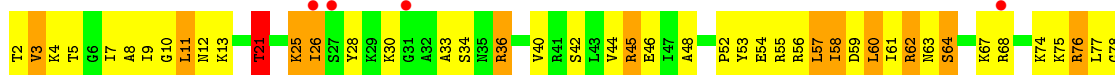
- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| A2 | G3 | V4 | K5 | A6 | Y7 | B8 | L9 | R10 | T11 | K12 | E15 | Q16 | L17 | D20 | L21 | V22 | D23 | L24 | K25 | V26 | E27 | L31 | K32 | L36 | L41 | P42 | K43 | L44 | K45 | T46 | V47 | R48 | K49 | S50 | V54 | L58 | N59 | B60 | Q61 | Q62 | R63 | V66 | R67 | Q68 | L69 | Y70 | K71 | G72 | K73 | V74 | V75 |
|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



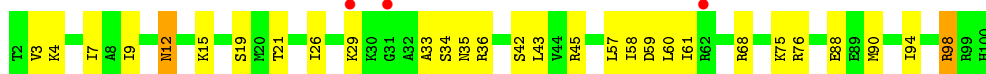
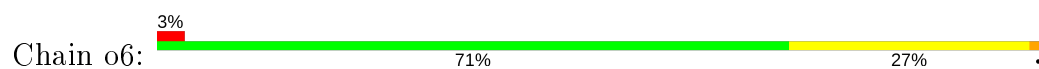
- Molecule 71: 60S ribosomal protein L35-A



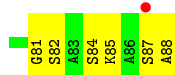
- Molecule 72: 60S ribosomal protein L36-A



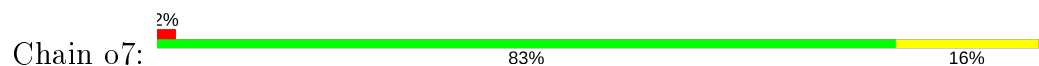
- Molecule 72: 60S ribosomal protein L36-A



- Molecule 73: 60S ribosomal protein L37-A

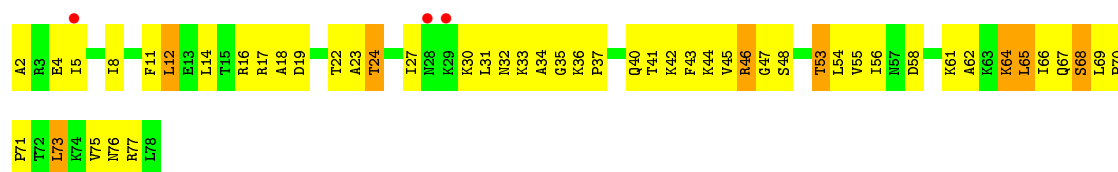


- Molecule 73: 60S ribosomal protein L37-A

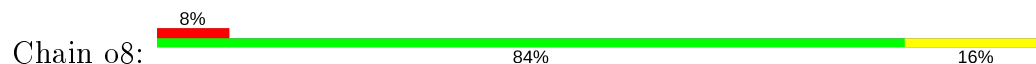


- Molecule 74: 60S ribosomal protein L38





- Molecule 74: 60S ribosomal protein L38



- Molecule 75: 60S ribosomal protein L39



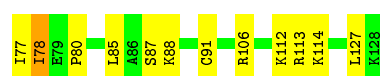
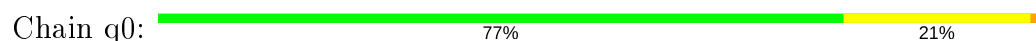
- Molecule 75: 60S ribosomal protein L39



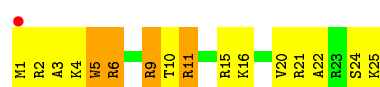
- Molecule 76: Ubiquitin-60S ribosomal protein L40



- Molecule 76: Ubiquitin-60S ribosomal protein L40



- Molecule 77: 60S ribosomal protein L41-A



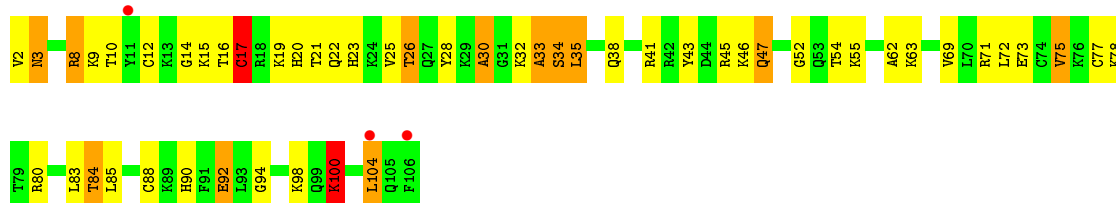
- Molecule 77: 60S ribosomal protein L41-A

Chain q1:  68% 32%




- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:  3% 50% 36% 11%



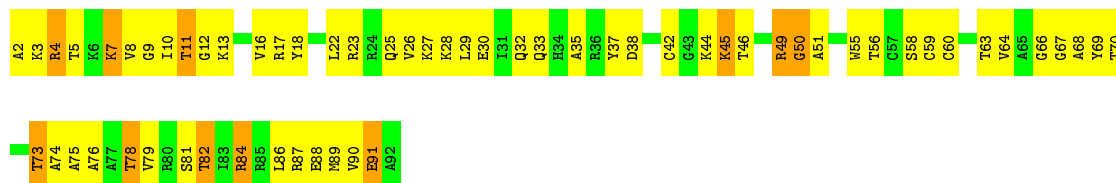
- Molecule 78: 60S ribosomal protein L42-A

Chain q2:  4% 84% 16%




- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:  33% 55% 12%



- Molecule 79: 60S ribosomal protein L43-A

Chain q3:  86% 11%

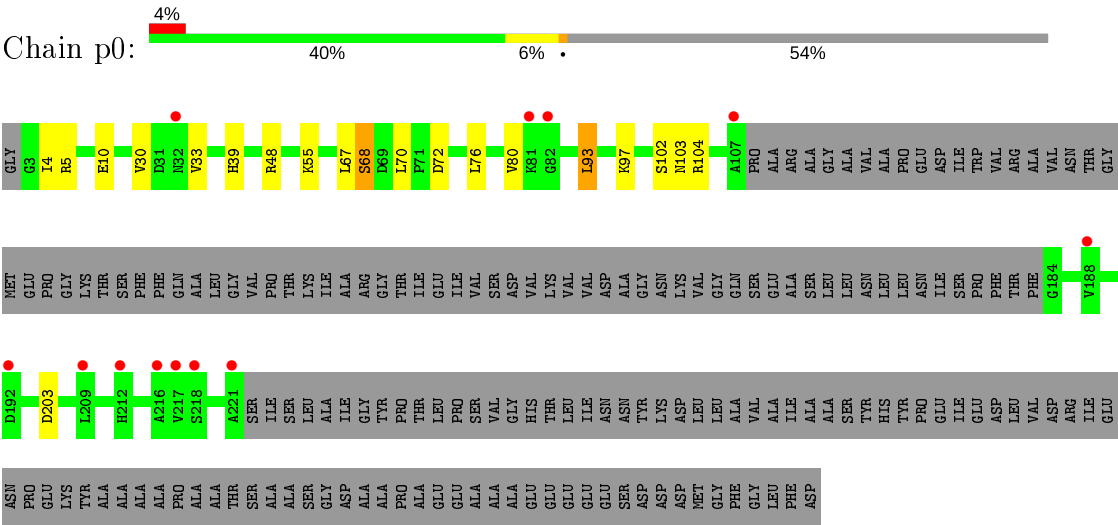


- Molecule 80: 60S ribosomal protein L12-A (uL11)

Chain m2:  100%

There are no outlier residues recorded for this chain.

- Molecule 81: 60S acidic ribosomal protein P0



- Molecule 82: 60S ribosomal protein P1 alpha



There are no outlier residues recorded for this chain.

- Molecule 83: 60S ribosomal protein P2 beta



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	436.11Å 287.31Å 303.99Å 90.00° 98.86° 90.00°	Depositor
Resolution (Å)	49.96 – 3.10 49.96 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.96-3.10) 89.6 (49.96-3.10)	Depositor EDS
R_{merge}	0.39	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.234 , 0.291 0.243 , 0.288	Depositor DCC
R_{free} test set	26664 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	63.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	410912	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% 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: ANM, ZN, OHX, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.50	0/42468	1.01	74/66173 (0.1%)
1	6	0.60	0/42790	1.06	102/66673 (0.2%)
2	S0	0.35	0/1617	0.56	0/2215
2	s0	0.34	0/1653	0.55	0/2261
3	S1	0.32	0/1735	0.59	0/2335
3	s1	0.36	0/1748	0.58	0/2352
4	S2	0.37	0/1665	0.57	0/2263
4	s2	0.42	0/1665	0.62	0/2263
5	S3	0.37	0/1759	0.55	0/2368
5	s3	0.33	0/1759	0.52	0/2368
6	S4	0.36	0/2109	0.59	0/2839
6	s4	0.39	0/2109	0.61	0/2839
7	S5	0.33	0/1629	0.55	0/2202
7	s5	0.33	0/1629	0.55	0/2202
8	S6	0.38	0/1823	0.55	0/2439
8	s6	0.39	0/1779	0.56	0/2379
9	S7	0.34	0/1506	0.57	0/2028
9	s7	0.34	0/1517	0.58	0/2044
10	S8	0.38	0/1514	0.59	1/2021 (0.0%)
10	s8	0.43	0/1514	0.58	0/2021
11	S9	0.36	0/1519	0.56	0/2035
11	s9	0.39	0/1519	0.57	0/2035
12	C0	0.34	0/730	0.52	0/985
12	c0	0.29	0/718	0.53	1/968 (0.1%)
13	C1	0.43	0/1195	0.57	0/1612
13	c1	0.44	0/1195	0.60	0/1612
14	C2	0.34	0/898	0.55	0/1220
14	c2	0.25	0/898	0.50	0/1220
15	C3	0.36	0/1215	0.57	1/1638 (0.1%)
15	c3	0.38	0/1215	0.58	0/1638
16	C4	0.30	0/901	0.56	0/1217
16	c4	0.39	0/960	0.62	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.34	0/998	0.57	0/1341
17	c5	0.38	0/1060	0.59	0/1426
18	C6	0.36	0/1125	0.62	3/1510 (0.2%)
18	c6	0.35	0/1131	0.57	0/1518
19	C7	0.37	0/935	0.60	0/1254
19	c7	0.31	0/953	0.53	0/1275
20	C8	0.36	0/1211	0.55	0/1628
20	c8	0.36	0/1211	0.58	0/1628
21	C9	0.33	0/1130	0.52	0/1517
21	c9	0.35	0/1130	0.55	0/1517
22	D0	0.36	0/865	0.57	0/1169
22	d0	0.36	0/892	0.58	0/1205
23	D1	0.36	0/693	0.54	0/935
23	d1	0.35	0/693	0.50	0/935
24	D2	0.37	0/1038	0.63	3/1395 (0.2%)
24	d2	0.44	0/1038	0.62	1/1395 (0.1%)
25	D3	0.44	0/1139	0.64	0/1518
25	d3	0.49	0/1139	0.66	1/1518 (0.1%)
26	D4	0.37	0/1087	0.55	0/1449
26	d4	0.40	0/1087	0.61	0/1449
27	D5	0.33	0/571	0.60	0/768
27	d5	0.33	0/566	0.54	0/761
28	D6	0.36	0/782	0.57	0/1047
28	d6	0.47	0/782	0.58	0/1047
29	D7	0.35	0/620	0.58	0/838
29	d7	0.36	0/620	0.56	0/838
30	D8	0.32	0/499	0.53	0/670
30	d8	0.34	0/499	0.54	0/670
31	D9	0.36	0/452	0.58	1/600 (0.2%)
31	d9	0.36	0/453	0.53	0/602
32	E0	0.37	0/483	0.54	0/643
32	e0	0.39	0/499	0.62	0/665
33	E1	0.35	0/577	0.61	0/770
33	e1	0.34	0/619	0.65	0/822
34	SR	0.31	0/2490	0.52	0/3389
34	sR	0.29	0/2498	0.49	0/3398
35	SM	0.38	0/984	0.56	0/1323
35	sM	0.40	0/480	0.60	0/642
36	1	0.78	3/75394 (0.0%)	1.21	317/117545 (0.3%)
36	5	0.82	7/75418 (0.0%)	1.21	316/117583 (0.3%)
37	3	0.65	0/2883	1.03	1/4491 (0.0%)
37	7	0.79	0/2883	1.20	8/4491 (0.2%)
38	4	0.73	0/3746	1.15	8/5832 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	8	0.68	0/3746	1.12	4/5832 (0.1%)
39	L2	0.50	0/1948	0.66	0/2617
39	l2	0.48	0/1952	0.69	2/2622 (0.1%)
40	L3	0.52	0/3136	0.64	0/4213
40	l3	0.59	1/3142 (0.0%)	0.68	1/4224 (0.0%)
41	L4	0.55	1/2800 (0.0%)	0.72	1/3790 (0.0%)
41	l4	0.53	0/2801	0.69	2/3792 (0.1%)
42	L5	0.43	0/2425	0.61	0/3271
42	l5	0.53	0/2408	0.65	0/3248
43	L6	0.53	0/1260	0.64	0/1694
43	l6	0.49	0/1269	0.62	0/1705
44	L7	0.53	0/1821	0.66	0/2451
44	l7	0.58	0/1828	0.70	1/2461 (0.0%)
45	L8	0.42	0/1836	0.60	0/2481
45	l8	0.40	0/1795	0.56	0/2429
46	L9	0.47	0/1539	0.59	0/2073
46	l9	0.54	0/1539	0.64	0/2073
47	M0	0.54	0/1741	0.66	0/2335
47	m0	0.55	0/1769	0.68	0/2372
48	M1	0.39	0/1374	0.59	0/1842
48	m1	0.47	0/1374	0.68	2/1842 (0.1%)
49	M3	0.51	0/1568	0.67	1/2106 (0.0%)
49	m3	0.47	0/1573	0.66	0/2113
50	M4	0.51	0/1068	0.64	0/1438
50	m4	0.53	0/1074	0.66	0/1446
51	M5	0.50	0/1757	0.64	0/2354
51	m5	0.47	0/1757	0.63	0/2354
52	M6	0.55	0/1585	0.69	1/2128 (0.0%)
52	m6	0.68	1/1585 (0.1%)	0.74	2/2128 (0.1%)
53	M7	0.53	0/1443	0.67	0/1944
53	m7	0.59	0/1250	0.69	0/1683
54	M8	0.51	0/1465	0.68	1/1965 (0.1%)
54	m8	0.53	0/1465	0.72	1/1965 (0.1%)
55	M9	0.38	0/1538	0.56	0/2050
55	m9	0.43	0/1538	0.57	0/2050
56	N0	0.55	0/1481	0.65	0/1990
56	n0	0.58	0/1481	0.70	0/1990
57	N1	0.56	0/1300	0.67	0/1743
57	n1	0.60	0/1300	0.62	0/1743
58	N2	0.36	0/812	0.54	0/1099
58	n2	0.39	0/794	0.60	0/1076
59	N3	0.53	0/1018	0.64	0/1369
59	n3	0.60	0/1018	0.74	0/1369

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	N4	0.42	0/712	0.57	0/958
60	n4	0.47	0/1103	0.60	0/1458
61	N5	0.44	0/979	0.64	1/1321 (0.1%)
61	n5	0.46	0/974	0.64	0/1314
62	N6	0.51	0/1004	0.69	0/1341
62	n6	0.45	0/1004	0.65	1/1341 (0.1%)
63	N7	0.40	0/1118	0.58	0/1497
63	n7	0.36	0/1118	0.53	0/1497
64	N8	0.54	0/1204	0.71	0/1612
64	n8	0.55	0/1204	0.71	0/1612
65	N9	0.48	0/473	0.68	1/629 (0.2%)
65	n9	0.54	0/473	0.82	1/629 (0.2%)
66	O0	0.38	0/751	0.51	0/1008
66	o0	0.40	0/775	0.58	1/1040 (0.1%)
67	O1	0.43	0/890	0.58	0/1196
67	o1	0.52	0/904	0.63	0/1213
68	O2	0.53	0/1041	0.67	0/1394
68	o2	0.57	0/1041	0.66	0/1394
69	O3	0.59	0/868	0.63	0/1168
69	o3	0.60	0/868	0.69	0/1168
70	O4	0.43	0/890	0.61	1/1189 (0.1%)
70	o4	0.43	0/891	0.63	0/1191
71	O5	0.49	0/978	0.64	0/1301
71	o5	0.42	0/978	0.54	0/1301
72	O6	0.46	0/778	0.62	0/1034
72	o6	0.43	0/778	0.58	0/1034
73	O7	0.57	0/696	0.70	1/923 (0.1%)
73	o7	0.49	0/696	0.66	0/923
74	O8	0.39	0/618	0.57	0/826
74	o8	0.34	0/618	0.50	0/826
75	O9	0.55	0/443	0.72	0/588
75	o9	0.47	0/443	0.66	0/588
76	Q0	0.52	0/423	0.69	0/562
76	q0	0.64	0/423	0.74	0/562
77	Q1	0.43	0/234	0.60	0/300
77	q1	0.49	0/234	0.71	0/300
78	Q2	0.65	1/860 (0.1%)	0.72	0/1136
78	q2	0.58	1/860 (0.1%)	0.69	1/1136 (0.1%)
79	Q3	0.52	0/701	0.66	0/934
79	q3	0.52	0/701	0.66	0/934
81	p0	0.34	0/1092	0.52	0/1474
All	All	0.62	15/430516 (0.0%)	0.98	865/632094 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	s5	0	1
9	S7	0	1
17	c5	0	1
19	C7	0	1
26	d4	0	1
27	D5	0	1
28	D6	0	1
44	l7	0	2
52	M6	0	1
56	N0	0	2
59	n3	0	1
64	n8	0	1
79	q3	0	1
All	All	0	15

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	11.25	2.01	1.82
36	5	1152	G	N9-C4	-9.21	1.30	1.38
78	q2	17	CYS	CB-SG	8.36	1.96	1.82
36	5	1152	G	N3-C4	-6.38	1.30	1.35
36	5	2941	A	N9-C4	-6.19	1.34	1.37

The worst 5 of 865 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-17.27	115.64	126.00
36	5	1152	G	N3-C4-C5	16.41	136.81	128.60
36	5	1152	G	C2-N3-C4	-11.50	106.15	111.90
36	1	2617	U	N3-C2-O2	-10.99	114.51	122.20
36	5	1307	G	P-O3'-C3'	10.06	131.77	119.70

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	C7	85	VAL	Peptide

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Mol	Chain	Res	Type	Group
27	D5	94	LYS	Peptide
28	D6	10	ARG	Peptide
52	M6	110	PRO	Peptide
9	S7	131	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37970	0	19104	888	1
1	6	38260	0	19251	812	0
2	S0	1577	0	1567	136	0
2	s0	1612	0	1623	0	0
3	S1	1709	0	1784	153	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	106	0
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	95	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	150	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	138	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	126	0
8	s6	1755	0	1845	0	0
9	S7	1481	0	1572	106	0
9	s7	1492	0	1581	0	0
10	S8	1489	0	1525	102	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	124	0
11	s9	1494	0	1573	0	0
12	C0	773	0	716	59	0
12	c0	762	0	691	0	0
13	C1	1214	0	1245	71	0
13	c1	1169	0	1235	0	0
14	C2	890	0	887	53	0
14	c2	890	0	887	0	0
15	C3	1192	0	1255	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	c3	1192	0	1255	0	0
16	C4	891	0	883	75	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	74	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	103	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	62	0
19	c7	944	0	1006	0	0
20	C8	1192	0	1222	105	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	86	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	69	0
22	d0	882	0	939	0	0
23	D1	684	0	672	56	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	64	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	87	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	69	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	57	0
27	d5	558	0	598	0	0
28	D6	769	0	814	81	0
28	d6	769	0	814	0	0
29	D7	610	0	631	30	0
29	d7	610	0	631	0	0
30	D8	497	0	535	43	0
30	d8	497	0	535	0	0
31	D9	442	0	428	26	0
31	d9	443	0	432	0	0
32	E0	475	0	525	46	0
32	e0	491	0	542	0	0
33	E1	566	0	602	48	0
33	e1	608	0	657	0	0
34	SR	2437	0	2386	157	0
34	sR	2445	0	2401	0	0
35	SM	1104	0	971	66	0
35	sM	680	0	539	0	0
36	1	67355	0	33846	1296	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	5	67377	0	33857	1249	1
37	3	2579	0	1304	54	0
37	7	2579	0	1304	59	0
38	4	3353	0	1695	71	0
38	8	3353	0	1695	84	0
39	L2	1914	0	1981	157	0
39	l2	1918	0	1987	0	0
40	L3	3067	0	3137	205	0
40	l3	3073	0	3160	0	0
41	L4	2748	0	2859	212	0
41	l4	2749	0	2863	0	0
42	L5	2375	0	2325	187	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	57	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	114	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	121	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	131	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1736	131	0
47	m0	1733	0	1776	0	0
48	M1	1353	0	1383	96	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	118	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	65	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	125	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	102	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	115	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	102	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	71	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	86	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	n1	1276	0	1323	0	0
58	N2	796	0	812	41	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	62	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	26	0
60	n4	1089	0	1183	0	0
61	N5	964	0	1025	62	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	69	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	76	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	114	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	37	0
65	n9	462	0	491	0	0
66	O0	743	0	797	59	0
66	o0	767	0	816	0	0
67	O1	876	0	912	46	0
67	o1	890	0	938	0	0
68	O2	1020	0	1090	71	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	44	0
69	o3	850	0	880	0	0
70	O4	880	0	945	73	0
70	o4	881	0	949	0	0
71	O5	969	0	1078	74	0
71	o5	969	0	1078	0	0
72	O6	771	0	849	65	0
72	o6	771	0	849	0	0
73	O7	681	0	683	45	0
73	o7	681	0	683	0	0
74	O8	612	0	682	40	0
74	o8	612	0	682	0	0
75	O9	436	0	475	33	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	24	0
76	q0	417	0	455	0	0
77	Q1	233	0	284	18	0
77	q1	233	0	284	0	0
78	Q2	847	0	914	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
78	q2	847	0	914	0	0
79	Q3	694	0	734	63	0
79	q3	694	0	734	0	0
80	m2	750	0	176	0	0
81	p0	1077	0	1041	0	0
82	p1	235	0	50	0	0
83	p2	230	0	50	0	0
84	1	330	0	0	0	0
84	2	82	0	0	0	0
84	3	10	0	0	0	0
84	4	14	0	0	0	0
84	5	349	0	0	0	0
84	6	110	0	0	0	0
84	7	10	0	0	0	0
84	8	10	0	0	0	0
84	D9	1	0	0	0	0
84	L2	2	0	0	0	0
84	L3	1	0	0	0	0
84	L6	1	0	0	0	0
84	L7	1	0	0	0	0
84	M0	1	0	0	0	0
84	M3	1	0	0	0	0
84	M5	1	0	0	0	0
84	M6	1	0	0	0	0
84	M7	4	0	0	0	0
84	N3	1	0	0	0	0
84	N8	2	0	0	0	0
84	O2	1	0	0	0	0
84	O3	1	0	0	0	0
84	O4	2	0	0	0	0
84	O7	2	0	0	0	0
84	Q2	1	0	0	0	0
84	S4	1	0	0	0	0
84	SM	1	0	0	0	0
84	c1	1	0	0	0	0
84	d6	1	0	0	0	0
84	l2	3	0	0	0	0
84	l3	5	0	0	0	0
84	l6	1	0	0	0	0
84	l7	1	0	0	0	0
84	l8	1	0	0	0	0
84	l9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	m1	1	0	0	0	0
84	m5	3	0	0	0	0
84	m6	1	0	0	0	0
84	m7	3	0	0	0	0
84	n0	2	0	0	0	0
84	n3	1	0	0	0	0
84	n6	2	0	0	0	0
84	n8	2	0	0	0	0
84	n9	1	0	0	0	0
84	o1	1	0	0	0	0
84	o3	1	0	0	0	0
84	o4	1	0	0	0	0
84	q0	1	0	0	0	0
84	q1	1	0	0	0	0
84	s8	1	0	0	0	0
84	sM	2	0	0	0	0
85	1	2191	0	0	228	0
85	2	959	0	0	120	0
85	3	70	0	0	5	0
85	4	119	0	0	10	0
85	5	2303	0	0	247	0
85	6	1050	0	0	107	0
85	7	77	0	0	7	0
85	8	105	0	0	15	0
85	C3	7	0	0	3	0
85	C5	7	0	0	3	0
85	C8	7	0	0	0	1
85	D9	7	0	0	3	0
85	L3	14	0	0	2	0
85	L4	7	0	0	5	0
85	M0	7	0	0	0	0
85	M5	7	0	0	0	0
85	M6	7	0	0	0	0
85	M7	7	0	0	1	0
85	M9	7	0	0	1	0
85	N1	7	0	0	0	0
85	N8	7	0	0	0	0
85	N9	7	0	0	0	0
85	O3	7	0	0	2	0
85	O7	14	0	0	1	0
85	O9	7	0	0	2	0
85	Q2	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	S6	7	0	0	1	0
85	S8	7	0	0	1	0
85	SR	7	0	0	0	0
85	c3	7	0	0	0	0
85	c5	7	0	0	0	0
85	c8	7	0	0	0	0
85	d4	7	0	0	0	0
85	l3	21	0	0	0	0
85	l4	14	0	0	0	0
85	l5	14	0	0	0	0
85	l9	7	0	0	0	0
85	m0	14	0	0	0	0
85	m1	7	0	0	0	0
85	m5	14	0	0	0	0
85	m7	7	0	0	0	0
85	n3	14	0	0	0	0
85	n9	7	0	0	0	0
85	o3	7	0	0	0	0
85	o7	7	0	0	0	0
85	o9	7	0	0	0	0
85	q2	7	0	0	0	0
85	s4	7	0	0	0	0
85	s8	7	0	0	0	0
85	s9	7	0	0	0	0
85	sR	7	0	0	0	0
86	D6	1	0	0	0	0
86	D7	1	0	0	0	0
86	D9	1	0	0	0	0
86	E1	1	0	0	0	0
86	O7	1	0	0	0	0
86	Q0	1	0	0	0	0
86	Q2	1	0	0	0	0
86	Q3	1	0	0	0	0
86	d6	1	0	0	0	0
86	d7	1	0	0	0	0
86	d9	1	0	0	0	0
86	e1	1	0	0	0	0
86	o7	1	0	0	0	0
86	q0	1	0	0	0	0
86	q2	1	0	0	0	0
86	q3	1	0	0	0	0
87	1	19	0	19	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	410912	0	297885	9383	2

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

The worst 5 of 9383 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1:1149:G:N7	85:1:4017:OHX:N6	2.05	1.04
1:6:1537:C:N3	85:6:2121:OHX:N5	2.06	1.03
36:1:1466:G:O6	85:1:3739:OHX:N4	1.93	1.01
36:1:1481:A:O2'	36:1:1858:A:N3	1.91	1.01
47:M0:38:LYS:HG2	47:M0:41:ALA:HB2	2.79	1.00

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1353:U:O2'	36:5:3165:A:OP1[2_546]	2.08	0.12
36:1:3195:U:OP1	85:C8:201:OHX:N6[2_555]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	157 (77%)	31 (15%)	16 (8%)	1	5
2	s0	204/251 (81%)	150 (74%)	39 (19%)	15 (7%)	1	6
3	S1	212/254 (84%)	155 (73%)	31 (15%)	26 (12%)	0	1
3	s1	214/254 (84%)	170 (79%)	28 (13%)	16 (8%)	1	6
4	S2	215/253 (85%)	180 (84%)	21 (10%)	14 (6%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	s2	215/253 (85%)	173 (80%)	32 (15%)	10 (5%)	2	14
5	S3	221/239 (92%)	187 (85%)	26 (12%)	8 (4%)	3	20
5	s3	221/239 (92%)	179 (81%)	29 (13%)	13 (6%)	1	10
6	S4	258/260 (99%)	205 (80%)	38 (15%)	15 (6%)	1	10
6	s4	258/260 (99%)	215 (83%)	23 (9%)	20 (8%)	1	5
7	S5	204/224 (91%)	155 (76%)	32 (16%)	17 (8%)	1	5
7	s5	204/224 (91%)	154 (76%)	37 (18%)	13 (6%)	1	8
8	S6	224/236 (95%)	187 (84%)	26 (12%)	11 (5%)	2	14
8	s6	216/236 (92%)	189 (88%)	18 (8%)	9 (4%)	3	16
9	S7	182/189 (96%)	133 (73%)	32 (18%)	17 (9%)	0	3
9	s7	184/189 (97%)	152 (83%)	22 (12%)	10 (5%)	2	12
10	S8	184/200 (92%)	158 (86%)	18 (10%)	8 (4%)	2	16
10	s8	184/200 (92%)	150 (82%)	29 (16%)	5 (3%)	5	25
11	S9	183/196 (93%)	142 (78%)	35 (19%)	6 (3%)	4	21
11	s9	183/196 (93%)	145 (79%)	32 (18%)	6 (3%)	4	21
12	C0	83/96 (86%)	71 (86%)	9 (11%)	3 (4%)	3	20
12	c0	82/96 (85%)	61 (74%)	11 (13%)	10 (12%)	0	1
13	C1	145/155 (94%)	121 (83%)	16 (11%)	8 (6%)	2	11
13	c1	144/155 (93%)	118 (82%)	21 (15%)	5 (4%)	3	20
14	C2	122/142 (86%)	72 (59%)	31 (25%)	19 (16%)	0	0
14	c2	122/142 (86%)	72 (59%)	33 (27%)	17 (14%)	0	1
15	C3	148/150 (99%)	130 (88%)	12 (8%)	6 (4%)	3	16
15	c3	148/150 (99%)	119 (80%)	21 (14%)	8 (5%)	2	12
16	C4	125/136 (92%)	99 (79%)	14 (11%)	12 (10%)	0	3
16	c4	126/136 (93%)	99 (79%)	17 (14%)	10 (8%)	1	5
17	C5	122/141 (86%)	89 (73%)	25 (20%)	8 (7%)	1	7
17	c5	133/141 (94%)	98 (74%)	17 (13%)	18 (14%)	0	1
18	C6	139/142 (98%)	111 (80%)	21 (15%)	7 (5%)	2	13
18	c6	140/142 (99%)	122 (87%)	10 (7%)	8 (6%)	1	10
19	C7	116/136 (85%)	83 (72%)	26 (22%)	7 (6%)	1	9
19	c7	113/136 (83%)	89 (79%)	16 (14%)	8 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	C8	143/145 (99%)	116 (81%)	14 (10%)	13 (9%)	1	4
20	c8	143/145 (99%)	117 (82%)	15 (10%)	11 (8%)	1	5
21	C9	141/143 (99%)	114 (81%)	20 (14%)	7 (5%)	2	13
21	c9	141/143 (99%)	119 (84%)	17 (12%)	5 (4%)	3	20
22	D0	105/120 (88%)	89 (85%)	10 (10%)	6 (6%)	1	10
22	d0	108/120 (90%)	81 (75%)	20 (18%)	7 (6%)	1	8
23	D1	85/87 (98%)	60 (71%)	15 (18%)	10 (12%)	0	1
23	d1	85/87 (98%)	69 (81%)	13 (15%)	3 (4%)	3	20
24	D2	127/129 (98%)	108 (85%)	17 (13%)	2 (2%)	9	37
24	d2	127/129 (98%)	113 (89%)	12 (9%)	2 (2%)	9	37
25	D3	142/144 (99%)	110 (78%)	19 (13%)	13 (9%)	1	4
25	d3	142/144 (99%)	127 (89%)	12 (8%)	3 (2%)	7	30
26	D4	132/134 (98%)	101 (76%)	19 (14%)	12 (9%)	1	4
26	d4	132/134 (98%)	102 (77%)	20 (15%)	10 (8%)	1	5
27	D5	68/107 (64%)	48 (71%)	15 (22%)	5 (7%)	1	6
27	d5	67/107 (63%)	54 (81%)	9 (13%)	4 (6%)	1	9
28	D6	95/97 (98%)	59 (62%)	23 (24%)	13 (14%)	0	1
28	d6	95/97 (98%)	71 (75%)	17 (18%)	7 (7%)	1	6
29	D7	79/81 (98%)	60 (76%)	16 (20%)	3 (4%)	3	19
29	d7	79/81 (98%)	65 (82%)	10 (13%)	4 (5%)	2	13
30	D8	61/66 (92%)	47 (77%)	10 (16%)	4 (7%)	1	7
30	d8	61/66 (92%)	48 (79%)	8 (13%)	5 (8%)	1	5
31	D9	51/55 (93%)	35 (69%)	12 (24%)	4 (8%)	1	5
31	d9	51/55 (93%)	43 (84%)	4 (8%)	4 (8%)	1	5
32	E0	58/62 (94%)	43 (74%)	12 (21%)	3 (5%)	2	12
32	e0	60/62 (97%)	46 (77%)	8 (13%)	6 (10%)	0	3
33	E1	69/76 (91%)	40 (58%)	13 (19%)	16 (23%)	0	0
33	e1	74/76 (97%)	34 (46%)	21 (28%)	19 (26%)	0	0
34	SR	316/318 (99%)	264 (84%)	38 (12%)	14 (4%)	2	15
34	sR	316/318 (99%)	266 (84%)	38 (12%)	12 (4%)	3	19
35	SM	131/182 (72%)	99 (76%)	18 (14%)	14 (11%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	sM	61/182 (34%)	39 (64%)	13 (21%)	9 (15%)	0	0
39	L2	250/253 (99%)	218 (87%)	24 (10%)	8 (3%)	4	22
39	l2	250/253 (99%)	213 (85%)	23 (9%)	14 (6%)	2	11
40	L3	384/386 (100%)	329 (86%)	48 (12%)	7 (2%)	8	34
40	l3	384/386 (100%)	346 (90%)	28 (7%)	10 (3%)	5	26
41	L4	359/361 (99%)	301 (84%)	38 (11%)	20 (6%)	2	11
41	l4	359/361 (99%)	289 (80%)	49 (14%)	21 (6%)	1	10
42	L5	294/296 (99%)	232 (79%)	41 (14%)	21 (7%)	1	6
42	l5	292/296 (99%)	249 (85%)	33 (11%)	10 (3%)	3	21
43	L6	152/175 (87%)	135 (89%)	15 (10%)	2 (1%)	12	42
43	l6	153/175 (87%)	130 (85%)	17 (11%)	6 (4%)	3	18
44	L7	220/243 (90%)	194 (88%)	20 (9%)	6 (3%)	5	25
44	l7	221/243 (91%)	199 (90%)	17 (8%)	5 (2%)	6	28
45	L8	231/255 (91%)	182 (79%)	34 (15%)	15 (6%)	1	8
45	l8	229/255 (90%)	178 (78%)	38 (17%)	13 (6%)	1	10
46	L9	189/191 (99%)	162 (86%)	23 (12%)	4 (2%)	7	30
46	l9	189/191 (99%)	170 (90%)	17 (9%)	2 (1%)	14	46
47	M0	207/220 (94%)	169 (82%)	28 (14%)	10 (5%)	2	14
47	m0	209/220 (95%)	168 (80%)	32 (15%)	9 (4%)	2	16
48	M1	167/173 (96%)	126 (75%)	24 (14%)	17 (10%)	0	3
48	m1	167/173 (96%)	142 (85%)	13 (8%)	12 (7%)	1	6
49	M3	191/198 (96%)	152 (80%)	26 (14%)	13 (7%)	1	7
49	m3	192/198 (97%)	157 (82%)	19 (10%)	16 (8%)	1	5
50	M4	134/137 (98%)	113 (84%)	14 (10%)	7 (5%)	2	12
50	m4	135/137 (98%)	116 (86%)	17 (13%)	2 (2%)	10	39
51	M5	201/203 (99%)	185 (92%)	10 (5%)	6 (3%)	4	23
51	m5	201/203 (99%)	179 (89%)	14 (7%)	8 (4%)	3	17
52	M6	195/198 (98%)	173 (89%)	17 (9%)	5 (3%)	5	26
52	m6	195/198 (98%)	183 (94%)	11 (6%)	1 (0%)	29	64
53	M7	181/183 (99%)	154 (85%)	20 (11%)	7 (4%)	3	18
53	m7	153/183 (84%)	134 (88%)	16 (10%)	3 (2%)	7	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	M8	183/185 (99%)	161 (88%)	17 (9%)	5 (3%)	5	25
54	m8	183/185 (99%)	149 (81%)	25 (14%)	9 (5%)	2	14
55	M9	186/188 (99%)	165 (89%)	20 (11%)	1 (0%)	29	64
55	m9	186/188 (99%)	165 (89%)	19 (10%)	2 (1%)	14	46
56	N0	170/172 (99%)	156 (92%)	10 (6%)	4 (2%)	6	27
56	n0	170/172 (99%)	154 (91%)	14 (8%)	2 (1%)	13	44
57	N1	157/159 (99%)	137 (87%)	17 (11%)	3 (2%)	8	33
57	n1	157/159 (99%)	141 (90%)	13 (8%)	3 (2%)	8	33
58	N2	98/120 (82%)	77 (79%)	18 (18%)	3 (3%)	4	23
58	n2	96/120 (80%)	80 (83%)	11 (12%)	5 (5%)	2	12
59	N3	134/136 (98%)	119 (89%)	12 (9%)	3 (2%)	6	29
59	n3	134/136 (98%)	123 (92%)	11 (8%)	0	100	100
60	N4	96/155 (62%)	68 (71%)	22 (23%)	6 (6%)	1	8
60	n4	133/155 (86%)	103 (77%)	23 (17%)	7 (5%)	2	12
61	N5	119/141 (84%)	99 (83%)	17 (14%)	3 (2%)	5	27
61	n5	118/141 (84%)	93 (79%)	16 (14%)	9 (8%)	1	5
62	N6	124/126 (98%)	106 (86%)	15 (12%)	3 (2%)	6	27
62	n6	124/126 (98%)	106 (86%)	13 (10%)	5 (4%)	3	17
63	N7	133/135 (98%)	109 (82%)	17 (13%)	7 (5%)	2	12
63	n7	133/135 (98%)	109 (82%)	13 (10%)	11 (8%)	1	5
64	N8	146/148 (99%)	121 (83%)	15 (10%)	10 (7%)	1	7
64	n8	146/148 (99%)	122 (84%)	17 (12%)	7 (5%)	2	14
65	N9	56/58 (97%)	47 (84%)	8 (14%)	1 (2%)	8	34
65	n9	56/58 (97%)	44 (79%)	6 (11%)	6 (11%)	0	2
66	O0	95/104 (91%)	84 (88%)	11 (12%)	0	100	100
66	o0	98/104 (94%)	84 (86%)	10 (10%)	4 (4%)	3	16
67	O1	107/112 (96%)	95 (89%)	7 (6%)	5 (5%)	2	14
67	o1	107/112 (96%)	92 (86%)	10 (9%)	5 (5%)	2	14
68	O2	125/129 (97%)	104 (83%)	14 (11%)	7 (6%)	2	11
68	o2	125/129 (97%)	105 (84%)	16 (13%)	4 (3%)	4	22
69	O3	104/106 (98%)	95 (91%)	8 (8%)	1 (1%)	15	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	o3	104/106 (98%)	94 (90%)	9 (9%)	1 (1%)	15	49
70	O4	110/120 (92%)	92 (84%)	16 (14%)	2 (2%)	8	34
70	o4	110/120 (92%)	96 (87%)	8 (7%)	6 (6%)	2	11
71	O5	117/119 (98%)	100 (86%)	12 (10%)	5 (4%)	2	16
71	o5	117/119 (98%)	100 (86%)	14 (12%)	3 (3%)	5	26
72	O6	97/99 (98%)	77 (79%)	12 (12%)	8 (8%)	1	5
72	o6	97/99 (98%)	82 (84%)	10 (10%)	5 (5%)	2	12
73	O7	85/87 (98%)	72 (85%)	13 (15%)	0	100	100
73	o7	85/87 (98%)	68 (80%)	12 (14%)	5 (6%)	1	10
74	O8	75/77 (97%)	64 (85%)	9 (12%)	2 (3%)	5	25
74	o8	75/77 (97%)	59 (79%)	13 (17%)	3 (4%)	3	17
75	O9	48/50 (96%)	41 (85%)	6 (12%)	1 (2%)	7	30
75	o9	48/50 (96%)	41 (85%)	6 (12%)	1 (2%)	7	30
76	Q0	50/52 (96%)	39 (78%)	9 (18%)	2 (4%)	3	17
76	q0	50/52 (96%)	48 (96%)	1 (2%)	1 (2%)	7	31
77	Q1	23/25 (92%)	20 (87%)	3 (13%)	0	100	100
77	q1	23/25 (92%)	23 (100%)	0	0	100	100
78	Q2	103/105 (98%)	82 (80%)	14 (14%)	7 (7%)	1	7
78	q2	103/105 (98%)	95 (92%)	6 (6%)	2 (2%)	8	33
79	Q3	89/91 (98%)	67 (75%)	15 (17%)	7 (8%)	1	5
79	q3	89/91 (98%)	78 (88%)	7 (8%)	4 (4%)	2	15
81	p0	139/311 (45%)	117 (84%)	16 (12%)	6 (4%)	2	16
All	All	22243/23945 (93%)	18323 (82%)	2769 (12%)	1151 (5%)	2	12

5 of 1151 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	158	VAL
2	S0	187	ALA
2	S0	191	ARG
2	S0	194	PRO

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%)	139 (85%)	25 (15%)	3	12
2	s0	173/209 (83%)	145 (84%)	28 (16%)	2	10
3	S1	191/223 (86%)	166 (87%)	25 (13%)	4	17
3	s1	192/223 (86%)	161 (84%)	31 (16%)	2	10
4	S2	176/204 (86%)	148 (84%)	28 (16%)	2	11
4	s2	176/204 (86%)	137 (78%)	39 (22%)	1	4
5	S3	182/194 (94%)	149 (82%)	33 (18%)	1	7
5	s3	182/194 (94%)	160 (88%)	22 (12%)	5	20
6	S4	221/221 (100%)	186 (84%)	35 (16%)	2	11
6	s4	221/221 (100%)	182 (82%)	39 (18%)	2	8
7	S5	173/190 (91%)	141 (82%)	32 (18%)	1	7
7	s5	173/190 (91%)	147 (85%)	26 (15%)	3	12
8	S6	188/201 (94%)	152 (81%)	36 (19%)	1	6
8	s6	187/201 (93%)	156 (83%)	31 (17%)	2	9
9	S7	165/169 (98%)	136 (82%)	29 (18%)	2	8
9	s7	166/169 (98%)	141 (85%)	25 (15%)	3	12
10	S8	150/161 (93%)	129 (86%)	21 (14%)	3	15
10	s8	150/161 (93%)	131 (87%)	19 (13%)	4	18
11	S9	158/165 (96%)	128 (81%)	30 (19%)	1	6
11	s9	158/165 (96%)	138 (87%)	20 (13%)	4	18
12	C0	77/78 (99%)	64 (83%)	13 (17%)	2	9
12	c0	73/78 (94%)	64 (88%)	9 (12%)	4	19
13	C1	129/129 (100%)	114 (88%)	15 (12%)	5	22
13	c1	129/129 (100%)	106 (82%)	23 (18%)	2	8
14	C2	88/118 (75%)	71 (81%)	17 (19%)	1	6
14	c2	88/118 (75%)	71 (81%)	17 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	C3	127/127 (100%)	104 (82%)	23 (18%)	1	7
15	c3	127/127 (100%)	103 (81%)	24 (19%)	1	6
16	C4	81/104 (78%)	64 (79%)	17 (21%)	1	5
16	c4	97/104 (93%)	78 (80%)	19 (20%)	1	6
17	C5	101/117 (86%)	87 (86%)	14 (14%)	3	15
17	c5	103/117 (88%)	90 (87%)	13 (13%)	4	18
18	C6	117/118 (99%)	98 (84%)	19 (16%)	2	10
18	c6	118/118 (100%)	101 (86%)	17 (14%)	3	14
19	C7	94/124 (76%)	75 (80%)	19 (20%)	1	5
19	c7	106/124 (86%)	91 (86%)	15 (14%)	3	14
20	C8	128/128 (100%)	102 (80%)	26 (20%)	1	5
20	c8	128/128 (100%)	102 (80%)	26 (20%)	1	5
21	C9	115/115 (100%)	93 (81%)	22 (19%)	1	6
21	c9	115/115 (100%)	98 (85%)	17 (15%)	3	13
22	D0	100/113 (88%)	83 (83%)	17 (17%)	2	9
22	d0	103/113 (91%)	79 (77%)	24 (23%)	1	3
23	D1	74/74 (100%)	62 (84%)	12 (16%)	2	10
23	d1	74/74 (100%)	64 (86%)	10 (14%)	4	16
24	D2	110/110 (100%)	91 (83%)	19 (17%)	2	9
24	d2	110/110 (100%)	95 (86%)	15 (14%)	3	16
25	D3	119/119 (100%)	103 (87%)	16 (13%)	4	16
25	d3	119/119 (100%)	103 (87%)	16 (13%)	4	16
26	D4	112/112 (100%)	96 (86%)	16 (14%)	3	14
26	d4	112/112 (100%)	96 (86%)	16 (14%)	3	14
27	D5	61/88 (69%)	45 (74%)	16 (26%)	0	1
27	d5	61/88 (69%)	56 (92%)	5 (8%)	11	38
28	D6	83/83 (100%)	63 (76%)	20 (24%)	0	2
28	d6	83/83 (100%)	73 (88%)	10 (12%)	5	20
29	D7	70/70 (100%)	58 (83%)	12 (17%)	2	9
29	d7	70/70 (100%)	61 (87%)	9 (13%)	4	18
30	D8	56/59 (95%)	45 (80%)	11 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	d8	56/59 (95%)	47 (84%)	9 (16%)	2	10
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2	9
31	d9	47/48 (98%)	42 (89%)	5 (11%)	6	26
32	E0	51/53 (96%)	45 (88%)	6 (12%)	5	21
32	e0	53/53 (100%)	41 (77%)	12 (23%)	1	3
33	E1	62/66 (94%)	48 (77%)	14 (23%)	1	3
33	e1	66/66 (100%)	54 (82%)	12 (18%)	1	7
34	SR	259/261 (99%)	226 (87%)	33 (13%)	4	18
34	sR	261/261 (100%)	238 (91%)	23 (9%)	10	36
35	SM	97/115 (84%)	77 (79%)	20 (21%)	1	5
35	sM	54/115 (47%)	43 (80%)	11 (20%)	1	5
39	L2	193/195 (99%)	152 (79%)	41 (21%)	1	5
39	l2	194/195 (100%)	160 (82%)	34 (18%)	2	8
40	L3	320/322 (99%)	256 (80%)	64 (20%)	1	5
40	l3	322/322 (100%)	270 (84%)	52 (16%)	2	10
41	L4	288/288 (100%)	237 (82%)	51 (18%)	2	8
41	l4	288/288 (100%)	244 (85%)	44 (15%)	2	12
42	L5	244/244 (100%)	207 (85%)	37 (15%)	3	12
42	l5	243/244 (100%)	202 (83%)	41 (17%)	2	9
43	L6	134/152 (88%)	115 (86%)	19 (14%)	3	14
43	l6	135/152 (89%)	112 (83%)	23 (17%)	2	9
44	L7	186/204 (91%)	169 (91%)	17 (9%)	9	33
44	l7	187/204 (92%)	163 (87%)	24 (13%)	4	18
45	L8	187/207 (90%)	163 (87%)	24 (13%)	4	18
45	l8	177/207 (86%)	146 (82%)	31 (18%)	2	8
46	L9	171/171 (100%)	134 (78%)	37 (22%)	1	4
46	l9	171/171 (100%)	133 (78%)	38 (22%)	1	4
47	M0	177/186 (95%)	146 (82%)	31 (18%)	2	8
47	m0	182/186 (98%)	151 (83%)	31 (17%)	2	9
48	M1	147/149 (99%)	117 (80%)	30 (20%)	1	5
48	m1	147/149 (99%)	119 (81%)	28 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	M3	154/158 (98%)	133 (86%)	21 (14%)	3	16
49	m3	154/158 (98%)	134 (87%)	20 (13%)	4	18
50	M4	107/108 (99%)	91 (85%)	16 (15%)	3	12
50	m4	108/108 (100%)	93 (86%)	15 (14%)	3	15
51	M5	175/175 (100%)	144 (82%)	31 (18%)	2	8
51	m5	175/175 (100%)	154 (88%)	21 (12%)	5	20
52	M6	160/161 (99%)	138 (86%)	22 (14%)	3	16
52	m6	160/161 (99%)	138 (86%)	22 (14%)	3	16
53	M7	140/145 (97%)	119 (85%)	21 (15%)	3	12
53	m7	125/145 (86%)	110 (88%)	15 (12%)	5	20
54	M8	150/150 (100%)	127 (85%)	23 (15%)	2	12
54	m8	150/150 (100%)	129 (86%)	21 (14%)	3	15
55	M9	153/153 (100%)	134 (88%)	19 (12%)	4	19
55	m9	153/153 (100%)	122 (80%)	31 (20%)	1	5
56	N0	156/156 (100%)	131 (84%)	25 (16%)	2	11
56	n0	156/156 (100%)	127 (81%)	29 (19%)	1	7
57	N1	136/136 (100%)	110 (81%)	26 (19%)	1	6
57	n1	136/136 (100%)	108 (79%)	28 (21%)	1	5
58	N2	87/106 (82%)	78 (90%)	9 (10%)	7	27
58	n2	85/106 (80%)	71 (84%)	14 (16%)	2	10
59	N3	104/104 (100%)	88 (85%)	16 (15%)	2	11
59	n3	104/104 (100%)	93 (89%)	11 (11%)	6	26
60	N4	57/129 (44%)	51 (90%)	6 (10%)	7	26
60	n4	114/129 (88%)	99 (87%)	15 (13%)	4	17
61	N5	104/117 (89%)	81 (78%)	23 (22%)	1	4
61	n5	104/117 (89%)	88 (85%)	16 (15%)	2	11
62	N6	109/109 (100%)	91 (84%)	18 (16%)	2	10
62	n6	109/109 (100%)	92 (84%)	17 (16%)	2	11
63	N7	115/115 (100%)	97 (84%)	18 (16%)	2	11
63	n7	115/115 (100%)	93 (81%)	22 (19%)	1	6
64	N8	118/118 (100%)	93 (79%)	25 (21%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	n8	118/118 (100%)	96 (81%)	22 (19%)	1	7
65	N9	46/46 (100%)	37 (80%)	9 (20%)	1	6
65	n9	46/46 (100%)	38 (83%)	8 (17%)	2	9
66	O0	81/87 (93%)	63 (78%)	18 (22%)	1	4
66	o0	84/87 (97%)	67 (80%)	17 (20%)	1	5
67	O1	92/96 (96%)	74 (80%)	18 (20%)	1	6
67	o1	96/96 (100%)	80 (83%)	16 (17%)	2	9
68	O2	109/110 (99%)	93 (85%)	16 (15%)	3	13
68	o2	109/110 (99%)	88 (81%)	21 (19%)	1	6
69	O3	90/90 (100%)	81 (90%)	9 (10%)	7	28
69	o3	90/90 (100%)	80 (89%)	10 (11%)	6	24
70	O4	95/102 (93%)	81 (85%)	14 (15%)	3	13
70	o4	95/102 (93%)	81 (85%)	14 (15%)	3	13
71	O5	104/104 (100%)	85 (82%)	19 (18%)	1	7
71	o5	104/104 (100%)	86 (83%)	18 (17%)	2	9
72	O6	81/81 (100%)	64 (79%)	17 (21%)	1	5
72	o6	81/81 (100%)	55 (68%)	26 (32%)	0	0
73	O7	70/70 (100%)	56 (80%)	14 (20%)	1	5
73	o7	70/70 (100%)	59 (84%)	11 (16%)	2	11
74	O8	68/68 (100%)	56 (82%)	12 (18%)	2	8
74	o8	68/68 (100%)	59 (87%)	9 (13%)	4	17
75	O9	45/45 (100%)	38 (84%)	7 (16%)	2	11
75	o9	45/45 (100%)	41 (91%)	4 (9%)	9	34
76	Q0	47/47 (100%)	40 (85%)	7 (15%)	3	13
76	q0	47/47 (100%)	35 (74%)	12 (26%)	0	1
77	Q1	23/23 (100%)	19 (83%)	4 (17%)	2	9
77	q1	23/23 (100%)	15 (65%)	8 (35%)	0	0
78	Q2	90/90 (100%)	74 (82%)	16 (18%)	2	8
78	q2	90/90 (100%)	76 (84%)	14 (16%)	2	11
79	Q3	71/71 (100%)	59 (83%)	12 (17%)	2	9
79	q3	71/71 (100%)	60 (84%)	11 (16%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
81	p0	105/253 (42%)	89 (85%)	16 (15%)	3	12
All	All	18777/19961 (94%)	15699 (84%)	3078 (16%)	2	10

5 of 3078 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
66	O0	89	VAL
7	s5	31	GLU
64	n8	8	THR
69	O3	58	GLU
2	s0	29	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
46	L9	156	GLN
74	O8	32	ASN
58	n2	101	ASN
51	M5	138	GLN
64	N8	28	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1777/1800 (98%)	461 (25%)	48 (2%)
1	6	1792/1800 (99%)	448 (25%)	45 (2%)
36	1	3145/3396 (92%)	658 (20%)	62 (1%)
36	5	3146/3396 (92%)	650 (20%)	68 (2%)
37	3	120/121 (99%)	13 (10%)	2 (1%)
37	7	120/121 (99%)	19 (15%)	1 (0%)
38	4	157/158 (99%)	37 (23%)	3 (1%)
38	8	157/158 (99%)	38 (24%)	1 (0%)
All	All	10414/10950 (95%)	2324 (22%)	230 (2%)

5 of 2324 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C

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Mol	Chain	Res	Type
1	2	25	C
1	2	26	A
1	2	27	U

5 of 230 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	3269	U
1	6	417	A
36	5	2873	U
36	1	3351	U
1	6	66	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2030 ligands modelled in this entry, 995 are monoatomic - leaving 1035 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	$\# Z > 2$
85	OHX	1	3893	-	0,6,6	0.00	-	-		
85	OHX	2	2052	-	0,6,6	0.00	-	-		
85	OHX	5	3789	-	0,6,6	0.00	-	-		
85	OHX	1	3733	-	0,6,6	0.00	-	-		
85	OHX	5	3817	-	0,6,6	0.00	-	-		
85	OHX	2	2043	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	2	2105	-	0,6,6	0.00	-	-		
85	OHX	6	2106	-	0,6,6	0.00	-	-		
85	OHX	6	2068	-	0,6,6	0.00	-	-		
85	OHX	1	3866	-	0,6,6	0.00	-	-		
85	OHX	m1	202	-	0,6,6	0.00	-	-		
85	OHX	5	3861	-	0,6,6	0.00	-	-		
85	OHX	5	3828	-	0,6,6	0.00	-	-		
85	OHX	5	4020	-	0,6,6	0.00	-	-		
85	OHX	5	3860	-	0,6,6	0.00	-	-		
85	OHX	6	2054	-	0,6,6	0.00	-	-		
85	OHX	6	2112	-	0,6,6	0.00	-	-		
85	OHX	5	3987	-	0,6,6	0.00	-	-		
85	OHX	5	3941	-	0,6,6	0.00	-	-		
85	OHX	4	218	-	0,6,6	0.00	-	-		
85	OHX	1	3942	-	0,6,6	0.00	-	-		
85	OHX	5	3771	-	0,6,6	0.00	-	-		
85	OHX	1	3774	-	0,6,6	0.00	-	-		
85	OHX	5	4068	-	0,6,6	0.00	-	-		
85	OHX	7	217	-	0,6,6	0.00	-	-		
85	OHX	4	228	-	0,6,6	0.00	-	-		
85	OHX	5	3927	-	0,6,6	0.00	-	-		
85	OHX	5	3772	-	0,6,6	0.00	-	-		
85	OHX	1	3858	-	0,6,6	0.00	-	-		
85	OHX	5	3930	-	0,6,6	0.00	-	-		
85	OHX	1	3811	-	0,6,6	0.00	-	-		
85	OHX	5	3757	-	0,6,6	0.00	-	-		
85	OHX	2	2028	-	0,6,6	0.00	-	-		
85	OHX	5	3818	-	0,6,6	0.00	-	-		
85	OHX	5	3812	-	0,6,6	0.00	-	-		
85	OHX	2	2118	-	0,6,6	0.00	-	-		
85	OHX	1	3825	-	0,6,6	0.00	-	-		
85	OHX	8	211	-	0,6,6	0.00	-	-		
85	OHX	1	3813	-	0,6,6	0.00	-	-		
85	OHX	5	3881	-	0,6,6	0.00	-	-		
85	OHX	1	4028	-	0,6,6	0.00	-	-		
85	OHX	5	3911	-	0,6,6	0.00	-	-		
85	OHX	1	3863	-	0,6,6	0.00	-	-		
85	OHX	2	2076	-	0,6,6	0.00	-	-		
85	OHX	5	3815	-	0,6,6	0.00	-	-		
85	OHX	1	3872	-	0,6,6	0.00	-	-		
85	OHX	1	3950	-	0,6,6	0.00	-	-		
85	OHX	1	3989	-	0,6,6	0.00	-	-		
85	OHX	6	2009	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	6	2145	-	0,6,6	0.00	-	-		
85	OHX	1	4024	-	0,6,6	0.00	-	-		
85	OHX	1	3756	-	0,6,6	0.00	-	-		
85	OHX	5	3973	-	0,6,6	0.00	-	-		
85	OHX	5	3893	-	0,6,6	0.00	-	-		
85	OHX	d4	201	-	0,6,6	0.00	-	-		
85	OHX	5	3765	-	0,6,6	0.00	-	-		
85	OHX	5	3923	-	0,6,6	0.00	-	-		
85	OHX	2	2085	-	0,6,6	0.00	-	-		
85	OHX	1	3920	-	0,6,6	0.00	-	-		
85	OHX	2	2108	-	0,6,6	0.00	-	-		
85	OHX	1	3895	-	0,6,6	0.00	-	-		
85	OHX	1	3775	-	0,6,6	0.00	-	-		
85	OHX	3	210	-	0,6,6	0.00	-	-		
85	OHX	6	2028	-	0,6,6	0.00	-	-		
85	OHX	5	3922	-	0,6,6	0.00	-	-		
85	OHX	5	3806	-	0,6,6	0.00	-	-		
85	OHX	1	3897	-	0,6,6	0.00	-	-		
85	OHX	1	3755	-	0,6,6	0.00	-	-		
85	OHX	6	2117	-	0,6,6	0.00	-	-		
85	OHX	5	3961	-	0,6,6	0.00	-	-		
85	OHX	1	3765	-	0,6,6	0.00	-	-		
85	OHX	6	2132	-	0,6,6	0.00	-	-		
85	OHX	6	2138	-	0,6,6	0.00	-	-		
85	OHX	1	3747	-	0,6,6	0.00	-	-		
85	OHX	1	3935	-	0,6,6	0.00	-	-		
85	OHX	2	2029	-	0,6,6	0.00	-	-		
85	OHX	1	3925	-	0,6,6	0.00	-	-		
85	OHX	2	1988	-	0,6,6	0.00	-	-		
85	OHX	1	3843	-	0,6,6	0.00	-	-		
85	OHX	2	1992	-	0,6,6	0.00	-	-		
85	OHX	1	3918	-	0,6,6	0.00	-	-		
85	OHX	1	3739	-	0,6,6	0.00	-	-		
85	OHX	6	2044	-	0,6,6	0.00	-	-		
85	OHX	6	2085	-	0,6,6	0.00	-	-		
85	OHX	2	2062	-	0,6,6	0.00	-	-		
85	OHX	5	3879	-	0,6,6	0.00	-	-		
85	OHX	1	3750	-	0,6,6	0.00	-	-		
85	OHX	1	4001	-	0,6,6	0.00	-	-		
85	OHX	c3	201	-	0,6,6	0.00	-	-		
85	OHX	1	3766	-	0,6,6	0.00	-	-		
85	OHX	1	3763	-	0,6,6	0.00	-	-		
85	OHX	5	3844	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	5	4032	-	0,6,6	0.00	-	-		
85	OHX	1	3799	-	0,6,6	0.00	-	-		
85	OHX	5	3932	-	0,6,6	0.00	-	-		
85	OHX	2	2058	-	0,6,6	0.00	-	-		
85	OHX	5	3993	-	0,6,6	0.00	-	-		
85	OHX	1	3792	-	0,6,6	0.00	-	-		
85	OHX	6	2144	-	0,6,6	0.00	-	-		
85	OHX	5	4021	-	0,6,6	0.00	-	-		
85	OHX	6	2039	-	0,6,6	0.00	-	-		
85	OHX	5	3986	-	0,6,6	0.00	-	-		
85	OHX	6	2022	-	0,6,6	0.00	-	-		
85	OHX	5	3891	-	0,6,6	0.00	-	-		
85	OHX	5	3769	-	0,6,6	0.00	-	-		
85	OHX	1	3840	-	0,6,6	0.00	-	-		
85	OHX	1	3815	-	0,6,6	0.00	-	-		
85	OHX	1	3865	-	0,6,6	0.00	-	-		
85	OHX	7	215	-	0,6,6	0.00	-	-		
85	OHX	1	3900	-	0,6,6	0.00	-	-		
85	OHX	3	216	-	0,6,6	0.00	-	-		
85	OHX	1	3979	-	0,6,6	0.00	-	-		
85	OHX	6	2089	-	0,6,6	0.00	-	-		
85	OHX	1	4009	-	0,6,6	0.00	-	-		
85	OHX	O7	105	-	0,6,6	0.00	-	-		
85	OHX	2	2001	-	0,6,6	0.00	-	-		
85	OHX	1	3945	-	0,6,6	0.00	-	-		
85	OHX	N1	201	-	0,6,6	0.00	-	-		
85	OHX	5	3942	-	0,6,6	0.00	-	-		
85	OHX	1	4026	-	0,6,6	0.00	-	-		
85	OHX	2	2067	-	0,6,6	0.00	-	-		
85	OHX	6	2091	-	0,6,6	0.00	-	-		
85	OHX	8	215	-	0,6,6	0.00	-	-		
85	OHX	5	3778	-	0,6,6	0.00	-	-		
85	OHX	1	3791	-	0,6,6	0.00	-	-		
85	OHX	6	2108	-	0,6,6	0.00	-	-		
85	OHX	5	3880	-	0,6,6	0.00	-	-		
85	OHX	5	3799	-	0,6,6	0.00	-	-		
85	OHX	5	3899	-	0,6,6	0.00	-	-		
85	OHX	1	3912	-	0,6,6	0.00	-	-		
85	OHX	3	211	-	0,6,6	0.00	-	-		
85	OHX	2	2061	-	0,6,6	0.00	-	-		
85	OHX	6	2031	-	0,6,6	0.00	-	-		
85	OHX	6	2121	-	0,6,6	0.00	-	-		
85	OHX	1	4016	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	1	4018	-	0,6,6	0.00	-	-		
85	OHX	2	2094	-	0,6,6	0.00	-	-		
85	OHX	5	4018	-	0,6,6	0.00	-	-		
85	OHX	5	3797	-	0,6,6	0.00	-	-		
85	OHX	1	3936	-	0,6,6	0.00	-	-		
85	OHX	2	2089	-	0,6,6	0.00	-	-		
85	OHX	3	212	-	0,6,6	0.00	-	-		
85	OHX	13	407	-	0,6,6	0.00	-	-		
85	OHX	5	3751	-	0,6,6	0.00	-	-		
85	OHX	5	3816	-	0,6,6	0.00	-	-		
85	OHX	1	3998	-	0,6,6	0.00	-	-		
85	OHX	2	2116	-	0,6,6	0.00	-	-		
85	OHX	2	1989	-	0,6,6	0.00	-	-		
85	OHX	2	1986	-	0,6,6	0.00	-	-		
85	OHX	1	3809	-	0,6,6	0.00	-	-		
85	OHX	5	3874	-	0,6,6	0.00	-	-		
85	OHX	1	3969	-	0,6,6	0.00	-	-		
85	OHX	6	2014	-	0,6,6	0.00	-	-		
85	OHX	5	3794	-	0,6,6	0.00	-	-		
85	OHX	5	3984	-	0,6,6	0.00	-	-		
85	OHX	1	3914	-	0,6,6	0.00	-	-		
85	OHX	5	3989	-	0,6,6	0.00	-	-		
85	OHX	1	3785	-	0,6,6	0.00	-	-		
85	OHX	1	4003	-	0,6,6	0.00	-	-		
85	OHX	1	3820	-	0,6,6	0.00	-	-		
85	OHX	6	2034	-	0,6,6	0.00	-	-		
85	OHX	1	3922	-	0,6,6	0.00	-	-		
85	OHX	1	3850	-	0,6,6	0.00	-	-		
85	OHX	5	4056	-	0,6,6	0.00	-	-		
85	OHX	1	3990	-	0,6,6	0.00	-	-		
85	OHX	5	3836	-	0,6,6	0.00	-	-		
85	OHX	5	4062	-	0,6,6	0.00	-	-		
85	OHX	5	3768	-	0,6,6	0.00	-	-		
85	OHX	n3	203	-	0,6,6	0.00	-	-		
85	OHX	1	3937	-	0,6,6	0.00	-	-		
85	OHX	2	2098	-	0,6,6	0.00	-	-		
85	OHX	1	3948	-	0,6,6	0.00	-	-		
85	OHX	L4	401	-	0,6,6	0.00	-	-		
85	OHX	1	3752	-	0,6,6	0.00	-	-		
85	OHX	2	2097	-	0,6,6	0.00	-	-		
85	OHX	2	2037	-	0,6,6	0.00	-	-		
85	OHX	5	3996	-	0,6,6	0.00	-	-		
85	OHX	2	2030	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	2	2009	-	0,6,6	0.00	-	-		
85	OHX	6	2064	-	0,6,6	0.00	-	-		
85	OHX	8	213	-	0,6,6	0.00	-	-		
85	OHX	2	2046	-	0,6,6	0.00	-	-		
85	OHX	2	2036	-	0,6,6	0.00	-	-		
85	OHX	5	3908	-	0,6,6	0.00	-	-		
85	OHX	1	3902	-	0,6,6	0.00	-	-		
85	OHX	O9	101	-	0,6,6	0.00	-	-		
85	OHX	5	3892	-	0,6,6	0.00	-	-		
85	OHX	5	3785	-	0,6,6	0.00	-	-		
85	OHX	6	2128	-	0,6,6	0.00	-	-		
85	OHX	2	2011	-	0,6,6	0.00	-	-		
85	OHX	5	3857	-	0,6,6	0.00	-	-		
85	OHX	5	3756	-	0,6,6	0.00	-	-		
85	OHX	1	3992	-	0,6,6	0.00	-	-		
85	OHX	1	3826	-	0,6,6	0.00	-	-		
85	OHX	1	3917	-	0,6,6	0.00	-	-		
85	OHX	5	4063	-	0,6,6	0.00	-	-		
85	OHX	1	4034	-	0,6,6	0.00	-	-		
85	OHX	1	3887	-	0,6,6	0.00	-	-		
85	OHX	2	2065	-	0,6,6	0.00	-	-		
85	OHX	5	3959	-	0,6,6	0.00	-	-		
85	OHX	1	3971	-	0,6,6	0.00	-	-		
85	OHX	6	2155	-	0,6,6	0.00	-	-		
85	OHX	1	3974	-	0,6,6	0.00	-	-		
85	OHX	6	2016	-	0,6,6	0.00	-	-		
85	OHX	6	2019	-	0,6,6	0.00	-	-		
85	OHX	2	2088	-	0,6,6	0.00	-	-		
85	OHX	1	3984	-	0,6,6	0.00	-	-		
85	OHX	6	2088	-	0,6,6	0.00	-	-		
85	OHX	4	217	-	0,6,6	0.00	-	-		
85	OHX	1	4025	-	0,6,6	0.00	-	-		
85	OHX	5	3822	-	0,6,6	0.00	-	-		
85	OHX	5	4019	-	0,6,6	0.00	-	-		
85	OHX	5	3767	-	0,6,6	0.00	-	-		
85	OHX	5	3835	-	0,6,6	0.00	-	-		
85	OHX	1	3994	-	0,6,6	0.00	-	-		
85	OHX	1	3810	-	0,6,6	0.00	-	-		
85	OHX	1	3818	-	0,6,6	0.00	-	-		
85	OHX	5	3742	-	0,6,6	0.00	-	-		
85	OHX	5	4060	-	0,6,6	0.00	-	-		
85	OHX	6	2146	-	0,6,6	0.00	-	-		
85	OHX	6	2045	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	5	4065	-	0,6,6	0.00	-	-		
85	OHX	6	2090	-	0,6,6	0.00	-	-		
85	OHX	3	215	-	0,6,6	0.00	-	-		
85	OHX	1	4007	-	0,6,6	0.00	-	-		
85	OHX	6	2080	-	0,6,6	0.00	-	-		
85	OHX	m0	301	-	0,6,6	0.00	-	-		
85	OHX	5	4038	-	0,6,6	0.00	-	-		
85	OHX	1	3973	-	0,6,6	0.00	-	-		
85	OHX	6	2157	-	0,6,6	0.00	-	-		
85	OHX	7	213	-	0,6,6	0.00	-	-		
85	OHX	1	3879	-	0,6,6	0.00	-	-		
85	OHX	1	3795	-	0,6,6	0.00	-	-		
85	OHX	6	2125	-	0,6,6	0.00	-	-		
85	OHX	5	3832	-	0,6,6	0.00	-	-		
85	OHX	1	3856	-	0,6,6	0.00	-	-		
85	OHX	5	3994	-	0,6,6	0.00	-	-		
85	OHX	5	3782	-	0,6,6	0.00	-	-		
85	OHX	6	2105	-	0,6,6	0.00	-	-		
85	OHX	6	2151	-	0,6,6	0.00	-	-		
85	OHX	8	216	-	0,6,6	0.00	-	-		
85	OHX	1	3946	-	0,6,6	0.00	-	-		
85	OHX	1	3943	-	0,6,6	0.00	-	-		
85	OHX	2	2091	-	0,6,6	0.00	-	-		
85	OHX	5	3854	-	0,6,6	0.00	-	-		
85	OHX	5	3976	-	0,6,6	0.00	-	-		
85	OHX	1	3823	-	0,6,6	0.00	-	-		
85	OHX	2	2063	-	0,6,6	0.00	-	-		
85	OHX	1	3958	-	0,6,6	0.00	-	-		
85	OHX	8	219	-	0,6,6	0.00	-	-		
85	OHX	6	2029	-	0,6,6	0.00	-	-		
85	OHX	5	3800	-	0,6,6	0.00	-	-		
85	OHX	5	3755	-	0,6,6	0.00	-	-		
85	OHX	2	2075	-	0,6,6	0.00	-	-		
85	OHX	2	2093	-	0,6,6	0.00	-	-		
85	OHX	1	4002	-	0,6,6	0.00	-	-		
85	OHX	5	3975	-	0,6,6	0.00	-	-		
85	OHX	2	2077	-	0,6,6	0.00	-	-		
85	OHX	1	4015	-	0,6,6	0.00	-	-		
85	OHX	2	2104	-	0,6,6	0.00	-	-		
85	OHX	2	2024	-	0,6,6	0.00	-	-		
85	OHX	5	3843	-	0,6,6	0.00	-	-		
85	OHX	1	3736	-	0,6,6	0.00	-	-		
85	OHX	6	2041	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	6	2095	-	0,6,6	0.00	-	-		
85	OHX	4	224	-	0,6,6	0.00	-	-		
85	OHX	5	4013	-	0,6,6	0.00	-	-		
85	OHX	1	3899	-	0,6,6	0.00	-	-		
85	OHX	1	3740	-	0,6,6	0.00	-	-		
85	OHX	5	3951	-	0,6,6	0.00	-	-		
85	OHX	6	2074	-	0,6,6	0.00	-	-		
85	OHX	5	3855	-	0,6,6	0.00	-	-		
85	OHX	5	3890	-	0,6,6	0.00	-	-		
85	OHX	5	4045	-	0,6,6	0.00	-	-		
85	OHX	4	219	-	0,6,6	0.00	-	-		
85	OHX	1	3746	-	0,6,6	0.00	-	-		
85	OHX	2	2022	-	0,6,6	0.00	-	-		
85	OHX	6	2021	-	0,6,6	0.00	-	-		
85	OHX	1	3857	-	0,6,6	0.00	-	-		
85	OHX	5	4054	-	0,6,6	0.00	-	-		
85	OHX	1	3876	-	0,6,6	0.00	-	-		
85	OHX	2	2100	-	0,6,6	0.00	-	-		
85	OHX	6	2070	-	0,6,6	0.00	-	-		
85	OHX	2	2102	-	0,6,6	0.00	-	-		
85	OHX	1	3985	-	0,6,6	0.00	-	-		
85	OHX	7	218	-	0,6,6	0.00	-	-		
85	OHX	6	2037	-	0,6,6	0.00	-	-		
85	OHX	1	3732	-	0,6,6	0.00	-	-		
85	OHX	2	2008	-	0,6,6	0.00	-	-		
85	OHX	5	3913	-	0,6,6	0.00	-	-		
85	OHX	sR	401	-	0,6,6	0.00	-	-		
85	OHX	5	3916	-	0,6,6	0.00	-	-		
85	OHX	4	226	-	0,6,6	0.00	-	-		
85	OHX	4	229	-	0,6,6	0.00	-	-		
85	OHX	1	3836	-	0,6,6	0.00	-	-		
85	OHX	6	2111	-	0,6,6	0.00	-	-		
85	OHX	1	3875	-	0,6,6	0.00	-	-		
85	OHX	7	216	-	0,6,6	0.00	-	-		
85	OHX	5	3770	-	0,6,6	0.00	-	-		
85	OHX	19	202	-	0,6,6	0.00	-	-		
85	OHX	1	3898	-	0,6,6	0.00	-	-		
85	OHX	6	2065	-	0,6,6	0.00	-	-		
85	OHX	5	3950	-	0,6,6	0.00	-	-		
85	OHX	5	3958	-	0,6,6	0.00	-	-		
85	OHX	1	3874	-	0,6,6	0.00	-	-		
85	OHX	6	2062	-	0,6,6	0.00	-	-		
85	OHX	M7	205	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	2	2014	-	0,6,6	0.00	-	-		
85	OHX	1	3735	-	0,6,6	0.00	-	-		
85	OHX	2	2096	-	0,6,6	0.00	-	-		
85	OHX	5	3952	-	0,6,6	0.00	-	-		
85	OHX	1	4033	-	0,6,6	0.00	-	-		
85	OHX	6	2073	-	0,6,6	0.00	-	-		
85	OHX	1	3929	-	0,6,6	0.00	-	-		
85	OHX	2	2053	-	0,6,6	0.00	-	-		
85	OHX	1	3997	-	0,6,6	0.00	-	-		
85	OHX	3	213	-	0,6,6	0.00	-	-		
85	OHX	Q2	503	-	0,6,6	0.00	-	-		
85	OHX	5	3870	-	0,6,6	0.00	-	-		
85	OHX	6	2120	-	0,6,6	0.00	-	-		
85	OHX	1	4022	-	0,6,6	0.00	-	-		
85	OHX	5	3945	-	0,6,6	0.00	-	-		
85	OHX	5	4055	-	0,6,6	0.00	-	-		
85	OHX	6	2081	-	0,6,6	0.00	-	-		
85	OHX	5	3997	-	0,6,6	0.00	-	-		
85	OHX	1	3770	-	0,6,6	0.00	-	-		
85	OHX	5	3753	-	0,6,6	0.00	-	-		
85	OHX	14	401	-	0,6,6	0.00	-	-		
85	OHX	5	3848	-	0,6,6	0.00	-	-		
85	OHX	6	2040	-	0,6,6	0.00	-	-		
85	OHX	5	3940	-	0,6,6	0.00	-	-		
85	OHX	1	3830	-	0,6,6	0.00	-	-		
85	OHX	5	3991	-	0,6,6	0.00	-	-		
85	OHX	1	3827	-	0,6,6	0.00	-	-		
85	OHX	5	4040	-	0,6,6	0.00	-	-		
85	OHX	6	2086	-	0,6,6	0.00	-	-		
85	OHX	6	2050	-	0,6,6	0.00	-	-		
85	OHX	6	2140	-	0,6,6	0.00	-	-		
85	OHX	5	3924	-	0,6,6	0.00	-	-		
85	OHX	5	4049	-	0,6,6	0.00	-	-		
85	OHX	5	3791	-	0,6,6	0.00	-	-		
85	OHX	2	2106	-	0,6,6	0.00	-	-		
85	OHX	5	3776	-	0,6,6	0.00	-	-		
85	OHX	4	223	-	0,6,6	0.00	-	-		
85	OHX	5	3864	-	0,6,6	0.00	-	-		
85	OHX	1	3955	-	0,6,6	0.00	-	-		
85	OHX	6	2113	-	0,6,6	0.00	-	-		
85	OHX	1	3819	-	0,6,6	0.00	-	-		
85	OHX	6	2154	-	0,6,6	0.00	-	-		
85	OHX	1	3890	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	5	3901	-	0,6,6	0.00	-	-		
85	OHX	2	2110	-	0,6,6	0.00	-	-		
85	OHX	2	2117	-	0,6,6	0.00	-	-		
85	OHX	6	2126	-	0,6,6	0.00	-	-		
85	OHX	1	3915	-	0,6,6	0.00	-	-		
85	OHX	1	4000	-	0,6,6	0.00	-	-		
85	OHX	1	3743	-	0,6,6	0.00	-	-		
85	OHX	5	3849	-	0,6,6	0.00	-	-		
85	OHX	8	220	-	0,6,6	0.00	-	-		
85	OHX	5	3834	-	0,6,6	0.00	-	-		
85	OHX	6	2057	-	0,6,6	0.00	-	-		
85	OHX	5	3936	-	0,6,6	0.00	-	-		
85	OHX	2	1997	-	0,6,6	0.00	-	-		
85	OHX	1	3957	-	0,6,6	0.00	-	-		
85	OHX	5	3968	-	0,6,6	0.00	-	-		
85	OHX	1	3835	-	0,6,6	0.00	-	-		
85	OHX	1	3773	-	0,6,6	0.00	-	-		
85	OHX	SR	401	-	0,6,6	0.00	-	-		
85	OHX	5	3969	-	0,6,6	0.00	-	-		
85	OHX	1	3751	-	0,6,6	0.00	-	-		
85	OHX	2	2031	-	0,6,6	0.00	-	-		
85	OHX	5	3833	-	0,6,6	0.00	-	-		
85	OHX	1	3744	-	0,6,6	0.00	-	-		
85	OHX	1	3841	-	0,6,6	0.00	-	-		
85	OHX	2	2090	-	0,6,6	0.00	-	-		
85	OHX	1	3760	-	0,6,6	0.00	-	-		
85	OHX	5	4014	-	0,6,6	0.00	-	-		
85	OHX	15	301	-	0,6,6	0.00	-	-		
85	OHX	6	2087	-	0,6,6	0.00	-	-		
85	OHX	5	3746	-	0,6,6	0.00	-	-		
87	ANM	1	3401	-	20,20,20	2.93	9 (45%)	22,27,27	2.80	10 (45%)
85	OHX	2	1990	-	0,6,6	0.00	-	-		
85	OHX	5	3777	-	0,6,6	0.00	-	-		
85	OHX	5	4025	-	0,6,6	0.00	-	-		
85	OHX	2	2066	-	0,6,6	0.00	-	-		
85	OHX	1	3869	-	0,6,6	0.00	-	-		
85	OHX	1	4011	-	0,6,6	0.00	-	-		
85	OHX	1	3802	-	0,6,6	0.00	-	-		
85	OHX	1	3924	-	0,6,6	0.00	-	-		
85	OHX	6	2026	-	0,6,6	0.00	-	-		
85	OHX	5	3963	-	0,6,6	0.00	-	-		
85	OHX	5	3837	-	0,6,6	0.00	-	-		
85	OHX	2	2021	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	5	3904	-	0,6,6	0.00	-	-		
85	OHX	2	2068	-	0,6,6	0.00	-	-		
85	OHX	6	2098	-	0,6,6	0.00	-	-		
85	OHX	6	2027	-	0,6,6	0.00	-	-		
85	OHX	n3	202	-	0,6,6	0.00	-	-		
85	OHX	m7	204	-	0,6,6	0.00	-	-		
85	OHX	6	2137	-	0,6,6	0.00	-	-		
85	OHX	6	2017	-	0,6,6	0.00	-	-		
85	OHX	5	3856	-	0,6,6	0.00	-	-		
85	OHX	1	4023	-	0,6,6	0.00	-	-		
85	OHX	5	3902	-	0,6,6	0.00	-	-		
85	OHX	1	3934	-	0,6,6	0.00	-	-		
85	OHX	5	3920	-	0,6,6	0.00	-	-		
85	OHX	5	3878	-	0,6,6	0.00	-	-		
85	OHX	1	3896	-	0,6,6	0.00	-	-		
85	OHX	2	2060	-	0,6,6	0.00	-	-		
85	OHX	6	2060	-	0,6,6	0.00	-	-		
85	OHX	5	4030	-	0,6,6	0.00	-	-		
85	OHX	1	3764	-	0,6,6	0.00	-	-		
85	OHX	5	3792	-	0,6,6	0.00	-	-		
85	OHX	2	2050	-	0,6,6	0.00	-	-		
85	OHX	1	3861	-	0,6,6	0.00	-	-		
85	OHX	2	2042	-	0,6,6	0.00	-	-		
85	OHX	5	4026	-	0,6,6	0.00	-	-		
85	OHX	6	2011	-	0,6,6	0.00	-	-		
85	OHX	2	2003	-	0,6,6	0.00	-	-		
85	OHX	6	2075	-	0,6,6	0.00	-	-		
85	OHX	2	2018	-	0,6,6	0.00	-	-		
85	OHX	1	3854	-	0,6,6	0.00	-	-		
85	OHX	6	2130	-	0,6,6	0.00	-	-		
85	OHX	5	3781	-	0,6,6	0.00	-	-		
85	OHX	2	2087	-	0,6,6	0.00	-	-		
85	OHX	1	3931	-	0,6,6	0.00	-	-		
85	OHX	1	3965	-	0,6,6	0.00	-	-		
85	OHX	6	2101	-	0,6,6	0.00	-	-		
85	OHX	1	3853	-	0,6,6	0.00	-	-		
85	OHX	5	3748	-	0,6,6	0.00	-	-		
85	OHX	6	2124	-	0,6,6	0.00	-	-		
85	OHX	1	4005	-	0,6,6	0.00	-	-		
85	OHX	s8	302	-	0,6,6	0.00	-	-		
85	OHX	5	3793	-	0,6,6	0.00	-	-		
85	OHX	1	3821	-	0,6,6	0.00	-	-		
85	OHX	1	3767	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	1	3803	-	0,6,6	0.00	-	-		
85	OHX	6	2148	-	0,6,6	0.00	-	-		
85	OHX	1	3978	-	0,6,6	0.00	-	-		
85	OHX	6	2058	-	0,6,6	0.00	-	-		
85	OHX	5	3935	-	0,6,6	0.00	-	-		
85	OHX	1	3982	-	0,6,6	0.00	-	-		
85	OHX	1	3880	-	0,6,6	0.00	-	-		
85	OHX	c8	201	-	0,6,6	0.00	-	-		
85	OHX	5	3883	-	0,6,6	0.00	-	-		
85	OHX	5	3909	-	0,6,6	0.00	-	-		
85	OHX	5	3867	-	0,6,6	0.00	-	-		
85	OHX	1	3877	-	0,6,6	0.00	-	-		
85	OHX	1	3907	-	0,6,6	0.00	-	-		
85	OHX	8	224	-	0,6,6	0.00	-	-		
85	OHX	1	4030	-	0,6,6	0.00	-	-		
85	OHX	1	4031	-	0,6,6	0.00	-	-		
85	OHX	5	3928	-	0,6,6	0.00	-	-		
85	OHX	5	3759	-	0,6,6	0.00	-	-		
85	OHX	1	3972	-	0,6,6	0.00	-	-		
85	OHX	1	3726	-	0,6,6	0.00	-	-		
85	OHX	6	2012	-	0,6,6	0.00	-	-		
85	OHX	5	3842	-	0,6,6	0.00	-	-		
85	OHX	5	3971	-	0,6,6	0.00	-	-		
85	OHX	6	2152	-	0,6,6	0.00	-	-		
85	OHX	1	3870	-	0,6,6	0.00	-	-		
85	OHX	5	3906	-	0,6,6	0.00	-	-		
85	OHX	5	3750	-	0,6,6	0.00	-	-		
85	OHX	1	3886	-	0,6,6	0.00	-	-		
85	OHX	1	3753	-	0,6,6	0.00	-	-		
85	OHX	5	3886	-	0,6,6	0.00	-	-		
85	OHX	5	4002	-	0,6,6	0.00	-	-		
85	OHX	5	4008	-	0,6,6	0.00	-	-		
85	OHX	5	4007	36	0,6,6	0.00	-	-		
85	OHX	6	2093	-	0,6,6	0.00	-	-		
85	OHX	1	3954	-	0,6,6	0.00	-	-		
85	OHX	4	216	-	0,6,6	0.00	-	-		
85	OHX	2	2023	-	0,6,6	0.00	-	-		
85	OHX	1	3995	-	0,6,6	0.00	-	-		
85	OHX	5	3830	-	0,6,6	0.00	-	-		
85	OHX	4	225	-	0,6,6	0.00	-	-		
85	OHX	2	2054	-	0,6,6	0.00	-	-		
85	OHX	2	2035	-	0,6,6	0.00	-	-		
85	OHX	5	3743	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	6	2158	-	0,6,6	0.00	-	-		
85	OHX	5	3838	-	0,6,6	0.00	-	-		
85	OHX	7	211	-	0,6,6	0.00	-	-		
85	OHX	2	2069	-	0,6,6	0.00	-	-		
85	OHX	6	2048	-	0,6,6	0.00	-	-		
85	OHX	5	3962	-	0,6,6	0.00	-	-		
85	OHX	5	4064	-	0,6,6	0.00	-	-		
85	OHX	5	3896	-	0,6,6	0.00	-	-		
85	OHX	1	3910	-	0,6,6	0.00	-	-		
85	OHX	1	3981	-	0,6,6	0.00	-	-		
85	OHX	5	4000	-	0,6,6	0.00	-	-		
85	OHX	5	3875	-	0,6,6	0.00	-	-		
85	OHX	1	3829	-	0,6,6	0.00	-	-		
85	OHX	1	3738	-	0,6,6	0.00	-	-		
85	OHX	6	2122	-	0,6,6	0.00	-	-		
85	OHX	5	4016	-	0,6,6	0.00	-	-		
85	OHX	5	3915	-	0,6,6	0.00	-	-		
85	OHX	6	2149	-	0,6,6	0.00	-	-		
85	OHX	5	4006	-	0,6,6	0.00	-	-		
85	OHX	4	231	-	0,6,6	0.00	-	-		
85	OHX	6	2025	-	0,6,6	0.00	-	-		
85	OHX	5	4027	-	0,6,6	0.00	-	-		
85	OHX	1	3777	-	0,6,6	0.00	-	-		
85	OHX	6	2020	-	0,6,6	0.00	-	-		
85	OHX	2	1985	-	0,6,6	0.00	-	-		
85	OHX	5	3978	-	0,6,6	0.00	-	-		
85	OHX	1	4004	-	0,6,6	0.00	-	-		
85	OHX	1	3986	-	0,6,6	0.00	-	-		
85	OHX	5	3900	-	0,6,6	0.00	-	-		
85	OHX	1	3961	-	0,6,6	0.00	-	-		
85	OHX	5	3949	-	0,6,6	0.00	-	-		
85	OHX	2	1991	-	0,6,6	0.00	-	-		
85	OHX	1	3771	-	0,6,6	0.00	-	-		
85	OHX	1	4037	-	0,6,6	0.00	-	-		
85	OHX	5	3990	-	0,6,6	0.00	-	-		
85	OHX	2	2083	-	0,6,6	0.00	-	-		
85	OHX	5	3907	-	0,6,6	0.00	-	-		
85	OHX	1	3867	-	0,6,6	0.00	-	-		
85	OHX	5	4066	-	0,6,6	0.00	-	-		
85	OHX	1	3817	-	0,6,6	0.00	-	-		
85	OHX	1	3728	-	0,6,6	0.00	-	-		
85	OHX	6	2055	-	0,6,6	0.00	-	-		
85	OHX	5	4048	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	1	4029	-	0,6,6	0.00	-	-		
85	OHX	1	3993	-	0,6,6	0.00	-	-		
85	OHX	2	2103	-	0,6,6	0.00	-	-		
85	OHX	1	3779	-	0,6,6	0.00	-	-		
85	OHX	6	2103	-	0,6,6	0.00	-	-		
85	OHX	5	3784	-	0,6,6	0.00	-	-		
85	OHX	1	3873	-	0,6,6	0.00	-	-		
85	OHX	5	4037	-	0,6,6	0.00	-	-		
85	OHX	2	2045	-	0,6,6	0.00	-	-		
85	OHX	1	3932	-	0,6,6	0.00	-	-		
85	OHX	6	2083	-	0,6,6	0.00	-	-		
85	OHX	2	2005	-	0,6,6	0.00	-	-		
85	OHX	5	3992	-	0,6,6	0.00	-	-		
85	OHX	1	3968	-	0,6,6	0.00	-	-		
85	OHX	2	2016	-	0,6,6	0.00	-	-		
85	OHX	1	3784	-	0,6,6	0.00	-	-		
85	OHX	1	3991	-	0,6,6	0.00	-	-		
85	OHX	2	2013	-	0,6,6	0.00	-	-		
85	OHX	2	2034	-	0,6,6	0.00	-	-		
85	OHX	1	3790	-	0,6,6	0.00	-	-		
85	OHX	5	4046	-	0,6,6	0.00	-	-		
85	OHX	13	406	-	0,6,6	0.00	-	-		
85	OHX	6	2114	-	0,6,6	0.00	-	-		
85	OHX	5	3803	-	0,6,6	0.00	-	-		
85	OHX	5	4024	-	0,6,6	0.00	-	-		
85	OHX	5	3744	-	0,6,6	0.00	-	-		
85	OHX	1	4020	-	0,6,6	0.00	-	-		
85	OHX	6	2056	-	0,6,6	0.00	-	-		
85	OHX	1	3960	-	0,6,6	0.00	-	-		
85	OHX	1	3838	-	0,6,6	0.00	-	-		
85	OHX	5	3982	-	0,6,6	0.00	-	-		
85	OHX	6	2116	-	0,6,6	0.00	-	-		
85	OHX	1	3759	-	0,6,6	0.00	-	-		
85	OHX	5	3965	-	0,6,6	0.00	-	-		
85	OHX	1	3901	-	0,6,6	0.00	-	-		
85	OHX	5	3841	-	0,6,6	0.00	-	-		
85	OHX	S8	301	-	0,6,6	0.00	-	-		
85	OHX	5	4070	-	0,6,6	0.00	-	-		
85	OHX	5	3847	-	0,6,6	0.00	-	-		
85	OHX	1	3980	-	0,6,6	0.00	-	-		
85	OHX	5	3749	-	0,6,6	0.00	-	-		
85	OHX	6	2084	-	0,6,6	0.00	-	-		
85	OHX	5	4061	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	1	3909	-	0,6,6	0.00	-	-		
85	OHX	L3	402	-	0,6,6	0.00	-	-		
85	OHX	1	4021	-	0,6,6	0.00	-	-		
85	OHX	2	2044	-	0,6,6	0.00	-	-		
85	OHX	2	2047	-	0,6,6	0.00	-	-		
85	OHX	5	3938	-	0,6,6	0.00	-	-		
85	OHX	6	2023	-	0,6,6	0.00	-	-		
85	OHX	1	3845	-	0,6,6	0.00	-	-		
85	OHX	1	3822	-	0,6,6	0.00	-	-		
85	OHX	2	2026	-	0,6,6	0.00	-	-		
85	OHX	5	3944	-	0,6,6	0.00	-	-		
85	OHX	6	2102	-	0,6,6	0.00	-	-		
85	OHX	5	3788	-	0,6,6	0.00	-	-		
85	OHX	5	4050	-	0,6,6	0.00	-	-		
85	OHX	2	2002	-	0,6,6	0.00	-	-		
85	OHX	2	2111	-	0,6,6	0.00	-	-		
85	OHX	5	3752	-	0,6,6	0.00	-	-		
85	OHX	1	3801	-	0,6,6	0.00	-	-		
85	OHX	6	2094	-	0,6,6	0.00	-	-		
85	OHX	1	3812	-	0,6,6	0.00	-	-		
85	OHX	1	3831	-	0,6,6	0.00	-	-		
85	OHX	5	3859	-	0,6,6	0.00	-	-		
85	OHX	N8	203	-	0,6,6	0.00	-	-		
85	OHX	1	3952	-	0,6,6	0.00	-	-		
85	OHX	1	3768	-	0,6,6	0.00	-	-		
85	OHX	5	3773	-	0,6,6	0.00	-	-		
85	OHX	5	3925	-	0,6,6	0.00	-	-		
85	OHX	1	3928	-	0,6,6	0.00	-	-		
85	OHX	m5	304	-	0,6,6	0.00	-	-		
85	OHX	5	4044	-	0,6,6	0.00	-	-		
85	OHX	o9	101	-	0,6,6	0.00	-	-		
85	OHX	5	4003	-	0,6,6	0.00	-	-		
85	OHX	2	1996	-	0,6,6	0.00	-	-		
85	OHX	5	3863	-	0,6,6	0.00	-	-		
85	OHX	5	3981	-	0,6,6	0.00	-	-		
85	OHX	1	3783	-	0,6,6	0.00	-	-		
85	OHX	1	3891	-	0,6,6	0.00	-	-		
85	OHX	6	2010	-	0,6,6	0.00	-	-		
85	OHX	5	4036	-	0,6,6	0.00	-	-		
85	OHX	1	3983	-	0,6,6	0.00	-	-		
85	OHX	1	3832	-	0,6,6	0.00	-	-		
85	OHX	1	3837	-	0,6,6	0.00	-	-		
85	OHX	5	3829	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	6	2067	-	0,6,6	0.00	-	-		
85	OHX	5	3921	-	0,6,6	0.00	-	-		
85	OHX	1	3793	-	0,6,6	0.00	-	-		
85	OHX	8	225	-	0,6,6	0.00	-	-		
85	OHX	1	3864	-	0,6,6	0.00	-	-		
85	OHX	6	2131	-	0,6,6	0.00	-	-		
85	OHX	1	3908	-	0,6,6	0.00	-	-		
85	OHX	2	2082	-	0,6,6	0.00	-	-		
85	OHX	6	2043	-	0,6,6	0.00	-	-		
85	OHX	5	3798	-	0,6,6	0.00	-	-		
85	OHX	5	4053	-	0,6,6	0.00	-	-		
85	OHX	c5	201	-	0,6,6	0.00	-	-		
85	OHX	1	3808	-	0,6,6	0.00	-	-		
85	OHX	6	2042	-	0,6,6	0.00	-	-		
85	OHX	2	2072	-	0,6,6	0.00	-	-		
85	OHX	5	3895	-	0,6,6	0.00	-	-		
85	OHX	5	3934	-	0,6,6	0.00	-	-		
85	OHX	5	3787	-	0,6,6	0.00	-	-		
85	OHX	1	3749	-	0,6,6	0.00	-	-		
85	OHX	8	212	-	0,6,6	0.00	-	-		
85	OHX	6	2143	-	0,6,6	0.00	-	-		
85	OHX	1	3996	-	0,6,6	0.00	-	-		
85	OHX	1	3947	-	0,6,6	0.00	-	-		
85	OHX	5	3898	-	0,6,6	0.00	-	-		
85	OHX	5	3912	-	0,6,6	0.00	-	-		
85	OHX	5	3905	-	0,6,6	0.00	-	-		
85	OHX	1	3988	-	0,6,6	0.00	-	-		
85	OHX	1	3987	-	0,6,6	0.00	-	-		
85	OHX	1	3906	-	0,6,6	0.00	-	-		
85	OHX	2	2000	-	0,6,6	0.00	-	-		
85	OHX	1	4027	-	0,6,6	0.00	-	-		
85	OHX	5	3955	-	0,6,6	0.00	-	-		
85	OHX	5	3779	-	0,6,6	0.00	-	-		
85	OHX	1	3786	-	0,6,6	0.00	-	-		
85	OHX	7	212	-	0,6,6	0.00	-	-		
85	OHX	5	3821	-	0,6,6	0.00	-	-		
85	OHX	o3	202	-	0,6,6	0.00	-	-		
85	OHX	2	2057	-	0,6,6	0.00	-	-		
85	OHX	5	4058	-	0,6,6	0.00	-	-		
85	OHX	2	2032	-	0,6,6	0.00	-	-		
85	OHX	6	2038	-	0,6,6	0.00	-	-		
85	OHX	5	3851	-	0,6,6	0.00	-	-		
85	OHX	5	4009	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	1	3964	-	0,6,6	0.00	-	-		
85	OHX	1	3780	-	0,6,6	0.00	-	-		
85	OHX	5	3790	-	0,6,6	0.00	-	-		
85	OHX	6	2153	-	0,6,6	0.00	-	-		
85	OHX	2	2038	-	0,6,6	0.00	-	-		
85	OHX	5	3903	-	0,6,6	0.00	-	-		
85	OHX	5	4015	-	0,6,6	0.00	-	-		
85	OHX	5	3840	-	0,6,6	0.00	-	-		
85	OHX	1	3903	-	0,6,6	0.00	-	-		
85	OHX	6	2036	-	0,6,6	0.00	-	-		
85	OHX	2	2119	-	0,6,6	0.00	-	-		
85	OHX	2	1993	-	0,6,6	0.00	-	-		
85	OHX	1	3849	-	0,6,6	0.00	-	-		
85	OHX	5	4069	-	0,6,6	0.00	-	-		
85	OHX	1	3889	-	0,6,6	0.00	-	-		
85	OHX	q2	502	-	0,6,6	0.00	-	-		
85	OHX	2	2051	-	0,6,6	0.00	-	-		
85	OHX	6	2076	-	0,6,6	0.00	-	-		
85	OHX	8	218	-	0,6,6	0.00	-	-		
85	OHX	6	2035	-	0,6,6	0.00	-	-		
85	OHX	5	4034	-	0,6,6	0.00	-	-		
85	OHX	15	302	-	0,6,6	0.00	-	-		
85	OHX	5	3988	-	0,6,6	0.00	-	-		
85	OHX	2	2064	-	0,6,6	0.00	-	-		
85	OHX	1	4006	-	0,6,6	0.00	-	-		
85	OHX	5	3917	-	0,6,6	0.00	-	-		
85	OHX	5	3918	-	0,6,6	0.00	-	-		
85	OHX	2	2019	-	0,6,6	0.00	-	-		
85	OHX	O7	104	-	0,6,6	0.00	-	-		
85	OHX	5	3795	-	0,6,6	0.00	-	-		
85	OHX	2	2033	-	0,6,6	0.00	-	-		
85	OHX	1	3916	-	0,6,6	0.00	-	-		
85	OHX	1	3842	-	0,6,6	0.00	-	-		
85	OHX	2	2115	-	0,6,6	0.00	-	-		
85	OHX	5	3966	-	0,6,6	0.00	-	-		
85	OHX	6	2096	-	0,6,6	0.00	-	-		
85	OHX	1	3940	-	0,6,6	0.00	-	-		
85	OHX	6	2051	-	0,6,6	0.00	-	-		
85	OHX	5	3762	-	0,6,6	0.00	-	-		
85	OHX	5	3910	-	0,6,6	0.00	-	-		
85	OHX	6	2061	-	0,6,6	0.00	-	-		
85	OHX	5	3885	-	0,6,6	0.00	-	-		
85	OHX	1	3806	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	5	3960	-	0,6,6	0.00	-	-		
85	OHX	5	3999	-	0,6,6	0.00	-	-		
85	OHX	1	3892	-	0,6,6	0.00	-	-		
85	OHX	6	2134	-	0,6,6	0.00	-	-		
85	OHX	5	3839	-	0,6,6	0.00	-	-		
85	OHX	5	4028	-	0,6,6	0.00	-	-		
85	OHX	1	3731	-	0,6,6	0.00	-	-		
85	OHX	7	214	-	0,6,6	0.00	-	-		
85	OHX	5	3884	-	0,6,6	0.00	-	-		
85	OHX	5	3866	-	0,6,6	0.00	-	-		
85	OHX	6	2092	-	0,6,6	0.00	-	-		
85	OHX	1	3859	-	0,6,6	0.00	-	-		
85	OHX	5	3974	-	0,6,6	0.00	-	-		
85	OHX	5	3853	-	0,6,6	0.00	-	-		
85	OHX	1	3797	-	0,6,6	0.00	-	-		
85	OHX	1	3805	-	0,6,6	0.00	-	-		
85	OHX	2	2007	-	0,6,6	0.00	-	-		
85	OHX	5	3852	-	0,6,6	0.00	-	-		
85	OHX	5	3802	-	0,6,6	0.00	-	-		
85	OHX	2	1998	-	0,6,6	0.00	-	-		
85	OHX	5	3929	-	0,6,6	0.00	-	-		
85	OHX	5	4033	-	0,6,6	0.00	-	-		
85	OHX	5	3894	-	0,6,6	0.00	-	-		
85	OHX	1	3772	-	0,6,6	0.00	-	-		
85	OHX	5	3954	-	0,6,6	0.00	-	-		
85	OHX	6	2059	-	0,6,6	0.00	-	-		
85	OHX	5	3826	-	0,6,6	0.00	-	-		
85	OHX	1	3727	-	0,6,6	0.00	-	-		
85	OHX	5	4005	-	0,6,6	0.00	-	-		
85	OHX	5	3869	-	0,6,6	0.00	-	-		
85	OHX	2	2056	-	0,6,6	0.00	-	-		
85	OHX	6	2066	-	0,6,6	0.00	-	-		
85	OHX	4	222	-	0,6,6	0.00	-	-		
85	OHX	4	227	-	0,6,6	0.00	-	-		
85	OHX	8	223	-	0,6,6	0.00	-	-		
85	OHX	1	3848	-	0,6,6	0.00	-	-		
85	OHX	6	2129	-	0,6,6	0.00	-	-		
85	OHX	2	2101	-	0,6,6	0.00	-	-		
85	OHX	5	3761	-	0,6,6	0.00	-	-		
85	OHX	5	4031	-	0,6,6	0.00	-	-		
85	OHX	6	2115	-	0,6,6	0.00	-	-		
85	OHX	5	3957	-	0,6,6	0.00	-	-		
85	OHX	2	2006	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	6	2156	-	0,6,6	0.00	-	-		
85	OHX	2	2080	-	0,6,6	0.00	-	-		
85	OHX	n9	102	-	0,6,6	0.00	-	-		
85	OHX	6	2049	-	0,6,6	0.00	-	-		
85	OHX	5	3872	-	0,6,6	0.00	-	-		
85	OHX	2	2074	-	0,6,6	0.00	-	-		
85	OHX	4	220	-	0,6,6	0.00	-	-		
85	OHX	1	4036	-	0,6,6	0.00	-	-		
85	OHX	5	3873	-	0,6,6	0.00	-	-		
85	OHX	8	214	-	0,6,6	0.00	-	-		
85	OHX	1	3846	-	0,6,6	0.00	-	-		
85	OHX	6	2069	-	0,6,6	0.00	-	-		
85	OHX	5	3786	-	0,6,6	0.00	-	-		
85	OHX	4	221	-	0,6,6	0.00	-	-		
85	OHX	1	3927	-	0,6,6	0.00	-	-		
85	OHX	1	3963	-	0,6,6	0.00	-	-		
85	OHX	5	3766	-	0,6,6	0.00	-	-		
85	OHX	6	2141	-	0,6,6	0.00	-	-		
85	OHX	6	2136	-	0,6,6	0.00	-	-		
85	OHX	2	2010	-	0,6,6	0.00	-	-		
85	OHX	2	2073	-	0,6,6	0.00	-	-		
85	OHX	4	230	-	0,6,6	0.00	-	-		
85	OHX	5	3827	-	0,6,6	0.00	-	-		
85	OHX	1	3860	-	0,6,6	0.00	-	-		
85	OHX	5	4057	-	0,6,6	0.00	-	-		
85	OHX	1	3778	-	0,6,6	0.00	-	-		
85	OHX	l3	408	-	0,6,6	0.00	-	-		
85	OHX	5	4010	-	0,6,6	0.00	-	-		
85	OHX	1	3782	-	0,6,6	0.00	-	-		
85	OHX	C5	201	-	0,6,6	0.00	-	-		
85	OHX	o7	502	-	0,6,6	0.00	-	-		
85	OHX	5	4051	-	0,6,6	0.00	-	-		
85	OHX	5	3754	-	0,6,6	0.00	-	-		
85	OHX	5	3801	-	0,6,6	0.00	-	-		
85	OHX	1	3828	-	0,6,6	0.00	-	-		
85	OHX	5	3887	-	0,6,6	0.00	-	-		
85	OHX	5	4012	-	0,6,6	0.00	-	-		
85	OHX	6	2052	-	0,6,6	0.00	-	-		
85	OHX	5	3882	-	0,6,6	0.00	-	-		
85	OHX	5	3919	-	0,6,6	0.00	-	-		
85	OHX	5	3820	-	0,6,6	0.00	-	-		
85	OHX	m0	302	-	0,6,6	0.00	-	-		
85	OHX	5	3970	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	5	3948	-	0,6,6	0.00	-	-		
85	OHX	6	2147	-	0,6,6	0.00	-	-		
85	OHX	2	2107	-	0,6,6	0.00	-	-		
85	OHX	1	3977	-	0,6,6	0.00	-	-		
85	OHX	2	2092	-	0,6,6	0.00	-	-		
85	OHX	1	3923	-	0,6,6	0.00	-	-		
85	OHX	1	3878	-	0,6,6	0.00	-	-		
85	OHX	6	2110	-	0,6,6	0.00	-	-		
85	OHX	5	3775	-	0,6,6	0.00	-	-		
85	OHX	1	3871	-	0,6,6	0.00	-	-		
85	OHX	1	3953	-	0,6,6	0.00	-	-		
85	OHX	1	3883	-	0,6,6	0.00	-	-		
85	OHX	1	3852	-	0,6,6	0.00	-	-		
85	OHX	5	4059	-	0,6,6	0.00	-	-		
85	OHX	1	3888	-	0,6,6	0.00	-	-		
85	OHX	5	3850	-	0,6,6	0.00	-	-		
85	OHX	5	3796	-	0,6,6	0.00	-	-		
85	OHX	5	3897	-	0,6,6	0.00	-	-		
85	OHX	1	4008	-	0,6,6	0.00	-	-		
85	OHX	1	3975	-	0,6,6	0.00	-	-		
85	OHX	1	3762	-	0,6,6	0.00	-	-		
85	OHX	1	3794	-	0,6,6	0.00	-	-		
85	OHX	7	221	-	0,6,6	0.00	-	-		
85	OHX	5	3819	-	0,6,6	0.00	-	-		
85	OHX	1	3814	-	0,6,6	0.00	-	-		
85	OHX	6	2079	-	0,6,6	0.00	-	-		
85	OHX	5	4043	-	0,6,6	0.00	-	-		
85	OHX	5	3824	-	0,6,6	0.00	-	-		
85	OHX	1	3938	-	0,6,6	0.00	-	-		
85	OHX	5	3745	-	0,6,6	0.00	-	-		
85	OHX	2	2040	-	0,6,6	0.00	-	-		
85	OHX	6	2078	-	0,6,6	0.00	-	-		
85	OHX	2	1999	-	0,6,6	0.00	-	-		
85	OHX	5	3947	-	0,6,6	0.00	-	-		
85	OHX	5	4041	-	0,6,6	0.00	-	-		
85	OHX	5	3931	-	0,6,6	0.00	-	-		
85	OHX	1	3999	-	0,6,6	0.00	-	-		
85	OHX	1	3734	-	0,6,6	0.00	-	-		
85	OHX	5	3888	-	0,6,6	0.00	-	-		
85	OHX	5	4017	-	0,6,6	0.00	-	-		
85	OHX	5	3747	-	0,6,6	0.00	-	-		
85	OHX	5	3831	-	0,6,6	0.00	-	-		
85	OHX	1	3926	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	6	2109	-	0,6,6	0.00	-	-		
85	OHX	2	1984	-	0,6,6	0.00	-	-		
85	OHX	5	3809	-	0,6,6	0.00	-	-		
85	OHX	2	1994	-	0,6,6	0.00	-	-		
85	OHX	5	3783	-	0,6,6	0.00	-	-		
85	OHX	M5	302	-	0,6,6	0.00	-	-		
85	OHX	2	2027	-	0,6,6	0.00	-	-		
85	OHX	6	2118	-	0,6,6	0.00	-	-		
85	OHX	1	3754	-	0,6,6	0.00	-	-		
85	OHX	6	2135	-	0,6,6	0.00	-	-		
85	OHX	1	3824	-	0,6,6	0.00	-	-		
85	OHX	5	3876	-	0,6,6	0.00	-	-		
85	OHX	5	3811	-	0,6,6	0.00	-	-		
85	OHX	5	3807	-	0,6,6	0.00	-	-		
85	OHX	1	3729	-	0,6,6	0.00	-	-		
85	OHX	1	3741	-	0,6,6	0.00	-	-		
85	OHX	2	2112	-	0,6,6	0.00	-	-		
85	OHX	1	3804	-	0,6,6	0.00	-	-		
85	OHX	6	2133	-	0,6,6	0.00	-	-		
85	OHX	4	215	-	0,6,6	0.00	-	-		
85	OHX	5	3972	-	0,6,6	0.00	-	-		
85	OHX	6	2030	-	0,6,6	0.00	-	-		
85	OHX	1	3730	-	0,6,6	0.00	-	-		
85	OHX	5	3825	-	0,6,6	0.00	-	-		
85	OHX	2	2004	-	0,6,6	0.00	-	-		
85	OHX	1	3970	-	0,6,6	0.00	-	-		
85	OHX	1	4010	-	0,6,6	0.00	-	-		
85	OHX	6	2119	-	0,6,6	0.00	-	-		
85	OHX	5	3939	-	0,6,6	0.00	-	-		
85	OHX	1	3816	-	0,6,6	0.00	-	-		
85	OHX	1	3745	-	0,6,6	0.00	-	-		
85	OHX	5	3977	-	0,6,6	0.00	-	-		
85	OHX	7	219	-	0,6,6	0.00	-	-		
85	OHX	1	4035	-	0,6,6	0.00	-	-		
85	OHX	3	219	-	0,6,6	0.00	-	-		
85	OHX	S6	301	-	0,6,6	0.00	-	-		
85	OHX	3	217	-	0,6,6	0.00	-	-		
85	OHX	2	2070	-	0,6,6	0.00	-	-		
85	OHX	1	3798	-	0,6,6	0.00	-	-		
85	OHX	5	3943	-	0,6,6	0.00	-	-		
85	OHX	1	3956	-	0,6,6	0.00	-	-		
85	OHX	1	3962	-	0,6,6	0.00	-	-		
85	OHX	2	2025	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	5	3774	-	0,6,6	0.00	-	-		
85	OHX	5	3845	-	0,6,6	0.00	-	-		
85	OHX	14	402	-	0,6,6	0.00	-	-		
85	OHX	5	3937	-	0,6,6	0.00	-	-		
85	OHX	5	3967	-	0,6,6	0.00	-	-		
85	OHX	5	3760	-	0,6,6	0.00	-	-		
85	OHX	1	3796	-	0,6,6	0.00	-	-		
85	OHX	8	221	-	0,6,6	0.00	-	-		
85	OHX	1	3944	-	0,6,6	0.00	-	-		
85	OHX	1	3742	-	0,6,6	0.00	-	-		
85	OHX	1	3761	-	0,6,6	0.00	-	-		
85	OHX	6	2104	-	0,6,6	0.00	-	-		
85	OHX	1	3941	-	0,6,6	0.00	-	-		
85	OHX	5	3889	-	0,6,6	0.00	-	-		
85	OHX	1	3748	-	0,6,6	0.00	-	-		
85	OHX	5	3810	-	0,6,6	0.00	-	-		
85	OHX	2	2041	-	0,6,6	0.00	-	-		
85	OHX	1	3758	-	0,6,6	0.00	-	-		
85	OHX	1	3951	-	0,6,6	0.00	-	-		
85	OHX	2	2081	-	0,6,6	0.00	-	-		
85	OHX	5	4047	-	0,6,6	0.00	-	-		
85	OHX	5	4011	-	0,6,6	0.00	-	-		
85	OHX	6	2063	-	0,6,6	0.00	-	-		
85	OHX	2	2095	-	0,6,6	0.00	-	-		
85	OHX	L3	403	-	0,6,6	0.00	-	-		
85	OHX	6	2024	-	0,6,6	0.00	-	-		
85	OHX	6	2053	-	0,6,6	0.00	-	-		
85	OHX	5	3953	-	0,6,6	0.00	-	-		
85	OHX	N9	101	-	0,6,6	0.00	-	-		
85	OHX	2	2017	-	0,6,6	0.00	-	-		
85	OHX	5	3823	-	0,6,6	0.00	-	-		
85	OHX	2	2086	-	0,6,6	0.00	-	-		
85	OHX	1	3787	-	0,6,6	0.00	-	-		
85	OHX	5	3865	-	0,6,6	0.00	-	-		
85	OHX	2	2055	-	0,6,6	0.00	-	-		
85	OHX	5	3998	-	0,6,6	0.00	-	-		
85	OHX	5	3979	-	0,6,6	0.00	-	-		
85	OHX	1	3921	-	0,6,6	0.00	-	-		
85	OHX	2	2099	-	0,6,6	0.00	-	-		
85	OHX	5	3763	-	0,6,6	0.00	-	-		
85	OHX	3	214	-	0,6,6	0.00	-	-		
85	OHX	1	3789	-	0,6,6	0.00	-	-		
85	OHX	M6	202	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	2	2020	-	0,6,6	0.00	-	-		
85	OHX	5	3846	-	0,6,6	0.00	-	-		
85	OHX	1	3855	-	0,6,6	0.00	-	-		
85	OHX	5	4022	-	0,6,6	0.00	-	-		
85	OHX	1	3834	-	0,6,6	0.00	-	-		
85	OHX	5	3995	-	0,6,6	0.00	-	-		
85	OHX	1	4019	-	0,6,6	0.00	-	-		
85	OHX	1	3769	-	0,6,6	0.00	-	-		
85	OHX	5	4004	-	0,6,6	0.00	-	-		
85	OHX	6	2046	-	0,6,6	0.00	-	-		
85	OHX	1	4014	-	0,6,6	0.00	-	-		
85	OHX	6	2150	-	0,6,6	0.00	-	-		
85	OHX	1	3781	-	0,6,6	0.00	-	-		
85	OHX	6	2142	-	0,6,6	0.00	-	-		
85	OHX	5	4023	-	0,6,6	0.00	-	-		
85	OHX	1	3933	-	0,6,6	0.00	-	-		
85	OHX	1	3885	-	0,6,6	0.00	-	-		
85	OHX	1	3939	-	0,6,6	0.00	-	-		
85	OHX	6	2033	-	0,6,6	0.00	-	-		
85	OHX	1	4017	-	0,6,6	0.00	-	-		
85	OHX	O3	202	-	0,6,6	0.00	-	-		
85	OHX	1	3868	-	0,6,6	0.00	-	-		
85	OHX	2	1987	-	0,6,6	0.00	-	-		
85	OHX	1	3884	-	0,6,6	0.00	-	-		
85	OHX	6	2099	-	0,6,6	0.00	-	-		
85	OHX	1	3894	-	0,6,6	0.00	-	-		
85	OHX	s9	201	-	0,6,6	0.00	-	-		
85	OHX	2	2079	-	0,6,6	0.00	-	-		
85	OHX	6	2018	-	0,6,6	0.00	-	-		
85	OHX	1	3911	-	0,6,6	0.00	-	-		
85	OHX	m5	305	-	0,6,6	0.00	-	-		
85	OHX	5	3808	-	0,6,6	0.00	-	-		
85	OHX	5	4029	-	0,6,6	0.00	-	-		
85	OHX	5	4035	-	0,6,6	0.00	-	-		
85	OHX	2	2012	-	0,6,6	0.00	-	-		
85	OHX	1	4038	-	0,6,6	0.00	-	-		
85	OHX	M0	302	-	0,6,6	0.00	-	-		
85	OHX	1	3847	-	0,6,6	0.00	-	-		
85	OHX	2	2109	-	0,6,6	0.00	-	-		
85	OHX	6	2013	-	0,6,6	0.00	-	-		
85	OHX	6	2082	-	0,6,6	0.00	-	-		
85	OHX	6	2047	-	0,6,6	0.00	-	-		
85	OHX	1	3776	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	5	3814	-	0,6,6	0.00	-	-		
85	OHX	C3	201	-	0,6,6	0.00	-	-		
85	OHX	1	3862	-	0,6,6	0.00	-	-		
85	OHX	5	3946	-	0,6,6	0.00	-	-		
85	OHX	1	3839	-	0,6,6	0.00	-	-		
85	OHX	2	2015	-	0,6,6	0.00	-	-		
85	OHX	6	2032	-	0,6,6	0.00	-	-		
85	OHX	5	3868	-	0,6,6	0.00	-	-		
85	OHX	1	3833	-	0,6,6	0.00	-	-		
85	OHX	1	3757	-	0,6,6	0.00	-	-		
85	OHX	5	3983	-	0,6,6	0.00	-	-		
85	OHX	1	3800	-	0,6,6	0.00	-	-		
85	OHX	2	2048	-	0,6,6	0.00	-	-		
85	OHX	6	2097	-	0,6,6	0.00	-	-		
85	OHX	8	222	-	0,6,6	0.00	-	-		
85	OHX	1	4032	-	0,6,6	0.00	-	-		
85	OHX	2	2071	-	0,6,6	0.00	-	-		
85	OHX	5	3926	-	0,6,6	0.00	-	-		
85	OHX	6	2107	-	0,6,6	0.00	-	-		
85	OHX	5	3758	-	0,6,6	0.00	-	-		
85	OHX	2	2049	-	0,6,6	0.00	-	-		
85	OHX	1	4012	-	0,6,6	0.00	-	-		
85	OHX	5	3780	-	0,6,6	0.00	-	-		
85	OHX	5	3933	-	0,6,6	0.00	-	-		
85	OHX	5	3964	-	0,6,6	0.00	-	-		
85	OHX	6	2139	-	0,6,6	0.00	-	-		
85	OHX	5	3914	-	0,6,6	0.00	-	-		
85	OHX	1	3881	-	0,6,6	0.00	-	-		
85	OHX	6	2127	-	0,6,6	0.00	-	-		
85	OHX	1	3737	-	0,6,6	0.00	-	-		
85	OHX	2	2114	-	0,6,6	0.00	-	-		
85	OHX	5	3805	-	0,6,6	0.00	-	-		
85	OHX	5	3985	-	0,6,6	0.00	-	-		
85	OHX	5	4052	-	0,6,6	0.00	-	-		
85	OHX	6	2071	-	0,6,6	0.00	-	-		
85	OHX	6	2123	-	0,6,6	0.00	-	-		
85	OHX	C8	201	-	0,6,6	0.00	-	-		
85	OHX	7	220	-	0,6,6	0.00	-	-		
85	OHX	D9	103	-	0,6,6	0.00	-	-		
85	OHX	5	3804	-	0,6,6	0.00	-	-		
85	OHX	1	3807	-	0,6,6	0.00	-	-		
85	OHX	5	4039	-	0,6,6	0.00	-	-		
85	OHX	1	3919	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	2	2113	-	0,6,6	0.00	-	-		
85	OHX	1	3913	-	0,6,6	0.00	-	-		
85	OHX	1	3851	-	0,6,6	0.00	-	-		
85	OHX	5	3764	-	0,6,6	0.00	-	-		
85	OHX	1	3976	-	0,6,6	0.00	-	-		
85	OHX	2	1983	-	0,6,6	0.00	-	-		
85	OHX	2	2039	-	0,6,6	0.00	-	-		
85	OHX	1	4013	-	0,6,6	0.00	-	-		
85	OHX	5	3813	-	0,6,6	0.00	-	-		
85	OHX	5	4042	-	0,6,6	0.00	-	-		
85	OHX	5	3956	-	0,6,6	0.00	-	-		
85	OHX	2	1995	-	0,6,6	0.00	-	-		
85	OHX	6	2072	-	0,6,6	0.00	-	-		
85	OHX	5	4001	-	0,6,6	0.00	-	-		
85	OHX	3	218	-	0,6,6	0.00	-	-		
85	OHX	6	2077	-	0,6,6	0.00	-	-		
85	OHX	1	3788	-	0,6,6	0.00	-	-		
85	OHX	5	3862	-	0,6,6	0.00	-	-		
85	OHX	1	3882	-	0,6,6	0.00	-	-		
85	OHX	1	3966	-	0,6,6	0.00	-	-		
85	OHX	5	3877	-	0,6,6	0.00	-	-		
85	OHX	1	3949	-	0,6,6	0.00	-	-		
85	OHX	1	3967	-	0,6,6	0.00	-	-		
85	OHX	M9	201	-	0,6,6	0.00	-	-		
85	OHX	5	4067	-	0,6,6	0.00	-	-		
85	OHX	1	3904	-	0,6,6	0.00	-	-		
85	OHX	2	2059	-	0,6,6	0.00	-	-		
85	OHX	s4	301	-	0,6,6	0.00	-	-		
85	OHX	2	2078	-	0,6,6	0.00	-	-		
85	OHX	1	3844	-	0,6,6	0.00	-	-		
85	OHX	5	3858	-	0,6,6	0.00	-	-		
85	OHX	1	3959	-	0,6,6	0.00	-	-		
85	OHX	5	3871	-	0,6,6	0.00	-	-		
85	OHX	1	3930	-	0,6,6	0.00	-	-		
85	OHX	1	3905	-	0,6,6	0.00	-	-		
85	OHX	8	217	-	0,6,6	0.00	-	-		
85	OHX	6	2015	-	0,6,6	0.00	-	-		
85	OHX	2	2084	-	0,6,6	0.00	-	-		
85	OHX	6	2100	-	0,6,6	0.00	-	-		
85	OHX	5	3980	-	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
87	ANM	1	3401	-	3/3/4/5	3/10/23/23	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)
87	1	3401	ANM	C4-C3	-6.47	1.43	1.53
87	1	3401	ANM	C3-C2	-6.41	1.40	1.53
87	1	3401	ANM	O2-C2	-4.67	1.37	1.44
87	1	3401	ANM	C16-N1	-4.41	1.38	1.48
87	1	3401	ANM	C15-C16	-3.10	1.47	1.53

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	1	3401	ANM	C15-C16-N1	-5.90	104.18	111.47
87	1	3401	ANM	C2-O2-C5	-5.34	109.46	117.72
87	1	3401	ANM	O2-C5-O3	-5.31	112.42	122.96
87	1	3401	ANM	C4-C3-C2	-4.14	97.94	103.29
87	1	3401	ANM	O4-C3-C4	-4.08	101.29	110.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
87	1	3401	ANM	C2
87	1	3401	ANM	C3
87	1	3401	ANM	C16

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	1	3401	ANM	C6-C5-O2-C2
87	1	3401	ANM	C10-C9-O1-C14
87	1	3401	ANM	C1-C9-O1-C14

There are no ring outliers.

496 monomers are involved in 773 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	1	3893	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	2	2052	OHX	1	0
85	5	3789	OHX	2	0
85	1	3733	OHX	1	0
85	2	2043	OHX	2	0
85	2	2105	OHX	1	0
85	6	2106	OHX	2	0
85	5	3861	OHX	1	0
85	5	4020	OHX	1	0
85	5	3860	OHX	1	0
85	6	2054	OHX	1	0
85	6	2112	OHX	3	0
85	5	3941	OHX	1	0
85	4	218	OHX	1	0
85	1	3774	OHX	1	0
85	5	4068	OHX	2	0
85	4	228	OHX	2	0
85	1	3858	OHX	1	0
85	5	3930	OHX	1	0
85	8	211	OHX	1	0
85	5	3911	OHX	1	0
85	1	3863	OHX	1	0
85	5	3815	OHX	1	0
85	1	3950	OHX	2	0
85	6	2009	OHX	1	0
85	5	3923	OHX	5	0
85	2	2085	OHX	1	0
85	2	2108	OHX	1	0
85	1	3895	OHX	2	0
85	3	210	OHX	1	0
85	5	3922	OHX	1	0
85	5	3806	OHX	4	0
85	6	2117	OHX	1	0
85	6	2138	OHX	2	0
85	1	3935	OHX	1	0
85	2	2029	OHX	2	0
85	1	3843	OHX	2	0
85	2	1992	OHX	2	0
85	1	3918	OHX	1	0
85	1	3739	OHX	2	0
85	6	2085	OHX	2	0
85	1	3766	OHX	1	0
85	5	3844	OHX	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	5	4032	OHX	2	0
85	5	3932	OHX	1	0
85	5	4021	OHX	1	0
85	5	3986	OHX	2	0
85	5	3891	OHX	1	0
85	5	3769	OHX	1	0
85	7	215	OHX	1	0
85	1	3900	OHX	1	0
85	1	3979	OHX	1	0
85	1	4009	OHX	8	0
85	2	2001	OHX	1	0
85	1	3945	OHX	1	0
85	1	4026	OHX	1	0
85	2	2067	OHX	1	0
85	8	215	OHX	1	0
85	1	3791	OHX	2	0
85	6	2108	OHX	1	0
85	1	3912	OHX	4	0
85	6	2121	OHX	4	0
85	1	4018	OHX	2	0
85	5	4018	OHX	1	0
85	5	3797	OHX	1	0
85	5	3751	OHX	2	0
85	5	3816	OHX	2	0
85	2	2116	OHX	1	0
85	2	1989	OHX	1	0
85	2	1986	OHX	1	0
85	1	3969	OHX	2	0
85	6	2014	OHX	1	0
85	5	3989	OHX	1	0
85	1	4003	OHX	1	0
85	1	3820	OHX	1	0
85	5	4056	OHX	1	0
85	5	3836	OHX	1	0
85	5	4062	OHX	3	0
85	5	3768	OHX	1	0
85	1	3948	OHX	1	0
85	L4	401	OHX	5	0
85	1	3752	OHX	1	0
85	2	2097	OHX	1	0
85	2	2037	OHX	2	0
85	5	3996	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	2	2030	OHX	2	0
85	2	2009	OHX	1	0
85	6	2064	OHX	2	0
85	8	213	OHX	1	0
85	2	2046	OHX	1	0
85	2	2036	OHX	1	0
85	5	3908	OHX	3	0
85	O9	101	OHX	2	0
85	5	3892	OHX	1	0
85	5	3857	OHX	1	0
85	5	3756	OHX	1	0
85	1	3826	OHX	1	0
85	1	3917	OHX	1	0
85	2	2065	OHX	2	0
85	1	3971	OHX	2	0
85	1	3974	OHX	1	0
85	6	2016	OHX	1	0
85	6	2019	OHX	2	0
85	6	2088	OHX	3	0
85	1	4025	OHX	1	0
85	5	3822	OHX	8	0
85	5	4019	OHX	1	0
85	5	3835	OHX	3	0
85	1	3818	OHX	6	0
85	5	3742	OHX	1	0
85	5	4060	OHX	1	0
85	6	2146	OHX	1	0
85	6	2090	OHX	1	0
85	3	215	OHX	1	0
85	1	4007	OHX	3	0
85	5	4038	OHX	5	0
85	6	2157	OHX	1	0
85	7	213	OHX	1	0
85	5	3782	OHX	1	0
85	6	2105	OHX	1	0
85	8	216	OHX	1	0
85	5	3854	OHX	6	0
85	5	3976	OHX	1	0
85	1	3823	OHX	2	0
85	8	219	OHX	2	0
85	6	2029	OHX	1	0
85	5	3800	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	2	2075	OHX	1	0
85	1	4002	OHX	1	0
85	1	4015	OHX	2	0
85	2	2024	OHX	2	0
85	1	3736	OHX	1	0
85	5	4013	OHX	1	0
85	1	3899	OHX	3	0
85	1	3740	OHX	1	0
85	5	3855	OHX	1	0
85	4	219	OHX	1	0
85	6	2021	OHX	1	0
85	5	4054	OHX	5	0
85	2	2100	OHX	1	0
85	2	2102	OHX	1	0
85	6	2037	OHX	2	0
85	1	3836	OHX	7	0
85	6	2111	OHX	1	0
85	1	3898	OHX	1	0
85	6	2065	OHX	1	0
85	5	3950	OHX	2	0
85	1	3874	OHX	2	0
85	6	2062	OHX	1	0
85	M7	205	OHX	1	0
85	1	3735	OHX	1	0
85	6	2073	OHX	1	0
85	1	3929	OHX	1	0
85	1	3997	OHX	3	0
85	6	2120	OHX	2	0
85	5	3848	OHX	1	0
85	6	2050	OHX	1	0
85	6	2140	OHX	1	0
85	5	4049	OHX	4	0
85	5	3776	OHX	1	0
85	5	3864	OHX	1	0
85	1	3955	OHX	1	0
85	6	2154	OHX	1	0
85	2	2110	OHX	1	0
85	6	2126	OHX	1	0
85	1	3915	OHX	3	0
85	1	3743	OHX	1	0
85	5	3849	OHX	2	0
85	5	3834	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	5	3968	OHX	1	0
85	1	3835	OHX	2	0
85	1	3751	OHX	3	0
85	2	2031	OHX	1	0
85	1	3744	OHX	2	0
85	1	3841	OHX	2	0
85	2	2090	OHX	1	0
85	6	2087	OHX	3	0
87	1	3401	ANM	16	0
85	5	4025	OHX	6	0
85	1	3869	OHX	1	0
85	1	4011	OHX	1	0
85	1	3924	OHX	1	0
85	5	3963	OHX	1	0
85	2	2021	OHX	2	0
85	2	2068	OHX	7	0
85	6	2098	OHX	1	0
85	6	2137	OHX	1	0
85	6	2017	OHX	1	0
85	5	3856	OHX	2	0
85	5	3902	OHX	1	0
85	1	3934	OHX	1	0
85	6	2060	OHX	2	0
85	5	4030	OHX	2	0
85	1	3764	OHX	1	0
85	5	3792	OHX	1	0
85	2	2050	OHX	1	0
85	2	2042	OHX	3	0
85	6	2075	OHX	1	0
85	2	2018	OHX	1	0
85	1	3854	OHX	3	0
85	5	3748	OHX	1	0
85	6	2124	OHX	2	0
85	1	3767	OHX	1	0
85	1	3978	OHX	1	0
85	5	3935	OHX	1	0
85	1	3880	OHX	4	0
85	5	3909	OHX	1	0
85	5	3867	OHX	1	0
85	1	3907	OHX	3	0
85	8	224	OHX	2	0
85	1	4031	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	5	3759	OHX	1	0
85	1	3726	OHX	1	0
85	6	2012	OHX	1	0
85	6	2152	OHX	5	0
85	5	3750	OHX	1	0
85	1	3753	OHX	1	0
85	5	3886	OHX	1	0
85	5	4002	OHX	1	0
85	5	4007	OHX	9	0
85	1	3954	OHX	1	0
85	4	216	OHX	1	0
85	2	2023	OHX	1	0
85	5	3830	OHX	1	0
85	2	2054	OHX	6	0
85	2	2035	OHX	1	0
85	2	2069	OHX	1	0
85	1	3910	OHX	1	0
85	5	3875	OHX	1	0
85	1	3829	OHX	1	0
85	5	4016	OHX	1	0
85	5	3915	OHX	1	0
85	4	231	OHX	1	0
85	6	2025	OHX	2	0
85	5	4027	OHX	7	0
85	1	4004	OHX	7	0
85	2	1991	OHX	2	0
85	1	3867	OHX	1	0
85	5	4066	OHX	2	0
85	1	3817	OHX	1	0
85	1	4029	OHX	1	0
85	1	3993	OHX	2	0
85	2	2103	OHX	1	0
85	1	3779	OHX	1	0
85	5	3784	OHX	1	0
85	5	4037	OHX	7	0
85	2	2045	OHX	2	0
85	1	3932	OHX	2	0
85	6	2083	OHX	1	0
85	2	2005	OHX	2	0
85	5	3992	OHX	1	0
85	2	2013	OHX	2	0
85	5	3803	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	6	2056	OHX	1	0
85	1	3838	OHX	1	0
85	6	2116	OHX	6	0
85	1	3759	OHX	1	0
85	1	3901	OHX	2	0
85	S8	301	OHX	1	0
85	1	3980	OHX	1	0
85	5	3749	OHX	1	0
85	L3	402	OHX	1	0
85	2	2044	OHX	3	0
85	6	2023	OHX	6	0
85	2	2026	OHX	1	0
85	5	3944	OHX	2	0
85	5	3788	OHX	1	0
85	2	2002	OHX	1	0
85	2	2111	OHX	2	0
85	5	3752	OHX	2	0
85	1	3801	OHX	1	0
85	1	3812	OHX	1	0
85	1	3831	OHX	1	0
85	1	3952	OHX	1	0
85	5	3773	OHX	1	0
85	5	4044	OHX	1	0
85	2	1996	OHX	1	0
85	1	3891	OHX	3	0
85	5	4036	OHX	7	0
85	1	3983	OHX	1	0
85	1	3832	OHX	7	0
85	1	3837	OHX	1	0
85	5	3829	OHX	1	0
85	5	3921	OHX	1	0
85	1	3793	OHX	1	0
85	1	3864	OHX	1	0
85	6	2043	OHX	1	0
85	5	3798	OHX	3	0
85	1	3808	OHX	1	0
85	5	3895	OHX	1	0
85	5	3934	OHX	5	0
85	8	212	OHX	2	0
85	1	3947	OHX	1	0
85	5	3898	OHX	6	0
85	5	3912	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	1	3987	OHX	2	0
85	2	2000	OHX	1	0
85	1	3786	OHX	1	0
85	5	4058	OHX	1	0
85	2	2032	OHX	1	0
85	1	3964	OHX	1	0
85	6	2153	OHX	1	0
85	5	4015	OHX	1	0
85	5	3840	OHX	1	0
85	1	3903	OHX	1	0
85	6	2036	OHX	1	0
85	2	2119	OHX	1	0
85	2	1993	OHX	1	0
85	1	3849	OHX	1	0
85	5	4069	OHX	1	0
85	2	2051	OHX	2	0
85	6	2076	OHX	1	0
85	8	218	OHX	2	0
85	6	2035	OHX	3	0
85	5	4034	OHX	1	0
85	2	2064	OHX	1	0
85	5	3917	OHX	2	0
85	O7	104	OHX	1	0
85	2	2033	OHX	1	0
85	1	3916	OHX	5	0
85	1	3842	OHX	1	0
85	5	3966	OHX	1	0
85	1	3940	OHX	6	0
85	6	2061	OHX	1	0
85	5	3999	OHX	2	0
85	5	3839	OHX	1	0
85	5	4028	OHX	1	0
85	1	3731	OHX	1	0
85	7	214	OHX	1	0
85	6	2092	OHX	1	0
85	1	3859	OHX	2	0
85	5	3974	OHX	1	0
85	5	3853	OHX	1	0
85	1	3797	OHX	1	0
85	2	2007	OHX	1	0
85	5	3852	OHX	1	0
85	2	1998	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	5	4033	OHX	1	0
85	5	3894	OHX	1	0
85	1	3772	OHX	2	0
85	5	3826	OHX	1	0
85	2	2056	OHX	3	0
85	6	2066	OHX	1	0
85	4	222	OHX	1	0
85	4	227	OHX	1	0
85	6	2129	OHX	1	0
85	2	2101	OHX	2	0
85	5	3761	OHX	1	0
85	5	4031	OHX	1	0
85	5	3957	OHX	1	0
85	2	2006	OHX	1	0
85	5	3872	OHX	1	0
85	2	2074	OHX	2	0
85	4	220	OHX	1	0
85	1	4036	OHX	1	0
85	8	214	OHX	1	0
85	1	3846	OHX	1	0
85	1	3927	OHX	5	0
85	5	3766	OHX	2	0
85	6	2141	OHX	1	0
85	6	2136	OHX	1	0
85	2	2010	OHX	1	0
85	5	3827	OHX	2	0
85	1	3860	OHX	2	0
85	5	4057	OHX	1	0
85	1	3778	OHX	1	0
85	1	3782	OHX	1	0
85	C5	201	OHX	3	0
85	5	4051	OHX	1	0
85	5	3754	OHX	2	0
85	5	3801	OHX	2	0
85	5	3882	OHX	1	0
85	5	3919	OHX	1	0
85	6	2147	OHX	2	0
85	2	2107	OHX	2	0
85	2	2092	OHX	1	0
85	1	3923	OHX	1	0
85	1	3878	OHX	1	0
85	6	2110	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	1	3852	OHX	1	0
85	5	4059	OHX	1	0
85	1	3888	OHX	1	0
85	5	3850	OHX	1	0
85	1	4008	OHX	6	0
85	1	3975	OHX	5	0
85	1	3794	OHX	1	0
85	1	3814	OHX	1	0
85	5	3745	OHX	1	0
85	2	1999	OHX	2	0
85	5	3947	OHX	2	0
85	1	3926	OHX	1	0
85	6	2109	OHX	7	0
85	5	3809	OHX	1	0
85	2	1994	OHX	1	0
85	6	2118	OHX	1	0
85	1	3824	OHX	2	0
85	5	3807	OHX	3	0
85	1	3729	OHX	1	0
85	2	2112	OHX	3	0
85	4	215	OHX	1	0
85	6	2030	OHX	1	0
85	1	3730	OHX	1	0
85	5	3825	OHX	1	0
85	2	2004	OHX	1	0
85	1	3970	OHX	1	0
85	5	3939	OHX	1	0
85	5	3977	OHX	1	0
85	7	219	OHX	4	0
85	3	219	OHX	1	0
85	S6	301	OHX	1	0
85	3	217	OHX	2	0
85	2	2070	OHX	3	0
85	1	3956	OHX	2	0
85	2	2025	OHX	1	0
85	5	3774	OHX	1	0
85	5	3937	OHX	1	0
85	8	221	OHX	2	0
85	1	3944	OHX	6	0
85	1	3742	OHX	1	0
85	1	3761	OHX	2	0
85	5	3889	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	1	3951	OHX	1	0
85	5	4011	OHX	1	0
85	2	2095	OHX	3	0
85	L3	403	OHX	1	0
85	6	2024	OHX	1	0
85	6	2053	OHX	1	0
85	5	3953	OHX	1	0
85	2	2017	OHX	1	0
85	2	2086	OHX	1	0
85	1	3787	OHX	1	0
85	5	3998	OHX	2	0
85	5	3979	OHX	2	0
85	2	2099	OHX	1	0
85	5	3763	OHX	1	0
85	5	3846	OHX	4	0
85	5	4022	OHX	1	0
85	5	3995	OHX	2	0
85	1	4019	OHX	3	0
85	6	2046	OHX	1	0
85	6	2150	OHX	1	0
85	6	2033	OHX	1	0
85	1	4017	OHX	5	0
85	O3	202	OHX	2	0
85	6	2099	OHX	2	0
85	1	3894	OHX	1	0
85	2	2079	OHX	5	0
85	6	2018	OHX	1	0
85	5	4029	OHX	1	0
85	5	4035	OHX	10	0
85	1	4038	OHX	1	0
85	6	2013	OHX	1	0
85	6	2082	OHX	1	0
85	6	2047	OHX	1	0
85	C3	201	OHX	3	0
85	1	3862	OHX	3	0
85	5	3868	OHX	2	0
85	1	3833	OHX	1	0
85	5	3983	OHX	2	0
85	1	3800	OHX	1	0
85	2	2048	OHX	4	0
85	6	2097	OHX	1	0
85	5	3926	OHX	1	0

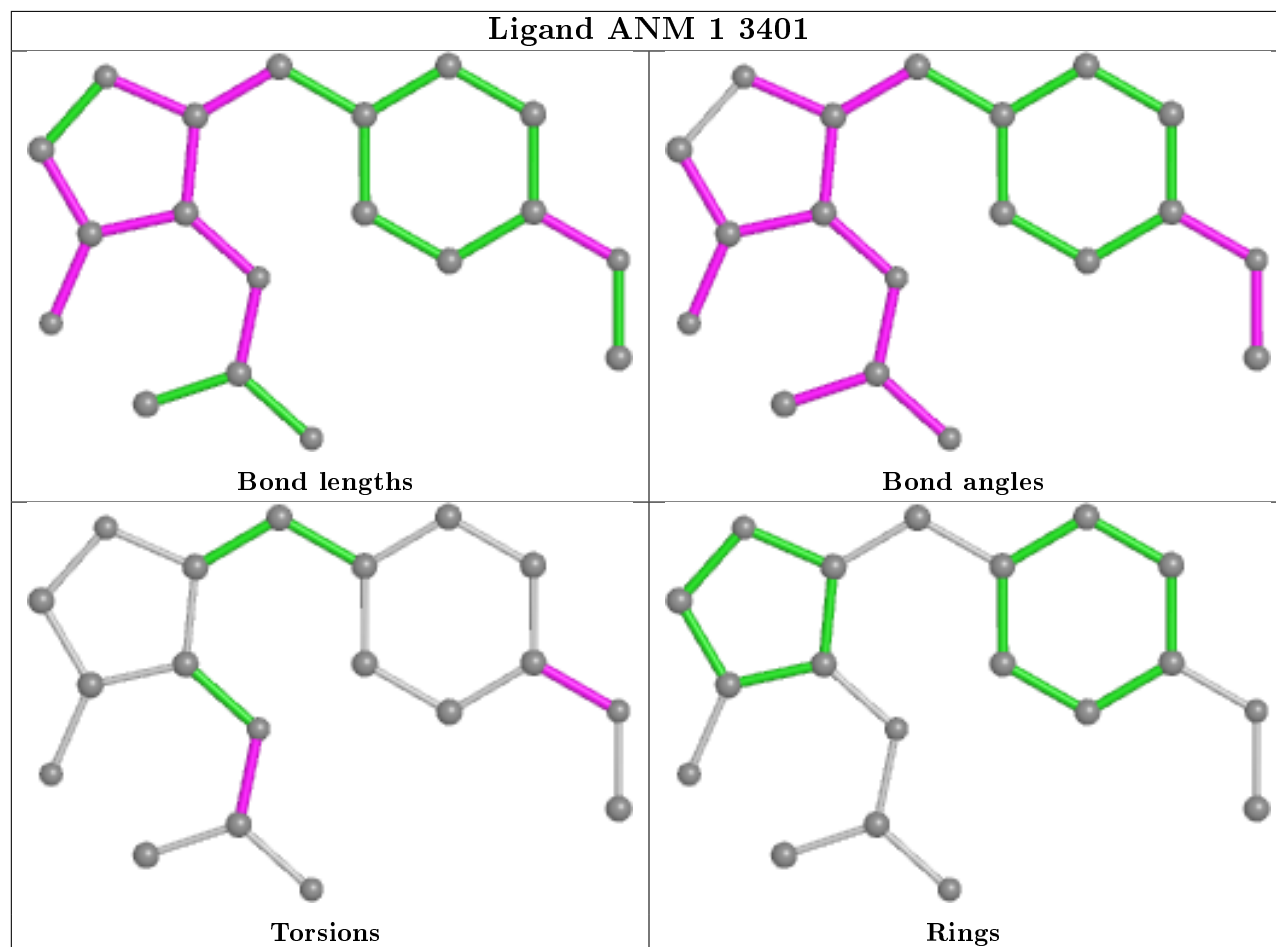
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	2	2049	OHX	1	0
85	1	4012	OHX	3	0
85	5	3780	OHX	1	0
85	5	3933	OHX	2	0
85	5	3964	OHX	2	0
85	1	3737	OHX	1	0
85	2	2114	OHX	1	0
85	5	4052	OHX	1	0
85	6	2071	OHX	2	0
85	C8	201	OHX	0	1
85	D9	103	OHX	3	0
85	5	4039	OHX	3	0
85	2	2113	OHX	1	0
85	1	3851	OHX	2	0
85	1	3976	OHX	1	0
85	2	1983	OHX	1	0
85	5	4042	OHX	3	0
85	2	1995	OHX	1	0
85	6	2072	OHX	1	0
85	6	2077	OHX	1	0
85	1	3788	OHX	1	0
85	1	3966	OHX	1	0
85	5	3877	OHX	6	0
85	1	3967	OHX	2	0
85	M9	201	OHX	1	0
85	1	3904	OHX	7	0
85	2	2059	OHX	1	0
85	2	2078	OHX	1	0
85	5	3858	OHX	1	0
85	1	3930	OHX	1	0
85	2	2084	OHX	1	0
85	6	2100	OHX	1	0
85	5	3980	OHX	1	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
80	m2	2
35	sM	1
12	c0	1
1	2	1
35	SM	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	139:UNK	C	155:UNK	N	37.86
1	SM	141:ALA	C	151:UNK	N	26.40
1	c0	84:GLU	C	87:UNK	N	8.00
1	2	1716:C	O3'	1717:G	P	3.94
1	m2	23:UNK	C	28:UNK	N	3.86

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	2	1781/1800 (98%)	0.47	141 (7%) 12 5	60, 86, 144, 179	0
1	6	1795/1800 (99%)	0.39	124 (6%) 16 7	43, 76, 145, 181	0
2	S0	206/251 (82%)	0.37	14 (6%) 17 7	87, 96, 101, 106	0
2	s0	206/251 (82%)	0.34	4 (1%) 66 46	78, 120, 181, 264	0
3	S1	214/254 (84%)	1.01	44 (20%) 1 0	96, 117, 134, 137	0
3	s1	216/254 (85%)	0.15	6 (2%) 53 30	71, 82, 95, 105	0
4	S2	217/253 (85%)	0.03	2 (0%) 84 69	73, 81, 90, 98	0
4	s2	217/253 (85%)	0.08	7 (3%) 47 25	58, 68, 84, 89	0
5	S3	223/239 (93%)	0.21	9 (4%) 38 19	76, 86, 104, 107	0
5	s3	223/239 (93%)	0.49	13 (5%) 23 10	77, 98, 120, 126	0
6	S4	260/260 (100%)	0.24	8 (3%) 49 26	64, 84, 91, 104	0
6	s4	260/260 (100%)	0.05	4 (1%) 73 54	49, 74, 82, 99	0
7	S5	206/224 (91%)	0.52	17 (8%) 11 4	94, 104, 110, 113	0
7	s5	206/224 (91%)	0.40	11 (5%) 26 12	74, 93, 100, 104	0
8	S6	226/236 (95%)	0.53	22 (9%) 7 2	67, 89, 106, 109	0
8	s6	218/236 (92%)	0.28	8 (3%) 41 21	51, 82, 94, 102	0
9	S7	184/189 (97%)	0.56	15 (8%) 11 4	83, 103, 119, 122	0
9	s7	186/189 (98%)	0.61	20 (10%) 5 2	71, 96, 123, 189	0
10	S8	188/200 (94%)	0.16	6 (3%) 47 25	61, 75, 106, 113	0
10	s8	188/200 (94%)	0.28	8 (4%) 35 17	46, 69, 110, 123	0
11	S9	185/196 (94%)	0.47	8 (4%) 35 17	77, 89, 111, 126	0
11	s9	185/196 (94%)	0.31	6 (3%) 47 25	62, 79, 104, 119	0
12	C0	84/96 (87%)	0.14	0 100 100	83, 96, 104, 107	0
12	c0	84/96 (87%)	0.77	10 (11%) 4 2	97, 122, 131, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	C1	146/155 (94%)	0.17	6 (4%) 37 18	64, 72, 90, 101	0
13	c1	146/155 (94%)	0.26	9 (6%) 20 9	51, 66, 97, 152	0
14	C2	124/142 (87%)	1.60	46 (37%) 0 0	118, 124, 129, 132	0
14	c2	124/142 (87%)	2.93	76 (61%) 0 0	170, 185, 193, 202	0
15	C3	150/150 (100%)	0.06	6 (4%) 38 19	71, 85, 93, 97	0
15	c3	150/150 (100%)	-0.12	0 100 100	56, 72, 87, 92	0
16	C4	127/136 (93%)	1.07	25 (19%) 1 0	74, 116, 124, 126	0
16	c4	128/136 (94%)	0.21	2 (1%) 72 51	54, 81, 85, 88	0
17	C5	124/141 (87%)	0.08	3 (2%) 59 37	77, 88, 107, 114	0
17	c5	135/141 (95%)	0.32	10 (7%) 14 5	61, 91, 108, 115	0
18	C6	141/142 (99%)	0.41	6 (4%) 35 17	81, 99, 102, 103	0
18	c6	142/142 (100%)	0.67	18 (12%) 3 1	69, 89, 101, 104	0
19	C7	120/136 (88%)	0.51	11 (9%) 9 3	89, 99, 106, 107	0
19	c7	117/136 (86%)	0.82	17 (14%) 2 1	79, 95, 321, 380	0
20	C8	145/145 (100%)	0.78	18 (12%) 4 1	76, 94, 109, 114	0
20	c8	145/145 (100%)	0.46	8 (5%) 25 11	69, 87, 98, 103	0
21	C9	143/143 (100%)	0.47	7 (4%) 29 14	86, 97, 105, 110	0
21	c9	143/143 (100%)	0.17	0 100 100	71, 83, 93, 98	0
22	D0	107/120 (89%)	1.21	26 (24%) 0 0	76, 98, 107, 109	0
22	d0	110/120 (91%)	1.24	30 (27%) 0 0	73, 103, 118, 121	0
23	D1	87/87 (100%)	0.35	5 (5%) 23 11	84, 87, 97, 100	0
23	d1	87/87 (100%)	0.11	2 (2%) 60 39	70, 86, 139, 157	0
24	D2	129/129 (100%)	0.01	2 (1%) 72 51	73, 81, 87, 95	0
24	d2	129/129 (100%)	-0.03	0 100 100	56, 67, 74, 81	0
25	D3	144/144 (100%)	0.02	2 (1%) 75 56	63, 66, 72, 75	0
25	d3	144/144 (100%)	-0.26	0 100 100	47, 52, 60, 65	0
26	D4	134/134 (100%)	0.60	12 (8%) 9 3	74, 90, 97, 100	0
26	d4	134/134 (100%)	0.27	6 (4%) 33 16	58, 78, 88, 101	0
27	D5	70/107 (65%)	0.39	2 (2%) 51 28	103, 109, 114, 114	0
27	d5	69/107 (64%)	0.78	10 (14%) 2 1	86, 97, 101, 102	0
28	D6	97/97 (100%)	0.55	4 (4%) 37 18	76, 85, 121, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	d6	97/97 (100%)	0.08	1 (1%) 82 67	56, 66, 87, 91	0
29	D7	81/81 (100%)	0.51	7 (8%) 10 4	84, 95, 107, 108	0
29	d7	81/81 (100%)	0.54	7 (8%) 10 4	72, 86, 101, 103	0
30	D8	63/66 (95%)	1.38	17 (26%) 0 0	101, 108, 112, 115	0
30	d8	63/66 (95%)	1.49	18 (28%) 0 0	88, 96, 101, 106	0
31	D9	53/55 (96%)	0.40	1 (1%) 66 46	78, 82, 94, 95	0
31	d9	53/55 (96%)	0.58	4 (7%) 14 5	73, 85, 114, 122	0
32	E0	60/62 (96%)	0.67	6 (10%) 7 2	65, 90, 102, 104	0
32	e0	62/62 (100%)	0.75	9 (14%) 2 1	53, 78, 95, 99	0
33	E1	71/76 (93%)	1.58	27 (38%) 0 0	89, 115, 125, 126	0
33	e1	76/76 (100%)	2.55	38 (50%) 0 0	96, 155, 181, 183	0
34	SR	318/318 (100%)	0.63	33 (10%) 6 2	95, 103, 114, 120	0
34	sR	318/318 (100%)	0.71	36 (11%) 5 2	102, 116, 127, 175	0
35	SM	133/182 (73%)	0.61	15 (11%) 5 2	56, 80, 122, 131	0
35	sM	63/182 (34%)	0.50	5 (7%) 12 5	44, 87, 93, 95	0
36	1	3149/3396 (92%)	0.05	123 (3%) 39 20	31, 53, 104, 189	0
36	5	3150/3396 (92%)	0.01	97 (3%) 49 26	29, 51, 105, 149	0
37	3	121/121 (100%)	-0.07	1 (0%) 86 72	43, 66, 77, 80	0
37	7	121/121 (100%)	-0.24	0 100 100	34, 52, 64, 69	0
38	4	158/158 (100%)	-0.17	3 (1%) 66 46	35, 54, 84, 107	0
38	8	158/158 (100%)	-0.04	3 (1%) 66 46	40, 61, 93, 104	0
39	L2	252/253 (99%)	-0.16	0 100 100	39, 52, 65, 70	0
39	l2	252/253 (99%)	-0.17	4 (1%) 72 51	37, 55, 73, 146	0
40	L3	386/386 (100%)	-0.25	1 (0%) 94 88	38, 53, 64, 73	0
40	l3	386/386 (100%)	-0.33	1 (0%) 94 88	30, 43, 58, 82	0
41	L4	361/361 (100%)	-0.37	0 100 100	33, 44, 56, 62	0
41	l4	361/361 (100%)	-0.25	3 (0%) 86 72	36, 51, 66, 72	0
42	L5	296/296 (100%)	0.13	5 (1%) 70 49	52, 69, 81, 90	0
42	l5	294/296 (99%)	-0.09	5 (1%) 70 49	37, 55, 77, 101	0
43	L6	156/175 (89%)	-0.29	0 100 100	42, 49, 58, 71	0
43	l6	157/175 (89%)	-0.24	2 (1%) 77 59	42, 54, 65, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	L7	222/243 (91%)	-0.44	1 (0%) 91 81	36, 42, 58, 72	0
44	l7	223/243 (91%)	-0.30	6 (2%) 54 31	33, 41, 69, 86	0
45	L8	233/255 (91%)	0.09	8 (3%) 45 24	58, 71, 89, 96	0
45	l8	231/255 (90%)	0.41	15 (6%) 18 8	65, 80, 101, 106	0
46	L9	191/191 (100%)	0.04	2 (1%) 82 67	51, 59, 67, 72	0
46	l9	191/191 (100%)	-0.30	1 (0%) 91 81	39, 47, 59, 67	0
47	M0	211/220 (95%)	-0.25	3 (1%) 75 56	39, 50, 74, 80	0
47	m0	213/220 (96%)	-0.16	4 (1%) 66 46	33, 46, 75, 167	0
48	M1	169/173 (97%)	0.30	7 (4%) 37 18	61, 74, 82, 86	0
48	m1	169/173 (97%)	-0.09	2 (1%) 79 61	44, 57, 67, 76	0
49	M3	193/198 (97%)	-0.14	6 (3%) 49 26	35, 52, 76, 98	0
49	m3	194/198 (97%)	0.08	6 (3%) 49 26	35, 63, 86, 93	0
50	M4	136/137 (99%)	-0.25	2 (1%) 73 54	46, 52, 62, 64	0
50	m4	137/137 (100%)	-0.40	1 (0%) 87 75	41, 46, 61, 67	0
51	M5	203/203 (100%)	-0.17	0 100 100	36, 49, 59, 60	0
51	m5	203/203 (100%)	-0.08	0 100 100	40, 56, 66, 69	0
52	M6	197/198 (99%)	-0.40	1 (0%) 91 81	37, 43, 57, 58	0
52	m6	197/198 (99%)	-0.46	0 100 100	30, 35, 55, 58	0
53	M7	183/183 (100%)	0.10	16 (8%) 10 4	39, 47, 73, 82	0
53	m7	155/183 (84%)	-0.29	0 100 100	36, 43, 53, 61	0
54	M8	185/185 (100%)	-0.42	0 100 100	37, 47, 59, 68	0
54	m8	185/185 (100%)	-0.26	1 (0%) 91 81	36, 52, 60, 66	0
55	M9	188/188 (100%)	0.30	10 (5%) 26 12	58, 67, 117, 123	0
55	m9	188/188 (100%)	0.23	8 (4%) 35 17	53, 61, 108, 121	0
56	N0	172/172 (100%)	-0.29	2 (1%) 79 61	43, 49, 57, 63	0
56	n0	172/172 (100%)	-0.37	0 100 100	35, 41, 49, 52	0
57	N1	159/159 (100%)	-0.20	3 (1%) 66 46	39, 49, 71, 75	0
57	n1	159/159 (100%)	-0.22	3 (1%) 66 46	34, 41, 66, 71	0
58	N2	100/120 (83%)	0.89	11 (11%) 5 2	81, 89, 92, 92	0
58	n2	98/120 (81%)	0.61	11 (11%) 5 2	70, 79, 83, 86	0
59	N3	136/136 (100%)	0.01	4 (2%) 51 28	43, 50, 55, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
59	n3	136/136 (100%)	-0.30	1 (0%) 87 75	30, 39, 48, 51	0
60	N4	98/155 (63%)	0.94	21 (21%) 0 0	49, 63, 112, 120	0
60	n4	135/155 (87%)	0.64	19 (14%) 2 1	38, 87, 303, 442	0
61	N5	121/141 (85%)	-0.04	1 (0%) 86 72	51, 60, 72, 88	0
61	n5	120/141 (85%)	0.14	6 (5%) 28 13	50, 65, 80, 86	0
62	N6	126/126 (100%)	0.20	4 (3%) 47 25	40, 53, 61, 64	0
62	n6	126/126 (100%)	0.03	1 (0%) 86 72	46, 60, 71, 75	0
63	N7	135/135 (100%)	0.26	3 (2%) 62 41	71, 79, 92, 98	0
63	n7	135/135 (100%)	0.19	4 (2%) 50 27	75, 86, 100, 107	0
64	N8	148/148 (100%)	-0.26	1 (0%) 87 75	30, 48, 62, 72	0
64	n8	148/148 (100%)	-0.25	0 100 100	31, 54, 63, 65	0
65	N9	58/58 (100%)	0.12	2 (3%) 45 24	35, 53, 81, 89	0
65	n9	58/58 (100%)	-0.13	0 100 100	32, 49, 69, 73	0
66	O0	97/104 (93%)	0.27	8 (8%) 11 4	67, 73, 84, 87	0
66	o0	100/104 (96%)	0.30	5 (5%) 28 13	66, 76, 86, 92	0
67	O1	109/112 (97%)	0.08	1 (0%) 84 69	52, 62, 76, 82	0
67	o1	109/112 (97%)	0.09	1 (0%) 84 69	44, 56, 81, 163	0
68	O2	127/129 (98%)	-0.18	2 (1%) 72 51	32, 44, 49, 53	0
68	o2	127/129 (98%)	-0.31	1 (0%) 86 72	31, 50, 57, 61	0
69	O3	106/106 (100%)	-0.32	0 100 100	37, 42, 56, 60	0
69	o3	106/106 (100%)	-0.33	0 100 100	34, 43, 59, 65	0
70	O4	112/120 (93%)	0.36	6 (5%) 25 12	52, 67, 82, 87	0
70	o4	112/120 (93%)	0.22	3 (2%) 54 31	51, 66, 88, 91	0
71	O5	119/119 (100%)	-0.03	1 (0%) 86 72	49, 60, 66, 70	0
71	o5	119/119 (100%)	-0.07	1 (0%) 86 72	57, 68, 76, 81	0
72	O6	99/99 (100%)	0.12	5 (5%) 28 13	51, 60, 77, 83	0
72	o6	99/99 (100%)	0.16	3 (3%) 50 27	59, 67, 77, 85	0
73	O7	87/87 (100%)	-0.09	1 (1%) 80 64	37, 43, 60, 73	0
73	o7	87/87 (100%)	0.04	2 (2%) 60 39	37, 46, 74, 90	0
74	O8	77/77 (100%)	0.22	3 (3%) 39 20	75, 80, 87, 87	0
74	o8	77/77 (100%)	0.62	6 (7%) 13 5	81, 89, 108, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	O9	50/50 (100%)	-0.26	2 (4%) 38 19	45, 49, 51, 52	0
75	o9	50/50 (100%)	-0.27	0 100 100	45, 50, 57, 66	0
76	Q0	52/52 (100%)	-0.01	0 100 100	48, 52, 61, 65	0
76	q0	52/52 (100%)	-0.27	0 100 100	36, 39, 47, 51	0
77	Q1	25/25 (100%)	0.52	1 (4%) 38 19	62, 63, 67, 68	0
77	q1	25/25 (100%)	-0.11	0 100 100	49, 51, 53, 55	0
78	Q2	105/105 (100%)	0.45	3 (2%) 51 28	39, 51, 63, 74	0
78	q2	105/105 (100%)	0.33	4 (3%) 40 20	38, 49, 59, 71	0
79	Q3	91/91 (100%)	-0.11	0 100 100	46, 53, 63, 69	0
79	q3	91/91 (100%)	-0.25	1 (1%) 80 64	43, 51, 65, 71	0
80	m2	0/150	-	-	-	-
81	p0	143/311 (45%)	0.41	12 (8%) 11 4	83, 101, 174, 180	0
82	p1	0/47	-	-	-	-
83	p2	0/46	-	-	-	-
All	All	32994/35138 (93%)	0.17	1617 (4%) 29 14	29, 66, 117, 442	0

The worst 5 of 1617 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	c2	20	ALA	27.1
47	m0	111	LEU	12.8
16	C4	15	GLY	12.0
1	2	1702	A	10.4
60	n4	68	ALA	10.3

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	6	1984	1/1	0.26	0.48	70,70,70,70	0
84	MG	1	3678	1/1	0.36	0.24	65,65,65,65	0
84	MG	M3	201	1/1	0.44	0.22	86,86,86,86	0
84	MG	5	3457	1/1	0.47	0.43	100,100,100,100	0
84	MG	2	1941	1/1	0.50	0.78	93,93,93,93	0
84	MG	2	1962	1/1	0.50	0.78	110,110,110,110	0
84	MG	5	3617	1/1	0.53	0.56	46,46,46,46	0
84	MG	l6	201	1/1	0.56	0.45	56,56,56,56	0
84	MG	5	3647	1/1	0.57	0.37	41,41,41,41	0
84	MG	5	3643	1/1	0.58	0.40	55,55,55,55	0
84	MG	SM	201	1/1	0.59	0.51	56,56,56,56	0
84	MG	1	3583	1/1	0.60	0.21	61,61,61,61	0
84	MG	6	1977	1/1	0.60	0.38	79,79,79,79	0
87	ANM	1	3401	19/19	0.61	0.52	62,62,62,62	19
84	MG	1	3494	1/1	0.62	0.38	52,52,52,52	0
84	MG	1	4043	1/1	0.62	0.72	33,33,33,33	0
84	MG	5	3613	1/1	0.63	0.34	58,58,58,58	0
84	MG	1	3714	1/1	0.64	0.22	45,45,45,45	0
84	MG	6	1971	1/1	0.64	0.60	90,90,90,90	0
84	MG	6	1996	1/1	0.64	0.36	54,54,54,54	0
84	MG	5	3460	1/1	0.65	0.29	44,44,44,44	0
84	MG	1	3722	1/1	0.65	0.37	60,60,60,60	0
84	MG	5	3462	1/1	0.65	0.29	58,58,58,58	0
84	MG	6	1961	1/1	0.66	0.43	61,61,61,61	0
84	MG	2	1904	1/1	0.66	0.67	77,77,77,77	0
84	MG	1	3570	1/1	0.66	0.69	67,67,67,67	0
84	MG	1	3599	1/1	0.66	0.49	59,59,59,59	0
84	MG	O7	103	1/1	0.67	0.61	64,64,64,64	0
84	MG	1	3624	1/1	0.68	0.23	44,44,44,44	0
84	MG	2	1970	1/1	0.68	0.56	76,76,76,76	0
84	MG	2	1912	1/1	0.68	0.55	74,74,74,74	0
84	MG	1	3496	1/1	0.69	0.48	39,39,39,39	0
84	MG	2	1969	1/1	0.69	0.71	66,66,66,66	0
84	MG	1	3673	1/1	0.69	0.51	65,65,65,65	0
84	MG	5	3426	1/1	0.69	0.30	36,36,36,36	0
84	MG	5	3715	1/1	0.69	0.29	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	5	3458	1/1	0.70	0.27	107,107,107,107	0
86	ZN	e1	501	1/1	0.70	0.07	160,160,160,160	0
84	MG	1	3667	1/1	0.70	0.66	62,62,62,62	0
84	MG	6	1969	1/1	0.71	0.48	65,65,65,65	0
84	MG	4	202	1/1	0.71	0.54	57,57,57,57	0
84	MG	5	3709	1/1	0.71	0.41	61,61,61,61	0
84	MG	1	3663	1/1	0.71	0.30	36,36,36,36	0
84	MG	2	1909	1/1	0.71	0.58	81,81,81,81	0
84	MG	5	3409	1/1	0.71	0.26	58,58,58,58	0
84	MG	1	3414	1/1	0.71	0.45	63,63,63,63	0
84	MG	2	1972	1/1	0.71	0.50	71,71,71,71	0
84	MG	2	1948	1/1	0.72	0.38	94,94,94,94	0
84	MG	5	3641	1/1	0.72	0.72	79,79,79,79	0
84	MG	3	201	1/1	0.72	0.24	71,71,71,71	0
84	MG	1	3487	1/1	0.72	0.62	49,49,49,49	0
84	MG	5	3693	1/1	0.72	0.40	80,80,80,80	0
84	MG	m7	201	1/1	0.73	0.31	37,37,37,37	0
84	MG	l3	402	1/1	0.73	0.24	32,32,32,32	0
84	MG	5	3404	1/1	0.73	0.24	33,33,33,33	0
84	MG	1	3715	1/1	0.73	0.78	48,48,48,48	0
84	MG	6	1998	1/1	0.73	0.23	58,58,58,58	0
84	MG	4	213	1/1	0.73	0.38	41,41,41,41	0
84	MG	1	3668	1/1	0.73	0.18	66,66,66,66	0
84	MG	6	1993	1/1	0.73	0.36	95,95,95,95	0
84	MG	6	2002	1/1	0.74	0.65	99,99,99,99	0
84	MG	2	1938	1/1	0.74	0.36	75,75,75,75	0
84	MG	5	3655	1/1	0.74	0.60	64,64,64,64	0
84	MG	1	3712	1/1	0.74	0.28	41,41,41,41	0
84	MG	2	1956	1/1	0.74	0.45	64,64,64,64	0
84	MG	6	1965	1/1	0.74	0.47	56,56,56,56	0
84	MG	1	3630	1/1	0.74	0.57	56,56,56,56	0
84	MG	1	3655	1/1	0.75	0.29	41,41,41,41	0
84	MG	1	3435	1/1	0.75	0.46	41,41,41,41	0
84	MG	1	3709	1/1	0.75	0.83	59,59,59,59	0
84	MG	5	3476	1/1	0.75	0.58	51,51,51,51	0
84	MG	2	1978	1/1	0.75	0.74	104,104,104,104	0
84	MG	6	2008	1/1	0.75	0.44	47,47,47,47	0
84	MG	8	207	1/1	0.76	0.45	51,51,51,51	0
84	MG	2	1979	1/1	0.76	0.40	72,72,72,72	0
84	MG	5	3697	1/1	0.76	0.29	50,50,50,50	0
84	MG	1	3508	1/1	0.76	0.39	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3639	1/1	0.76	0.43	59,59,59,59	0
84	MG	2	1915	1/1	0.77	0.59	76,76,76,76	0
84	MG	5	3438	1/1	0.77	0.36	45,45,45,45	0
84	MG	5	3738	1/1	0.77	0.38	45,45,45,45	0
84	MG	5	3731	1/1	0.77	0.57	37,37,37,37	0
84	MG	5	3614	1/1	0.77	0.25	55,55,55,55	0
84	MG	1	3408	1/1	0.77	0.33	50,50,50,50	0
84	MG	2	1923	1/1	0.77	0.51	56,56,56,56	0
84	MG	6	1938	1/1	0.77	0.50	99,99,99,99	0
84	MG	6	1917	1/1	0.77	1.38	75,75,75,75	0
84	MG	1	3701	1/1	0.78	0.27	40,40,40,40	0
84	MG	5	3645	1/1	0.78	0.31	33,33,33,33	0
84	MG	5	3732	1/1	0.78	0.30	52,52,52,52	0
84	MG	2	1949	1/1	0.78	0.40	96,96,96,96	0
84	MG	2	1913	1/1	0.78	0.32	63,63,63,63	0
84	MG	5	3635	1/1	0.78	0.18	66,66,66,66	0
84	MG	5	3463	1/1	0.78	0.37	41,41,41,41	0
84	MG	6	1908	1/1	0.78	0.20	51,51,51,51	0
84	MG	5	3722	1/1	0.78	0.31	55,55,55,55	0
84	MG	5	3678	1/1	0.78	0.31	58,58,58,58	0
84	MG	5	3688	1/1	0.78	0.40	33,33,33,33	0
84	MG	1	3707	1/1	0.78	0.35	53,53,53,53	0
84	MG	1	3666	1/1	0.79	0.24	45,45,45,45	0
84	MG	1	3568	1/1	0.79	0.52	40,40,40,40	0
84	MG	2	1946	1/1	0.79	0.63	93,93,93,93	0
84	MG	4	208	1/1	0.79	0.27	54,54,54,54	0
84	MG	1	3638	1/1	0.79	0.19	46,46,46,46	0
84	MG	2	1975	1/1	0.79	0.35	76,76,76,76	0
84	MG	5	3450	1/1	0.79	0.25	58,58,58,58	0
84	MG	2	1911	1/1	0.79	0.82	69,69,69,69	0
84	MG	5	3453	1/1	0.79	0.23	42,42,42,42	0
84	MG	6	1911	1/1	0.79	0.30	52,52,52,52	0
84	MG	O4	202	1/1	0.79	0.37	67,67,67,67	0
84	MG	5	3667	1/1	0.79	0.30	38,38,38,38	0
84	MG	6	2001	1/1	0.79	0.42	73,73,73,73	0
84	MG	5	3632	1/1	0.79	0.43	42,42,42,42	0
84	MG	6	1930	1/1	0.79	0.56	59,59,59,59	0
84	MG	1	3430	1/1	0.79	0.30	36,36,36,36	0
84	MG	1	3694	1/1	0.79	0.47	41,41,41,41	0
84	MG	5	3685	1/1	0.80	0.28	36,36,36,36	0
84	MG	5	3407	1/1	0.80	0.25	33,33,33,33	0
84	MG	1	3437	1/1	0.80	0.20	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	5	3598	1/1	0.80	0.17	42,42,42,42	0
84	MG	5	3467	1/1	0.80	0.62	65,65,65,65	0
84	MG	6	1903	1/1	0.80	0.50	45,45,45,45	0
84	MG	6	1946	1/1	0.80	0.56	49,49,49,49	0
84	MG	5	3585	1/1	0.80	0.30	39,39,39,39	0
84	MG	l9	201	1/1	0.80	0.22	45,45,45,45	0
84	MG	1	3685	1/1	0.80	0.29	39,39,39,39	0
84	MG	6	1994	1/1	0.80	0.25	49,49,49,49	0
84	MG	1	3442	1/1	0.80	0.15	41,41,41,41	0
84	MG	5	3636	1/1	0.80	0.45	44,44,44,44	0
84	MG	4	210	1/1	0.80	0.38	58,58,58,58	0
84	MG	5	3542	1/1	0.80	0.53	36,36,36,36	0
84	MG	Q2	502	1/1	0.81	0.14	55,55,55,55	0
84	MG	l2	302	1/1	0.81	0.37	42,42,42,42	0
84	MG	1	4039	1/1	0.81	0.42	46,46,46,46	0
84	MG	7	202	1/1	0.81	0.30	32,32,32,32	0
84	MG	5	3600	1/1	0.81	0.28	34,34,34,34	0
84	MG	1	3417	1/1	0.81	0.47	58,58,58,58	0
84	MG	n6	201	1/1	0.81	0.39	65,65,65,65	0
84	MG	1	3456	1/1	0.81	0.18	32,32,32,32	0
84	MG	5	3723	1/1	0.81	0.42	38,38,38,38	0
84	MG	2	1947	1/1	0.81	1.03	93,93,93,93	0
84	MG	6	1928	1/1	0.81	0.51	51,51,51,51	0
84	MG	5	3574	1/1	0.81	0.42	53,53,53,53	0
84	MG	1	3406	1/1	0.81	0.73	130,130,130,130	0
84	MG	2	1981	1/1	0.81	0.42	76,76,76,76	0
84	MG	1	3688	1/1	0.81	0.22	47,47,47,47	0
84	MG	6	1995	1/1	0.81	0.71	52,52,52,52	0
84	MG	2	1971	1/1	0.82	0.33	77,77,77,77	0
84	MG	6	1926	1/1	0.82	0.56	46,46,46,46	0
84	MG	5	3608	1/1	0.82	0.41	89,89,89,89	0
84	MG	1	3690	1/1	0.82	0.31	48,48,48,48	0
84	MG	1	3536	1/1	0.82	0.42	56,56,56,56	0
84	MG	5	3456	1/1	0.82	0.40	54,54,54,54	0
84	MG	1	3697	1/1	0.82	0.51	41,41,41,41	0
84	MG	5	3701	1/1	0.82	0.45	47,47,47,47	0
84	MG	5	3664	1/1	0.82	0.19	53,53,53,53	0
84	MG	5	3704	1/1	0.82	0.44	54,54,54,54	0
84	MG	5	3728	1/1	0.82	0.32	50,50,50,50	0
84	MG	1	3657	1/1	0.82	0.33	50,50,50,50	0
84	MG	2	1961	1/1	0.82	0.22	75,75,75,75	0
84	MG	5	3595	1/1	0.82	0.13	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	5	3461	1/1	0.82	0.19	40,40,40,40	0
84	MG	l8	301	1/1	0.83	0.65	83,83,83,83	0
84	MG	l3	405	1/1	0.83	0.69	34,34,34,34	0
84	MG	1	3457	1/1	0.83	0.46	42,42,42,42	0
84	MG	5	3604	1/1	0.83	0.42	36,36,36,36	0
84	MG	5	3470	1/1	0.83	0.37	32,32,32,32	0
84	MG	6	1956	1/1	0.83	0.64	60,60,60,60	0
84	MG	1	3720	1/1	0.83	0.18	56,56,56,56	0
84	MG	1	3692	1/1	0.83	0.35	45,45,45,45	0
84	MG	5	3471	1/1	0.83	0.34	68,68,68,68	0
84	MG	5	3640	1/1	0.83	0.27	51,51,51,51	0
84	MG	1	3611	1/1	0.83	0.26	39,39,39,39	0
84	MG	6	2006	1/1	0.83	0.56	61,61,61,61	0
84	MG	1	3424	1/1	0.83	0.45	45,45,45,45	0
84	MG	5	3485	1/1	0.83	0.34	37,37,37,37	0
84	MG	1	3710	1/1	0.83	0.32	40,40,40,40	0
84	MG	1	3637	1/1	0.83	0.42	42,42,42,42	0
84	MG	1	3629	1/1	0.83	0.46	74,74,74,74	0
84	MG	5	3727	1/1	0.83	0.23	62,62,62,62	0
84	MG	5	3674	1/1	0.83	0.30	49,49,49,49	0
84	MG	5	3605	1/1	0.83	0.21	37,37,37,37	0
84	MG	2	1937	1/1	0.84	0.39	79,79,79,79	0
84	MG	l7	301	1/1	0.84	0.18	37,37,37,37	0
84	MG	5	3532	1/1	0.84	0.68	50,50,50,50	0
84	MG	5	3651	1/1	0.84	0.37	46,46,46,46	0
84	MG	5	3541	1/1	0.84	0.39	50,50,50,50	0
84	MG	D9	102	1/1	0.84	0.45	86,86,86,86	0
84	MG	1	3479	1/1	0.84	0.61	64,64,64,64	0
84	MG	5	3642	1/1	0.84	0.32	37,37,37,37	0
84	MG	5	3675	1/1	0.84	0.18	59,59,59,59	0
84	MG	2	1921	1/1	0.84	0.69	81,81,81,81	0
84	MG	6	1970	1/1	0.84	0.47	98,98,98,98	0
84	MG	5	3644	1/1	0.84	0.32	72,72,72,72	0
84	MG	5	3624	1/1	0.84	0.21	41,41,41,41	0
84	MG	5	3681	1/1	0.84	0.49	40,40,40,40	0
84	MG	n6	202	1/1	0.84	0.39	52,52,52,52	0
84	MG	m5	303	1/1	0.84	0.51	46,46,46,46	0
84	MG	1	3560	1/1	0.84	0.34	40,40,40,40	0
84	MG	1	3618	1/1	0.84	0.29	62,62,62,62	0
84	MG	6	1922	1/1	0.84	0.54	48,48,48,48	0
84	MG	5	3413	1/1	0.84	0.33	41,41,41,41	0
84	MG	1	3696	1/1	0.84	0.32	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3527	1/1	0.84	0.23	64,64,64,64	0
84	MG	1	3516	1/1	0.84	0.65	40,40,40,40	0
84	MG	6	1990	1/1	0.84	0.18	61,61,61,61	0
84	MG	1	3411	1/1	0.85	0.44	51,51,51,51	0
84	MG	6	1916	1/1	0.85	0.46	46,46,46,46	0
84	MG	8	206	1/1	0.85	0.58	52,52,52,52	0
84	MG	1	3472	1/1	0.85	0.36	52,52,52,52	0
84	MG	5	3588	1/1	0.85	0.33	57,57,57,57	0
86	ZN	D7	101	1/1	0.85	0.35	115,115,115,115	0
84	MG	1	3439	1/1	0.85	0.26	60,60,60,60	0
84	MG	4	204	1/1	0.85	0.57	51,51,51,51	0
84	MG	d6	102	1/1	0.85	0.49	56,56,56,56	0
84	MG	1	3405	1/1	0.85	0.71	63,63,63,63	0
84	MG	5	3421	1/1	0.85	0.34	50,50,50,50	0
84	MG	5	3403	1/1	0.85	0.16	45,45,45,45	0
84	MG	1	3569	1/1	0.85	0.46	53,53,53,53	0
84	MG	6	1942	1/1	0.85	0.98	79,79,79,79	0
84	MG	1	3693	1/1	0.85	0.27	58,58,58,58	0
84	MG	5	3555	1/1	0.85	0.33	44,44,44,44	0
84	MG	1	3477	1/1	0.85	0.27	54,54,54,54	0
84	MG	5	3710	1/1	0.85	0.21	44,44,44,44	0
84	MG	5	3411	1/1	0.85	0.34	34,34,34,34	0
84	MG	M7	201	1/1	0.85	0.48	60,60,60,60	0
84	MG	2	1924	1/1	0.85	0.85	86,86,86,86	0
84	MG	1	3468	1/1	0.85	0.14	59,59,59,59	0
84	MG	5	3444	1/1	0.85	0.22	32,32,32,32	0
84	MG	1	3421	1/1	0.85	0.35	41,41,41,41	0
84	MG	5	3687	1/1	0.85	0.46	31,31,31,31	0
84	MG	6	1959	1/1	0.85	0.66	86,86,86,86	0
84	MG	5	3619	1/1	0.86	0.19	37,37,37,37	0
84	MG	2	1976	1/1	0.86	0.72	68,68,68,68	0
84	MG	4	214	1/1	0.86	0.41	53,53,53,53	0
84	MG	5	3540	1/1	0.86	0.54	28,28,28,28	0
84	MG	5	3616	1/1	0.86	0.37	40,40,40,40	0
84	MG	5	3406	1/1	0.86	0.13	47,47,47,47	0
84	MG	1	3684	1/1	0.86	0.82	51,51,51,51	0
84	MG	5	3621	1/1	0.86	0.34	40,40,40,40	0
84	MG	5	3666	1/1	0.86	0.21	37,37,37,37	0
84	MG	1	3598	1/1	0.86	0.29	39,39,39,39	0
84	MG	6	1982	1/1	0.86	0.22	46,46,46,46	0
84	MG	1	3610	1/1	0.86	0.61	42,42,42,42	0
84	MG	5	3544	1/1	0.86	0.46	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	5	3684	1/1	0.86	0.19	77,77,77,77	0
84	MG	6	2003	1/1	0.86	1.02	63,63,63,63	0
84	MG	5	3559	1/1	0.86	0.35	40,40,40,40	0
84	MG	5	3680	1/1	0.86	0.22	53,53,53,53	0
84	MG	5	3516	1/1	0.86	0.40	31,31,31,31	0
84	MG	5	3625	1/1	0.86	0.15	44,44,44,44	0
84	MG	5	3676	1/1	0.86	0.17	63,63,63,63	0
84	MG	5	3531	1/1	0.86	0.46	56,56,56,56	0
84	MG	2	1940	1/1	0.86	0.71	72,72,72,72	0
84	MG	5	3657	1/1	0.86	0.21	57,57,57,57	0
84	MG	1	3640	1/1	0.86	0.35	74,74,74,74	0
84	MG	2	1974	1/1	0.86	0.22	93,93,93,93	0
84	MG	2	1933	1/1	0.86	0.48	74,74,74,74	0
84	MG	L3	401	1/1	0.86	0.86	53,53,53,53	0
84	MG	6	1962	1/1	0.86	0.17	84,84,84,84	0
84	MG	1	3619	1/1	0.86	0.29	35,35,35,35	0
84	MG	5	4078	1/1	0.86	0.57	40,40,40,40	0
84	MG	1	3517	1/1	0.86	0.45	51,51,51,51	0
84	MG	1	3458	1/1	0.86	0.32	59,59,59,59	0
84	MG	7	206	1/1	0.87	0.45	42,42,42,42	0
84	MG	1	3471	1/1	0.87	0.24	58,58,58,58	0
84	MG	2	1932	1/1	0.87	0.58	68,68,68,68	0
84	MG	5	3638	1/1	0.87	0.24	37,37,37,37	0
84	MG	6	1919	1/1	0.87	0.66	67,67,67,67	0
84	MG	5	3686	1/1	0.87	0.25	44,44,44,44	0
84	MG	1	3649	1/1	0.87	0.26	43,43,43,43	0
84	MG	6	1947	1/1	0.87	0.53	53,53,53,53	0
84	MG	6	1924	1/1	0.87	0.70	56,56,56,56	0
84	MG	1	3552	1/1	0.87	0.67	44,44,44,44	0
84	MG	1	3626	1/1	0.87	0.27	44,44,44,44	0
84	MG	1	3589	1/1	0.87	0.14	64,64,64,64	0
84	MG	5	3408	1/1	0.87	0.39	42,42,42,42	0
84	MG	4	212	1/1	0.87	0.20	54,54,54,54	0
84	MG	1	3449	1/1	0.87	0.99	64,64,64,64	0
84	MG	1	3681	1/1	0.87	0.16	45,45,45,45	0
84	MG	6	1951	1/1	0.87	0.49	77,77,77,77	0
84	MG	1	3616	1/1	0.87	0.47	81,81,81,81	0
84	MG	6	1902	1/1	0.87	0.38	57,57,57,57	0
84	MG	O7	102	1/1	0.87	0.47	51,51,51,51	0
84	MG	1	3608	1/1	0.87	0.48	87,87,87,87	0
84	MG	5	3503	1/1	0.87	0.28	40,40,40,40	0
84	MG	6	1955	1/1	0.87	1.13	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3448	1/1	0.87	0.40	64,64,64,64	0
84	MG	5	3736	1/1	0.87	0.31	48,48,48,48	0
84	MG	1	3590	1/1	0.87	0.40	60,60,60,60	0
84	MG	1	3631	1/1	0.87	0.56	49,49,49,49	0
84	MG	2	1964	1/1	0.87	0.33	83,83,83,83	0
84	MG	1	3548	1/1	0.87	0.27	31,31,31,31	0
84	MG	5	3419	1/1	0.87	0.14	41,41,41,41	0
84	MG	5	3711	1/1	0.87	0.10	32,32,32,32	0
85	OHX	1	4012	7/7	0.87	0.38	116,116,116,116	0
84	MG	5	3526	1/1	0.87	0.37	38,38,38,38	0
84	MG	2	1936	1/1	0.87	0.67	73,73,73,73	0
84	MG	2	1965	1/1	0.88	0.72	60,60,60,60	0
84	MG	S4	301	1/1	0.88	0.32	79,79,79,79	0
84	MG	n9	101	1/1	0.88	0.38	33,33,33,33	0
84	MG	1	3431	1/1	0.88	0.17	51,51,51,51	0
84	MG	1	3650	1/1	0.88	0.56	81,81,81,81	0
84	MG	1	3708	1/1	0.88	0.28	60,60,60,60	0
84	MG	1	3679	1/1	0.88	0.24	34,34,34,34	0
84	MG	5	3402	1/1	0.88	0.66	61,61,61,61	0
84	MG	6	1932	1/1	0.88	0.76	62,62,62,62	0
84	MG	1	3429	1/1	0.88	0.53	51,51,51,51	0
84	MG	m5	301	1/1	0.88	0.26	48,48,48,48	0
84	MG	5	3482	1/1	0.88	0.12	33,33,33,33	0
84	MG	1	3689	1/1	0.88	0.32	57,57,57,57	0
84	MG	3	203	1/1	0.88	0.29	44,44,44,44	0
84	MG	n0	202	1/1	0.88	0.16	40,40,40,40	0
84	MG	6	1976	1/1	0.88	0.19	91,91,91,91	0
84	MG	5	3501	1/1	0.88	0.53	27,27,27,27	0
84	MG	1	3582	1/1	0.88	0.28	45,45,45,45	0
84	MG	6	1937	1/1	0.88	0.78	72,72,72,72	0
84	MG	3	202	1/1	0.88	0.68	67,67,67,67	0
84	MG	1	3601	1/1	0.88	0.32	65,65,65,65	0
84	MG	M7	204	1/1	0.88	0.23	40,40,40,40	0
84	MG	1	3652	1/1	0.88	0.25	57,57,57,57	0
84	MG	1	3510	1/1	0.88	0.36	31,31,31,31	0
84	MG	1	3615	1/1	0.88	0.33	31,31,31,31	0
84	MG	1	3656	1/1	0.88	0.44	46,46,46,46	0
84	MG	5	3610	1/1	0.88	0.29	37,37,37,37	0
84	MG	2	1954	1/1	0.88	0.49	90,90,90,90	0
84	MG	6	1927	1/1	0.88	0.40	50,50,50,50	0
84	MG	1	3620	1/1	0.88	0.42	54,54,54,54	0
84	MG	1	3724	1/1	0.88	0.46	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	5	3601	1/1	0.88	0.42	38,38,38,38	0
84	MG	1	3526	1/1	0.88	0.21	52,52,52,52	0
84	MG	c1	201	1/1	0.88	0.44	53,53,53,53	0
84	MG	1	3600	1/1	0.89	0.34	52,52,52,52	0
84	MG	5	3442	1/1	0.89	0.32	36,36,36,36	0
84	MG	1	3634	1/1	0.89	0.38	39,39,39,39	0
84	MG	5	3622	1/1	0.89	0.17	55,55,55,55	0
84	MG	2	1905	1/1	0.89	0.77	63,63,63,63	0
84	MG	1	3538	1/1	0.89	0.42	42,42,42,42	0
84	MG	1	3704	1/1	0.89	0.36	34,34,34,34	0
84	MG	2	1902	1/1	0.89	0.41	55,55,55,55	0
84	MG	l2	301	1/1	0.89	0.60	48,48,48,48	0
84	MG	1	3461	1/1	0.89	0.35	36,36,36,36	0
85	OHX	5	4068	7/7	0.89	0.27	96,96,96,96	0
84	MG	5	3428	1/1	0.89	0.52	39,39,39,39	0
84	MG	6	1966	1/1	0.89	0.40	53,53,53,53	0
84	MG	2	1919	1/1	0.89	0.70	73,73,73,73	0
84	MG	2	1943	1/1	0.89	0.75	71,71,71,71	0
84	MG	6	1910	1/1	0.89	0.40	74,74,74,74	0
84	MG	1	3700	1/1	0.89	0.46	36,36,36,36	0
84	MG	s8	301	1/1	0.89	0.32	47,47,47,47	0
84	MG	5	3581	1/1	0.89	0.57	35,35,35,35	0
84	MG	1	3721	1/1	0.89	0.56	42,42,42,42	0
84	MG	5	3587	1/1	0.89	0.32	39,39,39,39	0
84	MG	5	3445	1/1	0.89	0.60	49,49,49,49	0
84	MG	1	3416	1/1	0.89	0.41	48,48,48,48	0
84	MG	6	1963	1/1	0.89	0.32	76,76,76,76	0
84	MG	5	3662	1/1	0.89	0.26	34,34,34,34	0
84	MG	1	3466	1/1	0.89	0.74	57,57,57,57	0
85	OHX	2	2115	7/7	0.89	0.41	115,115,115,115	0
84	MG	5	3566	1/1	0.89	0.56	46,46,46,46	0
84	MG	6	2005	1/1	0.89	0.51	61,61,61,61	0
84	MG	2	1939	1/1	0.89	0.43	74,74,74,74	0
84	MG	1	3528	1/1	0.89	0.36	34,34,34,34	0
84	MG	5	3659	1/1	0.89	0.29	41,41,41,41	0
84	MG	5	3487	1/1	0.89	0.42	32,32,32,32	0
84	MG	5	3583	1/1	0.89	0.12	42,42,42,42	0
84	MG	5	3571	1/1	0.89	0.78	53,53,53,53	0
84	MG	N3	201	1/1	0.89	0.35	40,40,40,40	0
84	MG	5	3712	1/1	0.89	0.24	44,44,44,44	0
84	MG	1	3438	1/1	0.89	0.32	32,32,32,32	0
84	MG	1	3664	1/1	0.89	0.33	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3643	1/1	0.89	0.52	63,63,63,63	0
85	OHX	5	4043	7/7	0.89	0.43	96,96,96,96	0
84	MG	1	3723	1/1	0.89	0.30	37,37,37,37	0
84	MG	5	3615	1/1	0.89	0.56	56,56,56,56	0
84	MG	6	2007	1/1	0.89	0.29	61,61,61,61	0
84	MG	5	3507	1/1	0.89	0.43	44,44,44,44	0
84	MG	sM	201	1/1	0.89	0.32	44,44,44,44	0
84	MG	1	3441	1/1	0.89	0.32	31,31,31,31	0
84	MG	2	1955	1/1	0.89	0.33	68,68,68,68	0
84	MG	1	3587	1/1	0.89	0.20	42,42,42,42	0
84	MG	5	3671	1/1	0.89	0.28	35,35,35,35	0
84	MG	4	211	1/1	0.89	0.23	42,42,42,42	0
84	MG	1	3450	1/1	0.89	0.37	33,33,33,33	0
84	MG	5	3646	1/1	0.89	0.18	35,35,35,35	0
85	OHX	5	3938	7/7	0.89	0.22	115,115,115,115	0
84	MG	5	3705	1/1	0.89	0.14	36,36,36,36	0
84	MG	2	1982	1/1	0.89	0.27	65,65,65,65	0
84	MG	6	1975	1/1	0.89	0.32	79,79,79,79	0
84	MG	5	3478	1/1	0.89	0.21	45,45,45,45	0
84	MG	1	3462	1/1	0.89	0.31	38,38,38,38	0
84	MG	5	3707	1/1	0.89	0.16	43,43,43,43	0
84	MG	5	3477	1/1	0.90	0.21	42,42,42,42	0
84	MG	1	3452	1/1	0.90	0.43	38,38,38,38	0
84	MG	2	1901	1/1	0.90	1.24	85,85,85,85	0
84	MG	6	1915	1/1	0.90	0.27	72,72,72,72	0
84	MG	5	3480	1/1	0.90	0.21	36,36,36,36	0
84	MG	5	3698	1/1	0.90	0.35	73,73,73,73	0
84	MG	6	1988	1/1	0.90	0.27	73,73,73,73	0
84	MG	5	3737	1/1	0.90	0.08	52,52,52,52	0
84	MG	2	1910	1/1	0.90	0.43	64,64,64,64	0
84	MG	1	3484	1/1	0.90	0.40	52,52,52,52	0
84	MG	5	3696	1/1	0.90	0.21	31,31,31,31	0
84	MG	5	3650	1/1	0.90	0.11	46,46,46,46	0
84	MG	4	203	1/1	0.90	0.48	68,68,68,68	0
84	MG	5	3550	1/1	0.90	0.55	31,31,31,31	0
84	MG	5	3652	1/1	0.90	0.17	44,44,44,44	0
84	MG	5	3538	1/1	0.90	0.52	41,41,41,41	0
84	MG	5	3660	1/1	0.90	0.34	41,41,41,41	0
84	MG	5	3511	1/1	0.90	0.34	62,62,62,62	0
84	MG	1	3404	1/1	0.90	0.23	42,42,42,42	0
84	MG	5	4076	1/1	0.90	0.50	52,52,52,52	0
84	MG	5	3498	1/1	0.90	0.55	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	o3	201	1/1	0.90	0.29	49,49,49,49	0
84	MG	4	207	1/1	0.90	0.25	49,49,49,49	0
84	MG	1	3605	1/1	0.90	0.19	46,46,46,46	0
84	MG	5	3578	1/1	0.90	0.82	40,40,40,40	0
84	MG	5	3668	1/1	0.90	0.46	71,71,71,71	0
84	MG	1	4040	1/1	0.90	0.35	39,39,39,39	0
84	MG	5	3739	1/1	0.90	0.30	88,88,88,88	0
84	MG	q1	101	1/1	0.90	0.57	47,47,47,47	0
84	MG	1	3539	1/1	0.90	0.52	44,44,44,44	0
84	MG	6	1987	1/1	0.90	0.14	55,55,55,55	0
84	MG	1	3641	1/1	0.90	0.29	51,51,51,51	0
84	MG	6	1979	1/1	0.90	0.30	52,52,52,52	0
84	MG	2	1963	1/1	0.90	0.58	78,78,78,78	0
84	MG	1	3460	1/1	0.90	0.28	52,52,52,52	0
84	MG	1	3658	1/1	0.90	0.33	52,52,52,52	0
84	MG	5	3447	1/1	0.90	0.57	34,34,34,34	0
84	MG	8	205	1/1	0.90	0.25	48,48,48,48	0
84	MG	1	3561	1/1	0.90	0.43	43,43,43,43	0
84	MG	5	3597	1/1	0.90	0.27	29,29,29,29	0
84	MG	5	3515	1/1	0.90	0.45	52,52,52,52	0
84	MG	1	3549	1/1	0.90	0.38	53,53,53,53	0
85	OHX	1	3931	7/7	0.90	0.27	111,111,111,111	0
84	MG	5	3637	1/1	0.90	0.32	49,49,49,49	0
84	MG	1	3642	1/1	0.90	0.23	48,48,48,48	0
84	MG	5	3448	1/1	0.90	0.32	28,28,28,28	0
84	MG	1	3554	1/1	0.90	0.39	32,32,32,32	0
84	MG	1	3713	1/1	0.90	0.19	45,45,45,45	0
85	OHX	6	2158	7/7	0.90	0.35	140,140,140,140	0
84	MG	5	3509	1/1	0.90	0.36	47,47,47,47	0
84	MG	6	1934	1/1	0.90	0.29	67,67,67,67	0
84	MG	5	3446	1/1	0.90	0.33	45,45,45,45	0
84	MG	5	3631	1/1	0.90	0.24	41,41,41,41	0
84	MG	6	1981	1/1	0.90	0.38	57,57,57,57	0
84	MG	8	204	1/1	0.90	0.21	56,56,56,56	0
84	MG	1	3659	1/1	0.90	0.45	47,47,47,47	0
84	MG	1	3420	1/1	0.90	0.10	38,38,38,38	0
84	MG	5	3499	1/1	0.90	0.31	36,36,36,36	0
84	MG	m7	203	1/1	0.90	0.41	40,40,40,40	0
84	MG	1	3467	1/1	0.90	0.23	47,47,47,47	0
84	MG	6	1945	1/1	0.90	0.41	66,66,66,66	0
84	MG	2	1957	1/1	0.91	0.57	76,76,76,76	0
84	MG	1	3512	1/1	0.91	0.35	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	6	1929	1/1	0.91	0.30	67,67,67,67	0
84	MG	5	3529	1/1	0.91	0.67	58,58,58,58	0
84	MG	5	3425	1/1	0.91	0.19	31,31,31,31	0
84	MG	5	3500	1/1	0.91	0.38	47,47,47,47	0
84	MG	1	3531	1/1	0.91	0.72	45,45,45,45	0
84	MG	2	1918	1/1	0.91	0.77	64,64,64,64	0
84	MG	1	3623	1/1	0.91	0.19	51,51,51,51	0
84	MG	2	1952	1/1	0.91	0.98	77,77,77,77	0
85	OHX	5	4050	7/7	0.91	0.25	158,158,158,158	0
84	MG	5	4073	1/1	0.91	0.78	31,31,31,31	0
85	OHX	6	2131	7/7	0.91	0.34	121,121,121,121	0
84	MG	1	3427	1/1	0.91	0.41	48,48,48,48	0
84	MG	5	3741	1/1	0.91	0.31	54,54,54,54	0
84	MG	5	3418	1/1	0.91	0.31	41,41,41,41	0
84	MG	6	1913	1/1	0.91	0.53	51,51,51,51	0
84	MG	6	1980	1/1	0.91	0.28	68,68,68,68	0
84	MG	1	3407	1/1	0.91	0.45	45,45,45,45	0
84	MG	6	1957	1/1	0.91	0.46	63,63,63,63	0
84	MG	1	3585	1/1	0.91	0.70	59,59,59,59	0
84	MG	2	1935	1/1	0.91	0.35	68,68,68,68	0
84	MG	1	3584	1/1	0.91	0.88	54,54,54,54	0
84	MG	6	1901	1/1	0.91	0.37	50,50,50,50	0
84	MG	5	3690	1/1	0.91	0.43	30,30,30,30	0
84	MG	6	1985	1/1	0.91	0.29	65,65,65,65	0
84	MG	5	3653	1/1	0.91	0.17	67,67,67,67	0
84	MG	5	3672	1/1	0.91	0.34	40,40,40,40	0
84	MG	1	3506	1/1	0.91	0.53	42,42,42,42	0
84	MG	2	1953	1/1	0.91	0.94	84,84,84,84	0
84	MG	1	3595	1/1	0.91	0.28	50,50,50,50	0
84	MG	5	3593	1/1	0.91	0.36	54,54,54,54	0
86	ZN	d6	101	1/1	0.91	0.09	60,60,60,60	0
84	MG	1	3491	1/1	0.91	0.55	41,41,41,41	0
84	MG	1	3597	1/1	0.91	0.28	46,46,46,46	0
84	MG	5	3677	1/1	0.91	0.39	41,41,41,41	0
84	MG	2	1942	1/1	0.91	0.20	69,69,69,69	0
84	MG	5	3536	1/1	0.91	0.58	46,46,46,46	0
84	MG	6	2000	1/1	0.91	0.28	86,86,86,86	0
84	MG	5	3669	1/1	0.91	0.39	39,39,39,39	0
84	MG	1	3543	1/1	0.91	0.36	34,34,34,34	0
84	MG	6	2160	1/1	0.91	0.31	84,84,84,84	0
84	MG	1	3503	1/1	0.91	0.57	33,33,33,33	0
84	MG	2	1960	1/1	0.91	1.10	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3514	1/1	0.91	0.36	33,33,33,33	0
84	MG	5	3639	1/1	0.91	0.17	40,40,40,40	0
84	MG	l3	403	1/1	0.91	0.38	38,38,38,38	0
84	MG	q0	202	1/1	0.91	0.28	44,44,44,44	0
84	MG	1	3651	1/1	0.91	0.20	36,36,36,36	0
85	OHX	1	3921	7/7	0.91	0.32	110,110,110,110	0
84	MG	1	3645	1/1	0.91	0.21	69,69,69,69	0
84	MG	6	1912	1/1	0.91	0.32	79,79,79,79	0
84	MG	5	3594	1/1	0.91	0.25	40,40,40,40	0
84	MG	L6	201	1/1	0.91	0.14	48,48,48,48	0
84	MG	1	3542	1/1	0.91	0.33	46,46,46,46	0
84	MG	5	3520	1/1	0.91	0.44	40,40,40,40	0
85	OHX	2	2108	7/7	0.91	0.25	145,145,145,145	0
84	MG	7	204	1/1	0.91	0.49	40,40,40,40	0
84	MG	1	3556	1/1	0.91	0.52	30,30,30,30	0
84	MG	5	3729	1/1	0.91	0.22	52,52,52,52	0
84	MG	5	3714	1/1	0.91	0.24	34,34,34,34	0
85	OHX	2	2118	7/7	0.91	0.30	132,132,132,132	0
84	MG	5	3437	1/1	0.92	0.20	35,35,35,35	0
84	MG	5	4072	1/1	0.92	0.29	33,33,33,33	0
84	MG	5	3551	1/1	0.92	0.34	35,35,35,35	0
84	MG	5	3721	1/1	0.92	0.58	35,35,35,35	0
84	MG	n8	201	1/1	0.92	0.34	50,50,50,50	0
85	OHX	5	3860	7/7	0.92	0.16	122,122,122,122	0
84	MG	5	3423	1/1	0.92	0.56	45,45,45,45	0
84	MG	1	3447	1/1	0.92	0.48	37,37,37,37	0
84	MG	5	3716	1/1	0.92	0.40	29,29,29,29	0
84	MG	5	3633	1/1	0.92	0.86	36,36,36,36	0
84	MG	M6	201	1/1	0.92	0.16	45,45,45,45	0
84	MG	5	3730	1/1	0.92	0.37	43,43,43,43	0
84	MG	6	1999	1/1	0.92	0.28	49,49,49,49	0
84	MG	6	1958	1/1	0.92	0.68	47,47,47,47	0
84	MG	5	3429	1/1	0.92	0.15	78,78,78,78	0
84	MG	5	3553	1/1	0.92	0.42	38,38,38,38	0
84	MG	1	3497	1/1	0.92	0.56	33,33,33,33	0
84	MG	5	4071	1/1	0.92	0.23	43,43,43,43	0
85	OHX	6	2157	7/7	0.92	0.47	115,115,115,115	0
86	ZN	d7	101	1/1	0.92	0.17	106,106,106,106	0
86	ZN	q2	501	1/1	0.92	0.21	64,64,64,64	0
84	MG	5	3689	1/1	0.92	0.23	30,30,30,30	0
84	MG	5	3440	1/1	0.92	0.15	40,40,40,40	0
84	MG	5	3634	1/1	0.92	0.16	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	6	1964	1/1	0.92	0.33	73,73,73,73	0
84	MG	5	3451	1/1	0.92	0.35	33,33,33,33	0
84	MG	1	4044	1/1	0.92	0.30	51,51,51,51	0
84	MG	8	209	1/1	0.92	0.45	68,68,68,68	0
84	MG	2	1951	1/1	0.92	0.47	58,58,58,58	0
85	OHX	5	3969	7/7	0.92	0.25	138,138,138,138	0
85	OHX	2	2114	7/7	0.92	0.20	170,170,170,170	0
84	MG	6	1954	1/1	0.92	0.67	51,51,51,51	0
84	MG	1	3443	1/1	0.92	0.45	43,43,43,43	0
84	MG	1	3489	1/1	0.92	0.52	49,49,49,49	0
84	MG	1	3617	1/1	0.92	0.48	43,43,43,43	0
84	MG	5	4077	1/1	0.92	0.87	38,38,38,38	0
84	MG	1	3547	1/1	0.92	0.49	33,33,33,33	0
84	MG	5	3431	1/1	0.92	0.18	37,37,37,37	0
84	MG	5	3703	1/1	0.92	0.41	36,36,36,36	0
84	MG	6	1967	1/1	0.92	0.20	51,51,51,51	0
84	MG	12	303	1/1	0.92	1.08	46,46,46,46	0
84	MG	5	3427	1/1	0.92	0.11	47,47,47,47	0
85	OHX	5	4061	7/7	0.92	0.39	121,121,121,121	0
84	MG	1	3459	1/1	0.92	0.44	46,46,46,46	0
84	MG	5	3603	1/1	0.92	0.35	47,47,47,47	0
84	MG	1	3705	1/1	0.92	0.82	52,52,52,52	0
84	MG	1	3676	1/1	0.92	0.25	48,48,48,48	0
84	MG	5	3473	1/1	0.92	0.41	44,44,44,44	0
84	MG	5	3434	1/1	0.92	0.30	32,32,32,32	0
84	MG	1	3665	1/1	0.92	0.29	67,67,67,67	0
84	MG	O2	201	1/1	0.92	0.24	35,35,35,35	0
84	MG	5	3496	1/1	0.92	0.43	56,56,56,56	0
84	MG	5	3563	1/1	0.92	0.37	38,38,38,38	0
84	MG	o1	201	1/1	0.92	0.61	49,49,49,49	0
85	OHX	6	2146	7/7	0.92	0.36	108,108,108,108	0
84	MG	1	3541	1/1	0.92	0.45	55,55,55,55	0
85	OHX	2	2111	7/7	0.92	0.43	112,112,112,112	0
84	MG	6	1923	1/1	0.92	0.69	68,68,68,68	0
84	MG	1	3592	1/1	0.92	0.21	61,61,61,61	0
84	MG	2	1966	1/1	0.92	0.35	67,67,67,67	0
84	MG	5	3412	1/1	0.92	0.46	39,39,39,39	0
84	MG	1	3482	1/1	0.92	0.15	53,53,53,53	0
85	OHX	5	4020	7/7	0.92	0.41	101,101,101,101	0
84	MG	1	3662	1/1	0.92	0.24	45,45,45,45	0
84	MG	m6	201	1/1	0.92	0.28	37,37,37,37	0
84	MG	6	2159	1/1	0.92	0.59	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3672	1/1	0.92	0.28	42,42,42,42	0
84	MG	1	3593	1/1	0.92	0.18	39,39,39,39	0
84	MG	5	3740	1/1	0.93	0.15	41,41,41,41	0
84	MG	1	3612	1/1	0.93	0.29	40,40,40,40	0
84	MG	N8	202	1/1	0.93	0.14	35,35,35,35	0
84	MG	1	3604	1/1	0.93	0.17	47,47,47,47	0
84	MG	2	1922	1/1	0.93	0.97	74,74,74,74	0
84	MG	8	202	1/1	0.93	0.40	64,64,64,64	0
85	OHX	2	2100	7/7	0.93	0.20	116,116,116,116	0
84	MG	5	3549	1/1	0.93	0.41	48,48,48,48	0
85	OHX	6	2155	7/7	0.93	0.42	116,116,116,116	0
84	MG	1	3426	1/1	0.93	0.47	50,50,50,50	0
84	MG	5	3589	1/1	0.93	0.41	37,37,37,37	0
84	MG	5	3717	1/1	0.93	0.18	39,39,39,39	0
84	MG	5	3648	1/1	0.93	0.19	61,61,61,61	0
84	MG	1	3670	1/1	0.93	0.39	52,52,52,52	0
84	MG	1	3488	1/1	0.93	0.34	33,33,33,33	0
84	MG	l3	401	1/1	0.93	0.51	29,29,29,29	0
84	MG	5	3623	1/1	0.93	0.49	57,57,57,57	0
84	MG	5	3654	1/1	0.93	0.25	42,42,42,42	0
84	MG	5	3679	1/1	0.93	0.41	42,42,42,42	0
85	OHX	2	2034	7/7	0.93	0.26	113,113,113,113	0
84	MG	1	3719	1/1	0.93	0.71	45,45,45,45	0
84	MG	7	210	1/1	0.93	0.12	53,53,53,53	0
84	MG	5	3535	1/1	0.93	0.35	49,49,49,49	0
84	MG	sM	202	1/1	0.93	0.11	43,43,43,43	0
84	MG	1	3648	1/1	0.93	0.22	37,37,37,37	0
84	MG	5	3607	1/1	0.93	0.18	38,38,38,38	0
84	MG	2	1903	1/1	0.93	0.69	55,55,55,55	0
84	MG	1	3469	1/1	0.93	0.52	51,51,51,51	0
84	MG	1	3532	1/1	0.93	0.19	57,57,57,57	0
84	MG	8	210	1/1	0.93	0.23	57,57,57,57	0
84	MG	5	3518	1/1	0.93	0.38	41,41,41,41	0
85	OHX	2	2107	7/7	0.93	0.33	126,126,126,126	0
85	OHX	6	2127	7/7	0.93	0.25	138,138,138,138	0
84	MG	1	3575	1/1	0.93	0.45	40,40,40,40	0
84	MG	5	3708	1/1	0.93	0.26	44,44,44,44	0
84	MG	L7	301	1/1	0.93	0.36	42,42,42,42	0
84	MG	1	3501	1/1	0.93	0.53	43,43,43,43	0
85	OHX	5	3870	7/7	0.93	0.28	76,76,76,76	0
84	MG	2	1967	1/1	0.93	0.26	83,83,83,83	0
84	MG	6	1986	1/1	0.93	0.20	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3564	1/1	0.93	0.62	40,40,40,40	0
84	MG	6	1921	1/1	0.93	0.48	56,56,56,56	0
84	MG	6	1909	1/1	0.93	0.40	98,98,98,98	0
85	OHX	5	3932	7/7	0.93	0.26	75,75,75,75	0
84	MG	1	3444	1/1	0.93	0.27	51,51,51,51	0
85	OHX	2	2052	7/7	0.93	0.23	117,117,117,117	0
85	OHX	5	4005	7/7	0.93	0.27	104,104,104,104	0
84	MG	1	3518	1/1	0.93	0.43	52,52,52,52	0
84	MG	4	205	1/1	0.93	0.49	39,39,39,39	0
84	MG	1	3577	1/1	0.93	0.24	46,46,46,46	0
84	MG	5	3718	1/1	0.93	0.20	40,40,40,40	0
84	MG	5	3735	1/1	0.93	0.22	65,65,65,65	0
84	MG	5	3522	1/1	0.93	0.27	43,43,43,43	0
84	MG	5	3534	1/1	0.93	0.37	36,36,36,36	0
84	MG	5	3663	1/1	0.93	0.25	62,62,62,62	0
84	MG	n8	202	1/1	0.93	0.23	37,37,37,37	0
85	OHX	6	2068	7/7	0.93	0.22	90,90,90,90	0
84	MG	2	1973	1/1	0.93	0.45	64,64,64,64	0
84	MG	5	3673	1/1	0.93	0.51	34,34,34,34	0
84	MG	1	3602	1/1	0.93	0.52	41,41,41,41	0
84	MG	2	1928	1/1	0.93	0.39	71,71,71,71	0
84	MG	1	3423	1/1	0.93	0.23	36,36,36,36	0
84	MG	1	3614	1/1	0.93	0.14	55,55,55,55	0
84	MG	5	3609	1/1	0.93	0.42	55,55,55,55	0
84	MG	6	1973	1/1	0.93	0.21	78,78,78,78	0
85	OHX	6	2144	7/7	0.93	0.35	102,102,102,102	0
84	MG	2	1907	1/1	0.93	0.51	64,64,64,64	0
84	MG	7	209	1/1	0.93	0.34	51,51,51,51	0
85	OHX	7	220	7/7	0.93	0.31	110,110,110,110	0
84	MG	5	3596	1/1	0.93	0.43	40,40,40,40	0
85	OHX	5	4029	7/7	0.93	0.31	128,128,128,128	0
84	MG	5	3414	1/1	0.93	0.17	31,31,31,31	0
85	OHX	6	2135	7/7	0.93	0.39	92,92,92,92	0
84	MG	5	3401	1/1	0.94	0.26	32,32,32,32	0
85	OHX	2	2119	7/7	0.94	0.47	144,144,144,144	0
85	OHX	6	2137	7/7	0.94	0.27	127,127,127,127	0
85	OHX	5	4055	7/7	0.94	0.36	114,114,114,114	0
84	MG	5	3455	1/1	0.94	0.32	50,50,50,50	0
84	MG	5	3649	1/1	0.94	0.23	35,35,35,35	0
85	OHX	2	2106	7/7	0.94	0.35	123,123,123,123	0
85	OHX	1	3945	7/7	0.94	0.19	162,162,162,162	0
85	OHX	1	3889	7/7	0.94	0.21	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3661	1/1	0.94	0.47	55,55,55,55	0
84	MG	1	3520	1/1	0.94	0.32	42,42,42,42	0
84	MG	5	4075	1/1	0.94	0.46	33,33,33,33	0
84	MG	1	3682	1/1	0.94	0.50	33,33,33,33	0
85	OHX	5	4034	7/7	0.94	0.34	84,84,84,84	0
84	MG	1	3677	1/1	0.94	0.27	43,43,43,43	0
84	MG	4	209	1/1	0.94	0.29	54,54,54,54	0
84	MG	1	3613	1/1	0.94	0.13	45,45,45,45	0
84	MG	2	1925	1/1	0.94	0.76	74,74,74,74	0
85	OHX	1	3864	7/7	0.94	0.20	79,79,79,79	0
84	MG	5	3459	1/1	0.94	0.35	40,40,40,40	0
84	MG	6	1936	1/1	0.94	0.38	42,42,42,42	0
85	OHX	6	2142	7/7	0.94	0.24	117,117,117,117	0
84	MG	1	3644	1/1	0.94	0.72	41,41,41,41	0
84	MG	6	1952	1/1	0.94	0.51	54,54,54,54	0
84	MG	5	3439	1/1	0.94	0.33	33,33,33,33	0
84	MG	5	3628	1/1	0.94	0.27	49,49,49,49	0
84	MG	5	3492	1/1	0.94	0.56	41,41,41,41	0
84	MG	5	3530	1/1	0.94	0.31	41,41,41,41	0
84	MG	5	3665	1/1	0.94	0.45	39,39,39,39	0
84	MG	2	1934	1/1	0.94	0.32	72,72,72,72	0
84	MG	1	3545	1/1	0.94	0.54	36,36,36,36	0
84	MG	6	1972	1/1	0.94	0.31	51,51,51,51	0
84	MG	1	3428	1/1	0.94	0.44	48,48,48,48	0
84	MG	3	207	1/1	0.94	0.16	44,44,44,44	0
84	MG	1	3434	1/1	0.94	0.36	52,52,52,52	0
84	MG	5	3533	1/1	0.94	0.91	55,55,55,55	0
85	OHX	5	4008	7/7	0.94	0.26	144,144,144,144	0
84	MG	5	3495	1/1	0.94	0.17	35,35,35,35	0
85	OHX	1	4002	7/7	0.94	0.27	112,112,112,112	0
84	MG	4	201	1/1	0.94	0.52	53,53,53,53	0
84	MG	m1	201	1/1	0.94	0.40	48,48,48,48	0
84	MG	7	207	1/1	0.94	0.14	36,36,36,36	0
85	OHX	1	3918	7/7	0.94	0.29	121,121,121,121	0
84	MG	1	3455	1/1	0.94	0.34	32,32,32,32	0
84	MG	1	3476	1/1	0.94	0.20	42,42,42,42	0
84	MG	1	3660	1/1	0.94	0.09	47,47,47,47	0
85	OHX	2	2102	7/7	0.94	0.32	114,114,114,114	0
84	MG	6	1978	1/1	0.94	0.59	76,76,76,76	0
85	OHX	1	4029	7/7	0.94	0.42	89,89,89,89	0
85	OHX	5	4024	7/7	0.94	0.32	116,116,116,116	0
84	MG	1	3633	1/1	0.94	0.44	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3699	1/1	0.94	0.45	55,55,55,55	0
84	MG	1	3425	1/1	0.94	0.20	49,49,49,49	0
84	MG	1	3646	1/1	0.94	0.14	53,53,53,53	0
84	MG	3	205	1/1	0.94	0.24	66,66,66,66	0
84	MG	5	3725	1/1	0.94	0.28	38,38,38,38	0
85	OHX	1	4036	7/7	0.94	0.36	104,104,104,104	0
84	MG	1	3415	1/1	0.94	0.38	41,41,41,41	0
84	MG	2	1929	1/1	0.94	0.64	67,67,67,67	0
85	OHX	2	2110	7/7	0.94	0.38	130,130,130,130	0
84	MG	5	3733	1/1	0.94	0.43	32,32,32,32	0
84	MG	1	3687	1/1	0.94	0.19	48,48,48,48	0
84	MG	5	3629	1/1	0.94	0.35	35,35,35,35	0
85	OHX	2	2109	7/7	0.94	0.33	112,112,112,112	0
84	MG	2	1950	1/1	0.94	0.33	72,72,72,72	0
84	MG	1	3565	1/1	0.94	0.47	32,32,32,32	0
84	MG	1	3515	1/1	0.94	0.46	41,41,41,41	0
85	OHX	1	4003	7/7	0.94	0.39	108,108,108,108	0
84	MG	6	1918	1/1	0.94	0.48	58,58,58,58	0
84	MG	8	201	1/1	0.94	0.24	42,42,42,42	0
85	OHX	5	4044	7/7	0.94	0.24	116,116,116,116	0
85	OHX	5	4033	7/7	0.94	0.37	105,105,105,105	0
84	MG	1	3433	1/1	0.94	0.35	36,36,36,36	0
84	MG	1	3502	1/1	0.94	0.43	39,39,39,39	0
85	OHX	6	2088	7/7	0.94	0.46	81,81,81,81	0
84	MG	5	3582	1/1	0.94	0.23	49,49,49,49	0
85	OHX	5	3980	7/7	0.94	0.23	102,102,102,102	0
84	MG	5	3416	1/1	0.94	0.28	38,38,38,38	0
84	MG	5	3464	1/1	0.94	0.34	29,29,29,29	0
84	MG	1	3596	1/1	0.94	0.16	46,46,46,46	0
84	MG	3	204	1/1	0.94	0.60	40,40,40,40	0
84	MG	O3	201	1/1	0.94	0.21	42,42,42,42	0
85	OHX	2	2067	7/7	0.94	0.36	106,106,106,106	0
84	MG	1	3445	1/1	0.94	0.33	40,40,40,40	0
84	MG	5	3562	1/1	0.94	0.35	32,32,32,32	0
84	MG	6	1943	1/1	0.94	0.57	58,58,58,58	0
84	MG	1	3567	1/1	0.94	0.93	50,50,50,50	0
84	MG	5	3670	1/1	0.94	0.32	35,35,35,35	0
85	OHX	2	2089	7/7	0.94	0.42	113,113,113,113	0
84	MG	5	3417	1/1	0.94	0.20	84,84,84,84	0
84	MG	2	1920	1/1	0.94	0.69	74,74,74,74	0
84	MG	5	3415	1/1	0.94	0.59	29,29,29,29	0
85	OHX	5	3943	7/7	0.94	0.18	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3594	1/1	0.94	0.35	48,48,48,48	0
84	MG	5	3612	1/1	0.94	0.36	40,40,40,40	0
84	MG	1	3606	1/1	0.94	0.39	34,34,34,34	0
84	MG	1	3669	1/1	0.94	0.27	48,48,48,48	0
84	MG	6	1941	1/1	0.94	0.38	43,43,43,43	0
85	OHX	2	2027	7/7	0.94	0.20	128,128,128,128	0
85	OHX	6	2101	7/7	0.94	0.26	105,105,105,105	0
85	OHX	1	3997	7/7	0.94	0.39	82,82,82,82	0
84	MG	2	1906	1/1	0.94	0.45	63,63,63,63	0
85	OHX	6	2150	7/7	0.94	0.39	100,100,100,100	0
86	ZN	E1	501	1/1	0.94	0.05	115,115,115,115	0
84	MG	1	3432	1/1	0.94	0.22	49,49,49,49	0
85	OHX	2	2090	7/7	0.94	0.19	121,121,121,121	0
84	MG	5	3584	1/1	0.94	0.11	45,45,45,45	0
84	MG	5	3700	1/1	0.94	0.23	38,38,38,38	0
85	OHX	6	2123	7/7	0.94	0.33	102,102,102,102	0
84	MG	5	3502	1/1	0.94	0.46	32,32,32,32	0
85	OHX	2	2076	7/7	0.94	0.18	135,135,135,135	0
85	OHX	5	3976	7/7	0.94	0.25	107,107,107,107	0
84	MG	2	1926	1/1	0.94	0.33	74,74,74,74	0
85	OHX	2	2063	7/7	0.94	0.22	160,160,160,160	0
84	MG	5	3695	1/1	0.94	0.25	48,48,48,48	0
84	MG	5	3483	1/1	0.94	0.47	41,41,41,41	0
84	MG	2	1927	1/1	0.94	0.47	65,65,65,65	0
84	MG	5	3564	1/1	0.94	0.45	38,38,38,38	0
84	MG	1	3725	1/1	0.94	0.38	52,52,52,52	0
85	OHX	5	3909	7/7	0.94	0.18	88,88,88,88	0
85	OHX	5	3906	7/7	0.94	0.21	101,101,101,101	0
84	MG	5	3611	1/1	0.94	0.22	40,40,40,40	0
84	MG	1	3609	1/1	0.94	0.32	41,41,41,41	0
84	MG	6	1949	1/1	0.94	0.68	76,76,76,76	0
85	OHX	6	2128	7/7	0.94	0.31	112,112,112,112	0
84	MG	5	3472	1/1	0.94	0.47	50,50,50,50	0
85	OHX	S6	301	7/7	0.94	0.38	117,117,117,117	0
84	MG	6	1906	1/1	0.94	0.34	51,51,51,51	0
84	MG	2	1908	1/1	0.95	0.39	78,78,78,78	0
84	MG	L2	301	1/1	0.95	0.39	39,39,39,39	0
84	MG	5	3719	1/1	0.95	0.15	32,32,32,32	0
84	MG	1	3500	1/1	0.95	0.66	44,44,44,44	0
85	OHX	5	4031	7/7	0.95	0.27	106,106,106,106	0
84	MG	1	3588	1/1	0.95	0.41	42,42,42,42	0
85	OHX	5	4062	7/7	0.95	0.42	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	6	1904	1/1	0.95	0.62	76,76,76,76	0
84	MG	1	3403	1/1	0.95	0.65	51,51,51,51	0
85	OHX	4	225	7/7	0.95	0.16	113,113,113,113	0
85	OHX	O9	101	7/7	0.95	0.46	77,77,77,77	0
85	OHX	1	3858	7/7	0.95	0.11	128,128,128,128	0
84	MG	1	3422	1/1	0.95	0.35	55,55,55,55	0
84	MG	5	3575	1/1	0.95	0.47	31,31,31,31	0
85	OHX	5	3990	7/7	0.95	0.40	76,76,76,76	0
85	OHX	2	2092	7/7	0.95	0.32	106,106,106,106	0
85	OHX	6	2095	7/7	0.95	0.41	119,119,119,119	0
85	OHX	6	2154	7/7	0.95	0.38	100,100,100,100	0
85	OHX	1	3960	7/7	0.95	0.30	122,122,122,122	0
84	MG	n0	201	1/1	0.95	0.23	43,43,43,43	0
85	OHX	6	2132	7/7	0.95	0.30	112,112,112,112	0
84	MG	6	1920	1/1	0.95	0.49	42,42,42,42	0
85	OHX	6	2080	7/7	0.95	0.29	109,109,109,109	0
84	MG	5	3517	1/1	0.95	0.31	53,53,53,53	0
84	MG	5	3734	1/1	0.95	0.14	60,60,60,60	0
85	OHX	2	2085	7/7	0.95	0.29	114,114,114,114	0
84	MG	1	3627	1/1	0.95	0.23	45,45,45,45	0
85	OHX	1	4007	7/7	0.95	0.37	101,101,101,101	0
84	MG	L2	302	1/1	0.95	0.29	41,41,41,41	0
84	MG	5	3590	1/1	0.95	0.29	34,34,34,34	0
85	OHX	6	2133	7/7	0.95	0.25	85,85,85,85	0
84	MG	5	3572	1/1	0.95	0.55	28,28,28,28	0
85	OHX	m0	301	7/7	0.95	0.13	109,109,109,109	0
84	MG	5	3505	1/1	0.95	0.51	36,36,36,36	0
85	OHX	5	3997	7/7	0.95	0.37	87,87,87,87	0
84	MG	5	3479	1/1	0.95	0.27	35,35,35,35	0
84	MG	6	1933	1/1	0.95	0.41	84,84,84,84	0
86	ZN	D6	500	1/1	0.95	0.07	81,81,81,81	0
84	MG	1	3533	1/1	0.95	0.43	39,39,39,39	0
84	MG	5	3682	1/1	0.95	0.41	35,35,35,35	0
85	OHX	1	4013	7/7	0.95	0.26	104,104,104,104	0
85	OHX	5	4047	7/7	0.95	0.29	101,101,101,101	0
84	MG	1	3474	1/1	0.95	0.18	53,53,53,53	0
85	OHX	5	3849	7/7	0.95	0.15	90,90,90,90	0
85	OHX	1	3983	7/7	0.95	0.33	78,78,78,78	0
84	MG	6	1950	1/1	0.95	0.67	72,72,72,72	0
84	MG	5	3484	1/1	0.95	0.35	35,35,35,35	0
84	MG	1	3572	1/1	0.95	0.52	33,33,33,33	0
84	MG	5	3443	1/1	0.95	0.20	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	OHX	5	3983	7/7	0.95	0.30	83,83,83,83	0
85	OHX	6	2040	7/7	0.95	0.13	89,89,89,89	0
85	OHX	6	2027	7/7	0.95	0.15	78,78,78,78	0
85	OHX	6	2098	7/7	0.95	0.34	99,99,99,99	0
85	OHX	2	2075	7/7	0.95	0.35	115,115,115,115	0
84	MG	5	3527	1/1	0.95	0.33	69,69,69,69	0
85	OHX	5	4053	7/7	0.95	0.29	105,105,105,105	0
84	MG	5	3513	1/1	0.95	0.41	32,32,32,32	0
84	MG	6	1968	1/1	0.95	0.35	55,55,55,55	0
85	OHX	2	2012	7/7	0.95	0.14	107,107,107,107	0
85	OHX	2	2068	7/7	0.95	0.33	122,122,122,122	0
85	OHX	1	3969	7/7	0.95	0.33	103,103,103,103	0
84	MG	5	3405	1/1	0.95	0.27	43,43,43,43	0
84	MG	1	3607	1/1	0.95	0.23	42,42,42,42	0
84	MG	5	3592	1/1	0.95	0.19	42,42,42,42	0
85	OHX	5	4067	7/7	0.95	0.22	93,93,93,93	0
85	OHX	5	3978	7/7	0.95	0.27	92,92,92,92	0
84	MG	5	3441	1/1	0.95	0.35	65,65,65,65	0
85	OHX	2	2000	7/7	0.95	0.13	89,89,89,89	0
84	MG	2	1916	1/1	0.95	0.41	59,59,59,59	0
84	MG	1	3706	1/1	0.95	0.65	32,32,32,32	0
84	MG	1	3470	1/1	0.95	0.28	37,37,37,37	0
84	MG	5	3475	1/1	0.95	0.66	32,32,32,32	0
85	OHX	M9	201	7/7	0.95	0.35	124,124,124,124	0
84	MG	1	3446	1/1	0.95	0.17	47,47,47,47	0
84	MG	5	3602	1/1	0.95	0.50	49,49,49,49	0
84	MG	5	3702	1/1	0.95	0.13	35,35,35,35	0
85	OHX	l5	302	7/7	0.95	0.24	107,107,107,107	0
84	MG	1	3544	1/1	0.95	0.57	35,35,35,35	0
85	OHX	5	3864	7/7	0.95	0.17	78,78,78,78	0
84	MG	1	3493	1/1	0.95	0.49	30,30,30,30	0
85	OHX	5	3886	7/7	0.95	0.21	82,82,82,82	0
84	MG	1	3603	1/1	0.95	0.39	38,38,38,38	0
84	MG	1	3524	1/1	0.95	0.26	43,43,43,43	0
84	MG	5	3694	1/1	0.95	0.27	35,35,35,35	0
84	MG	5	3494	1/1	0.95	0.49	30,30,30,30	0
84	MG	5	3626	1/1	0.95	0.33	33,33,33,33	0
85	OHX	5	3989	7/7	0.95	0.36	81,81,81,81	0
85	OHX	1	3888	7/7	0.95	0.30	85,85,85,85	0
84	MG	1	3490	1/1	0.95	0.26	42,42,42,42	0
85	OHX	5	3988	7/7	0.95	0.28	116,116,116,116	0
85	OHX	1	3966	7/7	0.95	0.34	175,175,175,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	OHX	5	4018	7/7	0.95	0.35	105,105,105,105	0
84	MG	7	205	1/1	0.95	0.52	35,35,35,35	0
85	OHX	2	2093	7/7	0.95	0.31	103,103,103,103	0
84	MG	1	4042	1/1	0.95	0.15	45,45,45,45	0
84	MG	5	3713	1/1	0.95	0.34	33,33,33,33	0
84	MG	2	1959	1/1	0.95	0.34	67,67,67,67	0
85	OHX	5	4019	7/7	0.95	0.33	109,109,109,109	0
85	OHX	5	4056	7/7	0.95	0.33	104,104,104,104	0
85	OHX	1	4035	7/7	0.95	0.23	105,105,105,105	0
85	OHX	3	219	7/7	0.95	0.37	95,95,95,95	0
84	MG	1	3674	1/1	0.95	0.50	37,37,37,37	0
84	MG	5	3508	1/1	0.95	0.39	34,34,34,34	0
84	MG	5	3493	1/1	0.95	0.64	34,34,34,34	0
85	OHX	1	3949	7/7	0.95	0.30	101,101,101,101	0
84	MG	2	1968	1/1	0.95	0.44	85,85,85,85	0
86	ZN	Q0	500	1/1	0.95	0.10	48,48,48,48	0
84	MG	1	3559	1/1	0.95	0.47	48,48,48,48	0
85	OHX	2	2003	7/7	0.95	0.11	101,101,101,101	0
84	MG	5	3452	1/1	0.95	0.34	43,43,43,43	0
85	OHX	6	2116	7/7	0.95	0.18	111,111,111,111	0
85	OHX	1	3978	7/7	0.95	0.22	92,92,92,92	0
84	MG	1	3402	1/1	0.95	0.61	46,46,46,46	0
85	OHX	c3	201	7/7	0.95	0.24	113,113,113,113	0
84	MG	5	3558	1/1	0.95	0.47	37,37,37,37	0
84	MG	5	3570	1/1	0.95	0.29	31,31,31,31	0
85	OHX	2	2040	7/7	0.95	0.24	110,110,110,110	0
85	OHX	2	2026	7/7	0.95	0.19	118,118,118,118	0
85	OHX	5	3940	7/7	0.95	0.23	99,99,99,99	0
84	MG	1	3485	1/1	0.95	0.33	37,37,37,37	0
85	OHX	6	2109	7/7	0.95	0.26	84,84,84,84	0
84	MG	1	3511	1/1	0.95	0.50	39,39,39,39	0
85	OHX	2	2084	7/7	0.95	0.33	98,98,98,98	0
85	OHX	5	4058	7/7	0.95	0.35	115,115,115,115	0
85	OHX	1	4018	7/7	0.95	0.32	88,88,88,88	0
85	OHX	5	3897	7/7	0.95	0.32	81,81,81,81	0
85	OHX	6	2110	7/7	0.95	0.27	103,103,103,103	0
84	MG	M0	301	1/1	0.95	0.37	43,43,43,43	0
85	OHX	6	2143	7/7	0.95	0.34	97,97,97,97	0
85	OHX	2	2105	7/7	0.95	0.31	114,114,114,114	0
84	MG	5	3656	1/1	0.95	0.12	36,36,36,36	0
84	MG	5	3586	1/1	0.95	0.42	34,34,34,34	0
85	OHX	2	2025	7/7	0.95	0.14	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3418	1/1	0.95	0.22	66,66,66,66	0
85	OHX	6	2145	7/7	0.95	0.35	106,106,106,106	0
85	OHX	L4	401	7/7	0.95	0.30	92,92,92,92	0
85	OHX	5	3996	7/7	0.95	0.35	92,92,92,92	0
85	OHX	6	2081	7/7	0.95	0.19	110,110,110,110	0
84	MG	5	3658	1/1	0.95	0.31	46,46,46,46	0
85	OHX	1	3992	7/7	0.95	0.32	116,116,116,116	0
84	MG	5	3514	1/1	0.95	0.64	30,30,30,30	0
84	MG	5	3606	1/1	0.95	0.29	41,41,41,41	0
84	MG	1	3671	1/1	0.95	0.17	45,45,45,45	0
84	MG	8	203	1/1	0.95	0.43	43,43,43,43	0
85	OHX	1	3974	7/7	0.95	0.30	127,127,127,127	0
85	OHX	1	4031	7/7	0.95	0.23	102,102,102,102	0
85	OHX	4	228	7/7	0.95	0.36	85,85,85,85	0
85	OHX	1	4030	7/7	0.95	0.41	98,98,98,98	0
85	OHX	2	2098	7/7	0.95	0.38	125,125,125,125	0
84	MG	1	3436	1/1	0.95	0.38	38,38,38,38	0
84	MG	5	3580	1/1	0.95	0.57	37,37,37,37	0
85	OHX	5	3961	7/7	0.95	0.27	102,102,102,102	0
84	MG	5	3465	1/1	0.95	0.17	41,41,41,41	0
85	OHX	5	4001	7/7	0.95	0.27	130,130,130,130	0
85	OHX	6	2077	7/7	0.95	0.21	100,100,100,100	0
84	MG	M5	301	1/1	0.95	0.24	39,39,39,39	0
84	MG	5	3548	1/1	0.95	0.30	29,29,29,29	0
85	OHX	1	4017	7/7	0.95	0.41	68,68,68,68	0
84	MG	1	3698	1/1	0.95	0.26	49,49,49,49	0
85	OHX	1	3826	7/7	0.95	0.14	93,93,93,93	0
85	OHX	5	3982	7/7	0.96	0.30	80,80,80,80	0
85	OHX	1	4024	7/7	0.96	0.28	155,155,155,155	0
86	ZN	d9	101	1/1	0.96	0.13	86,86,86,86	0
84	MG	5	3627	1/1	0.96	0.39	34,34,34,34	0
85	OHX	1	4034	7/7	0.96	0.36	104,104,104,104	0
85	OHX	1	3828	7/7	0.96	0.10	104,104,104,104	0
84	MG	2	1958	1/1	0.96	0.49	96,96,96,96	0
84	MG	5	3661	1/1	0.96	0.23	33,33,33,33	0
85	OHX	2	2077	7/7	0.96	0.33	110,110,110,110	0
85	OHX	1	4015	7/7	0.96	0.36	91,91,91,91	0
85	OHX	2	2057	7/7	0.96	0.16	126,126,126,126	0
84	MG	4	206	1/1	0.96	0.27	35,35,35,35	0
85	OHX	6	2091	7/7	0.96	0.18	110,110,110,110	0
85	OHX	5	4009	7/7	0.96	0.27	115,115,115,115	0
84	MG	1	3711	1/1	0.96	0.23	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	OHX	6	2108	7/7	0.96	0.25	102,102,102,102	0
85	OHX	1	3879	7/7	0.96	0.24	101,101,101,101	0
85	OHX	1	4016	7/7	0.96	0.38	109,109,109,109	0
85	OHX	6	2141	7/7	0.96	0.35	109,109,109,109	0
85	OHX	6	2105	7/7	0.96	0.32	115,115,115,115	0
85	OHX	M0	302	7/7	0.96	0.18	86,86,86,86	0
85	OHX	1	3943	7/7	0.96	0.31	112,112,112,112	0
84	MG	1	3635	1/1	0.96	0.28	41,41,41,41	0
85	OHX	l3	408	7/7	0.96	0.35	111,111,111,111	0
85	OHX	1	4014	7/7	0.96	0.38	110,110,110,110	0
84	MG	1	3653	1/1	0.96	0.17	40,40,40,40	0
84	MG	5	3506	1/1	0.96	0.63	47,47,47,47	0
85	OHX	1	3981	7/7	0.96	0.24	95,95,95,95	0
84	MG	1	3530	1/1	0.96	0.66	41,41,41,41	0
84	MG	5	3488	1/1	0.96	0.32	53,53,53,53	0
84	MG	6	2004	1/1	0.96	0.24	70,70,70,70	0
85	OHX	1	3923	7/7	0.96	0.35	91,91,91,91	0
85	OHX	3	216	7/7	0.96	0.28	108,108,108,108	0
85	OHX	4	229	7/7	0.96	0.39	113,113,113,113	0
85	OHX	2	2060	7/7	0.96	0.25	122,122,122,122	0
85	OHX	2	2073	7/7	0.96	0.20	120,120,120,120	0
85	OHX	5	4032	7/7	0.96	0.33	86,86,86,86	0
85	OHX	1	3946	7/7	0.96	0.32	99,99,99,99	0
85	OHX	5	3802	7/7	0.96	0.12	70,70,70,70	0
84	MG	1	3498	1/1	0.96	0.46	32,32,32,32	0
84	MG	5	3618	1/1	0.96	0.61	40,40,40,40	0
85	OHX	8	223	7/7	0.96	0.33	95,95,95,95	0
84	MG	1	3574	1/1	0.96	0.41	33,33,33,33	0
85	OHX	5	3895	7/7	0.96	0.30	76,76,76,76	0
85	OHX	5	3878	7/7	0.96	0.15	80,80,80,80	0
85	OHX	5	3945	7/7	0.96	0.17	119,119,119,119	0
85	OHX	1	3950	7/7	0.96	0.26	121,121,121,121	0
84	MG	m7	202	1/1	0.96	0.36	36,36,36,36	0
85	OHX	1	3800	7/7	0.96	0.11	88,88,88,88	0
85	OHX	D9	103	7/7	0.96	0.38	108,108,108,108	0
84	MG	1	3702	1/1	0.96	0.44	36,36,36,36	0
85	OHX	5	4063	7/7	0.96	0.28	121,121,121,121	0
85	OHX	2	2091	7/7	0.96	0.20	122,122,122,122	0
84	MG	5	3424	1/1	0.96	0.37	32,32,32,32	0
85	OHX	4	223	7/7	0.96	0.24	97,97,97,97	0
85	OHX	1	3955	7/7	0.96	0.33	108,108,108,108	0
85	OHX	5	4051	7/7	0.96	0.36	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	3	209	1/1	0.96	0.17	74,74,74,74	0
85	OHX	6	2121	7/7	0.96	0.33	108,108,108,108	0
85	OHX	5	3919	7/7	0.96	0.28	97,97,97,97	0
85	OHX	1	4023	7/7	0.96	0.33	109,109,109,109	0
84	MG	5	3720	1/1	0.96	0.19	32,32,32,32	0
85	OHX	1	3835	7/7	0.96	0.18	85,85,85,85	0
85	OHX	1	3917	7/7	0.96	0.13	133,133,133,133	0
85	OHX	5	3963	7/7	0.96	0.23	108,108,108,108	0
84	MG	1	3409	1/1	0.96	0.39	40,40,40,40	0
85	OHX	5	4059	7/7	0.96	0.37	74,74,74,74	0
84	MG	M7	203	1/1	0.96	0.31	38,38,38,38	0
85	OHX	1	3905	7/7	0.96	0.20	79,79,79,79	0
84	MG	1	3703	1/1	0.96	0.26	33,33,33,33	0
84	MG	1	3465	1/1	0.96	0.21	42,42,42,42	0
85	OHX	1	3909	7/7	0.96	0.23	83,83,83,83	0
84	MG	5	3469	1/1	0.96	0.22	58,58,58,58	0
84	MG	6	1907	1/1	0.96	0.42	75,75,75,75	0
85	OHX	1	4037	7/7	0.96	0.45	98,98,98,98	0
84	MG	5	3537	1/1	0.96	0.42	36,36,36,36	0
85	OHX	2	2104	7/7	0.96	0.37	96,96,96,96	0
85	OHX	2	1991	7/7	0.96	0.12	97,97,97,97	0
84	MG	6	1953	1/1	0.96	0.63	43,43,43,43	0
84	MG	N8	201	1/1	0.96	0.21	37,37,37,37	0
85	OHX	5	4064	7/7	0.96	0.37	90,90,90,90	0
84	MG	1	3523	1/1	0.96	0.41	41,41,41,41	0
84	MG	6	1992	1/1	0.96	0.66	60,60,60,60	0
84	MG	1	3580	1/1	0.96	0.22	42,42,42,42	0
85	OHX	5	3984	7/7	0.96	0.31	86,86,86,86	0
84	MG	1	3654	1/1	0.96	0.16	45,45,45,45	0
85	OHX	2	2082	7/7	0.96	0.24	114,114,114,114	0
85	OHX	2	2059	7/7	0.96	0.23	119,119,119,119	0
85	OHX	2	2117	7/7	0.96	0.47	128,128,128,128	0
84	MG	5	3521	1/1	0.96	0.41	39,39,39,39	0
85	OHX	5	3972	7/7	0.96	0.33	87,87,87,87	0
84	MG	O4	201	1/1	0.96	0.52	51,51,51,51	0
84	MG	5	3410	1/1	0.96	0.62	42,42,42,42	0
85	OHX	2	2008	7/7	0.96	0.14	105,105,105,105	0
85	OHX	2	2070	7/7	0.96	0.24	95,95,95,95	0
84	MG	5	3576	1/1	0.96	0.41	34,34,34,34	0
85	OHX	sR	401	7/7	0.96	0.24	132,132,132,132	0
84	MG	1	3504	1/1	0.96	0.36	40,40,40,40	0
85	OHX	4	231	7/7	0.96	0.29	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	OHX	6	2062	7/7	0.96	0.12	126,126,126,126	0
85	OHX	m0	302	7/7	0.96	0.25	88,88,88,88	0
85	OHX	6	2103	7/7	0.96	0.21	131,131,131,131	0
84	MG	2	1914	1/1	0.96	0.56	73,73,73,73	0
85	OHX	N8	203	7/7	0.96	0.24	129,129,129,129	0
85	OHX	2	2086	7/7	0.96	0.35	104,104,104,104	0
85	OHX	1	3929	7/7	0.96	0.34	83,83,83,83	0
84	MG	1	3546	1/1	0.96	0.24	36,36,36,36	0
84	MG	5	3591	1/1	0.96	0.27	33,33,33,33	0
85	OHX	1	3873	7/7	0.96	0.18	112,112,112,112	0
85	OHX	5	4070	7/7	0.96	0.29	135,135,135,135	0
85	OHX	1	3770	7/7	0.96	0.18	74,74,74,74	0
85	OHX	2	2097	7/7	0.96	0.25	110,110,110,110	0
85	OHX	6	2151	7/7	0.96	0.33	127,127,127,127	0
84	MG	5	3435	1/1	0.96	0.21	34,34,34,34	0
85	OHX	1	3855	7/7	0.96	0.35	86,86,86,86	0
85	OHX	5	3995	7/7	0.96	0.33	80,80,80,80	0
85	OHX	1	3884	7/7	0.96	0.23	109,109,109,109	0
85	OHX	1	4000	7/7	0.96	0.31	109,109,109,109	0
84	MG	5	3726	1/1	0.96	0.13	33,33,33,33	0
84	MG	6	1948	1/1	0.96	0.48	47,47,47,47	0
85	OHX	1	3823	7/7	0.96	0.17	73,73,73,73	0
84	MG	1	3521	1/1	0.96	0.58	31,31,31,31	0
84	MG	1	3581	1/1	0.96	0.31	45,45,45,45	0
84	MG	2	1945	1/1	0.96	0.21	63,63,63,63	0
84	MG	5	3474	1/1	0.96	0.14	54,54,54,54	0
85	OHX	5	4017	7/7	0.96	0.27	128,128,128,128	0
85	OHX	6	2093	7/7	0.96	0.21	117,117,117,117	0
85	OHX	5	3884	7/7	0.96	0.10	129,129,129,129	0
85	OHX	s9	201	7/7	0.96	0.43	96,96,96,96	0
85	OHX	5	3914	7/7	0.96	0.24	93,93,93,93	0
84	MG	5	3420	1/1	0.96	0.54	60,60,60,60	0
84	MG	1	3647	1/1	0.96	0.20	49,49,49,49	0
84	MG	5	3512	1/1	0.96	0.14	31,31,31,31	0
85	OHX	1	4032	7/7	0.96	0.43	88,88,88,88	0
85	OHX	1	3856	7/7	0.96	0.15	107,107,107,107	0
85	OHX	7	221	7/7	0.96	0.32	110,110,110,110	0
85	OHX	5	4042	7/7	0.96	0.34	100,100,100,100	0
85	OHX	5	4014	7/7	0.96	0.28	96,96,96,96	0
85	OHX	3	218	7/7	0.96	0.37	125,125,125,125	0
85	OHX	1	3788	7/7	0.96	0.13	86,86,86,86	0
85	OHX	1	3916	7/7	0.96	0.30	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	OHX	6	2054	7/7	0.96	0.22	84,84,84,84	0
85	OHX	2	2015	7/7	0.96	0.15	106,106,106,106	0
84	MG	5	3432	1/1	0.96	0.21	31,31,31,31	0
84	MG	1	3691	1/1	0.96	0.16	54,54,54,54	0
85	OHX	1	3993	7/7	0.96	0.37	87,87,87,87	0
85	OHX	6	2084	7/7	0.96	0.19	117,117,117,117	0
84	MG	M7	202	1/1	0.96	0.36	41,41,41,41	0
84	MG	6	1997	1/1	0.96	0.20	63,63,63,63	0
85	OHX	2	2103	7/7	0.96	0.27	132,132,132,132	0
85	OHX	6	2149	7/7	0.96	0.31	132,132,132,132	0
84	MG	5	3422	1/1	0.96	0.34	37,37,37,37	0
85	OHX	m1	202	7/7	0.96	0.29	107,107,107,107	0
85	OHX	6	2112	7/7	0.96	0.27	115,115,115,115	0
84	MG	m5	302	1/1	0.96	0.17	53,53,53,53	0
85	OHX	2	2101	7/7	0.96	0.31	129,129,129,129	0
85	OHX	5	3843	7/7	0.96	0.14	91,91,91,91	0
85	OHX	6	2153	7/7	0.96	0.36	109,109,109,109	0
85	OHX	s8	302	7/7	0.96	0.38	132,132,132,132	0
85	OHX	1	3898	7/7	0.96	0.28	85,85,85,85	0
85	OHX	6	2148	7/7	0.96	0.51	114,114,114,114	0
84	MG	3	208	1/1	0.96	0.40	65,65,65,65	0
85	OHX	2	2112	7/7	0.96	0.34	116,116,116,116	0
85	OHX	2	2099	7/7	0.96	0.25	128,128,128,128	0
84	MG	5	3599	1/1	0.96	0.25	43,43,43,43	0
85	OHX	6	2152	7/7	0.96	0.29	107,107,107,107	0
84	MG	5	3486	1/1	0.96	0.36	48,48,48,48	0
85	OHX	6	2115	7/7	0.96	0.18	106,106,106,106	0
84	MG	1	3621	1/1	0.96	0.16	36,36,36,36	0
84	MG	5	3491	1/1	0.96	0.50	42,42,42,42	0
85	OHX	5	4007	7/7	0.96	0.32	63,63,63,63	0
85	OHX	5	3819	7/7	0.96	0.12	78,78,78,78	0
85	OHX	5	3871	7/7	0.96	0.21	77,77,77,77	0
84	MG	5	3692	1/1	0.96	0.44	68,68,68,68	0
85	OHX	4	230	7/7	0.96	0.40	108,108,108,108	0
85	OHX	c5	201	7/7	0.96	0.22	128,128,128,128	0
85	OHX	2	2096	7/7	0.96	0.30	122,122,122,122	0
85	OHX	5	3973	7/7	0.96	0.27	96,96,96,96	0
84	MG	6	1940	1/1	0.96	0.24	43,43,43,43	0
85	OHX	5	4000	7/7	0.96	0.24	106,106,106,106	0
85	OHX	8	221	7/7	0.96	0.33	92,92,92,92	0
85	OHX	5	4016	7/7	0.96	0.39	90,90,90,90	0
85	OHX	5	3955	7/7	0.96	0.23	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3622	1/1	0.96	0.23	35,35,35,35	0
84	MG	1	3573	1/1	0.96	0.69	33,33,33,33	0
85	OHX	1	3897	7/7	0.96	0.16	109,109,109,109	0
85	OHX	1	4006	7/7	0.96	0.43	102,102,102,102	0
85	OHX	1	3987	7/7	0.96	0.32	79,79,79,79	0
84	MG	l3	404	1/1	0.96	0.26	39,39,39,39	0
84	MG	1	3478	1/1	0.96	0.15	40,40,40,40	0
85	OHX	6	2136	7/7	0.96	0.37	108,108,108,108	0
84	MG	1	3563	1/1	0.96	0.83	54,54,54,54	0
85	OHX	1	3976	7/7	0.96	0.31	91,91,91,91	0
84	MG	5	3466	1/1	0.96	0.23	68,68,68,68	0
84	MG	1	3412	1/1	0.96	0.25	42,42,42,42	0
84	MG	1	3486	1/1	0.96	0.45	36,36,36,36	0
85	OHX	1	3869	7/7	0.96	0.21	91,91,91,91	0
85	OHX	5	3937	7/7	0.96	0.29	112,112,112,112	0
85	OHX	5	3967	7/7	0.96	0.14	116,116,116,116	0
85	OHX	5	3959	7/7	0.96	0.34	118,118,118,118	0
85	OHX	1	3964	7/7	0.96	0.28	89,89,89,89	0
85	OHX	1	3941	7/7	0.96	0.36	107,107,107,107	0
85	OHX	5	3968	7/7	0.96	0.22	86,86,86,86	0
85	OHX	1	3932	7/7	0.96	0.36	71,71,71,71	0
84	MG	5	3620	1/1	0.96	0.35	35,35,35,35	0
85	OHX	1	3877	7/7	0.96	0.12	126,126,126,126	0
84	MG	1	3475	1/1	0.96	0.45	40,40,40,40	0
85	OHX	1	3930	7/7	0.96	0.23	100,100,100,100	0
84	MG	5	3543	1/1	0.96	0.49	37,37,37,37	0
85	OHX	1	4038	7/7	0.96	0.45	100,100,100,100	0
85	OHX	5	3986	7/7	0.96	0.35	105,105,105,105	0
84	MG	5	3489	1/1	0.96	0.28	34,34,34,34	0
85	OHX	C3	201	7/7	0.96	0.18	115,115,115,115	0
85	OHX	1	4028	7/7	0.96	0.31	115,115,115,115	0
85	OHX	5	4054	7/7	0.96	0.33	87,87,87,87	0
84	MG	1	3632	1/1	0.96	0.53	50,50,50,50	0
85	OHX	1	3813	7/7	0.96	0.21	77,77,77,77	0
85	OHX	1	3920	7/7	0.96	0.17	121,121,121,121	0
85	OHX	1	3799	7/7	0.96	0.11	88,88,88,88	0
85	OHX	5	4023	7/7	0.96	0.32	89,89,89,89	0
84	MG	1	3525	1/1	0.96	0.39	46,46,46,46	0
85	OHX	1	3935	7/7	0.96	0.31	88,88,88,88	0
85	OHX	1	3919	7/7	0.96	0.24	99,99,99,99	0
85	OHX	6	2118	7/7	0.96	0.27	109,109,109,109	0
85	OHX	6	2089	7/7	0.96	0.32	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	OHX	2	2094	7/7	0.96	0.26	108,108,108,108	0
85	OHX	2	2058	7/7	0.96	0.11	89,89,89,89	0
85	OHX	1	3810	7/7	0.96	0.10	99,99,99,99	0
85	OHX	2	2113	7/7	0.96	0.34	110,110,110,110	0
85	OHX	5	3966	7/7	0.96	0.33	108,108,108,108	0
85	OHX	1	3914	7/7	0.96	0.16	111,111,111,111	0
85	OHX	s4	301	7/7	0.96	0.26	110,110,110,110	0
84	MG	7	201	1/1	0.96	0.68	49,49,49,49	0
84	MG	5	3724	1/1	0.96	0.14	42,42,42,42	0
85	OHX	6	2156	7/7	0.97	0.37	115,115,115,115	0
85	OHX	8	215	7/7	0.97	0.15	94,94,94,94	0
85	OHX	1	3936	7/7	0.97	0.23	98,98,98,98	0
84	MG	5	3449	1/1	0.97	0.23	34,34,34,34	0
85	OHX	l3	407	7/7	0.97	0.28	78,78,78,78	0
85	OHX	1	3910	7/7	0.97	0.24	84,84,84,84	0
84	MG	1	3507	1/1	0.97	0.41	34,34,34,34	0
85	OHX	5	3944	7/7	0.97	0.36	74,74,74,74	0
85	OHX	2	2116	7/7	0.97	0.42	109,109,109,109	0
85	OHX	5	4030	7/7	0.97	0.40	89,89,89,89	0
84	MG	1	3566	1/1	0.97	0.37	37,37,37,37	0
84	MG	1	3440	1/1	0.97	0.27	48,48,48,48	0
85	OHX	1	3977	7/7	0.97	0.29	98,98,98,98	0
85	OHX	5	3950	7/7	0.97	0.40	101,101,101,101	0
85	OHX	5	3998	7/7	0.97	0.44	83,83,83,83	0
85	OHX	5	3786	7/7	0.97	0.11	75,75,75,75	0
85	OHX	1	3967	7/7	0.97	0.35	94,94,94,94	0
85	OHX	2	2078	7/7	0.97	0.28	105,105,105,105	0
84	MG	3	206	1/1	0.97	0.79	59,59,59,59	0
85	OHX	1	3778	7/7	0.97	0.12	84,84,84,84	0
84	MG	1	3413	1/1	0.97	0.46	43,43,43,43	0
85	OHX	4	221	7/7	0.97	0.32	88,88,88,88	0
85	OHX	5	4028	7/7	0.97	0.32	86,86,86,86	0
85	OHX	2	2018	7/7	0.97	0.12	106,106,106,106	0
85	OHX	6	2079	7/7	0.97	0.23	110,110,110,110	0
85	OHX	6	2130	7/7	0.97	0.42	88,88,88,88	0
85	OHX	6	2124	7/7	0.97	0.27	89,89,89,89	0
85	OHX	1	3862	7/7	0.97	0.21	74,74,74,74	0
84	MG	1	3480	1/1	0.97	0.36	36,36,36,36	0
85	OHX	3	215	7/7	0.97	0.18	98,98,98,98	0
85	OHX	1	3953	7/7	0.97	0.26	108,108,108,108	0
84	MG	5	3454	1/1	0.97	0.40	37,37,37,37	0
85	OHX	5	3892	7/7	0.97	0.23	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	5	3573	1/1	0.97	0.32	37,37,37,37	0
85	OHX	5	3850	7/7	0.97	0.12	107,107,107,107	0
85	OHX	5	4057	7/7	0.97	0.34	96,96,96,96	0
85	OHX	1	3890	7/7	0.97	0.23	102,102,102,102	0
84	MG	1	3473	1/1	0.97	0.28	45,45,45,45	0
85	OHX	5	3824	7/7	0.97	0.13	82,82,82,82	0
85	OHX	5	3935	7/7	0.97	0.20	92,92,92,92	0
84	MG	o4	201	1/1	0.97	0.35	52,52,52,52	0
85	OHX	1	3807	7/7	0.97	0.12	76,76,76,76	0
84	MG	1	4041	1/1	0.97	0.30	41,41,41,41	0
85	OHX	2	1997	7/7	0.97	0.11	115,115,115,115	0
85	OHX	1	3982	7/7	0.97	0.32	107,107,107,107	0
85	OHX	8	224	7/7	0.97	0.45	94,94,94,94	0
85	OHX	15	301	7/7	0.97	0.17	106,106,106,106	0
85	OHX	1	3984	7/7	0.97	0.26	102,102,102,102	0
85	OHX	5	4002	7/7	0.97	0.33	102,102,102,102	0
85	OHX	1	3887	7/7	0.97	0.14	99,99,99,99	0
85	OHX	6	2037	7/7	0.97	0.09	112,112,112,112	0
84	MG	5	3525	1/1	0.97	0.53	36,36,36,36	0
85	OHX	6	2074	7/7	0.97	0.14	106,106,106,106	0
85	OHX	6	2119	7/7	0.97	0.24	106,106,106,106	0
85	OHX	5	3977	7/7	0.97	0.42	70,70,70,70	0
85	OHX	2	2021	7/7	0.97	0.17	99,99,99,99	0
85	OHX	2	2054	7/7	0.97	0.20	122,122,122,122	0
85	OHX	5	3970	7/7	0.97	0.37	90,90,90,90	0
85	OHX	5	3954	7/7	0.97	0.25	82,82,82,82	0
84	MG	1	3537	1/1	0.97	0.34	33,33,33,33	0
85	OHX	1	3928	7/7	0.97	0.24	95,95,95,95	0
85	OHX	7	218	7/7	0.97	0.30	92,92,92,92	0
85	OHX	6	2048	7/7	0.97	0.08	117,117,117,117	0
85	OHX	7	219	7/7	0.97	0.24	80,80,80,80	0
85	OHX	1	3822	7/7	0.97	0.11	95,95,95,95	0
85	OHX	5	3956	7/7	0.97	0.35	76,76,76,76	0
85	OHX	19	202	7/7	0.97	0.23	92,92,92,92	0
84	MG	1	3578	1/1	0.97	0.27	35,35,35,35	0
85	OHX	6	2058	7/7	0.97	0.17	99,99,99,99	0
85	OHX	5	4065	7/7	0.97	0.13	92,92,92,92	0
84	MG	2	1980	1/1	0.97	0.12	58,58,58,58	0
84	MG	1	3522	1/1	0.97	0.34	32,32,32,32	0
84	MG	1	3718	1/1	0.97	0.24	78,78,78,78	0
85	OHX	1	3973	7/7	0.97	0.40	105,105,105,105	0
85	OHX	2	2095	7/7	0.97	0.36	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	OHX	5	3810	7/7	0.97	0.11	87,87,87,87	0
85	OHX	2	2017	7/7	0.97	0.15	89,89,89,89	0
85	OHX	2	2035	7/7	0.97	0.17	95,95,95,95	0
85	OHX	7	213	7/7	0.97	0.13	79,79,79,79	0
84	MG	5	3524	1/1	0.97	0.66	34,34,34,34	0
84	MG	5	3630	1/1	0.97	0.15	31,31,31,31	0
85	OHX	5	4039	7/7	0.97	0.40	105,105,105,105	0
84	MG	6	1989	1/1	0.97	0.20	74,74,74,74	0
85	OHX	6	2129	7/7	0.97	0.25	152,152,152,152	0
85	OHX	5	3896	7/7	0.97	0.21	77,77,77,77	0
86	ZN	Q2	501	1/1	0.97	0.16	64,64,64,64	0
85	OHX	5	4004	7/7	0.97	0.29	119,119,119,119	0
85	OHX	5	3904	7/7	0.97	0.20	76,76,76,76	0
85	OHX	5	4027	7/7	0.97	0.28	92,92,92,92	0
85	OHX	5	3901	7/7	0.97	0.19	110,110,110,110	0
84	MG	n3	201	1/1	0.97	0.55	28,28,28,28	0
85	OHX	8	219	7/7	0.97	0.29	90,90,90,90	0
85	OHX	2	2045	7/7	0.97	0.23	90,90,90,90	0
85	OHX	1	4020	7/7	0.97	0.39	118,118,118,118	0
85	OHX	2	2028	7/7	0.97	0.22	94,94,94,94	0
85	OHX	2	2005	7/7	0.97	0.13	94,94,94,94	0
85	OHX	1	3991	7/7	0.97	0.28	119,119,119,119	0
85	OHX	2	2053	7/7	0.97	0.09	130,130,130,130	0
85	OHX	1	3934	7/7	0.97	0.33	94,94,94,94	0
85	OHX	m7	204	7/7	0.97	0.40	84,84,84,84	0
85	OHX	1	3795	7/7	0.97	0.13	83,83,83,83	0
84	MG	1	3636	1/1	0.97	0.27	46,46,46,46	0
85	OHX	5	3957	7/7	0.97	0.28	84,84,84,84	0
85	OHX	2	2047	7/7	0.97	0.22	101,101,101,101	0
85	OHX	5	4046	7/7	0.97	0.35	75,75,75,75	0
85	OHX	5	3941	7/7	0.97	0.28	90,90,90,90	0
85	OHX	1	3881	7/7	0.97	0.29	87,87,87,87	0
85	OHX	6	2066	7/7	0.97	0.17	83,83,83,83	0
85	OHX	5	3958	7/7	0.97	0.29	98,98,98,98	0
84	MG	6	1960	1/1	0.97	0.26	45,45,45,45	0
85	OHX	2	2080	7/7	0.97	0.31	112,112,112,112	0
84	MG	2	1931	1/1	0.97	0.54	65,65,65,65	0
85	OHX	8	212	7/7	0.97	0.10	91,91,91,91	0
85	OHX	1	3899	7/7	0.97	0.32	91,91,91,91	0
85	OHX	5	4026	7/7	0.97	0.37	105,105,105,105	0
85	OHX	2	2071	7/7	0.97	0.28	127,127,127,127	0
85	OHX	5	3946	7/7	0.97	0.23	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	OHX	1	3947	7/7	0.97	0.23	85,85,85,85	0
85	OHX	2	2049	7/7	0.97	0.23	100,100,100,100	0
85	OHX	5	4045	7/7	0.97	0.37	99,99,99,99	0
85	OHX	5	3874	7/7	0.97	0.16	87,87,87,87	0
85	OHX	14	402	7/7	0.97	0.52	99,99,99,99	0
85	OHX	5	4037	7/7	0.97	0.28	89,89,89,89	0
85	OHX	1	3970	7/7	0.97	0.31	94,94,94,94	0
85	OHX	1	3988	7/7	0.97	0.32	104,104,104,104	0
85	OHX	o9	101	7/7	0.97	0.28	87,87,87,87	0
85	OHX	5	4052	7/7	0.97	0.38	94,94,94,94	0
84	MG	1	3551	1/1	0.97	0.57	37,37,37,37	0
85	OHX	1	3986	7/7	0.97	0.19	112,112,112,112	0
85	OHX	1	3812	7/7	0.97	0.12	88,88,88,88	0
85	OHX	1	3972	7/7	0.97	0.31	77,77,77,77	0
85	OHX	6	2117	7/7	0.97	0.25	86,86,86,86	0
85	OHX	5	3951	7/7	0.97	0.27	92,92,92,92	0
85	OHX	6	2147	7/7	0.97	0.37	100,100,100,100	0
85	OHX	6	2120	7/7	0.97	0.24	85,85,85,85	0
85	OHX	5	3795	7/7	0.97	0.12	104,104,104,104	0
85	OHX	5	4003	7/7	0.97	0.25	86,86,86,86	0
84	MG	1	3419	1/1	0.97	0.53	44,44,44,44	0
85	OHX	1	3865	7/7	0.97	0.21	93,93,93,93	0
85	OHX	14	401	7/7	0.97	0.26	96,96,96,96	0
85	OHX	5	3913	7/7	0.97	0.21	88,88,88,88	0
85	OHX	1	3809	7/7	0.97	0.09	107,107,107,107	0
85	OHX	1	3806	7/7	0.97	0.10	92,92,92,92	0
85	OHX	5	3960	7/7	0.97	0.32	105,105,105,105	0
85	OHX	5	3947	7/7	0.97	0.36	79,79,79,79	0
85	OHX	1	3995	7/7	0.97	0.12	86,86,86,86	0
84	MG	1	3509	1/1	0.97	0.32	33,33,33,33	0
85	OHX	1	3985	7/7	0.97	0.41	97,97,97,97	0
85	OHX	1	3837	7/7	0.97	0.19	71,71,71,71	0
85	OHX	2	2032	7/7	0.97	0.15	121,121,121,121	0
85	OHX	5	3987	7/7	0.97	0.45	81,81,81,81	0
85	OHX	1	3942	7/7	0.97	0.30	88,88,88,88	0
85	OHX	5	4048	7/7	0.97	0.28	104,104,104,104	0
84	MG	1	3495	1/1	0.97	0.46	41,41,41,41	0
85	OHX	8	218	7/7	0.97	0.29	79,79,79,79	0
85	OHX	5	3818	7/7	0.97	0.11	90,90,90,90	0
85	OHX	4	227	7/7	0.97	0.39	85,85,85,85	0
85	OHX	1	3989	7/7	0.97	0.42	104,104,104,104	0
84	MG	1	3492	1/1	0.97	0.35	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	OHX	5	4040	7/7	0.97	0.41	102,102,102,102	0
85	OHX	8	217	7/7	0.97	0.20	101,101,101,101	0
85	OHX	1	3765	7/7	0.97	0.11	79,79,79,79	0
85	OHX	6	2140	7/7	0.97	0.30	101,101,101,101	0
85	OHX	5	3873	7/7	0.97	0.20	68,68,68,68	0
85	OHX	6	2100	7/7	0.97	0.20	96,96,96,96	0
84	MG	5	3490	1/1	0.97	0.60	39,39,39,39	0
85	OHX	1	3820	7/7	0.97	0.14	87,87,87,87	0
85	OHX	5	4010	7/7	0.97	0.38	75,75,75,75	0
84	MG	1	3571	1/1	0.97	0.43	35,35,35,35	0
85	OHX	2	2014	7/7	0.97	0.20	89,89,89,89	0
85	OHX	1	3971	7/7	0.97	0.41	98,98,98,98	0
85	OHX	6	2106	7/7	0.97	0.30	96,96,96,96	0
85	OHX	5	4021	7/7	0.97	0.38	82,82,82,82	0
85	OHX	C5	201	7/7	0.97	0.21	127,127,127,127	0
84	MG	1	3683	1/1	0.97	0.36	34,34,34,34	0
85	OHX	1	4033	7/7	0.97	0.27	100,100,100,100	0
85	OHX	1	4008	7/7	0.97	0.19	82,82,82,82	0
85	OHX	5	3879	7/7	0.97	0.16	103,103,103,103	0
85	OHX	1	3979	7/7	0.97	0.36	94,94,94,94	0
85	OHX	5	3869	7/7	0.97	0.15	79,79,79,79	0
85	OHX	1	3994	7/7	0.97	0.32	92,92,92,92	0
84	MG	2	1930	1/1	0.97	0.52	58,58,58,58	0
85	OHX	1	3915	7/7	0.97	0.28	69,69,69,69	0
85	OHX	5	4041	7/7	0.97	0.44	96,96,96,96	0
85	OHX	5	3930	7/7	0.97	0.37	75,75,75,75	0
85	OHX	6	2126	7/7	0.97	0.30	96,96,96,96	0
85	OHX	5	3911	7/7	0.97	0.27	80,80,80,80	0
85	OHX	1	3933	7/7	0.97	0.17	92,92,92,92	0
85	OHX	2	1993	7/7	0.97	0.14	99,99,99,99	0
85	OHX	S8	301	7/7	0.97	0.26	124,124,124,124	0
85	OHX	6	2087	7/7	0.97	0.34	109,109,109,109	0
85	OHX	5	3993	7/7	0.97	0.32	101,101,101,101	0
84	MG	6	1944	1/1	0.97	0.60	69,69,69,69	0
85	OHX	6	2107	7/7	0.97	0.26	99,99,99,99	0
85	OHX	6	2069	7/7	0.97	0.23	86,86,86,86	0
85	OHX	1	3962	7/7	0.97	0.20	101,101,101,101	0
85	OHX	d4	201	7/7	0.97	0.28	115,115,115,115	0
84	MG	5	3519	1/1	0.97	0.54	34,34,34,34	0
84	MG	1	3591	1/1	0.97	0.15	44,44,44,44	0
84	MG	1	3534	1/1	0.97	0.72	36,36,36,36	0
85	OHX	1	3840	7/7	0.97	0.15	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	3	220	1/1	0.97	0.42	46,46,46,46	0
84	MG	1	3529	1/1	0.97	0.48	50,50,50,50	0
84	MG	5	3468	1/1	0.97	0.49	51,51,51,51	0
84	MG	6	1974	1/1	0.97	0.14	50,50,50,50	0
85	OHX	6	2113	7/7	0.97	0.35	86,86,86,86	0
85	OHX	1	3937	7/7	0.97	0.43	88,88,88,88	0
85	OHX	5	3922	7/7	0.97	0.16	97,97,97,97	0
84	MG	1	3519	1/1	0.97	0.77	38,38,38,38	0
85	OHX	6	2057	7/7	0.97	0.12	108,108,108,108	0
84	MG	5	3433	1/1	0.97	0.34	42,42,42,42	0
85	OHX	1	3996	7/7	0.97	0.31	97,97,97,97	0
85	OHX	1	3998	7/7	0.97	0.42	102,102,102,102	0
84	MG	1	3680	1/1	0.97	0.13	40,40,40,40	0
85	OHX	2	2055	7/7	0.97	0.31	111,111,111,111	0
84	MG	1	3695	1/1	0.97	0.28	40,40,40,40	0
85	OHX	5	3905	7/7	0.97	0.26	93,93,93,93	0
85	OHX	1	4019	7/7	0.97	0.36	85,85,85,85	0
85	OHX	1	3906	7/7	0.97	0.30	85,85,85,85	0
84	MG	5	3481	1/1	0.97	0.44	35,35,35,35	0
85	OHX	1	4027	7/7	0.97	0.37	103,103,103,103	0
85	OHX	5	3903	7/7	0.97	0.11	110,110,110,110	0
85	OHX	5	3992	7/7	0.97	0.39	97,97,97,97	0
84	MG	1	3717	1/1	0.97	0.16	60,60,60,60	0
84	MG	5	3436	1/1	0.97	0.23	30,30,30,30	0
85	OHX	5	4038	7/7	0.97	0.30	91,91,91,91	0
85	OHX	1	3892	7/7	0.97	0.25	95,95,95,95	0
85	OHX	2	2036	7/7	0.97	0.14	103,103,103,103	0
85	OHX	1	3780	7/7	0.97	0.09	100,100,100,100	0
84	MG	5	3430	1/1	0.97	0.19	33,33,33,33	0
85	OHX	5	3889	7/7	0.97	0.25	72,72,72,72	0
85	OHX	1	3990	7/7	0.97	0.38	99,99,99,99	0
85	OHX	1	3903	7/7	0.97	0.24	77,77,77,77	0
85	OHX	8	222	7/7	0.97	0.27	114,114,114,114	0
85	OHX	5	3926	7/7	0.97	0.18	104,104,104,104	0
85	OHX	6	2036	7/7	0.97	0.10	110,110,110,110	0
85	OHX	5	4069	7/7	0.97	0.11	129,129,129,129	0
85	OHX	6	2139	7/7	0.97	0.44	84,84,84,84	0
85	OHX	2	2062	7/7	0.97	0.32	106,106,106,106	0
84	MG	2	1977	1/1	0.97	0.27	75,75,75,75	0
85	OHX	5	3852	7/7	0.97	0.18	71,71,71,71	0
85	OHX	5	3839	7/7	0.97	0.14	84,84,84,84	0
84	MG	5	3699	1/1	0.97	0.19	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3675	1/1	0.97	0.31	41,41,41,41	0
84	MG	5	3545	1/1	0.97	0.68	30,30,30,30	0
85	OHX	2	2039	7/7	0.97	0.19	133,133,133,133	0
84	MG	1	3586	1/1	0.97	0.56	68,68,68,68	0
85	OHX	1	3940	7/7	0.97	0.40	88,88,88,88	0
85	OHX	1	4010	7/7	0.97	0.45	104,104,104,104	0
85	OHX	5	3880	7/7	0.97	0.22	91,91,91,91	0
85	OHX	1	3912	7/7	0.97	0.25	110,110,110,110	0
85	OHX	1	4021	7/7	0.97	0.31	128,128,128,128	0
85	OHX	5	3975	7/7	0.97	0.39	85,85,85,85	0
85	OHX	6	2094	7/7	0.97	0.23	96,96,96,96	0
85	OHX	SR	401	7/7	0.97	0.13	134,134,134,134	0
85	OHX	5	3846	7/7	0.98	0.22	58,58,58,58	0
85	OHX	5	3912	7/7	0.98	0.30	108,108,108,108	0
85	OHX	6	2046	7/7	0.98	0.10	95,95,95,95	0
85	OHX	1	3907	7/7	0.98	0.21	96,96,96,96	0
85	OHX	7	211	7/7	0.98	0.09	74,74,74,74	0
84	MG	5	3691	1/1	0.98	0.12	43,43,43,43	0
85	OHX	1	3773	7/7	0.98	0.08	73,73,73,73	0
85	OHX	5	3994	7/7	0.98	0.30	97,97,97,97	0
85	OHX	6	2063	7/7	0.98	0.11	134,134,134,134	0
85	OHX	1	3944	7/7	0.98	0.18	100,100,100,100	0
84	MG	1	3410	1/1	0.98	0.45	35,35,35,35	0
85	OHX	1	3784	7/7	0.98	0.10	77,77,77,77	0
84	MG	5	3504	1/1	0.98	0.45	37,37,37,37	0
85	OHX	5	3854	7/7	0.98	0.21	80,80,80,80	0
85	OHX	O7	105	7/7	0.98	0.19	76,76,76,76	0
85	OHX	5	3964	7/7	0.98	0.34	106,106,106,106	0
85	OHX	5	4012	7/7	0.98	0.27	89,89,89,89	0
85	OHX	5	4035	7/7	0.98	0.18	63,63,63,63	0
85	OHX	5	3773	7/7	0.98	0.11	64,64,64,64	0
84	MG	5	3569	1/1	0.98	0.63	29,29,29,29	0
85	OHX	5	3827	7/7	0.98	0.20	76,76,76,76	0
85	OHX	2	1989	7/7	0.98	0.08	92,92,92,92	0
84	MG	1	3451	1/1	0.98	0.37	47,47,47,47	0
84	MG	5	4074	1/1	0.98	0.41	32,32,32,32	0
85	OHX	1	3870	7/7	0.98	0.22	97,97,97,97	0
85	OHX	1	3925	7/7	0.98	0.10	116,116,116,116	0
85	OHX	1	3965	7/7	0.98	0.20	109,109,109,109	0
85	OHX	2	2051	7/7	0.98	0.32	93,93,93,93	0
84	MG	2	1944	1/1	0.98	0.57	91,91,91,91	0
85	OHX	5	3883	7/7	0.98	0.19	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	OHX	5	3796	7/7	0.98	0.09	89,89,89,89	0
85	OHX	1	3836	7/7	0.98	0.21	83,83,83,83	0
85	OHX	6	2033	7/7	0.98	0.13	74,74,74,74	0
85	OHX	1	3814	7/7	0.98	0.14	71,71,71,71	0
85	OHX	1	3791	7/7	0.98	0.11	73,73,73,73	0
85	OHX	1	3833	7/7	0.98	0.20	78,78,78,78	0
86	ZN	D9	101	1/1	0.98	0.12	79,79,79,79	0
84	MG	1	3625	1/1	0.98	0.40	63,63,63,63	0
85	OHX	1	3792	7/7	0.98	0.11	80,80,80,80	0
85	OHX	5	3836	7/7	0.98	0.15	81,81,81,81	0
85	OHX	1	3868	7/7	0.98	0.23	83,83,83,83	0
85	OHX	5	3952	7/7	0.98	0.33	77,77,77,77	0
85	OHX	2	1988	7/7	0.98	0.17	90,90,90,90	0
85	OHX	3	213	7/7	0.98	0.18	97,97,97,97	0
85	OHX	5	3866	7/7	0.98	0.19	87,87,87,87	0
85	OHX	6	2049	7/7	0.98	0.14	85,85,85,85	0
85	OHX	5	3857	7/7	0.98	0.20	71,71,71,71	0
85	OHX	2	2007	7/7	0.98	0.14	94,94,94,94	0
85	OHX	2	2030	7/7	0.98	0.20	103,103,103,103	0
85	OHX	5	3787	7/7	0.98	0.10	63,63,63,63	0
85	OHX	2	1998	7/7	0.98	0.10	89,89,89,89	0
85	OHX	1	3999	7/7	0.98	0.25	82,82,82,82	0
85	OHX	6	2064	7/7	0.98	0.07	141,141,141,141	0
85	OHX	5	3942	7/7	0.98	0.25	98,98,98,98	0
85	OHX	5	3891	7/7	0.98	0.22	84,84,84,84	0
85	OHX	4	222	7/7	0.98	0.26	83,83,83,83	0
84	MG	5	3539	1/1	0.98	0.42	29,29,29,29	0
84	MG	1	3463	1/1	0.98	0.47	32,32,32,32	0
84	MG	1	3505	1/1	0.98	0.29	38,38,38,38	0
85	OHX	1	3789	7/7	0.98	0.10	88,88,88,88	0
85	OHX	6	2086	7/7	0.98	0.32	103,103,103,103	0
85	OHX	6	2061	7/7	0.98	0.18	98,98,98,98	0
85	OHX	1	3959	7/7	0.98	0.28	84,84,84,84	0
85	OHX	5	4060	7/7	0.98	0.30	125,125,125,125	0
85	OHX	1	4011	7/7	0.98	0.32	100,100,100,100	0
85	OHX	5	3933	7/7	0.98	0.30	77,77,77,77	0
85	OHX	6	2122	7/7	0.98	0.37	92,92,92,92	0
85	OHX	6	2075	7/7	0.98	0.24	96,96,96,96	0
85	OHX	5	3876	7/7	0.98	0.29	76,76,76,76	0
85	OHX	1	3927	7/7	0.98	0.29	92,92,92,92	0
85	OHX	5	3807	7/7	0.98	0.10	74,74,74,74	0
85	OHX	1	3831	7/7	0.98	0.18	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	6	1991	1/1	0.98	0.15	50,50,50,50	0
85	OHX	5	4022	7/7	0.98	0.38	94,94,94,94	0
85	OHX	2	2048	7/7	0.98	0.24	87,87,87,87	0
85	OHX	1	3829	7/7	0.98	0.15	82,82,82,82	0
85	OHX	6	2059	7/7	0.98	0.10	106,106,106,106	0
85	OHX	2	2023	7/7	0.98	0.22	90,90,90,90	0
85	OHX	5	3837	7/7	0.98	0.26	72,72,72,72	0
84	MG	5	3497	1/1	0.98	0.56	30,30,30,30	0
85	OHX	1	3952	7/7	0.98	0.23	111,111,111,111	0
85	OHX	5	3775	7/7	0.98	0.11	60,60,60,60	0
85	OHX	6	2065	7/7	0.98	0.11	94,94,94,94	0
85	OHX	6	2017	7/7	0.98	0.09	85,85,85,85	0
85	OHX	6	2029	7/7	0.98	0.08	110,110,110,110	0
85	OHX	1	3844	7/7	0.98	0.19	71,71,71,71	0
85	OHX	2	2024	7/7	0.98	0.20	89,89,89,89	0
85	OHX	6	2041	7/7	0.98	0.12	74,74,74,74	0
85	OHX	5	3931	7/7	0.98	0.18	68,68,68,68	0
85	OHX	2	1985	7/7	0.98	0.16	84,84,84,84	0
85	OHX	4	224	7/7	0.98	0.27	82,82,82,82	0
84	MG	2	1917	1/1	0.98	0.52	62,62,62,62	0
85	OHX	5	3900	7/7	0.98	0.24	103,103,103,103	0
85	OHX	5	3855	7/7	0.98	0.23	83,83,83,83	0
85	OHX	2	2087	7/7	0.98	0.26	119,119,119,119	0
85	OHX	1	3804	7/7	0.98	0.10	88,88,88,88	0
85	OHX	5	3845	7/7	0.98	0.11	87,87,87,87	0
85	OHX	1	3961	7/7	0.98	0.23	104,104,104,104	0
85	OHX	1	3968	7/7	0.98	0.28	86,86,86,86	0
85	OHX	6	2104	7/7	0.98	0.30	103,103,103,103	0
85	OHX	6	2090	7/7	0.98	0.23	115,115,115,115	0
84	MG	5	3561	1/1	0.98	0.93	48,48,48,48	0
85	OHX	6	2055	7/7	0.98	0.10	95,95,95,95	0
85	OHX	1	3880	7/7	0.98	0.23	89,89,89,89	0
85	OHX	O3	202	7/7	0.98	0.33	85,85,85,85	0
85	OHX	5	3840	7/7	0.98	0.20	73,73,73,73	0
85	OHX	1	3922	7/7	0.98	0.43	92,92,92,92	0
85	OHX	6	2134	7/7	0.98	0.29	112,112,112,112	0
85	OHX	2	2041	7/7	0.98	0.10	119,119,119,119	0
84	MG	1	3716	1/1	0.98	0.10	33,33,33,33	0
85	OHX	2	2081	7/7	0.98	0.28	109,109,109,109	0
85	OHX	3	210	7/7	0.98	0.09	77,77,77,77	0
85	OHX	M7	205	7/7	0.98	0.30	101,101,101,101	0
85	OHX	1	3954	7/7	0.98	0.37	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3628	1/1	0.98	0.72	50,50,50,50	0
85	OHX	6	2125	7/7	0.98	0.27	87,87,87,87	0
85	OHX	3	214	7/7	0.98	0.18	95,95,95,95	0
84	MG	8	208	1/1	0.98	0.10	63,63,63,63	0
85	OHX	2	2013	7/7	0.98	0.21	105,105,105,105	0
84	MG	1	3540	1/1	0.98	0.45	35,35,35,35	0
85	OHX	5	3923	7/7	0.98	0.20	85,85,85,85	0
86	ZN	q0	201	1/1	0.98	0.10	36,36,36,36	0
85	OHX	1	4022	7/7	0.98	0.41	77,77,77,77	0
85	OHX	1	4026	7/7	0.98	0.39	90,90,90,90	0
85	OHX	2	2037	7/7	0.98	0.22	106,106,106,106	0
85	OHX	1	4004	7/7	0.98	0.35	85,85,85,85	0
85	OHX	1	3975	7/7	0.98	0.34	85,85,85,85	0
85	OHX	5	3859	7/7	0.98	0.17	81,81,81,81	0
85	OHX	1	4025	7/7	0.98	0.44	101,101,101,101	0
85	OHX	5	3856	7/7	0.98	0.07	120,120,120,120	0
85	OHX	1	3866	7/7	0.98	0.26	91,91,91,91	0
85	OHX	5	3907	7/7	0.98	0.17	116,116,116,116	0
85	OHX	1	3867	7/7	0.98	0.20	75,75,75,75	0
85	OHX	1	3896	7/7	0.98	0.22	88,88,88,88	0
85	OHX	5	3924	7/7	0.98	0.28	77,77,77,77	0
85	OHX	5	3784	7/7	0.98	0.12	70,70,70,70	0
85	OHX	6	2083	7/7	0.98	0.19	116,116,116,116	0
85	OHX	5	4049	7/7	0.98	0.33	85,85,85,85	0
85	OHX	2	2016	7/7	0.98	0.20	108,108,108,108	0
85	OHX	1	3781	7/7	0.98	0.12	78,78,78,78	0
85	OHX	5	3800	7/7	0.98	0.09	78,78,78,78	0
84	MG	5	3557	1/1	0.98	0.68	42,42,42,42	0
85	OHX	1	3819	7/7	0.98	0.09	90,90,90,90	0
85	OHX	5	3934	7/7	0.98	0.26	91,91,91,91	0
84	MG	6	1983	1/1	0.98	0.19	73,73,73,73	0
85	OHX	1	3980	7/7	0.98	0.37	83,83,83,83	0
85	OHX	5	3979	7/7	0.98	0.28	85,85,85,85	0
85	OHX	5	3991	7/7	0.98	0.23	87,87,87,87	0
85	OHX	7	217	7/7	0.98	0.15	95,95,95,95	0
85	OHX	5	3831	7/7	0.98	0.11	77,77,77,77	0
85	OHX	1	3834	7/7	0.98	0.09	99,99,99,99	0
85	OHX	6	2102	7/7	0.98	0.27	104,104,104,104	0
85	OHX	5	3788	7/7	0.98	0.08	78,78,78,78	0
85	OHX	2	2002	7/7	0.98	0.08	84,84,84,84	0
85	OHX	1	3847	7/7	0.98	0.21	91,91,91,91	0
85	OHX	1	3764	7/7	0.98	0.15	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	OHX	5	3890	7/7	0.98	0.20	97,97,97,97	0
85	OHX	8	220	7/7	0.98	0.17	120,120,120,120	0
85	OHX	1	3771	7/7	0.98	0.09	76,76,76,76	0
85	OHX	C8	201	7/7	0.98	0.08	97,97,97,97	0
85	OHX	5	3925	7/7	0.98	0.22	81,81,81,81	0
84	MG	1	3550	1/1	0.98	0.26	40,40,40,40	0
85	OHX	1	3939	7/7	0.98	0.32	94,94,94,94	0
85	OHX	6	2097	7/7	0.98	0.19	103,103,103,103	0
85	OHX	5	3821	7/7	0.98	0.10	74,74,74,74	0
85	OHX	5	3875	7/7	0.98	0.10	112,112,112,112	0
84	MG	1	3558	1/1	0.98	0.32	45,45,45,45	0
85	OHX	1	3911	7/7	0.98	0.23	103,103,103,103	0
85	OHX	1	3891	7/7	0.98	0.22	81,81,81,81	0
85	OHX	8	225	7/7	0.98	0.37	101,101,101,101	0
85	OHX	5	3809	7/7	0.98	0.13	88,88,88,88	0
84	MG	1	3513	1/1	0.98	0.95	38,38,38,38	0
85	OHX	1	3751	7/7	0.98	0.13	67,67,67,67	0
85	OHX	5	4013	7/7	0.98	0.41	96,96,96,96	0
85	OHX	1	3776	7/7	0.98	0.13	69,69,69,69	0
85	OHX	6	2042	7/7	0.98	0.13	100,100,100,100	0
85	OHX	4	219	7/7	0.98	0.10	93,93,93,93	0
85	OHX	1	3757	7/7	0.98	0.11	70,70,70,70	0
84	MG	1	3579	1/1	0.98	0.42	40,40,40,40	0
85	OHX	5	3981	7/7	0.98	0.28	97,97,97,97	0
84	MG	5	3523	1/1	0.98	0.33	27,27,27,27	0
85	OHX	1	3783	7/7	0.98	0.11	70,70,70,70	0
85	OHX	2	1990	7/7	0.98	0.09	95,95,95,95	0
85	OHX	1	3846	7/7	0.98	0.19	97,97,97,97	0
85	OHX	6	2138	7/7	0.98	0.27	77,77,77,77	0
85	OHX	1	3756	7/7	0.98	0.12	68,68,68,68	0
85	OHX	1	3849	7/7	0.98	0.20	80,80,80,80	0
84	MG	5	3554	1/1	0.98	0.42	29,29,29,29	0
85	OHX	q2	502	7/7	0.98	0.16	61,61,61,61	0
85	OHX	4	218	7/7	0.98	0.18	77,77,77,77	0
85	OHX	1	3857	7/7	0.98	0.21	79,79,79,79	0
85	OHX	M5	302	7/7	0.98	0.22	88,88,88,88	0
85	OHX	2	2064	7/7	0.98	0.20	92,92,92,92	0
85	OHX	5	3902	7/7	0.98	0.27	87,87,87,87	0
84	MG	6	1905	1/1	0.98	0.83	61,61,61,61	0
84	MG	5	3579	1/1	0.98	0.55	32,32,32,32	0
85	OHX	6	2071	7/7	0.98	0.17	79,79,79,79	0
85	OHX	6	2051	7/7	0.98	0.12	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	OHX	2	1995	7/7	0.98	0.09	91,91,91,91	0
85	OHX	7	212	7/7	0.98	0.14	70,70,70,70	0
85	OHX	8	213	7/7	0.98	0.18	83,83,83,83	0
85	OHX	1	3882	7/7	0.98	0.19	90,90,90,90	0
85	OHX	6	2060	7/7	0.98	0.12	138,138,138,138	0
85	OHX	1	3853	7/7	0.98	0.14	93,93,93,93	0
85	OHX	2	2050	7/7	0.98	0.36	102,102,102,102	0
85	OHX	5	3804	7/7	0.98	0.11	63,63,63,63	0
85	OHX	2	2042	7/7	0.98	0.15	110,110,110,110	0
85	OHX	6	2070	7/7	0.98	0.28	98,98,98,98	0
85	OHX	7	214	7/7	0.98	0.15	71,71,71,71	0
85	OHX	1	3859	7/7	0.98	0.16	119,119,119,119	0
85	OHX	4	226	7/7	0.98	0.22	106,106,106,106	0
85	OHX	1	3816	7/7	0.98	0.12	84,84,84,84	0
84	MG	6	1925	1/1	0.98	0.38	72,72,72,72	0
85	OHX	3	217	7/7	0.98	0.31	85,85,85,85	0
85	OHX	1	3755	7/7	0.98	0.12	67,67,67,67	0
85	OHX	2	2072	7/7	0.98	0.29	106,106,106,106	0
85	OHX	5	4015	7/7	0.98	0.29	98,98,98,98	0
85	OHX	2	2056	7/7	0.98	0.09	127,127,127,127	0
85	OHX	1	3860	7/7	0.98	0.27	82,82,82,82	0
85	OHX	c8	201	7/7	0.98	0.15	117,117,117,117	0
85	OHX	5	3853	7/7	0.98	0.10	83,83,83,83	0
85	OHX	5	3928	7/7	0.98	0.22	91,91,91,91	0
84	MG	5	3683	1/1	0.98	0.11	46,46,46,46	0
85	OHX	1	3852	7/7	0.98	0.14	110,110,110,110	0
84	MG	1	3453	1/1	0.98	0.39	33,33,33,33	0
85	OHX	5	3816	7/7	0.98	0.13	66,66,66,66	0
85	OHX	5	3971	7/7	0.98	0.23	94,94,94,94	0
85	OHX	5	3872	7/7	0.98	0.18	65,65,65,65	0
85	OHX	2	2074	7/7	0.98	0.24	101,101,101,101	0
85	OHX	6	2028	7/7	0.98	0.09	89,89,89,89	0
85	OHX	1	3843	7/7	0.98	0.23	79,79,79,79	0
85	OHX	6	2096	7/7	0.98	0.21	100,100,100,100	0
84	MG	5	3568	1/1	0.98	0.56	35,35,35,35	0
85	OHX	1	3886	7/7	0.98	0.22	101,101,101,101	0
85	OHX	5	3916	7/7	0.98	0.32	85,85,85,85	0
85	OHX	o7	502	7/7	0.98	0.13	79,79,79,79	0
85	OHX	5	3887	7/7	0.98	0.23	72,72,72,72	0
84	MG	7	203	1/1	0.98	0.38	58,58,58,58	0
85	OHX	5	3948	7/7	0.98	0.31	92,92,92,92	0
85	OHX	6	2085	7/7	0.98	0.24	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	OHX	5	3917	7/7	0.98	0.23	86,86,86,86	0
85	OHX	2	2029	7/7	0.98	0.12	108,108,108,108	0
85	OHX	5	3939	7/7	0.98	0.26	83,83,83,83	0
84	MG	1	3686	1/1	0.98	0.11	37,37,37,37	0
85	OHX	1	3872	7/7	0.98	0.18	98,98,98,98	0
85	OHX	5	3962	7/7	0.98	0.23	111,111,111,111	0
84	MG	5	3510	1/1	0.98	0.56	36,36,36,36	0
85	OHX	O7	104	7/7	0.98	0.09	77,77,77,77	0
85	OHX	n3	203	7/7	0.98	0.21	76,76,76,76	0
85	OHX	2	2022	7/7	0.98	0.12	107,107,107,107	0
85	OHX	1	3827	7/7	0.98	0.20	72,72,72,72	0
85	OHX	2	1999	7/7	0.98	0.10	84,84,84,84	0
85	OHX	1	3902	7/7	0.98	0.26	88,88,88,88	0
85	OHX	5	3885	7/7	0.98	0.26	92,92,92,92	0
85	OHX	5	3893	7/7	0.98	0.15	111,111,111,111	0
85	OHX	5	3915	7/7	0.98	0.25	91,91,91,91	0
85	OHX	m5	305	7/7	0.98	0.18	94,94,94,94	0
85	OHX	1	3926	7/7	0.98	0.31	81,81,81,81	0
85	OHX	5	4006	7/7	0.98	0.37	89,89,89,89	0
85	OHX	1	3895	7/7	0.98	0.22	70,70,70,70	0
85	OHX	5	3820	7/7	0.98	0.12	81,81,81,81	0
85	OHX	1	3777	7/7	0.98	0.07	84,84,84,84	0
85	OHX	5	3806	7/7	0.98	0.08	74,74,74,74	0
84	MG	7	208	1/1	0.98	0.58	43,43,43,43	0
85	OHX	1	3805	7/7	0.98	0.10	72,72,72,72	0
84	MG	1	3555	1/1	0.98	0.16	35,35,35,35	0
85	OHX	L3	403	7/7	0.98	0.22	86,86,86,86	0
84	MG	6	1935	1/1	0.98	0.47	44,44,44,44	0
85	OHX	5	3974	7/7	0.98	0.36	89,89,89,89	0
85	OHX	2	2083	7/7	0.98	0.30	115,115,115,115	0
84	MG	1	3454	1/1	0.98	0.39	34,34,34,34	0
85	OHX	1	3817	7/7	0.98	0.16	75,75,75,75	0
85	OHX	5	3899	7/7	0.98	0.25	80,80,80,80	0
85	OHX	1	4001	7/7	0.98	0.25	108,108,108,108	0
85	OHX	6	2053	7/7	0.98	0.15	84,84,84,84	0
85	OHX	5	3918	7/7	0.98	0.33	84,84,84,84	0
85	OHX	5	3894	7/7	0.98	0.40	80,80,80,80	0
85	OHX	2	2033	7/7	0.98	0.27	94,94,94,94	0
85	OHX	1	3956	7/7	0.98	0.36	100,100,100,100	0
85	OHX	1	3863	7/7	0.98	0.16	95,95,95,95	0
85	OHX	1	3842	7/7	0.98	0.14	96,96,96,96	0
85	OHX	5	4036	7/7	0.98	0.22	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	OHX	1	3875	7/7	0.98	0.21	100,100,100,100	0
85	OHX	1	3963	7/7	0.98	0.26	88,88,88,88	0
85	OHX	1	3900	7/7	0.98	0.25	83,83,83,83	0
85	OHX	6	2072	7/7	0.98	0.23	92,92,92,92	0
85	OHX	5	3834	7/7	0.98	0.14	79,79,79,79	0
85	OHX	5	3823	7/7	0.98	0.13	76,76,76,76	0
85	OHX	6	2056	7/7	0.98	0.13	82,82,82,82	0
85	OHX	6	2114	7/7	0.98	0.26	114,114,114,114	0
85	OHX	5	3803	7/7	0.98	0.10	63,63,63,63	0
85	OHX	5	3770	7/7	0.98	0.13	63,63,63,63	0
85	OHX	m5	304	7/7	0.98	0.11	74,74,74,74	0
85	OHX	5	4025	7/7	0.98	0.37	93,93,93,93	0
84	MG	5	3706	1/1	0.98	0.23	37,37,37,37	0
85	OHX	6	2092	7/7	0.98	0.17	96,96,96,96	0
85	OHX	1	3901	7/7	0.98	0.19	106,106,106,106	0
85	OHX	2	2066	7/7	0.98	0.20	93,93,93,93	0
85	OHX	2	2079	7/7	0.98	0.23	115,115,115,115	0
85	OHX	2	2061	7/7	0.98	0.25	115,115,115,115	0
85	OHX	2	2020	7/7	0.98	0.09	103,103,103,103	0
85	OHX	1	3797	7/7	0.98	0.10	76,76,76,76	0
85	OHX	5	3985	7/7	0.98	0.39	97,97,97,97	0
85	OHX	6	2047	7/7	0.98	0.12	91,91,91,91	0
84	MG	6	1939	1/1	0.98	0.31	56,56,56,56	0
85	OHX	3	212	7/7	0.98	0.11	81,81,81,81	0
85	OHX	5	3936	7/7	0.98	0.23	98,98,98,98	0
85	OHX	2	2044	7/7	0.98	0.22	113,113,113,113	0
85	OHX	6	2032	7/7	0.98	0.09	87,87,87,87	0
85	OHX	1	3845	7/7	0.98	0.25	77,77,77,77	0
85	OHX	5	3910	7/7	0.98	0.12	95,95,95,95	0
85	OHX	1	3924	7/7	0.98	0.26	76,76,76,76	0
85	OHX	8	216	7/7	0.98	0.31	86,86,86,86	0
84	MG	5	3556	1/1	0.98	0.41	36,36,36,36	0
84	MG	5	3528	1/1	0.98	0.26	36,36,36,36	0
85	OHX	5	3908	7/7	0.98	0.23	84,84,84,84	0
85	OHX	5	3817	7/7	0.98	0.12	67,67,67,67	0
85	OHX	2	2009	7/7	0.98	0.15	95,95,95,95	0
85	OHX	2	2046	7/7	0.98	0.16	105,105,105,105	0
85	OHX	1	3894	7/7	0.98	0.14	114,114,114,114	0
84	MG	1	3557	1/1	0.98	0.70	37,37,37,37	0
85	OHX	5	3927	7/7	0.98	0.23	87,87,87,87	0
85	OHX	1	3913	7/7	0.98	0.27	70,70,70,70	0
85	OHX	5	3799	7/7	0.98	0.16	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	5	3546	1/1	0.98	0.67	39,39,39,39	0
84	MG	1	3499	1/1	0.98	0.47	39,39,39,39	0
85	OHX	6	2043	7/7	0.98	0.19	77,77,77,77	0
84	MG	5	3552	1/1	0.98	0.57	36,36,36,36	0
85	OHX	6	2039	7/7	0.98	0.11	83,83,83,83	0
86	ZN	Q3	501	1/1	0.98	0.06	58,58,58,58	0
85	OHX	2	2065	7/7	0.98	0.21	104,104,104,104	0
84	MG	5	3565	1/1	0.98	0.54	49,49,49,49	0
85	OHX	5	3877	7/7	0.98	0.19	80,80,80,80	0
85	OHX	4	220	7/7	0.98	0.17	96,96,96,96	0
85	OHX	8	214	7/7	0.98	0.13	102,102,102,102	0
85	OHX	5	3867	7/7	0.98	0.21	85,85,85,85	0
85	OHX	6	2067	7/7	0.98	0.16	98,98,98,98	0
85	OHX	2	2088	7/7	0.98	0.19	94,94,94,94	0
85	OHX	1	3790	7/7	0.99	0.11	72,72,72,72	0
85	OHX	1	3779	7/7	0.99	0.08	71,71,71,71	0
85	OHX	2	2011	7/7	0.99	0.16	98,98,98,98	0
85	OHX	2	1992	7/7	0.99	0.10	89,89,89,89	0
85	OHX	1	3739	7/7	0.99	0.07	62,62,62,62	0
85	OHX	6	2044	7/7	0.99	0.11	81,81,81,81	0
85	OHX	2	2031	7/7	0.99	0.18	95,95,95,95	0
85	OHX	1	3753	7/7	0.99	0.09	67,67,67,67	0
85	OHX	4	216	7/7	0.99	0.09	58,58,58,58	0
85	OHX	5	4066	7/7	0.99	0.43	114,114,114,114	0
85	OHX	1	3908	7/7	0.99	0.18	103,103,103,103	0
85	OHX	1	3878	7/7	0.99	0.21	88,88,88,88	0
85	OHX	5	3829	7/7	0.99	0.12	68,68,68,68	0
86	ZN	q3	501	1/1	0.99	0.10	57,57,57,57	0
85	OHX	5	3777	7/7	0.99	0.07	59,59,59,59	0
85	OHX	n3	202	7/7	0.99	0.08	72,72,72,72	0
85	OHX	1	3830	7/7	0.99	0.11	86,86,86,86	0
85	OHX	1	3871	7/7	0.99	0.22	100,100,100,100	0
85	OHX	5	3920	7/7	0.99	0.12	73,73,73,73	0
85	OHX	5	3765	7/7	0.99	0.10	59,59,59,59	0
84	MG	6	1914	1/1	0.99	0.46	41,41,41,41	0
85	OHX	5	3965	7/7	0.99	0.29	88,88,88,88	0
85	OHX	1	3731	7/7	0.99	0.11	50,50,50,50	0
85	OHX	5	3762	7/7	0.99	0.10	63,63,63,63	0
85	OHX	6	2022	7/7	0.99	0.09	87,87,87,87	0
85	OHX	5	3749	7/7	0.99	0.13	52,52,52,52	0
85	OHX	1	3774	7/7	0.99	0.06	74,74,74,74	0
86	ZN	O7	101	1/1	0.99	0.07	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	OHX	1	3841	7/7	0.99	0.17	62,62,62,62	0
85	OHX	6	2016	7/7	0.99	0.14	71,71,71,71	0
85	OHX	1	3742	7/7	0.99	0.11	65,65,65,65	0
85	OHX	6	2026	7/7	0.99	0.07	71,71,71,71	0
85	OHX	6	2019	7/7	0.99	0.13	77,77,77,77	0
85	OHX	1	3838	7/7	0.99	0.25	68,68,68,68	0
85	OHX	1	4009	7/7	0.99	0.20	83,83,83,83	0
85	OHX	1	3749	7/7	0.99	0.11	67,67,67,67	0
85	OHX	8	211	7/7	0.99	0.08	55,55,55,55	0
85	OHX	N1	201	7/7	0.99	0.08	59,59,59,59	0
85	OHX	5	3793	7/7	0.99	0.07	87,87,87,87	0
85	OHX	5	3848	7/7	0.99	0.20	80,80,80,80	0
85	OHX	1	3768	7/7	0.99	0.06	83,83,83,83	0
85	OHX	1	3767	7/7	0.99	0.12	69,69,69,69	0
85	OHX	1	3883	7/7	0.99	0.19	106,106,106,106	0
85	OHX	5	3778	7/7	0.99	0.06	64,64,64,64	0
85	OHX	5	3898	7/7	0.99	0.17	80,80,80,80	0
85	OHX	5	3999	7/7	0.99	0.28	76,76,76,76	0
85	OHX	5	3863	7/7	0.99	0.22	86,86,86,86	0
85	OHX	6	2031	7/7	0.99	0.13	76,76,76,76	0
85	OHX	6	2099	7/7	0.99	0.30	95,95,95,95	0
85	OHX	6	2011	7/7	0.99	0.09	61,61,61,61	0
85	OHX	5	3797	7/7	0.99	0.13	57,57,57,57	0
85	OHX	1	3762	7/7	0.99	0.07	66,66,66,66	0
85	OHX	5	3822	7/7	0.99	0.17	64,64,64,64	0
85	OHX	5	3767	7/7	0.99	0.11	63,63,63,63	0
85	OHX	6	2012	7/7	0.99	0.10	67,67,67,67	0
85	OHX	5	3881	7/7	0.99	0.11	106,106,106,106	0
85	OHX	5	3742	7/7	0.99	0.18	46,46,46,46	0
85	OHX	2	1986	7/7	0.99	0.10	81,81,81,81	0
85	OHX	1	3733	7/7	0.99	0.10	47,47,47,47	0
85	OHX	2	2001	7/7	0.99	0.09	83,83,83,83	0
85	OHX	5	4011	7/7	0.99	0.20	63,63,63,63	0
85	OHX	1	3734	7/7	0.99	0.09	56,56,56,56	0
85	OHX	6	2045	7/7	0.99	0.10	87,87,87,87	0
85	OHX	5	3779	7/7	0.99	0.06	65,65,65,65	0
85	OHX	5	3747	7/7	0.99	0.12	53,53,53,53	0
85	OHX	5	3813	7/7	0.99	0.09	81,81,81,81	0
85	OHX	2	1984	7/7	0.99	0.11	78,78,78,78	0
85	OHX	2	1994	7/7	0.99	0.11	99,99,99,99	0
84	MG	5	3547	1/1	0.99	0.53	33,33,33,33	0
85	OHX	5	3792	7/7	0.99	0.06	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	OHX	5	3838	7/7	0.99	0.15	101,101,101,101	0
85	OHX	5	3865	7/7	0.99	0.11	87,87,87,87	0
85	OHX	5	3830	7/7	0.99	0.14	64,64,64,64	0
85	OHX	1	3824	7/7	0.99	0.09	56,56,56,56	0
85	OHX	1	3758	7/7	0.99	0.05	67,67,67,67	0
85	OHX	5	3811	7/7	0.99	0.11	73,73,73,73	0
85	OHX	5	3794	7/7	0.99	0.08	69,69,69,69	0
85	OHX	5	3746	7/7	0.99	0.16	54,54,54,54	0
85	OHX	1	3746	7/7	0.99	0.10	65,65,65,65	0
85	OHX	1	3832	7/7	0.99	0.19	75,75,75,75	0
85	OHX	5	3921	7/7	0.99	0.24	95,95,95,95	0
85	OHX	1	3815	7/7	0.99	0.14	71,71,71,71	0
85	OHX	6	2023	7/7	0.99	0.06	71,71,71,71	0
85	OHX	6	2021	7/7	0.99	0.09	74,74,74,74	0
85	OHX	6	2035	7/7	0.99	0.19	71,71,71,71	0
85	OHX	5	3835	7/7	0.99	0.13	73,73,73,73	0
85	OHX	6	2030	7/7	0.99	0.19	74,74,74,74	0
85	OHX	5	3748	7/7	0.99	0.10	55,55,55,55	0
85	OHX	1	4005	7/7	0.99	0.25	95,95,95,95	0
85	OHX	5	3798	7/7	0.99	0.08	80,80,80,80	0
85	OHX	1	3839	7/7	0.99	0.18	80,80,80,80	0
85	OHX	5	3832	7/7	0.99	0.12	103,103,103,103	0
85	OHX	5	3929	7/7	0.99	0.18	76,76,76,76	0
85	OHX	6	2013	7/7	0.99	0.12	70,70,70,70	0
85	OHX	6	2020	7/7	0.99	0.09	69,69,69,69	0
85	OHX	1	3850	7/7	0.99	0.24	83,83,83,83	0
85	OHX	5	3814	7/7	0.99	0.07	84,84,84,84	0
85	OHX	4	217	7/7	0.99	0.08	68,68,68,68	0
85	OHX	1	3948	7/7	0.99	0.18	70,70,70,70	0
85	OHX	1	3772	7/7	0.99	0.06	74,74,74,74	0
85	OHX	2	2019	7/7	0.99	0.18	87,87,87,87	0
85	OHX	1	3951	7/7	0.99	0.29	81,81,81,81	0
85	OHX	5	3755	7/7	0.99	0.09	50,50,50,50	0
85	OHX	5	3949	7/7	0.99	0.18	63,63,63,63	0
85	OHX	1	3848	7/7	0.99	0.15	90,90,90,90	0
85	OHX	5	3833	7/7	0.99	0.07	61,61,61,61	0
85	OHX	5	3782	7/7	0.99	0.10	76,76,76,76	0
85	OHX	1	3766	7/7	0.99	0.08	76,76,76,76	0
85	OHX	6	2024	7/7	0.99	0.07	71,71,71,71	0
84	MG	6	1931	1/1	0.99	0.29	48,48,48,48	0
84	MG	1	3464	1/1	0.99	0.28	36,36,36,36	0
85	OHX	1	3735	7/7	0.99	0.11	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	OHX	1	3787	7/7	0.99	0.07	73,73,73,73	0
85	OHX	1	3763	7/7	0.99	0.09	68,68,68,68	0
85	OHX	5	3844	7/7	0.99	0.12	70,70,70,70	0
85	OHX	1	3732	7/7	0.99	0.13	57,57,57,57	0
85	OHX	5	3780	7/7	0.99	0.05	59,59,59,59	0
85	OHX	5	3825	7/7	0.99	0.12	68,68,68,68	0
85	OHX	5	3759	7/7	0.99	0.08	62,62,62,62	0
85	OHX	1	3738	7/7	0.99	0.08	56,56,56,56	0
85	OHX	1	3782	7/7	0.99	0.07	77,77,77,77	0
85	OHX	1	3854	7/7	0.99	0.17	74,74,74,74	0
85	OHX	1	3748	7/7	0.99	0.10	72,72,72,72	0
85	OHX	5	3750	7/7	0.99	0.11	54,54,54,54	0
85	OHX	1	3769	7/7	0.99	0.07	63,63,63,63	0
84	MG	5	3567	1/1	0.99	0.49	30,30,30,30	0
85	OHX	l3	406	7/7	0.99	0.14	79,79,79,79	0
85	OHX	2	2006	7/7	0.99	0.12	113,113,113,113	0
85	OHX	5	3751	7/7	0.99	0.12	52,52,52,52	0
85	OHX	1	3861	7/7	0.99	0.14	67,67,67,67	0
85	OHX	5	3783	7/7	0.99	0.06	77,77,77,77	0
85	OHX	1	3740	7/7	0.99	0.13	60,60,60,60	0
85	OHX	7	216	7/7	0.99	0.13	87,87,87,87	0
84	MG	1	3553	1/1	0.99	0.51	30,30,30,30	0
85	OHX	2	1987	7/7	0.99	0.10	74,74,74,74	0
84	MG	5	3577	1/1	0.99	0.50	45,45,45,45	0
85	OHX	Q2	503	7/7	0.99	0.20	59,59,59,59	0
84	MG	1	3481	1/1	0.99	0.21	45,45,45,45	0
84	MG	1	3535	1/1	0.99	0.37	43,43,43,43	0
85	OHX	5	3764	7/7	0.99	0.06	57,57,57,57	0
85	OHX	5	3776	7/7	0.99	0.10	86,86,86,86	0
85	OHX	5	3888	7/7	0.99	0.26	91,91,91,91	0
85	OHX	5	3761	7/7	0.99	0.08	55,55,55,55	0
85	OHX	1	3876	7/7	0.99	0.23	86,86,86,86	0
85	OHX	1	3775	7/7	0.99	0.10	83,83,83,83	0
85	OHX	1	3760	7/7	0.99	0.09	68,68,68,68	0
85	OHX	1	3885	7/7	0.99	0.22	78,78,78,78	0
85	OHX	n9	102	7/7	0.99	0.14	59,59,59,59	0
85	OHX	L3	402	7/7	0.99	0.27	86,86,86,86	0
85	OHX	5	3842	7/7	0.99	0.10	91,91,91,91	0
85	OHX	6	2052	7/7	0.99	0.09	110,110,110,110	0
85	OHX	5	3768	7/7	0.99	0.06	58,58,58,58	0
85	OHX	5	3851	7/7	0.99	0.08	52,52,52,52	0
85	OHX	1	3786	7/7	0.99	0.08	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	OHX	1	3904	7/7	0.99	0.16	82,82,82,82	0
85	OHX	4	215	7/7	0.99	0.10	54,54,54,54	0
85	OHX	1	3821	7/7	0.99	0.15	77,77,77,77	0
85	OHX	2	2038	7/7	0.99	0.24	93,93,93,93	0
85	OHX	3	211	7/7	0.99	0.20	85,85,85,85	0
85	OHX	5	3812	7/7	0.99	0.08	74,74,74,74	0
85	OHX	1	3730	7/7	0.99	0.18	55,55,55,55	0
85	OHX	2	2004	7/7	0.99	0.09	86,86,86,86	0
85	OHX	1	3801	7/7	0.99	0.11	81,81,81,81	0
85	OHX	1	3938	7/7	0.99	0.24	92,92,92,92	0
85	OHX	1	3798	7/7	0.99	0.08	75,75,75,75	0
85	OHX	1	3741	7/7	0.99	0.09	55,55,55,55	0
85	OHX	2	2010	7/7	0.99	0.17	88,88,88,88	0
85	OHX	2	1983	7/7	0.99	0.11	75,75,75,75	0
85	OHX	o3	202	7/7	0.99	0.19	82,82,82,82	0
85	OHX	6	2111	7/7	0.99	0.21	84,84,84,84	0
85	OHX	2	2043	7/7	0.99	0.19	89,89,89,89	0
85	OHX	6	2010	7/7	0.99	0.18	73,73,73,73	0
85	OHX	1	3793	7/7	0.99	0.06	89,89,89,89	0
85	OHX	5	3760	7/7	0.99	0.09	56,56,56,56	0
85	OHX	1	3796	7/7	0.99	0.07	79,79,79,79	0
85	OHX	5	3772	7/7	0.99	0.05	61,61,61,61	0
85	OHX	7	215	7/7	0.99	0.09	82,82,82,82	0
85	OHX	1	3874	7/7	0.99	0.20	91,91,91,91	0
85	OHX	6	2038	7/7	0.99	0.11	71,71,71,71	0
85	OHX	1	3808	7/7	0.99	0.10	93,93,93,93	0
85	OHX	5	3826	7/7	0.99	0.10	62,62,62,62	0
85	OHX	5	3790	7/7	0.99	0.08	58,58,58,58	0
85	OHX	5	3861	7/7	0.99	0.06	103,103,103,103	0
85	OHX	1	3750	7/7	0.99	0.12	76,76,76,76	0
85	OHX	6	2025	7/7	0.99	0.09	73,73,73,73	0
85	OHX	6	2073	7/7	0.99	0.28	86,86,86,86	0
85	OHX	5	3862	7/7	0.99	0.25	77,77,77,77	0
85	OHX	5	3789	7/7	0.99	0.06	59,59,59,59	0
85	OHX	5	3801	7/7	0.99	0.09	69,69,69,69	0
85	OHX	5	3781	7/7	0.99	0.09	65,65,65,65	0
85	OHX	1	3957	7/7	0.99	0.32	111,111,111,111	0
85	OHX	5	3808	7/7	0.99	0.09	67,67,67,67	0
85	OHX	1	3811	7/7	0.99	0.09	78,78,78,78	0
84	MG	5	3560	1/1	0.99	0.47	35,35,35,35	0
85	OHX	1	3851	7/7	0.99	0.23	82,82,82,82	0
85	OHX	1	3893	7/7	0.99	0.28	81,81,81,81	0

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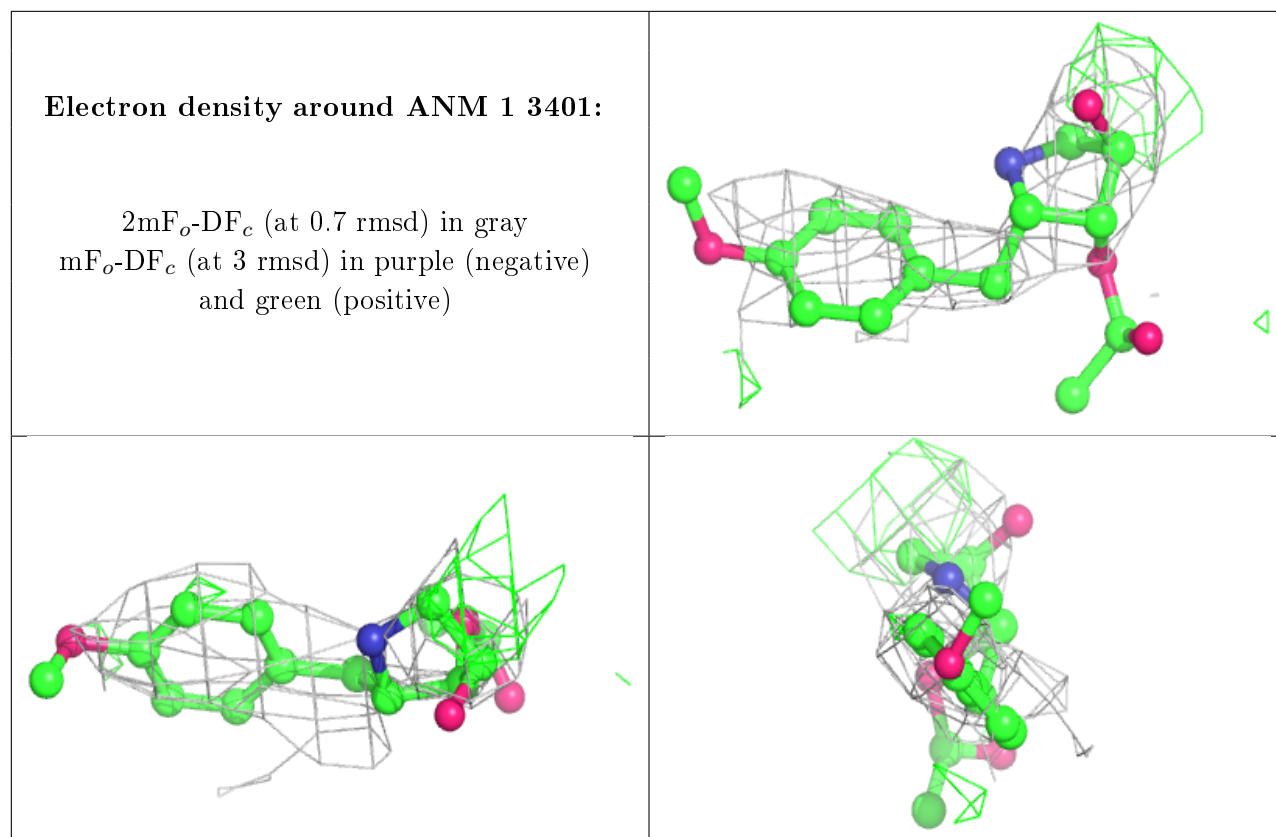
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	OHX	6	2015	7/7	0.99	0.11	75,75,75,75	0
85	OHX	5	3815	7/7	0.99	0.11	68,68,68,68	0
85	OHX	1	3818	7/7	0.99	0.16	58,58,58,58	0
85	OHX	1	3759	7/7	0.99	0.11	79,79,79,79	0
85	OHX	6	2082	7/7	0.99	0.21	91,91,91,91	0
85	OHX	5	3753	7/7	0.99	0.16	68,68,68,68	0
85	OHX	5	3841	7/7	0.99	0.08	97,97,97,97	0
85	OHX	1	3803	7/7	0.99	0.20	74,74,74,74	0
85	OHX	2	1996	7/7	0.99	0.10	83,83,83,83	0
84	MG	1	3576	1/1	0.99	0.57	28,28,28,28	0
85	OHX	5	3858	7/7	0.99	0.21	82,82,82,82	0
85	OHX	6	2050	7/7	0.99	0.12	92,92,92,92	0
85	OHX	1	3958	7/7	0.99	0.34	84,84,84,84	0
85	OHX	5	3868	7/7	0.99	0.07	96,96,96,96	0
85	OHX	6	2076	7/7	0.99	0.23	81,81,81,81	0
85	OHX	1	3794	7/7	0.99	0.06	62,62,62,62	0
85	OHX	5	3758	7/7	0.99	0.11	55,55,55,55	0
85	OHX	1	3802	7/7	0.99	0.13	75,75,75,75	0
85	OHX	5	3805	7/7	0.99	0.09	73,73,73,73	0
86	ZN	o7	501	1/1	0.99	0.07	45,45,45,45	0
85	OHX	6	2034	7/7	0.99	0.07	91,91,91,91	0
85	OHX	1	3825	7/7	0.99	0.15	83,83,83,83	0
85	OHX	6	2078	7/7	0.99	0.24	98,98,98,98	0
85	OHX	5	3953	7/7	0.99	0.20	81,81,81,81	0
84	MG	1	3562	1/1	0.99	0.56	48,48,48,48	0
85	OHX	5	3791	7/7	0.99	0.07	73,73,73,73	0
85	OHX	5	3754	7/7	0.99	0.09	50,50,50,50	0
85	OHX	5	3882	7/7	0.99	0.26	67,67,67,67	0
85	OHX	6	2018	7/7	0.99	0.10	60,60,60,60	0
85	OHX	2	2069	7/7	0.99	0.15	112,112,112,112	0
85	OHX	5	3828	7/7	0.99	0.19	73,73,73,73	0
85	OHX	1	3743	7/7	0.99	0.12	60,60,60,60	0
85	OHX	N9	101	7/7	0.99	0.11	56,56,56,56	0
85	OHX	5	3785	7/7	0.99	0.07	68,68,68,68	0
85	OHX	5	3847	7/7	0.99	0.12	67,67,67,67	0
85	OHX	1	3747	7/7	0.99	0.14	64,64,64,64	0
85	OHX	1	3736	7/7	0.99	0.11	63,63,63,63	0
84	MG	1	3483	1/1	0.99	0.31	45,45,45,45	0
85	OHX	5	3771	7/7	0.99	0.04	66,66,66,66	0
85	OHX	M6	202	7/7	0.99	0.18	80,80,80,80	0
85	OHX	1	3785	7/7	1.00	0.06	66,66,66,66	0
85	OHX	1	3761	7/7	1.00	0.06	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	OHX	1	3737	7/7	1.00	0.06	56,56,56,56	0
85	OHX	1	3729	7/7	1.00	0.14	53,53,53,53	0
85	OHX	1	3728	7/7	1.00	0.10	44,44,44,44	0
85	OHX	6	2009	7/7	1.00	0.12	57,57,57,57	0
85	OHX	1	3752	7/7	1.00	0.09	59,59,59,59	0
85	OHX	1	3745	7/7	1.00	0.09	66,66,66,66	0
85	OHX	5	3763	7/7	1.00	0.09	61,61,61,61	0
85	OHX	5	3743	7/7	1.00	0.14	43,43,43,43	0
85	OHX	1	3726	7/7	1.00	0.13	43,43,43,43	0
85	OHX	5	3752	7/7	1.00	0.09	40,40,40,40	0
85	OHX	5	3774	7/7	1.00	0.11	53,53,53,53	0
85	OHX	5	3757	7/7	1.00	0.10	58,58,58,58	0
85	OHX	5	3766	7/7	1.00	0.07	63,63,63,63	0
85	OHX	1	3744	7/7	1.00	0.04	54,54,54,54	0
85	OHX	5	3756	7/7	1.00	0.08	60,60,60,60	0
85	OHX	1	3754	7/7	1.00	0.05	63,63,63,63	0
85	OHX	5	3769	7/7	1.00	0.06	52,52,52,52	0
85	OHX	6	2014	7/7	1.00	0.09	62,62,62,62	0
85	OHX	5	3745	7/7	1.00	0.10	43,43,43,43	0
85	OHX	5	3744	7/7	1.00	0.12	40,40,40,40	0
85	OHX	1	3727	7/7	1.00	0.10	52,52,52,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.