



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2024 – 03:26 pm GMT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

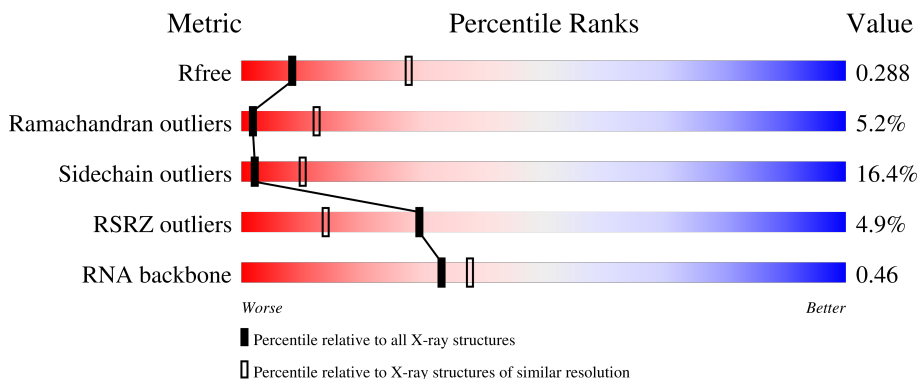
# 1 Overall quality at a glance

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)
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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 8% (poor fit), 72% (0-1 outliers), 26% (2-3 outliers), .. (not modelled)
1	6	1800	 7% (poor fit), 72% (0-1 outliers), 26% (2-3 outliers), . (not modelled)
2	S0	251	 6% (poor fit), 67% (0-1 outliers), 14% (2-3 outliers), 18% (not modelled)
2	s0	251	 2% (poor fit), 66% (0-1 outliers), 16% (2-3 outliers), 18% (not modelled)
3	S1	254	 17% (poor fit), 65% (0-1 outliers), 19% (2-3 outliers), 16% (not modelled)

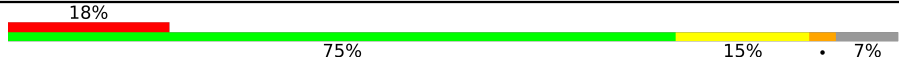
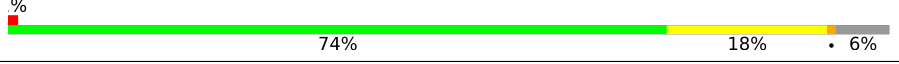
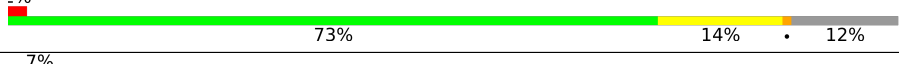


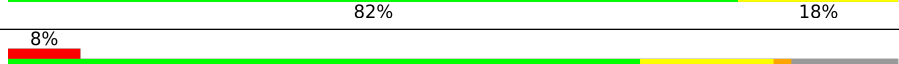
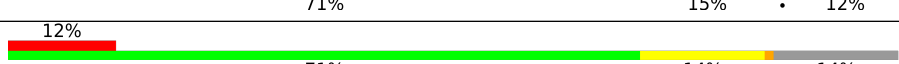
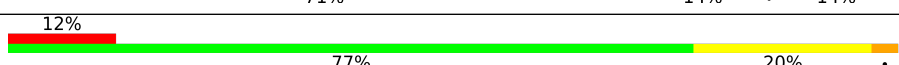
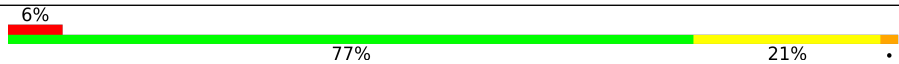


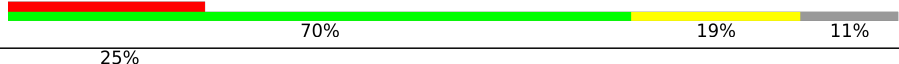
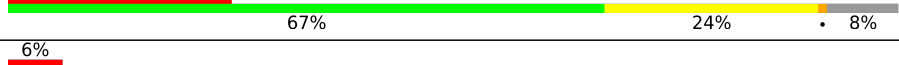

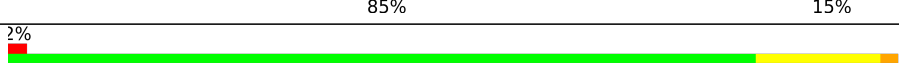










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Mol	Chain	Length	Quality of chain
3	s1	254	2% 69% 15% 15%
4	S2	253	% 70% 16% 14%
4	s2	253	3% 68% 17% 14%
5	S3	239	4% 77% 15% 7%
5	s3	239	5% 79% 14% 7%
6	S4	260	3% 82% 16%
6	s4	260	2% 79% 19%
7	S5	224	8% 71% 20% 8%
7	s5	224	5% 74% 18% 8%
8	S6	236	9% 78% 17%
8	s6	236	3% 76% 15% 8%
9	S7	189	8% 75% 21%
9	s7	189	11% 81% 15%
10	S8	200	3% 80% 13% 6%
10	s8	200	4% 82% 12% 6%
11	S9	196	4% 77% 17% 6%
11	s9	196	3% 82% 11% 6%
12	C0	96	84% 15%
12	c0	96	10% 82% 15%
13	C1	155	4% 86% 14%
13	c1	155	6% 77% 17% 6%
14	C2	142	32% 64% 21% 13%
14	c2	142	54% 65% 20% 13%
15	C3	150	4% 82% 16%
15	c3	150	81% 16%

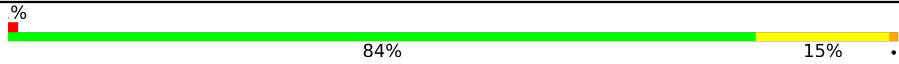
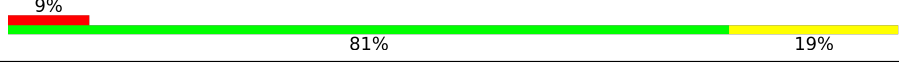
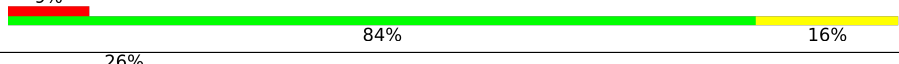


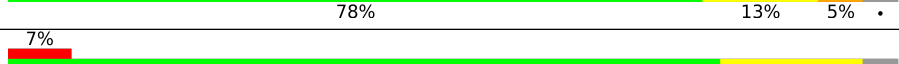
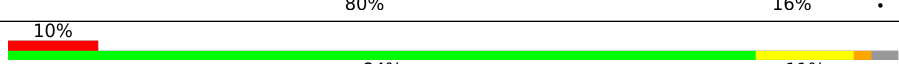
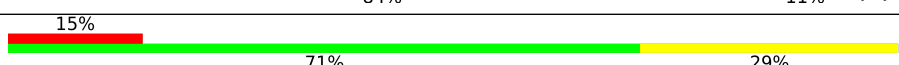
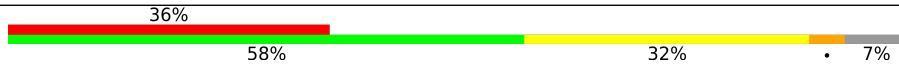


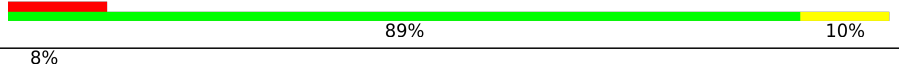
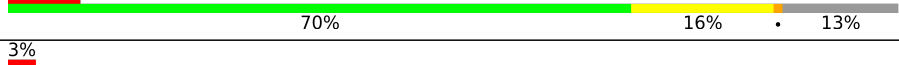
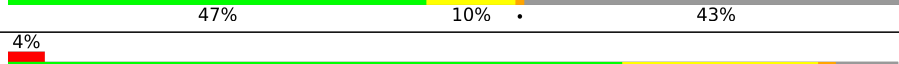
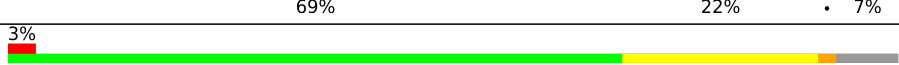










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Mol	Chain	Length	Quality of chain
16	C4	136	
16	c4	136	
17	C5	141	
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107	
27	d5	107	
28	D6	97	







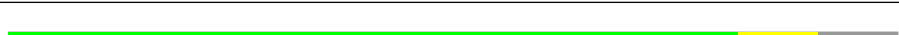
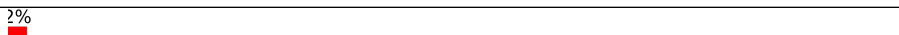
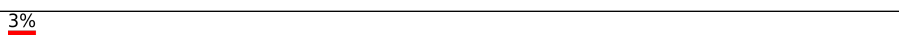
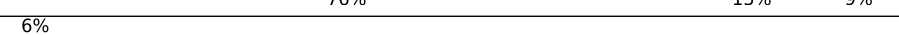
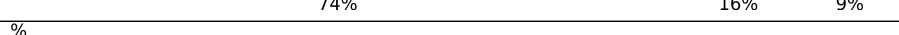
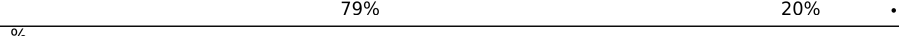













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Mol	Chain	Length	Quality of chain
28	d6	97	 % 84% 15%
29	D7	81	 9% 81% 19%
29	d7	81	 9% 84% 16%
30	D8	66	 26% 73% 23% 5%
30	d8	66	 27% 77% 15% 5%
31	D9	55	 2% 78% 13% 5%
31	d9	55	 7% 80% 16%
32	E0	62	 10% 84% 11%
32	e0	62	 15% 71% 29%
33	E1	76	 36% 58% 32% 7%
33	e1	76	 50% 66% 28% 7%
34	SR	318	 10% 86% 14%
34	sR	318	 11% 89% 10%
35	SM	182	 8% 70% 16% 13%
35	sM	182	 3% 47% 10% 43%
36	1	3396	 4% 69% 22% 7%
36	5	3396	 3% 69% 22% 7%
37	3	121	 % 88% 12%
37	7	121	 82% 16%
38	4	158	 2% 75% 23%
38	8	158	 2% 74% 25%
39	L2	253	 81% 18%
39	l2	253	 2% 81% 18%
40	L3	386	 82% 18%
40	l3	386	 84% 16%












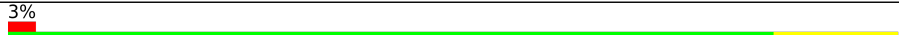

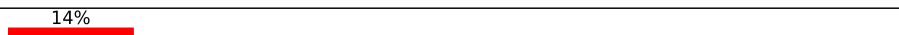
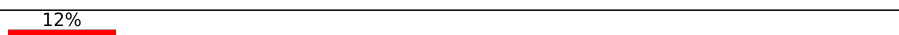
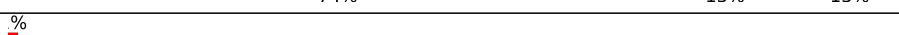

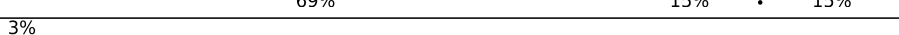







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Mol	Chain	Length	Quality of chain
41	L4	361	 81% 18%
41	l4	361	 83% 15%
42	L5	296	 81% 18%
42	l5	296	 82% 17%
43	L6	175	 78% 11% 11%
43	l6	175	 74% 14% 10%
44	L7	243	 82% 9% 9%
44	l7	243	 80% 10% 8%
45	L8	255	 76% 15% 9%
45	l8	255	 74% 16% 9%
46	L9	191	 79% 20%
46	l9	191	 80% 20%
47	M0	220	 78% 18%
47	m0	220	 79% 17%
48	M1	173	 73% 21%
48	m1	173	 77% 18%
49	M3	198	 80% 17%
49	m3	198	 80% 17%
50	M4	137	 83% 15%
50	m4	137	 88% 11%
51	M5	203	 82% 18%
51	m5	203	 86% 13%
52	M6	198	 86% 13%
52	m6	198	 87% 12%
53	M7	183	 85% 14%

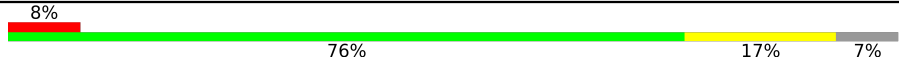

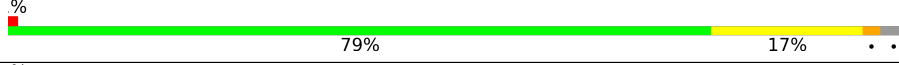

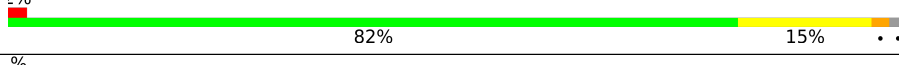
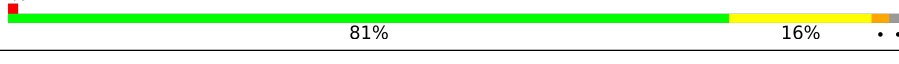
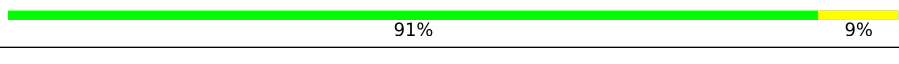
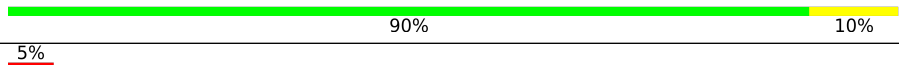
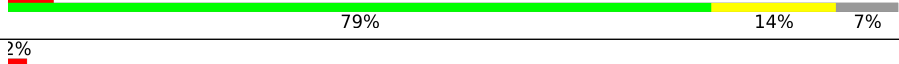


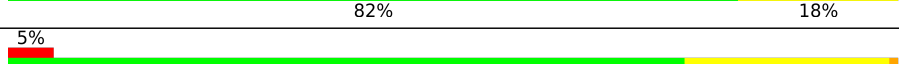
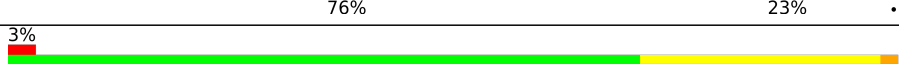
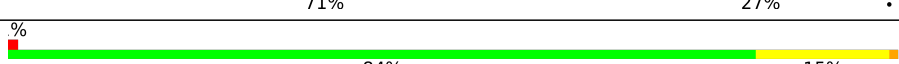

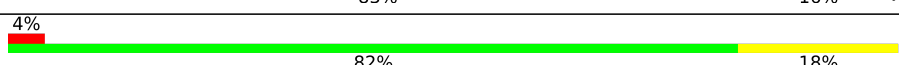
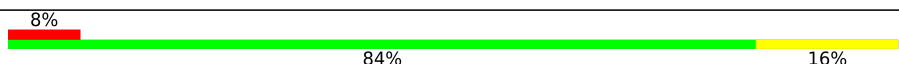
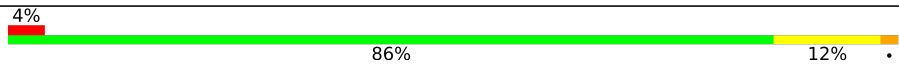
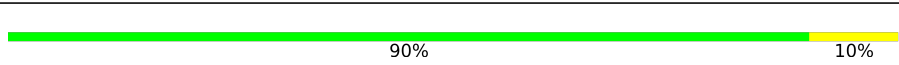


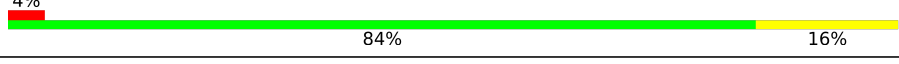
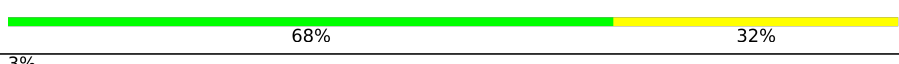


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Mol	Chain	Length	Quality of chain
53	m7	183	 75% 10% 15%
54	M8	185	 85% 14%
54	m8	185	 84% 15%
55	M9	188	 89% 11%
55	m9	188	 82% 18%
56	N0	172	 83% 17%
56	n0	172	 82% 18%
57	N1	159	 82% 18%
57	n1	159	 82% 17%
58	N2	120	 73% 10% 17%
58	n2	120	 68% 12% 18%
59	N3	136	 86% 14%
59	n3	136	 91% 9%
60	N4	155	 55% 8% 37%
60	n4	155	 74% 13% 13%
61	N5	141	 69% 15% 14%
61	n5	141	 69% 15% 15%
62	N6	126	 84% 15%
62	n6	126	 83% 15%
63	N7	135	 84% 14%
63	n7	135	 79% 17%
64	N8	148	 81% 14% 5%
64	n8	148	 80% 19%
65	N9	58	 83% 16%
65	n9	58	 78% 19%

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Mol	Chain	Length	Quality of chain
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	
78	Q2	105	

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Mol	Chain	Length	Quality of chain
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
84	MG	2	1956	-	-	-	X
84	MG	2	1962	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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
87	ANM	1	3401	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
			Total	C	N	O	P			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
4	S2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			
4	s2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	S7	184	Total	C	N	O	0	0	0
			1481	951	265	265			
9	s7	186	Total	C	N	O	0	0	0
			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
			Total	C	N	O	S			
10	s8	188	1489	925	298	264	2	0	0	0

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

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

- 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
			Total	C	N	O	S			
12	C0	96	773	500	126	145	2	0	0	0
12	c0	96	762	491	125	144	2	0	0	0

- 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
			Total	C	N	O	S			
13	C1	155	1214	775	230	206	3	0	0	0
13	c1	146	1169	748	221	197	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	C2	124	890	560	156	172	2	0	0	0
14	c2	124	890	560	156	172	2	0	0	0

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

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

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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
			Total	C	N	O	S			
21	C9	143	Total 1112	C 694	N 208	O 208	S 2	0	0	0
21	c9	143	Total 1112	C 694	N 208	O 208	S 2	0	0	0

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	P			
36	5	3150	67377	30095	12145	21987	3150	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	L2	252	1914	1191	388	334	1	0	0	0
39	l2	252	1918	1193	389	335	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	L3	386	3067	1942	583	533	9	0	0	0
40	l3	386	3073	1948	583	533	9	0	0	0

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
			Total	C	N	O	S			
46	19	191	1518	963	274	277	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	M0	211	1705	1083	322	294	6	0	0	0
47	m0	213	1733	1101	327	299	6	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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	0	0	0
			993	625	192	176			

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
67	O1	109	876	556	167	152	1	0	0	0
67	o1	109	890	565	168	156	1	0	0	0

- 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
			Total	C	N	O	S			
78	q2	105	847	534	170	138	5	0	0	0

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

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

- Molecule 80 is a protein called 60S ribosomal protein L12-A (uL11).

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
84	2	82	82	82	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	S4	1	Total Mg 1 1	0	0
84	D9	1	Total Mg 1 1	0	0
84	SM	1	Total Mg 1 1	0	0
84	1	330	Total Mg 330 330	0	0
84	3	10	Total Mg 10 10	0	0
84	4	14	Total Mg 14 14	0	0
84	L2	2	Total Mg 2 2	0	0
84	L3	1	Total Mg 1 1	0	0
84	L6	1	Total Mg 1 1	0	0
84	L7	1	Total Mg 1 1	0	0
84	M0	1	Total Mg 1 1	0	0
84	M3	1	Total Mg 1 1	0	0
84	M5	1	Total Mg 1 1	0	0
84	M6	1	Total Mg 1 1	0	0
84	M7	4	Total Mg 4 4	0	0
84	N3	1	Total Mg 1 1	0	0
84	N8	2	Total Mg 2 2	0	0
84	O2	1	Total Mg 1 1	0	0
84	O3	1	Total Mg 1 1	0	0
84	O4	2	Total Mg 2 2	0	0
84	O7	2	Total Mg 2 2	0	0

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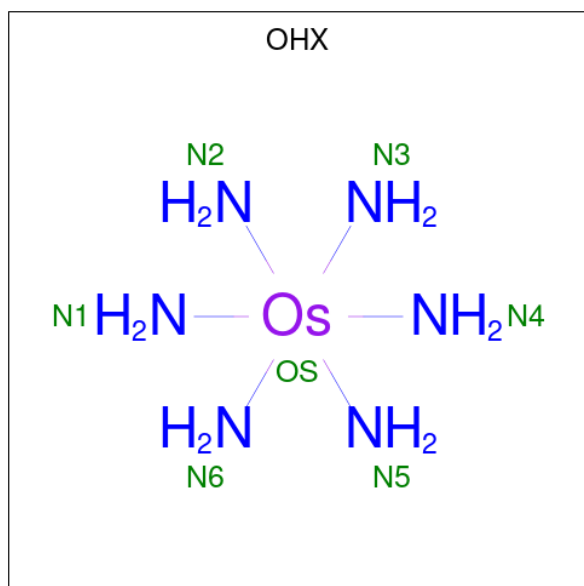
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	Q2	1	Total Mg 1 1	0	0
84	6	110	Total Mg 110 110	0	0
84	s8	1	Total Mg 1 1	0	0
84	c1	1	Total Mg 1 1	0	0
84	d6	1	Total Mg 1 1	0	0
84	sM	2	Total Mg 2 2	0	0
84	5	349	Total Mg 349 349	0	0
84	7	10	Total Mg 10 10	0	0
84	8	10	Total Mg 10 10	0	0
84	l2	3	Total Mg 3 3	0	0
84	l3	5	Total Mg 5 5	0	0
84	l6	1	Total Mg 1 1	0	0
84	l7	1	Total Mg 1 1	0	0
84	l8	1	Total Mg 1 1	0	0
84	l9	1	Total Mg 1 1	0	0
84	m1	1	Total Mg 1 1	0	0
84	m5	3	Total Mg 3 3	0	0
84	m6	1	Total Mg 1 1	0	0
84	m7	3	Total Mg 3 3	0	0
84	n0	2	Total Mg 2 2	0	0
84	n3	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	n6	2	Total Mg 2 2	0	0
84	n8	2	Total Mg 2 2	0	0
84	n9	1	Total Mg 1 1	0	0
84	o1	1	Total Mg 1 1	0	0
84	o3	1	Total Mg 1 1	0	0
84	o4	1	Total Mg 1 1	0	0
84	q0	1	Total Mg 1 1	0	0
84	q1	1	Total Mg 1 1	0	0

- Molecule 85 is osmium (III) hexammine (three-letter code: OHX) (formula:  $H_{12}N_6Os$ ).



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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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		

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	L4	1	7	6	1	0	0
85	M0	1	7	6	1	0	0
85	M5	1	7	6	1	0	0
85	M6	1	7	6	1	0	0
85	M7	1	7	6	1	0	0
85	M9	1	7	6	1	0	0
85	N1	1	7	6	1	0	0
85	N8	1	7	6	1	0	0
85	N9	1	7	6	1	0	0
85	O3	1	7	6	1	0	0
85	O7	1	7	6	1	0	0
85	O7	1	7	6	1	0	0
85	O9	1	7	6	1	0	0
85	Q2	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	s4	1	7	6	1	0	0
85	s8	1	7	6	1	0	0
85	s9	1	7	6	1	0	0
85	c3	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	c5	1	7	6	1	0	0
85	c8	1	7	6	1	0	0
85	d4	1	7	6	1	0	0
85	sR	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	O/s		
85	5	1	Total 7	N 6	O/s 1	0	0
85	5	1	Total 7	N 6	O/s 1	0	0
85	5	1	Total 7	N 6	O/s 1	0	0
85	5	1	Total 7	N 6	O/s 1	0	0
85	5	1	Total 7	N 6	O/s 1	0	0
85	5	1	Total 7	N 6	O/s 1	0	0
85	5	1	Total 7	N 6	O/s 1	0	0
85	5	1	Total 7	N 6	O/s 1	0	0
85	5	1	Total 7	N 6	O/s 1	0	0
85	5	1	Total 7	N 6	O/s 1	0	0
85	5	1	Total 7	N 6	O/s 1	0	0
85	5	1	Total 7	N 6	O/s 1	0	0
85	5	1	Total 7	N 6	O/s 1	0	0
85	5	1	Total 7	N 6	O/s 1	0	0
85	5	1	Total 7	N 6	O/s 1	0	0
85	5	1	Total 7	N 6	O/s 1	0	0
85	5	1	Total 7	N 6	O/s 1	0	0
85	5	1	Total 7	N 6	O/s 1	0	0
85	5	1	Total 7	N 6	O/s 1	0	0
85	5	1	Total 7	N 6	O/s 1	0	0
85	5	1	Total 7	N 6	O/s 1	0	0

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

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

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

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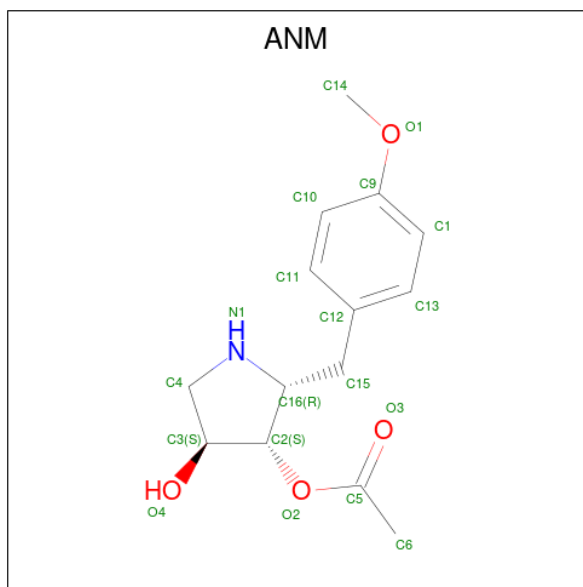
Continued from previous page...

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	D6	1	Total	Zn	0	0
			1	1		
86	D7	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	O7	1	Total	Zn	0	0
			1	1		
86	Q0	1	Total	Zn	0	0
			1	1		
86	Q2	1	Total	Zn	0	0
			1	1		
86	Q3	1	Total	Zn	0	0
			1	1		
86	d6	1	Total	Zn	0	0
			1	1		
86	d7	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	o7	1	Total	Zn	0	0
			1	1		
86	q0	1	Total	Zn	0	0
			1	1		
86	q2	1	Total	Zn	0	0
			1	1		
86	q3	1	Total	Zn	0	0
			1	1		

- Molecule 87 is ANISOMYCIN (three-letter code: ANM) (formula: C<sub>14</sub>H<sub>19</sub>NO<sub>4</sub>).



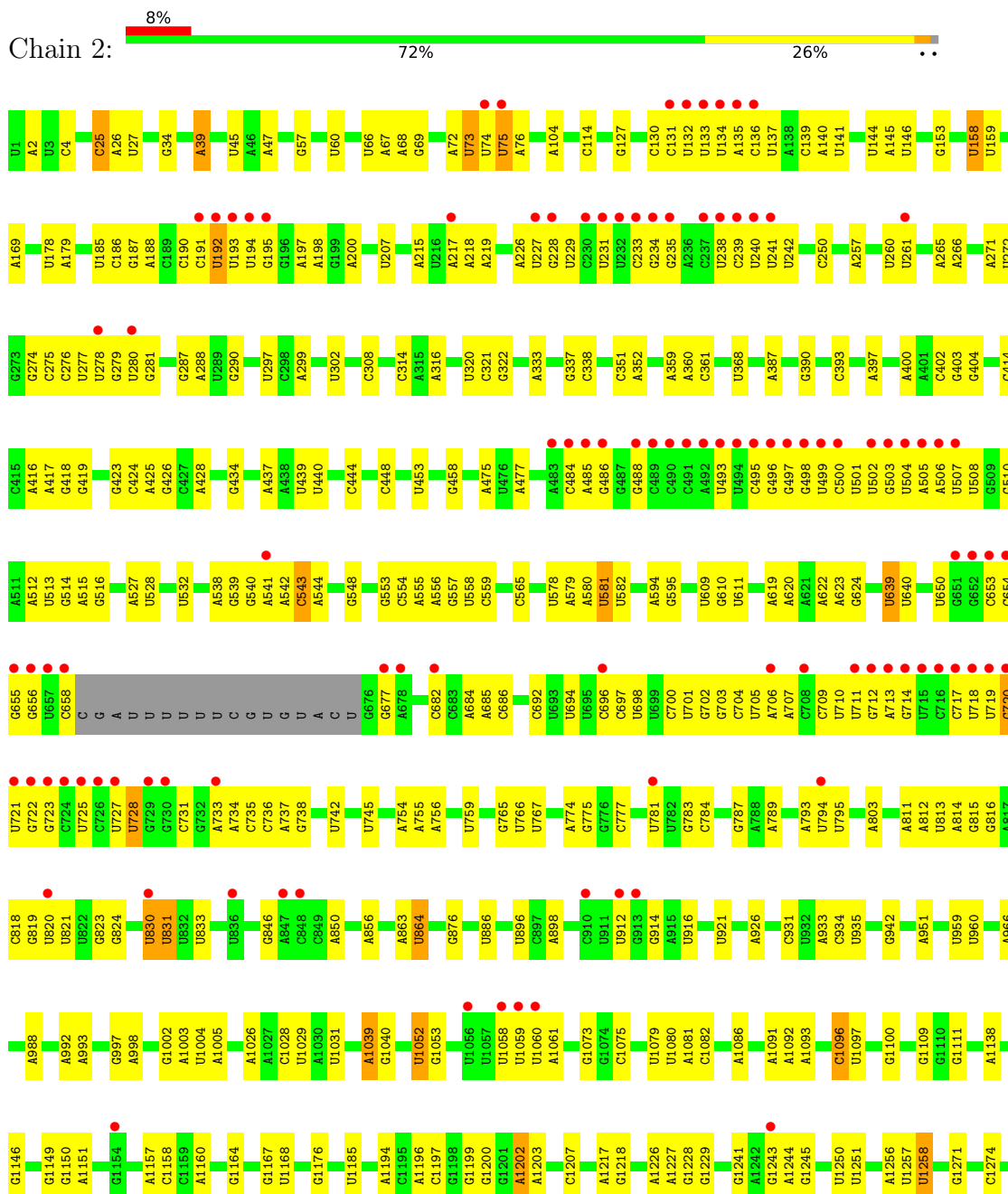
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
87	1	1	19	14	1	4	0	0



### 3 Residue-property plots i

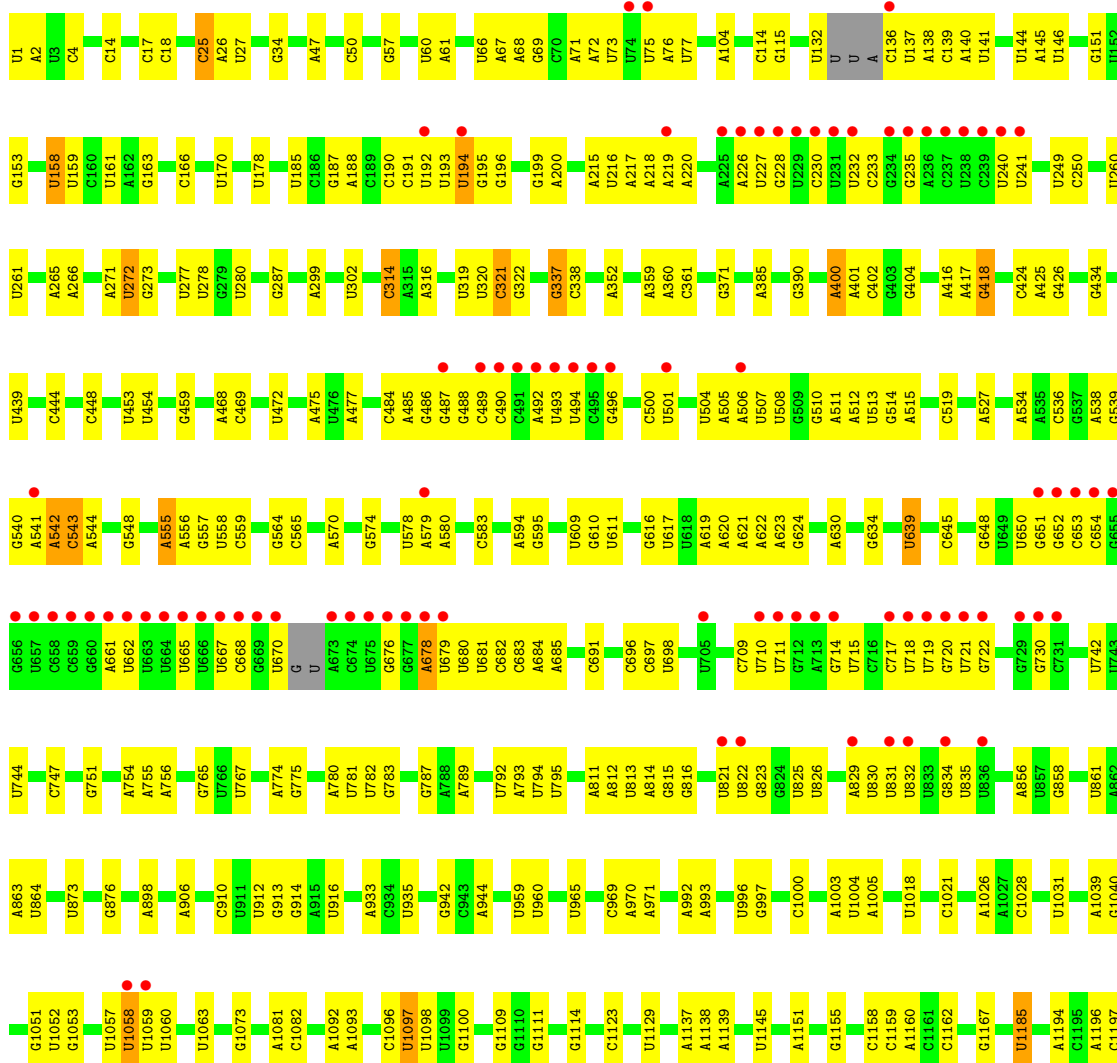
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

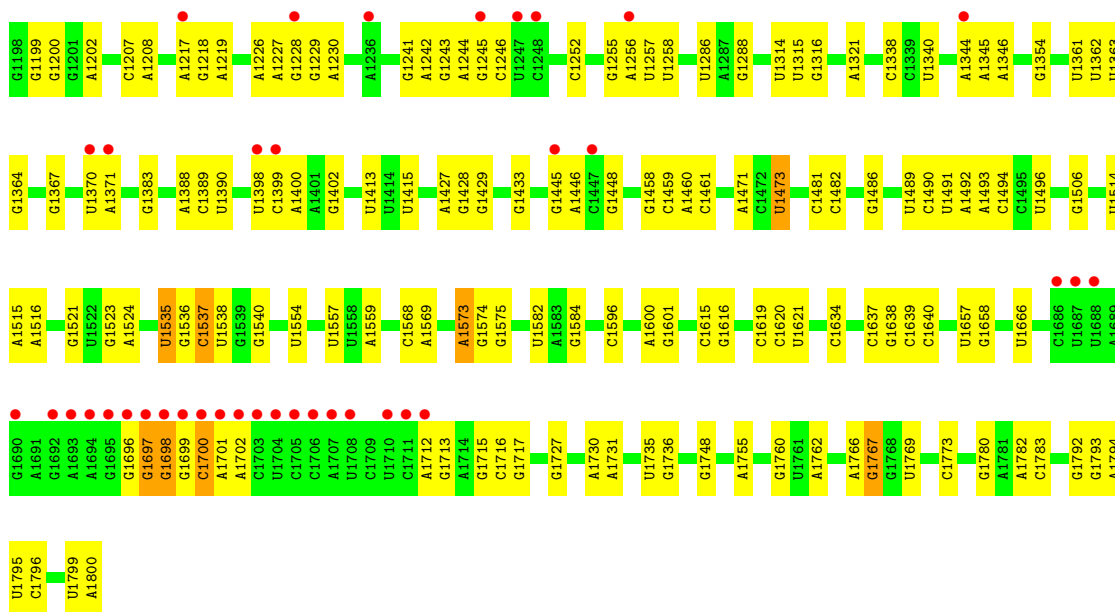
- Molecule 1: 18S ribosomal RNA



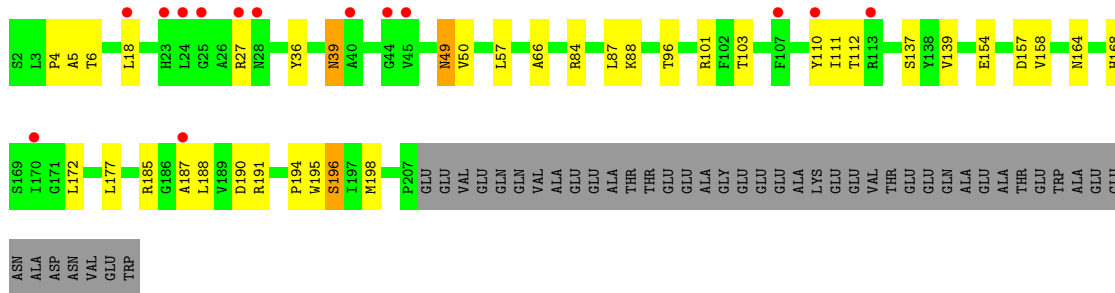


• Molecule 1: 18S ribosomal RNA

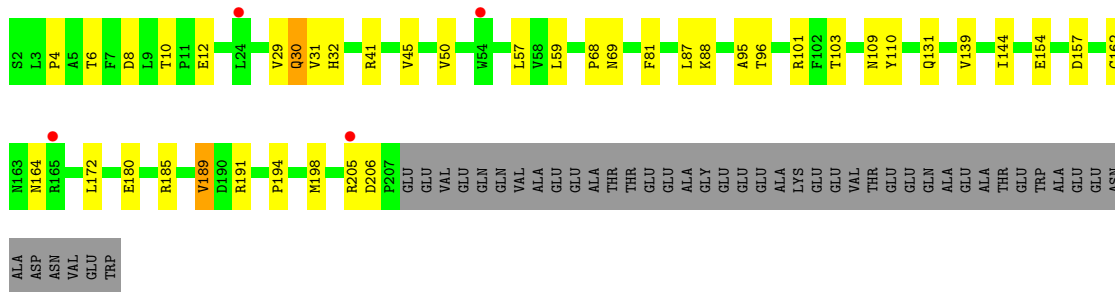




• Molecule 2: 40S ribosomal protein S0-A

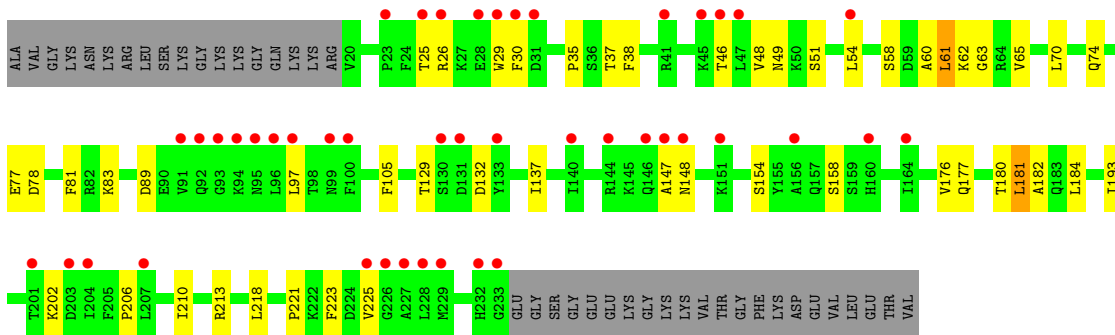


• Molecule 2: 40S ribosomal protein S0-A

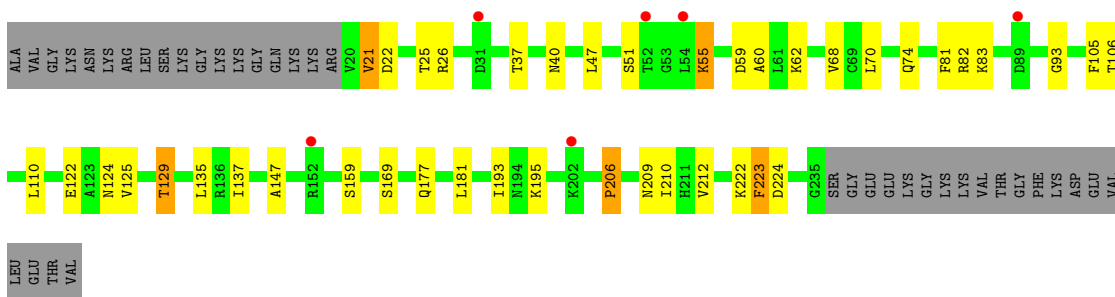


• Molecule 3: 40S ribosomal protein S1-A

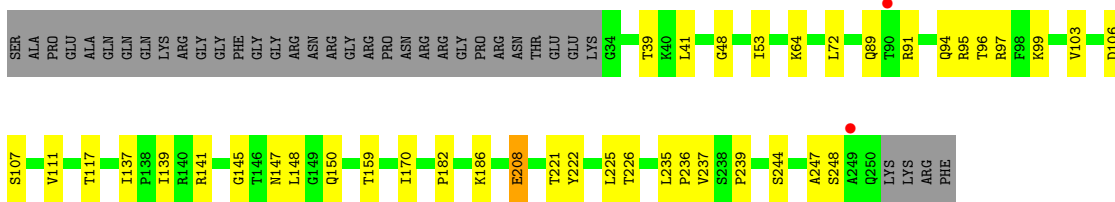




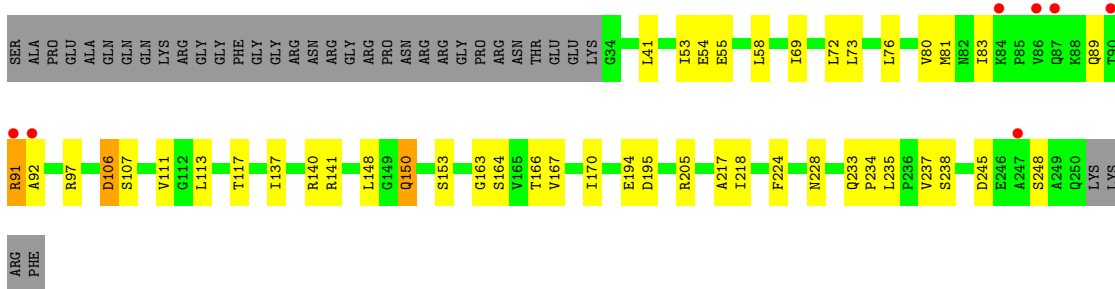
• Molecule 3: 40S ribosomal protein S1-A




• Molecule 4: 40S ribosomal protein S2

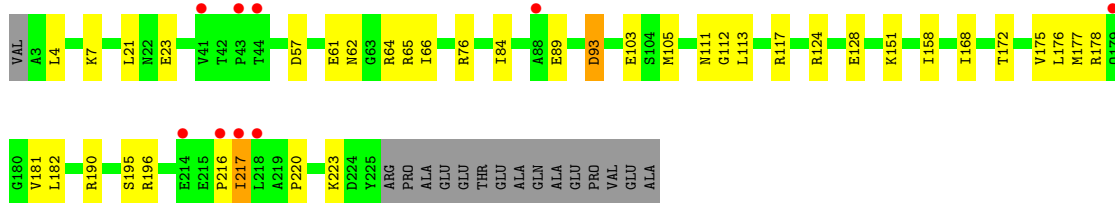


• Molecule 4: 40S ribosomal protein S2




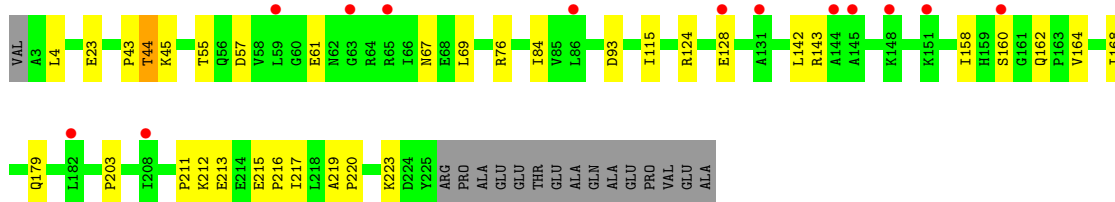
• Molecule 5: 40S ribosomal protein S3

Chain S3: 




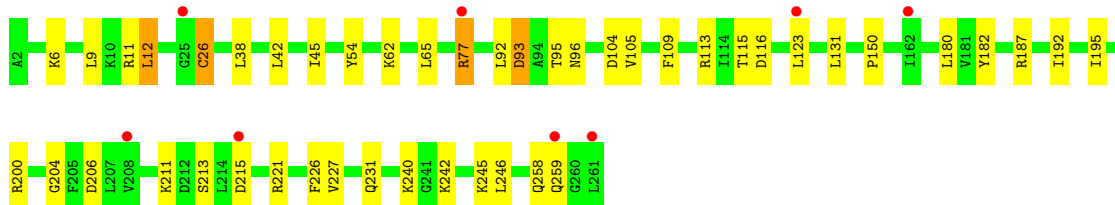
• Molecule 5: 40S ribosomal protein S3

Chain s3: 




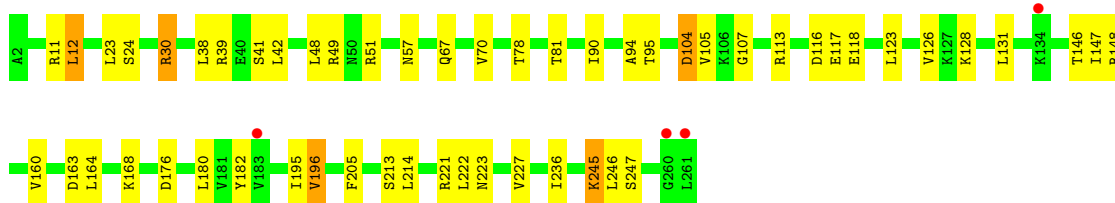
• Molecule 6: 40S ribosomal protein S4-A

Chain S4: 



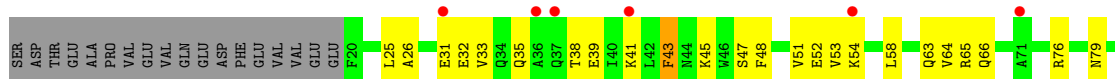
• Molecule 6: 40S ribosomal protein S4-A

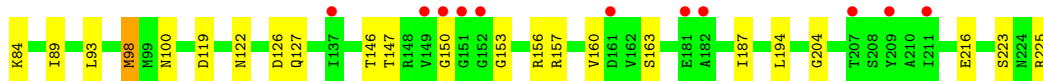
Chain s4: 



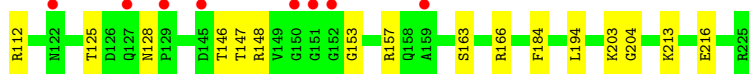
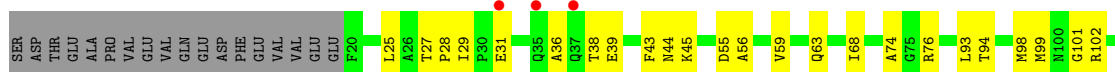
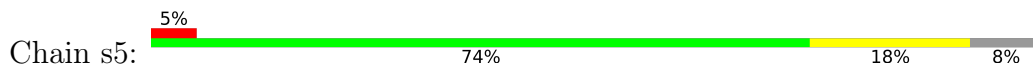
• Molecule 7: 40S ribosomal protein S5

Chain S5: 

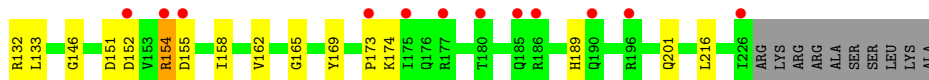
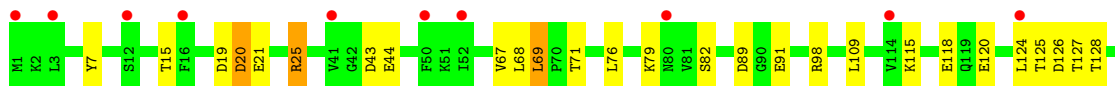
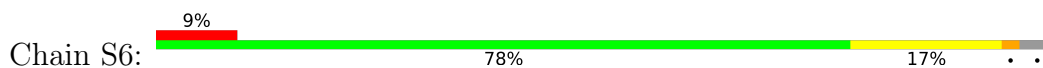




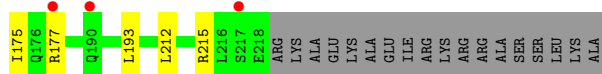
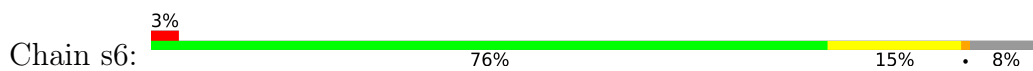
• Molecule 7: 40S ribosomal protein S5



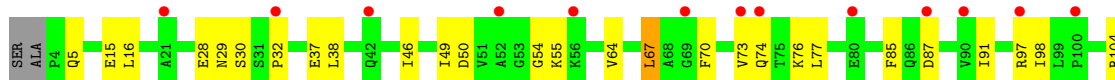
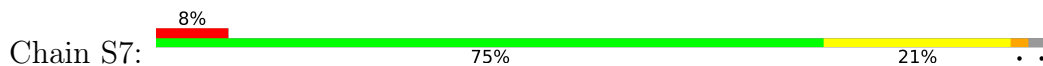
• Molecule 8: 40S ribosomal protein S6-A



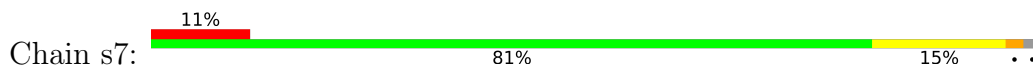
• Molecule 8: 40S ribosomal protein S6-A

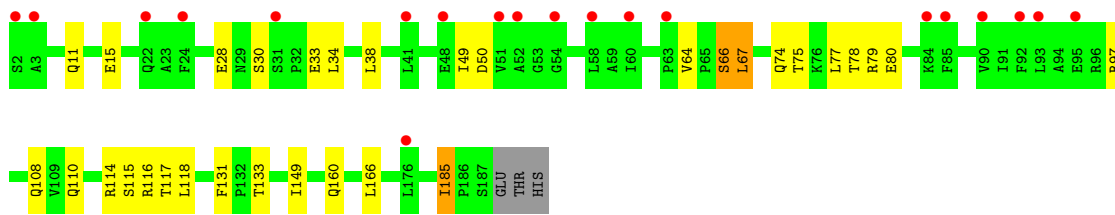


• Molecule 9: 40S ribosomal protein S7-A

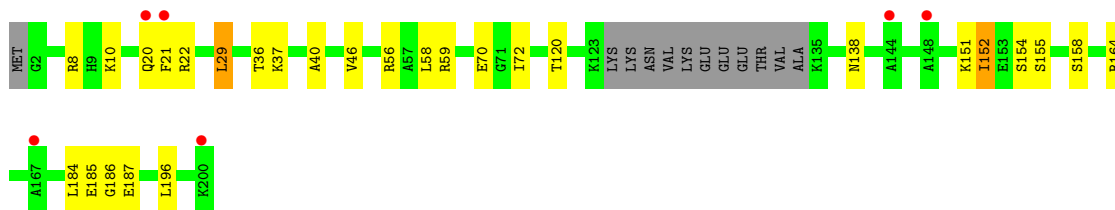
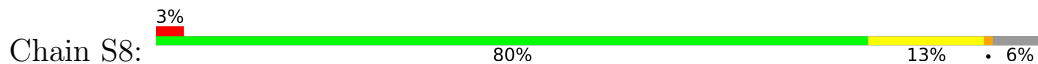


• Molecule 9: 40S ribosomal protein S7-A

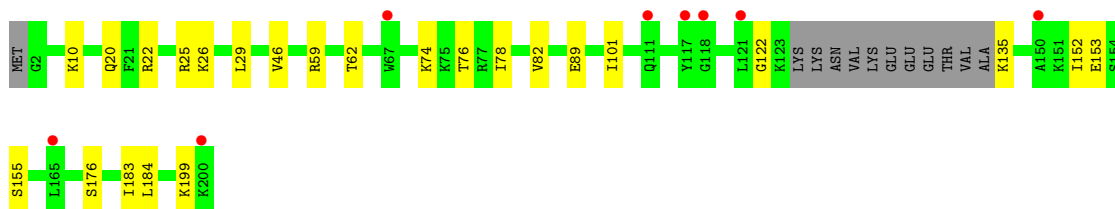
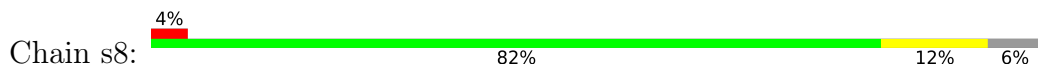




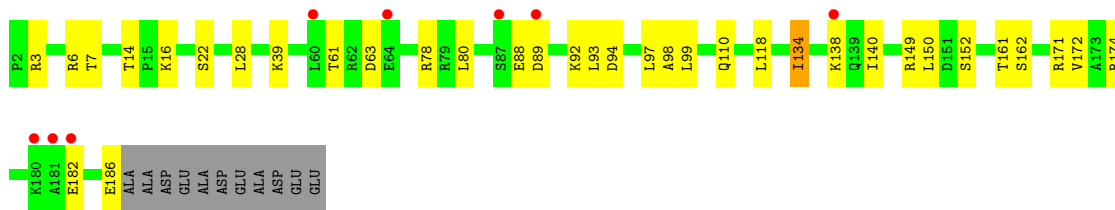
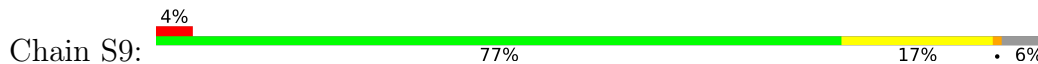
● Molecule 10: 40S ribosomal protein S8-A



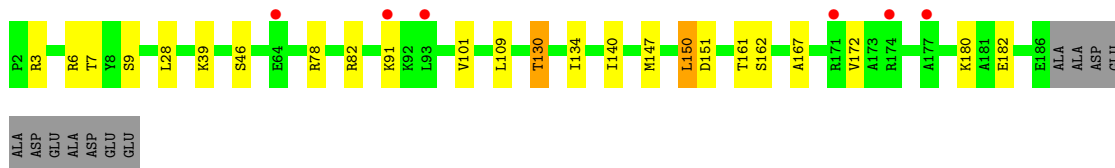
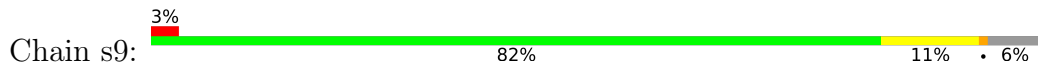
● Molecule 10: 40S ribosomal protein S8-A




● Molecule 11: 40S ribosomal protein S9-A

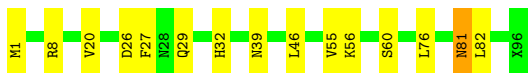


● Molecule 11: 40S ribosomal protein S9-A




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

Chain C0: 




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

Chain c0: 




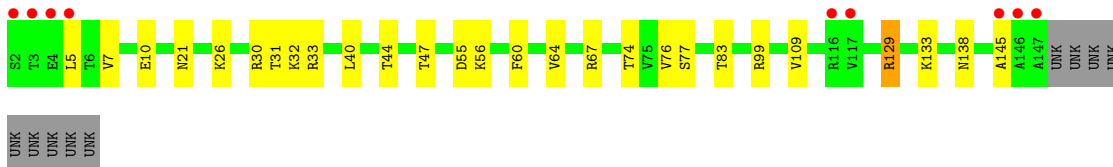
- Molecule 13: 40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A (uS17)

Chain C1: 



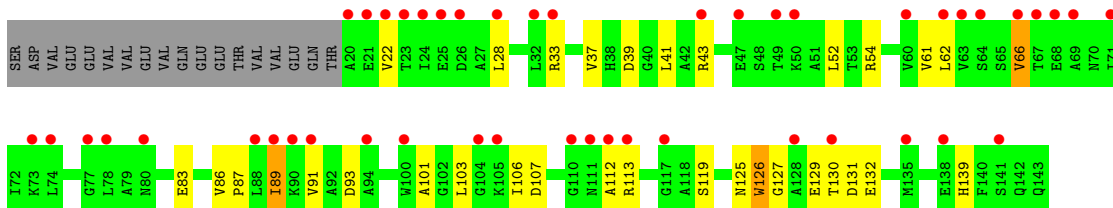
- Molecule 13: 40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A (uS17)

Chain c1: 



- Molecule 14: 40S ribosomal protein S12

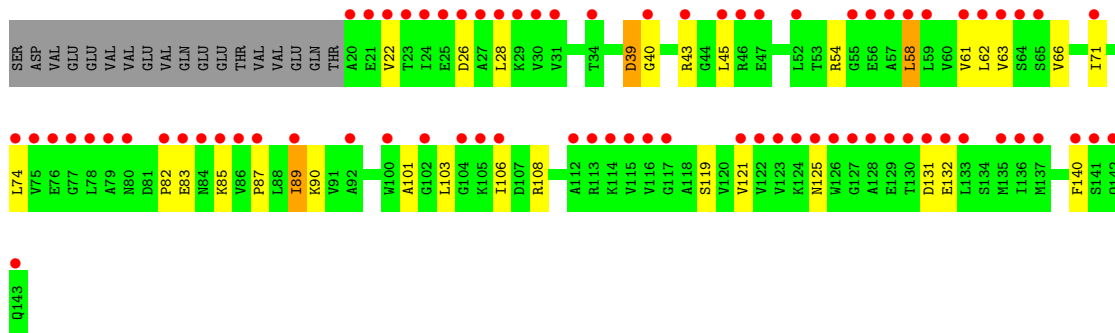
Chain C2: 



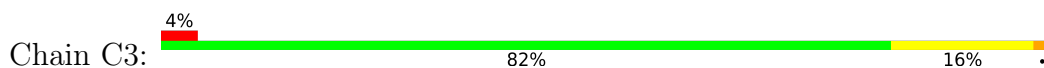
- Molecule 14: 40S ribosomal protein S12

Chain c2: 

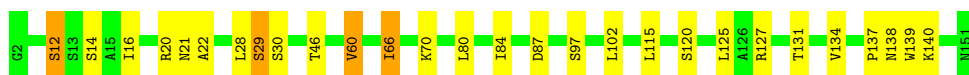
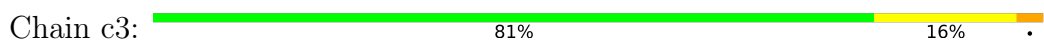




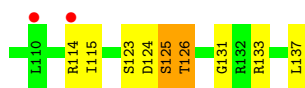
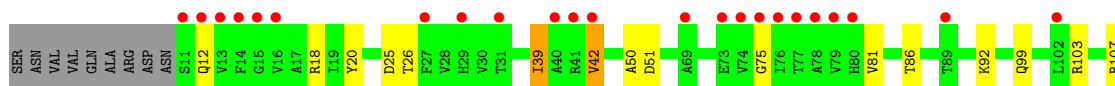
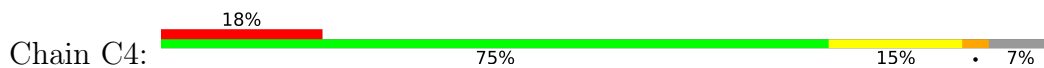
- Molecule 15: 40S ribosomal protein S13



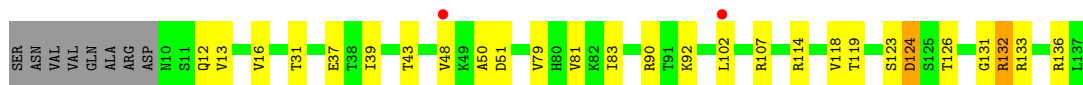
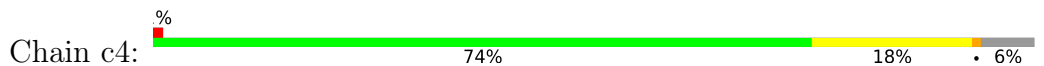
- Molecule 15: 40S ribosomal protein S13



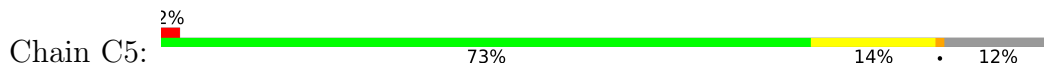
- Molecule 16: 40S ribosomal protein S14-A



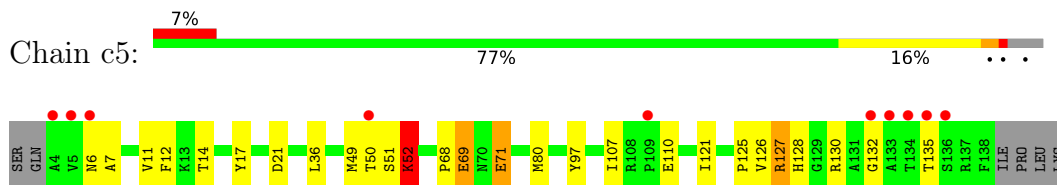
- Molecule 16: 40S ribosomal protein S14-A



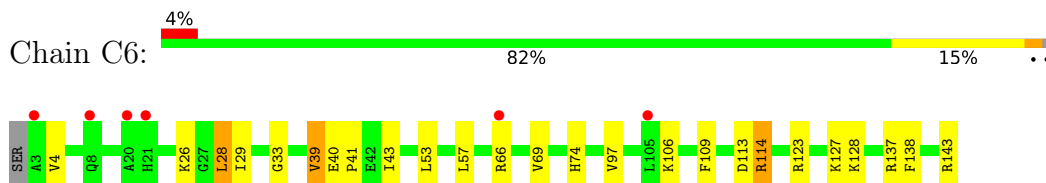
- Molecule 17: 40S ribosomal protein S15



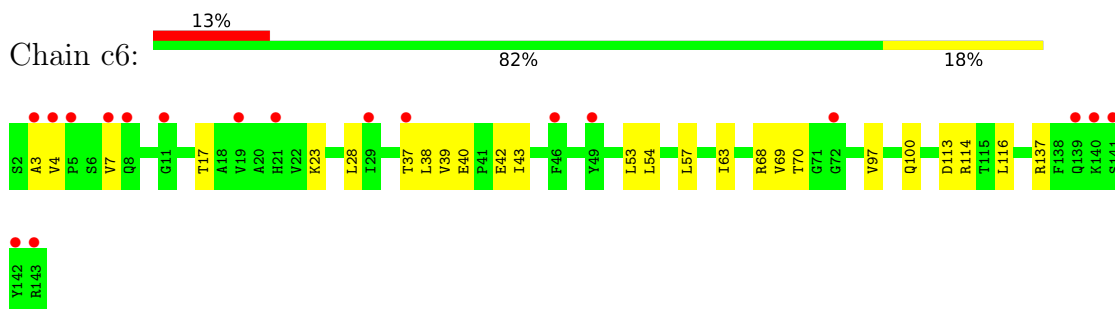
- Molecule 17: 40S ribosomal protein S15



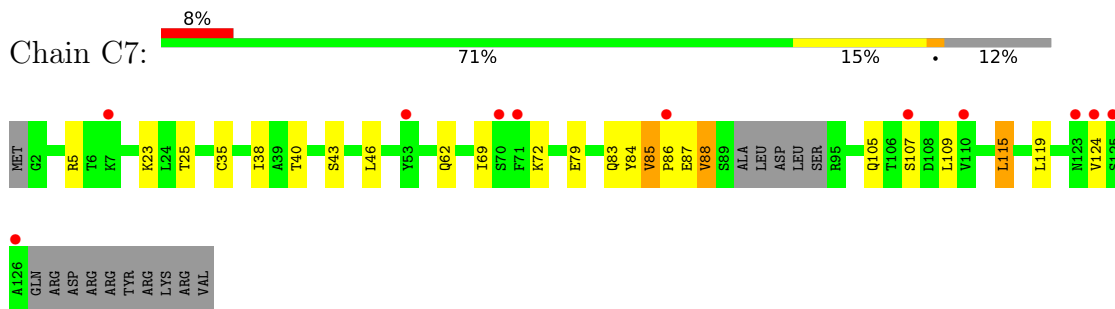
- Molecule 18: 40S ribosomal protein S16-A



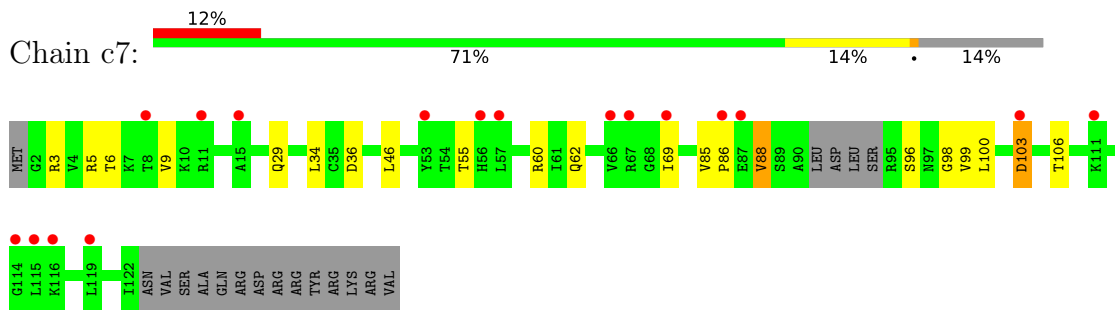
- Molecule 18: 40S ribosomal protein S16-A



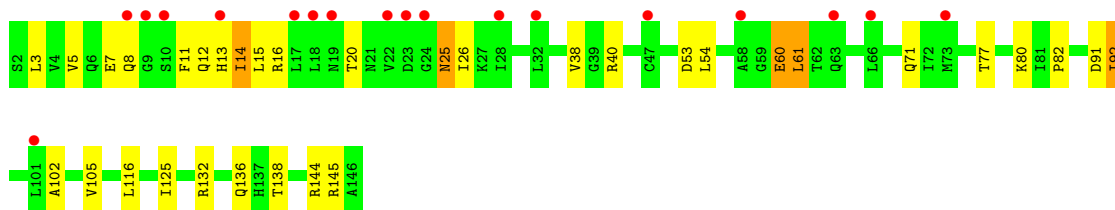
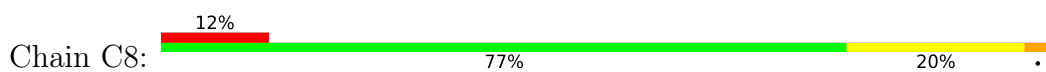
- Molecule 19: 40S ribosomal protein S17-A



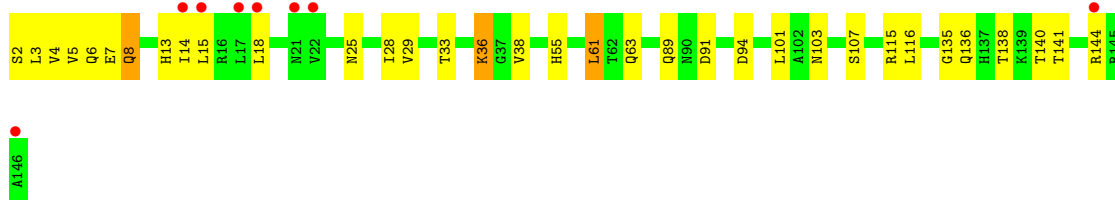
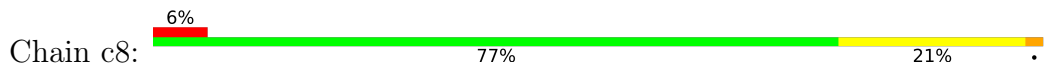
- Molecule 19: 40S ribosomal protein S17-A



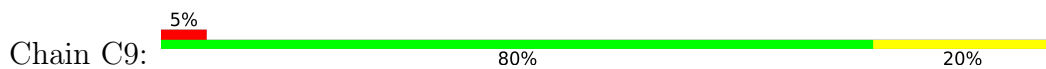
- Molecule 20: 40S ribosomal protein S18-A



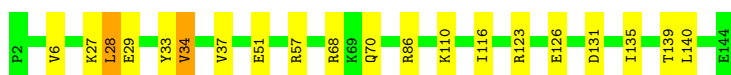
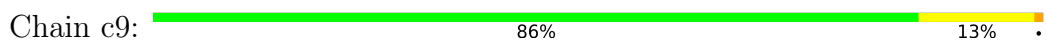
- Molecule 20: 40S ribosomal protein S18-A



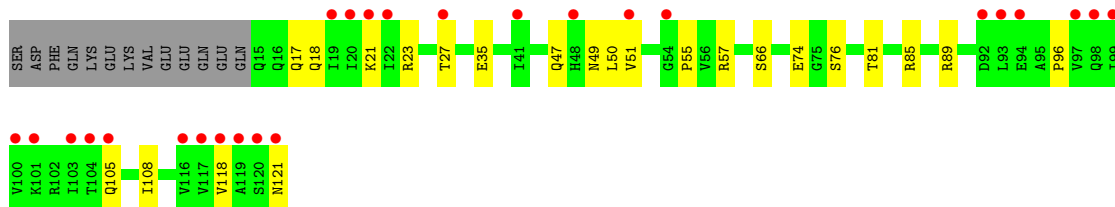
- Molecule 21: 40S ribosomal protein S19-A



- Molecule 21: 40S ribosomal protein S19-A

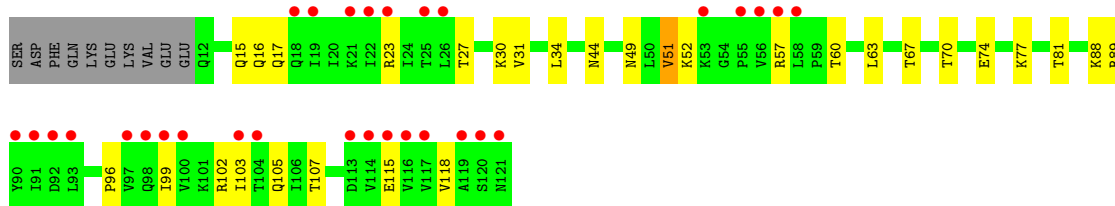


- Molecule 22: 40S ribosomal protein S20

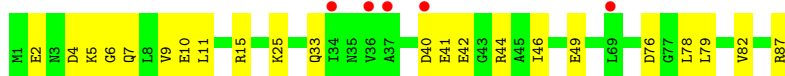
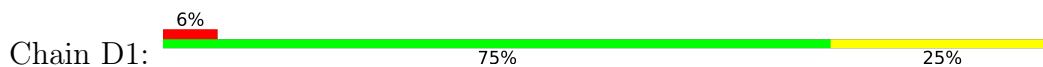


- Molecule 22: 40S ribosomal protein S20

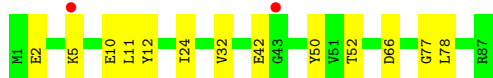
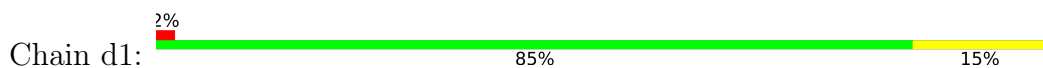




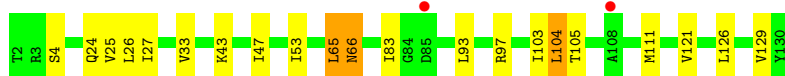
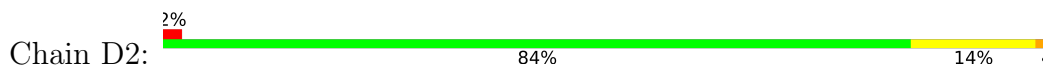
- Molecule 23: 40S ribosomal protein S21-A



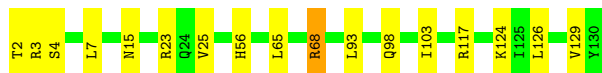
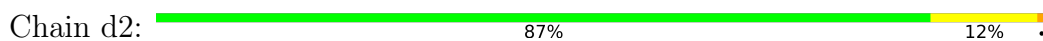
- Molecule 23: 40S ribosomal protein S21-A



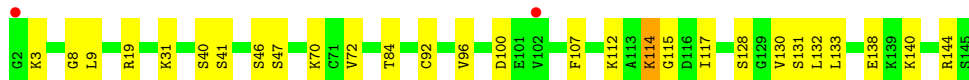
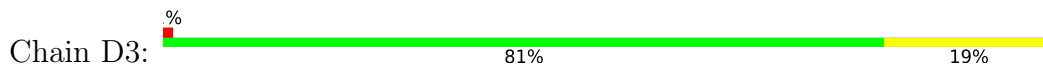
- Molecule 24: 40S ribosomal protein S22-A



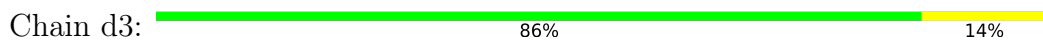
- Molecule 24: 40S ribosomal protein S22-A



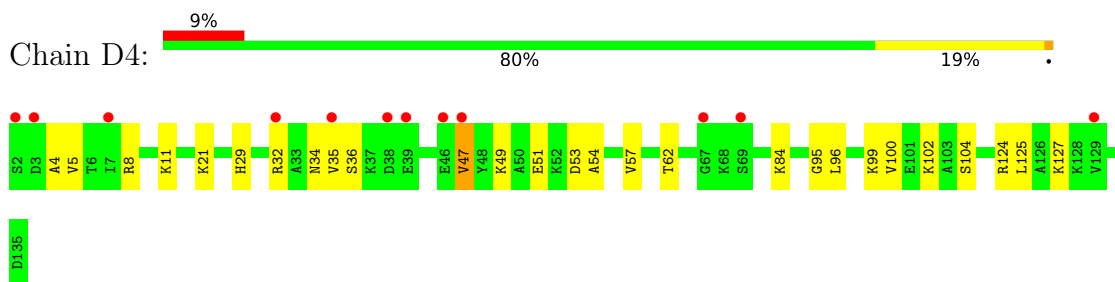
- Molecule 25: 40S ribosomal protein S23-A



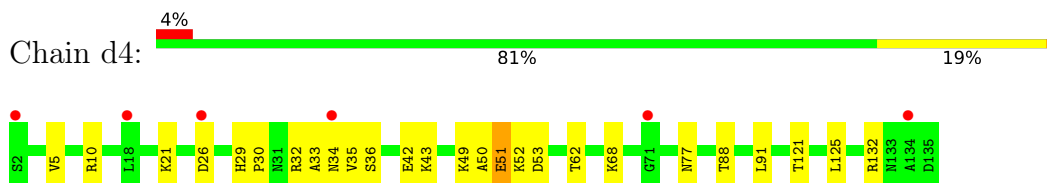
- Molecule 25: 40S ribosomal protein S23-A



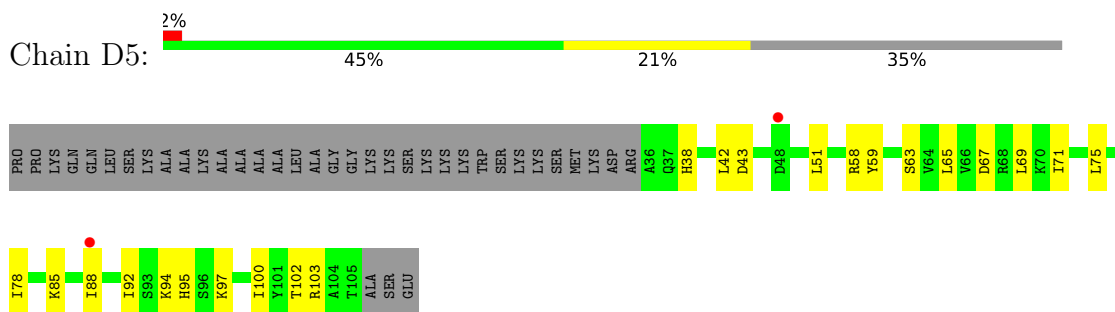
- Molecule 26: 40S ribosomal protein S24-A



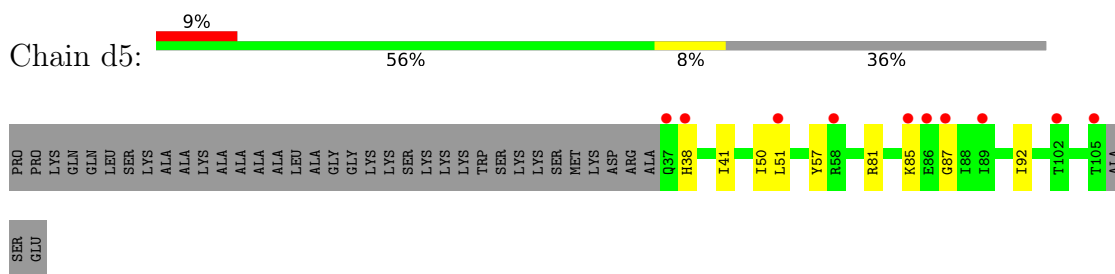
- Molecule 26: 40S ribosomal protein S24-A



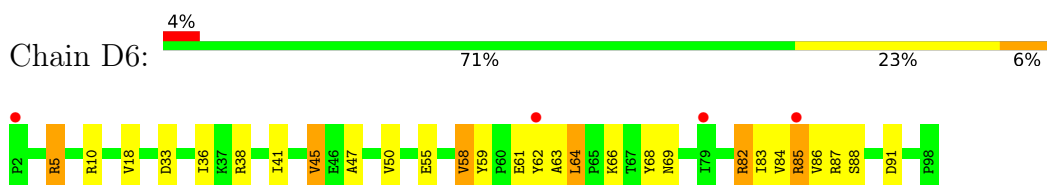
- Molecule 27: 40S ribosomal protein S25-A



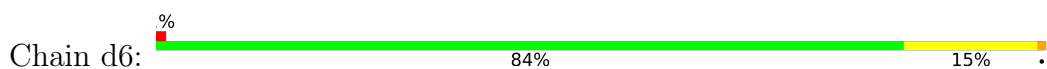
- Molecule 27: 40S ribosomal protein S25-A

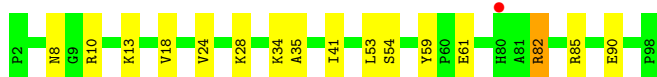


- Molecule 28: 40S ribosomal protein S26-B

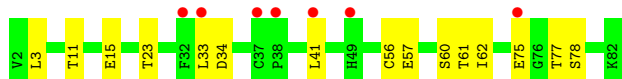
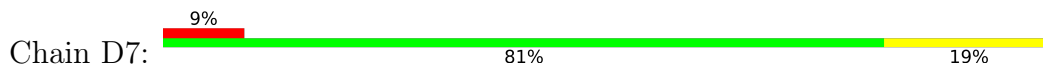


- Molecule 28: 40S ribosomal protein S26-B

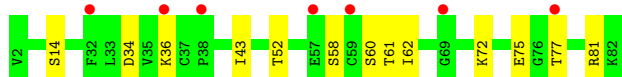
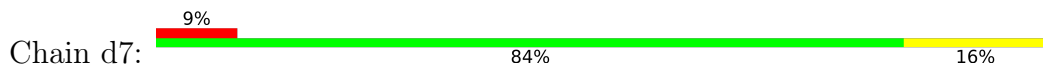




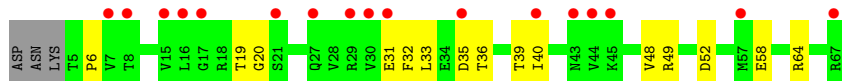
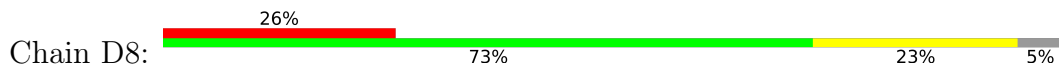
- Molecule 29: 40S ribosomal protein S27-A



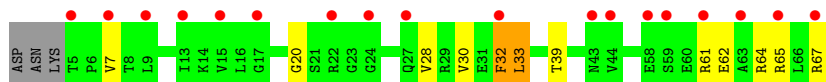
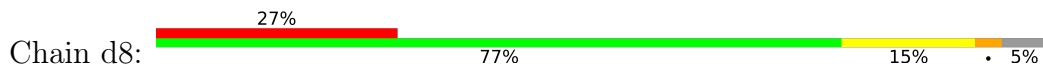
- Molecule 29: 40S ribosomal protein S27-A



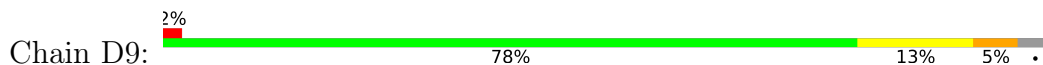
- Molecule 30: 40S ribosomal protein S28-A



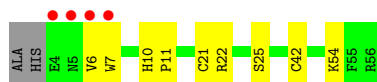
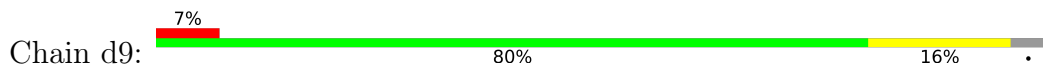
- Molecule 30: 40S ribosomal protein S28-A



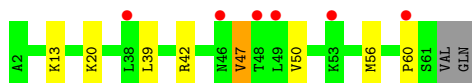
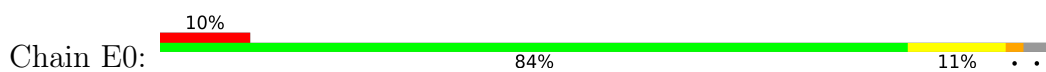
- Molecule 31: 40S ribosomal protein S29-A



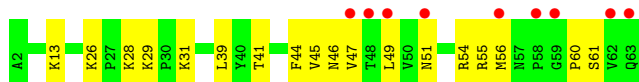
- Molecule 31: 40S ribosomal protein S29-A



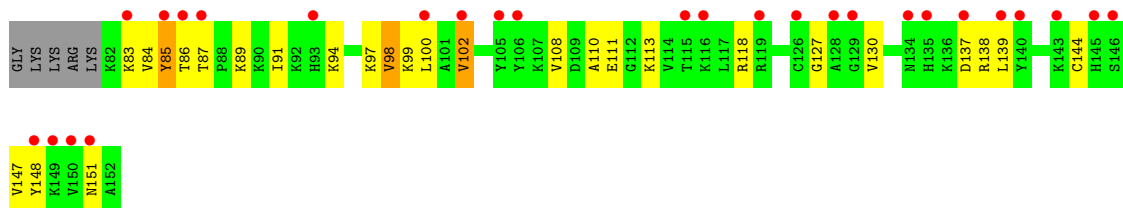
- Molecule 32: 40S ribosomal protein S30-A



- Molecule 32: 40S ribosomal protein S30-A



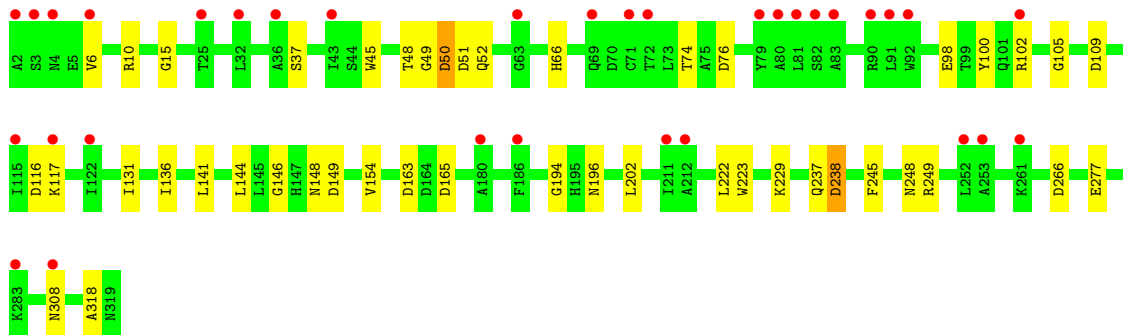
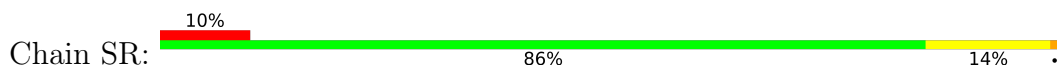
- Molecule 33: Ubiquitin-40S ribosomal protein S31



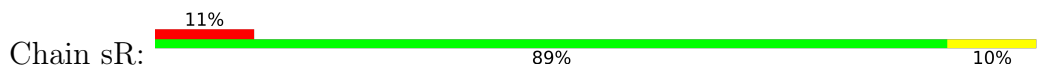
- Molecule 33: Ubiquitin-40S ribosomal protein S31

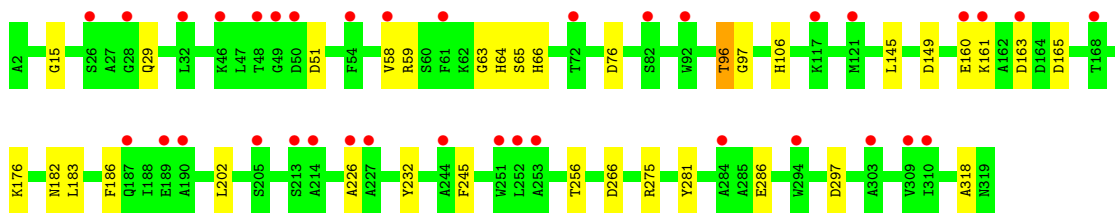


- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

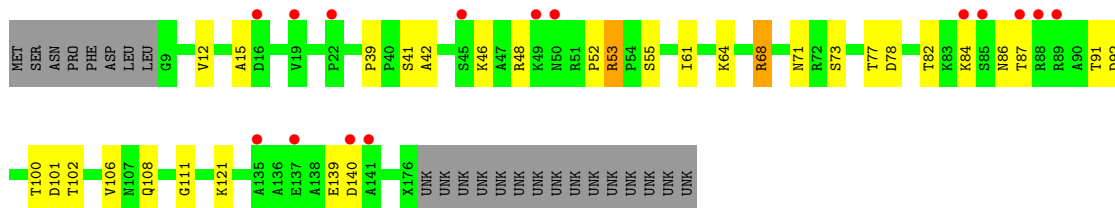
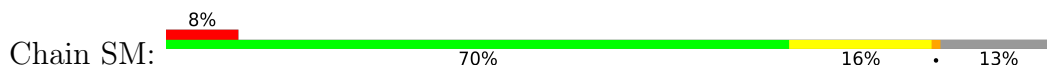


- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

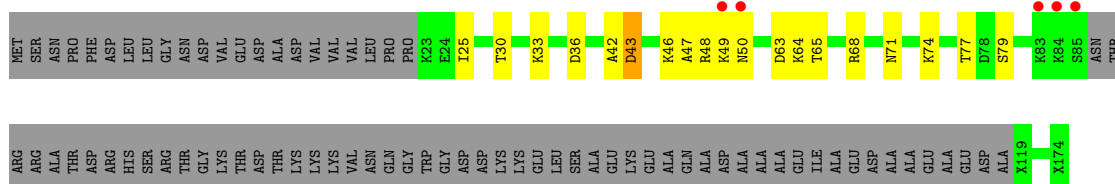




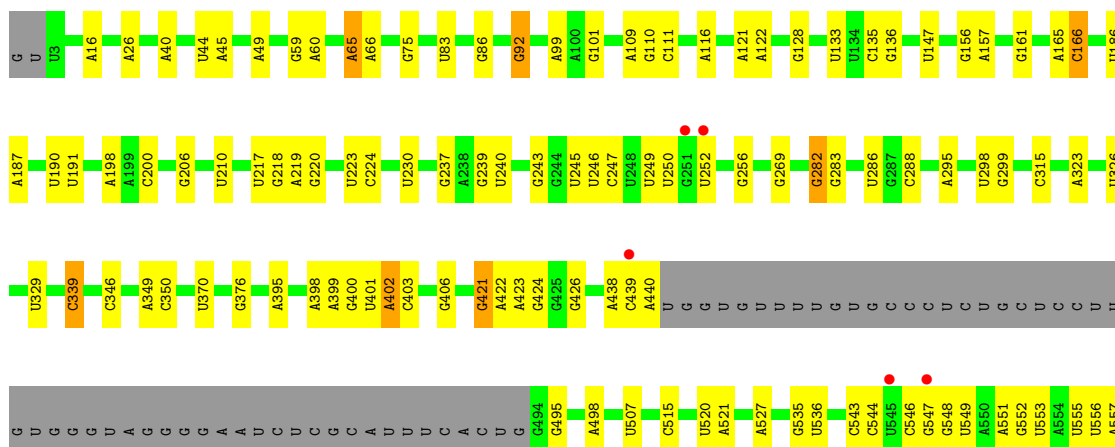
• Molecule 35: Suppressor protein STM1, Suppressor protein STM1, Suppressor protein STM1, Suppressor protein STM1, Suppressor protein STM1



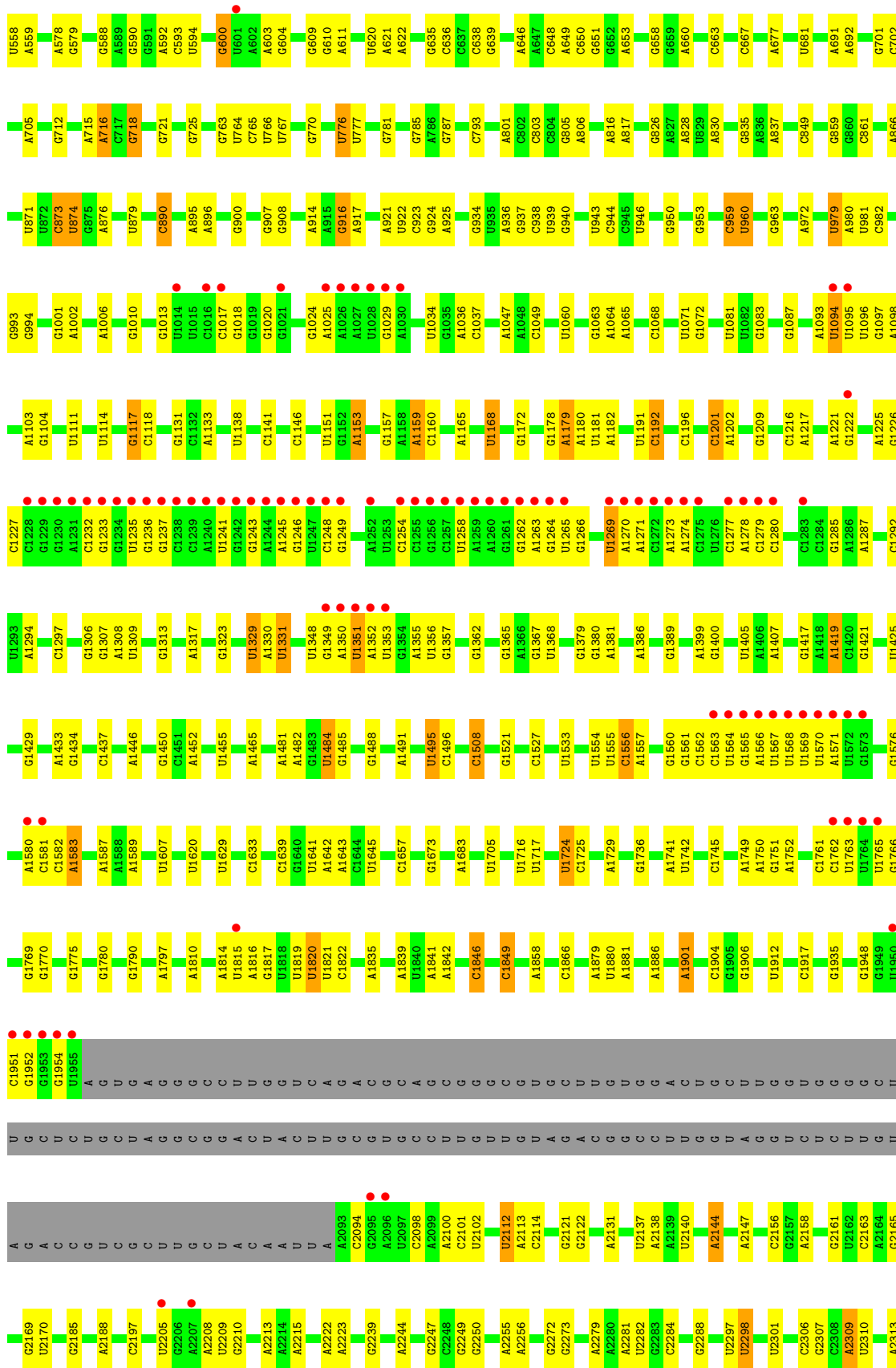
• Molecule 35: Suppressor protein STM1, Suppressor protein STM1, Suppressor protein STM1, Suppressor protein STM1, Suppressor protein STM1

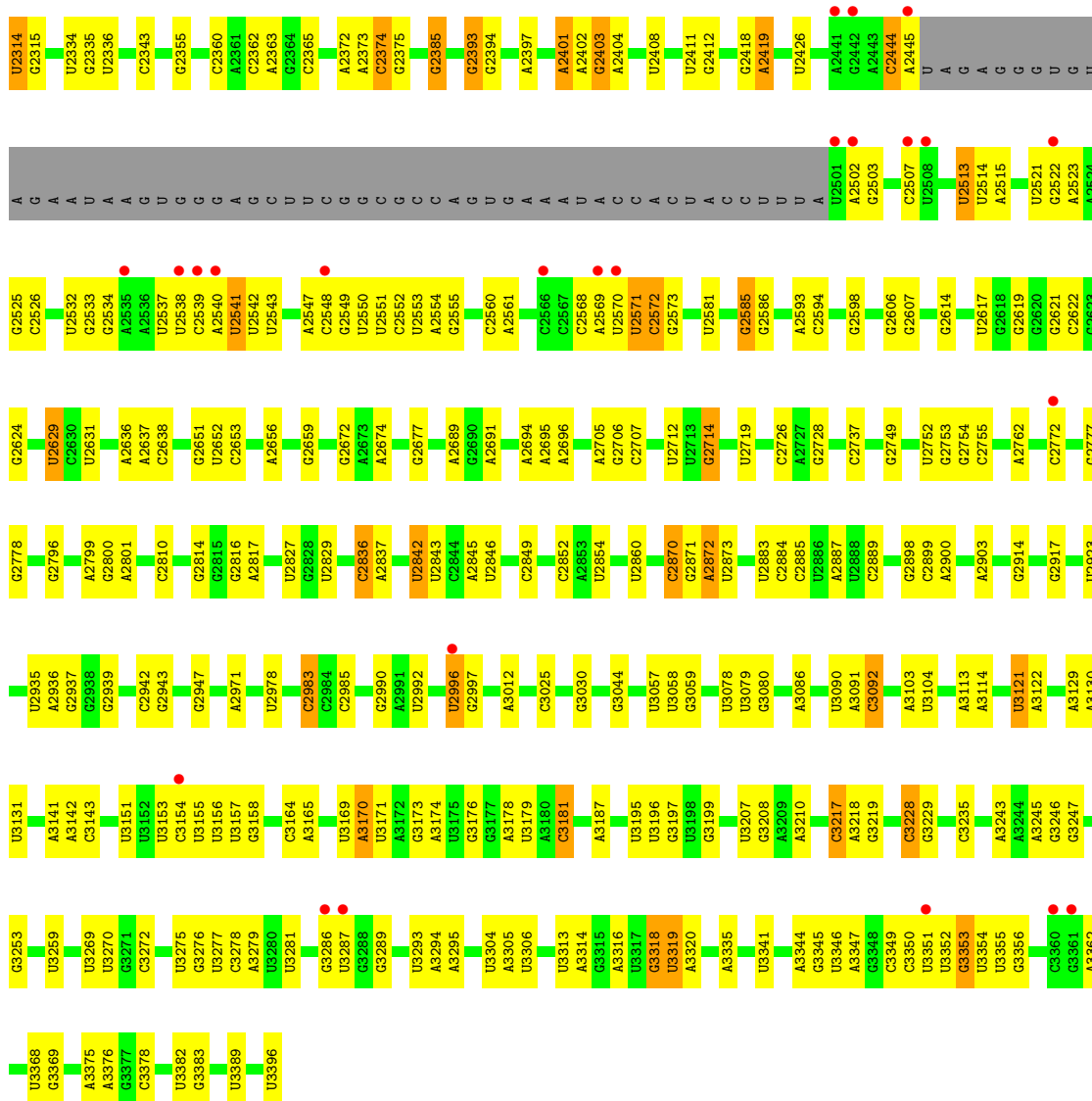


• Molecule 36: 25S ribosomal RNA

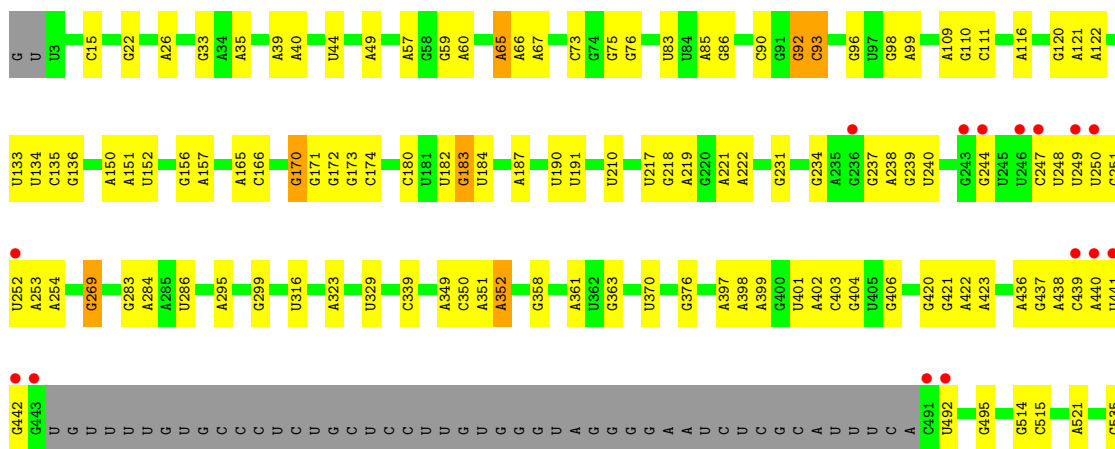


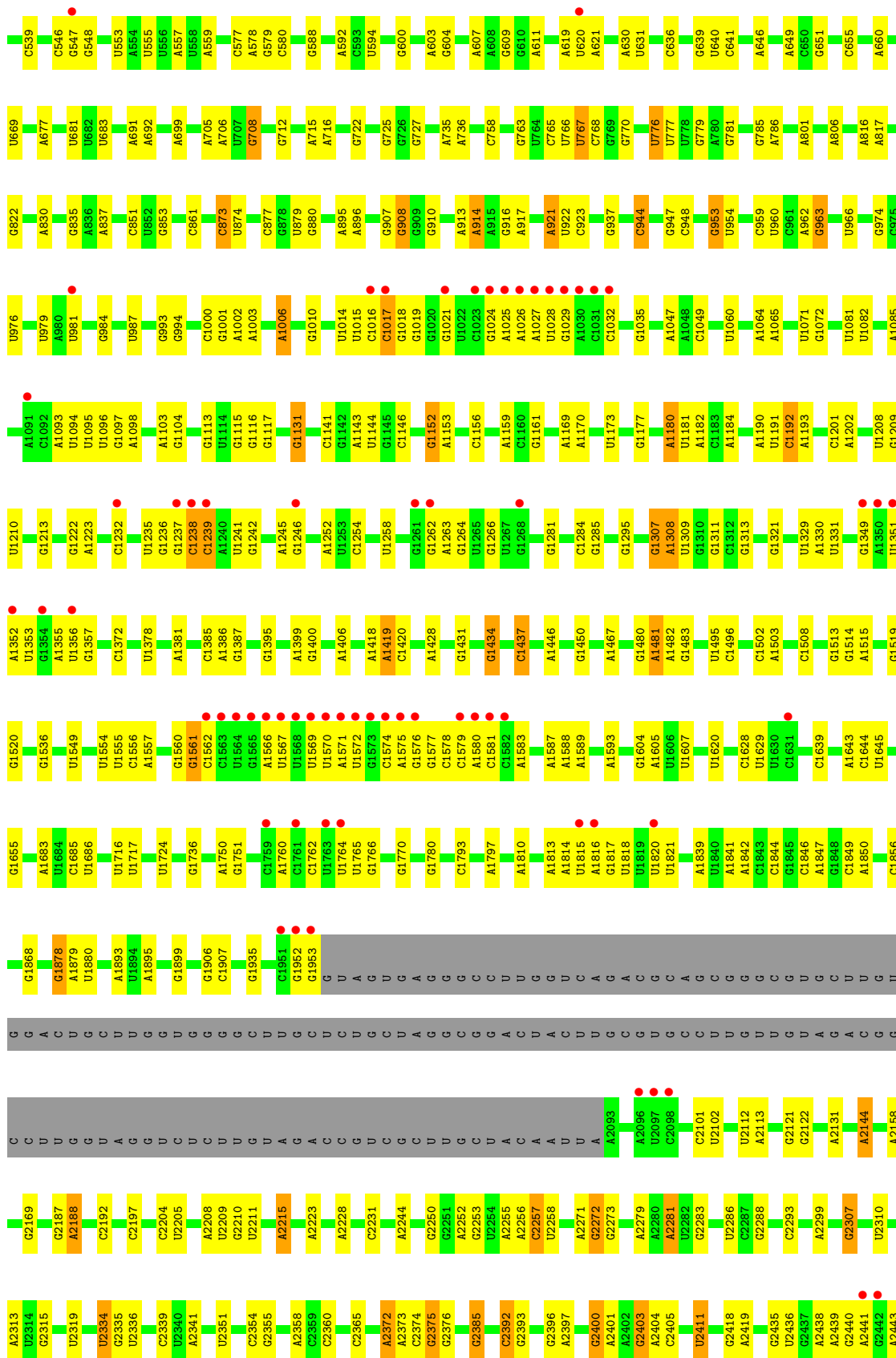


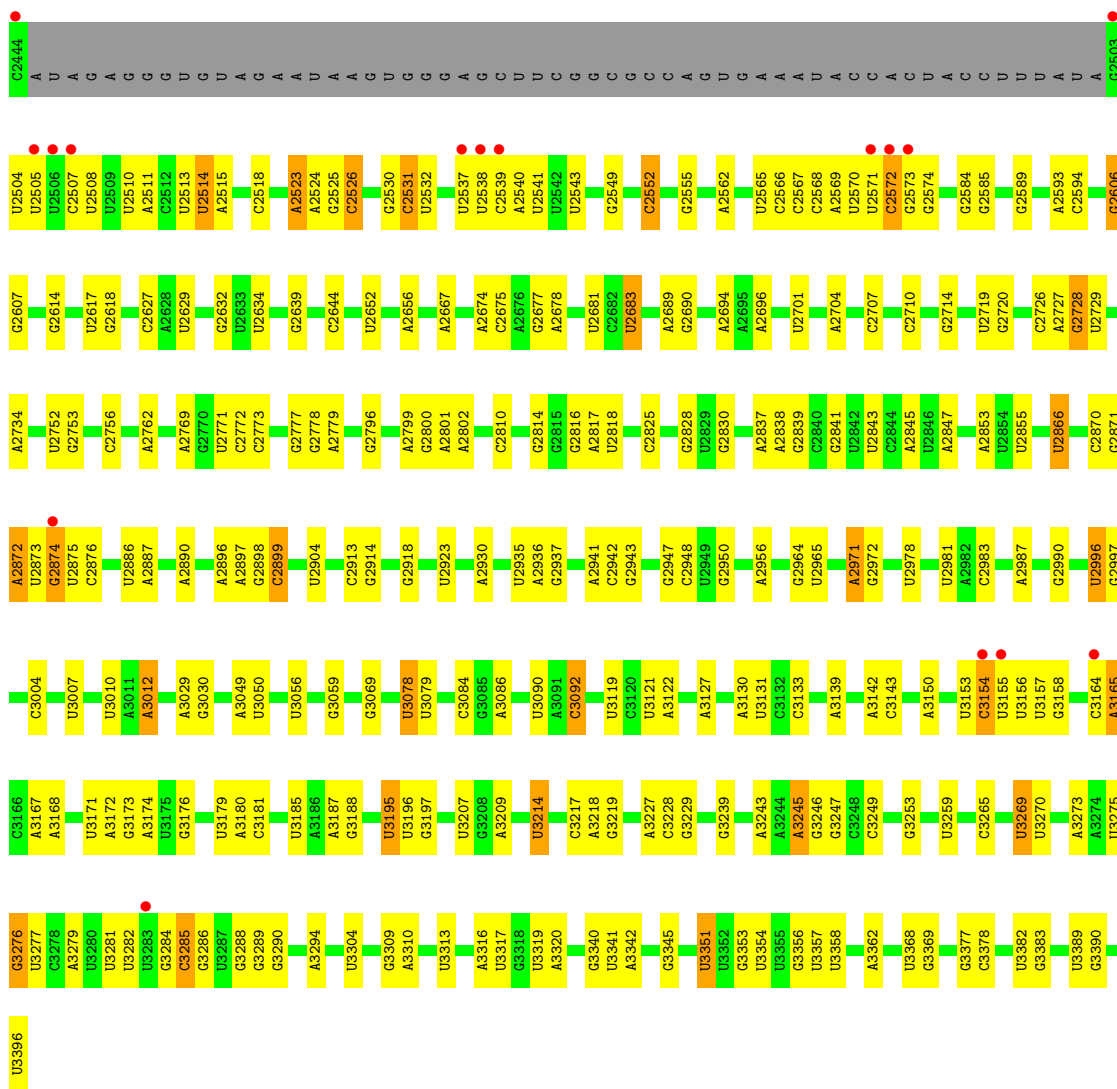




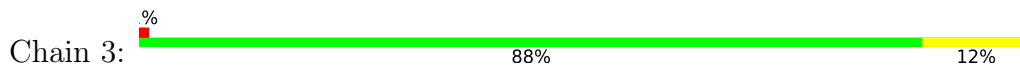
• Molecule 36: 25S ribosomal RNA



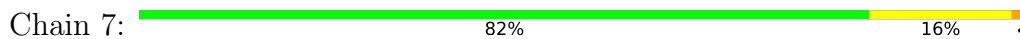




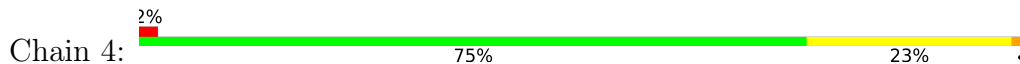
• Molecule 37: 5S ribosomal RNA

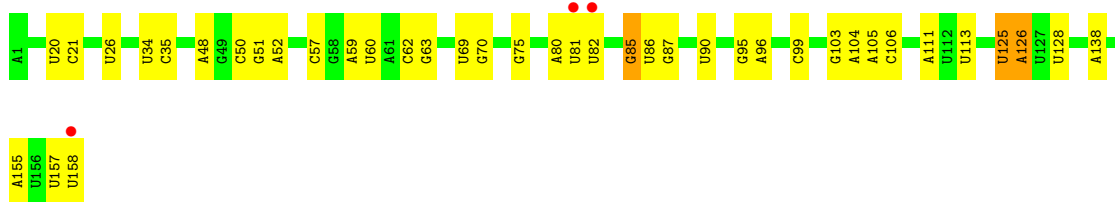


• Molecule 37: 5S ribosomal RNA

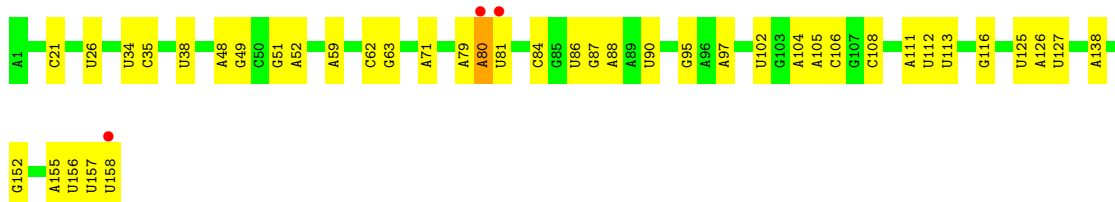
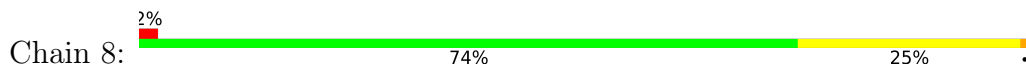


• Molecule 38: 5.8S ribosomal RNA

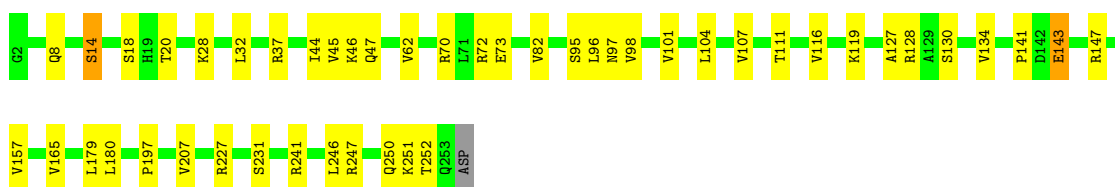
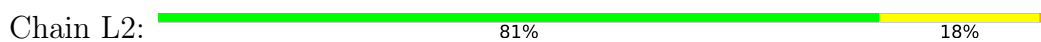




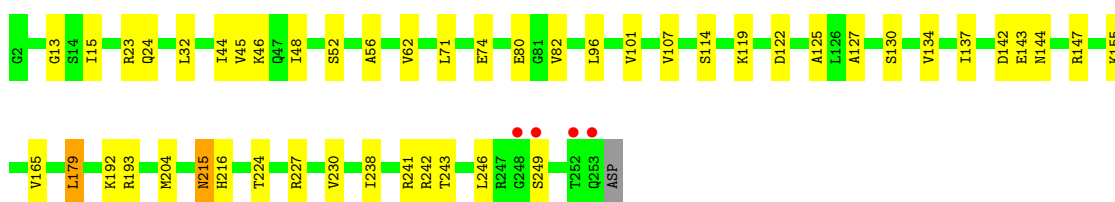
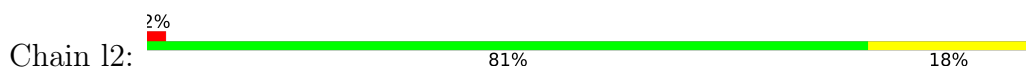
- Molecule 38: 5.8S ribosomal RNA



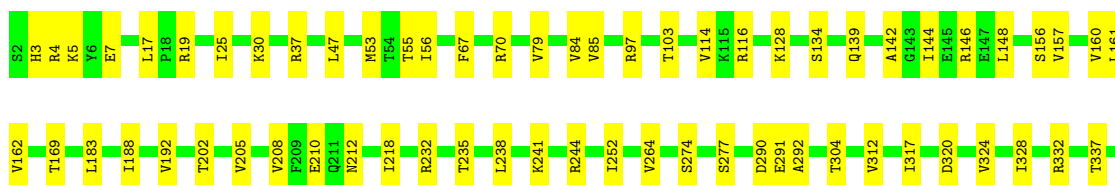
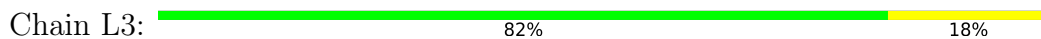
- Molecule 39: 60S ribosomal protein L2-A



- Molecule 39: 60S ribosomal protein L2-A



- Molecule 40: 60S ribosomal protein L3





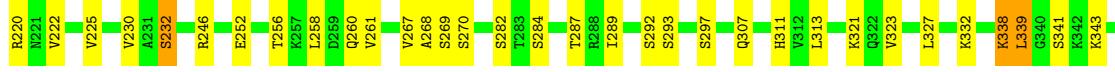
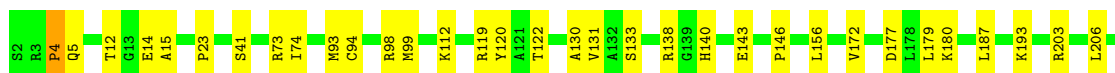
- Molecule 40: 60S ribosomal protein L3

Chain l3: 84% 16%



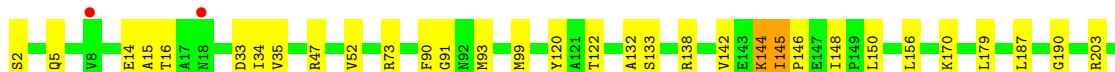
- Molecule 41: 60S ribosomal protein L4-A

Chain L4: 81% 18%



- Molecule 41: 60S ribosomal protein L4-A

Chain l4: 83% 15%

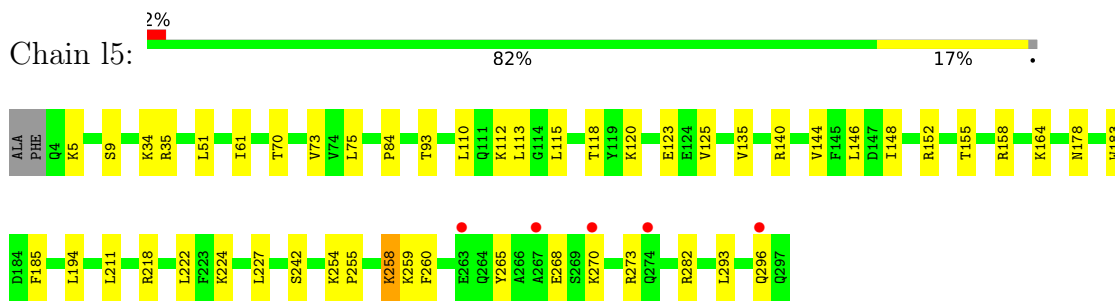


- Molecule 42: 60S ribosomal protein L5

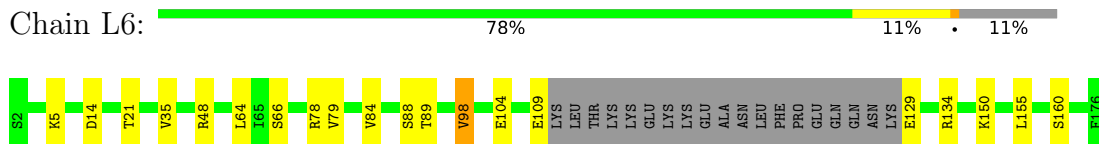
Chain L5: 81% 18%



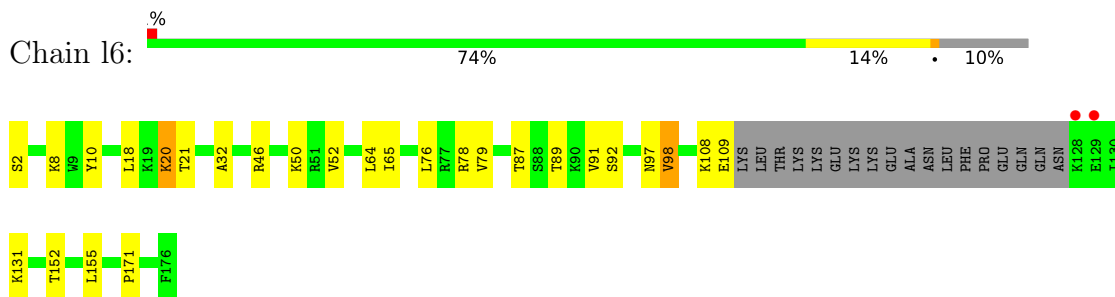
- Molecule 42: 60S ribosomal protein L5



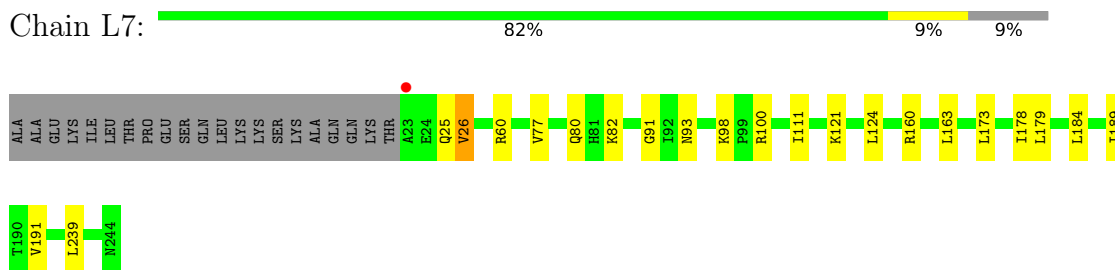
• Molecule 43: 60S ribosomal protein L6-A



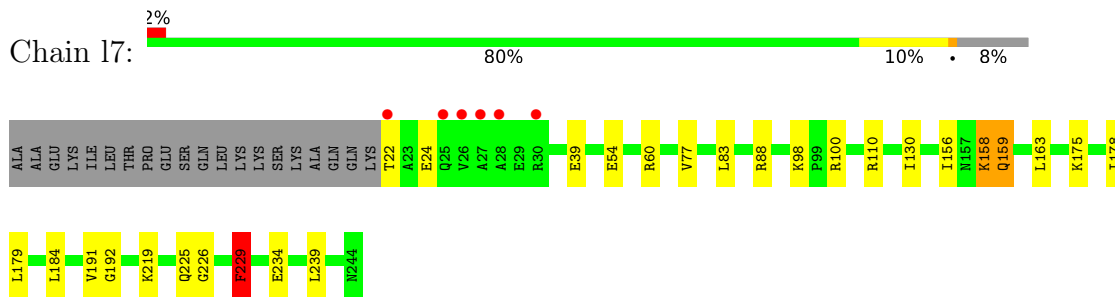
• Molecule 43: 60S ribosomal protein L6-A



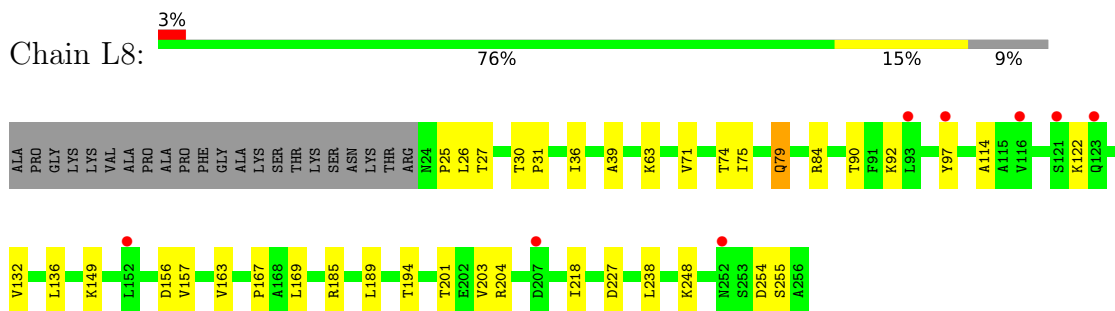
• Molecule 44: 60S ribosomal protein L7-A



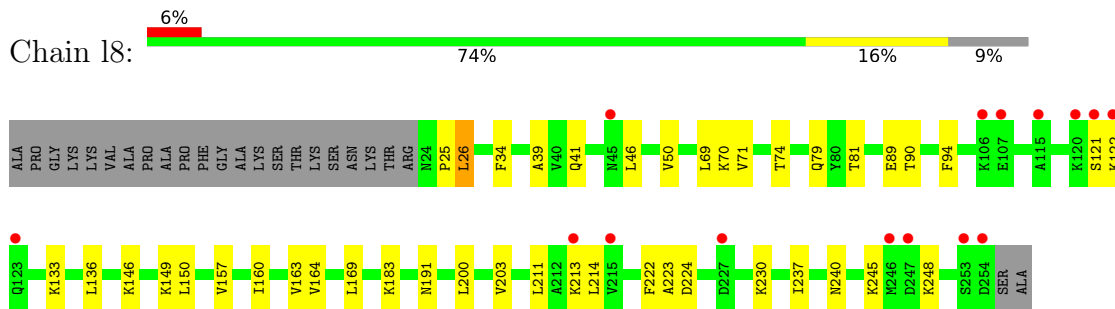
• Molecule 44: 60S ribosomal protein L7-A



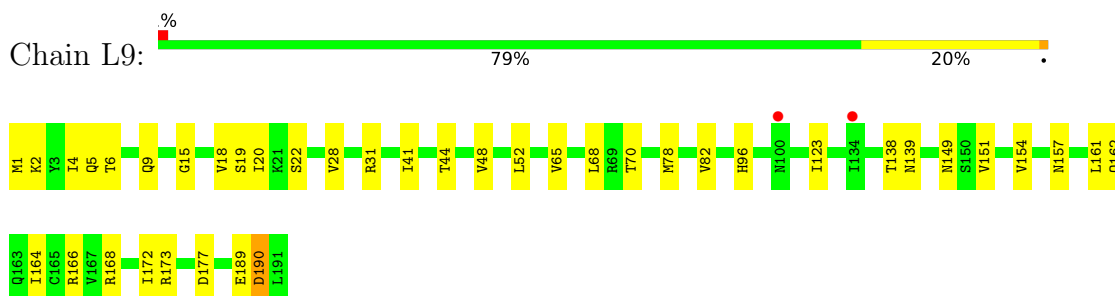
• Molecule 45: 60S ribosomal protein L8-A



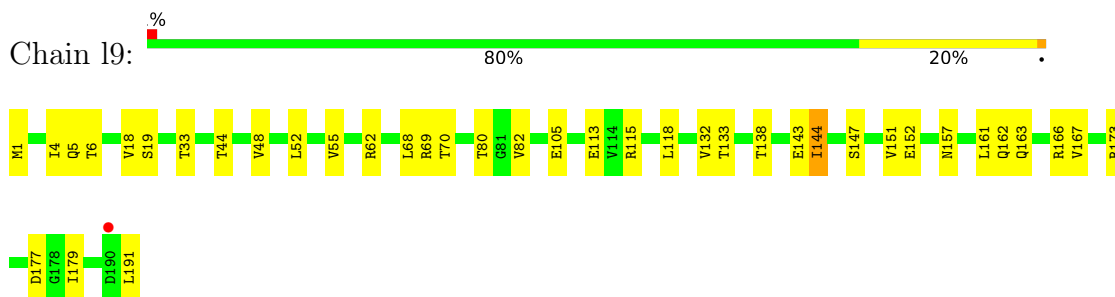
- Molecule 45: 60S ribosomal protein L8-A



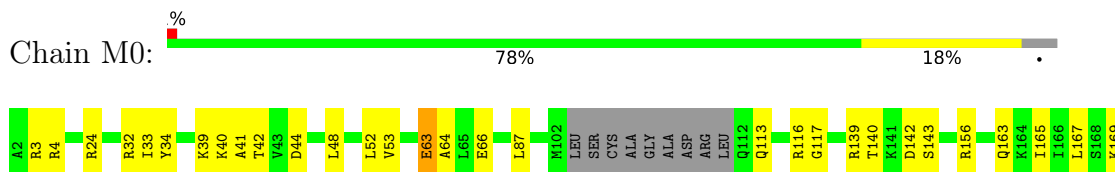
- Molecule 46: 60S ribosomal protein L9-A



- Molecule 46: 60S ribosomal protein L9-A



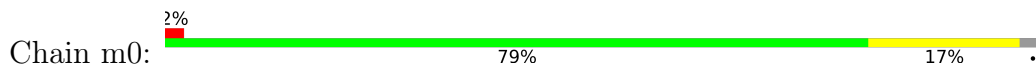
- Molecule 47: 60S ribosomal protein L10



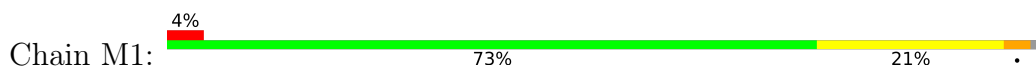




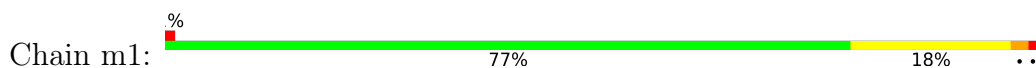
- Molecule 47: 60S ribosomal protein L10



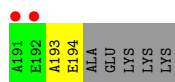
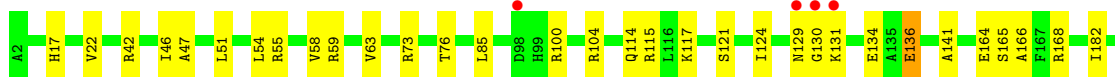
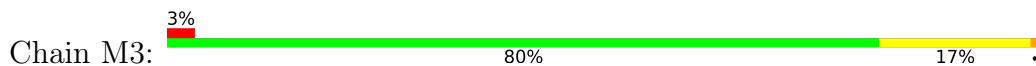
- Molecule 48: 60S ribosomal protein L11-A



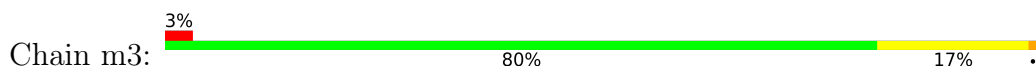
- Molecule 48: 60S ribosomal protein L11-A

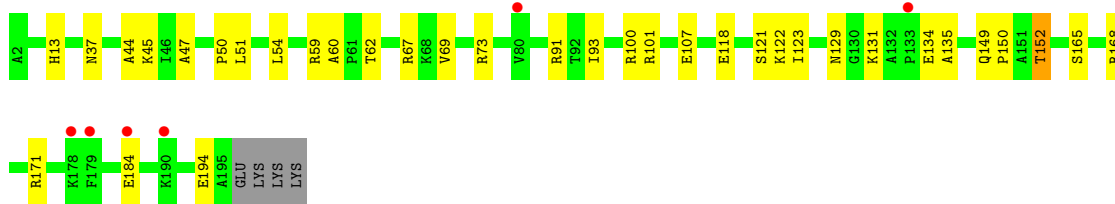


- Molecule 49: 60S ribosomal protein L13-A

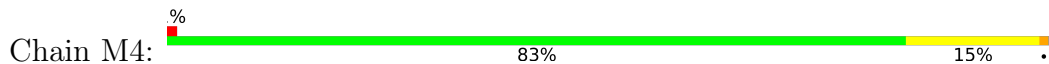


- Molecule 49: 60S ribosomal protein L13-A

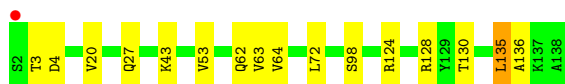
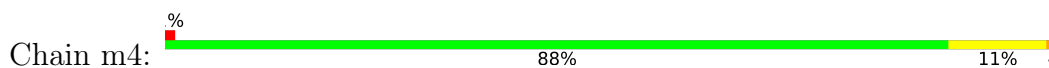




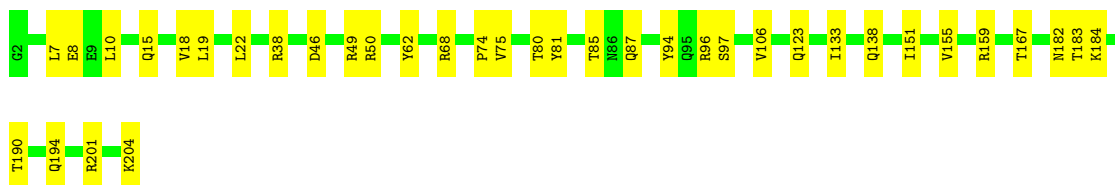
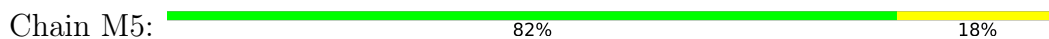
- Molecule 50: 60S ribosomal protein L14-A



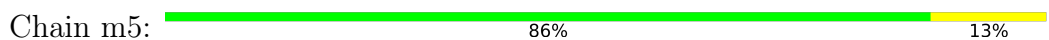
- Molecule 50: 60S ribosomal protein L14-A



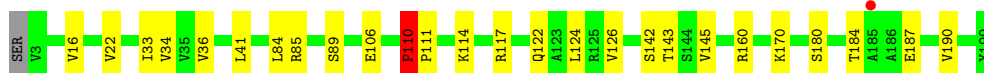
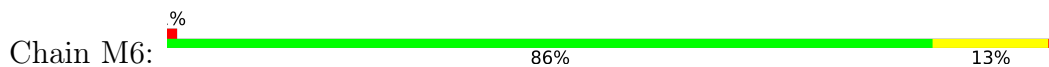
- Molecule 51: 60S ribosomal protein L15-A



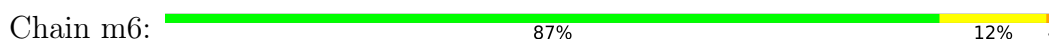
- Molecule 51: 60S ribosomal protein L15-A



- Molecule 52: 60S ribosomal protein L16-A

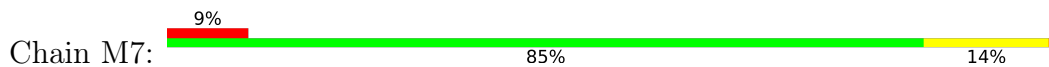


- Molecule 52: 60S ribosomal protein L16-A

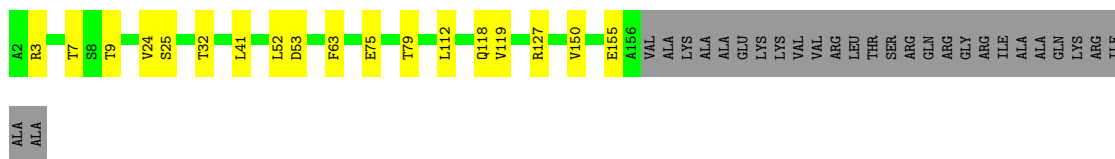
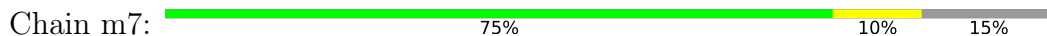




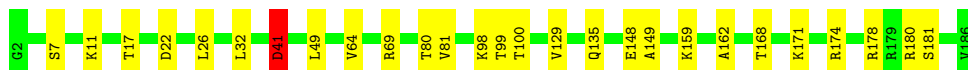
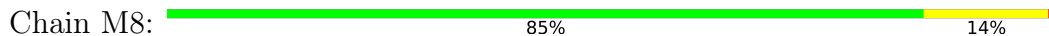
- Molecule 53: 60S ribosomal protein L17-A



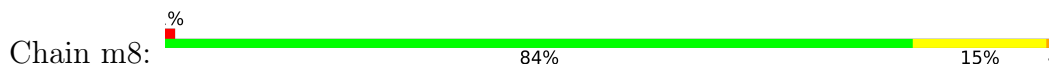
- Molecule 53: 60S ribosomal protein L17-A



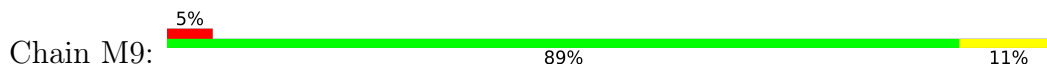
- Molecule 54: 60S ribosomal protein L18-A



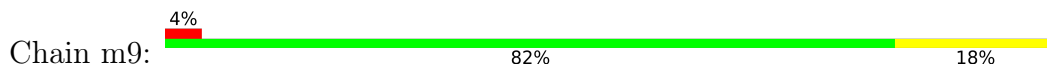
- Molecule 54: 60S ribosomal protein L18-A



- Molecule 55: 60S ribosomal protein L19-A

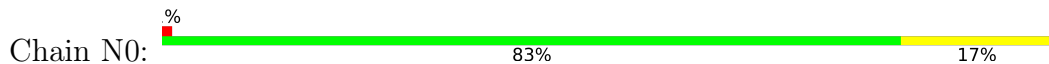


- Molecule 55: 60S ribosomal protein L19-A

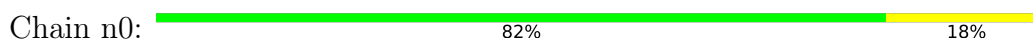




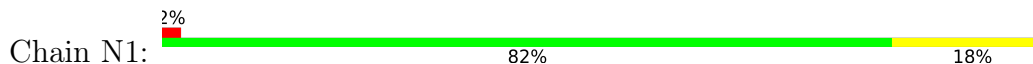
• Molecule 56: 60S ribosomal protein L20-A



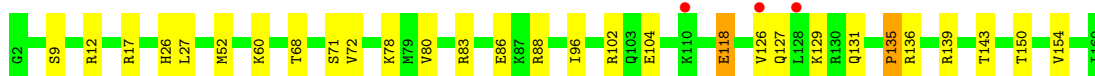
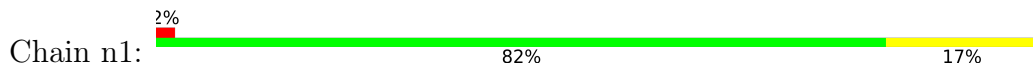
• Molecule 56: 60S ribosomal protein L20-A



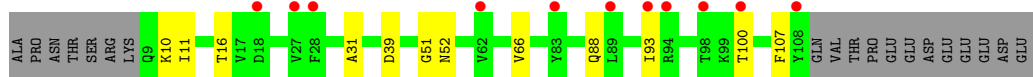
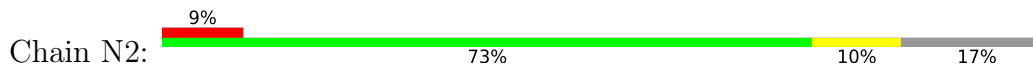
• Molecule 57: 60S ribosomal protein L21-A



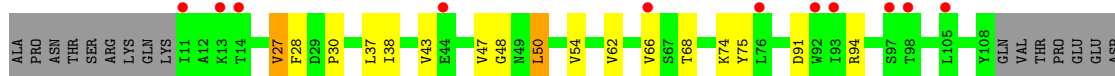
• Molecule 57: 60S ribosomal protein L21-A



• Molecule 58: 60S ribosomal protein L22-A

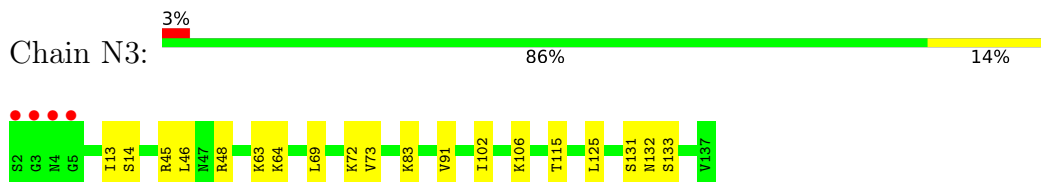


• Molecule 58: 60S ribosomal protein L22-A

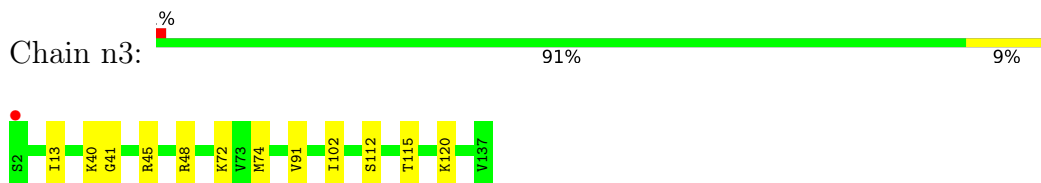


GLU  
GLU  
GLU  
ASP  
GLU  
GLU

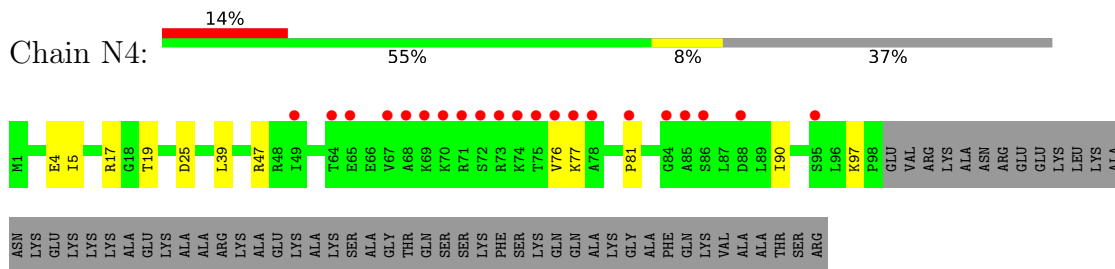
- Molecule 59: 60S ribosomal protein L23-A



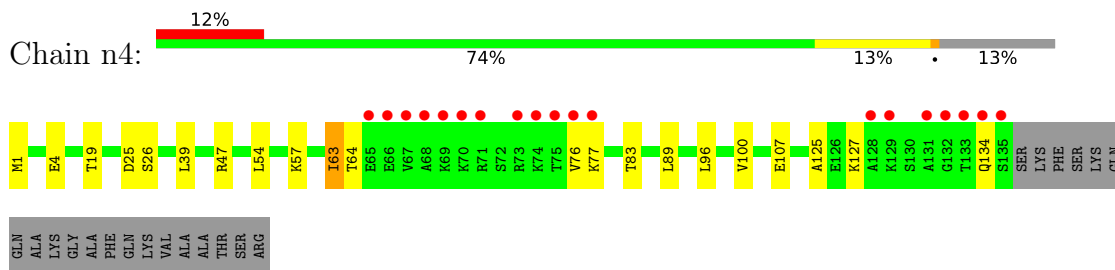
- Molecule 59: 60S ribosomal protein L23-A



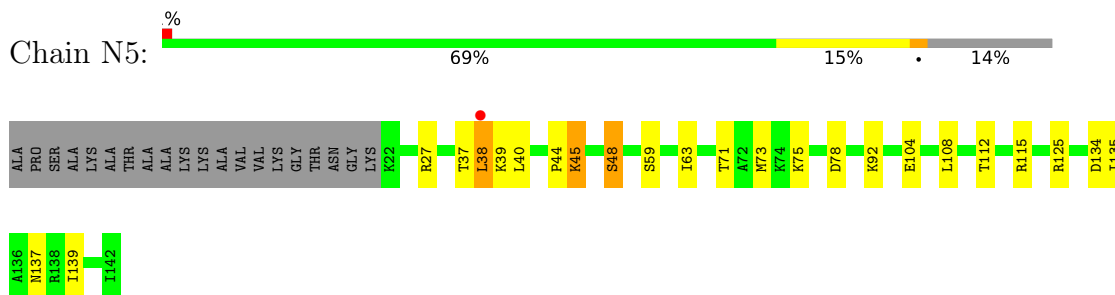
- Molecule 60: 60S ribosomal protein L24-A



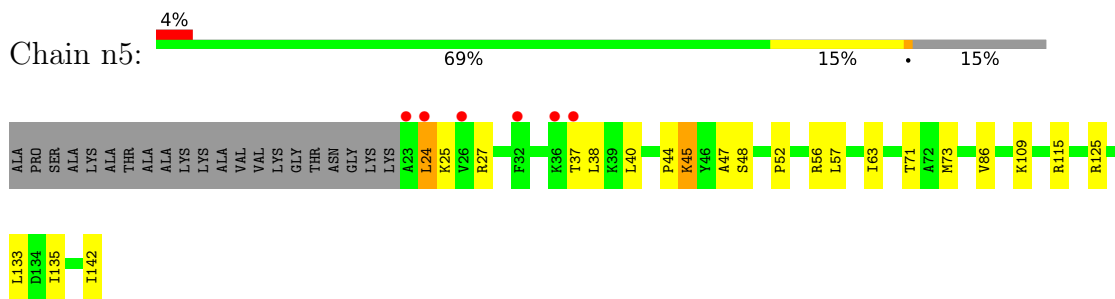
- Molecule 60: 60S ribosomal protein L24-A



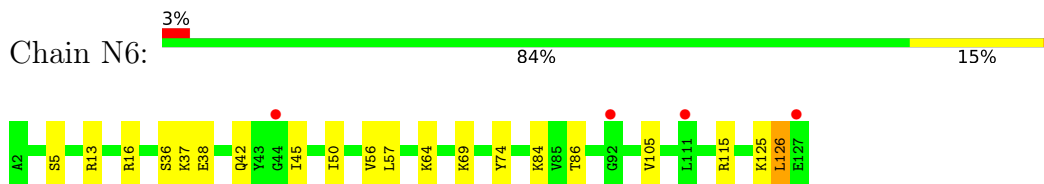
- Molecule 61: 60S ribosomal protein L25



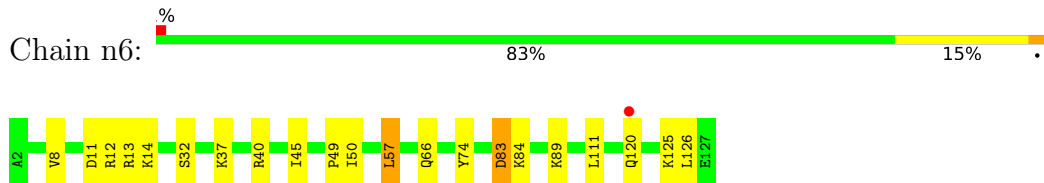
- Molecule 61: 60S ribosomal protein L25



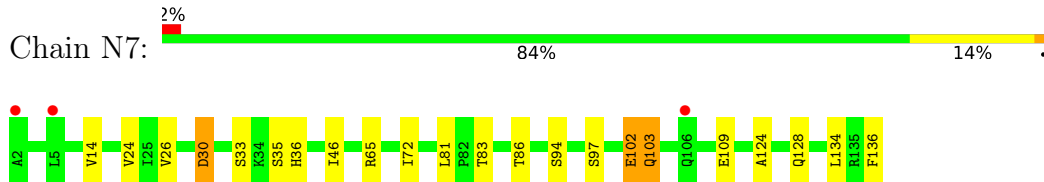
- Molecule 62: 60S ribosomal protein L26-A



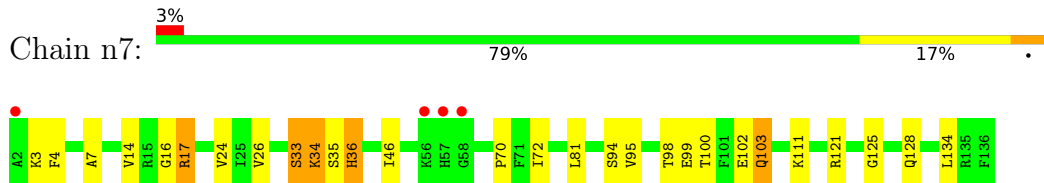
- Molecule 62: 60S ribosomal protein L26-A



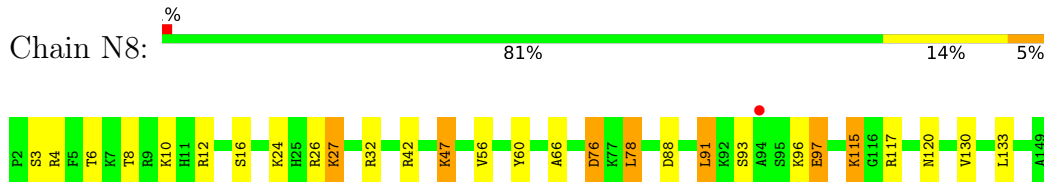
- Molecule 63: 60S ribosomal protein L27-A



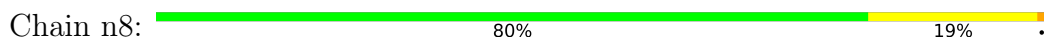
- Molecule 63: 60S ribosomal protein L27-A

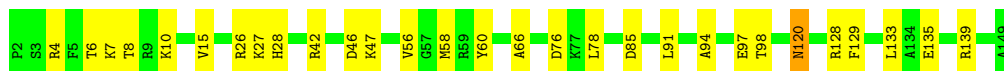


- Molecule 64: 60S ribosomal protein L28

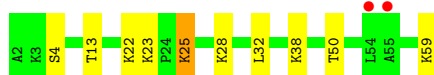
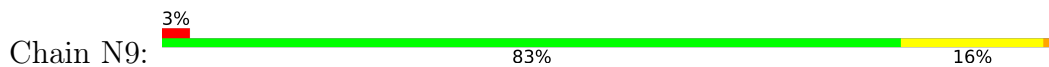


- Molecule 64: 60S ribosomal protein L28

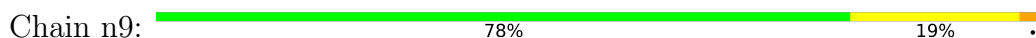




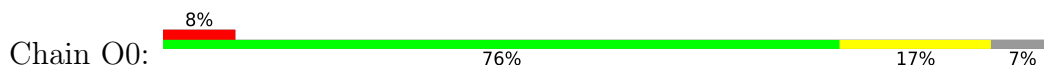
- Molecule 65: 60S ribosomal protein L29



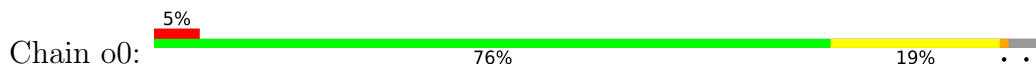
- Molecule 65: 60S ribosomal protein L29



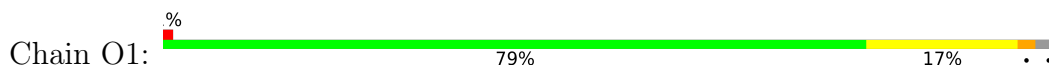
- Molecule 66: 60S ribosomal protein L30



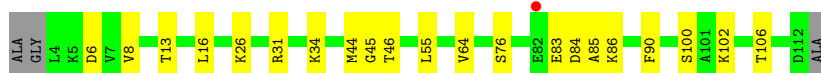
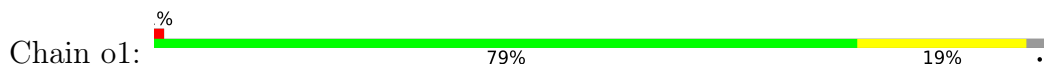
- Molecule 66: 60S ribosomal protein L30



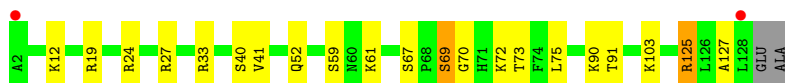
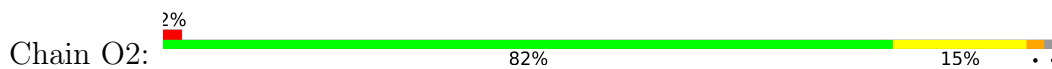
- Molecule 67: 60S ribosomal protein L31-A



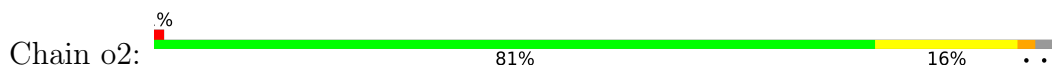
- Molecule 67: 60S ribosomal protein L31-A



- Molecule 68: 60S ribosomal protein L32



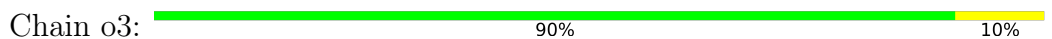
- Molecule 68: 60S ribosomal protein L32



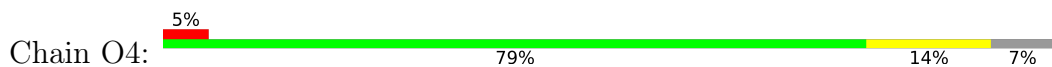
- Molecule 69: 60S ribosomal protein L33-A



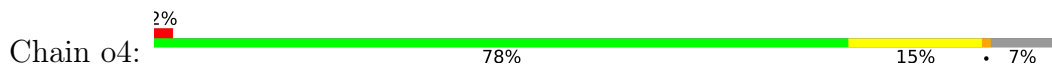
- Molecule 69: 60S ribosomal protein L33-A



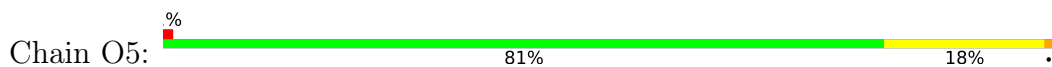
- Molecule 70: 60S ribosomal protein L34-A



- Molecule 70: 60S ribosomal protein L34-A

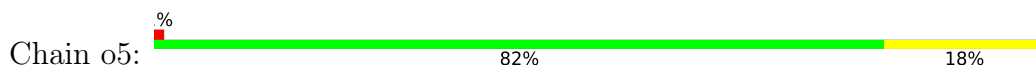


- Molecule 71: 60S ribosomal protein L35-A

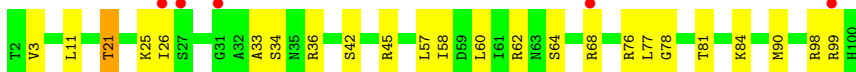
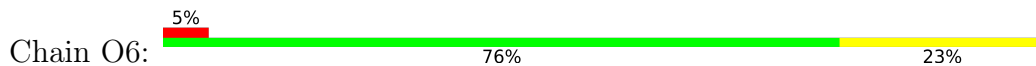


- Molecule 71: 60S ribosomal protein L35-A

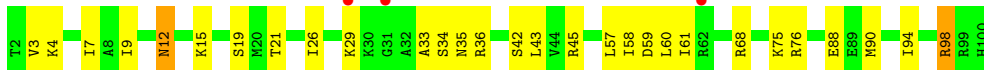




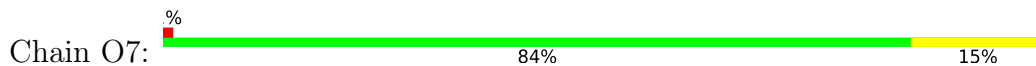
- Molecule 72: 60S ribosomal protein L36-A



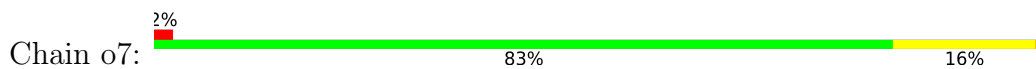
- Molecule 72: 60S ribosomal protein L36-A



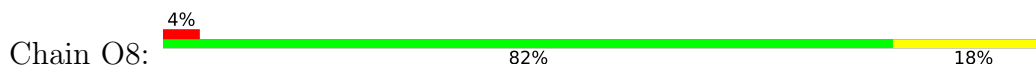
- Molecule 73: 60S ribosomal protein L37-A



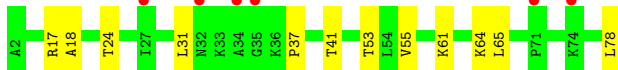
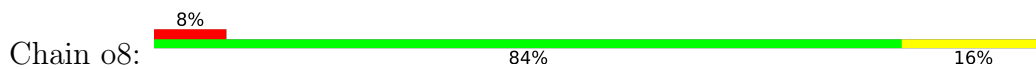
- Molecule 73: 60S ribosomal protein L37-A



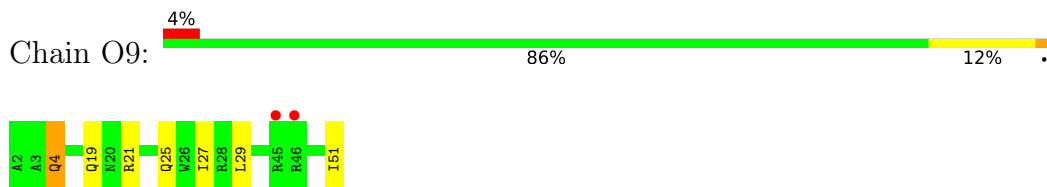
- Molecule 74: 60S ribosomal protein L38



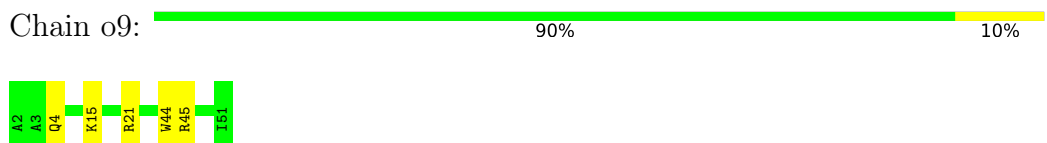
- Molecule 74: 60S ribosomal protein L38



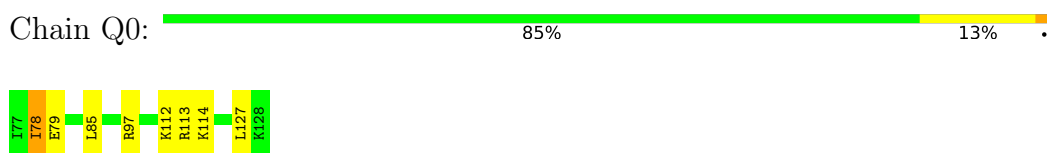
- Molecule 75: 60S ribosomal protein L39



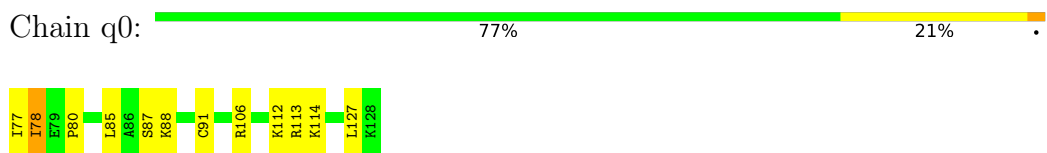
- Molecule 75: 60S ribosomal protein L39



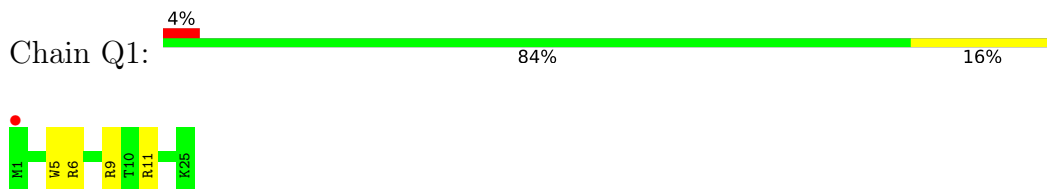
- Molecule 76: Ubiquitin-60S ribosomal protein L40



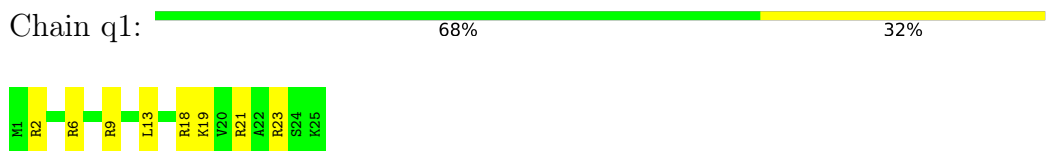
- Molecule 76: Ubiquitin-60S ribosomal protein L40



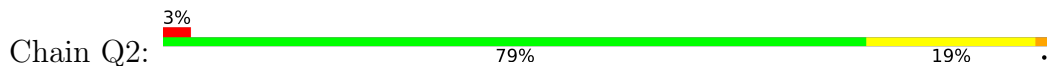
- Molecule 77: 60S ribosomal protein L41-A



- Molecule 77: 60S ribosomal protein L41-A

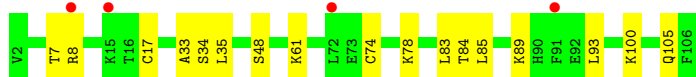
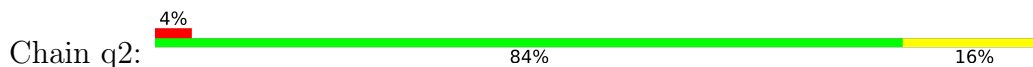


- Molecule 78: 60S ribosomal protein L42-A





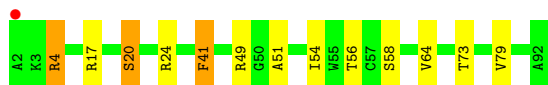
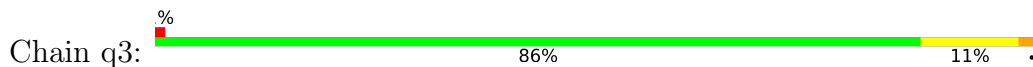
• Molecule 78: 60S ribosomal protein L42-A



• Molecule 79: 60S ribosomal protein L43-A



• Molecule 79: 60S ribosomal protein L43-A

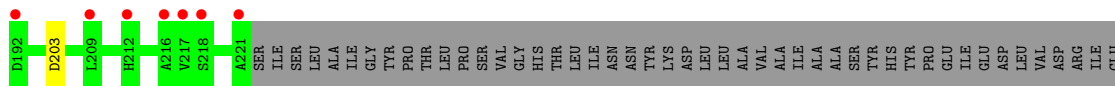
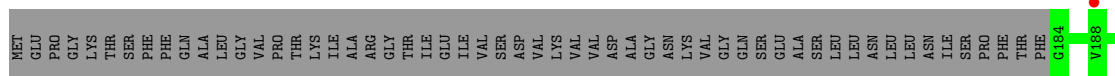
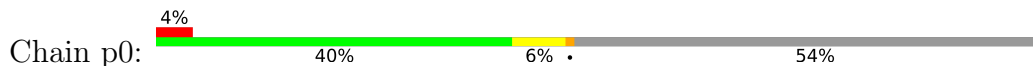


• Molecule 80: 60S ribosomal protein L12-A (uL11)



There are no outlier residues recorded for this chain.

• Molecule 81: 60S acidic ribosomal protein P0



• Molecule 82: 60S ribosomal protein P1 alpha

Chain p1:  100%

There are no outlier residues recorded for this chain.

- Molecule 83: 60S ribosomal protein P2 beta

Chain p2:  100%

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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.84 (at 3.12Å)	Xtrriage
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 <sup>2</sup> )	63.6	Xtrriage
Anisotropy	0.067	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 51.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	410912	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtrriage'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.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

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

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

All (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
36	5	1143	A	N9-C4	-5.83	1.34	1.37
36	1	2147	A	N9-C4	-5.68	1.34	1.37
36	1	2401	A	N3-C4	5.48	1.38	1.34
40	l3	255	CYS	CB-SG	-5.45	1.73	1.81
41	L4	94	CYS	CB-SG	-5.31	1.73	1.81
36	5	2358	A	N9-C4	-5.29	1.34	1.37
36	1	2971	A	N9-C4	5.27	1.41	1.37
36	5	1152	G	C2-N3	-5.24	1.28	1.32
52	m6	40	GLU	CG-CD	5.15	1.59	1.51
36	5	2769	A	N9-C4	-5.02	1.34	1.37

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
36	5	2617	U	O5'-P-OP2	-9.54	97.11	105.70
36	1	2996	U	C2-N1-C1'	9.16	128.69	117.70
36	5	1152	G	C8-N9-C1'	9.15	138.89	127.00
1	6	163	G	N3-C4-N9	-9.11	120.54	126.00
36	5	2728	G	O5'-P-OP2	-9.04	97.57	105.70
1	6	1	U	C2-N1-C1'	8.98	128.47	117.70
36	1	2622	C	C6-N1-C2	-8.89	116.74	120.30
36	1	3278	C	N1-C2-O2	8.88	124.23	118.90
1	6	1000	C	C2-N1-C1'	8.84	128.52	118.80
36	1	3217	C	C2-N1-C1'	8.59	128.25	118.80
36	5	406	G	O4'-C1'-N9	8.54	115.03	108.20
36	1	3278	C	N3-C2-O2	-8.49	115.96	121.90
1	6	453	U	C2-N1-C1'	8.49	127.89	117.70
36	1	2419	A	O5'-P-OP1	-8.48	98.07	105.70
36	5	2572	C	N1-C2-O2	8.44	123.96	118.90
36	5	1152	G	N3-C2-N2	-8.39	114.03	119.90
38	4	125	U	N1-C2-O2	8.39	128.67	122.80
36	5	1152	G	C5-N7-C8	-8.38	100.11	104.30
36	5	2272	G	O4'-C1'-N9	8.36	114.89	108.20
36	5	3276	G	O4'-C1'-N9	8.36	114.89	108.20
1	6	321	C	N3-C2-O2	-8.30	116.09	121.90
36	5	948	C	C6-N1-C2	8.28	123.61	120.30
36	5	2726	C	C6-N1-C2	-8.26	117.00	120.30
36	5	922	U	N3-C2-O2	-8.19	116.47	122.20
36	5	3154	C	N1-C2-O2	8.16	123.80	118.90
36	1	2572	C	N1-C2-O2	8.13	123.78	118.90
36	1	2403	G	N1-C6-O6	8.11	124.76	119.90
36	1	406	G	O4'-C1'-N9	8.07	114.65	108.20
1	6	1537	C	C5-C6-N1	8.06	125.03	121.00
36	5	1152	G	C4-N9-C1'	-7.99	116.11	126.50
1	6	194	U	C2-N1-C1'	7.95	127.24	117.70
36	1	2572	C	C2-N1-C1'	7.95	127.54	118.80
36	5	3245	A	C2-N3-C4	-7.93	106.63	110.60
36	5	3245	A	C5-N7-C8	-7.90	99.95	103.90
1	2	639	U	N3-C2-O2	-7.76	116.77	122.20
36	1	2726	C	N3-C2-O2	-7.74	116.48	121.90
36	5	283	G	C4-C5-N7	7.74	113.90	110.80
36	1	2617	U	C5-C4-O4	7.72	130.53	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	641	C	N1-C2-O2	-7.71	114.28	118.90
1	2	1096	C	C2-N1-C1'	7.69	127.26	118.80
36	5	3197	G	N3-C4-N9	-7.67	121.40	126.00
36	5	2816	G	C8-N9-C4	7.67	109.47	106.40
1	6	1537	C	C2-N3-C4	7.66	123.73	119.90
36	5	835	G	O4'-C1'-N9	7.65	114.32	108.20
36	5	2351	U	N3-C2-O2	-7.62	116.86	122.20
36	1	639	G	N1-C6-O6	7.60	124.46	119.90
36	5	3197	G	N3-C2-N2	-7.60	114.58	119.90
36	1	590	G	C5-C6-O6	-7.59	124.04	128.60
36	1	1365	G	N3-C4-C5	-7.59	124.80	128.60
36	1	1846	C	N1-C2-O2	-7.57	114.36	118.90
1	2	1052	U	C2-N1-C1'	7.55	126.76	117.70
48	m1	112	LEU	CA-CB-CG	7.53	132.61	115.30
36	5	2572	C	C2-N1-C1'	7.50	127.05	118.80
36	1	1365	G	C8-N9-C4	-7.47	103.41	106.40
36	1	1565	G	C8-N9-C4	-7.46	103.42	106.40
36	1	1904	C	C6-N1-C2	-7.45	117.32	120.30
36	5	2341	A	C8-N9-C4	7.42	108.77	105.80
36	5	3154	C	C2-N1-C1'	7.42	126.96	118.80
36	5	1208	U	N3-C2-O2	-7.39	117.03	122.20
36	1	2403	G	C5-C6-O6	-7.37	124.18	128.60
36	1	2870	C	C2-N1-C1'	-7.33	110.74	118.80
1	2	1537	C	C5-C6-N1	7.30	124.65	121.00
36	1	406	G	N1-C6-O6	-7.28	115.53	119.90
38	4	125	U	N3-C2-O2	-7.28	117.10	122.20
36	1	692	A	O5'-P-OP1	-7.27	99.15	105.70
36	5	708	G	C8-N9-C4	-7.26	103.49	106.40
36	5	639	G	N1-C6-O6	7.26	124.26	119.90
36	5	1208	U	C5-C4-O4	7.25	130.25	125.90
36	1	1389	G	C4-C5-N7	7.23	113.69	110.80
36	1	2314	U	C5-C6-N1	7.22	126.31	122.70
36	5	2726	C	C5-C4-N4	7.22	125.25	120.20
36	5	2874	G	P-O3'-C3'	7.21	128.35	119.70
36	1	1581	C	N1-C2-O2	7.20	123.22	118.90
18	C6	40	GLU	C-N-CD	-7.19	104.79	120.60
36	1	3319	U	P-O3'-C3'	7.17	128.31	119.70
36	1	2401	A	C2-N3-C4	-7.17	107.01	110.60
36	5	3245	A	N7-C8-N9	7.15	117.38	113.80
36	1	638	C	N1-C2-O2	7.10	123.16	118.90
1	2	728	U	C2-N1-C1'	7.06	126.17	117.70
36	1	2363	A	N1-C6-N6	-7.02	114.39	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	639	U	N1-C2-O2	7.00	127.70	122.80
36	1	2629	U	O5'-P-OP2	-7.00	99.40	105.70
1	2	73	U	O4'-C1'-N1	7.00	113.80	108.20
36	5	2701	U	C5-C4-O4	-7.00	121.70	125.90
36	1	1508	C	C6-N1-C2	-6.98	117.51	120.30
36	5	2704	A	O5'-P-OP1	-6.98	99.42	105.70
36	5	3012	A	C8-N9-C4	6.98	108.59	105.80
38	4	99	C	C6-N1-C2	6.95	123.08	120.30
36	5	987	U	O5'-P-OP1	-6.95	99.44	105.70
36	1	1269	U	C2-N1-C1'	6.92	126.00	117.70
36	5	2572	C	N3-C2-O2	-6.91	117.06	121.90
1	6	321	C	C6-N1-C2	-6.91	117.54	120.30
36	5	361	A	N1-C6-N6	-6.91	114.46	118.60
36	1	3306	U	N3-C2-O2	-6.90	117.37	122.20
78	q2	17	CYS	CA-CB-SG	6.90	126.42	114.00
36	1	2872	A	N1-C6-N6	6.89	122.74	118.60
36	1	2885	C	C6-N1-C2	6.88	123.05	120.30
1	6	1097	U	P-O3'-C3'	6.88	127.95	119.70
36	5	2231	C	C2-N1-C1'	6.86	126.34	118.80
1	6	1114	G	O4'-C1'-N9	6.86	113.69	108.20
36	5	1060	U	C6-N1-C2	6.85	125.11	121.00
36	5	2334	U	N3-C2-O2	-6.84	117.41	122.20
36	5	1495	U	C2-N1-C1'	6.84	125.91	117.70
1	6	194	U	N1-C2-O2	6.84	127.59	122.80
36	1	421	G	O5'-P-OP1	-6.82	99.56	105.70
1	2	959	U	N3-C2-O2	-6.82	117.42	122.20
1	6	1000	C	C6-N1-C1'	-6.82	112.62	120.80
1	2	830	U	N3-C2-O2	-6.81	117.43	122.20
36	5	3214	U	N3-C2-O2	-6.80	117.44	122.20
36	1	3362	A	O4'-C1'-N9	6.80	113.64	108.20
36	5	3092	C	O4'-C1'-N1	6.79	113.63	108.20
1	2	1096	C	N1-C2-O2	6.78	122.97	118.90
1	6	795	U	N3-C2-O2	-6.77	117.46	122.20
1	6	321	C	N1-C2-O2	6.74	122.94	118.90
36	1	2550	U	N3-C2-O2	-6.74	117.49	122.20
1	2	1039	A	O4'-C1'-N9	6.73	113.58	108.20
1	6	813	U	C2-N1-C1'	6.73	125.78	117.70
36	1	939	U	N1-C2-O2	-6.72	118.10	122.80
36	1	959	C	C6-N1-C2	6.71	122.98	120.30
36	5	1210	U	O5'-P-OP1	-6.70	99.67	105.70
36	1	2996	U	N1-C2-O2	6.69	127.48	122.80
1	2	1370	U	P-O3'-C3'	6.69	127.73	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1094	U	OP1-P-O3'	6.68	119.90	105.20
36	1	1495	U	C2-N1-C1'	-6.67	109.69	117.70
36	5	2644	C	O5'-P-OP1	-6.67	99.69	105.70
36	5	2726	C	N3-C2-O2	-6.67	117.23	121.90
36	5	921	A	C8-N9-C4	-6.67	103.13	105.80
36	1	92	G	C5-C6-N1	6.67	114.83	111.50
1	6	1	U	N1-C2-O2	6.65	127.46	122.80
1	2	728	U	N1-C2-O2	6.64	127.45	122.80
36	1	2572	C	N3-C2-O2	-6.63	117.26	121.90
1	2	75	U	C2-N1-C1'	6.62	125.65	117.70
36	1	402	A	N1-C6-N6	-6.62	114.63	118.60
36	1	282	G	O5'-P-OP1	-6.62	99.74	105.70
65	n9	23	LYS	C-N-CD	6.62	142.30	128.40
36	1	770	G	O4'-C1'-N9	6.61	113.49	108.20
36	1	3181	C	N3-C2-O2	-6.61	117.27	121.90
1	6	194	U	N3-C2-O2	-6.60	117.58	122.20
36	5	2403	G	O5'-P-OP2	-6.60	99.76	105.70
36	5	2978	U	O4'-C1'-N1	6.59	113.47	108.20
36	5	1308	A	O5'-P-OP1	-6.59	99.77	105.70
1	2	1698	G	P-O3'-C3'	6.58	127.60	119.70
36	1	1380	G	N3-C4-C5	6.56	131.88	128.60
36	5	2403	G	N1-C6-O6	6.56	123.84	119.90
38	4	125	U	C2-N1-C1'	6.54	125.55	117.70
36	5	1856	C	C6-N1-C2	-6.54	117.68	120.30
52	m6	78	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	2	728	U	N3-C2-O2	-6.52	117.64	122.20
31	D9	36	LEU	CA-CB-CG	6.52	130.30	115.30
36	5	1878	G	C4-N9-C1'	6.51	134.96	126.50
1	2	1600	A	O4'-C1'-N9	6.51	113.41	108.20
1	2	959	U	N1-C2-O2	6.50	127.35	122.80
1	2	831	U	C5-C6-N1	6.49	125.94	122.70
40	l3	4	ARG	NE-CZ-NH1	6.47	123.54	120.30
36	1	3306	U	C5-C4-O4	6.47	129.78	125.90
36	1	439	C	N1-C2-O2	6.47	122.78	118.90
36	1	702	C	C6-N1-C2	-6.47	117.71	120.30
1	6	163	G	N3-C2-N2	-6.47	115.37	119.90
36	1	646	A	C8-N9-C4	-6.46	103.21	105.80
36	1	2983	C	N3-C2-O2	-6.46	117.38	121.90
36	1	2827	U	C5-C4-O4	6.44	129.77	125.90
36	5	1208	U	N3-C4-O4	-6.44	114.89	119.40
36	1	1495	U	N1-C2-O2	-6.44	118.29	122.80
44	l7	229	PHE	CB-CG-CD1	6.44	125.31	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2306	C	N1-C2-O2	6.44	122.76	118.90
36	1	874	U	O5'-P-OP1	-6.43	99.91	105.70
36	1	2306	C	C2-N1-C1'	6.43	125.87	118.80
36	5	908	G	C4-N9-C1'	6.43	134.85	126.50
36	5	1115	G	C4-N9-C1'	6.42	134.85	126.50
36	1	2144	A	O4'-C1'-N9	6.42	113.33	108.20
36	1	65	A	P-O3'-C3'	6.41	127.40	119.70
36	1	1368	U	O5'-P-OP1	-6.41	99.93	105.70
36	5	1321	G	N1-C6-O6	6.40	123.74	119.90
36	1	3344	A	N7-C8-N9	6.40	117.00	113.80
36	5	2710	C	N1-C2-O2	-6.40	115.06	118.90
36	1	2872	A	C6-C5-N7	-6.39	127.83	132.30
1	6	610	G	C8-N9-C1'	-6.38	118.70	127.00
1	2	553	G	N1-C6-O6	6.38	123.73	119.90
36	1	2996	U	C6-N1-C1'	-6.38	112.27	121.20
36	1	1484	U	P-O3'-C3'	6.37	127.34	119.70
36	1	1904	C	C5-C6-N1	6.36	124.18	121.00
36	1	2298	U	C5-C4-O4	6.36	129.72	125.90
36	5	2231	C	O4'-C1'-N1	6.35	113.28	108.20
36	5	3050	U	C5-C4-O4	6.35	129.71	125.90
36	1	1849	C	O5'-P-OP1	-6.34	100.00	105.70
36	1	2714	G	C2-N3-C4	-6.33	108.73	111.90
36	1	3217	C	N3-C2-O2	-6.33	117.47	121.90
36	1	1820	U	P-O3'-C3'	6.31	127.27	119.70
24	d2	93	LEU	CA-CB-CG	6.31	129.81	115.30
36	1	890	C	C6-N1-C2	-6.31	117.78	120.30
36	5	1878	G	C8-N9-C1'	-6.31	118.80	127.00
36	1	2719	U	N1-C2-O2	-6.30	118.39	122.80
1	6	1773	C	N3-C4-C5	-6.29	119.38	121.90
36	1	2872	A	N7-C8-N9	6.29	116.94	113.80
36	1	3208	G	N3-C4-C5	-6.28	125.46	128.60
36	1	979	U	C6-N1-C2	-6.28	117.23	121.00
36	5	3310	A	N1-C6-N6	-6.28	114.83	118.60
36	1	3277	U	N3-C2-O2	-6.27	117.81	122.20
36	5	646	A	C8-N9-C4	-6.26	103.29	105.80
1	6	1	U	C5-C6-N1	6.26	125.83	122.70
36	1	2138	A	C8-N9-C4	-6.26	103.30	105.80
1	6	858	G	O4'-C1'-N9	6.26	113.21	108.20
36	5	1116	G	N3-C4-C5	-6.26	125.47	128.60
36	1	2156	C	C6-N1-C2	6.25	122.80	120.30
36	1	2714	G	N3-C4-C5	6.25	131.73	128.60
1	6	1767	G	C8-N9-C4	6.25	108.90	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1114	U	N1-C2-O2	6.24	127.17	122.80
1	2	1537	C	C6-N1-C2	-6.23	117.81	120.30
1	2	1560	U	N3-C2-O2	-6.23	117.84	122.20
36	5	2283	G	O5'-P-OP2	-6.22	100.10	105.70
36	1	1901	A	N1-C6-N6	-6.22	114.87	118.60
36	1	2314	U	C2-N1-C1'	6.22	125.16	117.70
36	5	92	G	C5-C6-N1	6.21	114.61	111.50
36	5	3078	U	N3-C2-O2	-6.21	117.85	122.20
36	1	1153	A	O5'-P-OP1	-6.21	100.11	105.70
1	6	163	G	N9-C4-C5	6.21	107.88	105.40
1	6	610	G	C4-N9-C1'	6.20	134.56	126.50
36	5	2816	G	N7-C8-N9	-6.20	110.00	113.10
36	1	1881	A	C8-N9-C4	6.20	108.28	105.80
36	5	776	U	C5-C6-N1	-6.20	119.60	122.70
36	1	950	G	C4-C5-N7	6.19	113.28	110.80
36	1	2385	G	N3-C4-C5	6.18	131.69	128.60
36	1	2983	C	C4-C5-C6	6.18	120.49	117.40
1	6	1000	C	N3-C2-O2	-6.17	117.58	121.90
36	1	2393	G	N3-C2-N2	-6.17	115.58	119.90
36	1	1556	C	C6-N1-C2	-6.17	117.83	120.30
38	4	126	A	O5'-P-OP1	-6.17	100.15	105.70
1	2	1052	U	N1-C2-O2	6.16	127.11	122.80
36	5	2411	U	C5-C6-N1	-6.15	119.63	122.70
36	5	1420	C	C6-N1-C2	6.15	122.76	120.30
36	5	963	G	N3-C4-C5	-6.14	125.53	128.60
36	1	2444	C	C2-N1-C1'	6.14	125.55	118.80
36	5	2271	A	N1-C6-N6	-6.14	114.92	118.60
1	6	1	U	C6-N1-C1'	-6.13	112.61	121.20
1	2	1761	U	P-O3'-C3'	6.13	127.06	119.70
36	1	2621	G	N3-C2-N2	-6.13	115.61	119.90
36	5	1141	C	O5'-P-OP1	-6.13	100.18	105.70
1	2	1096	C	C6-N1-C1'	-6.13	113.45	120.80
36	1	2836	C	C4-C5-C6	6.12	120.46	117.40
1	6	1698	G	P-O3'-C3'	6.12	127.05	119.70
36	1	2571	U	N3-C2-O2	-6.12	117.92	122.20
36	5	35	A	O5'-P-OP2	-6.12	100.19	105.70
36	1	2426	U	C5-C4-O4	6.11	129.56	125.90
36	5	2281	A	O5'-P-OP2	-6.10	100.21	105.70
36	1	1351	U	C2-N1-C1'	6.10	125.02	117.70
36	5	3269	U	P-O3'-C3'	6.10	127.02	119.70
12	c0	83	PRO	N-CA-CB	6.10	110.61	103.30
36	5	1437	C	C6-N1-C2	-6.09	117.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3217	C	N1-C2-O2	6.08	122.55	118.90
1	6	453	U	N1-C2-O2	6.08	127.06	122.80
1	6	1748	G	C8-N9-C4	6.07	108.83	106.40
39	12	216	HIS	N-CA-C	-6.07	94.60	111.00
1	6	542	A	O4'-C1'-N9	6.06	113.05	108.20
1	6	1340	U	N1-C2-O2	6.05	127.03	122.80
36	1	3217	C	C6-N1-C1'	-6.04	113.55	120.80
1	6	639	U	C2-N1-C1'	6.04	124.95	117.70
36	1	2343	C	N3-C4-C5	6.03	124.31	121.90
36	5	2841	G	N3-C4-C5	6.03	131.61	128.60
1	2	1274	C	N1-C2-O2	6.02	122.51	118.90
36	5	1483	G	O4'-C1'-N9	6.02	113.01	108.20
1	6	472	U	C2-N3-C4	-6.01	123.39	127.00
1	6	1340	U	N3-C2-O2	-6.01	117.99	122.20
36	5	1513	G	C8-N9-C4	-6.01	104.00	106.40
38	8	80	A	N7-C8-N9	6.01	116.80	113.80
36	1	2617	U	N1-C2-N3	6.00	118.50	114.90
54	M8	41	ASP	CB-CG-OD1	6.00	123.70	118.30
1	6	1535	U	C5-C6-N1	-6.00	119.70	122.70
36	1	400	G	C5-C6-O6	-6.00	125.00	128.60
41	L4	179	LEU	CA-CB-CG	6.00	129.09	115.30
36	5	3197	G	N3-C4-C5	5.99	131.60	128.60
36	1	946	U	O5'-P-OP2	-5.98	100.32	105.70
36	1	1297	C	O5'-P-OP1	-5.98	100.32	105.70
36	1	2617	U	N1-C2-O2	5.98	126.98	122.80
36	1	1495	U	N1-C2-N3	5.97	118.48	114.90
36	5	944	C	C6-N1-C2	5.97	122.69	120.30
36	1	1201	C	N3-C4-N4	5.97	122.18	118.00
1	6	337	G	C4-C5-N7	5.97	113.19	110.80
36	1	2827	U	O4'-C1'-N1	5.96	112.97	108.20
36	5	776	U	C5-C4-O4	5.96	129.48	125.90
1	6	1473	U	C2-N1-C1'	5.96	124.85	117.70
1	6	163	G	N3-C4-C5	5.96	131.58	128.60
36	5	2215	A	C8-N9-C4	5.95	108.18	105.80
1	2	1096	C	C5-C6-N1	5.95	123.97	121.00
36	1	2726	C	C6-N1-C2	-5.95	117.92	120.30
1	6	1389	C	C2-N1-C1'	5.94	125.33	118.80
1	6	621	A	O5'-P-OP1	-5.94	100.36	105.70
36	5	2950	G	O4'-C1'-N9	5.94	112.95	108.20
36	5	283	G	C6-C5-N7	-5.94	126.84	130.40
36	5	2405	C	N3-C2-O2	-5.93	117.75	121.90
36	1	1151	U	C6-N1-C2	-5.92	117.45	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	418	G	O5'-P-OP1	-5.91	100.38	105.70
36	1	2362	C	N1-C2-O2	5.91	122.45	118.90
36	5	1372	C	C6-N1-C2	5.91	122.66	120.30
15	C3	22	ALA	C-N-CD	-5.90	107.61	120.60
36	1	1157	G	N9-C4-C5	5.90	107.76	105.40
36	1	2403	G	N3-C4-N9	5.89	129.54	126.00
1	2	720	G	P-O3'-C3'	5.89	126.77	119.70
1	2	287	G	O4'-C1'-N9	5.89	112.91	108.20
36	1	439	C	C2-N1-C1'	5.87	125.26	118.80
36	1	2412	G	C5-C6-N1	5.87	114.44	111.50
36	1	776	U	C4-C5-C6	5.87	123.22	119.70
24	D2	93	LEU	CA-CB-CG	5.86	128.78	115.30
36	5	1239	C	C5-C6-N1	5.85	123.92	121.00
36	5	2629	U	C5-C4-O4	-5.85	122.39	125.90
1	6	1640	C	C5-C6-N1	5.84	123.92	121.00
36	1	1389	G	C5-C6-O6	-5.84	125.09	128.60
36	1	1495	U	C6-N1-C1'	5.84	129.38	121.20
36	5	2825	C	N3-C2-O2	5.84	125.98	121.90
36	5	1014	U	C2-N1-C1'	5.83	124.70	117.70
36	1	1508	C	N3-C4-C5	-5.82	119.57	121.90
36	5	767	U	O4'-C1'-N1	5.82	112.86	108.20
1	2	934	C	C2-N1-C1'	5.82	125.20	118.80
1	6	1058	U	OP1-P-O3'	5.82	118.00	105.20
36	5	2293	C	N1-C2-O2	5.82	122.39	118.90
36	5	2899	C	C6-N1-C2	-5.82	117.97	120.30
36	1	2903	A	C8-N9-C4	5.82	108.13	105.80
36	1	1351	U	C5-C6-N1	5.82	125.61	122.70
36	1	1269	U	N1-C2-O2	5.81	126.87	122.80
1	6	1	U	N3-C2-O2	-5.81	118.13	122.20
1	6	390	G	O5'-P-OP2	-5.81	100.47	105.70
36	5	2866	U	N3-C2-O2	-5.80	118.14	122.20
36	1	650	C	C6-N1-C2	5.80	122.62	120.30
36	1	1179	A	C8-N9-C4	5.80	108.12	105.80
36	1	1192	C	N1-C2-O2	5.80	122.38	118.90
1	6	795	U	N1-C2-O2	5.80	126.86	122.80
36	1	339	C	C5-C4-N4	5.80	124.26	120.20
36	5	1192	C	C2-N1-C1'	5.79	125.17	118.80
36	1	2365	C	C6-N1-C2	5.79	122.62	120.30
36	5	90	C	C6-N1-C2	-5.79	117.98	120.30
36	1	2306	C	N3-C2-O2	-5.79	117.85	121.90
36	1	2873	U	N3-C2-O2	-5.78	118.15	122.20
36	5	2392	C	C2-N1-C1'	-5.78	112.44	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2403	G	O5'-P-OP1	5.78	117.64	110.70
36	1	2571	U	N1-C2-O2	5.78	126.84	122.80
36	1	3318	G	C4-N9-C1'	5.78	134.01	126.50
36	1	805	G	C8-N9-C4	5.77	108.71	106.40
1	2	75	U	N1-C2-O2	5.77	126.84	122.80
36	1	3344	A	C8-N9-C4	-5.77	103.49	105.80
61	N5	38	LEU	CA-CB-CG	5.77	128.56	115.30
36	5	1628	C	C6-N1-C2	-5.77	117.99	120.30
36	5	3351	U	C2-N1-C1'	5.76	124.61	117.70
36	5	1467	A	O5'-P-OP2	-5.76	100.52	105.70
1	6	1123	C	C6-N1-C2	-5.76	118.00	120.30
36	1	2870	C	C6-N1-C1'	5.75	127.71	120.80
36	1	1157	G	C5-C6-O6	5.75	132.05	128.60
1	2	1052	U	N3-C2-O2	-5.75	118.18	122.20
36	1	101	G	O4'-C1'-N9	5.75	112.80	108.20
36	1	1157	G	N1-C6-O6	-5.74	116.46	119.90
36	1	282	G	C8-N9-C4	-5.74	104.11	106.40
36	1	1329	U	C6-N1-C2	-5.74	117.56	121.00
37	7	100	C	C5-C6-N1	-5.74	118.13	121.00
36	5	1308	A	O5'-P-OP2	5.74	117.58	110.70
36	1	2842	U	N1-C2-O2	5.73	126.81	122.80
36	1	2403	G	C6-C5-N7	-5.72	126.97	130.40
36	1	1117	G	O5'-P-OP1	-5.72	100.55	105.70
36	5	1307	G	OP2-P-O3'	5.72	117.78	105.20
36	5	1496	C	N1-C2-O2	5.72	122.33	118.90
36	5	966	U	C2-N1-C1'	5.71	124.56	117.70
36	5	2996	U	O5'-P-OP1	5.71	117.55	110.70
36	5	1381	A	C2-N3-C4	-5.70	107.75	110.60
36	5	2197	C	C6-N1-C2	5.70	122.58	120.30
36	5	1899	G	C5-C6-O6	5.70	132.02	128.60
36	5	2211	U	C4-C5-C6	5.70	123.12	119.70
36	1	922	U	N1-C2-O2	5.69	126.78	122.80
36	5	283	G	C5-N7-C8	-5.69	101.45	104.30
36	1	2971	A	C8-N9-C4	-5.69	103.52	105.80
1	6	151	G	N3-C2-N2	-5.68	115.92	119.90
1	6	194	U	C5-C6-N1	5.68	125.54	122.70
36	5	2866	U	N1-C2-O2	5.68	126.78	122.80
36	1	186	U	N1-C2-O2	5.68	126.78	122.80
36	1	1419	A	O5'-P-OP2	-5.68	100.59	105.70
36	5	3154	C	N3-C2-O2	-5.68	117.92	121.90
54	m8	127	LEU	CA-CB-CG	5.68	128.36	115.30
36	5	1844	C	C6-N1-C2	-5.67	118.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1157	G	C8-N9-C4	-5.67	104.13	106.40
52	m6	78	ARG	NE-CZ-NH2	-5.67	117.46	120.30
36	1	639	G	N3-C2-N2	-5.67	115.93	119.90
52	M6	110	PRO	C-N-CD	-5.66	108.14	120.60
10	S8	29	LEU	CA-CB-CG	5.66	128.32	115.30
36	5	708	G	N7-C8-N9	5.66	115.93	113.10
1	6	1123	C	C5-C6-N1	5.66	123.83	121.00
36	5	3050	U	N3-C2-O2	-5.66	118.24	122.20
36	1	716	A	N1-C6-N6	5.66	121.99	118.60
36	5	1481	A	P-O3'-C3'	5.66	126.49	119.70
36	1	515	C	C6-N1-C2	-5.65	118.04	120.30
48	m1	12	LEU	CA-CB-CG	5.65	128.30	115.30
36	1	1419	A	O5'-P-OP1	5.65	117.48	110.70
36	1	2513	U	OP1-P-O3'	5.65	117.63	105.20
36	1	2585	G	N3-C4-C5	-5.65	125.78	128.60
36	1	1111	U	C6-N1-C2	5.65	124.39	121.00
36	1	3208	G	N3-C4-N9	5.65	129.39	126.00
36	5	2606	G	C8-N9-C4	-5.65	104.14	106.40
36	5	2943	G	C6-C5-N7	-5.64	127.01	130.40
36	1	2363	A	C5-C6-N6	5.64	128.21	123.70
1	6	453	U	N3-C2-O2	-5.64	118.25	122.20
1	6	1596	C	N3-C2-O2	-5.64	117.95	121.90
1	2	1274	C	C2-N1-C1'	5.64	125.00	118.80
1	2	1596	C	N3-C2-O2	-5.64	117.95	121.90
36	1	2872	A	C5-N7-C8	-5.64	101.08	103.90
36	5	1006	A	O5'-P-OP2	-5.63	100.63	105.70
1	6	543	C	N1-C2-O2	5.63	122.28	118.90
36	5	3133	C	C6-N1-C2	-5.63	118.05	120.30
1	6	18	C	C6-N1-C2	-5.63	118.05	120.30
36	5	65	A	P-O3'-C3'	5.63	126.45	119.70
36	5	3351	U	N3-C2-O2	-5.62	118.26	122.20
1	6	400	A	N1-C6-N6	5.62	121.97	118.60
36	5	908	G	C8-N9-C1'	-5.62	119.69	127.00
36	1	1433	A	C8-N9-C4	-5.62	103.55	105.80
1	2	1456	C	C2-N1-C1'	5.61	124.97	118.80
36	1	424	G	N1-C6-O6	-5.61	116.54	119.90
36	1	610	G	O5'-P-OP1	-5.61	100.66	105.70
36	1	2572	C	C6-N1-C1'	-5.61	114.07	120.80
36	5	922	U	N1-C2-O2	5.60	126.72	122.80
41	14	339	LEU	CA-CB-CG	5.60	128.19	115.30
36	5	2365	C	O5'-P-OP1	-5.60	100.66	105.70
36	1	2978	U	O4'-C1'-N1	5.59	112.67	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3217	C	C6-N1-C2	-5.59	118.06	120.30
36	5	404	G	O5'-P-OP2	-5.59	100.67	105.70
36	1	2659	G	N1-C6-O6	5.59	123.25	119.90
36	1	639	G	C5-C6-O6	-5.58	125.25	128.60
1	2	192	U	N3-C2-O2	-5.58	118.29	122.20
36	1	2541	U	P-O3'-C3'	5.58	126.40	119.70
36	5	2531	C	N1-C2-O2	5.58	122.25	118.90
1	2	767	U	N3-C2-O2	-5.58	118.30	122.20
36	5	3050	U	N1-C2-O2	5.58	126.70	122.80
1	6	453	U	C6-N1-C1'	-5.57	113.40	121.20
36	1	859	G	C6-C5-N7	-5.57	127.06	130.40
36	5	1588	A	C8-N9-C4	5.57	108.03	105.80
36	5	1907	C	N1-C2-O2	-5.57	115.56	118.90
36	5	2899	C	N3-C2-O2	-5.57	118.00	121.90
1	2	543	C	N1-C2-O2	5.56	122.23	118.90
36	5	3007	U	N1-C2-O2	5.55	126.69	122.80
36	1	1362	G	C8-N9-C4	5.55	108.62	106.40
36	5	822	G	O5'-P-OP1	-5.55	100.71	105.70
36	5	1308	A	OP1-P-OP2	-5.55	111.28	119.60
36	1	1495	U	C5-C6-N1	-5.54	119.93	122.70
38	4	20	U	O5'-P-OP2	-5.54	100.72	105.70
36	5	2351	U	N1-C2-O2	5.54	126.67	122.80
1	2	1052	U	C5-C6-N1	5.53	125.47	122.70
36	5	1437	C	C2-N1-C1'	5.53	124.88	118.80
36	1	590	G	C4-C5-N7	5.52	113.01	110.80
36	5	98	G	O5'-P-OP2	-5.52	100.73	105.70
36	5	2898	G	C4-N9-C1'	-5.52	119.32	126.50
36	1	400	G	N1-C6-O6	5.52	123.21	119.90
36	1	590	G	N1-C6-O6	5.52	123.21	119.90
36	1	1556	C	C2-N1-C1'	5.52	124.87	118.80
36	5	1496	C	C2-N1-C1'	5.52	124.87	118.80
36	5	1604	G	C4-N9-C1'	5.52	133.67	126.50
36	5	1003	A	N1-C6-N6	5.51	121.91	118.60
36	1	2355	G	N1-C6-O6	5.51	123.21	119.90
36	5	1184	A	N1-C6-N6	-5.51	115.29	118.60
36	5	2403	G	N3-C2-N2	-5.51	116.04	119.90
36	5	3010	U	C5-C4-O4	5.51	129.21	125.90
36	1	166	C	N1-C2-O2	5.50	122.20	118.90
36	1	895	A	C4-C5-N7	5.50	113.45	110.70
36	1	1201	C	C5-C6-N1	5.50	123.75	121.00
38	4	85	G	C8-N9-C4	-5.50	104.20	106.40
1	2	581	U	C2-N1-C1'	5.50	124.30	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	653	A	N1-C6-N6	5.50	121.90	118.60
36	1	217	U	OP1-P-O3'	5.50	117.29	105.20
36	1	646	A	C4-C5-C6	5.49	119.75	117.00
36	1	3344	A	O4'-C1'-N9	5.49	112.59	108.20
1	6	813	U	N1-C2-O2	5.49	126.65	122.80
36	5	2354	C	N1-C2-O2	-5.49	115.60	118.90
36	5	2948	C	N3-C4-C5	5.49	124.10	121.90
36	5	67	A	C8-N9-C4	5.49	108.00	105.80
36	5	908	G	O4'-C1'-N9	-5.49	103.81	108.20
36	1	1294	A	O4'-C1'-N9	5.49	112.59	108.20
36	5	1152	G	N1-C6-O6	5.49	123.19	119.90
36	5	2211	U	N3-C2-O2	-5.49	118.36	122.20
36	5	2355	G	C6-C5-N7	-5.49	127.11	130.40
38	8	108	C	C6-N1-C2	-5.49	118.11	120.30
24	D2	65	LEU	CA-CB-CG	5.48	127.91	115.30
36	1	2571	U	C2-N1-C1'	5.48	124.28	117.70
1	2	830	U	N1-C2-O2	5.48	126.64	122.80
1	2	1202	A	C8-N9-C4	-5.48	103.61	105.80
36	1	2619	G	O5'-P-OP1	-5.48	100.77	105.70
36	5	170	G	C4-N9-C1'	5.48	133.62	126.50
1	2	1340	U	N1-C2-O2	5.48	126.63	122.80
1	2	720	G	OP1-P-O3'	5.47	117.24	105.20
36	1	803	C	C5-C6-N1	5.47	123.74	121.00
36	5	908	G	C6-C5-N7	-5.47	127.12	130.40
36	5	873	C	P-O3'-C3'	5.47	126.27	119.70
36	5	2816	G	C4-N9-C1'	-5.47	119.39	126.50
36	5	3007	U	N3-C2-O2	-5.47	118.37	122.20
36	5	640	U	N3-C4-O4	5.46	123.22	119.40
36	5	2981	U	N3-C2-O2	-5.46	118.38	122.20
36	1	939	U	C5-C4-O4	-5.46	122.62	125.90
1	6	1700	C	N1-C2-O2	5.46	122.17	118.90
36	5	880	G	C4-N9-C1'	-5.46	119.41	126.50
36	5	779	G	N1-C6-O6	5.45	123.17	119.90
36	5	640	U	N1-C2-N3	5.45	118.17	114.90
36	5	822	G	N3-C2-N2	-5.45	116.08	119.90
36	5	3154	C	C6-N1-C1'	-5.45	114.26	120.80
36	5	3245	A	C4-C5-N7	5.45	113.43	110.70
36	1	2996	U	C5-C6-N1	5.45	125.43	122.70
36	5	1152	G	N1-C2-N2	5.45	121.11	116.20
36	5	1192	C	N3-C4-N4	5.45	121.82	118.00
36	1	1133	A	O5'-P-OP2	-5.45	100.80	105.70
1	6	1473	U	N3-C2-O2	-5.45	118.39	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2197	C	C6-N1-C2	5.45	122.48	120.30
36	5	770	G	O4'-C1'-N9	5.45	112.56	108.20
36	1	895	A	C5-N7-C8	-5.44	101.18	103.90
1	6	1640	C	C2-N1-C1'	5.44	124.79	118.80
36	5	269	G	C8-N9-C4	5.44	108.58	106.40
36	5	85	A	O5'-P-OP2	-5.44	100.81	105.70
36	5	3004	C	OP2-P-O3'	5.44	117.16	105.20
36	1	3092	C	C6-N1-C2	5.43	122.47	120.30
36	1	701	G	OP2-P-O3'	5.43	117.15	105.20
36	5	1060	U	C5-C6-N1	-5.42	119.99	122.70
36	5	954	U	O5'-P-OP1	-5.42	100.82	105.70
36	5	2897	A	C5-C6-N6	-5.42	119.36	123.70
36	1	874	U	N3-C4-O4	-5.42	115.61	119.40
36	1	439	C	C5-C6-N1	5.42	123.71	121.00
36	1	1381	A	C8-N9-C4	5.42	107.97	105.80
1	6	542	A	P-O3'-C3'	5.41	126.19	119.70
36	5	3382	U	C2-N1-C1'	5.41	124.19	117.70
36	1	3275	U	C5-C6-N1	5.41	125.41	122.70
36	5	3188	G	N1-C6-O6	-5.41	116.65	119.90
36	1	2816	G	N1-C6-O6	5.41	123.14	119.90
36	1	3278	C	C6-N1-C2	-5.41	118.14	120.30
36	1	1858	A	C2-N3-C4	5.41	113.30	110.60
36	5	908	G	C5-C6-O6	-5.41	125.36	128.60
36	5	2552	C	C2-N1-C1'	5.41	124.75	118.80
36	1	421	G	N9-C4-C5	-5.40	103.24	105.40
36	1	3318	G	N3-C4-N9	5.40	129.24	126.00
39	12	179	LEU	CA-CB-CG	5.40	127.71	115.30
36	1	3141	A	C8-N9-C4	5.39	107.96	105.80
36	5	1868	G	N3-C4-N9	5.39	129.24	126.00
1	2	1274	C	N3-C2-O2	-5.39	118.12	121.90
36	1	2985	C	O5'-P-OP1	-5.39	100.85	105.70
1	6	158	U	P-O3'-C3'	5.39	126.17	119.70
36	1	2870	C	O4'-C1'-N1	5.39	112.51	108.20
1	6	25	C	P-O3'-C3'	5.39	126.17	119.70
36	5	577	C	C6-N1-C2	5.38	122.45	120.30
1	2	1458	G	N3-C4-N9	5.38	129.23	126.00
73	O7	65	ARG	NE-CZ-NH1	5.38	122.99	120.30
36	5	2964	G	N1-C6-O6	-5.38	116.67	119.90
36	1	873	C	P-O3'-C3'	5.37	126.15	119.70
1	6	163	G	C2-N3-C4	-5.37	109.21	111.90
1	2	1458	G	C4-N9-C1'	5.37	133.48	126.50
36	1	718	G	N3-C4-C5	5.37	131.28	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3305	A	N1-C6-N6	-5.37	115.38	118.60
36	5	1495	U	C6-N1-C2	-5.37	117.78	121.00
37	7	19	C	O5'-P-OP2	-5.37	100.87	105.70
36	5	640	U	C6-N1-C2	-5.36	117.78	121.00
36	5	1113	G	C2-N3-C4	-5.36	109.22	111.90
36	5	1520	G	C5-C6-O6	-5.36	125.38	128.60
1	2	297	U	N1-C2-O2	5.36	126.55	122.80
36	5	1152	G	N9-C4-C5	5.36	107.54	105.40
36	1	1565	G	N7-C8-N9	5.36	115.78	113.10
36	5	2634	U	C5-C4-O4	-5.36	122.69	125.90
36	1	2137	U	C2-N1-C1'	5.35	124.12	117.70
1	6	555	A	C8-N9-C4	-5.35	103.66	105.80
36	5	2971	A	C2-N3-C4	5.35	113.28	110.60
36	1	2298	U	N3-C4-O4	-5.35	115.65	119.40
36	1	1179	A	C2-N3-C4	-5.35	107.92	110.60
36	1	1725	C	C2-N1-C1'	-5.35	112.92	118.80
1	6	1698	G	N1-C6-O6	-5.35	116.69	119.90
36	1	1165	A	O5'-P-OP2	-5.34	100.89	105.70
36	1	2408	U	O5'-P-OP1	-5.34	100.89	105.70
1	2	453	U	C2-N1-C1'	5.34	124.11	117.70
36	5	646	A	C4-C5-C6	5.34	119.67	117.00
1	2	158	U	P-O3'-C3'	5.34	126.11	119.70
1	2	553	G	C6-C5-N7	-5.34	127.20	130.40
36	5	2286	U	N3-C2-O2	-5.33	118.47	122.20
36	5	3133	C	N3-C4-C5	-5.33	119.77	121.90
38	8	38	U	C2-N1-C1'	5.33	124.10	117.70
1	6	678	A	P-O3'-C3'	5.33	126.10	119.70
36	5	981	U	C6-N1-C2	-5.33	117.80	121.00
36	1	2631	U	C5-C6-N1	-5.33	120.04	122.70
1	2	831	U	C6-N1-C2	-5.33	117.80	121.00
36	1	2247	G	N1-C6-O6	5.33	123.10	119.90
36	1	3170	A	C8-N9-C4	-5.33	103.67	105.80
1	6	1700	C	C2-N1-C1'	5.33	124.66	118.80
36	5	966	U	N3-C2-O2	-5.33	118.47	122.20
1	2	1370	U	OP2-P-O3'	5.32	116.91	105.20
36	1	3181	C	C6-N1-C2	-5.32	118.17	120.30
36	5	580	C	C6-N1-C2	-5.32	118.17	120.30
36	1	426	G	N9-C4-C5	-5.32	103.27	105.40
36	5	2572	C	C6-N1-C2	-5.32	118.17	120.30
36	1	801	A	O4'-C1'-N9	-5.31	103.95	108.20
36	5	2629	U	N3-C4-O4	5.31	123.12	119.40
37	7	101	G	N9-C4-C5	-5.31	103.28	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1481	C	C6-N1-C2	-5.31	118.18	120.30
36	1	2816	G	C5-C6-O6	-5.31	125.42	128.60
1	2	75	U	N3-C2-O2	-5.30	118.49	122.20
36	1	198	A	C8-N9-C4	-5.30	103.68	105.80
1	6	1573	A	OP2-P-O3'	5.30	116.86	105.20
36	5	1604	G	C8-N9-C1'	-5.30	120.11	127.00
36	1	3178	A	C8-N9-C4	5.30	107.92	105.80
1	6	747	C	C6-N1-C2	-5.30	118.18	120.30
36	1	2163	C	C5-C6-N1	-5.30	118.35	121.00
36	5	2375	G	N1-C6-O6	-5.30	116.72	119.90
36	5	423	A	OP2-P-O3'	5.29	116.84	105.20
36	5	655	C	C6-N1-C2	-5.29	118.18	120.30
36	5	2514	U	C5-C6-N1	5.29	125.35	122.70
36	5	1131	G	N1-C6-O6	5.29	123.07	119.90
70	O4	51	LEU	CA-CB-CG	5.28	127.45	115.30
36	5	640	U	N1-C2-O2	-5.28	119.10	122.80
36	5	2307	G	N1-C6-O6	-5.28	116.73	119.90
36	5	2913	C	N1-C2-O2	-5.28	115.73	118.90
36	1	600	G	C4-N9-C1'	5.28	133.37	126.50
36	5	1192	C	C6-N1-C1'	-5.28	114.46	120.80
1	6	1596	C	C6-N1-C2	-5.28	118.19	120.30
36	1	2622	C	O5'-P-OP2	-5.28	100.95	105.70
1	6	1185	U	N1-C2-O2	5.28	126.49	122.80
1	2	39	A	O4'-C1'-N9	5.27	112.42	108.20
36	1	282	G	C2'-C3'-O3'	5.27	122.14	113.70
36	5	630	A	C8-N9-C4	5.27	107.91	105.80
1	2	1258	U	N3-C2-O2	-5.27	118.51	122.20
1	6	385	A	N1-C6-N6	-5.27	115.44	118.60
36	5	2144	A	O4'-C1'-N9	5.27	112.42	108.20
36	1	346	C	C5-C6-N1	-5.27	118.37	121.00
36	1	2598	G	C5-C6-O6	-5.27	125.44	128.60
36	1	2996	U	N3-C2-O2	-5.27	118.51	122.20
36	5	639	G	C5-C6-O6	-5.27	125.44	128.60
36	1	395	A	O5'-P-OP2	-5.26	100.96	105.70
36	1	1407	A	C8-N9-C4	5.26	107.91	105.80
36	1	2651	G	O5'-P-OP1	-5.26	100.96	105.70
36	1	2550	U	C5-C4-O4	5.26	129.06	125.90
36	1	1141	C	N1-C2-O2	-5.26	115.75	118.90
36	5	1604	G	N3-C4-N9	5.26	129.16	126.00
36	1	3306	U	N3-C4-O4	-5.26	115.72	119.40
36	5	3185	U	N3-C2-O2	-5.26	118.52	122.20
36	1	635	G	N3-C2-N2	-5.25	116.22	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3228	C	C2-N1-C1'	5.25	124.58	118.80
49	M3	85	LEU	CA-CB-CG	5.25	127.38	115.30
1	6	1	U	O4'-C1'-N1	5.25	112.40	108.20
1	6	1145	U	N1-C2-O2	-5.25	119.12	122.80
36	1	423	A	N1-C6-N6	5.25	121.75	118.60
36	1	3318	G	C6-C5-N7	-5.25	127.25	130.40
36	5	57	A	C8-N9-C4	5.25	107.90	105.80
36	1	2163	C	C4-C5-C6	5.25	120.02	117.40
36	5	2339	C	C2-N1-C1'	5.25	124.57	118.80
36	1	648	C	C2-N1-C1'	5.25	124.57	118.80
36	1	1201	C	C5-C4-N4	-5.25	116.53	120.20
36	5	699	A	N1-C6-N6	5.25	121.75	118.60
37	7	112	G	C8-N9-C4	-5.24	104.30	106.40
1	2	1202	A	C2-N3-C4	5.24	113.22	110.60
36	5	363	G	OP1-P-O3'	5.24	116.72	105.20
36	5	358	G	N3-C4-C5	5.24	131.22	128.60
41	14	340	GLY	N-CA-C	-5.24	100.01	113.10
36	1	940	G	N1-C6-O6	-5.23	116.76	119.90
36	1	2624	G	N1-C6-O6	5.23	123.04	119.90
36	1	1060	U	C5-C6-N1	-5.23	120.08	122.70
1	6	813	U	C6-N1-C1'	-5.23	113.88	121.20
36	5	2897	A	N1-C6-N6	5.22	121.73	118.60
36	1	2852	C	N3-C4-C5	5.22	123.99	121.90
36	1	339	C	N3-C4-N4	-5.22	114.35	118.00
36	1	2624	G	C5-C6-O6	-5.22	125.47	128.60
1	6	272	U	P-O3'-C3'	5.22	125.96	119.70
1	6	314	C	N3-C2-O2	-5.22	118.25	121.90
18	C6	40	GLU	C-N-CA	5.22	143.92	122.00
1	6	1537	C	C6-N1-C2	-5.22	118.21	120.30
1	2	1761	U	C6-N1-C2	-5.21	117.87	121.00
36	5	222	A	N1-C6-N6	5.21	121.73	118.60
36	1	1521	G	N3-C4-C5	5.21	131.21	128.60
36	1	1159	A	N1-C6-N6	-5.21	115.47	118.60
36	5	706	A	C8-N9-C4	5.21	107.89	105.80
36	1	2306	C	C6-N1-C2	-5.21	118.22	120.30
36	5	2726	C	N3-C4-N4	-5.21	114.35	118.00
1	2	25	C	OP2-P-O3'	5.21	116.65	105.20
36	5	2937	G	N1-C6-O6	5.21	123.02	119.90
1	2	1059	U	C2-N1-C1'	5.20	123.94	117.70
36	5	880	G	O4'-C1'-N9	5.20	112.36	108.20
36	1	1118	C	C6-N1-C2	-5.20	118.22	120.30
36	1	1367	G	N9-C4-C5	-5.20	103.32	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2444	C	C6-N1-C1'	-5.20	114.56	120.80
36	5	1437	C	C5-C6-N1	5.20	123.60	121.00
62	n6	57	LEU	CA-CB-CG	5.20	127.26	115.30
1	6	14	C	C6-N1-C2	-5.20	118.22	120.30
36	1	1165	A	C8-N9-C4	5.20	107.88	105.80
1	6	583	C	C5-C6-N1	5.20	123.60	121.00
1	6	1537	C	N3-C4-C5	-5.20	119.82	121.90
36	5	655	C	O5'-P-OP2	-5.20	101.03	105.70
1	6	864	U	N3-C2-O2	-5.19	118.56	122.20
36	1	793	C	C5-C4-N4	-5.19	116.57	120.20
36	1	934	G	C8-N9-C1'	-5.19	120.25	127.00
36	5	1419	A	O5'-P-OP2	-5.19	101.03	105.70
1	6	1129	U	N3-C4-O4	-5.19	115.77	119.40
24	D2	104	LEU	CA-CB-CG	5.19	127.23	115.30
1	6	1697	G	N3-C4-C5	-5.19	126.01	128.60
36	5	1017	C	C5-C6-N1	5.19	123.59	121.00
36	1	953	G	N3-C4-N9	-5.18	122.89	126.00
1	6	151	G	N3-C4-N9	-5.18	122.89	126.00
36	5	1655	G	C8-N9-C4	5.18	108.47	106.40
37	7	26	C	C4-C5-C6	5.18	119.99	117.40
1	6	1021	C	C6-N1-C2	-5.18	118.23	120.30
36	5	1213	G	C8-N9-C4	5.18	108.47	106.40
36	1	3208	G	N3-C2-N2	5.17	123.52	119.90
36	5	1014	U	C6-N1-C1'	-5.17	113.96	121.20
36	5	3285	C	C2-N1-C1'	5.17	124.49	118.80
36	1	1367	G	N3-C4-N9	5.17	129.10	126.00
36	5	1146	C	N1-C2-O2	5.17	122.00	118.90
36	5	217	U	OP1-P-O3'	5.17	116.58	105.20
36	5	2627	C	OP2-P-O3'	5.17	116.58	105.20
36	1	2622	C	N3-C4-C5	-5.17	119.83	121.90
65	N9	32	LEU	CA-CB-CG	5.17	127.19	115.30
36	1	600	G	C8-N9-C4	-5.17	104.33	106.40
36	1	1365	G	N7-C8-N9	5.17	115.68	113.10
36	1	2631	U	N3-C4-O4	-5.16	115.79	119.40
36	5	2683	U	C5-C6-N1	5.16	125.28	122.70
36	5	2965	U	N1-C2-O2	-5.16	119.19	122.80
36	5	2376	G	O5'-P-OP2	-5.16	101.05	105.70
36	1	2572	C	C6-N1-C2	-5.16	118.24	120.30
36	5	2351	U	C5-C4-O4	5.16	129.00	125.90
36	5	3351	U	N1-C2-O2	5.16	126.41	122.80
36	5	1307	G	C2'-C3'-O3'	5.16	121.95	113.70
36	5	1406	A	O5'-P-OP2	-5.16	101.06	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2309	A	N1-C6-N6	5.16	121.69	118.60
36	1	3318	G	N3-C4-C5	-5.16	126.02	128.60
1	6	1619	C	C6-N1-C2	-5.16	118.24	120.30
36	1	2401	A	O4'-C1'-N9	5.15	112.32	108.20
36	1	230	U	C2-N3-C4	-5.15	123.91	127.00
36	1	1146	C	O5'-P-OP2	-5.15	101.06	105.70
36	5	1170	A	N1-C6-N6	5.15	121.69	118.60
36	5	2531	C	C2-N1-C1'	5.15	124.47	118.80
36	5	3245	A	N1-C6-N6	5.15	121.69	118.60
1	6	337	G	C5-N7-C8	-5.15	101.72	104.30
1	6	965	U	N1-C2-O2	5.15	126.41	122.80
1	6	1698	G	C5-C6-O6	5.15	131.69	128.60
36	5	2987	A	C5-C6-N1	-5.15	115.13	117.70
36	1	803	C	C4-C5-C6	-5.15	114.83	117.40
36	1	3208	G	N1-C2-N2	-5.15	111.57	116.20
36	5	1131	G	N3-C2-N2	-5.15	116.30	119.90
36	1	1405	U	OP1-P-O3'	5.14	116.52	105.20
36	1	2872	A	C2-N3-C4	-5.14	108.03	110.60
36	1	2112	U	P-O3'-C3'	5.14	125.87	119.70
36	1	721	G	C5-C6-O6	-5.14	125.52	128.60
36	5	669	U	N3-C2-O2	-5.14	118.61	122.20
1	6	1573	A	P-O3'-C3'	5.13	125.86	119.70
36	5	183	G	P-O3'-C3'	5.13	125.86	119.70
1	2	25	C	P-O3'-C3'	5.13	125.86	119.70
1	2	1568	C	P-O3'-C3'	5.13	125.86	119.70
36	1	1172	G	O5'-P-OP1	-5.13	101.08	105.70
36	1	2215	A	C8-N9-C4	5.13	107.85	105.80
36	5	2899	C	C2-N1-C1'	5.13	124.44	118.80
1	2	1340	U	N3-C2-O2	-5.13	118.61	122.20
36	5	283	G	C5-C6-O6	-5.13	125.52	128.60
36	5	352	A	O4'-C1'-N9	5.12	112.30	108.20
38	4	103	G	N3-C4-C5	-5.12	126.04	128.60
36	5	361	A	C5-C6-N6	5.12	127.80	123.70
36	1	663	C	N3-C4-C5	-5.12	119.85	121.90
37	3	73	C	N1-C2-O2	5.12	121.97	118.90
36	1	1306	G	N1-C6-O6	5.12	122.97	119.90
36	5	2930	A	O4'-C1'-N9	5.12	112.30	108.20
36	5	3195	U	C2-N1-C1'	5.12	123.84	117.70
1	6	194	U	C6-N1-C2	-5.12	117.93	121.00
36	1	282	G	P-O3'-C3'	5.11	125.83	119.70
36	5	86	G	N3-C2-N2	5.11	123.48	119.90
1	6	996	U	O5'-P-OP1	-5.11	101.10	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	641	C	O4'-C1'-N1	5.11	112.29	108.20
36	5	1239	C	C2-N1-C1'	5.11	124.42	118.80
36	5	2403	G	C5-C6-O6	-5.11	125.54	128.60
37	7	100	C	C6-N1-C2	5.11	122.34	120.30
36	5	2830	G	N1-C2-N3	5.11	126.96	123.90
36	1	916	G	P-O3'-C3'	5.10	125.83	119.70
36	1	1269	U	N3-C2-O2	-5.10	118.63	122.20
18	C6	28	LEU	CA-CB-CG	5.10	127.04	115.30
36	5	3197	G	N1-C2-N2	5.10	120.79	116.20
36	5	976	U	N3-C2-O2	-5.10	118.63	122.20
36	1	1329	U	O4'-C1'-N1	5.10	112.28	108.20
36	1	1380	G	C2-N3-C4	-5.10	109.35	111.90
36	1	3121	U	OP1-P-O3'	5.10	116.41	105.20
36	5	2914	G	O5'-P-OP2	-5.10	101.11	105.70
36	1	960	U	C5-C4-O4	-5.09	122.84	125.90
36	5	3197	G	C8-N9-C1'	5.09	133.62	127.00
36	5	2572	C	C6-N1-C1'	-5.09	114.69	120.80
38	8	26	U	O5'-P-OP2	-5.09	101.12	105.70
36	1	2156	C	C5-C6-N1	-5.09	118.46	121.00
36	5	1180	A	O4'-C1'-N9	-5.09	104.13	108.20
36	5	2526	C	N1-C2-O2	5.09	121.95	118.90
1	2	864	U	N3-C2-O2	-5.09	118.64	122.20
1	6	1389	C	N1-C2-O2	5.08	121.95	118.90
1	2	1560	U	C6-N1-C2	-5.08	117.95	121.00
36	5	283	G	C4-N9-C1'	5.08	133.10	126.50
36	5	2552	C	N1-C2-O2	5.08	121.95	118.90
36	5	2283	G	C5-C6-O6	-5.08	125.55	128.60
36	1	900	G	C5-C6-O6	-5.08	125.55	128.60
36	1	1556	C	N3-C2-O2	-5.08	118.34	121.90
36	1	2161	G	N1-C6-O6	-5.08	116.85	119.90
36	5	1561	G	O4'-C1'-N9	5.07	112.26	108.20
36	5	3362	A	C5-N7-C8	-5.07	101.36	103.90
36	5	3377	G	C5-C6-O6	-5.07	125.56	128.60
36	5	358	G	N3-C4-N9	-5.07	122.96	126.00
36	5	776	U	C4-C5-C6	5.07	122.74	119.70
36	1	2846	U	N3-C2-O2	-5.07	118.65	122.20
36	5	1177	G	O4'-C1'-N9	5.07	112.25	108.20
36	5	776	U	N1-C2-N3	5.07	117.94	114.90
25	d3	45	GLY	N-CA-C	-5.06	100.44	113.10
36	5	3090	U	OP1-P-O3'	5.06	116.34	105.20
36	1	2884	C	N3-C4-C5	5.06	123.92	121.90
36	5	914	A	C2-N3-C4	-5.06	108.07	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2257	C	C6-N1-C2	-5.06	118.28	120.30
36	5	2400	G	N3-C4-C5	5.06	131.13	128.60
36	5	2769	A	C8-N9-C4	5.06	107.83	105.80
1	2	610	G	C4-N9-C1'	5.06	133.08	126.50
36	5	1434	G	N9-C4-C5	5.06	107.42	105.40
36	5	2188	A	C8-N9-C4	5.06	107.82	105.80
1	2	1458	G	C8-N9-C1'	-5.06	120.42	127.00
36	1	424	G	O5'-P-OP2	-5.06	101.15	105.70
36	5	2965	U	N3-C2-O2	5.06	125.74	122.20
36	1	1157	G	C4-C5-N7	-5.06	108.78	110.80
36	5	3309	G	C4-N9-C1'	5.06	133.07	126.50
36	1	2883	U	C5-C6-N1	5.05	125.23	122.70
36	5	1238	C	P-O3'-C3'	5.05	125.77	119.70
37	7	80	G	C6-C5-N7	-5.05	127.37	130.40
36	1	2374	C	O5'-P-OP2	-5.05	101.15	105.70
36	1	3353	G	P-O3'-C3'	5.05	125.76	119.70
36	5	1378	U	C6-N1-C2	5.05	124.03	121.00
1	6	453	U	C5-C6-N1	5.05	125.22	122.70
36	5	2523	A	OP2-P-O3'	5.05	116.31	105.20
36	5	801	A	O4'-C1'-N9	-5.04	104.16	108.20
36	5	1180	A	N9-C4-C5	5.04	107.82	105.80
36	1	86	G	O5'-P-OP2	-5.04	101.16	105.70
1	2	1389	C	N1-C2-O2	5.04	121.92	118.90
36	1	1790	G	N1-C6-O6	5.04	122.92	119.90
36	1	2983	C	C2-N1-C1'	5.04	124.34	118.80
66	o0	41	LEU	CA-CB-CG	5.04	126.89	115.30
36	5	1161	G	C8-N9-C4	5.04	108.41	106.40
36	5	2756	C	C6-N1-C2	-5.04	118.28	120.30
1	6	1619	C	C5-C6-N1	5.03	123.52	121.00
36	5	953	G	N3-C4-C5	5.03	131.12	128.60
36	1	1168	U	N1-C2-O2	5.03	126.32	122.80
36	5	2872	A	C5-C6-N1	-5.03	115.19	117.70
36	1	972	A	C8-N9-C4	5.03	107.81	105.80
36	5	2890	A	OP2-P-O3'	5.03	116.26	105.20
1	2	959	U	C2-N1-C1'	5.03	123.73	117.70
36	1	326	U	C5-C6-N1	5.03	125.21	122.70
1	2	1761	U	OP2-P-O3'	5.02	116.25	105.20
36	5	631	U	O5'-P-OP1	-5.02	101.18	105.70
36	5	2632	G	O5'-P-OP1	-5.02	101.18	105.70
36	1	835	G	O4'-C1'-N9	5.02	112.22	108.20
36	1	1331	U	N3-C4-O4	5.02	122.91	119.40
36	1	2403	G	N3-C4-C5	-5.02	126.09	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2553	U	C2-N1-C1'	5.02	123.72	117.70
1	6	459	G	N1-C6-O6	5.02	122.91	119.90
37	7	101	G	N1-C6-O6	5.02	122.91	119.90
36	1	206	G	N1-C6-O6	-5.02	116.89	119.90
36	5	93	C	C6-N1-C2	5.02	122.31	120.30
36	5	514	G	N1-C6-O6	5.02	122.91	119.90
36	5	2372	A	C8-N9-C4	-5.02	103.79	105.80
36	5	2710	C	N3-C2-O2	5.02	125.41	121.90
36	5	2211	U	N3-C4-C5	-5.01	111.59	114.60
36	1	421	G	N3-C4-N9	5.01	129.01	126.00
1	6	1197	C	C2-N1-C1'	5.01	124.31	118.80
36	5	1395	G	OP2-P-O3'	5.01	116.23	105.20
1	2	1060	U	C2-N1-C1'	5.01	123.71	117.70
36	1	1724	U	O4'-C1'-N1	5.01	112.21	108.20
36	5	2385	G	O5'-P-OP1	-5.01	101.19	105.70
36	1	2385	G	N3-C4-N9	-5.01	123.00	126.00
1	6	1000	C	N1-C2-O2	5.01	121.90	118.90
36	5	2319	U	C5-C6-N1	-5.01	120.20	122.70
36	5	22	G	N1-C6-O6	5.00	122.90	119.90
36	5	1169	A	OP2-P-O3'	5.00	116.21	105.20
1	2	414	C	C6-N1-C2	5.00	122.30	120.30
1	2	1339	C	C2-N1-C1'	5.00	124.30	118.80
36	1	1583	A	C8-N9-C4	-5.00	103.80	105.80
36	5	947	G	N1-C2-N2	-5.00	111.70	116.20

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	C7	85	VAL	Peptide
27	D5	94	LYS	Peptide
28	D6	10	ARG	Peptide
52	M6	110	PRO	Peptide
56	N0	166	LYS	Peptide
56	N0	22	PRO	Peptide
9	S7	131	PHE	Peptide
17	c5	52	LYS	Peptide
26	d4	29	HIS	Peptide
44	l7	192	GLY	Peptide
44	l7	226	GLY	Peptide
59	n3	41	GLY	Peptide
64	n8	66	ALA	Peptide

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Mol	Chain	Res	Type	Group
79	q3	41	PHE	Peptide
7	s5	44	ASN	Peptide

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
3	S1	37	THR
3	S1	132	ASP
3	S1	148	ASN
3	S1	158	SER
3	S1	181	LEU
3	S1	182	ALA
3	S1	213	ARG
3	S1	221	PRO
4	S2	48	GLY
4	S2	91	ARG
4	S2	147	ASN
5	S3	62	ASN
5	S3	93	ASP
5	S3	220	PRO
7	S5	31	GLU
7	S5	33	VAL
7	S5	35	GLN
7	S5	39	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	S5	100	ASN
8	S6	154	ARG
8	S6	165	GLY
8	S6	173	PRO
9	S7	30	SER
9	S7	64	VAL
9	S7	67	LEU
9	S7	111	LYS
9	S7	112	ARG
9	S7	116	ARG
9	S7	131	PHE
9	S7	134	GLU
11	S9	98	ALA
11	S9	134	ILE
11	S9	152	SER
13	C1	7	VAL
13	C1	30	ARG
13	C1	55	ASP
14	C2	83	GLU
14	C2	91	VAL
14	C2	113	ARG
14	C2	127	GLY
15	C3	24	ALA
15	C3	27	LYS
16	C4	42	VAL
16	C4	124	ASP
17	C5	54	ALA
17	C5	80	MET
17	C5	125	PRO
18	C6	39	VAL
18	C6	41	PRO
18	C6	97	VAL
18	C6	114	ARG
18	C6	138	PHE
19	C7	23	LYS
19	C7	85	VAL
19	C7	86	PRO
19	C7	88	VAL
19	C7	124	VAL
20	C8	14	ILE
20	C8	60	GLU
20	C8	144	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
21	C9	31	PRO
21	C9	53	TRP
22	D0	118	VAL
23	D1	4	ASP
24	D2	83	ILE
25	D3	128	SER
25	D3	131	SER
26	D4	53	ASP
27	D5	97	LYS
28	D6	45	VAL
28	D6	82	ARG
28	D6	84	VAL
28	D6	85	ARG
28	D6	86	VAL
29	D7	62	ILE
31	D9	25	SER
32	E0	47	VAL
33	E1	84	VAL
33	E1	98	VAL
33	E1	144	CYS
34	SR	50	ASP
34	SR	238	ASP
34	SR	318	ALA
35	SM	52	PRO
35	SM	68	ARG
35	SM	140	ASP
39	L2	14	SER
40	L3	5	LYS
40	L3	292	ALA
41	L4	4	PRO
41	L4	130	ALA
41	L4	131	VAL
41	L4	311	HIS
42	L5	221	GLU
42	L5	223	PHE
42	L5	233	ALA
42	L5	234	ASP
42	L5	252	ALA
42	L5	253	PHE
43	L6	98	VAL
44	L7	26	VAL
45	L8	25	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	L8	31	PRO
45	L8	255	SER
47	M0	218	ALA
48	M1	8	PRO
48	M1	11	ASP
48	M1	74	PRO
48	M1	94	ARG
48	M1	165	GLN
49	M3	141	ALA
49	M3	193	ALA
50	M4	8	LYS
50	M4	9	ALA
51	M5	75	VAL
52	M6	110	PRO
52	M6	111	PRO
53	M7	157	VAL
53	M7	163	LYS
56	N0	142	GLN
56	N0	167	ARG
57	N1	124	VAL
58	N2	11	ILE
59	N3	132	ASN
60	N4	81	PRO
61	N5	44	PRO
62	N6	84	LYS
63	N7	30	ASP
63	N7	128	GLN
64	N8	27	LYS
64	N8	76	ASP
64	N8	97	GLU
67	O1	5	LYS
67	O1	84	ASP
71	O5	97	ALA
72	O6	33	ALA
72	O6	77	LEU
74	O8	33	LYS
76	Q0	78	ILE
78	Q2	15	LYS
79	Q3	58	SER
2	s0	4	PRO
2	s0	68	PRO
2	s0	81	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	s0	95	ALA
2	s0	164	ASN
2	s0	189	VAL
2	s0	206	ASP
3	s1	26	ARG
3	s1	55	LYS
3	s1	206	PRO
3	s1	210	ILE
4	s2	91	ARG
4	s2	92	ALA
4	s2	107	SER
5	s3	61	GLU
5	s3	160	SER
5	s3	211	PRO
5	s3	216	PRO
5	s3	217	ILE
5	s3	220	PRO
6	s4	12	LEU
6	s4	24	SER
6	s4	104	ASP
6	s4	118	GLU
6	s4	163	ASP
6	s4	164	LEU
6	s4	195	ILE
6	s4	196	VAL
6	s4	205	PHE
7	s5	28	PRO
7	s5	39	GLU
7	s5	43	PHE
7	s5	101	GLY
7	s5	184	PHE
7	s5	204	GLY
8	s6	122	GLU
8	s6	153	VAL
8	s6	173	PRO
8	s6	174	LYS
9	s7	64	VAL
9	s7	66	SER
9	s7	67	LEU
9	s7	131	PHE
11	s9	91	LYS
12	c0	2	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	c0	83	PRO
13	c1	133	LYS
14	c2	101	ALA
15	c3	12	SER
15	c3	66	ILE
16	c4	126	THR
16	c4	132	ARG
17	c5	11	VAL
17	c5	17	TYR
17	c5	51	SER
17	c5	52	LYS
17	c5	126	VAL
17	c5	127	ARG
18	c6	39	VAL
18	c6	42	GLU
18	c6	116	LEU
19	c7	88	VAL
19	c7	103	ASP
20	c8	14	ILE
20	c8	55	HIS
21	c9	29	GLU
21	c9	34	VAL
22	d0	15	GLN
22	d0	49	ASN
22	d0	118	VAL
26	d4	30	PRO
26	d4	33	ALA
26	d4	35	VAL
27	d5	85	LYS
27	d5	87	GLY
28	d6	82	ARG
29	d7	60	SER
30	d8	32	PHE
31	d9	6	VAL
31	d9	7	TRP
32	e0	45	VAL
32	e0	60	PRO
33	e1	83	LYS
33	e1	87	THR
33	e1	92	LYS
33	e1	98	VAL
33	e1	102	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
33	e1	103	LEU
33	e1	137	ASP
34	sR	160	GLU
34	sR	163	ASP
34	sR	165	ASP
34	sR	318	ALA
39	l2	144	ASN
39	l2	215	ASN
39	l2	238	ILE
40	l3	23	ALA
40	l3	129	ALA
41	l4	15	ALA
41	l4	301	PRO
41	l4	311	HIS
41	l4	345	GLU
42	l5	178	ASN
42	l5	258	LYS
43	l6	98	VAL
44	l7	159	GLN
45	l8	25	PRO
45	l8	34	PHE
45	l8	122	LYS
45	l8	133	LYS
48	m1	8	PRO
48	m1	9	MET
48	m1	10	ARG
49	m3	44	ALA
49	m3	47	ALA
49	m3	93	ILE
49	m3	101	ARG
49	m3	134	GLU
49	m3	150	PRO
49	m3	152	THR
51	m5	76	PRO
54	m8	84	VAL
54	m8	99	THR
54	m8	112	ALA
54	m8	113	LYS
57	n1	118	GLU
57	n1	135	PRO
58	n2	27	VAL
58	n2	50	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
60	n4	26	SER
60	n4	63	ILE
61	n5	44	PRO
62	n6	83	ASP
62	n6	84	LYS
62	n6	125	LYS
63	n7	4	PHE
63	n7	7	ALA
63	n7	17	ARG
64	n8	47	LYS
64	n8	76	ASP
64	n8	120	ASN
65	n9	21	ILE
65	n9	23	LYS
65	n9	52	LYS
66	o0	100	ILE
67	o1	45	GLY
67	o1	84	ASP
68	o2	5	PRO
69	o3	88	ASN
70	o4	79	SER
71	o5	119	LYS
72	o6	4	LYS
72	o6	98	ARG
73	o7	84	SER
74	o8	17	ARG
74	o8	18	ALA
76	q0	78	ILE
81	p0	93	LEU
2	S0	5	ALA
2	S0	27	ARG
2	S0	39	ASN
2	S0	66	ALA
2	S0	190	ASP
2	S0	195	TRP
3	S1	35	PRO
3	S1	49	ASN
3	S1	60	ALA
3	S1	61	LEU
3	S1	62	LYS
3	S1	63	GLY
3	S1	177	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	S2	106	ASP
4	S2	247	ALA
5	S3	216	PRO
6	S4	12	LEU
6	S4	195	ILE
6	S4	258	GLN
7	S5	26	ALA
7	S5	43	PHE
7	S5	58	LEU
7	S5	63	GLN
7	S5	98	MET
7	S5	150	GLY
7	S5	153	GLY
8	S6	25	ARG
8	S6	118	GLU
8	S6	152	ASP
8	S6	174	LYS
9	S7	32	PRO
9	S7	98	ILE
10	S8	40	ALA
10	S8	120	THR
11	S9	118	LEU
12	C0	60	SER
13	C1	6	THR
14	C2	93	ASP
14	C2	101	ALA
14	C2	119	SER
14	C2	125	ASN
15	C3	22	ALA
15	C3	28	LEU
16	C4	126	THR
17	C5	126	VAL
19	C7	87	GLU
20	C8	7	GLU
20	C8	25	ASN
20	C8	91	ASP
20	C8	92	ILE
21	C9	69	LYS
23	D1	2	GLU
23	D1	15	ARG
23	D1	41	GLU
24	D2	66	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	D3	8	GLY
25	D3	46	SER
25	D3	70	LYS
25	D3	112	LYS
26	D4	4	ALA
26	D4	5	VAL
26	D4	35	VAL
26	D4	100	VAL
27	D5	43	ASP
27	D5	71	ILE
28	D6	5	ARG
28	D6	18	VAL
29	D7	57	GLU
30	D8	36	THR
31	D9	6	VAL
31	D9	8	PHE
33	E1	94	LYS
33	E1	111	GLU
33	E1	127	GLY
34	SR	237	GLN
35	SM	82	THR
35	SM	86	ASN
35	SM	111	GLY
39	L2	47	GLN
39	L2	251	LYS
40	L3	142	ALA
40	L3	291	GLU
41	L4	14	GLU
41	L4	15	ALA
41	L4	146	PRO
41	L4	232	SER
41	L4	268	ALA
41	L4	269	SER
41	L4	338	LYS
42	L5	57	ASN
42	L5	93	THR
42	L5	106	ALA
42	L5	137	ASP
44	L7	160	ARG
44	L7	163	LEU
45	L8	36	ILE
45	L8	39	ALA

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	L8	122	LYS
46	L9	190	ASP
47	M0	41	ALA
47	M0	63	GLU
47	M0	64	ALA
47	M0	194	GLY
48	M1	12	LEU
48	M1	24	GLY
48	M1	108	GLU
48	M1	115	LYS
48	M1	173	ASP
49	M3	47	ALA
49	M3	166	ALA
50	M4	28	SER
50	M4	29	ALA
50	M4	136	ALA
51	M5	74	PRO
51	M5	184	LYS
53	M7	161	ALA
53	M7	164	LYS
53	M7	182	ILE
54	M8	98	LYS
54	M8	149	ALA
55	M9	53	LYS
58	N2	31	ALA
58	N2	51	GLY
59	N3	131	SER
60	N4	97	LYS
61	N5	45	LYS
63	N7	35	SER
63	N7	102	GLU
64	N8	66	ALA
64	N8	96	LYS
64	N8	115	LYS
67	O1	6	ASP
68	O2	27	ARG
68	O2	40	SER
68	O2	125	ARG
70	O4	82	ALA
71	O5	119	LYS
72	O6	34	SER
72	O6	64	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
72	O6	98	ARG
75	O9	4	GLN
78	Q2	17	CYS
78	Q2	30	ALA
78	Q2	94	GLY
78	Q2	100	LYS
79	Q3	12	GLY
2	s0	8	ASP
2	s0	30	GLN
3	s1	21	VAL
3	s1	93	GLY
3	s1	106	THR
3	s1	147	ALA
3	s1	223	PHE
4	s2	106	ASP
4	s2	163	GLY
5	s3	179	GLN
6	s4	11	ARG
6	s4	94	ALA
6	s4	95	THR
7	s5	36	ALA
7	s5	74	ALA
7	s5	153	GLY
8	s6	138	ALA
8	s6	154	ARG
9	s7	34	LEU
10	s8	122	GLY
12	c0	82	LEU
13	c1	7	VAL
14	c2	22	VAL
14	c2	89	ILE
15	c3	137	PRO
15	c3	140	LYS
16	c4	51	ASP
17	c5	6	ASN
17	c5	50	THR
17	c5	69	GLU
17	c5	80	MET
17	c5	132	GLY
17	c5	135	THR
19	c7	99	VAL
20	c8	61	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
20	c8	135	GLY
21	c9	28	LEU
26	d4	32	ARG
27	d5	38	HIS
27	d5	50	ILE
28	d6	28	LYS
30	d8	61	ARG
33	e1	81	LYS
33	e1	84	VAL
33	e1	100	LEU
33	e1	106	TYR
33	e1	127	GLY
35	sM	42	ALA
35	sM	47	ALA
39	l2	24	GLN
39	l2	56	ALA
39	l2	80	GLU
39	l2	143	GLU
39	l2	249	SER
40	l3	3	HIS
40	l3	385	LYS
40	l3	386	ASP
41	l4	142	VAL
41	l4	247	PHE
41	l4	342	LYS
42	l5	270	LYS
43	l6	20	LYS
43	l6	32	ALA
43	l6	97	ASN
45	l8	26	LEU
45	l8	39	ALA
45	l8	121	SER
45	l8	223	ALA
45	l8	237	ILE
45	l8	240	ASN
46	l9	144	ILE
47	m0	25	ALA
47	m0	82	ARG
48	m1	39	GLN
48	m1	94	ARG
48	m1	115	LYS
49	m3	51	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	m3	129	ASN
51	m5	183	THR
51	m5	184	LYS
52	m6	16	VAL
53	m7	63	PHE
54	m8	21	SER
55	m9	35	ALA
55	m9	112	ALA
56	n0	129	ILE
57	n1	136	ARG
58	n2	48	GLY
60	n4	64	THR
60	n4	76	VAL
60	n4	83	THR
61	n5	38	LEU
61	n5	40	LEU
61	n5	45	LYS
61	n5	47	ALA
61	n5	48	SER
63	n7	16	GLY
63	n7	33	SER
63	n7	125	GLY
65	n9	39	PHE
66	o0	10	ILE
67	o1	85	ALA
68	o2	6	HIS
73	o7	85	LYS
78	q2	74	CYS
81	p0	68	SER
81	p0	102	SER
2	S0	36	TYR
2	S0	49	ASN
2	S0	196	SER
3	S1	26	ARG
3	S1	58	SER
3	S1	147	ALA
3	S1	206	PRO
6	S4	96	ASN
6	S4	104	ASP
6	S4	231	GLN
7	S5	54	LYS
7	S5	127	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	S6	20	ASP
8	S6	69	LEU
9	S7	5	GLN
10	S8	59	ARG
10	S8	152	ILE
13	C1	145	ALA
13	C1	146	ALA
14	C2	89	ILE
14	C2	112	ALA
16	C4	18	ARG
16	C4	51	ASP
16	C4	75	GLY
16	C4	125	SER
17	C5	52	LYS
17	C5	101	ALA
18	C6	33	GLY
20	C8	8	GLN
20	C8	61	LEU
21	C9	29	GLU
21	C9	50	ALA
22	D0	21	LYS
22	D0	49	ASN
23	D1	10	GLU
23	D1	42	GLU
23	D1	44	ARG
25	D3	3	LYS
25	D3	92	CYS
25	D3	114	LYS
26	D4	34	ASN
26	D4	47	VAL
26	D4	54	ALA
28	D6	47	ALA
28	D6	63	ALA
31	D9	11	PRO
32	E0	60	PRO
33	E1	87	THR
34	SR	98	GLU
34	SR	194	GLY
34	SR	249	ARG
35	SM	12	VAL
35	SM	15	ALA
35	SM	42	ALA

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	SM	87	THR
35	SM	139	GLU
39	L2	127	ALA
39	L2	141	PRO
39	L2	143	GLU
40	L3	347	SER
41	L4	270	SER
41	L4	293	SER
42	L5	110	LEU
42	L5	176	SER
42	L5	215	ASP
42	L5	259	LYS
42	L5	260	PHE
43	L6	150	LYS
45	L8	97	TYR
45	L8	114	ALA
45	L8	254	ASP
46	L9	2	LYS
46	L9	15	GLY
47	M0	207	GLU
48	M1	114	ILE
49	M3	129	ASN
49	M3	134	GLU
49	M3	136	GLU
51	M5	8	GLU
59	N3	69	LEU
62	N6	126	LEU
67	O1	82	GLU
68	O2	127	ALA
74	O8	19	ASP
79	Q3	50	GLY
79	Q3	51	ALA
79	Q3	91	GLU
3	s1	82	ARG
5	s3	44	THR
5	s3	219	ALA
6	s4	57	ASN
6	s4	168	LYS
7	s5	56	ALA
8	s6	152	ASP
9	s7	30	SER
9	s7	74	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	s8	199	LYS
11	s9	167	ALA
12	c0	30	ALA
12	c0	35	ILE
13	c1	145	ALA
14	c2	54	ARG
14	c2	58	LEU
14	c2	108	ARG
14	c2	119	SER
14	c2	131	ASP
15	c3	29	SER
15	c3	139	TRP
17	c5	7	ALA
17	c5	14	THR
17	c5	68	PRO
18	c6	113	ASP
20	c8	18	LEU
20	c8	33	THR
20	c8	36	LYS
21	c9	33	TYR
22	d0	52	LYS
22	d0	96	PRO
23	d1	42	GLU
25	d3	70	LYS
26	d4	51	GLU
26	d4	53	ASP
26	d4	68	LYS
28	d6	13	LYS
28	d6	34	LYS
29	d7	75	GLU
32	e0	51	ASN
32	e0	54	ARG
32	e0	61	SER
33	e1	85	TYR
33	e1	136	LYS
33	e1	145	HIS
34	sR	96	THR
34	sR	161	LYS
34	sR	226	ALA
35	sM	33	LYS
35	sM	50	ASN
35	sM	65	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	l2	96	LEU
39	l2	130	SER
39	l2	142	ASP
40	l3	187	SER
41	l4	14	GLU
41	l4	90	PHE
41	l4	144	LYS
41	l4	145	ILE
41	l4	233	LEU
41	l4	305	ALA
42	l5	123	GLU
42	l5	260	PHE
43	l6	10	TYR
44	l7	158	LYS
44	l7	229	PHE
45	l8	203	VAL
47	m0	3	ARG
47	m0	176	LEU
47	m0	207	GLU
47	m0	219	ALA
48	m1	167	TYR
49	m3	13	HIS
49	m3	37	ASN
49	m3	45	LYS
49	m3	50	PRO
49	m3	135	ALA
50	m4	136	ALA
51	m5	81	TYR
51	m5	187	ARG
53	m7	75	GLU
54	m8	127	LEU
63	n7	34	LYS
63	n7	134	LEU
64	n8	94	ALA
64	n8	129	PHE
65	n9	51	ALA
66	o0	104	LEU
67	o1	83	GLU
68	o2	122	PRO
68	o2	124	GLY
70	o4	14	ASN
70	o4	82	ALA

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
70	o4	93	PHE
71	o5	82	ALA
71	o5	84	LYS
72	o6	33	ALA
73	o7	67	LEU
73	o7	68	LYS
75	o9	44	TRP
79	q3	20	SER
81	p0	203	ASP
2	S0	103	THR
3	S1	38	PHE
3	S1	54	LEU
3	S1	210	ILE
4	S2	39	THR
4	S2	107	SER
4	S2	145	GLY
4	S2	150	GLN
4	S2	182	PRO
4	S2	208	GLU
4	S2	236	PRO
4	S2	248	SER
5	S3	89	GLU
5	S3	112	GLY
5	S3	217	ILE
6	S4	11	ARG
6	S4	26	CYS
6	S4	200	ARG
6	S4	213	SER
7	S5	51	VAL
7	S5	64	VAL
9	S7	29	ASN
9	S7	54	GLY
11	S9	16	LYS
11	S9	150	LEU
14	C2	39	ASP
14	C2	106	ILE
14	C2	107	ASP
14	C2	126	TRP
16	C4	50	ALA
16	C4	86	THR
17	C5	9	LYS
17	C5	69	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	C6	113	ASP
19	C7	115	LEU
20	C8	145	ARG
21	C9	116	ILE
22	D0	17	GLN
22	D0	96	PRO
23	D1	82	VAL
25	D3	40	SER
25	D3	115	GLY
26	D4	49	LYS
27	D5	38	HIS
30	D8	20	GLY
32	E0	13	LYS
33	E1	102	VAL
33	E1	118	ARG
34	SR	48	THR
34	SR	51	ASP
34	SR	105	GLY
34	SR	163	ASP
41	L4	138	ARG
41	L4	341	SER
42	L5	249	ALA
42	L5	258	LYS
42	L5	271	LYS
46	L9	96	HIS
48	M1	64	LYS
48	M1	117	ASP
48	M1	152	HIS
48	M1	167	TYR
49	M3	63	VAL
49	M3	165	SER
50	M4	10	SER
51	M5	81	TYR
53	M7	175	ARG
54	M8	162	ALA
56	N0	2	ALA
56	N0	24	LEU
60	N4	25	ASP
60	N4	77	LYS
61	N5	48	SER
62	N6	38	GLU
63	N7	103	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
64	N8	24	LYS
64	N8	47	LYS
64	N8	78	LEU
65	N9	25	LYS
68	O2	69	SER
68	O2	70	GLY
71	O5	75	TYR
71	O5	96	GLU
78	Q2	33	ALA
79	Q3	7	LYS
79	Q3	28	LYS
2	s0	139	VAL
2	s0	191	ARG
3	s1	60	ALA
3	s1	209	ASN
4	s2	150	GLN
4	s2	217	ALA
4	s2	234	PRO
4	s2	235	LEU
4	s2	238	SER
5	s3	45	LYS
5	s3	93	ASP
6	s4	117	GLU
6	s4	245	LYS
7	s5	55	ASP
7	s5	98	MET
9	s7	15	GLU
9	s7	133	THR
11	s9	130	THR
11	s9	147	MET
11	s9	162	SER
12	c0	23	ALA
12	c0	31	LYS
12	c0	32	HIS
14	c2	26	ASP
14	c2	39	ASP
14	c2	66	VAL
14	c2	87	PRO
14	c2	106	ILE
16	c4	12	GLN
16	c4	37	GLU
16	c4	124	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	c5	130	ARG
18	c6	3	ALA
20	c8	7	GLU
20	c8	8	GLN
20	c8	91	ASP
20	c8	115	ARG
24	d2	56	HIS
24	d2	68	ARG
25	d3	101	GLU
26	d4	50	ALA
26	d4	52	LYS
30	d8	62	GLU
31	d9	11	PRO
32	e0	47	VAL
33	e1	112	GLY
33	e1	128	ALA
33	e1	146	SER
34	sR	186	PHE
35	sM	36	ASP
35	sM	43	ASP
35	sM	46	LYS
39	l2	125	ALA
39	l2	127	ALA
40	l3	140	ASP
41	l4	5	GLN
41	l4	16	THR
41	l4	132	ALA
41	l4	146	PRO
42	l5	224	LYS
44	l7	191	VAL
45	l8	69	LEU
47	m0	220	GLN
48	m1	95	ASN
48	m1	108	GLU
48	m1	153	LYS
49	m3	60	ALA
53	m7	25	SER
54	m8	155	MET
56	n0	2	ALA
58	n2	91	ASP
60	n4	125	ALA
60	n4	134	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
61	n5	24	LEU
61	n5	25	LYS
62	n6	126	LEU
63	n7	103	GLN
67	o1	86	LYS
70	o4	47	CYS
78	q2	33	ALA
81	p0	33	VAL
3	S1	51	SER
3	S1	176	VAL
5	S3	196	ARG
6	S4	77	ARG
6	S4	93	ASP
6	S4	150	PRO
6	S4	245	LYS
8	S6	146	GLY
9	S7	73	VAL
9	S7	132	PRO
10	S8	10	LYS
10	S8	22	ARG
10	S8	154	SER
12	C0	26	ASP
12	C0	81	ASN
13	C1	40	LEU
14	C2	130	THR
15	C3	3	ARG
16	C4	114	ARG
16	C4	131	GLY
20	C8	102	ALA
21	C9	23	GLN
26	D4	11	LYS
28	D6	62	TYR
28	D6	64	LEU
29	D7	75	GLU
30	D8	35	ASP
33	E1	83	LYS
33	E1	85	TYR
33	E1	99	LYS
33	E1	110	ALA
33	E1	148	TYR
34	SR	146	GLY
35	SM	39	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	SM	53	ARG
35	SM	101	ASP
39	L2	98	VAL
40	L3	4	ARG
40	L3	317	ILE
41	L4	5	GLN
41	L4	140	HIS
41	L4	292	SER
41	L4	339	LEU
45	L8	75	ILE
45	L8	157	VAL
47	M0	113	GLN
47	M0	202	LYS
49	M3	46	ILE
49	M3	51	LEU
49	M3	76	THR
50	M4	6	ILE
52	M6	16	VAL
52	M6	89	SER
54	M8	41	ASP
63	N7	36	HIS
64	N8	91	LEU
67	O1	7	VAL
69	O3	91	ALA
72	O6	21	THR
72	O6	78	GLY
76	Q0	79	GLU
2	s0	10	THR
2	s0	103	THR
2	s0	109	ASN
2	s0	194	PRO
3	s1	22	ASP
3	s1	59	ASP
3	s1	129	THR
3	s1	224	ASP
6	s4	30	ARG
6	s4	90	ILE
6	s4	213	SER
7	s5	29	ILE
8	s6	70	PRO
10	s8	62	THR
10	s8	78	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	s8	101	ILE
11	s9	150	LEU
13	c1	55	ASP
14	c2	90	LYS
15	c3	22	ALA
16	c4	39	ILE
16	c4	50	ALA
17	c5	71	GLU
18	c6	40	GLU
19	c7	62	GLN
19	c7	86	PRO
19	c7	96	SER
19	c7	98	GLY
22	d0	17	GLN
22	d0	51	VAL
23	d1	10	GLU
25	d3	41	SER
28	d6	8	ASN
28	d6	35	ALA
29	d7	58	SER
30	d8	33	LEU
34	sR	281	TYR
35	sM	63	ASP
39	l2	13	GLY
40	l3	333	LYS
41	l4	220	ARG
41	l4	339	LEU
42	l5	265	TYR
42	l5	296	GLN
45	l8	70	LYS
46	l9	167	VAL
47	m0	204	GLY
48	m1	12	LEU
48	m1	114	ILE
49	m3	62	THR
50	m4	135	LEU
51	m5	42	PRO
51	m5	68	ARG
51	m5	74	PRO
54	m8	43	PRO
63	n7	70	PRO
66	o0	101	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
73	o7	86	ALA
74	o8	37	PRO
79	q3	51	ALA
3	S1	129	THR
4	S2	239	PRO
6	S4	204	GLY
14	C2	131	ASP
20	C8	82	PRO
22	D0	55	PRO
23	D1	46	ILE
25	D3	41	SER
25	D3	96	VAL
26	D4	36	SER
33	E1	100	LEU
39	L2	246	LEU
41	L4	23	PRO
42	L5	107	ARG
42	L5	136	GLU
44	L7	178	ILE
45	L8	30	THR
45	L8	79	GLN
47	M0	24	ARG
48	M1	95	ASN
51	M5	94	TYR
54	M8	99	THR
57	N1	18	ASP
57	N1	123	GLY
63	N7	124	ALA
68	O2	12	LYS
72	O6	3	VAL
78	Q2	34	SER
5	s3	203	PRO
8	s6	69	LEU
12	c0	24	LYS
13	c1	129	ARG
14	c2	40	GLY
14	c2	82	PRO
16	c4	48	VAL
18	c6	4	VAL
18	c6	97	VAL
21	c9	51	GLU
26	d4	77	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
31	d9	22	ARG
33	e1	148	TYR
34	sR	97	GLY
41	l4	91	GLY
44	l7	178	ILE
47	m0	194	GLY
62	n6	49	PRO
64	n8	56	VAL
65	n9	24	PRO
70	o4	78	GLY
72	o6	12	ASN
79	q3	4	ARG
79	q3	17	ARG
3	S1	48	VAL
10	S8	186	GLY
13	C1	130	PRO
34	SR	49	GLY
47	M0	117	GLY
48	M1	65	ILE
49	M3	130	GLY
52	M6	145	VAL
70	O4	77	GLY
12	c0	3	MET
17	c5	125	PRO
23	d1	77	GLY
40	l3	141	GLY
41	l4	190	GLY
2	S0	139	VAL
14	C2	22	VAL
14	C2	66	VAL
16	C4	39	ILE
28	D6	59	TYR
34	SR	15	GLY
42	L5	139	PRO
44	L7	91	GLY
45	L8	218	ILE
9	s7	185	ILE
14	c2	63	VAL
15	c3	60	VAL
16	c4	131	GLY
42	l5	125	VAL
58	n2	30	PRO

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Mol	Chain	Res	Type
61	n5	52	PRO
63	n7	36	HIS
8	S6	162	VAL
9	S7	144	VAL
9	S7	162	ILE
14	C2	87	PRO
20	C8	125	ILE
23	D1	6	GLY
27	D5	88	ILE
33	E1	91	ILE
53	M7	67	ILE
60	N4	76	VAL
6	s4	107	GLY
29	d7	62	ILE
34	sR	63	GLY
43	l6	171	PRO
54	m8	97	PRO
64	n8	28	HIS
72	o6	61	ILE
81	p0	80	VAL
7	S5	204	GLY
26	D4	95	GLY
30	D8	6	PRO
44	L7	191	VAL
45	L8	167	PRO
60	N4	90	ILE
5	s3	43	PRO
19	c7	9	VAL
30	d8	20	GLY
42	l5	255	PRO
15	C3	150	VAL
28	D6	58	VAL
71	O5	4	VAL
28	d6	59	TYR
34	sR	15	GLY
40	l3	186	GLY

### 5.3.2 Protein sidechains [i](#)

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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

All (3078) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	6	THR
2	S0	18	LEU
2	S0	39	ASN
2	S0	49	ASN
2	S0	50	VAL
2	S0	57	LEU
2	S0	84	ARG
2	S0	87	LEU
2	S0	88	LYS
2	S0	96	THR
2	S0	101	ARG
2	S0	110	TYR
2	S0	111	ILE
2	S0	112	THR
2	S0	137	SER
2	S0	154	GLU
2	S0	157	ASP
2	S0	164	ASN
2	S0	168	HIS
2	S0	172	LEU
2	S0	177	LEU
2	S0	185	ARG
2	S0	188	LEU
2	S0	196	SER
2	S0	198	MET
3	S1	25	THR
3	S1	29	TRP
3	S1	30	PHE
3	S1	46	THR
3	S1	61	LEU
3	S1	65	VAL
3	S1	70	LEU
3	S1	74	GLN
3	S1	77	GLU
3	S1	78	ASP
3	S1	81	PHE
3	S1	83	LYS
3	S1	89	ASP
3	S1	97	LEU
3	S1	105	PHE
3	S1	137	ILE
3	S1	154	SER
3	S1	180	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	S1	181	LEU
3	S1	184	LEU
3	S1	193	ILE
3	S1	202	LYS
3	S1	218	LEU
3	S1	223	PHE
3	S1	225	VAL
4	S2	41	LEU
4	S2	53	ILE
4	S2	64	LYS
4	S2	72	LEU
4	S2	89	GLN
4	S2	94	GLN
4	S2	95	ARG
4	S2	96	THR
4	S2	97	ARG
4	S2	99	LYS
4	S2	103	VAL
4	S2	111	VAL
4	S2	117	THR
4	S2	137	ILE
4	S2	139	ILE
4	S2	141	ARG
4	S2	148	LEU
4	S2	159	THR
4	S2	170	ILE
4	S2	186	LYS
4	S2	208	GLU
4	S2	221	THR
4	S2	222	TYR
4	S2	225	LEU
4	S2	226	THR
4	S2	235	LEU
4	S2	237	VAL
4	S2	244	SER
5	S3	4	LEU
5	S3	7	LYS
5	S3	21	LEU
5	S3	23	GLU
5	S3	57	ASP
5	S3	61	GLU
5	S3	64	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	S3	65	ARG
5	S3	66	ILE
5	S3	76	ARG
5	S3	84	ILE
5	S3	93	ASP
5	S3	103	GLU
5	S3	105	MET
5	S3	111	ASN
5	S3	113	LEU
5	S3	117	ARG
5	S3	124	ARG
5	S3	128	GLU
5	S3	151	LYS
5	S3	158	ILE
5	S3	168	ILE
5	S3	172	THR
5	S3	175	VAL
5	S3	176	LEU
5	S3	177	MET
5	S3	178	ARG
5	S3	181	VAL
5	S3	182	LEU
5	S3	190	ARG
5	S3	195	SER
5	S3	217	ILE
5	S3	223	LYS
6	S4	6	LYS
6	S4	9	LEU
6	S4	12	LEU
6	S4	26	CYS
6	S4	38	LEU
6	S4	42	LEU
6	S4	45	ILE
6	S4	54	TYR
6	S4	62	LYS
6	S4	65	LEU
6	S4	77	ARG
6	S4	92	LEU
6	S4	93	ASP
6	S4	95	THR
6	S4	105	VAL
6	S4	109	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	S4	113	ARG
6	S4	115	THR
6	S4	116	ASP
6	S4	123	LEU
6	S4	131	LEU
6	S4	180	LEU
6	S4	182	TYR
6	S4	187	ARG
6	S4	192	ILE
6	S4	206	ASP
6	S4	211	LYS
6	S4	215	ASP
6	S4	221	ARG
6	S4	226	PHE
6	S4	227	VAL
6	S4	240	LYS
6	S4	242	LYS
6	S4	246	LEU
6	S4	259	GLN
7	S5	25	LEU
7	S5	32	GLU
7	S5	38	THR
7	S5	41	LYS
7	S5	43	PHE
7	S5	45	LYS
7	S5	47	SER
7	S5	48	PHE
7	S5	52	GLU
7	S5	53	VAL
7	S5	65	ARG
7	S5	66	GLN
7	S5	76	ARG
7	S5	79	ASN
7	S5	84	LYS
7	S5	89	ILE
7	S5	93	LEU
7	S5	98	MET
7	S5	119	ASP
7	S5	122	ASN
7	S5	126	ASP
7	S5	146	THR
7	S5	147	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	S5	156	ARG
7	S5	157	ARG
7	S5	160	VAL
7	S5	163	SER
7	S5	187	ILE
7	S5	194	LEU
7	S5	216	GLU
7	S5	223	SER
7	S5	225	ARG
8	S6	7	TYR
8	S6	15	THR
8	S6	19	ASP
8	S6	20	ASP
8	S6	21	GLU
8	S6	25	ARG
8	S6	43	ASP
8	S6	44	GLU
8	S6	67	VAL
8	S6	68	LEU
8	S6	69	LEU
8	S6	71	THR
8	S6	76	LEU
8	S6	79	LYS
8	S6	82	SER
8	S6	89	ASP
8	S6	91	GLU
8	S6	98	ARG
8	S6	109	LEU
8	S6	115	LYS
8	S6	120	GLU
8	S6	124	LEU
8	S6	125	THR
8	S6	126	ASP
8	S6	127	THR
8	S6	128	THR
8	S6	132	ARG
8	S6	133	LEU
8	S6	151	ASP
8	S6	154	ARG
8	S6	155	ASP
8	S6	158	ILE
8	S6	169	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	S6	189	HIS
8	S6	201	GLN
8	S6	216	LEU
9	S7	15	GLU
9	S7	16	LEU
9	S7	28	GLU
9	S7	37	GLU
9	S7	38	LEU
9	S7	46	ILE
9	S7	49	ILE
9	S7	50	ASP
9	S7	55	LYS
9	S7	67	LEU
9	S7	70	PHE
9	S7	74	GLN
9	S7	76	LYS
9	S7	77	LEU
9	S7	85	PHE
9	S7	87	ASP
9	S7	91	ILE
9	S7	97	ARG
9	S7	104	ARG
9	S7	110	GLN
9	S7	114	ARG
9	S7	116	ARG
9	S7	122	HIS
9	S7	126	LEU
9	S7	136	VAL
9	S7	144	VAL
9	S7	158	ASP
9	S7	174	ASN
9	S7	185	ILE
10	S8	8	ARG
10	S8	20	GLN
10	S8	21	PHE
10	S8	29	LEU
10	S8	36	THR
10	S8	37	LYS
10	S8	46	VAL
10	S8	56	ARG
10	S8	58	LEU
10	S8	70	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	S8	72	ILE
10	S8	138	ASN
10	S8	151	LYS
10	S8	152	ILE
10	S8	155	SER
10	S8	158	SER
10	S8	164	ARG
10	S8	184	LEU
10	S8	185	GLU
10	S8	187	GLU
10	S8	196	LEU
11	S9	3	ARG
11	S9	6	ARG
11	S9	7	THR
11	S9	14	THR
11	S9	22	SER
11	S9	28	LEU
11	S9	39	LYS
11	S9	61	THR
11	S9	63	ASP
11	S9	78	ARG
11	S9	80	LEU
11	S9	88	GLU
11	S9	89	ASP
11	S9	92	LYS
11	S9	93	LEU
11	S9	94	ASP
11	S9	97	LEU
11	S9	99	LEU
11	S9	110	GLN
11	S9	134	ILE
11	S9	138	LYS
11	S9	140	ILE
11	S9	149	ARG
11	S9	161	THR
11	S9	162	SER
11	S9	171	ARG
11	S9	172	VAL
11	S9	174	ARG
11	S9	182	GLU
11	S9	186	GLU
12	C0	1	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	C0	8	ARG
12	C0	20	VAL
12	C0	27	PHE
12	C0	29	GLN
12	C0	32	HIS
12	C0	39	ASN
12	C0	46	LEU
12	C0	55	VAL
12	C0	56	LYS
12	C0	76	LEU
12	C0	81	ASN
12	C0	82	LEU
13	C1	4	GLU
13	C1	8	GLN
13	C1	16	GLN
13	C1	21	ASN
13	C1	37	ASN
13	C1	40	LEU
13	C1	44	THR
13	C1	67	ARG
13	C1	69	LYS
13	C1	72	THR
13	C1	80	MET
13	C1	83	THR
13	C1	91	LEU
13	C1	136	ARG
13	C1	140	VAL
14	C2	28	LEU
14	C2	33	ARG
14	C2	37	VAL
14	C2	41	LEU
14	C2	43	ARG
14	C2	52	LEU
14	C2	54	ARG
14	C2	61	VAL
14	C2	62	LEU
14	C2	66	VAL
14	C2	86	VAL
14	C2	89	ILE
14	C2	103	LEU
14	C2	126	TRP
14	C2	129	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	C2	132	GLU
14	C2	139	HIS
15	C3	3	ARG
15	C3	9	LYS
15	C3	19	SER
15	C3	21	ASN
15	C3	27	LYS
15	C3	33	VAL
15	C3	39	LYS
15	C3	56	ASP
15	C3	58	HIS
15	C3	64	ARG
15	C3	66	ILE
15	C3	76	LYS
15	C3	88	LEU
15	C3	98	VAL
15	C3	102	LEU
15	C3	105	ASN
15	C3	106	ARG
15	C3	114	ARG
15	C3	115	LEU
15	C3	120	SER
15	C3	125	LEU
15	C3	134	VAL
15	C3	140	LYS
16	C4	12	GLN
16	C4	20	TYR
16	C4	25	ASP
16	C4	26	THR
16	C4	39	ILE
16	C4	42	VAL
16	C4	81	VAL
16	C4	92	LYS
16	C4	99	GLN
16	C4	103	ARG
16	C4	107	ARG
16	C4	115	ILE
16	C4	123	SER
16	C4	125	SER
16	C4	126	THR
16	C4	133	ARG
16	C4	137	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	C5	11	VAL
17	C5	13	LYS
17	C5	14	THR
17	C5	22	LEU
17	C5	26	LEU
17	C5	31	GLU
17	C5	43	ARG
17	C5	44	ARG
17	C5	52	LYS
17	C5	60	LEU
17	C5	65	LEU
17	C5	84	ILE
17	C5	86	VAL
17	C5	110	GLU
18	C6	4	VAL
18	C6	26	LYS
18	C6	28	LEU
18	C6	29	ILE
18	C6	39	VAL
18	C6	43	ILE
18	C6	53	LEU
18	C6	57	LEU
18	C6	66	ARG
18	C6	69	VAL
18	C6	74	HIS
18	C6	106	LYS
18	C6	109	PHE
18	C6	114	ARG
18	C6	123	ARG
18	C6	127	LYS
18	C6	128	LYS
18	C6	137	ARG
18	C6	143	ARG
19	C7	5	ARG
19	C7	25	THR
19	C7	35	CYS
19	C7	38	ILE
19	C7	40	THR
19	C7	43	SER
19	C7	46	LEU
19	C7	62	GLN
19	C7	69	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
19	C7	72	LYS
19	C7	79	GLU
19	C7	83	GLN
19	C7	84	TYR
19	C7	88	VAL
19	C7	105	GLN
19	C7	107	SER
19	C7	109	LEU
19	C7	115	LEU
19	C7	119	LEU
20	C8	3	LEU
20	C8	5	VAL
20	C8	11	PHE
20	C8	12	GLN
20	C8	13	HIS
20	C8	14	ILE
20	C8	15	LEU
20	C8	16	ARG
20	C8	20	THR
20	C8	25	ASN
20	C8	26	ILE
20	C8	38	VAL
20	C8	40	ARG
20	C8	53	ASP
20	C8	54	LEU
20	C8	60	GLU
20	C8	61	LEU
20	C8	71	GLN
20	C8	77	THR
20	C8	80	LYS
20	C8	92	ILE
20	C8	105	VAL
20	C8	116	LEU
20	C8	132	ARG
20	C8	136	GLN
20	C8	138	THR
21	C9	4	VAL
21	C9	13	ASP
21	C9	18	TYR
21	C9	22	LEU
21	C9	28	LEU
21	C9	33	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
21	C9	35	ASP
21	C9	36	ILE
21	C9	37	VAL
21	C9	57	ARG
21	C9	63	ARG
21	C9	67	MET
21	C9	70	GLN
21	C9	125	SER
21	C9	126	GLU
21	C9	130	ARG
21	C9	131	ASP
21	C9	132	LEU
21	C9	133	ASP
21	C9	134	ARG
21	C9	139	THR
21	C9	144	GLU
22	D0	18	GLN
22	D0	23	ARG
22	D0	27	THR
22	D0	35	GLU
22	D0	47	GLN
22	D0	50	LEU
22	D0	51	VAL
22	D0	57	ARG
22	D0	66	SER
22	D0	74	GLU
22	D0	76	SER
22	D0	81	THR
22	D0	85	ARG
22	D0	89	ARG
22	D0	105	GLN
22	D0	108	ILE
22	D0	121	ASN
23	D1	5	LYS
23	D1	7	GLN
23	D1	9	VAL
23	D1	11	LEU
23	D1	25	LYS
23	D1	33	GLN
23	D1	40	ASP
23	D1	49	GLU
23	D1	76	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
23	D1	78	LEU
23	D1	79	LEU
23	D1	87	ARG
24	D2	4	SER
24	D2	24	GLN
24	D2	25	VAL
24	D2	26	LEU
24	D2	27	ILE
24	D2	33	VAL
24	D2	43	LYS
24	D2	47	ILE
24	D2	53	ILE
24	D2	65	LEU
24	D2	66	ASN
24	D2	97	ARG
24	D2	103	ILE
24	D2	104	LEU
24	D2	105	THR
24	D2	111	MET
24	D2	121	VAL
24	D2	126	LEU
24	D2	129	VAL
25	D3	9	LEU
25	D3	19	ARG
25	D3	31	LYS
25	D3	47	SER
25	D3	72	VAL
25	D3	84	THR
25	D3	100	ASP
25	D3	107	PHE
25	D3	114	LYS
25	D3	117	ILE
25	D3	130	VAL
25	D3	132	LEU
25	D3	133	LEU
25	D3	138	GLU
25	D3	140	LYS
25	D3	144	ARG
26	D4	8	ARG
26	D4	21	LYS
26	D4	29	HIS
26	D4	32	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
26	D4	47	VAL
26	D4	51	GLU
26	D4	57	VAL
26	D4	62	THR
26	D4	84	LYS
26	D4	96	LEU
26	D4	99	LYS
26	D4	102	LYS
26	D4	104	SER
26	D4	124	ARG
26	D4	125	LEU
26	D4	127	LYS
27	D5	42	LEU
27	D5	51	LEU
27	D5	58	ARG
27	D5	59	TYR
27	D5	63	SER
27	D5	65	LEU
27	D5	67	ASP
27	D5	69	LEU
27	D5	75	LEU
27	D5	78	ILE
27	D5	85	LYS
27	D5	92	ILE
27	D5	95	HIS
27	D5	100	ILE
27	D5	102	THR
27	D5	103	ARG
28	D6	5	ARG
28	D6	33	ASP
28	D6	36	ILE
28	D6	38	ARG
28	D6	41	ILE
28	D6	45	VAL
28	D6	50	VAL
28	D6	55	GLU
28	D6	58	VAL
28	D6	61	GLU
28	D6	64	LEU
28	D6	66	LYS
28	D6	68	TYR
28	D6	69	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
28	D6	82	ARG
28	D6	83	ILE
28	D6	85	ARG
28	D6	87	ARG
28	D6	88	SER
28	D6	91	ASP
29	D7	3	LEU
29	D7	11	THR
29	D7	15	GLU
29	D7	23	THR
29	D7	33	LEU
29	D7	34	ASP
29	D7	41	LEU
29	D7	56	CYS
29	D7	60	SER
29	D7	61	THR
29	D7	77	THR
29	D7	78	SER
30	D8	19	THR
30	D8	31	GLU
30	D8	32	PHE
30	D8	33	LEU
30	D8	39	THR
30	D8	40	ILE
30	D8	48	VAL
30	D8	49	ARG
30	D8	52	ASP
30	D8	58	GLU
30	D8	64	ARG
31	D9	7	TRP
31	D9	8	PHE
31	D9	19	ARG
31	D9	21	CYS
31	D9	25	SER
31	D9	30	LEU
31	D9	32	ARG
31	D9	36	LEU
32	E0	20	LYS
32	E0	39	LEU
32	E0	42	ARG
32	E0	47	VAL
32	E0	50	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	E0	56	MET
33	E1	85	TYR
33	E1	86	THR
33	E1	89	LYS
33	E1	97	LYS
33	E1	98	VAL
33	E1	102	VAL
33	E1	108	VAL
33	E1	113	LYS
33	E1	130	VAL
33	E1	137	ASP
33	E1	138	ARG
33	E1	139	LEU
33	E1	147	VAL
33	E1	151	ASN
34	SR	6	VAL
34	SR	10	ARG
34	SR	37	SER
34	SR	45	TRP
34	SR	50	ASP
34	SR	52	GLN
34	SR	66	HIS
34	SR	74	THR
34	SR	76	ASP
34	SR	100	TYR
34	SR	102	ARG
34	SR	109	ASP
34	SR	116	ASP
34	SR	117	LYS
34	SR	131	ILE
34	SR	136	ILE
34	SR	141	LEU
34	SR	144	LEU
34	SR	148	ASN
34	SR	149	ASP
34	SR	154	VAL
34	SR	165	ASP
34	SR	196	ASN
34	SR	202	LEU
34	SR	222	LEU
34	SR	223	TRP
34	SR	229	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	SR	238	ASP
34	SR	245	PHE
34	SR	248	ASN
34	SR	266	ASP
34	SR	277	GLU
34	SR	308	ASN
35	SM	41	SER
35	SM	46	LYS
35	SM	48	ARG
35	SM	53	ARG
35	SM	55	SER
35	SM	61	ILE
35	SM	64	LYS
35	SM	68	ARG
35	SM	71	ASN
35	SM	73	SER
35	SM	77	THR
35	SM	78	ASP
35	SM	84	LYS
35	SM	91	THR
35	SM	92	ASP
35	SM	100	THR
35	SM	102	THR
35	SM	106	VAL
35	SM	108	GLN
35	SM	121	LYS
39	L2	8	GLN
39	L2	14	SER
39	L2	18	SER
39	L2	20	THR
39	L2	28	LYS
39	L2	32	LEU
39	L2	37	ARG
39	L2	44	ILE
39	L2	45	VAL
39	L2	46	LYS
39	L2	62	VAL
39	L2	70	ARG
39	L2	72	ARG
39	L2	73	GLU
39	L2	82	VAL
39	L2	95	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	L2	96	LEU
39	L2	97	ASN
39	L2	101	VAL
39	L2	104	LEU
39	L2	107	VAL
39	L2	111	THR
39	L2	116	VAL
39	L2	119	LYS
39	L2	128	ARG
39	L2	130	SER
39	L2	134	VAL
39	L2	143	GLU
39	L2	147	ARG
39	L2	157	VAL
39	L2	165	VAL
39	L2	179	LEU
39	L2	180	LEU
39	L2	197	PRO
39	L2	207	VAL
39	L2	227	ARG
39	L2	231	SER
39	L2	241	ARG
39	L2	247	ARG
39	L2	250	GLN
39	L2	252	THR
40	L3	3	HIS
40	L3	7	GLU
40	L3	17	LEU
40	L3	19	ARG
40	L3	25	ILE
40	L3	30	LYS
40	L3	37	ARG
40	L3	47	LEU
40	L3	53	MET
40	L3	55	THR
40	L3	56	ILE
40	L3	67	PHE
40	L3	70	ARG
40	L3	79	VAL
40	L3	84	VAL
40	L3	85	VAL
40	L3	97	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
40	L3	103	THR
40	L3	114	VAL
40	L3	116	ARG
40	L3	128	LYS
40	L3	134	SER
40	L3	139	GLN
40	L3	144	ILE
40	L3	146	ARG
40	L3	148	LEU
40	L3	156	SER
40	L3	157	VAL
40	L3	160	VAL
40	L3	161	LEU
40	L3	162	VAL
40	L3	169	THR
40	L3	183	LEU
40	L3	188	ILE
40	L3	192	VAL
40	L3	202	THR
40	L3	205	VAL
40	L3	208	VAL
40	L3	210	GLU
40	L3	212	ASN
40	L3	218	ILE
40	L3	232	ARG
40	L3	235	THR
40	L3	238	LEU
40	L3	241	LYS
40	L3	244	ARG
40	L3	252	ILE
40	L3	264	VAL
40	L3	274	SER
40	L3	277	SER
40	L3	290	ASP
40	L3	304	THR
40	L3	312	VAL
40	L3	320	ASP
40	L3	324	VAL
40	L3	328	ILE
40	L3	332	ARG
40	L3	337	THR
40	L3	351	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
40	L3	354	VAL
40	L3	355	SER
40	L3	364	LYS
40	L3	380	MET
40	L3	386	ASP
41	L4	4	PRO
41	L4	12	THR
41	L4	41	SER
41	L4	73	ARG
41	L4	74	ILE
41	L4	93	MET
41	L4	98	ARG
41	L4	99	MET
41	L4	112	LYS
41	L4	119	ARG
41	L4	120	TYR
41	L4	122	THR
41	L4	133	SER
41	L4	143	GLU
41	L4	156	LEU
41	L4	172	VAL
41	L4	177	ASP
41	L4	180	LYS
41	L4	187	LEU
41	L4	193	LYS
41	L4	203	ARG
41	L4	206	LEU
41	L4	220	ARG
41	L4	222	VAL
41	L4	225	VAL
41	L4	230	VAL
41	L4	232	SER
41	L4	246	ARG
41	L4	252	GLU
41	L4	256	THR
41	L4	258	LEU
41	L4	260	GLN
41	L4	261	VAL
41	L4	267	VAL
41	L4	282	SER
41	L4	284	SER
41	L4	287	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
41	L4	289	ILE
41	L4	297	SER
41	L4	307	GLN
41	L4	313	LEU
41	L4	321	LYS
41	L4	323	VAL
41	L4	327	LEU
41	L4	332	LYS
41	L4	338	LYS
41	L4	339	LEU
41	L4	343	LYS
41	L4	346	LYS
41	L4	356	THR
41	L4	362	ASP
42	L5	8	LYS
42	L5	23	ARG
42	L5	41	LYS
42	L5	66	SER
42	L5	69	ILE
42	L5	75	LEU
42	L5	80	SER
42	L5	81	HIS
42	L5	89	THR
42	L5	92	LEU
42	L5	101	THR
42	L5	105	ILE
42	L5	112	LYS
42	L5	113	LEU
42	L5	115	LEU
42	L5	124	GLU
42	L5	126	GLU
42	L5	131	LEU
42	L5	140	ARG
42	L5	146	LEU
42	L5	151	GLN
42	L5	152	ARG
42	L5	155	THR
42	L5	158	ARG
42	L5	159	VAL
42	L5	163	LEU
42	L5	177	GLU
42	L5	185	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
42	L5	205	SER
42	L5	214	ASP
42	L5	222	LEU
42	L5	223	PHE
42	L5	236	LEU
42	L5	259	LYS
42	L5	263	GLU
42	L5	273	ARG
42	L5	290	ILE
43	L6	5	LYS
43	L6	14	ASP
43	L6	21	THR
43	L6	35	VAL
43	L6	48	ARG
43	L6	64	LEU
43	L6	66	SER
43	L6	78	ARG
43	L6	79	VAL
43	L6	84	VAL
43	L6	88	SER
43	L6	89	THR
43	L6	98	VAL
43	L6	104	GLU
43	L6	109	GLU
43	L6	129	GLU
43	L6	134	ARG
43	L6	155	LEU
43	L6	160	SER
44	L7	25	GLN
44	L7	26	VAL
44	L7	60	ARG
44	L7	77	VAL
44	L7	80	GLN
44	L7	82	LYS
44	L7	93	ASN
44	L7	98	LYS
44	L7	100	ARG
44	L7	111	ILE
44	L7	121	LYS
44	L7	124	LEU
44	L7	173	LEU
44	L7	179	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
44	L7	184	LEU
44	L7	189	ILE
44	L7	239	LEU
45	L8	26	LEU
45	L8	27	THR
45	L8	63	LYS
45	L8	71	VAL
45	L8	74	THR
45	L8	79	GLN
45	L8	84	ARG
45	L8	90	THR
45	L8	92	LYS
45	L8	132	VAL
45	L8	136	LEU
45	L8	149	LYS
45	L8	156	ASP
45	L8	163	VAL
45	L8	169	LEU
45	L8	185	ARG
45	L8	189	LEU
45	L8	194	THR
45	L8	201	THR
45	L8	203	VAL
45	L8	204	ARG
45	L8	227	ASP
45	L8	238	LEU
45	L8	248	LYS
46	L9	1	MET
46	L9	4	ILE
46	L9	5	GLN
46	L9	6	THR
46	L9	9	GLN
46	L9	18	VAL
46	L9	19	SER
46	L9	20	ILE
46	L9	22	SER
46	L9	28	VAL
46	L9	31	ARG
46	L9	41	ILE
46	L9	44	THR
46	L9	48	VAL
46	L9	52	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
46	L9	65	VAL
46	L9	68	LEU
46	L9	70	THR
46	L9	78	MET
46	L9	82	VAL
46	L9	123	ILE
46	L9	138	THR
46	L9	139	ASN
46	L9	149	ASN
46	L9	151	VAL
46	L9	154	VAL
46	L9	157	ASN
46	L9	161	LEU
46	L9	162	GLN
46	L9	164	ILE
46	L9	166	ARG
46	L9	168	ARG
46	L9	172	ILE
46	L9	173	ARG
46	L9	177	ASP
46	L9	189	GLU
46	L9	190	ASP
47	M0	3	ARG
47	M0	4	ARG
47	M0	32	ARG
47	M0	33	ILE
47	M0	34	TYR
47	M0	39	LYS
47	M0	40	LYS
47	M0	42	THR
47	M0	44	ASP
47	M0	48	LEU
47	M0	52	LEU
47	M0	53	VAL
47	M0	63	GLU
47	M0	66	GLU
47	M0	87	LEU
47	M0	116	ARG
47	M0	139	ARG
47	M0	140	THR
47	M0	142	ASP
47	M0	143	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
47	M0	156	ARG
47	M0	163	GLN
47	M0	165	ILE
47	M0	167	LEU
47	M0	169	LYS
47	M0	178	ARG
47	M0	185	ARG
47	M0	192	ASP
47	M0	197	VAL
47	M0	203	LYS
47	M0	208	ASN
48	M1	6	GLN
48	M1	10	ARG
48	M1	11	ASP
48	M1	12	LEU
48	M1	13	LYS
48	M1	19	LEU
48	M1	22	SER
48	M1	30	LEU
48	M1	44	THR
48	M1	46	VAL
48	M1	52	TYR
48	M1	56	THR
48	M1	61	ARG
48	M1	63	GLU
48	M1	65	ILE
48	M1	70	THR
48	M1	77	GLU
48	M1	80	LEU
48	M1	82	ARG
48	M1	94	ARG
48	M1	95	ASN
48	M1	106	ILE
48	M1	107	ASP
48	M1	112	LEU
48	M1	137	ARG
48	M1	138	VAL
48	M1	140	ARG
48	M1	159	THR
48	M1	166	LYS
48	M1	171	VAL
49	M3	17	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	M3	22	VAL
49	M3	42	ARG
49	M3	54	LEU
49	M3	55	ARG
49	M3	58	VAL
49	M3	59	ARG
49	M3	73	ARG
49	M3	100	ARG
49	M3	104	ARG
49	M3	114	GLN
49	M3	115	ARG
49	M3	117	LYS
49	M3	121	SER
49	M3	124	ILE
49	M3	131	LYS
49	M3	136	GLU
49	M3	164	GLU
49	M3	168	ARG
49	M3	182	ILE
49	M3	194	GLU
50	M4	8	LYS
50	M4	27	GLN
50	M4	38	ILE
50	M4	50	LYS
50	M4	53	VAL
50	M4	69	THR
50	M4	74	ARG
50	M4	90	VAL
50	M4	92	GLU
50	M4	93	LYS
50	M4	108	ARG
50	M4	125	LYS
50	M4	126	GLN
50	M4	130	THR
50	M4	133	LYS
50	M4	135	LEU
51	M5	7	LEU
51	M5	10	LEU
51	M5	15	GLN
51	M5	18	VAL
51	M5	19	LEU
51	M5	22	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
51	M5	38	ARG
51	M5	46	ASP
51	M5	49	ARG
51	M5	50	ARG
51	M5	62	TYR
51	M5	68	ARG
51	M5	80	THR
51	M5	85	THR
51	M5	87	GLN
51	M5	96	ARG
51	M5	97	SER
51	M5	106	VAL
51	M5	123	GLN
51	M5	133	ILE
51	M5	138	GLN
51	M5	151	ILE
51	M5	155	VAL
51	M5	159	ARG
51	M5	167	THR
51	M5	182	ASN
51	M5	183	THR
51	M5	190	THR
51	M5	194	GLN
51	M5	201	ARG
51	M5	204	LYS
52	M6	22	VAL
52	M6	33	ILE
52	M6	34	VAL
52	M6	36	VAL
52	M6	41	LEU
52	M6	84	LEU
52	M6	85	ARG
52	M6	106	GLU
52	M6	110	PRO
52	M6	114	LYS
52	M6	117	ARG
52	M6	122	GLN
52	M6	124	LEU
52	M6	126	VAL
52	M6	142	SER
52	M6	143	THR
52	M6	160	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	M6	170	LYS
52	M6	180	SER
52	M6	184	THR
52	M6	187	GLU
52	M6	190	VAL
53	M7	18	ARG
53	M7	24	VAL
53	M7	29	THR
53	M7	32	THR
53	M7	36	ILE
53	M7	42	THR
53	M7	52	LEU
53	M7	53	ASP
53	M7	54	HIS
53	M7	56	ARG
53	M7	69	ARG
53	M7	91	VAL
53	M7	111	LYS
53	M7	112	LEU
53	M7	119	VAL
53	M7	142	SER
53	M7	144	SER
53	M7	152	GLU
53	M7	153	LYS
53	M7	175	ARG
53	M7	181	ARG
54	M8	7	SER
54	M8	11	LYS
54	M8	17	THR
54	M8	22	ASP
54	M8	26	LEU
54	M8	32	LEU
54	M8	41	ASP
54	M8	49	LEU
54	M8	64	VAL
54	M8	69	ARG
54	M8	80	THR
54	M8	81	VAL
54	M8	100	THR
54	M8	129	VAL
54	M8	135	GLN
54	M8	148	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	M8	159	LYS
54	M8	168	THR
54	M8	171	LYS
54	M8	174	ARG
54	M8	178	ARG
54	M8	180	ARG
54	M8	181	SER
55	M9	19	LYS
55	M9	20	ARG
55	M9	25	ASP
55	M9	41	ILE
55	M9	42	ARG
55	M9	44	LEU
55	M9	55	VAL
55	M9	60	LYS
55	M9	69	SER
55	M9	74	ARG
55	M9	103	ARG
55	M9	104	ARG
55	M9	106	LEU
55	M9	138	LEU
55	M9	144	GLN
55	M9	155	LEU
55	M9	164	LEU
55	M9	175	GLN
55	M9	180	LYS
56	N0	16	THR
56	N0	21	GLU
56	N0	45	LEU
56	N0	51	VAL
56	N0	61	ILE
56	N0	71	LYS
56	N0	79	VAL
56	N0	80	ARG
56	N0	87	THR
56	N0	100	VAL
56	N0	105	THR
56	N0	115	ARG
56	N0	130	GLU
56	N0	131	LYS
56	N0	137	ARG
56	N0	145	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
56	N0	155	ARG
56	N0	156	VAL
56	N0	157	GLN
56	N0	160	THR
56	N0	161	LYS
56	N0	162	THR
56	N0	167	ARG
56	N0	169	SER
56	N0	172	TYR
57	N1	12	ARG
57	N1	16	GLN
57	N1	26	HIS
57	N1	27	LEU
57	N1	36	VAL
57	N1	38	ASP
57	N1	55	LYS
57	N1	71	SER
57	N1	75	ILE
57	N1	78	LYS
57	N1	79	MET
57	N1	80	VAL
57	N1	83	ARG
57	N1	88	ARG
57	N1	102	ARG
57	N1	104	GLU
57	N1	122	GLN
57	N1	126	VAL
57	N1	127	GLN
57	N1	128	LEU
57	N1	131	GLN
57	N1	139	ARG
57	N1	143	THR
57	N1	149	GLN
57	N1	158	THR
57	N1	159	PHE
58	N2	10	LYS
58	N2	16	THR
58	N2	39	ASP
58	N2	52	ASN
58	N2	66	VAL
58	N2	88	GLN
58	N2	93	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
58	N2	100	THR
58	N2	107	PHE
59	N3	13	ILE
59	N3	14	SER
59	N3	45	ARG
59	N3	46	LEU
59	N3	48	ARG
59	N3	63	LYS
59	N3	64	LYS
59	N3	72	LYS
59	N3	73	VAL
59	N3	83	LYS
59	N3	91	VAL
59	N3	102	ILE
59	N3	106	LYS
59	N3	115	THR
59	N3	125	LEU
59	N3	133	SER
60	N4	4	GLU
60	N4	5	ILE
60	N4	17	ARG
60	N4	19	THR
60	N4	39	LEU
60	N4	47	ARG
61	N5	27	ARG
61	N5	37	THR
61	N5	38	LEU
61	N5	39	LYS
61	N5	40	LEU
61	N5	45	LYS
61	N5	48	SER
61	N5	59	SER
61	N5	63	ILE
61	N5	71	THR
61	N5	73	MET
61	N5	75	LYS
61	N5	78	ASP
61	N5	92	LYS
61	N5	104	GLU
61	N5	108	LEU
61	N5	112	THR
61	N5	115	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
61	N5	125	ARG
61	N5	134	ASP
61	N5	135	ILE
61	N5	137	ASN
61	N5	139	ILE
62	N6	5	SER
62	N6	13	ARG
62	N6	16	ARG
62	N6	36	SER
62	N6	37	LYS
62	N6	42	GLN
62	N6	45	ILE
62	N6	50	ILE
62	N6	56	VAL
62	N6	57	LEU
62	N6	64	LYS
62	N6	69	LYS
62	N6	74	TYR
62	N6	86	THR
62	N6	105	VAL
62	N6	115	ARG
62	N6	125	LYS
62	N6	126	LEU
63	N7	14	VAL
63	N7	24	VAL
63	N7	26	VAL
63	N7	30	ASP
63	N7	33	SER
63	N7	46	ILE
63	N7	65	ARG
63	N7	72	ILE
63	N7	81	LEU
63	N7	83	THR
63	N7	86	THR
63	N7	94	SER
63	N7	97	SER
63	N7	102	GLU
63	N7	103	GLN
63	N7	109	GLU
63	N7	134	LEU
63	N7	136	PHE
64	N8	3	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
64	N8	4	ARG
64	N8	6	THR
64	N8	8	THR
64	N8	10	LYS
64	N8	12	ARG
64	N8	16	SER
64	N8	26	ARG
64	N8	27	LYS
64	N8	32	ARG
64	N8	42	ARG
64	N8	47	LYS
64	N8	56	VAL
64	N8	60	TYR
64	N8	76	ASP
64	N8	78	LEU
64	N8	88	ASP
64	N8	91	LEU
64	N8	93	SER
64	N8	97	GLU
64	N8	115	LYS
64	N8	117	ARG
64	N8	120	ASN
64	N8	130	VAL
64	N8	133	LEU
65	N9	4	SER
65	N9	13	THR
65	N9	22	LYS
65	N9	23	LYS
65	N9	25	LYS
65	N9	28	LYS
65	N9	38	LYS
65	N9	50	THR
65	N9	59	LYS
66	O0	14	LEU
66	O0	16	LEU
66	O0	20	SER
66	O0	30	THR
66	O0	33	SER
66	O0	40	LYS
66	O0	43	ILE
66	O0	48	THR
66	O0	54	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
66	O0	61	MET
66	O0	66	LYS
66	O0	79	THR
66	O0	83	LYS
66	O0	87	VAL
66	O0	89	VAL
66	O0	98	SER
66	O0	101	LEU
66	O0	104	LEU
67	O1	6	ASP
67	O1	26	LYS
67	O1	27	LYS
67	O1	31	ARG
67	O1	46	THR
67	O1	47	ASP
67	O1	65	LYS
67	O1	73	LEU
67	O1	76	SER
67	O1	79	ARG
67	O1	82	GLU
67	O1	83	GLU
67	O1	93	VAL
67	O1	96	VAL
67	O1	98	VAL
67	O1	104	LEU
67	O1	106	THR
67	O1	107	VAL
68	O2	19	ARG
68	O2	24	ARG
68	O2	33	ARG
68	O2	41	VAL
68	O2	52	GLN
68	O2	59	SER
68	O2	61	LYS
68	O2	67	SER
68	O2	69	SER
68	O2	72	LYS
68	O2	73	THR
68	O2	75	LEU
68	O2	90	LYS
68	O2	91	THR
68	O2	103	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
68	O2	125	ARG
69	O3	15	SER
69	O3	31	LYS
69	O3	45	LEU
69	O3	58	GLU
69	O3	59	VAL
69	O3	60	ARG
69	O3	70	LYS
69	O3	81	VAL
69	O3	98	VAL
70	O4	20	ILE
70	O4	23	VAL
70	O4	24	LYS
70	O4	35	VAL
70	O4	49	SER
70	O4	58	ARG
70	O4	61	GLN
70	O4	65	VAL
70	O4	68	THR
70	O4	71	THR
70	O4	79	SER
70	O4	80	ARG
70	O4	101	VAL
70	O4	104	VAL
71	O5	15	GLU
71	O5	21	LEU
71	O5	27	GLU
71	O5	31	LEU
71	O5	36	LEU
71	O5	45	LYS
71	O5	46	THR
71	O5	47	VAL
71	O5	48	ARG
71	O5	49	LYS
71	O5	50	SER
71	O5	73	LYS
71	O5	85	THR
71	O5	89	ARG
71	O5	90	ARG
71	O5	101	THR
71	O5	104	GLN
71	O5	107	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
71	O5	119	LYS
72	O6	11	LEU
72	O6	21	THR
72	O6	25	LYS
72	O6	26	ILE
72	O6	36	ARG
72	O6	42	SER
72	O6	45	ARG
72	O6	57	LEU
72	O6	58	ILE
72	O6	60	LEU
72	O6	62	ARG
72	O6	68	ARG
72	O6	76	ARG
72	O6	81	THR
72	O6	84	LYS
72	O6	90	MET
72	O6	99	ARG
73	O7	5	THR
73	O7	17	THR
73	O7	24	ARG
73	O7	25	ARG
73	O7	33	THR
73	O7	44	THR
73	O7	52	LYS
73	O7	55	ARG
73	O7	58	THR
73	O7	59	THR
73	O7	65	ARG
73	O7	67	LEU
73	O7	71	SER
73	O7	82	SER
74	O8	12	LEU
74	O8	22	THR
74	O8	24	THR
74	O8	45	VAL
74	O8	46	ARG
74	O8	53	THR
74	O8	64	LYS
74	O8	65	LEU
74	O8	67	GLN
74	O8	68	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
74	O8	73	LEU
74	O8	77	ARG
75	O9	4	GLN
75	O9	19	GLN
75	O9	21	ARG
75	O9	25	GLN
75	O9	27	ILE
75	O9	29	LEU
75	O9	51	ILE
76	Q0	78	ILE
76	Q0	85	LEU
76	Q0	97	ARG
76	Q0	112	LYS
76	Q0	113	ARG
76	Q0	114	LYS
76	Q0	127	LEU
77	Q1	5	TRP
77	Q1	6	ARG
77	Q1	9	ARG
77	Q1	11	ARG
78	Q2	3	ASN
78	Q2	8	ARG
78	Q2	9	LYS
78	Q2	21	THR
78	Q2	26	THR
78	Q2	35	LEU
78	Q2	38	GLN
78	Q2	47	GLN
78	Q2	75	VAL
78	Q2	78	LYS
78	Q2	83	LEU
78	Q2	84	THR
78	Q2	85	LEU
78	Q2	92	GLU
78	Q2	100	LYS
78	Q2	104	LEU
79	Q3	4	ARG
79	Q3	11	THR
79	Q3	25	GLN
79	Q3	42	CYS
79	Q3	45	LYS
79	Q3	46	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
79	Q3	49	ARG
79	Q3	73	THR
79	Q3	78	THR
79	Q3	82	THR
79	Q3	84	ARG
79	Q3	91	GLU
2	s0	6	THR
2	s0	12	GLU
2	s0	29	VAL
2	s0	30	GLN
2	s0	31	VAL
2	s0	32	HIS
2	s0	41	ARG
2	s0	45	VAL
2	s0	50	VAL
2	s0	57	LEU
2	s0	59	LEU
2	s0	69	ASN
2	s0	87	LEU
2	s0	88	LYS
2	s0	96	THR
2	s0	101	ARG
2	s0	110	TYR
2	s0	131	GLN
2	s0	144	ILE
2	s0	154	GLU
2	s0	157	ASP
2	s0	162	CYS
2	s0	172	LEU
2	s0	180	GLU
2	s0	185	ARG
2	s0	189	VAL
2	s0	198	MET
2	s0	205	ARG
3	s1	21	VAL
3	s1	25	THR
3	s1	37	THR
3	s1	40	ASN
3	s1	47	LEU
3	s1	51	SER
3	s1	55	LYS
3	s1	62	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	s1	68	VAL
3	s1	70	LEU
3	s1	74	GLN
3	s1	81	PHE
3	s1	83	LYS
3	s1	105	PHE
3	s1	110	LEU
3	s1	122	GLU
3	s1	124	ASN
3	s1	125	VAL
3	s1	129	THR
3	s1	135	LEU
3	s1	137	ILE
3	s1	159	SER
3	s1	169	SER
3	s1	177	GLN
3	s1	181	LEU
3	s1	193	ILE
3	s1	195	LYS
3	s1	206	PRO
3	s1	212	VAL
3	s1	222	LYS
3	s1	223	PHE
4	s2	41	LEU
4	s2	53	ILE
4	s2	54	GLU
4	s2	55	GLU
4	s2	58	LEU
4	s2	69	ILE
4	s2	72	LEU
4	s2	73	LEU
4	s2	76	LEU
4	s2	80	VAL
4	s2	81	MET
4	s2	83	ILE
4	s2	89	GLN
4	s2	91	ARG
4	s2	97	ARG
4	s2	106	ASP
4	s2	111	VAL
4	s2	113	LEU
4	s2	117	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	s2	137	ILE
4	s2	140	ARG
4	s2	141	ARG
4	s2	148	LEU
4	s2	150	GLN
4	s2	153	SER
4	s2	164	SER
4	s2	166	THR
4	s2	167	VAL
4	s2	170	ILE
4	s2	194	GLU
4	s2	195	ASP
4	s2	205	ARG
4	s2	218	ILE
4	s2	224	PHE
4	s2	228	ASN
4	s2	233	GLN
4	s2	237	VAL
4	s2	245	ASP
4	s2	248	SER
5	s3	4	LEU
5	s3	23	GLU
5	s3	44	THR
5	s3	55	THR
5	s3	57	ASP
5	s3	67	ASN
5	s3	69	LEU
5	s3	76	ARG
5	s3	84	ILE
5	s3	115	ILE
5	s3	124	ARG
5	s3	128	GLU
5	s3	142	LEU
5	s3	143	ARG
5	s3	158	ILE
5	s3	162	GLN
5	s3	164	VAL
5	s3	168	ILE
5	s3	212	LYS
5	s3	213	GLU
5	s3	215	GLU
5	s3	223	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	s4	12	LEU
6	s4	23	LEU
6	s4	30	ARG
6	s4	38	LEU
6	s4	39	ARG
6	s4	41	SER
6	s4	42	LEU
6	s4	48	LEU
6	s4	49	ARG
6	s4	51	ARG
6	s4	67	GLN
6	s4	70	VAL
6	s4	78	THR
6	s4	81	THR
6	s4	104	ASP
6	s4	105	VAL
6	s4	113	ARG
6	s4	116	ASP
6	s4	123	LEU
6	s4	126	VAL
6	s4	128	LYS
6	s4	131	LEU
6	s4	146	THR
6	s4	147	ILE
6	s4	148	ARG
6	s4	160	VAL
6	s4	176	ASP
6	s4	180	LEU
6	s4	182	TYR
6	s4	196	VAL
6	s4	214	LEU
6	s4	221	ARG
6	s4	222	LEU
6	s4	223	ASN
6	s4	227	VAL
6	s4	236	ILE
6	s4	245	LYS
6	s4	246	LEU
6	s4	247	SER
7	s5	25	LEU
7	s5	27	THR
7	s5	31	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	s5	38	THR
7	s5	45	LYS
7	s5	59	VAL
7	s5	63	GLN
7	s5	68	ILE
7	s5	76	ARG
7	s5	93	LEU
7	s5	94	THR
7	s5	99	MET
7	s5	102	ARG
7	s5	112	ARG
7	s5	125	THR
7	s5	128	ASN
7	s5	146	THR
7	s5	147	THR
7	s5	148	ARG
7	s5	157	ARG
7	s5	163	SER
7	s5	166	ARG
7	s5	194	LEU
7	s5	203	LYS
7	s5	213	LYS
7	s5	216	GLU
8	s6	10	ASN
8	s6	17	GLU
8	s6	29	ASP
8	s6	57	ASP
8	s6	69	LEU
8	s6	71	THR
8	s6	73	ILE
8	s6	76	LEU
8	s6	78	THR
8	s6	93	LYS
8	s6	97	VAL
8	s6	108	VAL
8	s6	109	LEU
8	s6	115	LYS
8	s6	121	LEU
8	s6	126	ASP
8	s6	127	THR
8	s6	128	THR
8	s6	129	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	s6	137	ARG
8	s6	143	LYS
8	s6	151	ASP
8	s6	153	VAL
8	s6	155	ASP
8	s6	156	PHE
8	s6	157	VAL
8	s6	175	ILE
8	s6	177	ARG
8	s6	193	LEU
8	s6	212	LEU
8	s6	215	ARG
9	s7	11	GLN
9	s7	28	GLU
9	s7	33	GLU
9	s7	38	LEU
9	s7	49	ILE
9	s7	50	ASP
9	s7	66	SER
9	s7	67	LEU
9	s7	75	THR
9	s7	77	LEU
9	s7	78	THR
9	s7	79	ARG
9	s7	80	GLU
9	s7	97	ARG
9	s7	108	GLN
9	s7	110	GLN
9	s7	114	ARG
9	s7	115	SER
9	s7	116	ARG
9	s7	117	THR
9	s7	118	LEU
9	s7	149	ILE
9	s7	160	GLN
9	s7	166	LEU
9	s7	185	ILE
10	s8	10	LYS
10	s8	20	GLN
10	s8	22	ARG
10	s8	25	ARG
10	s8	26	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	s8	29	LEU
10	s8	46	VAL
10	s8	59	ARG
10	s8	74	LYS
10	s8	76	THR
10	s8	82	VAL
10	s8	89	GLU
10	s8	135	LYS
10	s8	152	ILE
10	s8	153	GLU
10	s8	155	SER
10	s8	176	SER
10	s8	183	ILE
10	s8	184	LEU
11	s9	3	ARG
11	s9	6	ARG
11	s9	7	THR
11	s9	9	SER
11	s9	28	LEU
11	s9	39	LYS
11	s9	46	SER
11	s9	78	ARG
11	s9	82	ARG
11	s9	101	VAL
11	s9	109	LEU
11	s9	130	THR
11	s9	134	ILE
11	s9	140	ILE
11	s9	150	LEU
11	s9	151	ASP
11	s9	161	THR
11	s9	172	VAL
11	s9	180	LYS
11	s9	182	GLU
12	c0	2	LEU
12	c0	3	MET
12	c0	5	LYS
12	c0	15	LEU
12	c0	20	VAL
12	c0	22	VAL
12	c0	55	VAL
12	c0	57	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	c0	71	GLU
13	c1	5	LEU
13	c1	10	GLU
13	c1	21	ASN
13	c1	26	LYS
13	c1	30	ARG
13	c1	31	THR
13	c1	32	LYS
13	c1	33	ARG
13	c1	40	LEU
13	c1	44	THR
13	c1	47	THR
13	c1	56	LYS
13	c1	60	PHE
13	c1	64	VAL
13	c1	67	ARG
13	c1	74	THR
13	c1	76	VAL
13	c1	77	SER
13	c1	83	THR
13	c1	99	ARG
13	c1	109	VAL
13	c1	129	ARG
13	c1	138	ASN
14	c2	28	LEU
14	c2	39	ASP
14	c2	43	ARG
14	c2	45	LEU
14	c2	58	LEU
14	c2	61	VAL
14	c2	62	LEU
14	c2	71	ILE
14	c2	74	LEU
14	c2	83	GLU
14	c2	85	LYS
14	c2	89	ILE
14	c2	103	LEU
14	c2	121	VAL
14	c2	125	ASN
14	c2	132	GLU
14	c2	140	PHE
15	c3	12	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	c3	14	SER
15	c3	16	ILE
15	c3	20	ARG
15	c3	21	ASN
15	c3	28	LEU
15	c3	29	SER
15	c3	30	SER
15	c3	46	THR
15	c3	60	VAL
15	c3	66	ILE
15	c3	70	LYS
15	c3	80	LEU
15	c3	84	ILE
15	c3	87	ASP
15	c3	97	SER
15	c3	102	LEU
15	c3	115	LEU
15	c3	120	SER
15	c3	125	LEU
15	c3	127	ARG
15	c3	131	THR
15	c3	134	VAL
15	c3	138	ASN
16	c4	13	VAL
16	c4	16	VAL
16	c4	31	THR
16	c4	43	THR
16	c4	79	VAL
16	c4	81	VAL
16	c4	83	ILE
16	c4	90	ARG
16	c4	92	LYS
16	c4	102	LEU
16	c4	107	ARG
16	c4	114	ARG
16	c4	118	VAL
16	c4	119	THR
16	c4	123	SER
16	c4	124	ASP
16	c4	132	ARG
16	c4	133	ARG
16	c4	136	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	c5	12	PHE
17	c5	21	ASP
17	c5	36	LEU
17	c5	49	MET
17	c5	52	LYS
17	c5	69	GLU
17	c5	71	GLU
17	c5	97	TYR
17	c5	107	ILE
17	c5	110	GLU
17	c5	121	ILE
17	c5	127	ARG
17	c5	128	HIS
18	c6	7	VAL
18	c6	17	THR
18	c6	23	LYS
18	c6	28	LEU
18	c6	37	THR
18	c6	38	LEU
18	c6	43	ILE
18	c6	53	LEU
18	c6	54	LEU
18	c6	57	LEU
18	c6	63	ILE
18	c6	68	ARG
18	c6	69	VAL
18	c6	70	THR
18	c6	100	GLN
18	c6	114	ARG
18	c6	137	ARG
19	c7	3	ARG
19	c7	5	ARG
19	c7	6	THR
19	c7	29	GLN
19	c7	34	LEU
19	c7	36	ASP
19	c7	46	LEU
19	c7	55	THR
19	c7	60	ARG
19	c7	69	ILE
19	c7	85	VAL
19	c7	88	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
19	c7	100	LEU
19	c7	103	ASP
19	c7	106	THR
20	c8	2	SER
20	c8	3	LEU
20	c8	4	VAL
20	c8	5	VAL
20	c8	6	GLN
20	c8	8	GLN
20	c8	13	HIS
20	c8	15	LEU
20	c8	25	ASN
20	c8	28	ILE
20	c8	29	VAL
20	c8	36	LYS
20	c8	38	VAL
20	c8	61	LEU
20	c8	63	GLN
20	c8	89	GLN
20	c8	94	ASP
20	c8	101	LEU
20	c8	103	ASN
20	c8	107	SER
20	c8	116	LEU
20	c8	136	GLN
20	c8	138	THR
20	c8	140	THR
20	c8	141	THR
20	c8	144	ARG
21	c9	6	VAL
21	c9	27	LYS
21	c9	28	LEU
21	c9	34	VAL
21	c9	37	VAL
21	c9	57	ARG
21	c9	68	ARG
21	c9	70	GLN
21	c9	86	ARG
21	c9	110	LYS
21	c9	116	ILE
21	c9	123	ARG
21	c9	126	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
21	c9	131	ASP
21	c9	135	ILE
21	c9	139	THR
21	c9	140	LEU
22	d0	16	GLN
22	d0	23	ARG
22	d0	27	THR
22	d0	30	LYS
22	d0	31	VAL
22	d0	34	LEU
22	d0	44	ASN
22	d0	51	VAL
22	d0	57	ARG
22	d0	60	THR
22	d0	63	LEU
22	d0	67	THR
22	d0	70	THR
22	d0	74	GLU
22	d0	77	LYS
22	d0	81	THR
22	d0	88	LYS
22	d0	89	ARG
22	d0	99	ILE
22	d0	102	ARG
22	d0	103	ILE
22	d0	105	GLN
22	d0	107	THR
22	d0	115	GLU
23	d1	2	GLU
23	d1	5	LYS
23	d1	11	LEU
23	d1	12	TYR
23	d1	24	ILE
23	d1	32	VAL
23	d1	50	TYR
23	d1	52	THR
23	d1	66	ASP
23	d1	78	LEU
24	d2	2	THR
24	d2	3	ARG
24	d2	4	SER
24	d2	7	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
24	d2	15	ASN
24	d2	23	ARG
24	d2	25	VAL
24	d2	65	LEU
24	d2	68	ARG
24	d2	98	GLN
24	d2	103	ILE
24	d2	117	ARG
24	d2	124	LYS
24	d2	126	LEU
24	d2	129	VAL
25	d3	9	LEU
25	d3	16	ARG
25	d3	19	ARG
25	d3	33	LEU
25	d3	72	VAL
25	d3	73	ARG
25	d3	83	VAL
25	d3	84	THR
25	d3	99	ASN
25	d3	100	ASP
25	d3	107	PHE
25	d3	109	ARG
25	d3	125	VAL
25	d3	132	LEU
25	d3	133	LEU
25	d3	140	LYS
26	d4	5	VAL
26	d4	10	ARG
26	d4	21	LYS
26	d4	26	ASP
26	d4	34	ASN
26	d4	36	SER
26	d4	42	GLU
26	d4	43	LYS
26	d4	49	LYS
26	d4	51	GLU
26	d4	62	THR
26	d4	88	THR
26	d4	91	LEU
26	d4	121	THR
26	d4	125	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
26	d4	132	ARG
27	d5	41	ILE
27	d5	51	LEU
27	d5	57	TYR
27	d5	81	ARG
27	d5	92	ILE
28	d6	10	ARG
28	d6	18	VAL
28	d6	24	VAL
28	d6	41	ILE
28	d6	53	LEU
28	d6	54	SER
28	d6	61	GLU
28	d6	82	ARG
28	d6	85	ARG
28	d6	90	GLU
29	d7	14	SER
29	d7	34	ASP
29	d7	36	LYS
29	d7	43	ILE
29	d7	52	THR
29	d7	61	THR
29	d7	72	LYS
29	d7	77	THR
29	d7	81	ARG
30	d8	7	VAL
30	d8	28	VAL
30	d8	30	VAL
30	d8	32	PHE
30	d8	33	LEU
30	d8	39	THR
30	d8	64	ARG
30	d8	65	ARG
30	d8	67	ARG
31	d9	10	HIS
31	d9	21	CYS
31	d9	25	SER
31	d9	42	CYS
31	d9	54	LYS
32	e0	13	LYS
32	e0	26	LYS
32	e0	28	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	e0	29	LYS
32	e0	31	LYS
32	e0	39	LEU
32	e0	41	THR
32	e0	44	PHE
32	e0	46	ASN
32	e0	49	LEU
32	e0	55	ARG
32	e0	56	MET
33	e1	84	VAL
33	e1	86	THR
33	e1	90	LYS
33	e1	95	HIS
33	e1	96	LYS
33	e1	98	VAL
33	e1	100	LEU
33	e1	102	VAL
33	e1	106	TYR
33	e1	109	ASP
33	e1	113	LYS
33	e1	135	HIS
34	sR	29	GLN
34	sR	51	ASP
34	sR	58	VAL
34	sR	59	ARG
34	sR	64	HIS
34	sR	65	SER
34	sR	66	HIS
34	sR	76	ASP
34	sR	96	THR
34	sR	106	HIS
34	sR	145	LEU
34	sR	149	ASP
34	sR	176	LYS
34	sR	182	ASN
34	sR	183	LEU
34	sR	202	LEU
34	sR	232	TYR
34	sR	245	PHE
34	sR	256	THR
34	sR	266	ASP
34	sR	275	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	sR	286	GLU
34	sR	297	ASP
35	sM	25	ILE
35	sM	30	THR
35	sM	43	ASP
35	sM	48	ARG
35	sM	49	LYS
35	sM	64	LYS
35	sM	68	ARG
35	sM	71	ASN
35	sM	74	LYS
35	sM	77	THR
35	sM	79	SER
39	l2	15	ILE
39	l2	23	ARG
39	l2	32	LEU
39	l2	44	ILE
39	l2	45	VAL
39	l2	46	LYS
39	l2	48	ILE
39	l2	52	SER
39	l2	62	VAL
39	l2	71	LEU
39	l2	74	GLU
39	l2	82	VAL
39	l2	101	VAL
39	l2	107	VAL
39	l2	114	SER
39	l2	119	LYS
39	l2	122	ASP
39	l2	134	VAL
39	l2	137	ILE
39	l2	147	ARG
39	l2	155	LYS
39	l2	165	VAL
39	l2	179	LEU
39	l2	192	LYS
39	l2	193	ARG
39	l2	204	MET
39	l2	215	ASN
39	l2	224	THR
39	l2	227	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	12	230	VAL
39	12	241	ARG
39	12	242	ARG
39	12	243	THR
39	12	246	LEU
40	13	3	HIS
40	13	4	ARG
40	13	5	LYS
40	13	17	LEU
40	13	19	ARG
40	13	30	LYS
40	13	34	LYS
40	13	43	LEU
40	13	50	LYS
40	13	56	ILE
40	13	69	LYS
40	13	70	ARG
40	13	73	VAL
40	13	79	VAL
40	13	85	VAL
40	13	101	SER
40	13	103	THR
40	13	104	THR
40	13	110	LEU
40	13	114	VAL
40	13	120	LYS
40	13	139	GLN
40	13	145	GLU
40	13	148	LEU
40	13	150	ARG
40	13	157	VAL
40	13	160	VAL
40	13	167	ARG
40	13	169	THR
40	13	183	LEU
40	13	202	THR
40	13	205	VAL
40	13	208	VAL
40	13	211	GLN
40	13	213	GLU
40	13	222	LYS
40	13	227	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
40	13	232	ARG
40	13	235	THR
40	13	238	LEU
40	13	249	VAL
40	13	252	ILE
40	13	261	MET
40	13	274	SER
40	13	284	ARG
40	13	300	ARG
40	13	308	MET
40	13	324	VAL
40	13	327	CYS
40	13	328	ILE
40	13	332	ARG
40	13	348	ARG
41	14	2	SER
41	14	33	ASP
41	14	34	ILE
41	14	35	VAL
41	14	47	ARG
41	14	52	VAL
41	14	73	ARG
41	14	93	MET
41	14	99	MET
41	14	120	TYR
41	14	122	THR
41	14	133	SER
41	14	138	ARG
41	14	144	LYS
41	14	145	ILE
41	14	148	ILE
41	14	150	LEU
41	14	156	LEU
41	14	170	LYS
41	14	179	LEU
41	14	187	LEU
41	14	203	ARG
41	14	206	LEU
41	14	217	LYS
41	14	220	ARG
41	14	222	VAL
41	14	230	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
41	14	233	LEU
41	14	246	ARG
41	14	258	LEU
41	14	265	GLU
41	14	287	THR
41	14	289	ILE
41	14	292	SER
41	14	304	GLN
41	14	307	GLN
41	14	308	LYS
41	14	313	LEU
41	14	327	LEU
41	14	333	VAL
41	14	345	GLU
41	14	346	LYS
41	14	347	THR
41	14	356	THR
42	15	5	LYS
42	15	9	SER
42	15	34	LYS
42	15	35	ARG
42	15	51	LEU
42	15	61	ILE
42	15	70	THR
42	15	73	VAL
42	15	75	LEU
42	15	84	PRO
42	15	93	THR
42	15	110	LEU
42	15	112	LYS
42	15	113	LEU
42	15	115	LEU
42	15	118	THR
42	15	120	LYS
42	15	135	VAL
42	15	140	ARG
42	15	144	VAL
42	15	146	LEU
42	15	148	ILE
42	15	152	ARG
42	15	155	THR
42	15	158	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
42	15	164	LYS
42	15	183	TRP
42	15	185	PHE
42	15	194	LEU
42	15	211	LEU
42	15	218	ARG
42	15	222	LEU
42	15	227	LEU
42	15	242	SER
42	15	254	LYS
42	15	258	LYS
42	15	259	LYS
42	15	268	GLU
42	15	273	ARG
42	15	282	ARG
42	15	293	LEU
43	16	2	SER
43	16	8	LYS
43	16	18	LEU
43	16	20	LYS
43	16	21	THR
43	16	46	ARG
43	16	50	LYS
43	16	52	VAL
43	16	64	LEU
43	16	65	ILE
43	16	76	LEU
43	16	78	ARG
43	16	79	VAL
43	16	87	THR
43	16	89	THR
43	16	91	VAL
43	16	92	SER
43	16	98	VAL
43	16	108	LYS
43	16	109	GLU
43	16	131	LYS
43	16	152	THR
43	16	155	LEU
44	17	22	THR
44	17	24	GLU
44	17	39	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
44	17	54	GLU
44	17	60	ARG
44	17	77	VAL
44	17	83	LEU
44	17	88	ARG
44	17	98	LYS
44	17	100	ARG
44	17	110	ARG
44	17	130	ILE
44	17	156	ILE
44	17	158	LYS
44	17	159	GLN
44	17	163	LEU
44	17	175	LYS
44	17	179	LEU
44	17	184	LEU
44	17	219	LYS
44	17	225	GLN
44	17	229	PHE
44	17	234	GLU
44	17	239	LEU
45	18	26	LEU
45	18	41	GLN
45	18	46	LEU
45	18	50	VAL
45	18	71	VAL
45	18	74	THR
45	18	79	GLN
45	18	81	THR
45	18	89	GLU
45	18	90	THR
45	18	94	PHE
45	18	136	LEU
45	18	146	LYS
45	18	149	LYS
45	18	150	LEU
45	18	157	VAL
45	18	160	ILE
45	18	163	VAL
45	18	164	VAL
45	18	169	LEU
45	18	183	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	18	191	ASN
45	18	200	LEU
45	18	211	LEU
45	18	213	LYS
45	18	214	LEU
45	18	222	PHE
45	18	224	ASP
45	18	230	LYS
45	18	245	LYS
45	18	248	LYS
46	19	1	MET
46	19	4	ILE
46	19	5	GLN
46	19	6	THR
46	19	18	VAL
46	19	19	SER
46	19	33	THR
46	19	44	THR
46	19	48	VAL
46	19	52	LEU
46	19	55	VAL
46	19	62	ARG
46	19	68	LEU
46	19	69	ARG
46	19	70	THR
46	19	80	THR
46	19	82	VAL
46	19	105	GLU
46	19	113	GLU
46	19	115	ARG
46	19	118	LEU
46	19	132	VAL
46	19	133	THR
46	19	138	THR
46	19	143	GLU
46	19	144	ILE
46	19	147	SER
46	19	151	VAL
46	19	152	GLU
46	19	157	ASN
46	19	161	LEU
46	19	162	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
46	l9	163	GLN
46	l9	166	ARG
46	l9	173	ARG
46	l9	177	ASP
46	l9	179	ILE
46	l9	191	LEU
47	m0	7	ARG
47	m0	24	ARG
47	m0	31	ILE
47	m0	36	LEU
47	m0	38	LYS
47	m0	39	LYS
47	m0	42	THR
47	m0	44	ASP
47	m0	48	LEU
47	m0	52	LEU
47	m0	58	GLU
47	m0	63	GLU
47	m0	71	CYS
47	m0	74	LYS
47	m0	76	MET
47	m0	80	SER
47	m0	87	LEU
47	m0	91	VAL
47	m0	99	ILE
47	m0	139	ARG
47	m0	145	LYS
47	m0	154	ARG
47	m0	163	GLN
47	m0	169	LYS
47	m0	176	LEU
47	m0	197	VAL
47	m0	206	LEU
47	m0	211	ARG
47	m0	212	GLU
47	m0	215	GLU
47	m0	217	PHE
48	m1	6	GLN
48	m1	10	ARG
48	m1	11	ASP
48	m1	12	LEU
48	m1	13	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
48	m1	22	SER
48	m1	29	ARG
48	m1	30	LEU
48	m1	31	THR
48	m1	34	SER
48	m1	37	LEU
48	m1	44	THR
48	m1	80	LEU
48	m1	92	ARG
48	m1	101	ASN
48	m1	106	ILE
48	m1	107	ASP
48	m1	112	LEU
48	m1	115	LYS
48	m1	129	VAL
48	m1	130	VAL
48	m1	137	ARG
48	m1	140	ARG
48	m1	142	LYS
48	m1	145	LYS
48	m1	153	LYS
48	m1	155	THR
48	m1	160	VAL
49	m3	54	LEU
49	m3	59	ARG
49	m3	67	ARG
49	m3	69	VAL
49	m3	73	ARG
49	m3	91	ARG
49	m3	100	ARG
49	m3	107	GLU
49	m3	118	GLU
49	m3	121	SER
49	m3	122	LYS
49	m3	123	ILE
49	m3	131	LYS
49	m3	149	GLN
49	m3	152	THR
49	m3	165	SER
49	m3	168	ARG
49	m3	171	ARG
49	m3	184	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	m3	194	GLU
50	m4	3	THR
50	m4	4	ASP
50	m4	20	VAL
50	m4	27	GLN
50	m4	43	LYS
50	m4	53	VAL
50	m4	62	GLN
50	m4	63	VAL
50	m4	64	VAL
50	m4	72	LEU
50	m4	98	SER
50	m4	124	ARG
50	m4	128	ARG
50	m4	130	THR
50	m4	135	LEU
51	m5	15	GLN
51	m5	22	LEU
51	m5	24	ARG
51	m5	43	THR
51	m5	46	ASP
51	m5	61	ILE
51	m5	76	PRO
51	m5	80	THR
51	m5	92	LEU
51	m5	96	ARG
51	m5	104	GLU
51	m5	106	VAL
51	m5	117	ASN
51	m5	138	GLN
51	m5	153	ASP
51	m5	165	THR
51	m5	171	SER
51	m5	176	LYS
51	m5	182	ASN
51	m5	190	THR
51	m5	204	LYS
52	m6	41	LEU
52	m6	58	LEU
52	m6	67	THR
52	m6	68	ARG
52	m6	74	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	m6	78	ARG
52	m6	85	ARG
52	m6	106	GLU
52	m6	108	ILE
52	m6	110	PRO
52	m6	116	LYS
52	m6	117	ARG
52	m6	124	LEU
52	m6	128	ARG
52	m6	129	LEU
52	m6	134	LYS
52	m6	159	LYS
52	m6	160	ARG
52	m6	171	LYS
52	m6	175	THR
52	m6	182	ASN
52	m6	190	VAL
53	m7	3	ARG
53	m7	7	THR
53	m7	9	THR
53	m7	24	VAL
53	m7	32	THR
53	m7	41	LEU
53	m7	52	LEU
53	m7	53	ASP
53	m7	79	THR
53	m7	112	LEU
53	m7	118	GLN
53	m7	119	VAL
53	m7	127	ARG
53	m7	150	VAL
53	m7	155	GLU
54	m8	3	ILE
54	m8	7	SER
54	m8	12	ARG
54	m8	17	THR
54	m8	22	ASP
54	m8	26	LEU
54	m8	32	LEU
54	m8	34	THR
54	m8	49	LEU
54	m8	57	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	m8	69	ARG
54	m8	74	GLU
54	m8	80	THR
54	m8	81	VAL
54	m8	86	THR
54	m8	93	ILE
54	m8	113	LYS
54	m8	135	GLN
54	m8	138	LEU
54	m8	166	LEU
54	m8	170	ARG
55	m9	7	GLN
55	m9	9	ARG
55	m9	17	VAL
55	m9	20	ARG
55	m9	29	THR
55	m9	39	ASN
55	m9	43	LYS
55	m9	49	THR
55	m9	57	VAL
55	m9	70	LYS
55	m9	71	ARG
55	m9	74	ARG
55	m9	88	ARG
55	m9	92	GLN
55	m9	99	LEU
55	m9	106	LEU
55	m9	111	ASP
55	m9	117	LYS
55	m9	126	GLU
55	m9	127	SER
55	m9	128	LYS
55	m9	133	LYS
55	m9	134	HIS
55	m9	138	LEU
55	m9	148	ASP
55	m9	152	GLU
55	m9	153	LYS
55	m9	156	ASN
55	m9	164	LEU
55	m9	173	ARG
55	m9	180	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
56	n0	8	GLN
56	n0	13	ARG
56	n0	17	GLU
56	n0	21	GLU
56	n0	23	LYS
56	n0	40	ARG
56	n0	45	LEU
56	n0	50	LYS
56	n0	52	LYS
56	n0	80	ARG
56	n0	87	THR
56	n0	92	LYS
56	n0	97	VAL
56	n0	100	VAL
56	n0	105	THR
56	n0	107	TYR
56	n0	117	ARG
56	n0	120	SER
56	n0	130	GLU
56	n0	136	LYS
56	n0	137	ARG
56	n0	148	LEU
56	n0	149	LYS
56	n0	155	ARG
56	n0	159	SER
56	n0	160	THR
56	n0	162	THR
56	n0	167	ARG
56	n0	172	TYR
57	n1	9	SER
57	n1	12	ARG
57	n1	17	ARG
57	n1	26	HIS
57	n1	27	LEU
57	n1	52	MET
57	n1	60	LYS
57	n1	68	THR
57	n1	71	SER
57	n1	72	VAL
57	n1	78	LYS
57	n1	80	VAL
57	n1	83	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
57	n1	86	GLU
57	n1	88	ARG
57	n1	96	ILE
57	n1	102	ARG
57	n1	104	GLU
57	n1	118	GLU
57	n1	126	VAL
57	n1	127	GLN
57	n1	129	LYS
57	n1	131	GLN
57	n1	135	PRO
57	n1	139	ARG
57	n1	143	THR
57	n1	150	THR
57	n1	154	VAL
58	n2	27	VAL
58	n2	28	PHE
58	n2	37	LEU
58	n2	38	ILE
58	n2	43	VAL
58	n2	47	VAL
58	n2	50	LEU
58	n2	54	VAL
58	n2	62	VAL
58	n2	66	VAL
58	n2	68	THR
58	n2	74	LYS
58	n2	75	TYR
58	n2	94	ARG
59	n3	13	ILE
59	n3	40	LYS
59	n3	45	ARG
59	n3	48	ARG
59	n3	72	LYS
59	n3	74	MET
59	n3	91	VAL
59	n3	102	ILE
59	n3	112	SER
59	n3	115	THR
59	n3	120	LYS
60	n4	1	MET
60	n4	4	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
60	n4	19	THR
60	n4	25	ASP
60	n4	39	LEU
60	n4	47	ARG
60	n4	54	LEU
60	n4	57	LYS
60	n4	63	ILE
60	n4	77	LYS
60	n4	89	LEU
60	n4	96	LEU
60	n4	100	VAL
60	n4	107	GLU
60	n4	127	LYS
61	n5	24	LEU
61	n5	27	ARG
61	n5	37	THR
61	n5	45	LYS
61	n5	56	ARG
61	n5	57	LEU
61	n5	63	ILE
61	n5	71	THR
61	n5	73	MET
61	n5	86	VAL
61	n5	109	LYS
61	n5	115	ARG
61	n5	125	ARG
61	n5	133	LEU
61	n5	135	ILE
61	n5	142	ILE
62	n6	8	VAL
62	n6	11	ASP
62	n6	12	ARG
62	n6	13	ARG
62	n6	14	LYS
62	n6	32	SER
62	n6	37	LYS
62	n6	40	ARG
62	n6	45	ILE
62	n6	50	ILE
62	n6	57	LEU
62	n6	66	GLN
62	n6	74	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
62	n6	83	ASP
62	n6	89	LYS
62	n6	111	LEU
62	n6	120	GLN
63	n7	3	LYS
63	n7	14	VAL
63	n7	17	ARG
63	n7	24	VAL
63	n7	26	VAL
63	n7	33	SER
63	n7	34	LYS
63	n7	35	SER
63	n7	36	HIS
63	n7	46	ILE
63	n7	72	ILE
63	n7	81	LEU
63	n7	94	SER
63	n7	95	VAL
63	n7	98	THR
63	n7	99	GLU
63	n7	100	THR
63	n7	102	GLU
63	n7	103	GLN
63	n7	111	LYS
63	n7	121	ARG
63	n7	128	GLN
64	n8	4	ARG
64	n8	6	THR
64	n8	7	LYS
64	n8	8	THR
64	n8	10	LYS
64	n8	15	VAL
64	n8	26	ARG
64	n8	27	LYS
64	n8	42	ARG
64	n8	46	ASP
64	n8	58	MET
64	n8	60	TYR
64	n8	78	LEU
64	n8	85	ASP
64	n8	91	LEU
64	n8	97	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
64	n8	98	THR
64	n8	120	ASN
64	n8	128	ARG
64	n8	133	LEU
64	n8	135	GLU
64	n8	139	ARG
65	n9	19	ASN
65	n9	21	ILE
65	n9	22	LYS
65	n9	26	THR
65	n9	33	LYS
65	n9	38	LYS
65	n9	58	LYS
65	n9	59	LYS
66	o0	8	GLU
66	o0	12	GLN
66	o0	19	LYS
66	o0	32	LYS
66	o0	33	SER
66	o0	41	LEU
66	o0	48	THR
66	o0	50	VAL
66	o0	55	GLU
66	o0	61	MET
66	o0	74	ASN
66	o0	76	GLU
66	o0	81	VAL
66	o0	86	ARG
66	o0	87	VAL
66	o0	99	ASP
66	o0	103	THR
67	o1	6	ASP
67	o1	8	VAL
67	o1	13	THR
67	o1	16	LEU
67	o1	26	LYS
67	o1	31	ARG
67	o1	34	LYS
67	o1	44	MET
67	o1	46	THR
67	o1	55	LEU
67	o1	64	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
67	o1	76	SER
67	o1	90	PHE
67	o1	100	SER
67	o1	102	LYS
67	o1	106	THR
68	o2	4	LEU
68	o2	5	PRO
68	o2	6	HIS
68	o2	9	ILE
68	o2	19	ARG
68	o2	24	ARG
68	o2	31	ASN
68	o2	33	ARG
68	o2	34	LYS
68	o2	35	GLN
68	o2	51	SER
68	o2	54	LYS
68	o2	61	LYS
68	o2	68	PRO
68	o2	71	HIS
68	o2	73	THR
68	o2	75	LEU
68	o2	82	LEU
68	o2	91	THR
68	o2	125	ARG
68	o2	126	LEU
69	o3	4	SER
69	o3	15	SER
69	o3	28	SER
69	o3	37	THR
69	o3	59	VAL
69	o3	60	ARG
69	o3	70	LYS
69	o3	74	THR
69	o3	92	LYS
69	o3	98	VAL
70	o4	20	ILE
70	o4	24	LYS
70	o4	35	VAL
70	o4	41	ARG
70	o4	46	ASP
70	o4	47	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
70	o4	58	ARG
70	o4	65	VAL
70	o4	66	SER
70	o4	71	THR
70	o4	83	ASN
70	o4	85	VAL
70	o4	98	GLN
70	o4	104	VAL
71	o5	11	THR
71	o5	20	GLN
71	o5	27	GLU
71	o5	28	LEU
71	o5	30	GLU
71	o5	47	VAL
71	o5	48	ARG
71	o5	62	GLN
71	o5	67	ARG
71	o5	68	GLN
71	o5	69	LEU
71	o5	79	ASP
71	o5	81	ARG
71	o5	85	THR
71	o5	86	ARG
71	o5	89	ARG
71	o5	100	VAL
71	o5	101	THR
72	o6	3	VAL
72	o6	7	ILE
72	o6	9	ILE
72	o6	12	ASN
72	o6	15	LYS
72	o6	19	SER
72	o6	21	THR
72	o6	26	ILE
72	o6	29	LYS
72	o6	34	SER
72	o6	35	ASN
72	o6	36	ARG
72	o6	42	SER
72	o6	43	LEU
72	o6	45	ARG
72	o6	57	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
72	o6	58	ILE
72	o6	59	ASP
72	o6	60	LEU
72	o6	68	ARG
72	o6	75	LYS
72	o6	76	ARG
72	o6	88	GLU
72	o6	90	MET
72	o6	94	ILE
72	o6	98	ARG
73	o7	3	LYS
73	o7	15	SER
73	o7	17	THR
73	o7	21	ARG
73	o7	25	ARG
73	o7	33	THR
73	o7	35	SER
73	o7	44	THR
73	o7	55	ARG
73	o7	67	LEU
73	o7	80	THR
74	o8	24	THR
74	o8	31	LEU
74	o8	41	THR
74	o8	53	THR
74	o8	55	VAL
74	o8	61	LYS
74	o8	64	LYS
74	o8	65	LEU
74	o8	78	LEU
75	o9	4	GLN
75	o9	15	LYS
75	o9	21	ARG
75	o9	45	ARG
76	q0	77	ILE
76	q0	78	ILE
76	q0	80	PRO
76	q0	85	LEU
76	q0	87	SER
76	q0	88	LYS
76	q0	91	CYS
76	q0	106	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
76	q0	112	LYS
76	q0	113	ARG
76	q0	114	LYS
76	q0	127	LEU
77	q1	2	ARG
77	q1	6	ARG
77	q1	9	ARG
77	q1	13	LEU
77	q1	18	ARG
77	q1	19	LYS
77	q1	21	ARG
77	q1	23	ARG
78	q2	7	THR
78	q2	8	ARG
78	q2	34	SER
78	q2	35	LEU
78	q2	48	SER
78	q2	61	LYS
78	q2	78	LYS
78	q2	83	LEU
78	q2	84	THR
78	q2	85	LEU
78	q2	89	LYS
78	q2	93	LEU
78	q2	100	LYS
78	q2	105	GLN
79	q3	4	ARG
79	q3	20	SER
79	q3	24	ARG
79	q3	41	PHE
79	q3	49	ARG
79	q3	54	ILE
79	q3	56	THR
79	q3	58	SER
79	q3	64	VAL
79	q3	73	THR
79	q3	79	VAL
81	p0	4	ILE
81	p0	5	ARG
81	p0	10	GLU
81	p0	30	VAL
81	p0	39	HIS

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Mol	Chain	Res	Type
81	p0	48	ARG
81	p0	55	LYS
81	p0	67	LEU
81	p0	68	SER
81	p0	70	LEU
81	p0	72	ASP
81	p0	76	LEU
81	p0	93	LEU
81	p0	97	LYS
81	p0	103	ASN
81	p0	104	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
2	S0	83	GLN
3	S1	183	GLN
4	S2	89	GLN
5	S3	162	GLN
10	S8	32	GLN
11	S9	110	GLN
18	C6	83	GLN
20	C8	89	GLN
20	C8	99	HIS
22	D0	121	ASN
23	D1	75	ASN
30	D8	51	ASN
39	L2	8	GLN
39	L2	216	HIS
40	L3	279	ASN
41	L4	304	GLN
42	L5	32	GLN
43	L6	102	ASN
46	L9	156	GLN
51	M5	138	GLN
55	M9	175	GLN
64	N8	28	HIS
65	N9	17	HIS
74	O8	32	ASN
3	s1	209	ASN
4	s2	228	ASN
11	s9	123	HIS

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Mol	Chain	Res	Type
20	c8	89	GLN
21	c9	25	GLN
22	d0	16	GLN
24	d2	56	HIS
34	sR	148	ASN
39	l2	194	ASN
46	l9	8	GLN
51	m5	156	HIS
52	m6	72	HIS
53	m7	120	ASN
55	m9	36	ASN
58	n2	101	ASN
61	n5	55	ASN
75	o9	50	ASN
81	p0	37	GLN

### 5.3.3 RNA [i](#)

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%)

All (2324) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	25	C
1	2	26	A
1	2	27	U
1	2	34	G
1	2	39	A
1	2	45	U
1	2	47	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	57	G
1	2	60	U
1	2	66	U
1	2	67	A
1	2	68	A
1	2	69	G
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	76	A
1	2	104	A
1	2	114	C
1	2	127	G
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	137	U
1	2	140	A
1	2	141	U
1	2	144	U
1	2	145	A
1	2	146	U
1	2	153	G
1	2	158	U
1	2	159	U
1	2	169	A
1	2	178	U
1	2	179	A
1	2	185	U
1	2	186	C
1	2	187	G
1	2	188	A
1	2	190	C
1	2	191	C
1	2	192	U
1	2	193	U
1	2	194	U
1	2	195	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	197	A
1	2	198	A
1	2	200	A
1	2	207	U
1	2	215	A
1	2	217	A
1	2	218	A
1	2	219	A
1	2	226	A
1	2	227	U
1	2	228	G
1	2	229	U
1	2	231	U
1	2	233	C
1	2	234	G
1	2	235	G
1	2	238	U
1	2	239	C
1	2	240	U
1	2	241	U
1	2	242	U
1	2	250	C
1	2	257	A
1	2	260	U
1	2	261	U
1	2	265	A
1	2	266	A
1	2	271	A
1	2	272	U
1	2	274	G
1	2	275	C
1	2	276	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	288	A
1	2	290	G
1	2	299	A
1	2	302	U
1	2	308	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	314	C
1	2	316	A
1	2	320	U
1	2	321	C
1	2	322	G
1	2	333	A
1	2	337	G
1	2	338	C
1	2	351	C
1	2	352	A
1	2	359	A
1	2	360	A
1	2	361	C
1	2	368	U
1	2	387	A
1	2	390	G
1	2	393	C
1	2	397	A
1	2	400	A
1	2	402	C
1	2	403	G
1	2	404	G
1	2	416	A
1	2	418	G
1	2	419	G
1	2	423	G
1	2	424	C
1	2	425	A
1	2	426	G
1	2	428	A
1	2	434	G
1	2	437	A
1	2	439	U
1	2	440	U
1	2	444	C
1	2	448	C
1	2	458	G
1	2	475	A
1	2	477	A
1	2	484	C
1	2	485	A
1	2	486	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	488	G
1	2	493	U
1	2	495	C
1	2	496	G
1	2	497	G
1	2	498	G
1	2	499	U
1	2	500	C
1	2	502	U
1	2	503	G
1	2	504	U
1	2	505	A
1	2	506	A
1	2	507	U
1	2	508	U
1	2	510	G
1	2	513	U
1	2	514	G
1	2	515	A
1	2	516	G
1	2	527	A
1	2	528	U
1	2	532	U
1	2	538	A
1	2	539	G
1	2	540	G
1	2	541	A
1	2	542	A
1	2	543	C
1	2	544	A
1	2	548	G
1	2	554	C
1	2	555	A
1	2	556	A
1	2	557	G
1	2	558	U
1	2	559	C
1	2	565	C
1	2	578	U
1	2	579	A
1	2	580	A
1	2	581	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	582	U
1	2	594	A
1	2	595	G
1	2	609	U
1	2	611	U
1	2	619	A
1	2	620	A
1	2	622	A
1	2	623	A
1	2	624	G
1	2	639	U
1	2	640	U
1	2	650	U
1	2	653	C
1	2	654	C
1	2	655	G
1	2	656	G
1	2	658	C
1	2	677	G
1	2	682	C
1	2	684	A
1	2	685	A
1	2	686	C
1	2	692	C
1	2	694	U
1	2	696	C
1	2	697	C
1	2	698	U
1	2	700	C
1	2	701	U
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	706	A
1	2	707	A
1	2	709	C
1	2	710	U
1	2	711	U
1	2	712	G
1	2	713	A
1	2	714	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	717	C
1	2	718	U
1	2	719	U
1	2	721	U
1	2	722	G
1	2	723	G
1	2	725	U
1	2	727	U
1	2	728	U
1	2	731	C
1	2	733	A
1	2	734	A
1	2	735	C
1	2	736	C
1	2	737	A
1	2	738	G
1	2	742	U
1	2	745	U
1	2	754	A
1	2	755	A
1	2	756	A
1	2	759	U
1	2	765	G
1	2	766	U
1	2	774	A
1	2	775	G
1	2	777	C
1	2	781	U
1	2	783	G
1	2	784	C
1	2	787	G
1	2	789	A
1	2	793	A
1	2	794	U
1	2	795	U
1	2	803	A
1	2	812	A
1	2	813	U
1	2	814	A
1	2	815	G
1	2	816	G
1	2	818	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	819	G
1	2	820	U
1	2	821	U
1	2	823	G
1	2	824	G
1	2	830	U
1	2	831	U
1	2	833	U
1	2	846	G
1	2	850	A
1	2	856	A
1	2	863	A
1	2	864	U
1	2	876	G
1	2	886	U
1	2	896	U
1	2	898	A
1	2	912	U
1	2	914	G
1	2	916	U
1	2	921	U
1	2	926	A
1	2	931	C
1	2	933	A
1	2	935	U
1	2	942	G
1	2	951	A
1	2	960	U
1	2	966	A
1	2	988	A
1	2	992	A
1	2	993	A
1	2	997	G
1	2	998	A
1	2	1002	G
1	2	1003	A
1	2	1004	U
1	2	1005	A
1	2	1026	A
1	2	1028	C
1	2	1029	U
1	2	1031	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	1039	A
1	2	1040	G
1	2	1052	U
1	2	1053	G
1	2	1058	U
1	2	1061	A
1	2	1073	G
1	2	1075	C
1	2	1079	U
1	2	1080	U
1	2	1082	C
1	2	1086	A
1	2	1091	A
1	2	1092	A
1	2	1093	A
1	2	1096	C
1	2	1097	U
1	2	1100	G
1	2	1109	G
1	2	1111	G
1	2	1138	A
1	2	1146	G
1	2	1149	G
1	2	1150	G
1	2	1151	A
1	2	1157	A
1	2	1158	C
1	2	1160	A
1	2	1164	G
1	2	1167	G
1	2	1168	U
1	2	1176	G
1	2	1185	U
1	2	1194	A
1	2	1196	A
1	2	1197	C
1	2	1199	G
1	2	1200	G
1	2	1202	A
1	2	1203	A
1	2	1207	C
1	2	1217	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	1218	G
1	2	1227	A
1	2	1228	G
1	2	1229	G
1	2	1241	G
1	2	1243	G
1	2	1244	A
1	2	1245	G
1	2	1251	U
1	2	1256	A
1	2	1257	U
1	2	1258	U
1	2	1271	G
1	2	1285	U
1	2	1286	U
1	2	1291	G
1	2	1301	U
1	2	1307	U
1	2	1314	U
1	2	1315	U
1	2	1320	U
1	2	1321	A
1	2	1337	A
1	2	1339	C
1	2	1340	U
1	2	1341	A
1	2	1344	A
1	2	1345	A
1	2	1346	A
1	2	1355	C
1	2	1361	U
1	2	1363	U
1	2	1370	U
1	2	1371	A
1	2	1372	U
1	2	1388	A
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1412	G
1	2	1413	U
1	2	1415	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	1427	A
1	2	1428	G
1	2	1431	C
1	2	1446	A
1	2	1457	C
1	2	1458	G
1	2	1459	C
1	2	1461	C
1	2	1471	A
1	2	1473	U
1	2	1474	G
1	2	1482	C
1	2	1486	G
1	2	1489	U
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1499	G
1	2	1514	U
1	2	1516	A
1	2	1517	U
1	2	1518	C
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1526	A
1	2	1535	U
1	2	1536	G
1	2	1537	C
1	2	1538	U
1	2	1542	G
1	2	1557	U
1	2	1559	A
1	2	1569	A
1	2	1574	G
1	2	1584	G
1	2	1601	G
1	2	1614	A
1	2	1616	G
1	2	1626	U
1	2	1631	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	1657	U
1	2	1658	G
1	2	1680	G
1	2	1683	C
1	2	1684	U
1	2	1686	C
1	2	1697	G
1	2	1698	G
1	2	1699	G
1	2	1700	C
1	2	1701	A
1	2	1702	A
1	2	1703	C
1	2	1704	U
1	2	1711	C
1	2	1712	A
1	2	1713	G
1	2	1715	G
1	2	1731	A
1	2	1760	G
1	2	1762	A
1	2	1766	A
1	2	1769	U
1	2	1770	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U
1	2	1796	C
36	1	16	A
36	1	26	A
36	1	40	A
36	1	44	U
36	1	45	A
36	1	49	A
36	1	59	G
36	1	60	A
36	1	65	A
36	1	66	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	1	75	G
36	1	83	U
36	1	92	G
36	1	99	A
36	1	109	A
36	1	110	G
36	1	111	C
36	1	116	A
36	1	121	A
36	1	122	A
36	1	128	G
36	1	133	U
36	1	135	C
36	1	136	G
36	1	147	U
36	1	156	G
36	1	157	A
36	1	161	G
36	1	165	A
36	1	166	C
36	1	187	A
36	1	190	U
36	1	191	U
36	1	200	C
36	1	210	U
36	1	218	G
36	1	219	A
36	1	220	G
36	1	224	C
36	1	237	G
36	1	240	U
36	1	243	G
36	1	245	U
36	1	246	U
36	1	247	C
36	1	249	U
36	1	250	U
36	1	252	U
36	1	256	G
36	1	269	G
36	1	283	G
36	1	286	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	1	288	C
36	1	295	A
36	1	298	U
36	1	299	G
36	1	315	C
36	1	323	A
36	1	329	U
36	1	339	C
36	1	349	A
36	1	350	C
36	1	370	U
36	1	376	G
36	1	398	A
36	1	399	A
36	1	401	U
36	1	402	A
36	1	403	C
36	1	421	G
36	1	422	A
36	1	438	A
36	1	440	A
36	1	495	G
36	1	498	A
36	1	507	U
36	1	520	U
36	1	521	A
36	1	527	A
36	1	535	G
36	1	536	U
36	1	543	C
36	1	544	C
36	1	546	C
36	1	547	G
36	1	548	G
36	1	549	U
36	1	551	A
36	1	552	G
36	1	553	U
36	1	555	U
36	1	556	U
36	1	557	A
36	1	558	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	1	559	A
36	1	578	A
36	1	579	G
36	1	592	A
36	1	593	C
36	1	600	G
36	1	603	A
36	1	604	G
36	1	609	G
36	1	611	A
36	1	620	U
36	1	621	A
36	1	622	A
36	1	636	C
36	1	649	A
36	1	651	G
36	1	658	G
36	1	660	A
36	1	667	C
36	1	677	A
36	1	681	U
36	1	691	A
36	1	705	A
36	1	712	G
36	1	715	A
36	1	716	A
36	1	718	G
36	1	725	G
36	1	763	G
36	1	764	U
36	1	765	C
36	1	766	U
36	1	767	U
36	1	776	U
36	1	777	U
36	1	781	G
36	1	785	G
36	1	787	G
36	1	806	A
36	1	816	A
36	1	817	A
36	1	826	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	1	828	A
36	1	830	A
36	1	837	A
36	1	849	C
36	1	861	C
36	1	866	A
36	1	871	U
36	1	874	U
36	1	876	A
36	1	879	U
36	1	890	C
36	1	896	A
36	1	907	G
36	1	908	G
36	1	914	A
36	1	916	G
36	1	917	A
36	1	921	A
36	1	923	C
36	1	924	G
36	1	925	A
36	1	936	A
36	1	937	G
36	1	938	C
36	1	943	U
36	1	944	C
36	1	959	C
36	1	960	U
36	1	963	G
36	1	979	U
36	1	980	A
36	1	981	U
36	1	982	C
36	1	994	G
36	1	1001	G
36	1	1002	A
36	1	1006	A
36	1	1010	G
36	1	1013	G
36	1	1017	C
36	1	1018	G
36	1	1020	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	1	1024	G
36	1	1025	A
36	1	1029	G
36	1	1034	U
36	1	1036	A
36	1	1037	C
36	1	1047	A
36	1	1049	C
36	1	1063	G
36	1	1064	A
36	1	1065	A
36	1	1068	C
36	1	1071	U
36	1	1072	G
36	1	1081	U
36	1	1083	G
36	1	1087	G
36	1	1093	A
36	1	1094	U
36	1	1095	U
36	1	1096	U
36	1	1097	G
36	1	1098	A
36	1	1103	A
36	1	1104	G
36	1	1117	G
36	1	1131	G
36	1	1138	U
36	1	1153	A
36	1	1159	A
36	1	1160	C
36	1	1168	U
36	1	1178	G
36	1	1179	A
36	1	1180	A
36	1	1181	U
36	1	1182	A
36	1	1191	U
36	1	1192	C
36	1	1201	C
36	1	1202	A
36	1	1209	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	1	1216	C
36	1	1217	A
36	1	1221	A
36	1	1222	G
36	1	1225	A
36	1	1226	G
36	1	1227	C
36	1	1232	C
36	1	1233	G
36	1	1235	U
36	1	1236	G
36	1	1237	G
36	1	1241	U
36	1	1243	G
36	1	1245	A
36	1	1246	G
36	1	1248	C
36	1	1249	G
36	1	1254	C
36	1	1258	U
36	1	1262	G
36	1	1263	A
36	1	1264	G
36	1	1265	U
36	1	1266	G
36	1	1269	U
36	1	1270	A
36	1	1271	A
36	1	1274	A
36	1	1277	C
36	1	1278	A
36	1	1279	C
36	1	1280	C
36	1	1285	G
36	1	1287	A
36	1	1292	C
36	1	1307	G
36	1	1308	A
36	1	1309	U
36	1	1313	G
36	1	1323	G
36	1	1329	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	1	1330	A
36	1	1331	U
36	1	1348	U
36	1	1349	G
36	1	1350	A
36	1	1351	U
36	1	1352	A
36	1	1353	U
36	1	1355	A
36	1	1356	U
36	1	1357	G
36	1	1379	G
36	1	1386	A
36	1	1399	A
36	1	1400	G
36	1	1417	G
36	1	1419	A
36	1	1421	G
36	1	1425	U
36	1	1429	G
36	1	1434	G
36	1	1437	C
36	1	1446	A
36	1	1450	G
36	1	1452	A
36	1	1455	U
36	1	1465	A
36	1	1481	A
36	1	1482	A
36	1	1485	G
36	1	1488	G
36	1	1491	A
36	1	1495	U
36	1	1496	C
36	1	1508	C
36	1	1527	C
36	1	1533	U
36	1	1555	U
36	1	1556	C
36	1	1557	A
36	1	1560	G
36	1	1561	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	1	1562	C
36	1	1563	C
36	1	1564	U
36	1	1566	A
36	1	1567	U
36	1	1568	U
36	1	1569	U
36	1	1570	U
36	1	1571	A
36	1	1576	G
36	1	1580	A
36	1	1583	A
36	1	1587	A
36	1	1589	A
36	1	1607	U
36	1	1620	U
36	1	1629	U
36	1	1633	C
36	1	1639	C
36	1	1641	U
36	1	1642	A
36	1	1643	A
36	1	1645	U
36	1	1657	C
36	1	1673	G
36	1	1683	A
36	1	1705	U
36	1	1716	U
36	1	1717	U
36	1	1724	U
36	1	1729	A
36	1	1736	G
36	1	1741	A
36	1	1742	U
36	1	1745	C
36	1	1749	A
36	1	1750	A
36	1	1751	G
36	1	1752	A
36	1	1761	C
36	1	1762	C
36	1	1763	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	1	1765	U
36	1	1766	G
36	1	1769	G
36	1	1770	G
36	1	1775	G
36	1	1780	G
36	1	1797	A
36	1	1810	A
36	1	1814	A
36	1	1815	U
36	1	1816	A
36	1	1817	G
36	1	1819	U
36	1	1820	U
36	1	1821	U
36	1	1822	C
36	1	1835	A
36	1	1839	A
36	1	1841	A
36	1	1842	A
36	1	1846	C
36	1	1849	C
36	1	1866	C
36	1	1879	A
36	1	1880	U
36	1	1886	A
36	1	1901	A
36	1	1906	G
36	1	1912	U
36	1	1917	C
36	1	1935	G
36	1	1948	G
36	1	1951	C
36	1	1952	G
36	1	1954	G
36	1	2094	C
36	1	2098	C
36	1	2100	A
36	1	2101	C
36	1	2102	U
36	1	2112	U
36	1	2113	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	1	2114	C
36	1	2121	G
36	1	2122	G
36	1	2131	A
36	1	2140	U
36	1	2144	A
36	1	2158	A
36	1	2165	G
36	1	2169	G
36	1	2170	U
36	1	2185	G
36	1	2188	A
36	1	2205	U
36	1	2208	A
36	1	2210	G
36	1	2213	A
36	1	2222	A
36	1	2223	A
36	1	2239	G
36	1	2244	A
36	1	2249	G
36	1	2250	G
36	1	2255	A
36	1	2256	A
36	1	2272	G
36	1	2273	G
36	1	2279	A
36	1	2281	A
36	1	2282	U
36	1	2284	C
36	1	2288	G
36	1	2298	U
36	1	2301	U
36	1	2307	G
36	1	2309	A
36	1	2310	U
36	1	2313	A
36	1	2314	U
36	1	2315	G
36	1	2334	U
36	1	2335	G
36	1	2336	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	1	2360	C
36	1	2372	A
36	1	2373	A
36	1	2374	C
36	1	2375	G
36	1	2385	G
36	1	2393	G
36	1	2394	G
36	1	2397	A
36	1	2401	A
36	1	2402	A
36	1	2403	G
36	1	2404	A
36	1	2411	U
36	1	2418	G
36	1	2419	A
36	1	2444	C
36	1	2445	A
36	1	2502	A
36	1	2503	G
36	1	2507	C
36	1	2514	U
36	1	2515	A
36	1	2521	U
36	1	2522	G
36	1	2523	A
36	1	2526	C
36	1	2532	U
36	1	2533	G
36	1	2534	G
36	1	2537	U
36	1	2538	U
36	1	2539	C
36	1	2540	A
36	1	2541	U
36	1	2542	U
36	1	2543	U
36	1	2547	A
36	1	2548	C
36	1	2549	G
36	1	2551	U
36	1	2552	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	1	2554	A
36	1	2555	G
36	1	2560	C
36	1	2561	A
36	1	2568	C
36	1	2569	A
36	1	2570	U
36	1	2571	U
36	1	2572	C
36	1	2573	G
36	1	2581	U
36	1	2585	G
36	1	2586	G
36	1	2593	A
36	1	2594	C
36	1	2606	G
36	1	2607	G
36	1	2614	G
36	1	2629	U
36	1	2636	A
36	1	2637	A
36	1	2638	C
36	1	2652	U
36	1	2653	C
36	1	2656	A
36	1	2672	G
36	1	2674	A
36	1	2677	G
36	1	2689	A
36	1	2691	A
36	1	2694	A
36	1	2695	A
36	1	2696	A
36	1	2705	A
36	1	2706	G
36	1	2707	C
36	1	2712	U
36	1	2714	G
36	1	2728	G
36	1	2737	C
36	1	2749	G
36	1	2752	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	1	2753	G
36	1	2754	G
36	1	2755	C
36	1	2762	A
36	1	2772	C
36	1	2777	G
36	1	2778	G
36	1	2796	G
36	1	2799	A
36	1	2800	G
36	1	2801	A
36	1	2810	C
36	1	2814	G
36	1	2817	A
36	1	2829	U
36	1	2836	C
36	1	2837	A
36	1	2842	U
36	1	2843	U
36	1	2845	A
36	1	2849	C
36	1	2854	U
36	1	2860	U
36	1	2870	C
36	1	2871	G
36	1	2872	A
36	1	2887	A
36	1	2889	C
36	1	2898	G
36	1	2899	C
36	1	2900	A
36	1	2914	G
36	1	2917	G
36	1	2923	U
36	1	2935	U
36	1	2936	A
36	1	2937	G
36	1	2939	G
36	1	2942	C
36	1	2943	G
36	1	2947	G
36	1	2983	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	1	2990	G
36	1	2992	U
36	1	2996	U
36	1	2997	G
36	1	3012	A
36	1	3025	C
36	1	3030	G
36	1	3044	G
36	1	3057	U
36	1	3058	U
36	1	3059	G
36	1	3078	U
36	1	3079	U
36	1	3080	G
36	1	3086	A
36	1	3090	U
36	1	3091	A
36	1	3092	C
36	1	3103	A
36	1	3104	U
36	1	3113	A
36	1	3114	A
36	1	3122	A
36	1	3129	A
36	1	3130	A
36	1	3131	U
36	1	3142	A
36	1	3143	C
36	1	3151	U
36	1	3153	U
36	1	3154	C
36	1	3155	U
36	1	3156	U
36	1	3157	U
36	1	3158	G
36	1	3164	C
36	1	3165	A
36	1	3169	U
36	1	3170	A
36	1	3171	U
36	1	3173	G
36	1	3174	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	1	3176	G
36	1	3179	U
36	1	3181	C
36	1	3187	A
36	1	3196	U
36	1	3197	G
36	1	3199	G
36	1	3207	U
36	1	3210	A
36	1	3217	C
36	1	3218	A
36	1	3219	G
36	1	3228	C
36	1	3229	G
36	1	3235	C
36	1	3243	A
36	1	3245	A
36	1	3246	G
36	1	3247	G
36	1	3253	G
36	1	3259	U
36	1	3270	U
36	1	3272	C
36	1	3276	G
36	1	3279	A
36	1	3281	U
36	1	3286	G
36	1	3287	U
36	1	3289	G
36	1	3293	U
36	1	3294	A
36	1	3295	A
36	1	3304	U
36	1	3313	U
36	1	3314	A
36	1	3316	A
36	1	3318	G
36	1	3319	U
36	1	3320	A
36	1	3335	A
36	1	3341	U
36	1	3345	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	1	3346	U
36	1	3347	A
36	1	3349	C
36	1	3351	U
36	1	3352	U
36	1	3353	G
36	1	3354	U
36	1	3355	U
36	1	3356	G
36	1	3368	U
36	1	3369	G
36	1	3375	A
36	1	3376	A
36	1	3378	C
36	1	3382	U
36	1	3383	G
36	1	3389	U
36	1	3396	U
37	3	7	G
37	3	10	C
37	3	13	A
37	3	14	U
37	3	22	A
37	3	41	G
37	3	54	U
37	3	65	G
37	3	76	A
37	3	91	G
37	3	102	A
37	3	112	G
37	3	121	U
38	4	21	C
38	4	26	U
38	4	34	U
38	4	35	C
38	4	48	A
38	4	50	C
38	4	51	G
38	4	52	A
38	4	57	C
38	4	59	A
38	4	60	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
38	4	62	C
38	4	63	G
38	4	69	U
38	4	70	G
38	4	75	G
38	4	80	A
38	4	81	U
38	4	82	U
38	4	85	G
38	4	86	U
38	4	87	G
38	4	90	U
38	4	95	G
38	4	96	A
38	4	104	A
38	4	105	A
38	4	106	C
38	4	111	A
38	4	113	U
38	4	125	U
38	4	126	A
38	4	128	U
38	4	138	A
38	4	155	A
38	4	157	U
38	4	158	U
1	6	2	A
1	6	4	C
1	6	17	C
1	6	25	C
1	6	26	A
1	6	27	U
1	6	34	G
1	6	47	A
1	6	50	C
1	6	57	G
1	6	60	U
1	6	61	A
1	6	66	U
1	6	67	A
1	6	68	A
1	6	69	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	6	71	A
1	6	72	A
1	6	73	U
1	6	75	U
1	6	76	A
1	6	77	U
1	6	104	A
1	6	114	C
1	6	115	G
1	6	132	U
1	6	137	U
1	6	138	A
1	6	140	A
1	6	141	U
1	6	144	U
1	6	145	A
1	6	146	U
1	6	153	G
1	6	158	U
1	6	159	U
1	6	161	U
1	6	166	C
1	6	170	U
1	6	178	U
1	6	185	U
1	6	188	A
1	6	190	C
1	6	191	C
1	6	192	U
1	6	193	U
1	6	194	U
1	6	195	G
1	6	196	G
1	6	199	G
1	6	200	A
1	6	215	A
1	6	216	U
1	6	217	A
1	6	218	A
1	6	219	A
1	6	220	A
1	6	226	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	6	227	U
1	6	228	G
1	6	230	C
1	6	232	U
1	6	233	C
1	6	235	G
1	6	240	U
1	6	241	U
1	6	249	U
1	6	250	C
1	6	260	U
1	6	261	U
1	6	265	A
1	6	266	A
1	6	271	A
1	6	272	U
1	6	273	G
1	6	277	U
1	6	278	U
1	6	280	U
1	6	287	G
1	6	299	A
1	6	302	U
1	6	314	C
1	6	316	A
1	6	319	U
1	6	320	U
1	6	321	C
1	6	322	G
1	6	337	G
1	6	338	C
1	6	352	A
1	6	359	A
1	6	360	A
1	6	361	C
1	6	371	G
1	6	400	A
1	6	401	A
1	6	402	C
1	6	404	G
1	6	416	A
1	6	417	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	6	418	G
1	6	424	C
1	6	425	A
1	6	426	G
1	6	434	G
1	6	439	U
1	6	444	C
1	6	448	C
1	6	454	U
1	6	468	A
1	6	469	C
1	6	475	A
1	6	477	A
1	6	484	C
1	6	485	A
1	6	486	G
1	6	487	G
1	6	488	G
1	6	489	C
1	6	490	C
1	6	492	A
1	6	493	U
1	6	494	U
1	6	496	G
1	6	500	C
1	6	501	U
1	6	504	U
1	6	505	A
1	6	506	A
1	6	507	U
1	6	508	U
1	6	510	G
1	6	511	A
1	6	512	A
1	6	513	U
1	6	514	G
1	6	515	A
1	6	519	C
1	6	527	A
1	6	534	A
1	6	536	C
1	6	538	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	6	539	G
1	6	540	G
1	6	541	A
1	6	542	A
1	6	543	C
1	6	544	A
1	6	548	G
1	6	555	A
1	6	556	A
1	6	557	G
1	6	558	U
1	6	559	C
1	6	564	G
1	6	565	C
1	6	570	A
1	6	574	G
1	6	578	U
1	6	579	A
1	6	580	A
1	6	594	A
1	6	595	G
1	6	609	U
1	6	611	U
1	6	616	G
1	6	617	U
1	6	619	A
1	6	620	A
1	6	622	A
1	6	623	A
1	6	624	G
1	6	630	A
1	6	634	G
1	6	639	U
1	6	645	C
1	6	648	G
1	6	650	U
1	6	652	G
1	6	653	C
1	6	654	C
1	6	661	A
1	6	662	U
1	6	665	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	6	667	U
1	6	668	C
1	6	670	U
1	6	676	G
1	6	678	A
1	6	679	U
1	6	680	U
1	6	681	U
1	6	682	C
1	6	683	C
1	6	684	A
1	6	685	A
1	6	691	C
1	6	696	C
1	6	697	C
1	6	698	U
1	6	709	C
1	6	710	U
1	6	711	U
1	6	714	G
1	6	715	U
1	6	718	U
1	6	719	U
1	6	720	G
1	6	721	U
1	6	722	G
1	6	730	G
1	6	742	U
1	6	744	U
1	6	751	G
1	6	754	A
1	6	755	A
1	6	756	A
1	6	765	G
1	6	767	U
1	6	774	A
1	6	775	G
1	6	780	A
1	6	781	U
1	6	782	U
1	6	783	G
1	6	787	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	6	789	A
1	6	792	U
1	6	793	A
1	6	794	U
1	6	811	A
1	6	812	A
1	6	814	A
1	6	815	G
1	6	816	G
1	6	821	U
1	6	822	U
1	6	823	G
1	6	825	U
1	6	826	U
1	6	829	A
1	6	830	U
1	6	831	U
1	6	832	U
1	6	834	G
1	6	835	U
1	6	856	A
1	6	861	U
1	6	863	A
1	6	873	U
1	6	876	G
1	6	898	A
1	6	906	A
1	6	910	C
1	6	912	U
1	6	913	G
1	6	914	G
1	6	916	U
1	6	933	A
1	6	935	U
1	6	942	G
1	6	944	A
1	6	959	U
1	6	960	U
1	6	969	C
1	6	970	A
1	6	971	A
1	6	992	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	6	993	A
1	6	997	G
1	6	1003	A
1	6	1004	U
1	6	1005	A
1	6	1018	U
1	6	1026	A
1	6	1028	C
1	6	1031	U
1	6	1039	A
1	6	1040	G
1	6	1052	U
1	6	1053	G
1	6	1057	U
1	6	1058	U
1	6	1059	U
1	6	1060	U
1	6	1063	U
1	6	1073	G
1	6	1082	C
1	6	1092	A
1	6	1093	A
1	6	1096	C
1	6	1097	U
1	6	1098	U
1	6	1100	G
1	6	1109	G
1	6	1111	G
1	6	1137	A
1	6	1138	A
1	6	1139	A
1	6	1151	A
1	6	1155	G
1	6	1158	C
1	6	1159	C
1	6	1160	A
1	6	1162	C
1	6	1167	G
1	6	1185	U
1	6	1194	A
1	6	1196	A
1	6	1199	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	6	1200	G
1	6	1202	A
1	6	1207	C
1	6	1208	A
1	6	1217	A
1	6	1218	G
1	6	1219	A
1	6	1226	A
1	6	1227	A
1	6	1228	G
1	6	1229	G
1	6	1230	A
1	6	1241	G
1	6	1242	A
1	6	1243	G
1	6	1244	A
1	6	1245	G
1	6	1246	C
1	6	1252	C
1	6	1255	G
1	6	1256	A
1	6	1257	U
1	6	1258	U
1	6	1286	U
1	6	1288	G
1	6	1314	U
1	6	1315	U
1	6	1316	G
1	6	1321	A
1	6	1338	C
1	6	1344	A
1	6	1345	A
1	6	1346	A
1	6	1354	G
1	6	1361	U
1	6	1362	U
1	6	1363	U
1	6	1364	G
1	6	1367	G
1	6	1370	U
1	6	1371	A
1	6	1383	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	6	1388	A
1	6	1390	U
1	6	1398	U
1	6	1399	C
1	6	1400	A
1	6	1402	G
1	6	1413	U
1	6	1415	U
1	6	1427	A
1	6	1428	G
1	6	1429	G
1	6	1433	G
1	6	1445	G
1	6	1446	A
1	6	1448	G
1	6	1458	G
1	6	1459	C
1	6	1460	A
1	6	1461	C
1	6	1471	A
1	6	1473	U
1	6	1481	C
1	6	1482	C
1	6	1486	G
1	6	1489	U
1	6	1490	C
1	6	1491	U
1	6	1492	A
1	6	1493	A
1	6	1494	C
1	6	1496	U
1	6	1506	G
1	6	1514	U
1	6	1515	A
1	6	1516	A
1	6	1521	G
1	6	1523	G
1	6	1524	A
1	6	1535	U
1	6	1536	G
1	6	1537	C
1	6	1538	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	6	1540	G
1	6	1554	U
1	6	1557	U
1	6	1559	A
1	6	1569	A
1	6	1573	A
1	6	1574	G
1	6	1575	G
1	6	1582	U
1	6	1584	G
1	6	1600	A
1	6	1601	G
1	6	1615	C
1	6	1616	G
1	6	1621	U
1	6	1634	C
1	6	1637	C
1	6	1638	G
1	6	1639	C
1	6	1657	U
1	6	1658	G
1	6	1666	U
1	6	1697	G
1	6	1698	G
1	6	1699	G
1	6	1700	C
1	6	1701	A
1	6	1702	A
1	6	1712	A
1	6	1713	G
1	6	1715	G
1	6	1716	C
1	6	1717	G
1	6	1727	G
1	6	1730	A
1	6	1731	A
1	6	1735	U
1	6	1736	G
1	6	1755	A
1	6	1760	G
1	6	1762	A
1	6	1766	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	6	1767	G
1	6	1769	U
1	6	1780	G
1	6	1782	A
1	6	1783	C
1	6	1792	G
1	6	1793	G
1	6	1794	A
1	6	1795	U
1	6	1796	C
1	6	1799	U
1	6	1800	A
36	5	15	C
36	5	26	A
36	5	33	G
36	5	39	A
36	5	40	A
36	5	44	U
36	5	49	A
36	5	59	G
36	5	60	A
36	5	65	A
36	5	66	A
36	5	73	C
36	5	75	G
36	5	76	G
36	5	83	U
36	5	92	G
36	5	93	C
36	5	96	G
36	5	99	A
36	5	109	A
36	5	110	G
36	5	111	C
36	5	116	A
36	5	120	G
36	5	121	A
36	5	122	A
36	5	133	U
36	5	134	U
36	5	135	C
36	5	136	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	5	150	A
36	5	152	U
36	5	156	G
36	5	157	A
36	5	165	A
36	5	166	C
36	5	170	G
36	5	171	G
36	5	172	G
36	5	173	G
36	5	174	C
36	5	180	C
36	5	182	U
36	5	183	G
36	5	184	U
36	5	187	A
36	5	190	U
36	5	191	U
36	5	210	U
36	5	218	G
36	5	219	A
36	5	221	A
36	5	231	G
36	5	234	G
36	5	237	G
36	5	238	A
36	5	239	G
36	5	240	U
36	5	244	G
36	5	247	C
36	5	248	U
36	5	249	U
36	5	250	U
36	5	251	G
36	5	252	U
36	5	253	A
36	5	254	A
36	5	269	G
36	5	284	A
36	5	286	U
36	5	295	A
36	5	299	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	5	316	U
36	5	323	A
36	5	329	U
36	5	339	C
36	5	349	A
36	5	350	C
36	5	351	A
36	5	352	A
36	5	370	U
36	5	376	G
36	5	397	A
36	5	398	A
36	5	399	A
36	5	401	U
36	5	402	A
36	5	403	C
36	5	420	G
36	5	421	G
36	5	422	A
36	5	436	A
36	5	437	G
36	5	438	A
36	5	439	C
36	5	440	A
36	5	441	U
36	5	442	G
36	5	492	U
36	5	495	G
36	5	515	C
36	5	521	A
36	5	535	G
36	5	539	C
36	5	546	C
36	5	547	G
36	5	548	G
36	5	553	U
36	5	555	U
36	5	557	A
36	5	559	A
36	5	578	A
36	5	579	G
36	5	592	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	5	594	U
36	5	600	G
36	5	603	A
36	5	604	G
36	5	609	G
36	5	611	A
36	5	619	A
36	5	620	U
36	5	621	A
36	5	636	C
36	5	649	A
36	5	651	G
36	5	660	A
36	5	677	A
36	5	681	U
36	5	683	U
36	5	691	A
36	5	692	A
36	5	705	A
36	5	708	G
36	5	712	G
36	5	715	A
36	5	716	A
36	5	722	G
36	5	725	G
36	5	727	G
36	5	735	A
36	5	736	A
36	5	758	C
36	5	763	G
36	5	766	U
36	5	767	U
36	5	768	C
36	5	776	U
36	5	777	U
36	5	781	G
36	5	785	G
36	5	786	A
36	5	806	A
36	5	816	A
36	5	817	A
36	5	830	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	5	837	A
36	5	851	C
36	5	853	G
36	5	861	C
36	5	874	U
36	5	877	C
36	5	879	U
36	5	895	A
36	5	896	A
36	5	907	G
36	5	908	G
36	5	910	G
36	5	913	A
36	5	914	A
36	5	916	G
36	5	917	A
36	5	921	A
36	5	923	C
36	5	937	G
36	5	944	C
36	5	953	G
36	5	959	C
36	5	960	U
36	5	962	A
36	5	963	G
36	5	974	G
36	5	979	U
36	5	984	G
36	5	993	G
36	5	994	G
36	5	1000	C
36	5	1001	G
36	5	1002	A
36	5	1006	A
36	5	1010	G
36	5	1015	U
36	5	1016	C
36	5	1017	C
36	5	1018	G
36	5	1019	G
36	5	1021	G
36	5	1024	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	5	1025	A
36	5	1026	A
36	5	1027	A
36	5	1028	U
36	5	1029	G
36	5	1032	C
36	5	1035	G
36	5	1047	A
36	5	1049	C
36	5	1064	A
36	5	1065	A
36	5	1071	U
36	5	1072	G
36	5	1081	U
36	5	1082	U
36	5	1085	A
36	5	1093	A
36	5	1094	U
36	5	1095	U
36	5	1096	U
36	5	1097	G
36	5	1098	A
36	5	1103	A
36	5	1104	G
36	5	1117	G
36	5	1131	G
36	5	1144	U
36	5	1152	G
36	5	1153	A
36	5	1156	C
36	5	1159	A
36	5	1173	U
36	5	1180	A
36	5	1181	U
36	5	1182	A
36	5	1190	A
36	5	1191	U
36	5	1192	C
36	5	1193	A
36	5	1201	C
36	5	1202	A
36	5	1209	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	5	1222	G
36	5	1223	A
36	5	1232	C
36	5	1235	U
36	5	1236	G
36	5	1237	G
36	5	1238	C
36	5	1239	C
36	5	1241	U
36	5	1242	G
36	5	1245	A
36	5	1246	G
36	5	1252	A
36	5	1254	C
36	5	1258	U
36	5	1262	G
36	5	1263	A
36	5	1264	G
36	5	1266	G
36	5	1281	G
36	5	1285	G
36	5	1295	G
36	5	1307	G
36	5	1308	A
36	5	1309	U
36	5	1311	G
36	5	1313	G
36	5	1330	A
36	5	1349	G
36	5	1351	U
36	5	1352	A
36	5	1353	U
36	5	1355	A
36	5	1356	U
36	5	1357	G
36	5	1385	C
36	5	1386	A
36	5	1387	G
36	5	1399	A
36	5	1400	G
36	5	1418	A
36	5	1419	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	5	1428	A
36	5	1431	G
36	5	1434	G
36	5	1437	C
36	5	1446	A
36	5	1450	G
36	5	1480	G
36	5	1481	A
36	5	1482	A
36	5	1502	C
36	5	1503	A
36	5	1508	C
36	5	1514	G
36	5	1515	A
36	5	1519	G
36	5	1536	G
36	5	1549	U
36	5	1554	U
36	5	1555	U
36	5	1556	C
36	5	1557	A
36	5	1560	G
36	5	1561	G
36	5	1562	C
36	5	1566	A
36	5	1567	U
36	5	1569	U
36	5	1570	U
36	5	1571	A
36	5	1572	U
36	5	1574	C
36	5	1575	A
36	5	1576	G
36	5	1577	G
36	5	1578	C
36	5	1579	C
36	5	1581	C
36	5	1583	A
36	5	1587	A
36	5	1589	A
36	5	1593	A
36	5	1605	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	5	1607	U
36	5	1620	U
36	5	1629	U
36	5	1639	C
36	5	1643	A
36	5	1644	C
36	5	1645	U
36	5	1683	A
36	5	1685	C
36	5	1686	U
36	5	1716	U
36	5	1717	U
36	5	1724	U
36	5	1736	G
36	5	1750	A
36	5	1751	G
36	5	1760	A
36	5	1762	C
36	5	1764	U
36	5	1765	U
36	5	1766	G
36	5	1770	G
36	5	1780	G
36	5	1793	C
36	5	1797	A
36	5	1810	A
36	5	1813	A
36	5	1814	A
36	5	1815	U
36	5	1816	A
36	5	1817	G
36	5	1818	U
36	5	1820	U
36	5	1821	U
36	5	1839	A
36	5	1841	A
36	5	1842	A
36	5	1846	C
36	5	1847	A
36	5	1849	C
36	5	1850	A
36	5	1878	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	5	1879	A
36	5	1880	U
36	5	1893	A
36	5	1895	A
36	5	1906	G
36	5	1935	G
36	5	1952	G
36	5	1953	G
36	5	2101	C
36	5	2102	U
36	5	2112	U
36	5	2113	A
36	5	2121	G
36	5	2122	G
36	5	2131	A
36	5	2144	A
36	5	2158	A
36	5	2169	G
36	5	2187	G
36	5	2188	A
36	5	2192	C
36	5	2205	U
36	5	2208	A
36	5	2210	G
36	5	2215	A
36	5	2223	A
36	5	2228	A
36	5	2244	A
36	5	2250	G
36	5	2252	A
36	5	2253	G
36	5	2255	A
36	5	2256	A
36	5	2258	U
36	5	2272	G
36	5	2273	G
36	5	2279	A
36	5	2281	A
36	5	2288	G
36	5	2299	A
36	5	2307	G
36	5	2310	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	5	2313	A
36	5	2315	G
36	5	2334	U
36	5	2335	G
36	5	2336	U
36	5	2360	C
36	5	2372	A
36	5	2373	A
36	5	2374	C
36	5	2375	G
36	5	2385	G
36	5	2392	C
36	5	2393	G
36	5	2396	G
36	5	2397	A
36	5	2401	A
36	5	2403	G
36	5	2404	A
36	5	2411	U
36	5	2418	G
36	5	2419	A
36	5	2435	G
36	5	2436	U
36	5	2438	A
36	5	2439	A
36	5	2440	G
36	5	2441	A
36	5	2443	A
36	5	2504	U
36	5	2505	U
36	5	2508	U
36	5	2510	U
36	5	2511	A
36	5	2514	U
36	5	2515	A
36	5	2518	C
36	5	2523	A
36	5	2524	A
36	5	2525	G
36	5	2526	C
36	5	2530	G
36	5	2531	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	5	2532	U
36	5	2537	U
36	5	2538	U
36	5	2539	C
36	5	2540	A
36	5	2541	U
36	5	2543	U
36	5	2549	G
36	5	2552	C
36	5	2555	G
36	5	2562	A
36	5	2565	U
36	5	2566	C
36	5	2567	C
36	5	2568	C
36	5	2569	A
36	5	2570	U
36	5	2571	U
36	5	2572	C
36	5	2573	G
36	5	2574	G
36	5	2584	G
36	5	2585	G
36	5	2589	G
36	5	2593	A
36	5	2594	C
36	5	2606	G
36	5	2607	G
36	5	2614	G
36	5	2618	G
36	5	2639	G
36	5	2652	U
36	5	2656	A
36	5	2667	A
36	5	2674	A
36	5	2675	C
36	5	2677	G
36	5	2678	A
36	5	2681	U
36	5	2683	U
36	5	2689	A
36	5	2690	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	5	2694	A
36	5	2696	A
36	5	2707	C
36	5	2714	G
36	5	2719	U
36	5	2720	G
36	5	2727	A
36	5	2728	G
36	5	2729	U
36	5	2734	A
36	5	2752	U
36	5	2753	G
36	5	2762	A
36	5	2771	U
36	5	2772	C
36	5	2773	C
36	5	2777	G
36	5	2778	G
36	5	2779	A
36	5	2796	G
36	5	2799	A
36	5	2800	G
36	5	2801	A
36	5	2802	A
36	5	2810	C
36	5	2814	G
36	5	2817	A
36	5	2818	U
36	5	2828	G
36	5	2837	A
36	5	2838	A
36	5	2839	G
36	5	2843	U
36	5	2845	A
36	5	2847	A
36	5	2853	A
36	5	2855	U
36	5	2866	U
36	5	2870	C
36	5	2871	G
36	5	2872	A
36	5	2873	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	5	2874	G
36	5	2875	U
36	5	2876	C
36	5	2886	U
36	5	2887	A
36	5	2896	A
36	5	2899	C
36	5	2904	U
36	5	2918	G
36	5	2923	U
36	5	2935	U
36	5	2936	A
36	5	2942	C
36	5	2947	G
36	5	2956	A
36	5	2971	A
36	5	2972	G
36	5	2983	C
36	5	2990	G
36	5	2996	U
36	5	2997	G
36	5	3012	A
36	5	3029	A
36	5	3030	G
36	5	3049	A
36	5	3056	U
36	5	3059	G
36	5	3069	G
36	5	3078	U
36	5	3079	U
36	5	3084	C
36	5	3086	A
36	5	3092	C
36	5	3119	U
36	5	3122	A
36	5	3127	A
36	5	3130	A
36	5	3131	U
36	5	3139	A
36	5	3142	A
36	5	3143	C
36	5	3150	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	5	3153	U
36	5	3154	C
36	5	3155	U
36	5	3156	U
36	5	3157	U
36	5	3158	G
36	5	3164	C
36	5	3165	A
36	5	3167	A
36	5	3168	A
36	5	3171	U
36	5	3172	A
36	5	3173	G
36	5	3174	A
36	5	3176	G
36	5	3179	U
36	5	3180	A
36	5	3181	C
36	5	3187	A
36	5	3195	U
36	5	3196	U
36	5	3207	U
36	5	3209	A
36	5	3214	U
36	5	3217	C
36	5	3218	A
36	5	3219	G
36	5	3227	A
36	5	3229	G
36	5	3239	G
36	5	3243	A
36	5	3245	A
36	5	3246	G
36	5	3247	G
36	5	3249	C
36	5	3253	G
36	5	3259	U
36	5	3265	C
36	5	3270	U
36	5	3273	A
36	5	3275	U
36	5	3276	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	5	3277	U
36	5	3279	A
36	5	3281	U
36	5	3282	U
36	5	3284	G
36	5	3285	C
36	5	3286	G
36	5	3288	G
36	5	3289	G
36	5	3290	G
36	5	3294	A
36	5	3304	U
36	5	3313	U
36	5	3316	A
36	5	3317	U
36	5	3319	U
36	5	3320	A
36	5	3341	U
36	5	3342	A
36	5	3345	G
36	5	3351	U
36	5	3353	G
36	5	3354	U
36	5	3356	G
36	5	3358	U
36	5	3368	U
36	5	3369	G
36	5	3378	C
36	5	3383	G
36	5	3389	U
36	5	3390	G
36	5	3396	U
37	7	7	G
37	7	19	C
37	7	22	A
37	7	42	A
37	7	45	A
37	7	49	G
37	7	51	A
37	7	54	U
37	7	60	G
37	7	65	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
37	7	73	C
37	7	74	C
37	7	93	C
37	7	99	G
37	7	101	G
37	7	102	A
37	7	103	A
37	7	104	A
37	7	112	G
38	8	21	C
38	8	34	U
38	8	35	C
38	8	48	A
38	8	49	G
38	8	51	G
38	8	52	A
38	8	59	A
38	8	62	C
38	8	63	G
38	8	71	A
38	8	79	A
38	8	80	A
38	8	81	U
38	8	84	C
38	8	86	U
38	8	87	G
38	8	88	A
38	8	90	U
38	8	95	G
38	8	97	A
38	8	102	U
38	8	104	A
38	8	105	A
38	8	106	C
38	8	111	A
38	8	112	U
38	8	113	U
38	8	116	G
38	8	125	U
38	8	126	A
38	8	127	U
38	8	138	A

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Mol	Chain	Res	Type
38	8	152	G
38	8	155	A
38	8	156	U
38	8	157	U
38	8	158	U

All (230) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	25	C
1	2	45	U
1	2	68	A
1	2	73	U
1	2	114	C
1	2	130	C
1	2	131	C
1	2	139	C
1	2	158	U
1	2	218	A
1	2	240	U
1	2	277	U
1	2	278	U
1	2	280	U
1	2	417	A
1	2	497	G
1	2	499	U
1	2	501	U
1	2	503	G
1	2	512	A
1	2	555	A
1	2	558	U
1	2	685	A
1	2	704	C
1	2	720	G
1	2	721	U
1	2	755	A
1	2	794	U
1	2	811	A
1	2	1081	A
1	2	1150	G
1	2	1157	A
1	2	1196	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	1226	A
1	2	1244	A
1	2	1250	U
1	2	1344	A
1	2	1370	U
1	2	1481	C
1	2	1489	U
1	2	1490	C
1	2	1568	C
1	2	1573	A
1	2	1615	C
1	2	1657	U
1	2	1698	G
1	2	1711	C
1	2	1761	U
36	1	65	A
36	1	210	U
36	1	223	U
36	1	239	G
36	1	282	G
36	1	547	G
36	1	588	G
36	1	594	U
36	1	715	A
36	1	763	G
36	1	873	C
36	1	896	A
36	1	916	G
36	1	979	U
36	1	981	U
36	1	993	G
36	1	1064	A
36	1	1094	U
36	1	1097	G
36	1	1103	A
36	1	1196	C
36	1	1273	A
36	1	1317	A
36	1	1329	U
36	1	1352	A
36	1	1355	A
36	1	1481	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	1	1484	U
36	1	1554	U
36	1	1562	C
36	1	1582	C
36	1	1589	A
36	1	1716	U
36	1	1815	U
36	1	1820	U
36	1	1842	A
36	1	2101	C
36	1	2112	U
36	1	2209	U
36	1	2249	G
36	1	2281	A
36	1	2297	U
36	1	2372	A
36	1	2513	U
36	1	2525	G
36	1	2537	U
36	1	2541	U
36	1	2554	A
36	1	2585	G
36	1	2593	A
36	1	3078	U
36	1	3121	U
36	1	3157	U
36	1	3169	U
36	1	3218	A
36	1	3228	C
36	1	3269	U
36	1	3319	U
36	1	3350	C
36	1	3351	U
36	1	3353	G
36	1	3375	A
37	3	13	A
37	3	49	G
38	4	85	G
38	4	111	A
38	4	125	U
1	6	25	C
1	6	66	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	6	76	A
1	6	114	C
1	6	136	C
1	6	139	C
1	6	158	U
1	6	187	G
1	6	192	U
1	6	217	A
1	6	240	U
1	6	272	U
1	6	277	U
1	6	417	A
1	6	512	A
1	6	542	A
1	6	555	A
1	6	651	G
1	6	678	A
1	6	697	C
1	6	717	C
1	6	755	A
1	6	829	A
1	6	834	G
1	6	1051	G
1	6	1058	U
1	6	1081	A
1	6	1097	U
1	6	1207	C
1	6	1227	A
1	6	1244	A
1	6	1255	G
1	6	1344	A
1	6	1481	C
1	6	1489	U
1	6	1491	U
1	6	1535	U
1	6	1568	C
1	6	1573	A
1	6	1615	C
1	6	1620	C
1	6	1657	U
1	6	1696	G
1	6	1698	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	6	1700	C
36	5	65	A
36	5	93	C
36	5	151	A
36	5	183	G
36	5	238	A
36	5	588	G
36	5	594	U
36	5	607	A
36	5	715	A
36	5	735	A
36	5	765	C
36	5	873	C
36	5	896	A
36	5	916	G
36	5	993	G
36	5	1027	A
36	5	1064	A
36	5	1081	U
36	5	1152	G
36	5	1192	C
36	5	1222	G
36	5	1238	C
36	5	1241	U
36	5	1284	C
36	5	1307	G
36	5	1308	A
36	5	1329	U
36	5	1331	U
36	5	1352	A
36	5	1355	A
36	5	1481	A
36	5	1554	U
36	5	1560	G
36	5	1580	A
36	5	1716	U
36	5	1816	A
36	5	1846	C
36	5	2101	C
36	5	2112	U
36	5	2204	C
36	5	2209	U

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Mol	Chain	Res	Type
36	5	2255	A
36	5	2257	C
36	5	2372	A
36	5	2400	G
36	5	2440	G
36	5	2507	C
36	5	2513	U
36	5	2728	G
36	5	2772	C
36	5	2801	A
36	5	2818	U
36	5	2873	U
36	5	2874	G
36	5	2887	A
36	5	2896	A
36	5	2971	A
36	5	3078	U
36	5	3121	U
36	5	3154	C
36	5	3195	U
36	5	3207	U
36	5	3228	C
36	5	3269	U
36	5	3289	G
36	5	3340	G
36	5	3341	U
36	5	3357	U
37	7	49	G
38	8	126	A

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

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

#### 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	3795	-	0,6,6	-	-	-		
85	OHX	8	224	-	0,6,6	-	-	-		
85	OHX	6	2068	-	0,6,6	-	-	-		
85	OHX	5	3915	-	0,6,6	-	-	-		
85	OHX	1	4015	-	0,6,6	-	-	-		
85	OHX	1	3994	-	0,6,6	-	-	-		
85	OHX	5	3957	-	0,6,6	-	-	-		
85	OHX	1	3850	-	0,6,6	-	-	-		
85	OHX	1	4005	-	0,6,6	-	-	-		
85	OHX	6	2098	-	0,6,6	-	-	-		
85	OHX	5	3964	-	0,6,6	-	-	-		
85	OHX	1	3929	-	0,6,6	-	-	-		
85	OHX	6	2058	-	0,6,6	-	-	-		
85	OHX	1	3999	-	0,6,6	-	-	-		
85	OHX	5	3991	-	0,6,6	-	-	-		
85	OHX	1	3933	-	0,6,6	-	-	-		
85	OHX	2	2034	-	0,6,6	-	-	-		
85	OHX	2	1994	-	0,6,6	-	-	-		
85	OHX	5	4044	-	0,6,6	-	-	-		
85	OHX	1	3836	-	0,6,6	-	-	-		
85	OHX	2	2048	-	0,6,6	-	-	-		
85	OHX	6	2136	-	0,6,6	-	-	-		
85	OHX	1	3927	-	0,6,6	-	-	-		
85	OHX	2	2031	-	0,6,6	-	-	-		
85	OHX	1	3808	-	0,6,6	-	-	-		
85	OHX	1	3888	-	0,6,6	-	-	-		
85	OHX	6	2099	-	0,6,6	-	-	-		
85	OHX	5	3822	-	0,6,6	-	-	-		
85	OHX	2	2094	-	0,6,6	-	-	-		
85	OHX	6	2095	-	0,6,6	-	-	-		
85	OHX	5	3841	-	0,6,6	-	-	-		
85	OHX	5	3891	-	0,6,6	-	-	-		
85	OHX	2	2006	-	0,6,6	-	-	-		
85	OHX	1	3797	-	0,6,6	-	-	-		
85	OHX	1	3759	-	0,6,6	-	-	-		
85	OHX	2	2005	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	5	3850	-	0,6,6	-	-	-		
85	OHX	5	3885	-	0,6,6	-	-	-		
85	OHX	5	3970	-	0,6,6	-	-	-		
85	OHX	15	302	-	0,6,6	-	-	-		
85	OHX	5	3835	-	0,6,6	-	-	-		
85	OHX	5	3895	-	0,6,6	-	-	-		
85	OHX	1	3855	-	0,6,6	-	-	-		
85	OHX	1	3902	-	0,6,6	-	-	-		
85	OHX	5	3932	-	0,6,6	-	-	-		
85	OHX	5	3981	-	0,6,6	-	-	-		
85	OHX	C8	201	-	0,6,6	-	-	-		
85	OHX	1	3818	-	0,6,6	-	-	-		
85	OHX	2	2046	-	0,6,6	-	-	-		
85	OHX	2	1985	-	0,6,6	-	-	-		
85	OHX	1	3832	-	0,6,6	-	-	-		
85	OHX	1	3971	-	0,6,6	-	-	-		
85	OHX	1	3758	-	0,6,6	-	-	-		
85	OHX	5	3761	-	0,6,6	-	-	-		
85	OHX	m7	204	-	0,6,6	-	-	-		
85	OHX	6	2148	-	0,6,6	-	-	-		
85	OHX	5	4061	-	0,6,6	-	-	-		
85	OHX	5	3872	-	0,6,6	-	-	-		
85	OHX	7	213	-	0,6,6	-	-	-		
85	OHX	6	2062	-	0,6,6	-	-	-		
85	OHX	2	2084	-	0,6,6	-	-	-		
85	OHX	6	2022	-	0,6,6	-	-	-		
85	OHX	5	4015	-	0,6,6	-	-	-		
85	OHX	1	3750	-	0,6,6	-	-	-		
85	OHX	1	4031	-	0,6,6	-	-	-		
85	OHX	8	217	-	0,6,6	-	-	-		
85	OHX	6	2080	-	0,6,6	-	-	-		
85	OHX	6	2084	-	0,6,6	-	-	-		
85	OHX	2	2077	-	0,6,6	-	-	-		
85	OHX	1	3742	-	0,6,6	-	-	-		
85	OHX	1	3809	-	0,6,6	-	-	-		
85	OHX	6	2050	-	0,6,6	-	-	-		
85	OHX	6	2138	-	0,6,6	-	-	-		
85	OHX	6	2065	-	0,6,6	-	-	-		
85	OHX	2	2022	-	0,6,6	-	-	-		
85	OHX	2	2051	-	0,6,6	-	-	-		
85	OHX	s4	301	-	0,6,6	-	-	-		
85	OHX	5	3751	-	0,6,6	-	-	-		
85	OHX	5	3839	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	1	3769	-	0,6,6	-	-	-		
85	OHX	5	3972	-	0,6,6	-	-	-		
85	OHX	q2	502	-	0,6,6	-	-	-		
85	OHX	sR	401	-	0,6,6	-	-	-		
85	OHX	1	3923	-	0,6,6	-	-	-		
85	OHX	1	4002	-	0,6,6	-	-	-		
85	OHX	5	3833	-	0,6,6	-	-	-		
85	OHX	2	2020	-	0,6,6	-	-	-		
85	OHX	5	3893	-	0,6,6	-	-	-		
85	OHX	5	3746	-	0,6,6	-	-	-		
85	OHX	7	216	-	0,6,6	-	-	-		
85	OHX	5	3883	-	0,6,6	-	-	-		
85	OHX	5	4052	-	0,6,6	-	-	-		
85	OHX	6	2028	-	0,6,6	-	-	-		
85	OHX	1	3877	-	0,6,6	-	-	-		
85	OHX	1	3978	-	0,6,6	-	-	-		
85	OHX	1	3918	-	0,6,6	-	-	-		
85	OHX	5	4003	-	0,6,6	-	-	-		
85	OHX	5	3861	-	0,6,6	-	-	-		
85	OHX	6	2072	-	0,6,6	-	-	-		
85	OHX	1	3752	-	0,6,6	-	-	-		
85	OHX	1	3827	-	0,6,6	-	-	-		
85	OHX	3	212	-	0,6,6	-	-	-		
85	OHX	5	3809	-	0,6,6	-	-	-		
85	OHX	8	215	-	0,6,6	-	-	-		
85	OHX	1	4036	-	0,6,6	-	-	-		
85	OHX	o3	202	-	0,6,6	-	-	-		
85	OHX	5	3921	-	0,6,6	-	-	-		
85	OHX	1	3948	-	0,6,6	-	-	-		
85	OHX	d4	201	-	0,6,6	-	-	-		
85	OHX	8	219	-	0,6,6	-	-	-		
85	OHX	5	4060	-	0,6,6	-	-	-		
85	OHX	5	3843	-	0,6,6	-	-	-		
85	OHX	O3	202	-	0,6,6	-	-	-		
85	OHX	6	2036	-	0,6,6	-	-	-		
85	OHX	1	3866	-	0,6,6	-	-	-		
85	OHX	5	4029	-	0,6,6	-	-	-		
85	OHX	1	4008	-	0,6,6	-	-	-		
85	OHX	5	3886	-	0,6,6	-	-	-		
85	OHX	2	2021	-	0,6,6	-	-	-		
85	OHX	1	3908	-	0,6,6	-	-	-		
85	OHX	5	3904	-	0,6,6	-	-	-		
85	OHX	8	220	-	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	1	3892	-	0,6,6	-	-	-	-	-
85	OHX	5	4011	-	0,6,6	-	-	-	-	-
85	OHX	1	3938	-	0,6,6	-	-	-	-	-
85	OHX	5	3936	-	0,6,6	-	-	-	-	-
85	OHX	1	3779	-	0,6,6	-	-	-	-	-
85	OHX	5	4037	-	0,6,6	-	-	-	-	-
85	OHX	5	3801	-	0,6,6	-	-	-	-	-
85	OHX	1	4028	-	0,6,6	-	-	-	-	-
85	OHX	2	2070	-	0,6,6	-	-	-	-	-
85	OHX	2	2044	-	0,6,6	-	-	-	-	-
85	OHX	6	2087	-	0,6,6	-	-	-	-	-
85	OHX	5	4035	-	0,6,6	-	-	-	-	-
85	OHX	1	3756	-	0,6,6	-	-	-	-	-
85	OHX	4	216	-	0,6,6	-	-	-	-	-
85	OHX	1	3822	-	0,6,6	-	-	-	-	-
85	OHX	5	3958	-	0,6,6	-	-	-	-	-
85	OHX	1	3760	-	0,6,6	-	-	-	-	-
85	OHX	5	3999	-	0,6,6	-	-	-	-	-
85	OHX	5	3826	-	0,6,6	-	-	-	-	-
85	OHX	5	3776	-	0,6,6	-	-	-	-	-
85	OHX	5	4057	-	0,6,6	-	-	-	-	-
85	OHX	1	4017	-	0,6,6	-	-	-	-	-
85	OHX	2	2037	-	0,6,6	-	-	-	-	-
85	OHX	1	3767	-	0,6,6	-	-	-	-	-
85	OHX	1	3868	-	0,6,6	-	-	-	-	-
85	OHX	1	3959	-	0,6,6	-	-	-	-	-
85	OHX	5	3772	-	0,6,6	-	-	-	-	-
85	OHX	5	4043	-	0,6,6	-	-	-	-	-
85	OHX	2	2004	-	0,6,6	-	-	-	-	-
85	OHX	2	2012	-	0,6,6	-	-	-	-	-
85	OHX	5	4008	-	0,6,6	-	-	-	-	-
85	OHX	1	3859	-	0,6,6	-	-	-	-	-
85	OHX	1	3928	-	0,6,6	-	-	-	-	-
85	OHX	6	2053	-	0,6,6	-	-	-	-	-
85	OHX	1	3911	-	0,6,6	-	-	-	-	-
85	OHX	5	3844	-	0,6,6	-	-	-	-	-
85	OHX	5	3775	-	0,6,6	-	-	-	-	-
85	OHX	L4	401	-	0,6,6	-	-	-	-	-
85	OHX	5	4039	-	0,6,6	-	-	-	-	-
85	OHX	1	3845	-	0,6,6	-	-	-	-	-
85	OHX	1	3776	-	0,6,6	-	-	-	-	-
85	OHX	5	3778	-	0,6,6	-	-	-	-	-
85	OHX	5	3988	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	1	4022	-	0,6,6	-	-	-		
85	OHX	1	3968	-	0,6,6	-	-	-		
85	OHX	6	2019	-	0,6,6	-	-	-		
85	OHX	5	3881	-	0,6,6	-	-	-		
85	OHX	5	3830	-	0,6,6	-	-	-		
85	OHX	2	2049	-	0,6,6	-	-	-		
85	OHX	5	3817	-	0,6,6	-	-	-		
85	OHX	1	3785	-	0,6,6	-	-	-		
85	OHX	6	2140	-	0,6,6	-	-	-		
85	OHX	1	3986	-	0,6,6	-	-	-		
85	OHX	5	3848	-	0,6,6	-	-	-		
85	OHX	5	3832	-	0,6,6	-	-	-		
85	OHX	5	3758	-	0,6,6	-	-	-		
85	OHX	5	3851	-	0,6,6	-	-	-		
85	OHX	1	3988	-	0,6,6	-	-	-		
85	OHX	5	3790	-	0,6,6	-	-	-		
85	OHX	5	4042	-	0,6,6	-	-	-		
85	OHX	5	3940	-	0,6,6	-	-	-		
85	OHX	2	2098	-	0,6,6	-	-	-		
85	OHX	1	3805	-	0,6,6	-	-	-		
85	OHX	5	3820	-	0,6,6	-	-	-		
85	OHX	2	2015	-	0,6,6	-	-	-		
85	OHX	2	2058	-	0,6,6	-	-	-		
85	OHX	1	3946	-	0,6,6	-	-	-		
85	OHX	5	3879	-	0,6,6	-	-	-		
85	OHX	1	3789	-	0,6,6	-	-	-		
85	OHX	5	4050	-	0,6,6	-	-	-		
85	OHX	1	3858	-	0,6,6	-	-	-		
85	OHX	m0	302	-	0,6,6	-	-	-		
85	OHX	1	3874	-	0,6,6	-	-	-		
85	OHX	8	212	-	0,6,6	-	-	-		
85	OHX	5	3742	-	0,6,6	-	-	-		
85	OHX	1	3903	-	0,6,6	-	-	-		
85	OHX	1	3990	-	0,6,6	-	-	-		
85	OHX	1	3787	-	0,6,6	-	-	-		
85	OHX	1	3955	-	0,6,6	-	-	-		
85	OHX	5	3871	-	0,6,6	-	-	-		
85	OHX	1	4010	-	0,6,6	-	-	-		
85	OHX	5	4048	-	0,6,6	-	-	-		
85	OHX	5	3961	-	0,6,6	-	-	-		
85	OHX	6	2041	-	0,6,6	-	-	-		
85	OHX	1	3952	-	0,6,6	-	-	-		
85	OHX	1	3817	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	2	2116	-	0,6,6	-	-	-		
85	OHX	1	3914	-	0,6,6	-	-	-		
85	OHX	1	3953	-	0,6,6	-	-	-		
85	OHX	6	2014	-	0,6,6	-	-	-		
85	OHX	8	211	-	0,6,6	-	-	-		
85	OHX	5	3877	-	0,6,6	-	-	-		
85	OHX	2	2075	-	0,6,6	-	-	-		
85	OHX	1	3848	-	0,6,6	-	-	-		
85	OHX	6	2118	-	0,6,6	-	-	-		
85	OHX	1	3989	-	0,6,6	-	-	-		
85	OHX	1	3921	-	0,6,6	-	-	-		
85	OHX	1	3950	-	0,6,6	-	-	-		
85	OHX	1	3824	-	0,6,6	-	-	-		
85	OHX	1	3917	-	0,6,6	-	-	-		
85	OHX	2	2073	-	0,6,6	-	-	-		
85	OHX	6	2147	-	0,6,6	-	-	-		
85	OHX	1	3747	-	0,6,6	-	-	-		
85	OHX	5	3774	-	0,6,6	-	-	-		
85	OHX	2	2000	-	0,6,6	-	-	-		
85	OHX	5	3955	-	0,6,6	-	-	-		
85	OHX	5	3971	-	0,6,6	-	-	-		
85	OHX	1	3873	-	0,6,6	-	-	-		
85	OHX	5	3944	-	0,6,6	-	-	-		
85	OHX	5	3764	-	0,6,6	-	-	-		
85	OHX	5	3831	-	0,6,6	-	-	-		
85	OHX	2	2079	-	0,6,6	-	-	-		
85	OHX	1	3847	-	0,6,6	-	-	-		
85	OHX	6	2158	-	0,6,6	-	-	-		
85	OHX	5	3866	-	0,6,6	-	-	-		
85	OHX	6	2128	-	0,6,6	-	-	-		
85	OHX	1	4011	-	0,6,6	-	-	-		
85	OHX	6	2031	-	0,6,6	-	-	-		
85	OHX	5	4018	-	0,6,6	-	-	-		
85	OHX	2	2101	-	0,6,6	-	-	-		
85	OHX	6	2035	-	0,6,6	-	-	-		
85	OHX	8	225	-	0,6,6	-	-	-		
85	OHX	1	3788	-	0,6,6	-	-	-		
85	OHX	D9	103	-	0,6,6	-	-	-		
85	OHX	2	2024	-	0,6,6	-	-	-		
85	OHX	5	3779	-	0,6,6	-	-	-		
85	OHX	5	3993	-	0,6,6	-	-	-		
85	OHX	7	212	-	0,6,6	-	-	-		
85	OHX	1	3867	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	6	2078	-	0,6,6	-	-	-		
85	OHX	2	1988	-	0,6,6	-	-	-		
85	OHX	5	3874	-	0,6,6	-	-	-		
85	OHX	1	3761	-	0,6,6	-	-	-		
85	OHX	2	2074	-	0,6,6	-	-	-		
85	OHX	N8	203	-	0,6,6	-	-	-		
85	OHX	5	3782	-	0,6,6	-	-	-		
85	OHX	5	4066	-	0,6,6	-	-	-		
85	OHX	2	2019	-	0,6,6	-	-	-		
85	OHX	1	3798	-	0,6,6	-	-	-		
85	OHX	2	2010	-	0,6,6	-	-	-		
85	OHX	1	3974	-	0,6,6	-	-	-		
85	OHX	2	1998	-	0,6,6	-	-	-		
85	OHX	1	3957	-	0,6,6	-	-	-		
85	OHX	2	2066	-	0,6,6	-	-	-		
85	OHX	1	4020	-	0,6,6	-	-	-		
85	OHX	1	3942	-	0,6,6	-	-	-		
85	OHX	3	215	-	0,6,6	-	-	-		
85	OHX	6	2038	-	0,6,6	-	-	-		
85	OHX	5	3899	-	0,6,6	-	-	-		
85	OHX	5	4063	-	0,6,6	-	-	-		
85	OHX	1	3913	-	0,6,6	-	-	-		
85	OHX	1	3813	-	0,6,6	-	-	-		
85	OHX	1	3768	-	0,6,6	-	-	-		
85	OHX	3	217	-	0,6,6	-	-	-		
85	OHX	4	221	-	0,6,6	-	-	-		
85	OHX	1	3782	-	0,6,6	-	-	-		
85	OHX	6	2045	-	0,6,6	-	-	-		
85	OHX	1	3922	-	0,6,6	-	-	-		
85	OHX	5	3875	-	0,6,6	-	-	-		
85	OHX	1	3733	-	0,6,6	-	-	-		
85	OHX	1	3735	-	0,6,6	-	-	-		
85	OHX	6	2051	-	0,6,6	-	-	-		
85	OHX	5	3898	-	0,6,6	-	-	-		
85	OHX	5	4022	-	0,6,6	-	-	-		
85	OHX	5	4068	-	0,6,6	-	-	-		
85	OHX	6	2132	-	0,6,6	-	-	-		
85	OHX	1	3820	-	0,6,6	-	-	-		
85	OHX	2	2030	-	0,6,6	-	-	-		
85	OHX	6	2049	-	0,6,6	-	-	-		
85	OHX	8	221	-	0,6,6	-	-	-		
85	OHX	2	2026	-	0,6,6	-	-	-		
85	OHX	1	3889	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	5	3974	-	0,6,6	-	-	-		
85	OHX	2	1989	-	0,6,6	-	-	-		
85	OHX	2	2016	-	0,6,6	-	-	-		
85	OHX	5	3986	-	0,6,6	-	-	-		
85	OHX	6	2009	-	0,6,6	-	-	-		
85	OHX	2	2111	-	0,6,6	-	-	-		
85	OHX	1	3734	-	0,6,6	-	-	-		
85	OHX	6	2039	-	0,6,6	-	-	-		
85	OHX	M9	201	-	0,6,6	-	-	-		
85	OHX	1	3800	-	0,6,6	-	-	-		
85	OHX	1	3894	-	0,6,6	-	-	-		
85	OHX	c5	201	-	0,6,6	-	-	-		
85	OHX	1	3794	-	0,6,6	-	-	-		
85	OHX	2	2008	-	0,6,6	-	-	-		
85	OHX	5	3813	-	0,6,6	-	-	-		
85	OHX	6	2104	-	0,6,6	-	-	-		
85	OHX	N1	201	-	0,6,6	-	-	-		
85	OHX	2	2039	-	0,6,6	-	-	-		
85	OHX	5	3949	-	0,6,6	-	-	-		
85	OHX	5	3989	-	0,6,6	-	-	-		
85	OHX	5	3829	-	0,6,6	-	-	-		
85	OHX	5	4046	-	0,6,6	-	-	-		
85	OHX	5	3792	-	0,6,6	-	-	-		
85	OHX	4	223	-	0,6,6	-	-	-		
85	OHX	6	2024	-	0,6,6	-	-	-		
85	OHX	2	2118	-	0,6,6	-	-	-		
85	OHX	1	3885	-	0,6,6	-	-	-		
85	OHX	2	2071	-	0,6,6	-	-	-		
85	OHX	6	2075	-	0,6,6	-	-	-		
85	OHX	1	3925	-	0,6,6	-	-	-		
85	OHX	5	3783	-	0,6,6	-	-	-		
85	OHX	S6	301	-	0,6,6	-	-	-		
85	OHX	5	3980	-	0,6,6	-	-	-		
85	OHX	6	2021	-	0,6,6	-	-	-		
85	OHX	2	2103	-	0,6,6	-	-	-		
85	OHX	2	2105	-	0,6,6	-	-	-		
85	OHX	5	3794	-	0,6,6	-	-	-		
85	OHX	6	2037	-	0,6,6	-	-	-		
85	OHX	5	3786	-	0,6,6	-	-	-		
85	OHX	5	3873	-	0,6,6	-	-	-		
85	OHX	5	3750	-	0,6,6	-	-	-		
85	OHX	L3	402	-	0,6,6	-	-	-		
85	OHX	6	2012	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	1	3771	-	0,6,6	-	-	-		
85	OHX	5	3807	-	0,6,6	-	-	-		
85	OHX	5	3894	-	0,6,6	-	-	-		
85	OHX	1	3898	-	0,6,6	-	-	-		
85	OHX	6	2124	-	0,6,6	-	-	-		
85	OHX	1	3745	-	0,6,6	-	-	-		
85	OHX	5	3796	-	0,6,6	-	-	-		
85	OHX	1	3932	-	0,6,6	-	-	-		
85	OHX	6	2046	-	0,6,6	-	-	-		
85	OHX	1	3980	-	0,6,6	-	-	-		
85	OHX	8	214	-	0,6,6	-	-	-		
85	OHX	1	4026	-	0,6,6	-	-	-		
85	OHX	2	2088	-	0,6,6	-	-	-		
85	OHX	1	3821	-	0,6,6	-	-	-		
85	OHX	6	2073	-	0,6,6	-	-	-		
85	OHX	1	3982	-	0,6,6	-	-	-		
85	OHX	8	213	-	0,6,6	-	-	-		
85	OHX	5	4058	-	0,6,6	-	-	-		
85	OHX	6	2063	-	0,6,6	-	-	-		
85	OHX	1	3977	-	0,6,6	-	-	-		
85	OHX	1	3944	-	0,6,6	-	-	-		
85	OHX	2	2113	-	0,6,6	-	-	-		
85	OHX	1	4027	-	0,6,6	-	-	-		
85	OHX	5	3929	-	0,6,6	-	-	-		
85	OHX	5	3853	-	0,6,6	-	-	-		
85	OHX	1	3886	-	0,6,6	-	-	-		
85	OHX	1	3764	-	0,6,6	-	-	-		
85	OHX	5	3757	-	0,6,6	-	-	-		
85	OHX	1	3746	-	0,6,6	-	-	-		
85	OHX	1	3791	-	0,6,6	-	-	-		
85	OHX	1	3831	-	0,6,6	-	-	-		
85	OHX	6	2102	-	0,6,6	-	-	-		
85	OHX	5	3744	-	0,6,6	-	-	-		
85	OHX	5	3997	-	0,6,6	-	-	-		
85	OHX	2	2080	-	0,6,6	-	-	-		
85	OHX	2	2007	-	0,6,6	-	-	-		
85	OHX	5	3827	-	0,6,6	-	-	-		
85	OHX	5	4038	-	0,6,6	-	-	-		
85	OHX	5	3996	-	0,6,6	-	-	-		
85	OHX	5	3965	-	0,6,6	-	-	-		
85	OHX	2	1991	-	0,6,6	-	-	-		
85	OHX	6	2015	-	0,6,6	-	-	-		
85	OHX	1	3833	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	n9	102	-	0,6,6	-	-	-		
85	OHX	1	3899	-	0,6,6	-	-	-		
85	OHX	6	2130	-	0,6,6	-	-	-		
85	OHX	1	3853	-	0,6,6	-	-	-		
85	OHX	1	3972	-	0,6,6	-	-	-		
85	OHX	1	3983	-	0,6,6	-	-	-		
85	OHX	5	3834	-	0,6,6	-	-	-		
85	OHX	1	3905	-	0,6,6	-	-	-		
85	OHX	5	3909	-	0,6,6	-	-	-		
85	OHX	5	3884	-	0,6,6	-	-	-		
85	OHX	1	3900	-	0,6,6	-	-	-		
85	OHX	6	2123	-	0,6,6	-	-	-		
85	OHX	2	2001	-	0,6,6	-	-	-		
85	OHX	6	2040	-	0,6,6	-	-	-		
85	OHX	5	3912	-	0,6,6	-	-	-		
85	OHX	6	2142	-	0,6,6	-	-	-		
85	OHX	1	3854	-	0,6,6	-	-	-		
85	OHX	1	3926	-	0,6,6	-	-	-		
85	OHX	6	2105	-	0,6,6	-	-	-		
85	OHX	2	2029	-	0,6,6	-	-	-		
85	OHX	1	4003	-	0,6,6	-	-	-		
85	OHX	6	2108	-	0,6,6	-	-	-		
85	OHX	5	3987	-	0,6,6	-	-	-		
85	OHX	1	3741	-	0,6,6	-	-	-		
85	OHX	5	3959	-	0,6,6	-	-	-		
85	OHX	2	1993	-	0,6,6	-	-	-		
85	OHX	1	3775	-	0,6,6	-	-	-		
85	OHX	1	3901	-	0,6,6	-	-	-		
85	OHX	2	1999	-	0,6,6	-	-	-		
85	OHX	6	2079	-	0,6,6	-	-	-		
85	OHX	1	3792	-	0,6,6	-	-	-		
85	OHX	6	2096	-	0,6,6	-	-	-		
85	OHX	6	2122	-	0,6,6	-	-	-		
85	OHX	1	4021	-	0,6,6	-	-	-		
85	OHX	5	3878	-	0,6,6	-	-	-		
85	OHX	5	4055	-	0,6,6	-	-	-		
85	OHX	6	2017	-	0,6,6	-	-	-		
85	OHX	1	3728	-	0,6,6	-	-	-		
85	OHX	1	3816	-	0,6,6	-	-	-		
85	OHX	6	2013	-	0,6,6	-	-	-		
85	OHX	5	3754	-	0,6,6	-	-	-		
85	OHX	6	2026	-	0,6,6	-	-	-		
85	OHX	1	3949	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	5	3860	-	0,6,6	-	-	-		
85	OHX	1	3839	-	0,6,6	-	-	-		
85	OHX	5	3890	-	0,6,6	-	-	-		
85	OHX	1	3995	-	0,6,6	-	-	-		
85	OHX	1	3840	-	0,6,6	-	-	-		
85	OHX	5	4000	-	0,6,6	-	-	-		
85	OHX	3	210	-	0,6,6	-	-	-		
85	OHX	2	2011	-	0,6,6	-	-	-		
85	OHX	3	211	-	0,6,6	-	-	-		
85	OHX	5	3975	-	0,6,6	-	-	-		
85	OHX	2	2038	-	0,6,6	-	-	-		
85	OHX	1	3784	-	0,6,6	-	-	-		
85	OHX	6	2081	-	0,6,6	-	-	-		
85	OHX	2	2082	-	0,6,6	-	-	-		
85	OHX	5	3759	-	0,6,6	-	-	-		
85	OHX	5	3865	-	0,6,6	-	-	-		
85	OHX	1	3807	-	0,6,6	-	-	-		
85	OHX	1	3811	-	0,6,6	-	-	-		
85	OHX	1	3835	-	0,6,6	-	-	-		
85	OHX	1	3943	-	0,6,6	-	-	-		
85	OHX	4	218	-	0,6,6	-	-	-		
85	OHX	2	2081	-	0,6,6	-	-	-		
85	OHX	1	3778	-	0,6,6	-	-	-		
85	OHX	5	3979	-	0,6,6	-	-	-		
85	OHX	1	3984	-	0,6,6	-	-	-		
85	OHX	1	4038	-	0,6,6	-	-	-		
85	OHX	1	3801	-	0,6,6	-	-	-		
85	OHX	6	2088	-	0,6,6	-	-	-		
85	OHX	1	3732	-	0,6,6	-	-	-		
85	OHX	6	2094	-	0,6,6	-	-	-		
85	OHX	5	3941	-	0,6,6	-	-	-		
85	OHX	5	3905	-	0,6,6	-	-	-		
85	OHX	6	2056	-	0,6,6	-	-	-		
85	OHX	5	3859	-	0,6,6	-	-	-		
85	OHX	5	4027	-	0,6,6	-	-	-		
85	OHX	1	3865	-	0,6,6	-	-	-		
85	OHX	1	4001	-	0,6,6	-	-	-		
85	OHX	2	2018	-	0,6,6	-	-	-		
85	OHX	5	3760	-	0,6,6	-	-	-		
85	OHX	2	2092	-	0,6,6	-	-	-		
85	OHX	1	3834	-	0,6,6	-	-	-		
85	OHX	13	406	-	0,6,6	-	-	-		
85	OHX	5	3984	-	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	4	222	-	0,6,6	-	-	-		
85	OHX	7	215	-	0,6,6	-	-	-		
85	OHX	5	4030	-	0,6,6	-	-	-		
85	OHX	5	4024	-	0,6,6	-	-	-		
85	OHX	5	3948	-	0,6,6	-	-	-		
85	OHX	1	3904	-	0,6,6	-	-	-		
85	OHX	6	2042	-	0,6,6	-	-	-		
85	OHX	5	3919	-	0,6,6	-	-	-		
85	OHX	1	4016	-	0,6,6	-	-	-		
85	OHX	7	217	-	0,6,6	-	-	-		
85	OHX	6	2144	-	0,6,6	-	-	-		
85	OHX	6	2010	-	0,6,6	-	-	-		
85	OHX	5	4070	-	0,6,6	-	-	-		
85	OHX	5	3810	-	0,6,6	-	-	-		
85	OHX	5	3876	-	0,6,6	-	-	-		
85	OHX	6	2070	-	0,6,6	-	-	-		
85	OHX	6	2113	-	0,6,6	-	-	-		
85	OHX	2	1987	-	0,6,6	-	-	-		
85	OHX	6	2052	-	0,6,6	-	-	-		
85	OHX	5	3855	-	0,6,6	-	-	-		
85	OHX	5	3916	-	0,6,6	-	-	-		
85	OHX	1	3856	-	0,6,6	-	-	-		
85	OHX	5	3745	-	0,6,6	-	-	-		
85	OHX	5	3803	-	0,6,6	-	-	-		
85	OHX	1	3802	-	0,6,6	-	-	-		
85	OHX	1	3979	-	0,6,6	-	-	-		
85	OHX	1	3786	-	0,6,6	-	-	-		
85	OHX	6	2134	-	0,6,6	-	-	-		
85	OHX	5	3748	-	0,6,6	-	-	-		
85	OHX	6	2150	-	0,6,6	-	-	-		
85	OHX	2	2002	-	0,6,6	-	-	-		
85	OHX	5	3977	-	0,6,6	-	-	-		
85	OHX	6	2125	-	0,6,6	-	-	-		
85	OHX	5	3766	-	0,6,6	-	-	-		
85	OHX	6	2057	-	0,6,6	-	-	-		
85	OHX	1	3992	-	0,6,6	-	-	-		
85	OHX	5	3816	-	0,6,6	-	-	-		
85	OHX	5	3856	-	0,6,6	-	-	-		
85	OHX	5	3902	-	0,6,6	-	-	-		
85	OHX	1	3830	-	0,6,6	-	-	-		
85	OHX	1	3966	-	0,6,6	-	-	-		
85	OHX	5	4051	-	0,6,6	-	-	-		
85	OHX	n3	202	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	6	2155	-	0,6,6	-	-	-		
85	OHX	5	3780	-	0,6,6	-	-	-		
85	OHX	6	2157	-	0,6,6	-	-	-		
85	OHX	7	220	-	0,6,6	-	-	-		
85	OHX	5	3968	-	0,6,6	-	-	-		
85	OHX	5	3901	-	0,6,6	-	-	-		
85	OHX	1	3748	-	0,6,6	-	-	-		
85	OHX	6	2114	-	0,6,6	-	-	-		
85	OHX	5	4006	-	0,6,6	-	-	-		
85	OHX	5	3952	-	0,6,6	-	-	-		
85	OHX	5	3927	-	0,6,6	-	-	-		
85	OHX	6	2091	-	0,6,6	-	-	-		
85	OHX	1	4029	-	0,6,6	-	-	-		
85	OHX	2	2100	-	0,6,6	-	-	-		
85	OHX	4	219	-	0,6,6	-	-	-		
85	OHX	5	3943	-	0,6,6	-	-	-		
85	OHX	5	3947	-	0,6,6	-	-	-		
85	OHX	5	3918	-	0,6,6	-	-	-		
85	OHX	1	3825	-	0,6,6	-	-	-		
85	OHX	1	3852	-	0,6,6	-	-	-		
85	OHX	5	3951	-	0,6,6	-	-	-		
85	OHX	2	2068	-	0,6,6	-	-	-		
85	OHX	5	4023	-	0,6,6	-	-	-		
85	OHX	8	223	-	0,6,6	-	-	-		
85	OHX	2	2072	-	0,6,6	-	-	-		
85	OHX	5	3900	-	0,6,6	-	-	-		
85	OHX	1	3963	-	0,6,6	-	-	-		
85	OHX	6	2115	-	0,6,6	-	-	-		
85	OHX	5	3934	-	0,6,6	-	-	-		
85	OHX	1	3814	-	0,6,6	-	-	-		
85	OHX	5	3917	-	0,6,6	-	-	-		
85	OHX	6	2145	-	0,6,6	-	-	-		
85	OHX	2	1984	-	0,6,6	-	-	-		
85	OHX	2	2040	-	0,6,6	-	-	-		
85	OHX	1	3793	-	0,6,6	-	-	-		
85	OHX	1	4035	-	0,6,6	-	-	-		
85	OHX	5	3762	-	0,6,6	-	-	-		
85	OHX	8	216	-	0,6,6	-	-	-		
85	OHX	2	2099	-	0,6,6	-	-	-		
85	OHX	6	2133	-	0,6,6	-	-	-		
85	OHX	1	3951	-	0,6,6	-	-	-		
85	OHX	5	3892	-	0,6,6	-	-	-		
85	OHX	m5	304	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	5	3837	-	0,6,6	-	-	-		
85	OHX	6	2061	-	0,6,6	-	-	-		
85	OHX	1	3893	-	0,6,6	-	-	-		
85	OHX	1	3919	-	0,6,6	-	-	-		
85	OHX	4	231	-	0,6,6	-	-	-		
85	OHX	2	2055	-	0,6,6	-	-	-		
85	OHX	6	2011	-	0,6,6	-	-	-		
85	OHX	2	2061	-	0,6,6	-	-	-		
85	OHX	1	3910	-	0,6,6	-	-	-		
85	OHX	5	3806	-	0,6,6	-	-	-		
85	OHX	5	4045	-	0,6,6	-	-	-		
85	OHX	2	2009	-	0,6,6	-	-	-		
85	OHX	5	4049	-	0,6,6	-	-	-		
85	OHX	6	2126	-	0,6,6	-	-	-		
85	OHX	15	301	-	0,6,6	-	-	-		
85	OHX	6	2110	-	0,6,6	-	-	-		
85	OHX	1	4030	-	0,6,6	-	-	-		
85	OHX	2	2097	-	0,6,6	-	-	-		
85	OHX	5	3985	-	0,6,6	-	-	-		
85	OHX	1	3837	-	0,6,6	-	-	-		
85	OHX	2	2104	-	0,6,6	-	-	-		
85	OHX	5	3787	-	0,6,6	-	-	-		
85	OHX	5	3768	-	0,6,6	-	-	-		
85	OHX	1	4032	-	0,6,6	-	-	-		
85	OHX	6	2117	-	0,6,6	-	-	-		
85	OHX	5	3870	-	0,6,6	-	-	-		
85	OHX	6	2034	-	0,6,6	-	-	-		
85	OHX	1	3812	-	0,6,6	-	-	-		
85	OHX	4	215	-	0,6,6	-	-	-		
85	OHX	4	229	-	0,6,6	-	-	-		
85	OHX	5	3953	-	0,6,6	-	-	-		
85	OHX	1	3878	-	0,6,6	-	-	-		
85	OHX	5	3924	-	0,6,6	-	-	-		
85	OHX	6	2156	-	0,6,6	-	-	-		
85	OHX	2	2062	-	0,6,6	-	-	-		
85	OHX	1	3881	-	0,6,6	-	-	-		
85	OHX	3	219	-	0,6,6	-	-	-		
85	OHX	5	3795	-	0,6,6	-	-	-		
85	OHX	5	4054	-	0,6,6	-	-	-		
85	OHX	6	2033	-	0,6,6	-	-	-		
85	OHX	2	1992	-	0,6,6	-	-	-		
85	OHX	6	2074	-	0,6,6	-	-	-		
85	OHX	7	211	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	1	3842	-	0,6,6	-	-	-		
85	OHX	2	2043	-	0,6,6	-	-	-		
85	OHX	2	2033	-	0,6,6	-	-	-		
85	OHX	5	3802	-	0,6,6	-	-	-		
85	OHX	6	2154	-	0,6,6	-	-	-		
85	OHX	6	2082	-	0,6,6	-	-	-		
85	OHX	8	218	-	0,6,6	-	-	-		
85	OHX	1	3774	-	0,6,6	-	-	-		
85	OHX	2	2064	-	0,6,6	-	-	-		
85	OHX	1	3936	-	0,6,6	-	-	-		
85	OHX	5	3973	-	0,6,6	-	-	-		
85	OHX	1	3909	-	0,6,6	-	-	-		
85	OHX	2	2108	-	0,6,6	-	-	-		
85	OHX	5	3950	-	0,6,6	-	-	-		
85	OHX	5	3946	-	0,6,6	-	-	-		
85	OHX	5	3747	-	0,6,6	-	-	-		
85	OHX	2	2023	-	0,6,6	-	-	-		
85	OHX	1	3766	-	0,6,6	-	-	-		
85	OHX	6	2048	-	0,6,6	-	-	-		
85	OHX	5	3939	-	0,6,6	-	-	-		
85	OHX	5	3994	-	0,6,6	-	-	-		
85	OHX	5	3828	-	0,6,6	-	-	-		
85	OHX	5	3770	-	0,6,6	-	-	-		
85	OHX	1	3826	-	0,6,6	-	-	-		
85	OHX	1	3947	-	0,6,6	-	-	-		
85	OHX	1	4019	-	0,6,6	-	-	-		
85	OHX	5	3926	-	0,6,6	-	-	-		
85	OHX	5	4064	-	0,6,6	-	-	-		
85	OHX	8	222	-	0,6,6	-	-	-		
85	OHX	o9	101	-	0,6,6	-	-	-		
85	OHX	5	4062	-	0,6,6	-	-	-		
85	OHX	2	2093	-	0,6,6	-	-	-		
85	OHX	2	2095	-	0,6,6	-	-	-		
85	OHX	1	3920	-	0,6,6	-	-	-		
85	OHX	1	3828	-	0,6,6	-	-	-		
85	OHX	2	2013	-	0,6,6	-	-	-		
85	OHX	6	2020	-	0,6,6	-	-	-		
85	OHX	6	2151	-	0,6,6	-	-	-		
85	OHX	5	3935	-	0,6,6	-	-	-		
85	OHX	5	3818	-	0,6,6	-	-	-		
85	OHX	1	4018	-	0,6,6	-	-	-		
85	OHX	5	3976	-	0,6,6	-	-	-		
85	OHX	1	3790	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	1	3960	-	0,6,6	-	-	-		
85	OHX	1	3849	-	0,6,6	-	-	-		
85	OHX	2	2102	-	0,6,6	-	-	-		
85	OHX	6	2116	-	0,6,6	-	-	-		
85	OHX	5	4019	-	0,6,6	-	-	-		
85	OHX	5	4021	-	0,6,6	-	-	-		
85	OHX	6	2018	-	0,6,6	-	-	-		
85	OHX	5	3938	-	0,6,6	-	-	-		
85	OHX	1	4009	-	0,6,6	-	-	-		
85	OHX	1	3879	-	0,6,6	-	-	-		
85	OHX	2	2017	-	0,6,6	-	-	-		
85	OHX	5	3920	-	0,6,6	-	-	-		
85	OHX	1	3841	-	0,6,6	-	-	-		
85	OHX	2	2014	-	0,6,6	-	-	-		
85	OHX	1	3803	-	0,6,6	-	-	-		
85	OHX	1	3757	-	0,6,6	-	-	-		
85	OHX	1	3985	-	0,6,6	-	-	-		
85	OHX	1	3970	-	0,6,6	-	-	-		
85	OHX	M7	205	-	0,6,6	-	-	-		
85	OHX	6	2120	-	0,6,6	-	-	-		
85	OHX	5	3907	-	0,6,6	-	-	-		
85	OHX	5	4002	-	0,6,6	-	-	-		
85	OHX	1	3975	-	0,6,6	-	-	-		
85	OHX	1	3864	-	0,6,6	-	-	-		
85	OHX	2	2025	-	0,6,6	-	-	-		
85	OHX	1	3906	-	0,6,6	-	-	-		
85	OHX	5	3847	-	0,6,6	-	-	-		
85	OHX	C3	201	-	0,6,6	-	-	-		
85	OHX	6	2109	-	0,6,6	-	-	-		
85	OHX	6	2137	-	0,6,6	-	-	-		
85	OHX	5	3815	-	0,6,6	-	-	-		
85	OHX	n3	203	-	0,6,6	-	-	-		
85	OHX	5	3880	-	0,6,6	-	-	-		
85	OHX	5	4053	-	0,6,6	-	-	-		
85	OHX	c3	201	-	0,6,6	-	-	-		
85	OHX	6	2083	-	0,6,6	-	-	-		
85	OHX	1	3896	-	0,6,6	-	-	-		
85	OHX	1	3806	-	0,6,6	-	-	-		
85	OHX	6	2146	-	0,6,6	-	-	-		
85	OHX	5	4036	-	0,6,6	-	-	-		
85	OHX	1	3895	-	0,6,6	-	-	-		
85	OHX	1	4034	-	0,6,6	-	-	-		
85	OHX	2	2087	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	6	2032	-	0,6,6	-	-	-		
85	OHX	Q2	503	-	0,6,6	-	-	-		
85	OHX	2	1990	-	0,6,6	-	-	-		
85	OHX	1	3915	-	0,6,6	-	-	-		
85	OHX	1	3973	-	0,6,6	-	-	-		
85	OHX	6	2093	-	0,6,6	-	-	-		
85	OHX	C5	201	-	0,6,6	-	-	-		
85	OHX	1	3872	-	0,6,6	-	-	-		
85	OHX	5	3781	-	0,6,6	-	-	-		
85	OHX	4	225	-	0,6,6	-	-	-		
85	OHX	2	2041	-	0,6,6	-	-	-		
85	OHX	2	2050	-	0,6,6	-	-	-		
85	OHX	5	3842	-	0,6,6	-	-	-		
85	OHX	5	4016	-	0,6,6	-	-	-		
85	OHX	5	3882	-	0,6,6	-	-	-		
85	OHX	1	3937	-	0,6,6	-	-	-		
85	OHX	5	4034	-	0,6,6	-	-	-		
85	OHX	5	3913	-	0,6,6	-	-	-		
85	OHX	O7	104	-	0,6,6	-	-	-		
85	OHX	1	3727	-	0,6,6	-	-	-		
85	OHX	M6	202	-	0,6,6	-	-	-		
85	OHX	2	2035	-	0,6,6	-	-	-		
85	OHX	1	3880	-	0,6,6	-	-	-		
85	OHX	1	3941	-	0,6,6	-	-	-		
85	OHX	5	3908	-	0,6,6	-	-	-		
85	OHX	5	4025	-	0,6,6	-	-	-		
85	OHX	1	3876	-	0,6,6	-	-	-		
85	OHX	2	2056	-	0,6,6	-	-	-		
85	OHX	1	3869	-	0,6,6	-	-	-		
85	OHX	1	3804	-	0,6,6	-	-	-		
85	OHX	4	226	-	0,6,6	-	-	-		
85	OHX	1	3916	-	0,6,6	-	-	-		
85	OHX	1	3998	-	0,6,6	-	-	-		
85	OHX	3	214	-	0,6,6	-	-	-		
85	OHX	5	3791	-	0,6,6	-	-	-		
85	OHX	5	3911	-	0,6,6	-	-	-		
85	OHX	5	3960	-	0,6,6	-	-	-		
85	OHX	1	3823	-	0,6,6	-	-	-		
85	OHX	2	2117	-	0,6,6	-	-	-		
85	OHX	6	2025	-	0,6,6	-	-	-		
85	OHX	1	3736	-	0,6,6	-	-	-		
85	OHX	2	2065	-	0,6,6	-	-	-		
85	OHX	1	3954	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	5	3755	-	0,6,6	-	-	-		
85	OHX	5	3771	-	0,6,6	-	-	-		
85	OHX	6	2139	-	0,6,6	-	-	-		
85	OHX	6	2023	-	0,6,6	-	-	-		
85	OHX	5	3862	-	0,6,6	-	-	-		
85	OHX	6	2112	-	0,6,6	-	-	-		
85	OHX	6	2055	-	0,6,6	-	-	-		
85	OHX	5	3967	-	0,6,6	-	-	-		
85	OHX	1	3754	-	0,6,6	-	-	-		
85	OHX	1	3965	-	0,6,6	-	-	-		
85	OHX	N9	101	-	0,6,6	-	-	-		
85	OHX	5	3765	-	0,6,6	-	-	-		
85	OHX	5	3749	-	0,6,6	-	-	-		
85	OHX	1	4006	-	0,6,6	-	-	-		
85	OHX	5	3769	-	0,6,6	-	-	-		
85	OHX	6	2097	-	0,6,6	-	-	-		
85	OHX	1	3912	-	0,6,6	-	-	-		
85	OHX	5	3773	-	0,6,6	-	-	-		
85	OHX	5	3982	-	0,6,6	-	-	-		
85	OHX	1	3863	-	0,6,6	-	-	-		
85	OHX	1	3755	-	0,6,6	-	-	-		
85	OHX	5	4009	-	0,6,6	-	-	-		
85	OHX	1	3964	-	0,6,6	-	-	-		
85	OHX	1	3935	-	0,6,6	-	-	-		
85	OHX	5	3937	-	0,6,6	-	-	-		
85	OHX	6	2090	-	0,6,6	-	-	-		
85	OHX	5	3797	-	0,6,6	-	-	-		
85	OHX	5	3963	-	0,6,6	-	-	-		
85	OHX	5	3852	-	0,6,6	-	-	-		
85	OHX	5	3903	-	0,6,6	-	-	-		
85	OHX	1	3773	-	0,6,6	-	-	-		
85	OHX	5	3814	-	0,6,6	-	-	-		
87	ANM	1	3401	-	20,20,20	2.93	9 (45%)	22,27,27	2.80	10 (45%)
85	OHX	6	2029	-	0,6,6	-	-	-		
85	OHX	1	3924	-	0,6,6	-	-	-		
85	OHX	5	3888	-	0,6,6	-	-	-		
85	OHX	2	1983	-	0,6,6	-	-	-		
85	OHX	1	3796	-	0,6,6	-	-	-		
85	OHX	1	3956	-	0,6,6	-	-	-		
85	OHX	6	2016	-	0,6,6	-	-	-		
85	OHX	1	3762	-	0,6,6	-	-	-		
85	OHX	6	2047	-	0,6,6	-	-	-		
85	OHX	5	3887	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	6	2101	-	0,6,6	-	-	-		
85	OHX	1	3751	-	0,6,6	-	-	-		
85	OHX	2	2085	-	0,6,6	-	-	-		
85	OHX	2	2047	-	0,6,6	-	-	-		
85	OHX	1	3860	-	0,6,6	-	-	-		
85	OHX	1	3969	-	0,6,6	-	-	-		
85	OHX	2	2078	-	0,6,6	-	-	-		
85	OHX	5	4032	-	0,6,6	-	-	-		
85	OHX	1	3744	-	0,6,6	-	-	-		
85	OHX	2	2053	-	0,6,6	-	-	-		
85	OHX	5	4026	-	0,6,6	-	-	-		
85	OHX	6	2127	-	0,6,6	-	-	-		
85	OHX	6	2119	-	0,6,6	-	-	-		
85	OHX	2	1996	-	0,6,6	-	-	-		
85	OHX	3	213	-	0,6,6	-	-	-		
85	OHX	3	218	-	0,6,6	-	-	-		
85	OHX	5	3767	-	0,6,6	-	-	-		
85	OHX	5	3868	-	0,6,6	-	-	-		
85	OHX	5	3978	-	0,6,6	-	-	-		
85	OHX	2	2067	-	0,6,6	-	-	-		
85	OHX	1	3997	-	0,6,6	-	-	-		
85	OHX	1	4014	-	0,6,6	-	-	-		
85	OHX	5	3954	-	0,6,6	-	-	-		
85	OHX	5	4033	-	0,6,6	-	-	-		
85	OHX	1	3883	-	0,6,6	-	-	-		
85	OHX	2	2110	-	0,6,6	-	-	-		
85	OHX	2	2086	-	0,6,6	-	-	-		
85	OHX	5	3756	-	0,6,6	-	-	-		
85	OHX	6	2066	-	0,6,6	-	-	-		
85	OHX	1	4025	-	0,6,6	-	-	-		
85	OHX	5	3869	-	0,6,6	-	-	-		
85	OHX	13	408	-	0,6,6	-	-	-		
85	OHX	2	2032	-	0,6,6	-	-	-		
85	OHX	2	2109	-	0,6,6	-	-	-		
85	OHX	O7	105	-	0,6,6	-	-	-		
85	OHX	5	3825	-	0,6,6	-	-	-		
85	OHX	5	3896	-	0,6,6	-	-	-		
85	OHX	2	2083	-	0,6,6	-	-	-		
85	OHX	1	3780	-	0,6,6	-	-	-		
85	OHX	1	4033	-	0,6,6	-	-	-		
85	OHX	5	3840	-	0,6,6	-	-	-		
85	OHX	m5	305	-	0,6,6	-	-	-		
85	OHX	5	3752	-	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	1	3743	-	0,6,6	-	-	-	-	-
85	OHX	4	224	-	0,6,6	-	-	-	-	-
85	OHX	2	2003	-	0,6,6	-	-	-	-	-
85	OHX	1	3875	-	0,6,6	-	-	-	-	-
85	OHX	1	3967	-	0,6,6	-	-	-	-	-
85	OHX	2	2063	-	0,6,6	-	-	-	-	-
85	OHX	1	3940	-	0,6,6	-	-	-	-	-
85	OHX	6	2071	-	0,6,6	-	-	-	-	-
85	OHX	5	3863	-	0,6,6	-	-	-	-	-
85	OHX	2	2089	-	0,6,6	-	-	-	-	-
85	OHX	2	2054	-	0,6,6	-	-	-	-	-
85	OHX	1	3738	-	0,6,6	-	-	-	-	-
85	OHX	1	3843	-	0,6,6	-	-	-	-	-
85	OHX	6	2152	-	0,6,6	-	-	-	-	-
85	OHX	5	3811	-	0,6,6	-	-	-	-	-
85	OHX	m0	301	-	0,6,6	-	-	-	-	-
85	OHX	1	4037	-	0,6,6	-	-	-	-	-
85	OHX	s8	302	-	0,6,6	-	-	-	-	-
85	OHX	5	3942	-	0,6,6	-	-	-	-	-
85	OHX	5	4069	-	0,6,6	-	-	-	-	-
85	OHX	5	4067	-	0,6,6	-	-	-	-	-
85	OHX	m1	202	-	0,6,6	-	-	-	-	-
85	OHX	1	3749	-	0,6,6	-	-	-	-	-
85	OHX	6	2143	-	0,6,6	-	-	-	-	-
85	OHX	7	214	-	0,6,6	-	-	-	-	-
85	OHX	5	3753	-	0,6,6	-	-	-	-	-
85	OHX	6	2103	-	0,6,6	-	-	-	-	-
85	OHX	5	4020	-	0,6,6	-	-	-	-	-
85	OHX	5	3956	-	0,6,6	-	-	-	-	-
85	OHX	5	4031	-	0,6,6	-	-	-	-	-
85	OHX	1	3961	-	0,6,6	-	-	-	-	-
85	OHX	1	3897	-	0,6,6	-	-	-	-	-
85	OHX	1	3810	-	0,6,6	-	-	-	-	-
85	OHX	M5	302	-	0,6,6	-	-	-	-	-
85	OHX	5	3784	-	0,6,6	-	-	-	-	-
85	OHX	5	4065	-	0,6,6	-	-	-	-	-
85	OHX	1	3976	-	0,6,6	-	-	-	-	-
85	OHX	2	2107	-	0,6,6	-	-	-	-	-
85	OHX	1	3857	-	0,6,6	-	-	-	-	-
85	OHX	5	3923	-	0,6,6	-	-	-	-	-
85	OHX	1	3882	-	0,6,6	-	-	-	-	-
85	OHX	1	3772	-	0,6,6	-	-	-	-	-
85	OHX	2	2069	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	1	3770	-	0,6,6	-	-	-	-	-
85	OHX	1	3887	-	0,6,6	-	-	-	-	-
85	OHX	5	3743	-	0,6,6	-	-	-	-	-
85	OHX	5	3793	-	0,6,6	-	-	-	-	-
85	OHX	1	3777	-	0,6,6	-	-	-	-	-
85	OHX	1	3753	-	0,6,6	-	-	-	-	-
85	OHX	1	3783	-	0,6,6	-	-	-	-	-
85	OHX	5	3925	-	0,6,6	-	-	-	-	-
85	OHX	5	3812	-	0,6,6	-	-	-	-	-
85	OHX	6	2131	-	0,6,6	-	-	-	-	-
85	OHX	1	4004	-	0,6,6	-	-	-	-	-
85	OHX	5	3889	-	0,6,6	-	-	-	-	-
85	OHX	1	3799	-	0,6,6	-	-	-	-	-
85	OHX	1	3931	-	0,6,6	-	-	-	-	-
85	OHX	6	2129	-	0,6,6	-	-	-	-	-
85	OHX	5	3823	-	0,6,6	-	-	-	-	-
85	OHX	2	2045	-	0,6,6	-	-	-	-	-
85	OHX	1	3844	-	0,6,6	-	-	-	-	-
85	OHX	1	4013	-	0,6,6	-	-	-	-	-
85	OHX	6	2106	-	0,6,6	-	-	-	-	-
85	OHX	7	221	-	0,6,6	-	-	-	-	-
85	OHX	14	401	-	0,6,6	-	-	-	-	-
85	OHX	4	230	-	0,6,6	-	-	-	-	-
85	OHX	1	3890	-	0,6,6	-	-	-	-	-
85	OHX	2	2027	-	0,6,6	-	-	-	-	-
85	OHX	1	3726	-	0,6,6	-	-	-	-	-
85	OHX	1	3958	-	0,6,6	-	-	-	-	-
85	OHX	c8	201	-	0,6,6	-	-	-	-	-
85	OHX	1	3737	-	0,6,6	-	-	-	-	-
85	OHX	5	4059	-	0,6,6	-	-	-	-	-
85	OHX	2	2106	-	0,6,6	-	-	-	-	-
85	OHX	1	3819	-	0,6,6	-	-	-	-	-
85	OHX	1	3729	-	0,6,6	-	-	-	-	-
85	OHX	1	4007	-	0,6,6	-	-	-	-	-
85	OHX	SR	401	-	0,6,6	-	-	-	-	-
85	OHX	4	217	-	0,6,6	-	-	-	-	-
85	OHX	5	3906	-	0,6,6	-	-	-	-	-
85	OHX	2	2112	-	0,6,6	-	-	-	-	-
85	OHX	s9	201	-	0,6,6	-	-	-	-	-
85	OHX	5	3846	-	0,6,6	-	-	-	-	-
85	OHX	5	3864	-	0,6,6	-	-	-	-	-
85	OHX	5	3990	-	0,6,6	-	-	-	-	-
85	OHX	5	3777	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	1	3815	-	0,6,6	-	-	-		
85	OHX	2	2096	-	0,6,6	-	-	-		
85	OHX	6	2149	-	0,6,6	-	-	-		
85	OHX	6	2111	-	0,6,6	-	-	-		
85	OHX	1	3739	-	0,6,6	-	-	-		
85	OHX	5	3836	-	0,6,6	-	-	-		
85	OHX	1	3993	-	0,6,6	-	-	-		
85	OHX	6	2085	-	0,6,6	-	-	-		
85	OHX	1	3740	-	0,6,6	-	-	-		
85	OHX	5	3798	-	0,6,6	-	-	-		
85	OHX	2	2090	-	0,6,6	-	-	-		
85	OHX	1	3939	-	0,6,6	-	-	-		
85	OHX	5	3945	-	0,6,6	-	-	-		
85	OHX	5	3962	-	0,6,6	-	-	-		
85	OHX	6	2076	-	0,6,6	-	-	-		
85	OHX	14	402	-	0,6,6	-	-	-		
85	OHX	5	3910	-	0,6,6	-	-	-		
85	OHX	6	2153	-	0,6,6	-	-	-		
85	OHX	5	4014	-	0,6,6	-	-	-		
85	OHX	1	3871	-	0,6,6	-	-	-		
85	OHX	1	4024	-	0,6,6	-	-	-		
85	OHX	5	3983	-	0,6,6	-	-	-		
85	OHX	5	3824	-	0,6,6	-	-	-		
85	OHX	2	2076	-	0,6,6	-	-	-		
85	OHX	6	2060	-	0,6,6	-	-	-		
85	OHX	1	3930	-	0,6,6	-	-	-		
85	OHX	6	2107	-	0,6,6	-	-	-		
85	OHX	2	2042	-	0,6,6	-	-	-		
85	OHX	5	3789	-	0,6,6	-	-	-		
85	OHX	5	3992	-	0,6,6	-	-	-		
85	OHX	S8	301	-	0,6,6	-	-	-		
85	OHX	1	3884	-	0,6,6	-	-	-		
85	OHX	1	4012	-	0,6,6	-	-	-		
85	OHX	5	3763	-	0,6,6	-	-	-		
85	OHX	2	2060	-	0,6,6	-	-	-		
85	OHX	5	3858	-	0,6,6	-	-	-		
85	OHX	4	220	-	0,6,6	-	-	-		
85	OHX	1	3731	-	0,6,6	-	-	-		
85	OHX	5	3897	-	0,6,6	-	-	-		
85	OHX	2	2114	-	0,6,6	-	-	-		
85	OHX	5	3933	-	0,6,6	-	-	-		
85	OHX	3	216	-	0,6,6	-	-	-		
85	OHX	5	3805	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	2	2052	-	0,6,6	-	-	-		
85	OHX	5	4005	-	0,6,6	-	-	-		
85	OHX	6	2064	-	0,6,6	-	-	-		
85	OHX	5	3969	-	0,6,6	-	-	-		
85	OHX	5	3800	-	0,6,6	-	-	-		
85	OHX	6	2044	-	0,6,6	-	-	-		
85	OHX	13	407	-	0,6,6	-	-	-		
85	OHX	5	3804	-	0,6,6	-	-	-		
85	OHX	5	3857	-	0,6,6	-	-	-		
85	OHX	2	2036	-	0,6,6	-	-	-		
85	OHX	2	1995	-	0,6,6	-	-	-		
85	OHX	1	3962	-	0,6,6	-	-	-		
85	OHX	6	2077	-	0,6,6	-	-	-		
85	OHX	5	3998	-	0,6,6	-	-	-		
85	OHX	1	3934	-	0,6,6	-	-	-		
85	OHX	2	2119	-	0,6,6	-	-	-		
85	OHX	6	2141	-	0,6,6	-	-	-		
85	OHX	5	4041	-	0,6,6	-	-	-		
85	OHX	5	3838	-	0,6,6	-	-	-		
85	OHX	5	3966	-	0,6,6	-	-	-		
85	OHX	1	3907	-	0,6,6	-	-	-		
85	OHX	5	3867	-	0,6,6	-	-	-		
85	OHX	07	502	-	0,6,6	-	-	-		
85	OHX	2	2028	-	0,6,6	-	-	-		
85	OHX	6	2121	-	0,6,6	-	-	-		
85	OHX	6	2089	-	0,6,6	-	-	-		
85	OHX	7	218	-	0,6,6	-	-	-		
85	OHX	6	2100	-	0,6,6	-	-	-		
85	OHX	09	101	-	0,6,6	-	-	-		
85	OHX	5	3819	-	0,6,6	-	-	-		
85	OHX	6	2067	-	0,6,6	-	-	-		
85	OHX	5	4007	36	0,6,6	-	-	-		
85	OHX	1	3829	-	0,6,6	-	-	-		
85	OHX	4	228	-	0,6,6	-	-	-		
85	OHX	6	2092	-	0,6,6	-	-	-		
85	OHX	1	3987	-	0,6,6	-	-	-		
85	OHX	1	3991	-	0,6,6	-	-	-		
85	OHX	1	3838	-	0,6,6	-	-	-		
85	OHX	5	3808	-	0,6,6	-	-	-		
85	OHX	5	4013	-	0,6,6	-	-	-		
85	OHX	1	3981	-	0,6,6	-	-	-		
85	OHX	1	3765	-	0,6,6	-	-	-		
85	OHX	5	4028	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	6	2135	-	0,6,6	-	-	-		
85	OHX	2	1997	-	0,6,6	-	-	-		
85	OHX	6	2086	-	0,6,6	-	-	-		
85	OHX	5	4017	-	0,6,6	-	-	-		
85	OHX	5	3931	-	0,6,6	-	-	-		
85	OHX	6	2059	-	0,6,6	-	-	-		
85	OHX	1	4023	-	0,6,6	-	-	-		
85	OHX	1	3846	-	0,6,6	-	-	-		
85	OHX	5	3845	-	0,6,6	-	-	-		
85	OHX	5	3928	-	0,6,6	-	-	-		
85	OHX	6	2027	-	0,6,6	-	-	-		
85	OHX	5	4056	-	0,6,6	-	-	-		
85	OHX	2	2059	-	0,6,6	-	-	-		
85	OHX	1	3851	-	0,6,6	-	-	-		
85	OHX	5	3995	-	0,6,6	-	-	-		
85	OHX	2	2057	-	0,6,6	-	-	-		
85	OHX	19	202	-	0,6,6	-	-	-		
85	OHX	5	3785	-	0,6,6	-	-	-		
85	OHX	5	3922	-	0,6,6	-	-	-		
85	OHX	2	1986	-	0,6,6	-	-	-		
85	OHX	6	2054	-	0,6,6	-	-	-		
85	OHX	5	3914	-	0,6,6	-	-	-		
85	OHX	5	4001	-	0,6,6	-	-	-		
85	OHX	6	2043	-	0,6,6	-	-	-		
85	OHX	2	2115	-	0,6,6	-	-	-		
85	OHX	1	3996	-	0,6,6	-	-	-		
85	OHX	2	2091	-	0,6,6	-	-	-		
85	OHX	1	3730	-	0,6,6	-	-	-		
85	OHX	M0	302	-	0,6,6	-	-	-		
85	OHX	5	4040	-	0,6,6	-	-	-		
85	OHX	5	4047	-	0,6,6	-	-	-		
85	OHX	1	3781	-	0,6,6	-	-	-		
85	OHX	5	3788	-	0,6,6	-	-	-		
85	OHX	1	3945	-	0,6,6	-	-	-		
85	OHX	1	3891	-	0,6,6	-	-	-		
85	OHX	5	3930	-	0,6,6	-	-	-		
85	OHX	1	3861	-	0,6,6	-	-	-		
85	OHX	5	3854	-	0,6,6	-	-	-		
85	OHX	1	3870	-	0,6,6	-	-	-		
85	OHX	6	2069	-	0,6,6	-	-	-		
85	OHX	5	3821	-	0,6,6	-	-	-		
85	OHX	5	4004	-	0,6,6	-	-	-		
85	OHX	5	4010	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	OHX	1	3763	-	0,6,6	-	-	-	-	-
85	OHX	1	4000	-	0,6,6	-	-	-	-	-
85	OHX	5	3799	-	0,6,6	-	-	-	-	-
85	OHX	7	219	-	0,6,6	-	-	-	-	-
85	OHX	4	227	-	0,6,6	-	-	-	-	-
85	OHX	5	4012	-	0,6,6	-	-	-	-	-
85	OHX	L3	403	-	0,6,6	-	-	-	-	-
85	OHX	5	3849	-	0,6,6	-	-	-	-	-
85	OHX	1	3862	-	0,6,6	-	-	-	-	-
85	OHX	6	2030	-	0,6,6	-	-	-	-	-

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

All (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
87	1	3401	ANM	C2-C16	-2.91	1.47	1.53
87	1	3401	ANM	O4-C3	-2.83	1.37	1.43
87	1	3401	ANM	O1-C9	2.79	1.43	1.37
87	1	3401	ANM	O2-C5	2.62	1.41	1.35

All (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
87	1	3401	ANM	O2-C5-C6	3.33	117.21	111.09
87	1	3401	ANM	O4-C3-C2	-2.88	103.16	111.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	1	3401	ANM	O3-C5-C6	-2.56	115.49	124.81
87	1	3401	ANM	C3-C2-C16	-2.33	100.92	104.29
87	1	3401	ANM	C14-O1-C9	-2.28	112.56	117.51

All (3) chirality outliers are listed below:

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

All (3) torsion outliers are listed below:

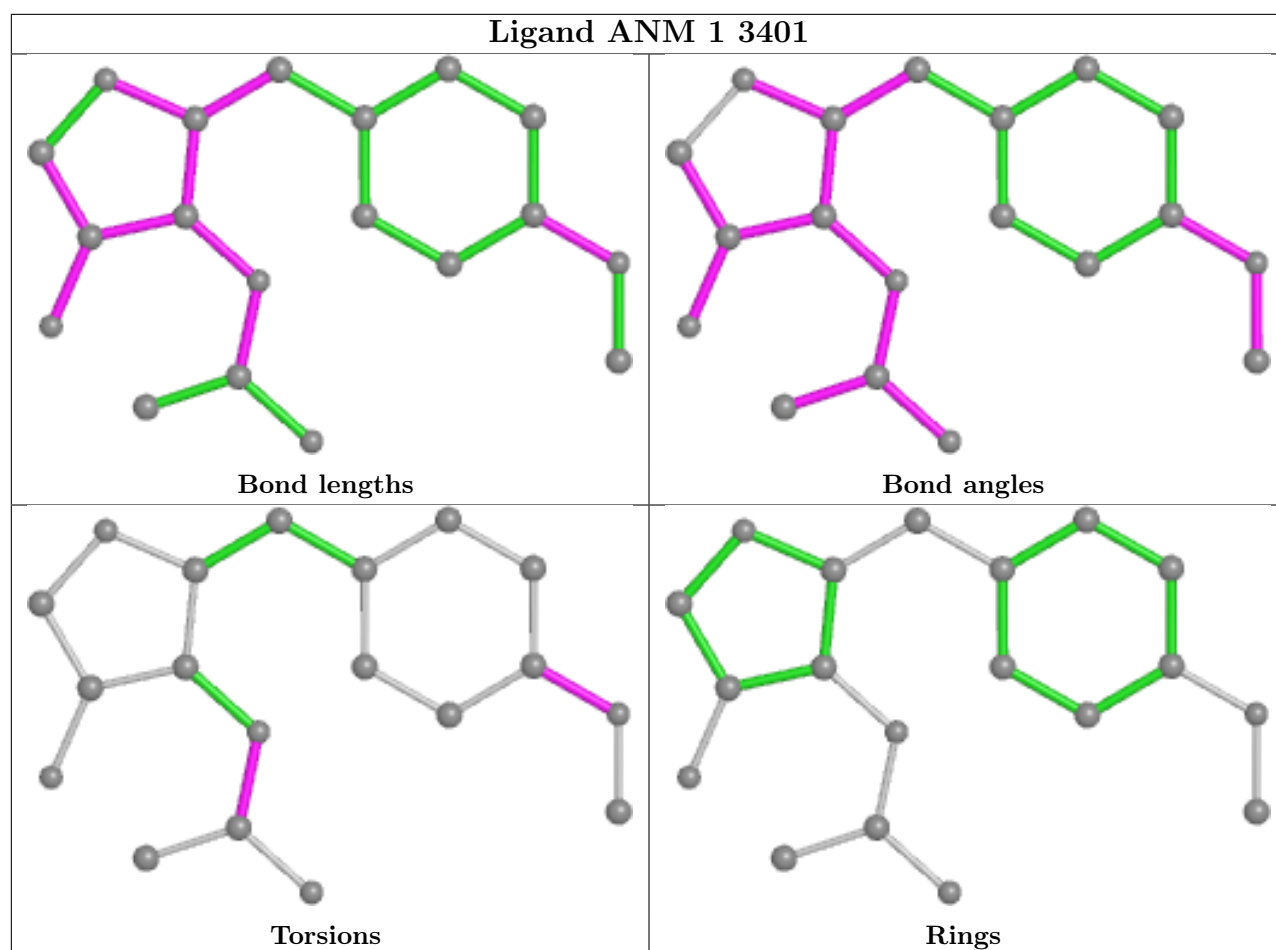
Mol	Chain	Res	Type	Atoms
87	1	3401	ANM	C6-C5-O2-C2
87	1	3401	ANM	C10-C9-O1-C14
87	1	3401	ANM	C1-C9-O1-C14

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	C8	201	OHX	0	1

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
35	SM	1
12	c0	1
1	2	1

All 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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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
1	m2	52:UNK	C	54:UNK	N	3.08

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	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 <sup>2</sup> )	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 <sup>2</sup> )	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, 60, 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 <sup>2</sup> )	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 <sup>2</sup> )	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

All (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
33	e1	145	HIS	10.1
33	e1	77	GLY	10.1
36	1	1237	G	9.5
60	n4	73	ARG	9.4
1	2	194	U	9.4
14	c2	21	GLU	9.3
1	6	662	U	9.1
13	c1	147	ALA	8.7
1	6	663	U	8.6
60	N4	75	THR	8.3
1	6	658	C	8.1
1	2	656	G	8.1
33	e1	95	HIS	8.0
36	1	1952	G	8.0

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Mol	Chain	Res	Type	RSRZ
14	c2	30	VAL	7.9
1	2	1700	C	7.9
1	6	239	C	7.9
14	C2	62	LEU	7.9
1	6	718	U	7.9
3	S1	93	GLY	7.7
1	6	668	C	7.7
36	1	1236	G	7.6
14	c2	80	ASN	7.5
36	1	1243	G	7.3
58	N2	27	VAL	7.3
14	c2	23	THR	7.2
1	2	1699	G	7.2
36	1	1955	U	7.1
11	S9	181	ALA	7.1
1	6	1707	A	7.0
14	c2	63	VAL	7.0
14	c2	126	TRP	7.0
30	D8	21	SER	6.9
22	d0	121	ASN	6.9
1	6	229	U	6.8
14	c2	86	VAL	6.8
1	2	1704	U	6.7
33	e1	85	TYR	6.7
39	l2	253	GLN	6.6
73	o7	87	SER	6.6
60	N4	86	SER	6.5
1	2	491	C	6.4
17	c5	133	ALA	6.4
14	c2	85	LYS	6.4
36	1	1238	C	6.3
1	6	661	A	6.3
60	N4	76	VAL	6.3
27	d5	37	GLN	6.3
36	5	2503	G	6.3
1	6	659	C	6.3
1	2	1709	C	6.2
33	e1	134	ASN	6.2
60	n4	65	GLU	6.2
1	6	667	U	6.2
5	S3	217	ILE	6.2
3	S1	226	GLY	6.2

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Mol	Chain	Res	Type	RSRZ
1	2	714	G	6.2
1	2	1703	C	6.2
3	S1	92	GLN	6.2
33	e1	78	LYS	6.2
36	1	1245	A	6.1
1	6	669	G	6.1
60	n4	70	LYS	6.1
14	c2	123	VAL	6.1
39	l2	252	THR	6.0
27	d5	87	GLY	6.0
1	2	1698	G	6.0
60	n4	69	LYS	6.0
1	2	238	U	6.0
1	2	1711	C	6.0
1	2	506	A	6.0
1	6	1702	A	6.0
36	1	1568	U	6.0
60	N4	72	SER	5.9
22	d0	119	ALA	5.9
36	1	1234	G	5.9
1	2	1708	U	5.9
1	6	240	U	5.9
14	c2	57	ALA	5.9
1	2	493	U	5.9
1	2	715	U	5.8
35	sM	84	LYS	5.8
16	C4	14	PHE	5.8
19	C7	125	SER	5.8
3	S1	94	LYS	5.8
1	2	713	A	5.6
1	2	913	G	5.6
1	6	656	G	5.6
14	c2	29	LYS	5.6
31	d9	4	GLU	5.6
33	e1	80	ARG	5.6
3	S1	96	LEU	5.6
1	6	232	U	5.6
34	SR	79	TYR	5.6
5	S3	44	THR	5.5
1	2	1701	A	5.5
36	1	2539	C	5.5
47	m0	112	GLN	5.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	6	1711	C	5.4
1	2	1694	A	5.4
1	6	1712	A	5.4
1	6	490	C	5.4
1	2	1692	G	5.4
13	C1	146	ALA	5.4
1	6	238	U	5.3
1	2	657	U	5.3
36	1	1260	A	5.3
14	c2	64	SER	5.3
1	2	725	U	5.3
71	O5	120	ALA	5.3
1	6	660	G	5.3
14	c2	114	LYS	5.3
36	1	1349	G	5.2
22	D0	120	SER	5.2
2	S0	28	ASN	5.2
1	6	665	U	5.2
36	1	1242	G	5.2
12	c0	84	GLU	5.2
1	2	1705	C	5.2
1	6	1696	G	5.2
1	6	228	G	5.1
1	6	1697	G	5.1
3	S1	46	THR	5.1
33	e1	86	THR	5.1
22	D0	121	ASN	5.1
1	2	658	C	5.1
3	S1	25	THR	5.1
33	e1	102	VAL	5.1
22	d0	57	ARG	5.1
1	2	132	U	5.1
20	C8	8	GLN	5.1
1	2	1707	A	5.0
73	o7	88	ALA	5.1
1	2	1687	U	5.0
1	6	666	U	5.0
14	c2	124	LYS	5.0
1	6	664	U	5.0
22	D0	93	LEU	5.0
14	c2	59	LEU	5.0
17	c5	4	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
60	N4	70	LYS	5.0
33	e1	143	LYS	5.0
13	C1	147	ALA	5.0
35	SM	141	ALA	5.0
1	6	1371	A	4.9
14	c2	128	ALA	4.9
34	SR	36	ALA	4.9
1	2	1693	A	4.9
3	S1	45	LYS	4.9
58	N2	94	ARG	4.9
20	c8	146	ALA	4.9
36	5	249	U	4.9
1	2	712	G	4.9
1	6	1699	G	4.9
19	C7	126	ALA	4.9
22	d0	92	ASP	4.8
36	1	1239	C	4.8
14	c2	79	ALA	4.8
36	5	1569	U	4.8
30	d8	17	GLY	4.8
35	SM	84	LYS	4.8
19	C7	123	ASN	4.8
36	1	1256	G	4.8
13	c1	146	ALA	4.8
70	O4	113	LYS	4.8
1	2	1686	C	4.8
1	6	719	U	4.8
1	2	716	C	4.7
1	2	494	U	4.7
1	2	1691	A	4.7
22	D0	51	VAL	4.7
12	c0	79	TYR	4.7
30	d8	5	THR	4.7
1	2	718	U	4.7
36	5	1031	C	4.7
1	2	505	A	4.7
1	6	491	C	4.7
36	1	1569	U	4.7
81	p0	209	LEU	4.7
8	S6	180	THR	4.7
1	2	280	U	4.7
33	e1	79	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
7	S5	161	ASP	4.7
1	2	1690	G	4.7
1	2	1712	A	4.6
29	D7	38	PRO	4.6
14	c2	137	MET	4.6
1	2	135	A	4.6
14	c2	136	ILE	4.6
68	O2	2	ALA	4.6
16	C4	16	VAL	4.6
1	6	493	U	4.6
9	s7	3	ALA	4.6
3	S1	47	LEU	4.6
3	S1	28	GLU	4.6
8	S6	124	LEU	4.6
1	6	194	U	4.6
36	5	1580	A	4.6
22	d0	90	TYR	4.6
14	c2	56	GLU	4.5
14	c2	28	LEU	4.5
36	1	1235	U	4.5
14	C2	32	LEU	4.5
22	D0	19	ILE	4.5
14	C2	50	LYS	4.5
16	C4	75	GLY	4.5
16	C4	11	SER	4.5
9	s7	93	LEU	4.5
16	C4	89	THR	4.5
17	c5	50	THR	4.5
33	e1	147	VAL	4.5
1	2	721	U	4.5
14	c2	125	ASN	4.5
1	2	1713	G	4.5
1	2	719	U	4.5
36	1	1762	C	4.5
14	C2	111	ASN	4.5
1	2	134	U	4.5
9	S7	52	ALA	4.5
1	6	721	U	4.5
36	5	1567	U	4.5
36	5	2506	U	4.5
20	C8	10	SER	4.5
1	6	226	A	4.4

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Mol	Chain	Res	Type	RSRZ
1	2	729	G	4.4
60	n4	71	ARG	4.4
1	2	492	A	4.4
81	p0	217	VAL	4.4
14	c2	43	ARG	4.4
1	6	1698	G	4.4
33	e1	90	LYS	4.4
12	c0	78	GLU	4.4
30	d8	13	ILE	4.4
35	SM	87	THR	4.4
3	S1	54	LEU	4.4
7	S5	41	LYS	4.4
5	s3	145	ALA	4.4
36	1	1269	U	4.4
36	1	1271	A	4.4
1	6	496	G	4.4
36	5	442	G	4.4
14	c2	84	ASN	4.4
60	n4	128	ALA	4.4
1	6	1217	A	4.3
45	l8	254	ASP	4.3
30	D8	44	VAL	4.3
36	5	1566	A	4.3
58	N2	93	ILE	4.3
1	6	225	A	4.3
36	1	1571	A	4.3
36	1	1567	U	4.3
8	s6	169	TYR	4.3
36	1	1273	A	4.3
1	6	75	U	4.3
1	6	657	U	4.3
42	L5	213	ASP	4.3
60	N4	73	ARG	4.3
22	D0	20	ILE	4.3
35	SM	88	ARG	4.3
27	d5	86	GLU	4.2
33	E1	116	LYS	4.2
36	1	1261	G	4.2
36	1	1572	U	4.2
1	2	1689	A	4.2
1	6	506	A	4.2
1	2	136	C	4.2

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Mol	Chain	Res	Type	RSRZ
18	c6	19	VAL	4.2
60	N4	77	LYS	4.2
30	D8	7	VAL	4.2
36	1	1240	A	4.2
9	s7	2	SER	4.2
36	1	1255	C	4.2
3	S1	29	TRP	4.2
55	M9	181	ARG	4.2
53	M7	162	GLU	4.2
20	c8	18	LEU	4.2
26	d4	2	SER	4.2
33	e1	110	ALA	4.2
60	N4	78	ALA	4.2
36	1	1263	A	4.2
36	1	1570	U	4.2
31	d9	5	ASN	4.2
33	E1	149	LYS	4.2
53	M7	159	LYS	4.2
36	5	1025	A	4.2
14	C2	25	GLU	4.2
14	c2	106	ILE	4.2
36	1	1351	U	4.1
13	c1	3	THR	4.1
1	2	499	U	4.1
1	6	1059	U	4.1
13	C1	27	THR	4.1
34	sR	168	THR	4.1
14	c2	22	VAL	4.1
36	5	1017	C	4.1
53	M7	174	GLY	4.1
60	N4	69	LYS	4.1
65	N9	54	LEU	4.1
22	D0	92	ASP	4.1
35	SM	49	LYS	4.1
36	5	1349	G	4.1
36	1	1028	U	4.1
1	2	495	C	4.1
1	6	673	A	4.1
16	C4	27	PHE	4.1
14	c2	75	VAL	4.1
36	5	1026	A	4.1
21	C9	5	SER	4.1

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Mol	Chain	Res	Type	RSRZ
33	e1	104	SER	4.1
16	C4	80	HIS	4.1
33	e1	112	GLY	4.1
34	SR	3	SER	4.1
14	c2	105	LYS	4.1
15	C3	61	THR	4.1
1	6	731	C	4.1
35	SM	89	ARG	4.1
36	5	2505	U	4.1
36	5	443	G	4.1
20	C8	22	VAL	4.1
60	n4	76	VAL	4.1
10	S8	21	PHE	4.1
58	n2	14	THR	4.1
1	6	492	A	4.1
22	d0	93	LEU	4.1
1	2	1688	U	4.0
14	c2	82	PRO	4.0
1	6	1694	A	4.0
18	c6	139	GLN	4.0
14	c2	47	GLU	4.0
1	6	1710	U	4.0
36	5	620	U	4.0
36	1	1233	G	4.0
19	c7	87	GLU	4.0
1	6	1703	C	4.0
1	6	676	G	4.0
1	2	490	C	4.0
47	m0	103	LEU	4.0
1	2	488	G	4.0
36	5	1024	G	4.0
22	d0	56	VAL	4.0
2	s0	205	ARG	4.0
7	S5	54	LYS	4.0
22	D0	48	HIS	4.0
33	e1	113	LYS	4.0
36	1	1259	A	4.0
60	n4	67	VAL	4.0
34	sR	244	ALA	4.0
1	6	717	C	4.0
3	S1	225	VAL	3.9
1	6	489	C	3.9

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Mol	Chain	Res	Type	RSRZ
26	D4	2	SER	3.9
7	s5	37	GLN	3.9
36	1	1016	C	3.9
60	N4	64	THR	3.9
1	6	711	U	3.9
9	s7	52	ALA	3.9
26	D4	7	ILE	3.9
1	2	1697	G	3.9
36	1	1350	A	3.9
60	N4	95	SER	3.9
13	c1	4	GLU	3.9
36	5	1016	C	3.9
1	2	720	G	3.9
36	1	1270	A	3.9
22	D0	22	ILE	3.9
5	s3	128	GLU	3.9
66	o0	100	ILE	3.9
36	1	1953	G	3.9
14	c2	121	VAL	3.9
33	E1	146	SER	3.9
18	C6	3	ALA	3.9
28	D6	2	PRO	3.9
1	6	651	G	3.9
7	s5	159	ALA	3.9
59	N3	4	ASN	3.9
1	6	1704	U	3.8
35	sM	49	LYS	3.8
58	N2	89	LEU	3.8
7	S5	152	GLY	3.8
1	2	507	U	3.8
36	5	1764	U	3.8
66	o0	6	SER	3.8
34	sR	160	GLU	3.8
36	1	1241	U	3.8
14	c2	143	GLN	3.8
19	c7	119	LEU	3.8
14	C2	67	THR	3.8
36	1	1352	A	3.8
1	2	239	C	3.8
1	6	230	C	3.8
36	1	1566	A	3.8
55	M9	182	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	2	234	G	3.8
59	N3	2	SER	3.8
35	sM	83	LYS	3.8
53	M7	168	LEU	3.8
31	d9	6	VAL	3.8
14	c2	76	GLU	3.8
33	e1	146	SER	3.8
81	p0	81	LYS	3.8
1	6	722	G	3.8
36	1	1278	A	3.8
1	2	500	C	3.8
30	d8	43	ASN	3.8
1	2	484	C	3.8
22	D0	21	LYS	3.7
1	6	227	U	3.7
14	c2	133	LEU	3.7
1	2	486	G	3.7
18	c6	3	ALA	3.7
22	D0	104	THR	3.7
33	e1	111	GLU	3.7
1	2	1059	U	3.7
1	6	1370	U	3.7
30	D8	17	GLY	3.7
27	D5	88	ILE	3.7
18	c6	4	VAL	3.7
49	M3	129	ASN	3.7
14	c2	132	GLU	3.7
36	1	1265	U	3.7
6	S4	261	LEU	3.7
14	c2	34	THR	3.7
45	l8	121	SER	3.7
67	o1	82	GLU	3.7
14	c2	58	LEU	3.7
3	S1	227	ALA	3.7
1	2	498	G	3.7
36	5	491	C	3.7
36	1	1229	G	3.6
18	c6	142	TYR	3.6
34	SR	4	ASN	3.6
67	O1	4	LEU	3.6
1	2	192	U	3.6
8	S6	1	MET	3.6

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Mol	Chain	Res	Type	RSRZ
22	d0	120	SER	3.6
36	1	1954	G	3.6
30	D8	45	LYS	3.6
48	M1	96	PHE	3.6
1	2	74	U	3.6
33	E1	87	THR	3.6
1	6	720	G	3.6
32	e0	63	GLN	3.6
79	q3	2	ALA	3.6
1	2	678	A	3.6
36	5	1574	C	3.6
1	2	261	U	3.6
14	c2	122	VAL	3.6
81	p0	221	ALA	3.6
10	s8	200	LYS	3.6
14	c2	140	PHE	3.6
34	sR	48	THR	3.6
1	2	485	A	3.6
36	1	1274	A	3.6
18	c6	5	PRO	3.6
18	c6	8	GLN	3.6
7	s5	145	ASP	3.6
60	n4	66	GLU	3.6
20	C8	13	HIS	3.6
1	6	1705	C	3.6
34	sR	46	LYS	3.6
19	c7	57	LEU	3.6
33	e1	89	LYS	3.5
16	C4	79	VAL	3.5
34	SR	6	VAL	3.5
36	1	1279	C	3.5
18	c6	141	SER	3.5
22	d0	100	VAL	3.5
33	e1	127	GLY	3.5
60	N4	85	ALA	3.5
36	5	1027	A	3.5
33	e1	81	LYS	3.5
3	S1	95	ASN	3.5
17	c5	134	THR	3.5
22	d0	18	GLN	3.5
34	sR	205	SER	3.5
14	c2	77	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
30	D8	40	ILE	3.5
2	S0	44	GLY	3.5
9	S7	97	ARG	3.5
60	n4	135	SER	3.5
22	D0	94	GLU	3.5
36	5	1562	C	3.5
19	c7	115	LEU	3.5
1	2	653	C	3.5
27	D5	48	ASP	3.5
1	2	1370	U	3.5
1	2	1710	U	3.5
34	SR	212	ALA	3.5
33	E1	85	TYR	3.5
36	1	2445	A	3.5
33	E1	115	THR	3.5
39	l2	249	SER	3.5
14	C2	63	VAL	3.4
60	N4	81	PRO	3.4
36	1	1951	C	3.4
1	6	834	G	3.4
14	c2	26	ASP	3.4
33	E1	134	ASN	3.4
22	d0	22	ILE	3.4
5	s3	151	LYS	3.4
36	1	1021	G	3.4
2	S0	25	GLY	3.4
20	C8	9	GLY	3.4
60	n4	132	GLY	3.4
8	S6	186	ARG	3.4
34	sR	72	THR	3.4
36	5	1032	C	3.4
7	s5	151	GLY	3.4
58	N2	28	PHE	3.4
45	l8	115	ALA	3.4
36	1	1232	C	3.4
8	s6	35	GLU	3.4
34	sR	121	MET	3.4
5	s3	144	ALA	3.4
1	2	497	G	3.4
14	c2	142	GLN	3.4
60	N4	74	LYS	3.4
1	6	1700	C	3.4

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Mol	Chain	Res	Type	RSRZ
35	SM	16	ASP	3.4
60	n4	133	THR	3.4
1	6	710	U	3.4
16	C4	40	ALA	3.4
22	d0	117	VAL	3.4
14	c2	141	SER	3.4
58	N2	108	TYR	3.4
36	5	252	U	3.4
30	d8	9	LEU	3.4
61	n5	23	ALA	3.4
1	2	230	C	3.4
9	s7	22	GLN	3.4
45	L8	121	SER	3.4
36	5	1815	U	3.4
68	o2	128	LEU	3.4
18	C6	20	ALA	3.4
1	2	489	C	3.4
7	S5	37	GLN	3.4
14	C2	112	ALA	3.3
36	1	1231	A	3.3
10	s8	121	LEU	3.3
14	C2	23	THR	3.3
22	d0	25	THR	3.3
5	S3	88	ALA	3.3
34	SR	115	ILE	3.3
26	D4	47	VAL	3.3
32	e0	62	VAL	3.3
14	C2	47	GLU	3.3
1	2	1362	U	3.3
36	5	1028	U	3.3
45	l8	120	LYS	3.3
20	c8	22	VAL	3.3
36	1	1573	G	3.3
13	C1	2	SER	3.3
71	o5	120	ALA	3.3
36	1	1272	C	3.3
19	C7	71	PHE	3.3
34	SR	71	CYS	3.3
53	M7	160	ALA	3.3
1	2	677	G	3.3
14	C2	78	LEU	3.3
26	d4	18	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
36	1	1280	C	3.3
10	S8	144	ALA	3.3
11	S9	180	LYS	3.3
17	C5	14	THR	3.3
53	M7	163	LYS	3.3
1	6	655	G	3.3
65	N9	55	ALA	3.3
27	d5	105	THR	3.3
58	n2	97	SER	3.3
36	5	2874	G	3.3
21	C9	72	GLY	3.3
33	E1	151	ASN	3.3
3	S1	146	GLN	3.3
36	5	1572	U	3.3
34	SR	81	LEU	3.3
33	E1	143	LYS	3.3
3	S1	41	ARG	3.2
30	d8	61	ARG	3.2
1	2	1060	U	3.2
8	S6	175	ILE	3.2
14	c2	55	GLY	3.2
1	2	237	C	3.2
1	6	487	G	3.2
61	n5	36	LYS	3.2
2	S0	23	HIS	3.2
1	2	193	U	3.2
1	2	727	U	3.2
1	6	1693	A	3.2
34	SR	2	ALA	3.2
1	6	1228	G	3.2
36	5	244	G	3.2
17	c5	132	GLY	3.2
2	S0	24	LEU	3.2
63	n7	2	ALA	3.2
1	2	504	U	3.2
36	1	1763	U	3.2
8	S6	190	GLN	3.2
9	s7	60	ILE	3.2
45	l8	246	MET	3.2
14	c2	74	LEU	3.2
30	D8	43	ASN	3.2
35	SM	85	SER	3.2

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Mol	Chain	Res	Type	RSRZ
53	M7	165	VAL	3.2
11	S9	87	SER	3.2
34	sR	161	LYS	3.2
32	e0	56	MET	3.2
36	5	246	U	3.2
10	S8	148	ALA	3.2
14	C2	90	LYS	3.2
14	C2	100	TRP	3.2
1	2	131	C	3.2
3	S1	233	GLY	3.2
13	C1	3	THR	3.2
1	6	494	U	3.2
17	c5	5	VAL	3.2
1	2	1696	G	3.2
36	1	3361	G	3.2
1	6	678	A	3.2
14	C2	128	ALA	3.2
44	l7	26	VAL	3.2
34	SR	122	ILE	3.2
36	5	1352	A	3.2
16	C4	42	VAL	3.2
53	M7	161	ALA	3.2
33	e1	96	LYS	3.2
1	2	730	G	3.2
1	2	1625	C	3.1
14	c2	24	ILE	3.1
36	1	1764	U	3.1
7	S5	181	GLU	3.1
14	C2	91	VAL	3.1
34	sR	303	ALA	3.1
34	sR	49	GLY	3.1
34	sR	294	TRP	3.1
2	S0	40	ALA	3.1
3	S1	91	VAL	3.1
74	o8	34	ALA	3.1
4	s2	90	THR	3.1
1	6	1701	A	3.1
14	c2	116	VAL	3.1
63	n7	56	LYS	3.1
1	2	496	G	3.1
1	6	234	G	3.1
22	d0	98	GLN	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
14	C2	28	LEU	3.1
16	C4	29	HIS	3.1
35	SM	135	ALA	3.1
1	2	502	U	3.1
16	C4	12	GLN	3.1
53	M7	166	VAL	3.1
36	5	2444	C	3.1
58	n2	11	ILE	3.1
1	2	217	A	3.1
32	E0	60	PRO	3.1
19	c7	116	LYS	3.1
32	E0	49	LEU	3.1
36	1	1264	G	3.1
20	C8	66	LEU	3.1
20	c8	15	LEU	3.1
33	E1	86	THR	3.1
33	e1	106	TYR	3.1
1	6	1399	C	3.1
36	5	1571	A	3.1
1	6	705	U	3.1
7	S5	71	ALA	3.1
40	l3	387	LEU	3.1
36	5	1581	C	3.1
7	S5	36	ALA	3.1
13	C1	145	ALA	3.1
29	d7	38	PRO	3.1
33	e1	103	LEU	3.1
14	c2	46	ARG	3.1
1	6	495	C	3.1
14	C2	74	LEU	3.1
36	1	2096	A	3.1
14	c2	87	PRO	3.0
36	5	2538	U	3.0
36	5	1029	G	3.0
33	e1	135	HIS	3.0
3	s1	202	LYS	3.0
5	S3	216	PRO	3.0
6	S4	259	GLN	3.0
36	5	1570	U	3.0
17	c5	136	SER	3.0
36	5	2539	C	3.0
42	l5	296	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
49	m3	80	VAL	3.0
9	s7	51	VAL	3.0
22	D0	97	VAL	3.0
81	p0	218	SER	3.0
14	C2	20	ALA	3.0
22	D0	98	GLN	3.0
7	S5	207	THR	3.0
33	E1	129	GLY	3.0
1	2	1361	U	3.0
36	5	1237	G	3.0
36	5	1350	A	3.0
42	l5	263	GLU	3.0
78	Q2	11	TYR	3.0
33	E1	150	VAL	3.0
34	sR	61	PHE	3.0
14	C2	68	GLU	3.0
70	O4	109	THR	3.0
36	1	2508	U	3.0
1	6	1695	G	3.0
28	D6	85	ARG	3.0
11	S9	64	GLU	3.0
44	l7	28	ALA	3.0
1	6	674	C	3.0
4	s2	87	GLN	3.0
36	5	439	C	3.0
36	1	2502	A	3.0
14	c2	83	GLU	3.0
66	O0	94	GLU	3.0
81	p0	32	ASN	3.0
19	c7	67	ARG	3.0
21	C9	2	PRO	3.0
1	6	1398	U	3.0
6	S4	215	ASP	3.0
20	C8	17	LEU	3.0
14	C2	94	ALA	3.0
19	c7	15	ALA	3.0
36	1	1247	U	3.0
1	6	136	C	3.0
3	S1	207	LEU	3.0
55	M9	185	LEU	3.0
19	C7	107	SER	3.0
36	1	2535	A	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
12	c0	74	GLU	2.9
14	C2	21	GLU	2.9
1	6	1058	U	2.9
38	8	81	U	2.9
2	S0	113	ARG	2.9
47	M0	209	ASN	2.9
33	E1	93	HIS	2.9
36	1	2507	C	2.9
36	5	247	C	2.9
5	S3	218	LEU	2.9
45	L8	93	LEU	2.9
55	M9	188	ASP	2.9
36	1	1275	C	2.9
3	S1	100	PHE	2.9
34	sR	189	GLU	2.9
1	2	133	U	2.9
1	2	241	U	2.9
1	2	912	U	2.9
36	1	3287	U	2.9
49	m3	133	PRO	2.9
74	O8	29	LYS	2.9
14	c2	127	GLY	2.9
22	D0	100	VAL	2.9
43	l6	128	LYS	2.9
58	n2	98	THR	2.9
7	S5	211	ILE	2.9
36	5	243	G	2.9
36	5	1576	G	2.9
60	N4	88	ASP	2.9
14	c2	27	ALA	2.9
34	sR	214	ALA	2.9
1	6	231	U	2.9
3	S1	23	PRO	2.9
30	d8	59	SER	2.9
36	5	250	U	2.9
72	O6	27	SER	2.9
74	O8	28	ASN	2.9
29	d7	57	GLU	2.9
28	D6	79	ILE	2.9
36	1	2772	C	2.9
36	1	3360	C	2.9
36	5	3154	C	2.9

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Mol	Chain	Res	Type	RSRZ
1	2	722	G	2.9
1	2	723	G	2.9
36	5	1565	G	2.9
2	S0	187	ALA	2.9
14	C2	26	ASP	2.9
45	l8	247	ASP	2.9
60	N4	68	ALA	2.9
1	6	501	U	2.9
1	6	729	G	2.9
32	E0	46	ASN	2.9
60	N4	84	GLY	2.9
17	C5	50	THR	2.9
34	SR	253	ALA	2.9
36	5	1351	U	2.9
8	S6	50	PHE	2.9
49	M3	131	LYS	2.9
3	S1	97	LEU	2.9
4	s2	91	ARG	2.8
57	N1	121	ALA	2.8
62	N6	127	GLU	2.8
36	5	1261	G	2.8
36	5	1262	G	2.8
18	c6	29	ILE	2.8
26	D4	35	VAL	2.8
46	L9	134	ILE	2.8
1	2	1716	C	2.8
33	e1	140	TYR	2.8
9	s7	58	LEU	2.8
78	Q2	104	LEU	2.8
1	6	1256	A	2.8
1	6	235	G	2.8
18	C6	8	GLN	2.8
30	d8	58	GLU	2.8
23	D1	36	VAL	2.8
34	sR	284	ALA	2.8
81	p0	107	ALA	2.8
1	6	241	U	2.8
33	E1	83	LYS	2.8
36	5	441	U	2.8
55	m9	165	LYS	2.8
35	SM	140	ASP	2.8
36	1	1581	C	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
10	s8	117	TYR	2.8
4	s2	84	LYS	2.8
11	s9	171	ARG	2.8
3	S1	30	PHE	2.8
1	6	714	G	2.8
58	N2	18	ASP	2.8
1	6	1248	C	2.8
30	d8	24	GLY	2.8
68	O2	128	LEU	2.8
8	s6	217	SER	2.8
16	C4	74	VAL	2.8
19	C7	70	SER	2.8
16	C4	31	THR	2.8
58	n2	44	GLU	2.8
55	M9	186	LYS	2.8
30	D8	16	LEU	2.8
40	L3	387	LEU	2.8
14	C2	89	ILE	2.8
36	5	2507	C	2.8
45	l8	253	SER	2.8
26	D4	39	GLU	2.8
45	l8	106	LYS	2.8
1	2	830	U	2.8
20	C8	32	LEU	2.8
22	D0	119	ALA	2.8
33	E1	105	TYR	2.8
36	5	1238	C	2.8
42	l5	270	LYS	2.8
49	m3	184	GLU	2.8
55	M9	187	GLU	2.8
14	c2	52	LEU	2.8
7	S5	151	GLY	2.8
33	E1	102	VAL	2.8
8	S6	177	ARG	2.8
30	d8	63	ALA	2.8
36	1	1277	C	2.8
57	N1	125	ALA	2.8
33	E1	100	LEU	2.8
42	l5	267	ALA	2.8
9	S7	100	PRO	2.8
22	d0	19	ILE	2.7
45	l8	227	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
60	N4	65	GLU	2.7
36	1	1262	G	2.7
23	d1	43	GLY	2.7
3	S1	140	ILE	2.7
26	d4	26	ASP	2.7
36	1	1017	C	2.7
34	SR	252	LEU	2.7
19	C7	53	TYR	2.7
1	2	1371	A	2.7
7	S5	31	GLU	2.7
36	5	2441	A	2.7
6	s4	261	LEU	2.7
14	c2	115	VAL	2.7
34	SR	80	ALA	2.7
44	L7	23	ALA	2.7
20	C8	19	ASN	2.7
49	m3	178	LYS	2.7
1	2	191	C	2.7
1	2	724	C	2.7
1	6	1706	C	2.7
1	2	227	U	2.7
36	1	252	U	2.7
38	4	82	U	2.7
14	c2	135	MET	2.7
17	c5	135	THR	2.7
42	L5	214	ASP	2.7
1	2	235	G	2.7
7	s5	152	GLY	2.7
33	e1	98	VAL	2.7
22	D0	41	ILE	2.7
1	2	233	C	2.7
2	S0	18	LEU	2.7
13	c1	5	LEU	2.7
30	D8	30	VAL	2.7
3	S1	204	ILE	2.7
27	d5	58	ARG	2.7
60	N4	49	ILE	2.7
5	s3	86	LEU	2.7
29	D7	33	LEU	2.7
36	1	1565	G	2.7
36	1	3286	G	2.7
35	SM	45	SER	2.7

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Mol	Chain	Res	Type	RSRZ
61	n5	24	LEU	2.7
14	C2	113	ARG	2.7
25	D3	102	VAL	2.7
33	e1	94	LYS	2.7
34	sR	163	ASP	2.7
72	O6	99	ARG	2.7
29	D7	49	HIS	2.7
33	e1	84	VAL	2.7
36	1	2522	G	2.7
14	C2	130	THR	2.7
16	C4	77	THR	2.7
21	C9	134	ARG	2.7
72	o6	29	LYS	2.7
3	S1	99	ASN	2.7
3	S1	147	ALA	2.7
34	sR	226	ALA	2.7
36	1	2207	A	2.7
1	6	1690	G	2.7
27	d5	85	LYS	2.7
36	1	2442	G	2.7
60	n4	77	LYS	2.7
29	D7	75	GLU	2.7
22	d0	99	ILE	2.7
23	D1	37	ALA	2.7
3	S1	31	ASP	2.7
14	c2	131	ASP	2.7
34	sR	252	LEU	2.7
75	O9	46	ARG	2.7
22	D0	105	GLN	2.7
60	N4	67	VAL	2.7
16	C4	41	ARG	2.6
2	S0	107	PHE	2.6
14	C2	49	THR	2.6
19	c7	8	THR	2.6
20	C8	24	GLY	2.6
11	S9	182	GLU	2.6
61	n5	26	VAL	2.6
36	5	1023	C	2.6
60	n4	131	ALA	2.6
36	5	1021	G	2.6
55	M9	164	LEU	2.6
8	S6	41	VAL	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
43	l6	129	GLU	2.6
58	n2	13	LYS	2.6
58	n2	66	VAL	2.6
5	s3	182	LEU	2.6
32	e0	49	LEU	2.6
1	2	717	C	2.6
1	2	726	C	2.6
34	SR	186	PHE	2.6
14	C2	105	LYS	2.6
18	c6	140	LYS	2.6
26	D4	3	ASP	2.6
14	C2	71	ILE	2.6
38	8	158	U	2.6
3	S1	232	HIS	2.6
1	6	237	C	2.6
34	SR	82	SER	2.6
8	S6	114	VAL	2.6
8	S6	152	ASP	2.6
8	S6	196	ARG	2.6
21	C9	71	VAL	2.6
36	1	1254	C	2.6
9	S7	74	GLN	2.6
60	n4	134	GLN	2.6
62	N6	111	LEU	2.6
22	d0	55	PRO	2.6
36	1	1230	G	2.6
31	d9	7	TRP	2.6
35	sM	85	SER	2.6
36	5	1816	A	2.6
38	8	80	A	2.6
1	2	654	C	2.6
3	S1	156	ALA	2.6
3	s1	52	THR	2.6
53	M7	178	ALA	2.6
9	s7	90	VAL	2.6
36	5	1953	G	2.6
34	SR	91	LEU	2.6
7	s5	129	PRO	2.6
14	c2	129	GLU	2.6
26	D4	67	GLY	2.6
48	M1	85	LYS	2.6
53	M7	167	ARG	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
36	5	1239	C	2.6
1	6	675	U	2.6
33	E1	139	LEU	2.6
77	Q1	1	MET	2.6
12	c0	64	TYR	2.6
14	c2	92	ALA	2.6
34	sR	26	SER	2.6
35	SM	19	VAL	2.6
36	5	1573	G	2.6
36	1	1026	A	2.6
36	1	2540	A	2.6
1	2	1706	C	2.6
10	s8	67	TRP	2.6
14	C2	88	LEU	2.6
36	5	1763	U	2.6
19	c7	114	GLY	2.6
66	O0	93	LEU	2.6
1	2	682	C	2.6
36	5	2571	U	2.6
14	c2	102	GLY	2.6
48	M1	148	VAL	2.6
33	E1	135	HIS	2.6
34	sR	227	ALA	2.5
5	S3	214	GLU	2.5
14	C2	117	GLY	2.5
34	SR	102	ARG	2.5
36	1	2095	G	2.5
36	1	2205	U	2.5
29	D7	37	CYS	2.5
70	o4	68	THR	2.5
6	s4	183	VAL	2.5
58	N2	62	VAL	2.5
1	6	236	A	2.5
36	5	1575	A	2.5
22	d0	91	ILE	2.5
10	S8	20	GLN	2.5
30	D8	27	GLN	2.5
32	E0	48	THR	2.5
33	e1	148	TYR	2.5
50	M4	138	ALA	2.5
53	M7	184	ALA	2.5
60	n4	75	THR	2.5

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Mol	Chain	Res	Type	RSRZ
63	N7	2	ALA	2.5
26	D4	38	ASP	2.5
36	1	2501	U	2.5
36	5	492	U	2.5
56	N0	1	MET	2.5
35	sM	50	ASN	2.5
1	6	677	G	2.5
1	6	1692	G	2.5
7	s5	150	GLY	2.5
44	l7	25	GLN	2.5
72	o6	31	GLY	2.5
11	S9	138	LYS	2.5
78	q2	15	LYS	2.5
9	s7	54	GLY	2.5
36	5	1579	C	2.5
39	l2	248	GLY	2.5
70	O4	66	SER	2.5
1	2	794	U	2.5
13	c1	117	VAL	2.5
14	c2	112	ALA	2.5
16	C4	78	ALA	2.5
34	SR	180	ALA	2.5
36	5	1564	U	2.5
61	n5	37	THR	2.5
30	d8	32	PHE	2.5
36	1	1025	A	2.5
36	1	1228	C	2.5
36	5	1232	C	2.5
3	s1	89	ASP	2.5
34	SR	117	LYS	2.5
34	sR	309	VAL	2.5
35	SM	22	PRO	2.5
13	c1	2	SER	2.5
55	m9	151	ARG	2.5
20	C8	73	MET	2.5
23	d1	5	LYS	2.5
34	SR	72	THR	2.5
3	s1	152	ARG	2.5
16	C4	114	ARG	2.5
10	s8	150	ALA	2.5
12	c0	76	LEU	2.5
22	D0	116	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
30	d8	15	VAL	2.5
33	E1	148	TYR	2.5
81	p0	192	ASP	2.5
50	M4	8	LYS	2.5
14	c2	89	ILE	2.5
45	L8	252	ASN	2.5
21	C9	83	ALA	2.5
7	s5	35	GLN	2.5
19	c7	86	PRO	2.5
24	D2	85	ASP	2.5
14	C2	24	ILE	2.5
36	1	1244	A	2.5
36	1	2548	C	2.5
36	1	3154	C	2.5
58	n2	92	TRP	2.5
1	2	240	U	2.5
1	6	822	U	2.5
5	s3	63	GLY	2.5
14	C2	60	VAL	2.5
61	n5	32	PHE	2.5
14	C2	64	SER	2.5
35	SM	137	GLU	2.5
1	6	1236	A	2.4
22	d0	21	LYS	2.4
59	N3	3	GLY	2.4
61	N5	38	LEU	2.4
66	O0	38	LYS	2.4
1	2	711	U	2.4
1	6	670	U	2.4
72	O6	68	ARG	2.4
12	c0	70	GLU	2.4
30	D8	31	GLU	2.4
26	D4	69	SER	2.4
1	6	1245	G	2.4
7	S5	150	GLY	2.4
18	C6	105	LEU	2.4
29	d7	36	LYS	2.4
30	d8	7	VAL	2.4
34	sR	92	TRP	2.4
45	l8	45	ASN	2.4
52	M6	185	ALA	2.4
66	o0	105	ALA	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
10	s8	111	GLN	2.4
16	C4	73	GLU	2.4
18	c6	11	GLY	2.4
25	D3	2	GLY	2.4
66	O0	91	SER	2.4
14	c2	113	ARG	2.4
20	C8	28	ILE	2.4
36	5	1246	G	2.4
36	5	1952	G	2.4
1	6	829	A	2.4
3	S1	229	MET	2.4
5	s3	65	ARG	2.4
46	L9	100	ASN	2.4
10	s8	165	LEU	2.4
20	c8	144	ARG	2.4
36	1	3351	U	2.4
1	2	503	G	2.4
33	E1	137	ASP	2.4
10	S8	200	LYS	2.4
16	C4	69	ALA	2.4
45	l8	213	LYS	2.4
53	M7	177	ALA	2.4
14	C2	138	GLU	2.4
19	C7	110	VAL	2.4
33	E1	119	ARG	2.4
34	sR	28	GLY	2.4
19	C7	7	LYS	2.4
20	C8	23	ASP	2.4
8	S6	12	SER	2.4
14	C2	141	SER	2.4
36	5	2573	G	2.4
5	S3	179	GLN	2.4
11	s9	174	ARG	2.4
20	C8	63	GLN	2.4
44	l7	30	ARG	2.4
14	C2	80	ASN	2.4
32	e0	58	PRO	2.4
60	n4	129	LYS	2.4
26	d4	134	ALA	2.4
33	E1	145	HIS	2.4
36	1	1564	U	2.4
36	1	2570	U	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
81	p0	212	HIS	2.4
2	s0	165	ARG	2.4
14	c2	71	ILE	2.4
23	D1	34	ILE	2.4
36	1	2569	A	2.4
58	N2	98	THR	2.4
3	S1	144	ARG	2.4
1	2	75	U	2.4
1	6	74	U	2.4
7	S5	137	ILE	2.4
36	5	2097	U	2.4
36	1	1563	C	2.4
36	5	1631	C	2.4
59	n3	2	SER	2.4
6	S4	25	GLY	2.4
22	D0	27	THR	2.4
44	l7	22	THR	2.4
33	e1	82	LYS	2.4
34	sR	50	ASP	2.4
1	6	1708	U	2.4
16	C4	102	LEU	2.4
36	1	1014	U	2.4
36	1	1094	U	2.4
14	c2	104	GLY	2.4
45	l8	123	GLN	2.4
1	2	910	C	2.4
19	c7	11	ARG	2.4
36	1	439	C	2.4
36	1	2566	C	2.4
70	O4	110	GLU	2.4
5	s3	208	ILE	2.4
66	o0	32	LYS	2.4
11	s9	93	LEU	2.4
16	c4	102	LEU	2.4
20	C8	101	LEU	2.4
9	s7	85	PHE	2.4
36	1	547	G	2.4
36	1	1246	G	2.4
36	1	2538	U	2.4
59	N3	5	GLY	2.4
18	c6	143	ARG	2.4
78	q2	8	ARG	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
8	S6	173	PRO	2.4
19	c7	111	LYS	2.4
20	C8	47	CYS	2.4
3	s1	31	ASP	2.3
8	S6	154	ARG	2.3
13	c1	116	ARG	2.3
19	C7	124	VAL	2.3
19	c7	103	ASP	2.3
22	d0	23	ARG	2.3
45	L8	116	VAL	2.3
45	L8	123	GLN	2.3
78	Q2	106	PHE	2.3
7	s5	31	GLU	2.3
73	O7	87	SER	2.3
1	2	655	G	2.3
1	6	1445	G	2.3
36	5	1354	G	2.3
57	n1	128	LEU	2.3
16	c4	48	VAL	2.3
19	c7	56	HIS	2.3
60	N4	71	ARG	2.3
30	D8	35	ASP	2.3
42	L5	185	PHE	2.3
1	6	219	A	2.3
34	SR	69	GLN	2.3
36	1	1027	A	2.3
17	C5	51	SER	2.3
33	E1	106	TYR	2.3
34	SR	211	ILE	2.3
3	S1	148	ASN	2.3
26	d4	71	GLY	2.3
62	N6	92	GLY	2.3
36	5	1761	C	2.3
36	5	440	A	2.3
36	5	1030	A	2.3
1	2	1058	U	2.3
34	sR	117	LYS	2.3
36	5	1356	U	2.3
18	c6	46	PHE	2.3
66	o0	67	VAL	2.3
34	SR	25	THR	2.3
35	SM	50	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
14	C2	33	ARG	2.3
34	sR	190	ALA	2.3
36	5	1563	C	2.3
7	S5	149	VAL	2.3
12	c0	10	LYS	2.3
55	m9	2	ALA	2.3
29	d7	32	PHE	2.3
36	1	2996	U	2.3
36	5	3155	U	2.3
36	5	3283	U	2.3
14	C2	43	ARG	2.3
22	d0	104	THR	2.3
3	S1	203	ASP	2.3
5	s3	59	LEU	2.3
53	M7	182	ILE	2.3
14	c2	61	VAL	2.3
22	d0	97	VAL	2.3
1	6	652	G	2.3
34	SR	63	GLY	2.3
27	d5	38	HIS	2.3
34	sR	251	TRP	2.3
19	c7	69	ILE	2.3
42	L5	2	ALA	2.3
26	D4	129	VAL	2.3
9	s7	31	SER	2.3
18	C6	66	ARG	2.3
70	O4	16	ARG	2.3
22	d0	53	LYS	2.3
36	1	1248	C	2.3
70	o4	106	LYS	2.3
1	6	679	U	2.3
36	1	1222	G	2.3
33	E1	140	TYR	2.3
55	m9	115	ILE	2.3
49	m3	179	PHE	2.3
14	c2	40	GLY	2.3
22	D0	101	LYS	2.3
34	SR	261	LYS	2.3
1	6	654	C	2.3
8	S6	185	GLN	2.3
14	c2	62	LEU	2.3
1	2	278	U	2.3

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Mol	Chain	Res	Type	RSRZ
20	c8	14	ILE	2.3
30	D8	8	THR	2.3
32	e0	47	VAL	2.3
48	M1	127	PHE	2.3
1	2	228	G	2.3
14	C2	110	GLY	2.3
22	D0	54	GLY	2.3
1	2	706	A	2.3
57	n1	110	LYS	2.3
2	s0	24	LEU	2.3
14	c2	65	SER	2.3
20	c8	17	LEU	2.3
22	d0	103	ILE	2.3
9	S7	21	ALA	2.3
14	c2	31	VAL	2.3
22	D0	118	VAL	2.3
30	D8	15	VAL	2.3
41	l4	8	VAL	2.3
55	M9	177	VAL	2.3
1	2	847	A	2.3
3	s1	54	LEU	2.3
30	d8	65	ARG	2.3
36	1	251	G	2.3
34	SR	43	ILE	2.3
3	S1	160	HIS	2.3
26	d4	34	ASN	2.3
38	4	158	U	2.3
20	C8	18	LEU	2.3
2	S0	170	ILE	2.3
5	s3	148	LYS	2.3
45	l8	122	LYS	2.3
58	N2	83	TYR	2.3
66	O0	23	TYR	2.3
31	D9	4	GLU	2.2
55	m9	152	GLU	2.2
15	C3	104	ARG	2.2
22	d0	26	LEU	2.2
36	1	1765	U	2.2
36	1	1815	U	2.2
36	5	2537	U	2.2
6	S4	208	VAL	2.2
47	M0	217	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
78	q2	91	PHE	2.2
34	sR	213	SER	2.2
66	O0	105	ALA	2.2
36	1	1252	A	2.2
1	2	652	G	2.2
14	C2	135	MET	2.2
34	SR	32	LEU	2.2
58	n2	76	LEU	2.2
58	n2	105	LEU	2.2
36	1	1029	G	2.2
1	2	836	U	2.2
3	S1	133	TYR	2.2
22	D0	117	VAL	2.2
9	S7	42	GLN	2.2
36	5	1951	C	2.2
36	5	2098	C	2.2
63	n7	57	HIS	2.2
1	6	541	A	2.2
8	S6	226	ILE	2.2
58	n2	93	ILE	2.2
1	2	195	G	2.2
1	6	831	U	2.2
5	s3	131	ALA	2.2
34	SR	90	ARG	2.2
34	sR	187	GLN	2.2
47	M0	191	LYS	2.2
1	2	696	C	2.2
36	5	3164	C	2.2
8	S6	80	ASN	2.2
6	s4	134	LYS	2.2
15	C3	23	PRO	2.2
8	s6	190	GLN	2.2
55	M9	165	LYS	2.2
56	N0	2	ALA	2.2
1	2	820	U	2.2
36	1	601	U	2.2
72	O6	26	ILE	2.2
2	S0	110	TYR	2.2
6	s4	260	GLY	2.2
9	S7	87	ASP	2.2
21	C9	141	GLU	2.2
22	d0	113	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
26	D4	46	GLU	2.2
81	p0	82	GLY	2.2
33	e1	87	THR	2.2
3	S1	130	SER	2.2
15	C3	66	ILE	2.2
9	s7	95	GLU	2.2
74	o8	71	PRO	2.2
33	e1	115	THR	2.2
34	sR	32	LEU	2.2
14	C2	73	LYS	2.2
28	d6	80	HIS	2.2
66	O0	90	VAL	2.2
19	C7	86	PRO	2.2
23	D1	40	ASP	2.2
1	2	651	G	2.2
4	S2	90	THR	2.2
7	s5	122	ASN	2.2
37	3	73	C	2.2
14	c2	130	THR	2.2
18	c6	37	THR	2.2
58	N2	100	THR	2.2
74	o8	32	ASN	2.2
9	S7	90	VAL	2.2
1	6	836	U	2.2
22	d0	115	GLU	2.2
70	o4	110	GLU	2.2
32	e0	59	GLY	2.2
33	E1	126	CYS	2.2
36	5	2096	A	2.2
81	p0	216	ALA	2.2
1	2	708	C	2.2
30	d8	44	VAL	2.2
36	5	1582	C	2.2
18	c6	21	HIS	2.2
1	2	1243	G	2.2
1	6	712	G	2.2
36	1	1249	G	2.2
36	5	1268	G	2.2
49	M3	130	GLY	2.2
55	m9	113	GLY	2.2
72	O6	31	GLY	2.2
4	s2	247	ALA	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
10	S8	167	ALA	2.2
11	s9	177	ALA	2.2
66	O0	101	LEU	2.2
8	S6	16	PHE	2.2
3	S1	164	ILE	2.2
8	s6	162	VAL	2.2
19	c7	66	VAL	2.2
14	C2	104	GLY	2.2
3	S1	26	ARG	2.2
18	c6	49	TYR	2.2
44	l7	27	ALA	2.2
1	6	192	U	2.2
1	6	1247	U	2.2
1	6	1688	U	2.2
50	m4	2	SER	2.2
9	s7	63	PRO	2.2
1	2	733	A	2.2
8	s6	166	GLU	2.2
74	o8	27	ILE	2.2
14	C2	77	GLY	2.2
27	d5	51	LEU	2.1
1	6	1686	C	2.1
1	6	730	G	2.1
18	c6	72	GLY	2.1
9	s7	24	PHE	2.1
9	S7	73	VAL	2.1
1	2	781	U	2.1
1	2	1056	U	2.1
11	S9	89	ASP	2.1
30	D8	57	MET	2.1
36	5	1820	U	2.1
38	4	81	U	2.1
45	L8	207	ASP	2.1
62	N6	44	GLY	2.1
63	N7	5	LEU	2.1
27	d5	102	THR	2.1
29	d7	77	THR	2.1
41	l4	18	ASN	2.1
7	s5	127	GLN	2.1
8	s6	143	LYS	2.1
9	s7	48	GLU	2.1
55	m9	157	GLU	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
60	n4	74	LYS	2.1
14	C2	22	VAL	2.1
17	c5	109	PRO	2.1
34	sR	82	SER	2.1
1	2	1624	C	2.1
1	6	1687	U	2.1
6	S4	123	LEU	2.1
22	d0	58	LEU	2.1
36	5	981	U	2.1
2	S0	27	ARG	2.1
4	s2	92	ALA	2.1
9	S7	56	LYS	2.1
14	c2	100	TRP	2.1
48	M1	159	THR	2.1
49	M3	192	GLU	2.1
1	6	1344	A	2.1
14	c2	78	LEU	2.1
36	1	1580	A	2.1
1	6	821	U	2.1
26	D4	32	ARG	2.1
29	D7	32	PHE	2.1
33	E1	128	ALA	2.1
34	sR	253	ALA	2.1
36	1	545	U	2.1
36	1	1353	U	2.1
36	5	1568	U	2.1
49	M3	98	ASP	2.1
7	S5	182	ALA	2.1
14	c2	25	GLU	2.1
54	m8	95	GLU	2.1
55	m9	27	ASN	2.1
48	M1	90	GLN	2.1
9	S7	69	GLY	2.1
29	D7	41	LEU	2.1
29	d7	69	GLY	2.1
55	M9	4	LEU	2.1
3	S1	151	LYS	2.1
32	E0	53	LYS	2.1
72	o6	62	ARG	2.1
16	C4	13	VAL	2.1
17	c5	6	ASN	2.1
20	c8	21	ASN	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
9	S7	126	LEU	2.1
9	s7	176	LEU	2.1
30	D8	29	ARG	2.1
48	m1	174	LYS	2.1
9	S7	32	PRO	2.1
20	C8	58	ALA	2.1
46	l9	190	ASP	2.1
1	2	231	U	2.1
1	2	483	A	2.1
15	C3	5	HIS	2.1
18	c6	7	VAL	2.1
1	6	832	U	2.1
36	1	1030	A	2.1
36	1	2441	A	2.1
6	S4	77	ARG	2.1
8	s6	177	ARG	2.1
9	S7	105	THR	2.1
16	C4	110	LEU	2.1
30	d8	67	ARG	2.1
32	e0	48	THR	2.1
33	e1	92	LYS	2.1
74	o8	35	GLY	2.1
36	5	2572	C	2.1
34	SR	83	ALA	2.1
45	l8	107	GLU	2.1
30	d8	22	ARG	2.1
33	e1	83	LYS	2.1
33	e1	150	VAL	2.1
57	n1	126	VAL	2.1
36	1	1095	U	2.1
45	L8	152	LEU	2.1
62	n6	120	GLN	2.1
1	6	653	C	2.1
9	S7	80	GLU	2.1
36	5	547	G	2.1
9	s7	84	LYS	2.1
41	l4	346	LYS	2.1
53	M7	158	ALA	2.1
34	sR	310	ILE	2.1
75	O9	45	ARG	2.1
10	s8	118	GLY	2.1
18	C6	21	HIS	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
63	n7	58	GLY	2.1
1	2	232	U	2.1
3	S1	201	THR	2.1
34	SR	308	ASN	2.1
4	S2	249	ALA	2.1
24	D2	108	ALA	2.1
30	D8	67	ARG	2.1
49	M3	191	ALA	2.1
8	S6	3	LEU	2.1
47	m0	194	GLY	2.1
29	d7	59	CYS	2.1
33	e1	97	LYS	2.1
28	D6	62	TYR	2.1
14	c2	45	LEU	2.1
74	O8	5	ILE	2.1
1	2	848	C	2.1
2	s0	54	TRP	2.0
15	C3	108	ASP	2.1
2	S0	45	VAL	2.0
19	c7	53	TYR	2.0
36	5	2442	G	2.0
48	M1	167	TYR	2.0
32	e0	51	ASN	2.0
11	S9	60	LEU	2.0
14	c2	117	GLY	2.0
32	E0	38	LEU	2.0
30	d8	27	GLN	2.0
34	sR	54	PHE	2.0
36	1	1257	C	2.0
36	1	1283	C	2.0
12	c0	57	THR	2.0
1	2	1154	G	2.0
36	5	236	G	2.0
8	S6	155	ASP	2.0
11	s9	64	GLU	2.0
42	l5	274	GLN	2.0
63	N7	106	GLN	2.0
70	O4	73	SER	2.0
4	s2	86	VAL	2.0
45	l8	215	VAL	2.0
6	S4	162	ILE	2.0
8	S6	52	ILE	2.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
16	C4	76	ILE	2.0
22	D0	99	ILE	2.0
22	D0	103	ILE	2.0
23	D1	69	LEU	2.0
27	d5	89	ILE	2.0
36	5	1759	C	2.0
64	N8	94	ALA	2.0
78	q2	72	LEU	2.0
12	c0	77	ARG	2.0
42	L5	297	GLN	2.0
5	s3	160	SER	2.0
5	S3	41	VAL	2.0
7	S5	209	TYR	2.0
34	SR	283	LYS	2.0
34	sR	58	VAL	2.0
3	S1	228	LEU	2.0
14	C2	69	ALA	2.0
49	m3	190	LYS	2.0
1	2	541	A	2.0
1	6	713	A	2.0
57	N1	148	PRO	2.0
36	1	1258	U	2.0
36	1	1950	U	2.0
3	S1	131	ASP	2.0
34	SR	92	TRP	2.0
45	L8	97	TYR	2.0
53	M7	164	LYS	2.0
81	p0	188	VAL	2.0
9	s7	41	LEU	2.0
13	c1	145	ALA	2.0
1	2	1486	G	2.0
1	2	1601	G	2.0
9	s7	92	PHE	2.0
5	S3	43	PRO	2.0
1	2	1346	A	2.0
1	6	579	A	2.0
36	5	1091	A	2.0
48	m1	108	GLU	2.0
1	6	1447	C	2.0
11	s9	91	LYS	2.0
74	o8	74	LYS	2.0
14	C2	66	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
22	d0	114	VAL	2.0
22	d0	116	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	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	16	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	4043	1/1	0.62	0.72	33,33,33,33	0
84	MG	1	3494	1/1	0.62	0.38	52,52,52,52	0
84	MG	5	3613	1/1	0.63	0.34	58,58,58,58	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	1	3714	1/1	0.64	0.22	45,45,45,45	0
84	MG	1	3722	1/1	0.65	0.37	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	MG	5	3460	1/1	0.65	0.29	44,44,44,44	0
84	MG	5	3462	1/1	0.65	0.29	58,58,58,58	0
84	MG	1	3570	1/1	0.66	0.69	67,67,67,67	0
84	MG	2	1904	1/1	0.66	0.67	77,77,77,77	0
84	MG	6	1961	1/1	0.66	0.43	61,61,61,61	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	2	1969	1/1	0.69	0.71	66,66,66,66	0
84	MG	1	3496	1/1	0.69	0.48	39,39,39,39	0
84	MG	5	3715	1/1	0.69	0.29	39,39,39,39	0
84	MG	5	3426	1/1	0.69	0.30	36,36,36,36	0
84	MG	1	3673	1/1	0.69	0.51	65,65,65,65	0
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	5	3409	1/1	0.71	0.26	58,58,58,58	0
84	MG	2	1972	1/1	0.71	0.50	71,71,71,71	0
84	MG	6	1969	1/1	0.71	0.48	65,65,65,65	0
84	MG	5	3709	1/1	0.71	0.41	61,61,61,61	0
84	MG	2	1909	1/1	0.71	0.58	81,81,81,81	0
84	MG	4	202	1/1	0.71	0.54	57,57,57,57	0
84	MG	1	3414	1/1	0.71	0.45	63,63,63,63	0
84	MG	1	3663	1/1	0.71	0.30	36,36,36,36	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	5	3404	1/1	0.73	0.24	33,33,33,33	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	l3	402	1/1	0.73	0.24	32,32,32,32	0
84	MG	6	1993	1/1	0.73	0.36	95,95,95,95	0
84	MG	m7	201	1/1	0.73	0.31	37,37,37,37	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	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	2	1938	1/1	0.74	0.36	75,75,75,75	0
84	MG	1	3712	1/1	0.74	0.28	41,41,41,41	0
84	MG	6	2002	1/1	0.74	0.65	99,99,99,99	0
84	MG	5	3655	1/1	0.74	0.60	64,64,64,64	0
84	MG	1	3630	1/1	0.74	0.57	56,56,56,56	0
84	MG	6	2008	1/1	0.75	0.44	47,47,47,47	0
84	MG	1	3655	1/1	0.75	0.29	41,41,41,41	0
84	MG	2	1978	1/1	0.75	0.74	104,104,104,104	0
84	MG	5	3476	1/1	0.75	0.58	51,51,51,51	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	1	3508	1/1	0.76	0.39	43,43,43,43	0
84	MG	5	3697	1/1	0.76	0.29	50,50,50,50	0
84	MG	2	1979	1/1	0.76	0.40	72,72,72,72	0
84	MG	1	3639	1/1	0.76	0.43	59,59,59,59	0
84	MG	8	207	1/1	0.76	0.45	51,51,51,51	0
84	MG	1	3408	1/1	0.77	0.33	50,50,50,50	0
84	MG	5	3731	1/1	0.77	0.57	37,37,37,37	0
84	MG	5	3738	1/1	0.77	0.38	45,45,45,45	0
84	MG	2	1923	1/1	0.77	0.51	56,56,56,56	0
84	MG	2	1915	1/1	0.77	0.59	76,76,76,76	0
84	MG	6	1917	1/1	0.77	1.38	75,75,75,75	0
84	MG	5	3438	1/1	0.77	0.36	45,45,45,45	0
84	MG	5	3614	1/1	0.77	0.25	55,55,55,55	0
84	MG	6	1938	1/1	0.77	0.50	99,99,99,99	0
84	MG	5	3635	1/1	0.78	0.18	66,66,66,66	0
84	MG	1	3707	1/1	0.78	0.35	53,53,53,53	0
84	MG	5	3722	1/1	0.78	0.31	55,55,55,55	0
84	MG	5	3463	1/1	0.78	0.37	41,41,41,41	0
84	MG	5	3732	1/1	0.78	0.30	52,52,52,52	0
84	MG	5	3645	1/1	0.78	0.31	33,33,33,33	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	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	3701	1/1	0.78	0.27	40,40,40,40	0
84	MG	6	1908	1/1	0.78	0.20	51,51,51,51	0
84	MG	5	3667	1/1	0.79	0.30	38,38,38,38	0
84	MG	1	3666	1/1	0.79	0.24	45,45,45,45	0
84	MG	2	1975	1/1	0.79	0.35	76,76,76,76	0
84	MG	O4	202	1/1	0.79	0.37	67,67,67,67	0
84	MG	1	3568	1/1	0.79	0.52	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	MG	1	3638	1/1	0.79	0.19	46,46,46,46	0
84	MG	6	1911	1/1	0.79	0.30	52,52,52,52	0
84	MG	6	2001	1/1	0.79	0.42	73,73,73,73	0
84	MG	2	1946	1/1	0.79	0.63	93,93,93,93	0
84	MG	6	1930	1/1	0.79	0.56	59,59,59,59	0
84	MG	5	3632	1/1	0.79	0.43	42,42,42,42	0
84	MG	1	3694	1/1	0.79	0.47	41,41,41,41	0
84	MG	2	1911	1/1	0.79	0.82	69,69,69,69	0
84	MG	1	3430	1/1	0.79	0.30	36,36,36,36	0
84	MG	4	208	1/1	0.79	0.27	54,54,54,54	0
84	MG	5	3450	1/1	0.79	0.25	58,58,58,58	0
84	MG	5	3453	1/1	0.79	0.23	42,42,42,42	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	1	3442	1/1	0.80	0.15	41,41,41,41	0
84	MG	5	3407	1/1	0.80	0.25	33,33,33,33	0
84	MG	5	3636	1/1	0.80	0.45	44,44,44,44	0
84	MG	6	1994	1/1	0.80	0.25	49,49,49,49	0
84	MG	1	3437	1/1	0.80	0.20	45,45,45,45	0
84	MG	5	3467	1/1	0.80	0.62	65,65,65,65	0
84	MG	1	3685	1/1	0.80	0.29	39,39,39,39	0
84	MG	5	3542	1/1	0.80	0.53	36,36,36,36	0
84	MG	5	3585	1/1	0.80	0.30	39,39,39,39	0
84	MG	19	201	1/1	0.80	0.22	45,45,45,45	0
84	MG	5	3598	1/1	0.80	0.17	42,42,42,42	0
84	MG	5	3685	1/1	0.80	0.28	36,36,36,36	0
84	MG	4	210	1/1	0.80	0.38	58,58,58,58	0
84	MG	2	1947	1/1	0.81	1.03	93,93,93,93	0
84	MG	6	1995	1/1	0.81	0.71	52,52,52,52	0
84	MG	5	3723	1/1	0.81	0.42	38,38,38,38	0
84	MG	5	3574	1/1	0.81	0.42	53,53,53,53	0
84	MG	1	3417	1/1	0.81	0.47	58,58,58,58	0
84	MG	Q2	502	1/1	0.81	0.14	55,55,55,55	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	12	302	1/1	0.81	0.37	42,42,42,42	0
84	MG	1	3456	1/1	0.81	0.18	32,32,32,32	0
84	MG	1	3688	1/1	0.81	0.22	47,47,47,47	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	n6	201	1/1	0.81	0.39	65,65,65,65	0
84	MG	6	1928	1/1	0.81	0.51	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	4039	1/1	0.81	0.42	46,46,46,46	0
84	MG	5	3461	1/1	0.82	0.19	40,40,40,40	0
84	MG	5	3728	1/1	0.82	0.32	50,50,50,50	0
84	MG	5	3608	1/1	0.82	0.41	89,89,89,89	0
84	MG	5	3664	1/1	0.82	0.19	53,53,53,53	0
84	MG	2	1971	1/1	0.82	0.33	77,77,77,77	0
84	MG	1	3697	1/1	0.82	0.51	41,41,41,41	0
84	MG	2	1961	1/1	0.82	0.22	75,75,75,75	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	3657	1/1	0.82	0.33	50,50,50,50	0
84	MG	5	3701	1/1	0.82	0.45	47,47,47,47	0
84	MG	5	3704	1/1	0.82	0.44	54,54,54,54	0
84	MG	1	3690	1/1	0.82	0.31	48,48,48,48	0
84	MG	5	3595	1/1	0.82	0.13	60,60,60,60	0
84	MG	6	1926	1/1	0.82	0.56	46,46,46,46	0
84	MG	5	3640	1/1	0.83	0.27	51,51,51,51	0
84	MG	1	3720	1/1	0.83	0.18	56,56,56,56	0
84	MG	1	3611	1/1	0.83	0.26	39,39,39,39	0
84	MG	5	3727	1/1	0.83	0.23	62,62,62,62	0
84	MG	6	2006	1/1	0.83	0.56	61,61,61,61	0
84	MG	1	3457	1/1	0.83	0.46	42,42,42,42	0
84	MG	1	3629	1/1	0.83	0.46	74,74,74,74	0
84	MG	1	3710	1/1	0.83	0.32	40,40,40,40	0
84	MG	5	3604	1/1	0.83	0.42	36,36,36,36	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	1	3692	1/1	0.83	0.35	45,45,45,45	0
84	MG	13	405	1/1	0.83	0.69	34,34,34,34	0
84	MG	6	1956	1/1	0.83	0.64	60,60,60,60	0
84	MG	18	301	1/1	0.83	0.65	83,83,83,83	0
84	MG	1	3424	1/1	0.83	0.45	45,45,45,45	0
84	MG	5	3470	1/1	0.83	0.37	32,32,32,32	0
84	MG	5	3471	1/1	0.83	0.34	68,68,68,68	0
84	MG	1	3637	1/1	0.83	0.42	42,42,42,42	0
84	MG	5	3485	1/1	0.83	0.34	37,37,37,37	0
84	MG	1	3527	1/1	0.84	0.23	64,64,64,64	0
84	MG	1	3618	1/1	0.84	0.29	62,62,62,62	0
84	MG	5	3642	1/1	0.84	0.32	37,37,37,37	0
84	MG	2	1937	1/1	0.84	0.39	79,79,79,79	0
84	MG	5	3644	1/1	0.84	0.32	72,72,72,72	0
84	MG	1	3560	1/1	0.84	0.34	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	6	1970	1/1	0.84	0.47	98,98,98,98	0
84	MG	5	3651	1/1	0.84	0.37	46,46,46,46	0
84	MG	6	1922	1/1	0.84	0.54	48,48,48,48	0
84	MG	2	1921	1/1	0.84	0.69	81,81,81,81	0
84	MG	1	3696	1/1	0.84	0.32	55,55,55,55	0
84	MG	6	1990	1/1	0.84	0.18	61,61,61,61	0
84	MG	5	3675	1/1	0.84	0.18	59,59,59,59	0
84	MG	5	3413	1/1	0.84	0.33	41,41,41,41	0
84	MG	5	3681	1/1	0.84	0.49	40,40,40,40	0
84	MG	17	301	1/1	0.84	0.18	37,37,37,37	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	m5	303	1/1	0.84	0.51	46,46,46,46	0
84	MG	5	3624	1/1	0.84	0.21	41,41,41,41	0
84	MG	1	3516	1/1	0.84	0.65	40,40,40,40	0
84	MG	n6	202	1/1	0.84	0.39	52,52,52,52	0
84	MG	5	3532	1/1	0.84	0.68	50,50,50,50	0
84	MG	5	3541	1/1	0.84	0.39	50,50,50,50	0
84	MG	5	3710	1/1	0.85	0.21	44,44,44,44	0
84	MG	2	1924	1/1	0.85	0.85	86,86,86,86	0
84	MG	6	1916	1/1	0.85	0.46	46,46,46,46	0
84	MG	5	3411	1/1	0.85	0.34	34,34,34,34	0
84	MG	4	204	1/1	0.85	0.57	51,51,51,51	0
84	MG	5	3421	1/1	0.85	0.34	50,50,50,50	0
84	MG	5	3555	1/1	0.85	0.33	44,44,44,44	0
84	MG	1	3405	1/1	0.85	0.71	63,63,63,63	0
84	MG	1	3468	1/1	0.85	0.14	59,59,59,59	0
84	MG	5	3588	1/1	0.85	0.33	57,57,57,57	0
84	MG	8	206	1/1	0.85	0.58	52,52,52,52	0
84	MG	5	3444	1/1	0.85	0.22	32,32,32,32	0
84	MG	1	3472	1/1	0.85	0.36	52,52,52,52	0
84	MG	1	3693	1/1	0.85	0.27	58,58,58,58	0
84	MG	M7	201	1/1	0.85	0.48	60,60,60,60	0
84	MG	6	1942	1/1	0.85	0.98	79,79,79,79	0
84	MG	1	3477	1/1	0.85	0.27	54,54,54,54	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	1	3439	1/1	0.85	0.26	60,60,60,60	0
84	MG	1	3569	1/1	0.85	0.46	53,53,53,53	0
84	MG	d6	102	1/1	0.85	0.49	56,56,56,56	0
86	ZN	D7	101	1/1	0.85	0.35	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	5	3403	1/1	0.85	0.16	45,45,45,45	0
84	MG	1	3411	1/1	0.85	0.44	51,51,51,51	0
84	MG	1	3619	1/1	0.86	0.29	35,35,35,35	0
84	MG	5	3619	1/1	0.86	0.19	37,37,37,37	0
84	MG	5	3621	1/1	0.86	0.34	40,40,40,40	0
84	MG	2	1976	1/1	0.86	0.72	68,68,68,68	0
84	MG	5	3625	1/1	0.86	0.15	44,44,44,44	0
84	MG	5	3516	1/1	0.86	0.40	31,31,31,31	0
84	MG	5	3531	1/1	0.86	0.46	56,56,56,56	0
84	MG	1	3517	1/1	0.86	0.45	51,51,51,51	0
84	MG	5	3540	1/1	0.86	0.54	28,28,28,28	0
84	MG	1	3458	1/1	0.86	0.32	59,59,59,59	0
84	MG	1	3598	1/1	0.86	0.29	39,39,39,39	0
84	MG	5	3544	1/1	0.86	0.46	32,32,32,32	0
84	MG	2	1940	1/1	0.86	0.71	72,72,72,72	0
84	MG	5	3559	1/1	0.86	0.35	40,40,40,40	0
84	MG	5	4078	1/1	0.86	0.57	40,40,40,40	0
84	MG	6	1962	1/1	0.86	0.17	84,84,84,84	0
84	MG	6	2003	1/1	0.86	1.02	63,63,63,63	0
84	MG	1	3684	1/1	0.86	0.82	51,51,51,51	0
84	MG	5	3657	1/1	0.86	0.21	57,57,57,57	0
84	MG	1	3610	1/1	0.86	0.61	42,42,42,42	0
84	MG	5	3666	1/1	0.86	0.21	37,37,37,37	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	4	214	1/1	0.86	0.41	53,53,53,53	0
84	MG	5	3676	1/1	0.86	0.17	63,63,63,63	0
84	MG	5	3406	1/1	0.86	0.13	47,47,47,47	0
84	MG	5	3680	1/1	0.86	0.22	53,53,53,53	0
84	MG	6	1982	1/1	0.86	0.22	46,46,46,46	0
84	MG	5	3684	1/1	0.86	0.19	77,77,77,77	0
84	MG	L3	401	1/1	0.86	0.86	53,53,53,53	0
84	MG	2	1933	1/1	0.86	0.48	74,74,74,74	0
84	MG	5	3616	1/1	0.86	0.37	40,40,40,40	0
84	MG	5	3503	1/1	0.87	0.28	40,40,40,40	0
84	MG	2	1964	1/1	0.87	0.33	83,83,83,83	0
84	MG	5	3526	1/1	0.87	0.37	38,38,38,38	0
84	MG	5	3638	1/1	0.87	0.24	37,37,37,37	0
84	MG	5	3711	1/1	0.87	0.10	32,32,32,32	0
84	MG	1	3626	1/1	0.87	0.27	44,44,44,44	0
84	MG	2	1936	1/1	0.87	0.67	73,73,73,73	0
84	MG	5	3408	1/1	0.87	0.39	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	MG	O7	102	1/1	0.87	0.47	51,51,51,51	0
84	MG	1	3681	1/1	0.87	0.16	45,45,45,45	0
84	MG	1	3589	1/1	0.87	0.14	64,64,64,64	0
84	MG	5	3419	1/1	0.87	0.14	41,41,41,41	0
84	MG	5	3736	1/1	0.87	0.31	48,48,48,48	0
84	MG	6	1902	1/1	0.87	0.38	57,57,57,57	0
84	MG	1	3631	1/1	0.87	0.56	49,49,49,49	0
84	MG	1	3590	1/1	0.87	0.40	60,60,60,60	0
84	MG	7	206	1/1	0.87	0.45	42,42,42,42	0
84	MG	1	3448	1/1	0.87	0.40	64,64,64,64	0
84	MG	1	3548	1/1	0.87	0.27	31,31,31,31	0
84	MG	1	3608	1/1	0.87	0.48	87,87,87,87	0
84	MG	6	1919	1/1	0.87	0.66	67,67,67,67	0
84	MG	1	3649	1/1	0.87	0.26	43,43,43,43	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	3471	1/1	0.87	0.24	58,58,58,58	0
84	MG	4	212	1/1	0.87	0.20	54,54,54,54	0
84	MG	1	3616	1/1	0.87	0.47	81,81,81,81	0
84	MG	1	3449	1/1	0.87	0.99	64,64,64,64	0
84	MG	5	3686	1/1	0.87	0.25	44,44,44,44	0
84	MG	2	1932	1/1	0.87	0.58	68,68,68,68	0
85	OHX	1	4012	7/7	0.87	0.38	116,116,116,116	0
84	MG	6	1947	1/1	0.87	0.53	53,53,53,53	0
84	MG	6	1951	1/1	0.87	0.49	77,77,77,77	0
84	MG	6	1955	1/1	0.87	1.13	67,67,67,67	0
84	MG	1	3429	1/1	0.88	0.53	51,51,51,51	0
84	MG	1	3510	1/1	0.88	0.36	31,31,31,31	0
84	MG	1	3650	1/1	0.88	0.56	81,81,81,81	0
84	MG	1	3724	1/1	0.88	0.46	49,49,49,49	0
84	MG	1	3689	1/1	0.88	0.32	57,57,57,57	0
84	MG	1	3652	1/1	0.88	0.25	57,57,57,57	0
84	MG	1	3620	1/1	0.88	0.42	54,54,54,54	0
84	MG	3	202	1/1	0.88	0.68	67,67,67,67	0
84	MG	6	1976	1/1	0.88	0.19	91,91,91,91	0
84	MG	3	203	1/1	0.88	0.29	44,44,44,44	0
84	MG	1	3656	1/1	0.88	0.44	46,46,46,46	0
84	MG	2	1965	1/1	0.88	0.72	60,60,60,60	0
84	MG	1	3431	1/1	0.88	0.17	51,51,51,51	0
84	MG	1	3601	1/1	0.88	0.32	65,65,65,65	0
84	MG	6	1927	1/1	0.88	0.40	50,50,50,50	0
84	MG	1	3526	1/1	0.88	0.21	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	5	3601	1/1	0.88	0.42	38,38,38,38	0
84	MG	S4	301	1/1	0.88	0.32	79,79,79,79	0
84	MG	6	1932	1/1	0.88	0.76	62,62,62,62	0
84	MG	6	1937	1/1	0.88	0.78	72,72,72,72	0
84	MG	5	3610	1/1	0.88	0.29	37,37,37,37	0
84	MG	1	3708	1/1	0.88	0.28	60,60,60,60	0
84	MG	1	3582	1/1	0.88	0.28	45,45,45,45	0
84	MG	m5	301	1/1	0.88	0.26	48,48,48,48	0
84	MG	1	3615	1/1	0.88	0.33	31,31,31,31	0
84	MG	1	3679	1/1	0.88	0.24	34,34,34,34	0
84	MG	n0	202	1/1	0.88	0.16	40,40,40,40	0
84	MG	c1	201	1/1	0.88	0.44	53,53,53,53	0
84	MG	M7	204	1/1	0.88	0.23	40,40,40,40	0
84	MG	n9	101	1/1	0.88	0.38	33,33,33,33	0
84	MG	5	3482	1/1	0.88	0.12	33,33,33,33	0
84	MG	5	3402	1/1	0.88	0.66	61,61,61,61	0
84	MG	5	3501	1/1	0.88	0.53	27,27,27,27	0
84	MG	2	1954	1/1	0.88	0.49	90,90,90,90	0
84	MG	1	3704	1/1	0.89	0.36	34,34,34,34	0
84	MG	5	3671	1/1	0.89	0.28	35,35,35,35	0
84	MG	2	1943	1/1	0.89	0.75	71,71,71,71	0
84	MG	1	3441	1/1	0.89	0.32	31,31,31,31	0
84	MG	1	3664	1/1	0.89	0.33	36,36,36,36	0
84	MG	N3	201	1/1	0.89	0.35	40,40,40,40	0
84	MG	2	1955	1/1	0.89	0.33	68,68,68,68	0
84	MG	5	3566	1/1	0.89	0.56	46,46,46,46	0
84	MG	5	3571	1/1	0.89	0.78	53,53,53,53	0
84	MG	2	1902	1/1	0.89	0.41	55,55,55,55	0
84	MG	5	3581	1/1	0.89	0.57	35,35,35,35	0
84	MG	5	3583	1/1	0.89	0.12	42,42,42,42	0
84	MG	6	1963	1/1	0.89	0.32	76,76,76,76	0
84	MG	5	3587	1/1	0.89	0.32	39,39,39,39	0
84	MG	2	1939	1/1	0.89	0.43	74,74,74,74	0
84	MG	6	1966	1/1	0.89	0.40	53,53,53,53	0
84	MG	1	3450	1/1	0.89	0.37	33,33,33,33	0
84	MG	5	3705	1/1	0.89	0.14	36,36,36,36	0
84	MG	5	3707	1/1	0.89	0.16	43,43,43,43	0
84	MG	2	1919	1/1	0.89	0.70	73,73,73,73	0
84	MG	5	3428	1/1	0.89	0.52	39,39,39,39	0
84	MG	1	3721	1/1	0.89	0.56	42,42,42,42	0
84	MG	5	3712	1/1	0.89	0.24	44,44,44,44	0
84	MG	5	3442	1/1	0.89	0.32	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	6	1975	1/1	0.89	0.32	79,79,79,79	0
84	MG	5	3445	1/1	0.89	0.60	49,49,49,49	0
84	MG	1	3587	1/1	0.89	0.20	42,42,42,42	0
84	MG	6	1910	1/1	0.89	0.40	74,74,74,74	0
84	MG	5	3615	1/1	0.89	0.56	56,56,56,56	0
84	MG	1	3723	1/1	0.89	0.30	37,37,37,37	0
84	MG	2	1982	1/1	0.89	0.27	65,65,65,65	0
84	MG	1	3634	1/1	0.89	0.38	39,39,39,39	0
84	MG	2	1905	1/1	0.89	0.77	63,63,63,63	0
84	MG	5	3622	1/1	0.89	0.17	55,55,55,55	0
84	MG	1	3461	1/1	0.89	0.35	36,36,36,36	0
84	MG	1	3462	1/1	0.89	0.31	38,38,38,38	0
84	MG	1	3600	1/1	0.89	0.34	52,52,52,52	0
84	MG	12	301	1/1	0.89	0.60	48,48,48,48	0
84	MG	1	3643	1/1	0.89	0.52	63,63,63,63	0
84	MG	1	3466	1/1	0.89	0.74	57,57,57,57	0
84	MG	1	3528	1/1	0.89	0.36	34,34,34,34	0
84	MG	1	3416	1/1	0.89	0.41	48,48,48,48	0
84	MG	5	3478	1/1	0.89	0.21	45,45,45,45	0
84	MG	6	2005	1/1	0.89	0.51	61,61,61,61	0
84	MG	4	211	1/1	0.89	0.23	42,42,42,42	0
84	MG	5	3487	1/1	0.89	0.42	32,32,32,32	0
84	MG	6	2007	1/1	0.89	0.29	61,61,61,61	0
84	MG	5	3646	1/1	0.89	0.18	35,35,35,35	0
84	MG	1	3538	1/1	0.89	0.42	42,42,42,42	0
84	MG	5	3507	1/1	0.89	0.43	44,44,44,44	0
84	MG	s8	301	1/1	0.89	0.32	47,47,47,47	0
84	MG	1	3700	1/1	0.89	0.46	36,36,36,36	0
85	OHX	2	2115	7/7	0.89	0.41	115,115,115,115	0
84	MG	5	3659	1/1	0.89	0.29	41,41,41,41	0
85	OHX	5	3938	7/7	0.89	0.22	115,115,115,115	0
85	OHX	5	4043	7/7	0.89	0.43	96,96,96,96	0
85	OHX	5	4068	7/7	0.89	0.27	96,96,96,96	0
84	MG	5	3662	1/1	0.89	0.26	34,34,34,34	0
84	MG	1	3438	1/1	0.89	0.32	32,32,32,32	0
84	MG	sM	201	1/1	0.89	0.32	44,44,44,44	0
84	MG	1	3460	1/1	0.90	0.28	52,52,52,52	0
84	MG	4	207	1/1	0.90	0.25	49,49,49,49	0
84	MG	5	3477	1/1	0.90	0.21	42,42,42,42	0
84	MG	5	3696	1/1	0.90	0.21	31,31,31,31	0
84	MG	2	1963	1/1	0.90	0.58	78,78,78,78	0
84	MG	5	3698	1/1	0.90	0.35	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	5	3480	1/1	0.90	0.21	36,36,36,36	0
84	MG	1	3484	1/1	0.90	0.40	52,52,52,52	0
84	MG	1	3641	1/1	0.90	0.29	51,51,51,51	0
84	MG	1	3642	1/1	0.90	0.23	48,48,48,48	0
84	MG	5	3498	1/1	0.90	0.55	41,41,41,41	0
84	MG	5	3499	1/1	0.90	0.31	36,36,36,36	0
84	MG	1	3713	1/1	0.90	0.19	45,45,45,45	0
84	MG	6	1979	1/1	0.90	0.30	52,52,52,52	0
84	MG	6	1981	1/1	0.90	0.38	57,57,57,57	0
84	MG	5	3631	1/1	0.90	0.24	41,41,41,41	0
84	MG	5	3509	1/1	0.90	0.36	47,47,47,47	0
84	MG	5	3511	1/1	0.90	0.34	62,62,62,62	0
84	MG	5	3515	1/1	0.90	0.45	52,52,52,52	0
84	MG	5	3637	1/1	0.90	0.32	49,49,49,49	0
84	MG	2	1901	1/1	0.90	1.24	85,85,85,85	0
84	MG	1	3452	1/1	0.90	0.43	38,38,38,38	0
84	MG	5	3737	1/1	0.90	0.08	52,52,52,52	0
84	MG	6	1987	1/1	0.90	0.14	55,55,55,55	0
84	MG	5	3739	1/1	0.90	0.30	88,88,88,88	0
84	MG	5	4076	1/1	0.90	0.50	52,52,52,52	0
84	MG	6	1988	1/1	0.90	0.27	73,73,73,73	0
84	MG	5	3538	1/1	0.90	0.52	41,41,41,41	0
84	MG	1	3467	1/1	0.90	0.23	47,47,47,47	0
84	MG	8	204	1/1	0.90	0.21	56,56,56,56	0
84	MG	8	205	1/1	0.90	0.25	48,48,48,48	0
84	MG	6	1934	1/1	0.90	0.29	67,67,67,67	0
84	MG	1	3539	1/1	0.90	0.52	44,44,44,44	0
84	MG	1	3420	1/1	0.90	0.10	38,38,38,38	0
84	MG	5	3650	1/1	0.90	0.11	46,46,46,46	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	1	3549	1/1	0.90	0.38	53,53,53,53	0
84	MG	5	3446	1/1	0.90	0.33	45,45,45,45	0
84	MG	5	3447	1/1	0.90	0.57	34,34,34,34	0
84	MG	5	3660	1/1	0.90	0.34	41,41,41,41	0
84	MG	5	3448	1/1	0.90	0.32	28,28,28,28	0
84	MG	6	1945	1/1	0.90	0.41	66,66,66,66	0
84	MG	5	3578	1/1	0.90	0.82	40,40,40,40	0
84	MG	m7	203	1/1	0.90	0.41	40,40,40,40	0
84	MG	1	3404	1/1	0.90	0.23	42,42,42,42	0
84	MG	5	3668	1/1	0.90	0.46	71,71,71,71	0
84	MG	1	3658	1/1	0.90	0.33	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	MG	1	4040	1/1	0.90	0.35	39,39,39,39	0
84	MG	o3	201	1/1	0.90	0.29	49,49,49,49	0
84	MG	q1	101	1/1	0.90	0.57	47,47,47,47	0
84	MG	1	3659	1/1	0.90	0.45	47,47,47,47	0
85	OHX	1	3931	7/7	0.90	0.27	111,111,111,111	0
84	MG	1	3554	1/1	0.90	0.39	32,32,32,32	0
85	OHX	6	2158	7/7	0.90	0.35	140,140,140,140	0
84	MG	2	1910	1/1	0.90	0.43	64,64,64,64	0
84	MG	5	3597	1/1	0.90	0.27	29,29,29,29	0
84	MG	1	3605	1/1	0.90	0.19	46,46,46,46	0
84	MG	1	3561	1/1	0.90	0.43	43,43,43,43	0
84	MG	4	203	1/1	0.90	0.48	68,68,68,68	0
84	MG	6	1915	1/1	0.90	0.27	72,72,72,72	0
84	MG	2	1960	1/1	0.91	1.10	72,72,72,72	0
84	MG	5	3639	1/1	0.91	0.17	40,40,40,40	0
84	MG	5	3714	1/1	0.91	0.24	34,34,34,34	0
84	MG	6	1929	1/1	0.91	0.30	67,67,67,67	0
84	MG	2	1952	1/1	0.91	0.98	77,77,77,77	0
84	MG	1	3407	1/1	0.91	0.45	45,45,45,45	0
84	MG	1	3623	1/1	0.91	0.19	51,51,51,51	0
84	MG	L6	201	1/1	0.91	0.14	48,48,48,48	0
84	MG	5	3729	1/1	0.91	0.22	52,52,52,52	0
84	MG	1	3427	1/1	0.91	0.41	48,48,48,48	0
84	MG	2	1953	1/1	0.91	0.94	84,84,84,84	0
84	MG	6	2000	1/1	0.91	0.28	86,86,86,86	0
84	MG	1	3584	1/1	0.91	0.88	54,54,54,54	0
84	MG	1	3585	1/1	0.91	0.70	59,59,59,59	0
84	MG	1	3531	1/1	0.91	0.72	45,45,45,45	0
84	MG	5	3741	1/1	0.91	0.31	54,54,54,54	0
84	MG	5	4073	1/1	0.91	0.78	31,31,31,31	0
84	MG	5	3653	1/1	0.91	0.17	67,67,67,67	0
84	MG	1	3491	1/1	0.91	0.55	41,41,41,41	0
84	MG	2	1942	1/1	0.91	0.20	69,69,69,69	0
84	MG	7	204	1/1	0.91	0.49	40,40,40,40	0
84	MG	1	3595	1/1	0.91	0.28	50,50,50,50	0
84	MG	6	1957	1/1	0.91	0.46	63,63,63,63	0
84	MG	6	2160	1/1	0.91	0.31	84,84,84,84	0
84	MG	5	3593	1/1	0.91	0.36	54,54,54,54	0
84	MG	5	3594	1/1	0.91	0.25	40,40,40,40	0
84	MG	6	1901	1/1	0.91	0.37	50,50,50,50	0
84	MG	1	3597	1/1	0.91	0.28	46,46,46,46	0
84	MG	5	3669	1/1	0.91	0.39	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	l3	403	1/1	0.91	0.38	38,38,38,38	0
84	MG	2	1918	1/1	0.91	0.77	64,64,64,64	0
84	MG	5	3672	1/1	0.91	0.34	40,40,40,40	0
84	MG	1	3542	1/1	0.91	0.33	46,46,46,46	0
84	MG	1	3543	1/1	0.91	0.36	34,34,34,34	0
84	MG	1	3503	1/1	0.91	0.57	33,33,33,33	0
84	MG	5	3677	1/1	0.91	0.39	41,41,41,41	0
84	MG	6	1912	1/1	0.91	0.32	79,79,79,79	0
84	MG	6	1913	1/1	0.91	0.53	51,51,51,51	0
84	MG	1	3645	1/1	0.91	0.21	69,69,69,69	0
84	MG	1	3506	1/1	0.91	0.53	42,42,42,42	0
84	MG	5	3500	1/1	0.91	0.38	47,47,47,47	0
84	MG	2	1935	1/1	0.91	0.35	68,68,68,68	0
84	MG	1	3651	1/1	0.91	0.20	36,36,36,36	0
84	MG	2	1957	1/1	0.91	0.57	76,76,76,76	0
84	MG	q0	202	1/1	0.91	0.28	44,44,44,44	0
84	MG	5	3690	1/1	0.91	0.43	30,30,30,30	0
85	OHX	2	2108	7/7	0.91	0.25	145,145,145,145	0
84	MG	5	3418	1/1	0.91	0.31	41,41,41,41	0
85	OHX	2	2118	7/7	0.91	0.30	132,132,132,132	0
85	OHX	1	3921	7/7	0.91	0.32	110,110,110,110	0
84	MG	6	1980	1/1	0.91	0.28	68,68,68,68	0
84	MG	1	3556	1/1	0.91	0.52	30,30,30,30	0
85	OHX	6	2131	7/7	0.91	0.34	121,121,121,121	0
84	MG	5	3425	1/1	0.91	0.19	31,31,31,31	0
84	MG	5	3520	1/1	0.91	0.44	40,40,40,40	0
84	MG	1	3512	1/1	0.91	0.35	55,55,55,55	0
85	OHX	5	4050	7/7	0.91	0.25	158,158,158,158	0
84	MG	5	3529	1/1	0.91	0.67	58,58,58,58	0
84	MG	1	3514	1/1	0.91	0.36	33,33,33,33	0
86	ZN	d6	101	1/1	0.91	0.09	60,60,60,60	0
84	MG	6	1985	1/1	0.91	0.29	65,65,65,65	0
84	MG	5	3536	1/1	0.91	0.58	46,46,46,46	0
84	MG	5	3412	1/1	0.92	0.46	39,39,39,39	0
84	MG	1	3547	1/1	0.92	0.49	33,33,33,33	0
84	MG	1	3665	1/1	0.92	0.29	67,67,67,67	0
84	MG	6	1958	1/1	0.92	0.68	47,47,47,47	0
84	MG	5	4071	1/1	0.92	0.23	43,43,43,43	0
84	MG	5	4072	1/1	0.92	0.29	33,33,33,33	0
84	MG	1	3447	1/1	0.92	0.48	37,37,37,37	0
84	MG	5	3496	1/1	0.92	0.43	56,56,56,56	0
84	MG	5	4077	1/1	0.92	0.87	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	5	3423	1/1	0.92	0.56	45,45,45,45	0
84	MG	5	3603	1/1	0.92	0.35	47,47,47,47	0
84	MG	2	1951	1/1	0.92	0.47	58,58,58,58	0
84	MG	6	1999	1/1	0.92	0.28	49,49,49,49	0
84	MG	5	3427	1/1	0.92	0.11	47,47,47,47	0
84	MG	M6	201	1/1	0.92	0.16	45,45,45,45	0
84	MG	5	3429	1/1	0.92	0.15	78,78,78,78	0
84	MG	5	3431	1/1	0.92	0.18	37,37,37,37	0
84	MG	8	209	1/1	0.92	0.45	68,68,68,68	0
84	MG	5	3434	1/1	0.92	0.30	32,32,32,32	0
84	MG	5	3437	1/1	0.92	0.20	35,35,35,35	0
84	MG	l2	303	1/1	0.92	1.08	46,46,46,46	0
84	MG	6	1923	1/1	0.92	0.69	68,68,68,68	0
84	MG	5	3440	1/1	0.92	0.15	40,40,40,40	0
84	MG	6	1964	1/1	0.92	0.33	73,73,73,73	0
84	MG	1	3489	1/1	0.92	0.52	49,49,49,49	0
84	MG	1	3672	1/1	0.92	0.28	42,42,42,42	0
84	MG	6	1967	1/1	0.92	0.20	51,51,51,51	0
84	MG	5	3689	1/1	0.92	0.23	30,30,30,30	0
84	MG	1	4044	1/1	0.92	0.30	51,51,51,51	0
84	MG	O2	201	1/1	0.92	0.24	35,35,35,35	0
84	MG	m6	201	1/1	0.92	0.28	37,37,37,37	0
84	MG	5	3633	1/1	0.92	0.86	36,36,36,36	0
84	MG	5	3634	1/1	0.92	0.16	31,31,31,31	0
84	MG	6	2159	1/1	0.92	0.59	58,58,58,58	0
84	MG	5	3451	1/1	0.92	0.35	33,33,33,33	0
84	MG	5	3703	1/1	0.92	0.41	36,36,36,36	0
84	MG	n8	201	1/1	0.92	0.34	50,50,50,50	0
84	MG	2	1966	1/1	0.92	0.35	67,67,67,67	0
84	MG	o1	201	1/1	0.92	0.61	49,49,49,49	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	3551	1/1	0.92	0.34	35,35,35,35	0
84	MG	5	3553	1/1	0.92	0.42	38,38,38,38	0
85	OHX	2	2111	7/7	0.92	0.43	112,112,112,112	0
85	OHX	2	2114	7/7	0.92	0.20	170,170,170,170	0
84	MG	1	3443	1/1	0.92	0.45	43,43,43,43	0
84	MG	1	3459	1/1	0.92	0.44	46,46,46,46	0
84	MG	5	3563	1/1	0.92	0.37	38,38,38,38	0
84	MG	1	3541	1/1	0.92	0.45	55,55,55,55	0
84	MG	5	3716	1/1	0.92	0.40	29,29,29,29	0
84	MG	5	3721	1/1	0.92	0.58	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	OHX	6	2146	7/7	0.92	0.36	108,108,108,108	0
85	OHX	6	2157	7/7	0.92	0.47	115,115,115,115	0
84	MG	1	3592	1/1	0.92	0.21	61,61,61,61	0
85	OHX	5	3860	7/7	0.92	0.16	122,122,122,122	0
84	MG	1	3593	1/1	0.92	0.18	39,39,39,39	0
85	OHX	5	3969	7/7	0.92	0.25	138,138,138,138	0
85	OHX	5	4020	7/7	0.92	0.41	101,101,101,101	0
84	MG	1	3617	1/1	0.92	0.48	43,43,43,43	0
84	MG	1	3497	1/1	0.92	0.56	33,33,33,33	0
85	OHX	5	4061	7/7	0.92	0.39	121,121,121,121	0
84	MG	1	3662	1/1	0.92	0.24	45,45,45,45	0
84	MG	5	3730	1/1	0.92	0.37	43,43,43,43	0
84	MG	5	3473	1/1	0.92	0.41	44,44,44,44	0
86	ZN	d7	101	1/1	0.92	0.17	106,106,106,106	0
84	MG	6	1954	1/1	0.92	0.67	51,51,51,51	0
86	ZN	q2	501	1/1	0.92	0.21	64,64,64,64	0
84	MG	1	3482	1/1	0.92	0.15	53,53,53,53	0
84	MG	8	202	1/1	0.93	0.40	64,64,64,64	0
84	MG	1	3469	1/1	0.93	0.52	51,51,51,51	0
84	MG	2	1973	1/1	0.93	0.45	64,64,64,64	0
84	MG	5	3623	1/1	0.93	0.49	57,57,57,57	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
84	MG	8	210	1/1	0.93	0.23	57,57,57,57	0
84	MG	5	3549	1/1	0.93	0.41	48,48,48,48	0
84	MG	1	3501	1/1	0.93	0.53	43,43,43,43	0
84	MG	1	3532	1/1	0.93	0.19	57,57,57,57	0
84	MG	l3	401	1/1	0.93	0.51	29,29,29,29	0
84	MG	5	3414	1/1	0.93	0.17	31,31,31,31	0
84	MG	1	3564	1/1	0.93	0.62	40,40,40,40	0
84	MG	1	3444	1/1	0.93	0.27	51,51,51,51	0
84	MG	2	1907	1/1	0.93	0.51	64,64,64,64	0
84	MG	2	1903	1/1	0.93	0.69	55,55,55,55	0
84	MG	6	1909	1/1	0.93	0.40	98,98,98,98	0
84	MG	1	3602	1/1	0.93	0.52	41,41,41,41	0
84	MG	4	205	1/1	0.93	0.49	39,39,39,39	0
84	MG	1	3604	1/1	0.93	0.17	47,47,47,47	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	1	3670	1/1	0.93	0.39	52,52,52,52	0
84	MG	1	3577	1/1	0.93	0.24	46,46,46,46	0
84	MG	1	3423	1/1	0.93	0.23	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	5	3589	1/1	0.93	0.41	37,37,37,37	0
84	MG	5	3648	1/1	0.93	0.19	61,61,61,61	0
84	MG	n8	202	1/1	0.93	0.23	37,37,37,37	0
84	MG	2	1928	1/1	0.93	0.39	71,71,71,71	0
84	MG	6	1921	1/1	0.93	0.48	56,56,56,56	0
84	MG	5	3717	1/1	0.93	0.18	39,39,39,39	0
84	MG	5	3718	1/1	0.93	0.20	40,40,40,40	0
84	MG	1	3612	1/1	0.93	0.29	40,40,40,40	0
85	OHX	2	2034	7/7	0.93	0.26	113,113,113,113	0
85	OHX	2	2052	7/7	0.93	0.23	117,117,117,117	0
85	OHX	2	2100	7/7	0.93	0.20	116,116,116,116	0
85	OHX	2	2107	7/7	0.93	0.33	126,126,126,126	0
84	MG	5	3596	1/1	0.93	0.43	40,40,40,40	0
84	MG	5	3654	1/1	0.93	0.25	42,42,42,42	0
84	MG	1	3614	1/1	0.93	0.14	55,55,55,55	0
84	MG	1	3719	1/1	0.93	0.71	45,45,45,45	0
84	MG	L7	301	1/1	0.93	0.36	42,42,42,42	0
84	MG	6	1973	1/1	0.93	0.21	78,78,78,78	0
84	MG	5	3518	1/1	0.93	0.38	41,41,41,41	0
84	MG	5	3663	1/1	0.93	0.25	62,62,62,62	0
85	OHX	6	2068	7/7	0.93	0.22	90,90,90,90	0
85	OHX	6	2127	7/7	0.93	0.25	138,138,138,138	0
84	MG	5	3735	1/1	0.93	0.22	65,65,65,65	0
85	OHX	6	2135	7/7	0.93	0.39	92,92,92,92	0
85	OHX	6	2144	7/7	0.93	0.35	102,102,102,102	0
84	MG	1	3648	1/1	0.93	0.22	37,37,37,37	0
85	OHX	6	2155	7/7	0.93	0.42	116,116,116,116	0
84	MG	5	3522	1/1	0.93	0.27	43,43,43,43	0
84	MG	5	3607	1/1	0.93	0.18	38,38,38,38	0
84	MG	1	3488	1/1	0.93	0.34	33,33,33,33	0
85	OHX	5	3870	7/7	0.93	0.28	76,76,76,76	0
85	OHX	5	3932	7/7	0.93	0.26	75,75,75,75	0
84	MG	5	3740	1/1	0.93	0.15	41,41,41,41	0
84	MG	5	3609	1/1	0.93	0.42	55,55,55,55	0
85	OHX	5	4005	7/7	0.93	0.27	104,104,104,104	0
84	MG	sM	202	1/1	0.93	0.11	43,43,43,43	0
85	OHX	5	4029	7/7	0.93	0.31	128,128,128,128	0
84	MG	1	3426	1/1	0.93	0.47	50,50,50,50	0
84	MG	5	3673	1/1	0.93	0.51	34,34,34,34	0
84	MG	2	1922	1/1	0.93	0.97	74,74,74,74	0
84	MG	5	3534	1/1	0.93	0.37	36,36,36,36	0
85	OHX	7	220	7/7	0.93	0.31	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	5	3535	1/1	0.93	0.35	49,49,49,49	0
84	MG	1	3518	1/1	0.93	0.43	52,52,52,52	0
84	MG	N8	202	1/1	0.93	0.14	35,35,35,35	0
84	MG	5	3679	1/1	0.93	0.41	42,42,42,42	0
84	MG	7	209	1/1	0.93	0.34	51,51,51,51	0
84	MG	7	210	1/1	0.93	0.12	53,53,53,53	0
84	MG	1	3660	1/1	0.94	0.09	47,47,47,47	0
84	MG	O3	201	1/1	0.94	0.21	42,42,42,42	0
84	MG	5	3415	1/1	0.94	0.59	29,29,29,29	0
84	MG	5	4075	1/1	0.94	0.46	33,33,33,33	0
84	MG	5	3416	1/1	0.94	0.28	38,38,38,38	0
84	MG	5	3530	1/1	0.94	0.31	41,41,41,41	0
84	MG	5	3417	1/1	0.94	0.20	84,84,84,84	0
84	MG	1	3661	1/1	0.94	0.47	55,55,55,55	0
84	MG	5	3533	1/1	0.94	0.91	55,55,55,55	0
84	MG	5	3649	1/1	0.94	0.23	35,35,35,35	0
84	MG	7	207	1/1	0.94	0.14	36,36,36,36	0
84	MG	1	3502	1/1	0.94	0.43	39,39,39,39	0
84	MG	1	3445	1/1	0.94	0.33	40,40,40,40	0
84	MG	8	201	1/1	0.94	0.24	42,42,42,42	0
84	MG	1	3415	1/1	0.94	0.38	41,41,41,41	0
84	MG	1	3545	1/1	0.94	0.54	36,36,36,36	0
84	MG	2	1920	1/1	0.94	0.69	74,74,74,74	0
84	MG	6	1972	1/1	0.94	0.31	51,51,51,51	0
84	MG	2	1925	1/1	0.94	0.76	74,74,74,74	0
84	MG	6	1906	1/1	0.94	0.34	51,51,51,51	0
84	MG	1	3594	1/1	0.94	0.35	48,48,48,48	0
84	MG	1	3669	1/1	0.94	0.27	48,48,48,48	0
84	MG	6	1978	1/1	0.94	0.59	76,76,76,76	0
84	MG	1	3476	1/1	0.94	0.20	42,42,42,42	0
84	MG	5	3665	1/1	0.94	0.45	39,39,39,39	0
84	MG	5	3439	1/1	0.94	0.33	33,33,33,33	0
84	MG	1	3725	1/1	0.94	0.38	52,52,52,52	0
84	MG	5	3562	1/1	0.94	0.35	32,32,32,32	0
84	MG	1	3596	1/1	0.94	0.16	46,46,46,46	0
84	MG	5	3670	1/1	0.94	0.32	35,35,35,35	0
84	MG	5	3564	1/1	0.94	0.45	38,38,38,38	0
84	MG	1	3633	1/1	0.94	0.44	56,56,56,56	0
84	MG	m1	201	1/1	0.94	0.40	48,48,48,48	0
84	MG	1	3432	1/1	0.94	0.22	49,49,49,49	0
84	MG	1	3677	1/1	0.94	0.27	43,43,43,43	0
84	MG	1	3515	1/1	0.94	0.46	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	6	1918	1/1	0.94	0.48	58,58,58,58	0
84	MG	5	3582	1/1	0.94	0.23	49,49,49,49	0
84	MG	1	3433	1/1	0.94	0.35	36,36,36,36	0
84	MG	5	3584	1/1	0.94	0.11	45,45,45,45	0
84	MG	1	3455	1/1	0.94	0.34	32,32,32,32	0
84	MG	3	204	1/1	0.94	0.60	40,40,40,40	0
84	MG	5	3455	1/1	0.94	0.32	50,50,50,50	0
84	MG	3	205	1/1	0.94	0.24	66,66,66,66	0
84	MG	3	207	1/1	0.94	0.16	44,44,44,44	0
84	MG	4	201	1/1	0.94	0.52	53,53,53,53	0
84	MG	5	3459	1/1	0.94	0.35	40,40,40,40	0
84	MG	1	3682	1/1	0.94	0.50	33,33,33,33	0
85	OHX	2	2027	7/7	0.94	0.20	128,128,128,128	0
84	MG	1	3434	1/1	0.94	0.36	52,52,52,52	0
84	MG	1	3520	1/1	0.94	0.32	42,42,42,42	0
85	OHX	2	2063	7/7	0.94	0.22	160,160,160,160	0
85	OHX	2	2067	7/7	0.94	0.36	106,106,106,106	0
85	OHX	2	2076	7/7	0.94	0.18	135,135,135,135	0
85	OHX	2	2089	7/7	0.94	0.42	113,113,113,113	0
85	OHX	2	2090	7/7	0.94	0.19	121,121,121,121	0
84	MG	5	3695	1/1	0.94	0.25	48,48,48,48	0
85	OHX	2	2102	7/7	0.94	0.32	114,114,114,114	0
85	OHX	2	2106	7/7	0.94	0.35	123,123,123,123	0
84	MG	1	3687	1/1	0.94	0.19	48,48,48,48	0
84	MG	5	3464	1/1	0.94	0.34	29,29,29,29	0
85	OHX	2	2109	7/7	0.94	0.33	112,112,112,112	0
85	OHX	2	2110	7/7	0.94	0.38	130,130,130,130	0
84	MG	1	3565	1/1	0.94	0.47	32,32,32,32	0
84	MG	5	3700	1/1	0.94	0.23	38,38,38,38	0
84	MG	1	3567	1/1	0.94	0.93	50,50,50,50	0
84	MG	6	1936	1/1	0.94	0.38	42,42,42,42	0
85	OHX	2	2119	7/7	0.94	0.47	144,144,144,144	0
85	OHX	S6	301	7/7	0.94	0.38	117,117,117,117	0
85	OHX	1	3864	7/7	0.94	0.20	79,79,79,79	0
85	OHX	1	3889	7/7	0.94	0.21	99,99,99,99	0
85	OHX	1	3918	7/7	0.94	0.29	121,121,121,121	0
84	MG	5	3472	1/1	0.94	0.47	50,50,50,50	0
84	MG	4	209	1/1	0.94	0.29	54,54,54,54	0
85	OHX	1	3945	7/7	0.94	0.19	162,162,162,162	0
85	OHX	1	3997	7/7	0.94	0.39	82,82,82,82	0
85	OHX	1	4002	7/7	0.94	0.27	112,112,112,112	0
85	OHX	1	4003	7/7	0.94	0.39	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3644	1/1	0.94	0.72	41,41,41,41	0
85	OHX	1	4029	7/7	0.94	0.42	89,89,89,89	0
85	OHX	1	4036	7/7	0.94	0.36	104,104,104,104	0
84	MG	6	1941	1/1	0.94	0.38	43,43,43,43	0
85	OHX	6	2088	7/7	0.94	0.46	81,81,81,81	0
85	OHX	6	2101	7/7	0.94	0.26	105,105,105,105	0
85	OHX	6	2123	7/7	0.94	0.33	102,102,102,102	0
84	MG	5	3611	1/1	0.94	0.22	40,40,40,40	0
85	OHX	6	2128	7/7	0.94	0.31	112,112,112,112	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
85	OHX	6	2137	7/7	0.94	0.27	127,127,127,127	0
85	OHX	6	2142	7/7	0.94	0.24	117,117,117,117	0
84	MG	6	1943	1/1	0.94	0.57	58,58,58,58	0
84	MG	1	3646	1/1	0.94	0.14	53,53,53,53	0
85	OHX	6	2150	7/7	0.94	0.39	100,100,100,100	0
84	MG	5	3483	1/1	0.94	0.47	41,41,41,41	0
84	MG	2	1950	1/1	0.94	0.33	72,72,72,72	0
84	MG	1	3609	1/1	0.94	0.32	41,41,41,41	0
84	MG	5	3492	1/1	0.94	0.56	41,41,41,41	0
84	MG	5	3495	1/1	0.94	0.17	35,35,35,35	0
85	OHX	5	3906	7/7	0.94	0.21	101,101,101,101	0
85	OHX	5	3909	7/7	0.94	0.18	88,88,88,88	0
84	MG	6	1949	1/1	0.94	0.68	76,76,76,76	0
84	MG	2	1934	1/1	0.94	0.32	72,72,72,72	0
85	OHX	5	3943	7/7	0.94	0.18	116,116,116,116	0
84	MG	5	3725	1/1	0.94	0.28	38,38,38,38	0
85	OHX	5	3976	7/7	0.94	0.25	107,107,107,107	0
85	OHX	5	3980	7/7	0.94	0.23	102,102,102,102	0
84	MG	5	3401	1/1	0.94	0.26	32,32,32,32	0
85	OHX	5	4008	7/7	0.94	0.26	144,144,144,144	0
84	MG	5	3628	1/1	0.94	0.27	49,49,49,49	0
85	OHX	5	4024	7/7	0.94	0.32	116,116,116,116	0
84	MG	5	3629	1/1	0.94	0.35	35,35,35,35	0
85	OHX	5	4033	7/7	0.94	0.37	105,105,105,105	0
85	OHX	5	4034	7/7	0.94	0.34	84,84,84,84	0
84	MG	6	1952	1/1	0.94	0.51	54,54,54,54	0
85	OHX	5	4044	7/7	0.94	0.24	116,116,116,116	0
84	MG	1	3699	1/1	0.94	0.45	55,55,55,55	0
85	OHX	5	4055	7/7	0.94	0.36	114,114,114,114	0
84	MG	5	3502	1/1	0.94	0.46	32,32,32,32	0
84	MG	5	3733	1/1	0.94	0.43	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	2	1926	1/1	0.94	0.33	74,74,74,74	0
84	MG	2	1927	1/1	0.94	0.47	65,65,65,65	0
86	ZN	E1	501	1/1	0.94	0.05	115,115,115,115	0
84	MG	1	3613	1/1	0.94	0.13	45,45,45,45	0
84	MG	1	3425	1/1	0.94	0.20	49,49,49,49	0
84	MG	2	1906	1/1	0.94	0.45	63,63,63,63	0
84	MG	2	1929	1/1	0.94	0.64	67,67,67,67	0
84	MG	1	3428	1/1	0.94	0.44	48,48,48,48	0
85	OHX	2	2003	7/7	0.95	0.11	101,101,101,101	0
85	OHX	2	2012	7/7	0.95	0.14	107,107,107,107	0
85	OHX	2	2025	7/7	0.95	0.14	108,108,108,108	0
85	OHX	2	2026	7/7	0.95	0.19	118,118,118,118	0
84	MG	2	1908	1/1	0.95	0.39	78,78,78,78	0
84	MG	1	3588	1/1	0.95	0.41	42,42,42,42	0
85	OHX	2	2040	7/7	0.95	0.24	110,110,110,110	0
84	MG	5	3713	1/1	0.95	0.34	33,33,33,33	0
84	MG	1	3490	1/1	0.95	0.26	42,42,42,42	0
84	MG	M0	301	1/1	0.95	0.37	43,43,43,43	0
85	OHX	2	2068	7/7	0.95	0.33	122,122,122,122	0
85	OHX	2	2075	7/7	0.95	0.35	115,115,115,115	0
84	MG	5	3548	1/1	0.95	0.30	29,29,29,29	0
85	OHX	2	2084	7/7	0.95	0.33	98,98,98,98	0
85	OHX	2	2085	7/7	0.95	0.29	114,114,114,114	0
84	MG	5	3465	1/1	0.95	0.17	41,41,41,41	0
84	MG	1	3470	1/1	0.95	0.28	37,37,37,37	0
85	OHX	2	2092	7/7	0.95	0.32	106,106,106,106	0
85	OHX	2	2093	7/7	0.95	0.31	103,103,103,103	0
85	OHX	2	2098	7/7	0.95	0.38	125,125,125,125	0
84	MG	5	3719	1/1	0.95	0.15	32,32,32,32	0
84	MG	M5	301	1/1	0.95	0.24	39,39,39,39	0
85	OHX	2	2105	7/7	0.95	0.31	114,114,114,114	0
84	MG	1	3493	1/1	0.95	0.49	30,30,30,30	0
84	MG	6	1933	1/1	0.95	0.41	84,84,84,84	0
84	MG	5	3558	1/1	0.95	0.47	37,37,37,37	0
84	MG	2	1916	1/1	0.95	0.41	59,59,59,59	0
84	MG	5	3475	1/1	0.95	0.66	32,32,32,32	0
84	MG	1	3524	1/1	0.95	0.26	43,43,43,43	0
84	MG	1	3559	1/1	0.95	0.47	48,48,48,48	0
84	MG	1	3418	1/1	0.95	0.22	66,66,66,66	0
84	MG	5	3570	1/1	0.95	0.29	31,31,31,31	0
84	MG	5	3479	1/1	0.95	0.27	35,35,35,35	0
84	MG	5	3734	1/1	0.95	0.14	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	OHX	1	3826	7/7	0.95	0.14	93,93,93,93	0
85	OHX	1	3858	7/7	0.95	0.11	128,128,128,128	0
84	MG	5	3572	1/1	0.95	0.55	28,28,28,28	0
85	OHX	1	3888	7/7	0.95	0.30	85,85,85,85	0
84	MG	1	4042	1/1	0.95	0.15	45,45,45,45	0
84	MG	5	3575	1/1	0.95	0.47	31,31,31,31	0
84	MG	1	3474	1/1	0.95	0.18	53,53,53,53	0
84	MG	5	3580	1/1	0.95	0.57	37,37,37,37	0
84	MG	1	3500	1/1	0.95	0.66	44,44,44,44	0
85	OHX	1	3949	7/7	0.95	0.30	101,101,101,101	0
85	OHX	1	3960	7/7	0.95	0.30	122,122,122,122	0
85	OHX	1	3966	7/7	0.95	0.34	175,175,175,175	0
85	OHX	1	3969	7/7	0.95	0.33	103,103,103,103	0
85	OHX	1	3974	7/7	0.95	0.30	127,127,127,127	0
85	OHX	1	3978	7/7	0.95	0.22	92,92,92,92	0
85	OHX	1	3983	7/7	0.95	0.33	78,78,78,78	0
85	OHX	1	3992	7/7	0.95	0.32	116,116,116,116	0
84	MG	5	3656	1/1	0.95	0.12	36,36,36,36	0
84	MG	5	3484	1/1	0.95	0.35	35,35,35,35	0
84	MG	5	3658	1/1	0.95	0.31	46,46,46,46	0
85	OHX	1	4007	7/7	0.95	0.37	101,101,101,101	0
84	MG	1	3627	1/1	0.95	0.23	45,45,45,45	0
85	OHX	1	4013	7/7	0.95	0.26	104,104,104,104	0
85	OHX	1	4017	7/7	0.95	0.41	68,68,68,68	0
85	OHX	1	4018	7/7	0.95	0.32	88,88,88,88	0
84	MG	1	3446	1/1	0.95	0.17	47,47,47,47	0
85	OHX	1	4030	7/7	0.95	0.41	98,98,98,98	0
85	OHX	1	4031	7/7	0.95	0.23	102,102,102,102	0
85	OHX	1	4035	7/7	0.95	0.23	105,105,105,105	0
84	MG	1	3436	1/1	0.95	0.38	38,38,38,38	0
85	OHX	3	219	7/7	0.95	0.37	95,95,95,95	0
85	OHX	4	225	7/7	0.95	0.16	113,113,113,113	0
85	OHX	4	228	7/7	0.95	0.36	85,85,85,85	0
85	OHX	L4	401	7/7	0.95	0.30	92,92,92,92	0
85	OHX	M9	201	7/7	0.95	0.35	124,124,124,124	0
85	OHX	O9	101	7/7	0.95	0.46	77,77,77,77	0
85	OHX	6	2027	7/7	0.95	0.15	78,78,78,78	0
85	OHX	6	2040	7/7	0.95	0.13	89,89,89,89	0
84	MG	5	3586	1/1	0.95	0.42	34,34,34,34	0
85	OHX	6	2077	7/7	0.95	0.21	100,100,100,100	0
85	OHX	6	2080	7/7	0.95	0.29	109,109,109,109	0
85	OHX	6	2081	7/7	0.95	0.19	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	5	3493	1/1	0.95	0.64	34,34,34,34	0
85	OHX	6	2095	7/7	0.95	0.41	119,119,119,119	0
85	OHX	6	2098	7/7	0.95	0.34	99,99,99,99	0
84	MG	5	3494	1/1	0.95	0.49	30,30,30,30	0
85	OHX	6	2109	7/7	0.95	0.26	84,84,84,84	0
85	OHX	6	2110	7/7	0.95	0.27	103,103,103,103	0
85	OHX	6	2116	7/7	0.95	0.18	111,111,111,111	0
84	MG	1	3533	1/1	0.95	0.43	39,39,39,39	0
84	MG	7	205	1/1	0.95	0.52	35,35,35,35	0
84	MG	5	3590	1/1	0.95	0.29	34,34,34,34	0
84	MG	5	3592	1/1	0.95	0.19	42,42,42,42	0
85	OHX	6	2132	7/7	0.95	0.30	112,112,112,112	0
85	OHX	6	2133	7/7	0.95	0.25	85,85,85,85	0
84	MG	6	1950	1/1	0.95	0.67	72,72,72,72	0
84	MG	1	3698	1/1	0.95	0.26	49,49,49,49	0
84	MG	1	3402	1/1	0.95	0.61	46,46,46,46	0
85	OHX	6	2143	7/7	0.95	0.34	97,97,97,97	0
84	MG	6	1904	1/1	0.95	0.62	76,76,76,76	0
85	OHX	6	2145	7/7	0.95	0.35	106,106,106,106	0
84	MG	8	203	1/1	0.95	0.43	43,43,43,43	0
84	MG	1	3603	1/1	0.95	0.39	38,38,38,38	0
85	OHX	6	2154	7/7	0.95	0.38	100,100,100,100	0
84	MG	1	3403	1/1	0.95	0.65	51,51,51,51	0
84	MG	1	3572	1/1	0.95	0.52	33,33,33,33	0
84	MG	5	3505	1/1	0.95	0.51	36,36,36,36	0
85	OHX	c3	201	7/7	0.95	0.24	113,113,113,113	0
85	OHX	5	3849	7/7	0.95	0.15	90,90,90,90	0
84	MG	5	3602	1/1	0.95	0.50	49,49,49,49	0
85	OHX	5	3864	7/7	0.95	0.17	78,78,78,78	0
84	MG	5	3441	1/1	0.95	0.35	65,65,65,65	0
85	OHX	5	3886	7/7	0.95	0.21	82,82,82,82	0
85	OHX	5	3897	7/7	0.95	0.32	81,81,81,81	0
84	MG	5	3508	1/1	0.95	0.39	34,34,34,34	0
84	MG	1	3422	1/1	0.95	0.35	55,55,55,55	0
84	MG	5	3606	1/1	0.95	0.29	41,41,41,41	0
84	MG	5	3682	1/1	0.95	0.41	35,35,35,35	0
85	OHX	5	3940	7/7	0.95	0.23	99,99,99,99	0
84	MG	5	3443	1/1	0.95	0.20	38,38,38,38	0
85	OHX	5	3961	7/7	0.95	0.27	102,102,102,102	0
84	MG	5	3513	1/1	0.95	0.41	32,32,32,32	0
84	MG	5	3514	1/1	0.95	0.64	30,30,30,30	0
85	OHX	5	3978	7/7	0.95	0.27	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3706	1/1	0.95	0.65	32,32,32,32	0
85	OHX	5	3983	7/7	0.95	0.30	83,83,83,83	0
85	OHX	5	3988	7/7	0.95	0.28	116,116,116,116	0
85	OHX	5	3989	7/7	0.95	0.36	81,81,81,81	0
85	OHX	5	3990	7/7	0.95	0.40	76,76,76,76	0
85	OHX	5	3996	7/7	0.95	0.35	92,92,92,92	0
85	OHX	5	3997	7/7	0.95	0.37	87,87,87,87	0
85	OHX	5	4001	7/7	0.95	0.27	130,130,130,130	0
84	MG	1	3607	1/1	0.95	0.23	42,42,42,42	0
84	MG	5	3517	1/1	0.95	0.31	53,53,53,53	0
85	OHX	5	4018	7/7	0.95	0.35	105,105,105,105	0
85	OHX	5	4019	7/7	0.95	0.33	109,109,109,109	0
84	MG	1	3485	1/1	0.95	0.33	37,37,37,37	0
84	MG	1	3671	1/1	0.95	0.17	45,45,45,45	0
84	MG	5	3694	1/1	0.95	0.27	35,35,35,35	0
85	OHX	5	4031	7/7	0.95	0.27	106,106,106,106	0
84	MG	1	3511	1/1	0.95	0.50	39,39,39,39	0
84	MG	2	1968	1/1	0.95	0.44	85,85,85,85	0
84	MG	5	3527	1/1	0.95	0.33	69,69,69,69	0
84	MG	1	3674	1/1	0.95	0.50	37,37,37,37	0
85	OHX	5	4047	7/7	0.95	0.29	101,101,101,101	0
84	MG	n0	201	1/1	0.95	0.23	43,43,43,43	0
85	OHX	5	4053	7/7	0.95	0.29	105,105,105,105	0
84	MG	5	3452	1/1	0.95	0.34	43,43,43,43	0
85	OHX	5	4056	7/7	0.95	0.33	104,104,104,104	0
85	OHX	5	4058	7/7	0.95	0.35	115,115,115,115	0
84	MG	1	3544	1/1	0.95	0.57	35,35,35,35	0
85	OHX	5	4062	7/7	0.95	0.42	84,84,84,84	0
85	OHX	5	4067	7/7	0.95	0.22	93,93,93,93	0
84	MG	5	3702	1/1	0.95	0.13	35,35,35,35	0
84	MG	6	1968	1/1	0.95	0.35	55,55,55,55	0
85	OHX	l5	302	7/7	0.95	0.24	107,107,107,107	0
85	OHX	m0	301	7/7	0.95	0.13	109,109,109,109	0
86	ZN	D6	500	1/1	0.95	0.07	81,81,81,81	0
84	MG	6	1920	1/1	0.95	0.49	42,42,42,42	0
84	MG	2	1959	1/1	0.95	0.34	67,67,67,67	0
86	ZN	Q0	500	1/1	0.95	0.10	48,48,48,48	0
84	MG	5	3626	1/1	0.95	0.33	33,33,33,33	0
84	MG	L2	301	1/1	0.95	0.39	39,39,39,39	0
84	MG	L2	302	1/1	0.95	0.29	41,41,41,41	0
84	MG	5	3405	1/1	0.95	0.27	43,43,43,43	0
85	OHX	2	2000	7/7	0.95	0.13	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	OHX	1	3898	7/7	0.96	0.28	85,85,85,85	0
85	OHX	1	3905	7/7	0.96	0.20	79,79,79,79	0
85	OHX	1	3909	7/7	0.96	0.23	83,83,83,83	0
85	OHX	1	3914	7/7	0.96	0.16	111,111,111,111	0
85	OHX	1	3916	7/7	0.96	0.30	87,87,87,87	0
85	OHX	1	3917	7/7	0.96	0.13	133,133,133,133	0
84	MG	1	3478	1/1	0.96	0.15	40,40,40,40	0
85	OHX	1	3919	7/7	0.96	0.24	99,99,99,99	0
85	OHX	1	3920	7/7	0.96	0.17	121,121,121,121	0
84	MG	1	3504	1/1	0.96	0.36	40,40,40,40	0
85	OHX	1	3923	7/7	0.96	0.35	91,91,91,91	0
85	OHX	1	3929	7/7	0.96	0.34	83,83,83,83	0
85	OHX	1	3930	7/7	0.96	0.23	100,100,100,100	0
84	MG	4	206	1/1	0.96	0.27	35,35,35,35	0
85	OHX	1	3932	7/7	0.96	0.36	71,71,71,71	0
85	OHX	1	3935	7/7	0.96	0.31	88,88,88,88	0
85	OHX	1	3941	7/7	0.96	0.36	107,107,107,107	0
85	OHX	1	3943	7/7	0.96	0.31	112,112,112,112	0
84	MG	5	3521	1/1	0.96	0.41	39,39,39,39	0
85	OHX	1	3946	7/7	0.96	0.32	99,99,99,99	0
84	MG	1	3521	1/1	0.96	0.58	31,31,31,31	0
85	OHX	1	3950	7/7	0.96	0.26	121,121,121,121	0
85	OHX	1	3955	7/7	0.96	0.33	108,108,108,108	0
84	MG	1	3523	1/1	0.96	0.41	41,41,41,41	0
85	OHX	1	3964	7/7	0.96	0.28	89,89,89,89	0
84	MG	2	1958	1/1	0.96	0.49	96,96,96,96	0
84	MG	1	3525	1/1	0.96	0.39	46,46,46,46	0
84	MG	1	3711	1/1	0.96	0.23	46,46,46,46	0
85	OHX	1	3976	7/7	0.96	0.31	91,91,91,91	0
84	MG	1	3647	1/1	0.96	0.20	49,49,49,49	0
85	OHX	1	3981	7/7	0.96	0.24	95,95,95,95	0
84	MG	1	3546	1/1	0.96	0.24	36,36,36,36	0
85	OHX	1	3987	7/7	0.96	0.32	79,79,79,79	0
84	MG	1	3573	1/1	0.96	0.69	33,33,33,33	0
85	OHX	1	3993	7/7	0.96	0.37	87,87,87,87	0
84	MG	5	3692	1/1	0.96	0.44	68,68,68,68	0
85	OHX	1	4000	7/7	0.96	0.31	109,109,109,109	0
84	MG	5	3618	1/1	0.96	0.61	40,40,40,40	0
84	MG	13	404	1/1	0.96	0.26	39,39,39,39	0
85	OHX	1	4006	7/7	0.96	0.43	102,102,102,102	0
84	MG	1	3621	1/1	0.96	0.16	36,36,36,36	0
84	MG	5	3620	1/1	0.96	0.35	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3622	1/1	0.96	0.23	35,35,35,35	0
85	OHX	1	4014	7/7	0.96	0.38	110,110,110,110	0
85	OHX	1	4015	7/7	0.96	0.36	91,91,91,91	0
85	OHX	1	4016	7/7	0.96	0.38	109,109,109,109	0
84	MG	1	3574	1/1	0.96	0.41	33,33,33,33	0
84	MG	5	3537	1/1	0.96	0.42	36,36,36,36	0
85	OHX	1	4023	7/7	0.96	0.33	109,109,109,109	0
85	OHX	1	4024	7/7	0.96	0.28	155,155,155,155	0
85	OHX	1	4028	7/7	0.96	0.31	115,115,115,115	0
84	MG	1	3653	1/1	0.96	0.17	40,40,40,40	0
84	MG	1	3654	1/1	0.96	0.16	45,45,45,45	0
84	MG	m5	302	1/1	0.96	0.17	53,53,53,53	0
85	OHX	1	4032	7/7	0.96	0.43	88,88,88,88	0
85	OHX	1	4034	7/7	0.96	0.36	104,104,104,104	0
84	MG	5	3466	1/1	0.96	0.23	68,68,68,68	0
84	MG	5	3627	1/1	0.96	0.39	34,34,34,34	0
85	OHX	1	4037	7/7	0.96	0.45	98,98,98,98	0
85	OHX	1	4038	7/7	0.96	0.45	100,100,100,100	0
85	OHX	3	216	7/7	0.96	0.28	108,108,108,108	0
85	OHX	3	218	7/7	0.96	0.37	125,125,125,125	0
84	MG	1	3465	1/1	0.96	0.21	42,42,42,42	0
85	OHX	4	223	7/7	0.96	0.24	97,97,97,97	0
84	MG	m7	202	1/1	0.96	0.36	36,36,36,36	0
84	MG	5	3543	1/1	0.96	0.49	37,37,37,37	0
85	OHX	4	229	7/7	0.96	0.39	113,113,113,113	0
85	OHX	4	230	7/7	0.96	0.40	108,108,108,108	0
85	OHX	4	231	7/7	0.96	0.29	103,103,103,103	0
84	MG	5	3469	1/1	0.96	0.22	58,58,58,58	0
85	OHX	M0	302	7/7	0.96	0.18	86,86,86,86	0
84	MG	5	3410	1/1	0.96	0.62	42,42,42,42	0
85	OHX	N8	203	7/7	0.96	0.24	129,129,129,129	0
84	MG	1	3412	1/1	0.96	0.25	42,42,42,42	0
84	MG	1	3580	1/1	0.96	0.22	42,42,42,42	0
84	MG	1	3581	1/1	0.96	0.31	45,45,45,45	0
85	OHX	6	2054	7/7	0.96	0.22	84,84,84,84	0
85	OHX	6	2062	7/7	0.96	0.12	126,126,126,126	0
84	MG	5	3474	1/1	0.96	0.14	54,54,54,54	0
84	MG	1	3691	1/1	0.96	0.16	54,54,54,54	0
84	MG	M7	202	1/1	0.96	0.36	41,41,41,41	0
84	MG	M7	203	1/1	0.96	0.31	38,38,38,38	0
85	OHX	6	2084	7/7	0.96	0.19	117,117,117,117	0
84	MG	2	1914	1/1	0.96	0.56	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	OHX	6	2089	7/7	0.96	0.32	85,85,85,85	0
85	OHX	6	2091	7/7	0.96	0.18	110,110,110,110	0
85	OHX	6	2093	7/7	0.96	0.21	117,117,117,117	0
84	MG	1	3530	1/1	0.96	0.66	41,41,41,41	0
85	OHX	2	1991	7/7	0.96	0.12	97,97,97,97	0
84	MG	N8	201	1/1	0.96	0.21	37,37,37,37	0
85	OHX	6	2103	7/7	0.96	0.21	131,131,131,131	0
85	OHX	6	2105	7/7	0.96	0.32	115,115,115,115	0
85	OHX	6	2108	7/7	0.96	0.25	102,102,102,102	0
84	MG	5	3420	1/1	0.96	0.54	60,60,60,60	0
85	OHX	2	2008	7/7	0.96	0.14	105,105,105,105	0
85	OHX	6	2112	7/7	0.96	0.27	115,115,115,115	0
85	OHX	6	2115	7/7	0.96	0.18	106,106,106,106	0
84	MG	5	3720	1/1	0.96	0.19	32,32,32,32	0
85	OHX	6	2118	7/7	0.96	0.27	109,109,109,109	0
85	OHX	6	2121	7/7	0.96	0.33	108,108,108,108	0
85	OHX	2	2015	7/7	0.96	0.15	106,106,106,106	0
84	MG	1	3632	1/1	0.96	0.53	50,50,50,50	0
84	MG	5	3422	1/1	0.96	0.34	37,37,37,37	0
84	MG	6	1940	1/1	0.96	0.24	43,43,43,43	0
84	MG	5	3724	1/1	0.96	0.14	42,42,42,42	0
84	MG	5	3486	1/1	0.96	0.36	48,48,48,48	0
84	MG	5	3726	1/1	0.96	0.13	33,33,33,33	0
85	OHX	6	2136	7/7	0.96	0.37	108,108,108,108	0
85	OHX	2	2057	7/7	0.96	0.16	126,126,126,126	0
85	OHX	6	2141	7/7	0.96	0.35	109,109,109,109	0
85	OHX	2	2058	7/7	0.96	0.11	89,89,89,89	0
85	OHX	2	2059	7/7	0.96	0.23	119,119,119,119	0
85	OHX	2	2060	7/7	0.96	0.25	122,122,122,122	0
84	MG	5	3424	1/1	0.96	0.37	32,32,32,32	0
84	MG	5	3576	1/1	0.96	0.41	34,34,34,34	0
85	OHX	6	2148	7/7	0.96	0.51	114,114,114,114	0
85	OHX	6	2149	7/7	0.96	0.31	132,132,132,132	0
84	MG	5	3488	1/1	0.96	0.32	53,53,53,53	0
85	OHX	6	2151	7/7	0.96	0.33	127,127,127,127	0
85	OHX	6	2152	7/7	0.96	0.29	107,107,107,107	0
85	OHX	6	2153	7/7	0.96	0.36	109,109,109,109	0
85	OHX	2	2070	7/7	0.96	0.24	95,95,95,95	0
85	OHX	2	2073	7/7	0.96	0.20	120,120,120,120	0
84	MG	5	3489	1/1	0.96	0.28	34,34,34,34	0
84	MG	5	3491	1/1	0.96	0.50	42,42,42,42	0
85	OHX	s4	301	7/7	0.96	0.26	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	OHX	s8	302	7/7	0.96	0.38	132,132,132,132	0
85	OHX	s9	201	7/7	0.96	0.43	96,96,96,96	0
85	OHX	2	2077	7/7	0.96	0.33	110,110,110,110	0
85	OHX	c5	201	7/7	0.96	0.22	128,128,128,128	0
85	OHX	sR	401	7/7	0.96	0.24	132,132,132,132	0
85	OHX	5	3802	7/7	0.96	0.12	70,70,70,70	0
85	OHX	5	3819	7/7	0.96	0.12	78,78,78,78	0
85	OHX	5	3843	7/7	0.96	0.14	91,91,91,91	0
85	OHX	2	2082	7/7	0.96	0.24	114,114,114,114	0
84	MG	1	3486	1/1	0.96	0.45	36,36,36,36	0
84	MG	1	3498	1/1	0.96	0.46	32,32,32,32	0
85	OHX	2	2086	7/7	0.96	0.35	104,104,104,104	0
85	OHX	5	3871	7/7	0.96	0.21	77,77,77,77	0
85	OHX	5	3878	7/7	0.96	0.15	80,80,80,80	0
85	OHX	5	3884	7/7	0.96	0.10	129,129,129,129	0
84	MG	6	1992	1/1	0.96	0.66	60,60,60,60	0
85	OHX	5	3895	7/7	0.96	0.30	76,76,76,76	0
84	MG	O4	201	1/1	0.96	0.52	51,51,51,51	0
85	OHX	2	2091	7/7	0.96	0.20	122,122,122,122	0
84	MG	1	3635	1/1	0.96	0.28	41,41,41,41	0
85	OHX	5	3914	7/7	0.96	0.24	93,93,93,93	0
85	OHX	5	3919	7/7	0.96	0.28	97,97,97,97	0
84	MG	1	3475	1/1	0.96	0.45	40,40,40,40	0
85	OHX	5	3937	7/7	0.96	0.29	112,112,112,112	0
85	OHX	2	2094	7/7	0.96	0.26	108,108,108,108	0
85	OHX	2	2096	7/7	0.96	0.30	122,122,122,122	0
85	OHX	2	2097	7/7	0.96	0.25	110,110,110,110	0
85	OHX	5	3945	7/7	0.96	0.17	119,119,119,119	0
85	OHX	5	3955	7/7	0.96	0.23	104,104,104,104	0
85	OHX	5	3959	7/7	0.96	0.34	118,118,118,118	0
84	MG	5	3432	1/1	0.96	0.21	31,31,31,31	0
85	OHX	5	3963	7/7	0.96	0.23	108,108,108,108	0
85	OHX	5	3966	7/7	0.96	0.33	108,108,108,108	0
85	OHX	5	3967	7/7	0.96	0.14	116,116,116,116	0
85	OHX	5	3968	7/7	0.96	0.22	86,86,86,86	0
85	OHX	2	2099	7/7	0.96	0.25	128,128,128,128	0
85	OHX	5	3972	7/7	0.96	0.33	87,87,87,87	0
85	OHX	5	3973	7/7	0.96	0.27	96,96,96,96	0
84	MG	2	1945	1/1	0.96	0.21	63,63,63,63	0
85	OHX	2	2101	7/7	0.96	0.31	129,129,129,129	0
84	MG	5	3661	1/1	0.96	0.23	33,33,33,33	0
85	OHX	5	3982	7/7	0.96	0.30	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	OHX	2	2103	7/7	0.96	0.27	132,132,132,132	0
85	OHX	5	3984	7/7	0.96	0.31	86,86,86,86	0
85	OHX	5	3986	7/7	0.96	0.35	105,105,105,105	0
85	OHX	2	2104	7/7	0.96	0.37	96,96,96,96	0
84	MG	5	3435	1/1	0.96	0.21	34,34,34,34	0
84	MG	5	3591	1/1	0.96	0.27	33,33,33,33	0
85	OHX	5	3995	7/7	0.96	0.33	80,80,80,80	0
84	MG	6	1997	1/1	0.96	0.20	63,63,63,63	0
84	MG	6	1948	1/1	0.96	0.48	47,47,47,47	0
85	OHX	5	4000	7/7	0.96	0.24	106,106,106,106	0
84	MG	1	3409	1/1	0.96	0.39	40,40,40,40	0
84	MG	5	3506	1/1	0.96	0.63	47,47,47,47	0
85	OHX	5	4007	7/7	0.96	0.32	63,63,63,63	0
84	MG	3	208	1/1	0.96	0.40	65,65,65,65	0
85	OHX	5	4009	7/7	0.96	0.27	115,115,115,115	0
85	OHX	5	4014	7/7	0.96	0.28	96,96,96,96	0
85	OHX	5	4016	7/7	0.96	0.39	90,90,90,90	0
85	OHX	5	4017	7/7	0.96	0.27	128,128,128,128	0
85	OHX	2	2112	7/7	0.96	0.34	116,116,116,116	0
85	OHX	2	2113	7/7	0.96	0.34	110,110,110,110	0
84	MG	3	209	1/1	0.96	0.17	74,74,74,74	0
85	OHX	5	4023	7/7	0.96	0.32	89,89,89,89	0
84	MG	7	201	1/1	0.96	0.68	49,49,49,49	0
85	OHX	2	2117	7/7	0.96	0.47	128,128,128,128	0
84	MG	1	3702	1/1	0.96	0.44	36,36,36,36	0
85	OHX	5	4032	7/7	0.96	0.33	86,86,86,86	0
84	MG	5	3599	1/1	0.96	0.25	43,43,43,43	0
84	MG	6	1953	1/1	0.96	0.63	43,43,43,43	0
85	OHX	5	4042	7/7	0.96	0.34	100,100,100,100	0
85	OHX	C3	201	7/7	0.96	0.18	115,115,115,115	0
85	OHX	D9	103	7/7	0.96	0.38	108,108,108,108	0
85	OHX	1	3770	7/7	0.96	0.18	74,74,74,74	0
85	OHX	1	3788	7/7	0.96	0.13	86,86,86,86	0
85	OHX	5	4051	7/7	0.96	0.36	100,100,100,100	0
85	OHX	1	3799	7/7	0.96	0.11	88,88,88,88	0
85	OHX	5	4054	7/7	0.96	0.33	87,87,87,87	0
85	OHX	1	3800	7/7	0.96	0.11	88,88,88,88	0
85	OHX	1	3810	7/7	0.96	0.10	99,99,99,99	0
85	OHX	1	3813	7/7	0.96	0.21	77,77,77,77	0
85	OHX	5	4059	7/7	0.96	0.37	74,74,74,74	0
85	OHX	1	3823	7/7	0.96	0.17	73,73,73,73	0
84	MG	5	3512	1/1	0.96	0.14	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	OHX	5	4063	7/7	0.96	0.28	121,121,121,121	0
85	OHX	5	4064	7/7	0.96	0.37	90,90,90,90	0
85	OHX	1	3828	7/7	0.96	0.10	104,104,104,104	0
85	OHX	1	3835	7/7	0.96	0.18	85,85,85,85	0
85	OHX	5	4070	7/7	0.96	0.29	135,135,135,135	0
85	OHX	1	3855	7/7	0.96	0.35	86,86,86,86	0
85	OHX	7	221	7/7	0.96	0.32	110,110,110,110	0
85	OHX	8	221	7/7	0.96	0.33	92,92,92,92	0
85	OHX	8	223	7/7	0.96	0.33	95,95,95,95	0
85	OHX	13	408	7/7	0.96	0.35	111,111,111,111	0
85	OHX	1	3856	7/7	0.96	0.15	107,107,107,107	0
84	MG	6	2004	1/1	0.96	0.24	70,70,70,70	0
85	OHX	m0	302	7/7	0.96	0.25	88,88,88,88	0
85	OHX	m1	202	7/7	0.96	0.29	107,107,107,107	0
84	MG	1	3703	1/1	0.96	0.26	33,33,33,33	0
85	OHX	1	3869	7/7	0.96	0.21	91,91,91,91	0
85	OHX	1	3873	7/7	0.96	0.18	112,112,112,112	0
85	OHX	1	3877	7/7	0.96	0.12	126,126,126,126	0
85	OHX	1	3879	7/7	0.96	0.24	101,101,101,101	0
85	OHX	1	3884	7/7	0.96	0.23	109,109,109,109	0
86	ZN	d9	101	1/1	0.96	0.13	86,86,86,86	0
84	MG	1	3563	1/1	0.96	0.83	54,54,54,54	0
84	MG	6	1907	1/1	0.96	0.42	75,75,75,75	0
85	OHX	1	3897	7/7	0.96	0.16	109,109,109,109	0
85	OHX	1	3837	7/7	0.97	0.19	71,71,71,71	0
85	OHX	1	3840	7/7	0.97	0.15	82,82,82,82	0
84	MG	5	3525	1/1	0.97	0.53	36,36,36,36	0
85	OHX	6	2087	7/7	0.97	0.34	109,109,109,109	0
85	OHX	2	2028	7/7	0.97	0.22	94,94,94,94	0
85	OHX	2	2032	7/7	0.97	0.15	121,121,121,121	0
85	OHX	1	3862	7/7	0.97	0.21	74,74,74,74	0
84	MG	5	3699	1/1	0.97	0.19	42,42,42,42	0
85	OHX	6	2094	7/7	0.97	0.23	96,96,96,96	0
85	OHX	1	3865	7/7	0.97	0.21	93,93,93,93	0
85	OHX	2	2035	7/7	0.97	0.17	95,95,95,95	0
85	OHX	6	2100	7/7	0.97	0.20	96,96,96,96	0
85	OHX	2	2036	7/7	0.97	0.14	103,103,103,103	0
85	OHX	2	2039	7/7	0.97	0.19	133,133,133,133	0
84	MG	1	3507	1/1	0.97	0.41	34,34,34,34	0
85	OHX	6	2106	7/7	0.97	0.30	96,96,96,96	0
85	OHX	6	2107	7/7	0.97	0.26	99,99,99,99	0
85	OHX	1	3881	7/7	0.97	0.29	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	OHX	2	2045	7/7	0.97	0.23	90,90,90,90	0
85	OHX	1	3887	7/7	0.97	0.14	99,99,99,99	0
85	OHX	2	2047	7/7	0.97	0.22	101,101,101,101	0
85	OHX	6	2113	7/7	0.97	0.35	86,86,86,86	0
85	OHX	2	2049	7/7	0.97	0.23	100,100,100,100	0
85	OHX	1	3890	7/7	0.97	0.23	102,102,102,102	0
85	OHX	6	2117	7/7	0.97	0.25	86,86,86,86	0
85	OHX	1	3892	7/7	0.97	0.25	95,95,95,95	0
85	OHX	6	2119	7/7	0.97	0.24	106,106,106,106	0
85	OHX	6	2120	7/7	0.97	0.24	85,85,85,85	0
84	MG	5	3430	1/1	0.97	0.19	33,33,33,33	0
85	OHX	2	2053	7/7	0.97	0.09	130,130,130,130	0
85	OHX	6	2124	7/7	0.97	0.27	89,89,89,89	0
85	OHX	6	2126	7/7	0.97	0.30	96,96,96,96	0
85	OHX	1	3899	7/7	0.97	0.32	91,91,91,91	0
85	OHX	1	3903	7/7	0.97	0.24	77,77,77,77	0
85	OHX	6	2129	7/7	0.97	0.25	152,152,152,152	0
85	OHX	6	2130	7/7	0.97	0.42	88,88,88,88	0
85	OHX	2	2054	7/7	0.97	0.20	122,122,122,122	0
85	OHX	1	3906	7/7	0.97	0.30	85,85,85,85	0
85	OHX	2	2055	7/7	0.97	0.31	111,111,111,111	0
85	OHX	1	3910	7/7	0.97	0.24	84,84,84,84	0
85	OHX	1	3912	7/7	0.97	0.25	110,110,110,110	0
84	MG	1	3473	1/1	0.97	0.28	45,45,45,45	0
85	OHX	6	2139	7/7	0.97	0.44	84,84,84,84	0
85	OHX	6	2140	7/7	0.97	0.30	101,101,101,101	0
85	OHX	1	3915	7/7	0.97	0.28	69,69,69,69	0
84	MG	1	3571	1/1	0.97	0.43	35,35,35,35	0
84	MG	5	3433	1/1	0.97	0.34	42,42,42,42	0
84	MG	3	206	1/1	0.97	0.79	59,59,59,59	0
85	OHX	2	2062	7/7	0.97	0.32	106,106,106,106	0
84	MG	1	3509	1/1	0.97	0.32	33,33,33,33	0
85	OHX	6	2147	7/7	0.97	0.37	100,100,100,100	0
84	MG	5	3436	1/1	0.97	0.23	30,30,30,30	0
84	MG	5	3481	1/1	0.97	0.44	35,35,35,35	0
85	OHX	1	3928	7/7	0.97	0.24	95,95,95,95	0
84	MG	1	3675	1/1	0.97	0.31	41,41,41,41	0
85	OHX	2	2071	7/7	0.97	0.28	127,127,127,127	0
84	MG	1	3495	1/1	0.97	0.46	41,41,41,41	0
84	MG	3	220	1/1	0.97	0.42	46,46,46,46	0
85	OHX	1	3933	7/7	0.97	0.17	92,92,92,92	0
85	OHX	6	2156	7/7	0.97	0.37	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	OHX	1	3934	7/7	0.97	0.33	94,94,94,94	0
84	MG	6	1974	1/1	0.97	0.14	50,50,50,50	0
85	OHX	1	3936	7/7	0.97	0.23	98,98,98,98	0
85	OHX	1	3937	7/7	0.97	0.43	88,88,88,88	0
85	OHX	1	3940	7/7	0.97	0.40	88,88,88,88	0
84	MG	1	3440	1/1	0.97	0.27	48,48,48,48	0
85	OHX	1	3942	7/7	0.97	0.30	88,88,88,88	0
85	OHX	d4	201	7/7	0.97	0.28	115,115,115,115	0
85	OHX	2	2078	7/7	0.97	0.28	105,105,105,105	0
85	OHX	5	3786	7/7	0.97	0.11	75,75,75,75	0
85	OHX	5	3795	7/7	0.97	0.12	104,104,104,104	0
85	OHX	2	2080	7/7	0.97	0.31	112,112,112,112	0
85	OHX	5	3810	7/7	0.97	0.11	87,87,87,87	0
85	OHX	5	3818	7/7	0.97	0.11	90,90,90,90	0
84	MG	2	1930	1/1	0.97	0.52	58,58,58,58	0
85	OHX	5	3824	7/7	0.97	0.13	82,82,82,82	0
85	OHX	5	3839	7/7	0.97	0.14	84,84,84,84	0
85	OHX	1	3947	7/7	0.97	0.23	85,85,85,85	0
84	MG	1	3529	1/1	0.97	0.48	50,50,50,50	0
85	OHX	5	3850	7/7	0.97	0.12	107,107,107,107	0
85	OHX	5	3852	7/7	0.97	0.18	71,71,71,71	0
84	MG	1	3680	1/1	0.97	0.13	40,40,40,40	0
85	OHX	1	3953	7/7	0.97	0.26	108,108,108,108	0
85	OHX	5	3869	7/7	0.97	0.15	79,79,79,79	0
84	MG	5	3545	1/1	0.97	0.68	30,30,30,30	0
84	MG	5	3490	1/1	0.97	0.60	39,39,39,39	0
85	OHX	5	3873	7/7	0.97	0.20	68,68,68,68	0
85	OHX	5	3874	7/7	0.97	0.16	87,87,87,87	0
85	OHX	1	3962	7/7	0.97	0.20	101,101,101,101	0
85	OHX	5	3879	7/7	0.97	0.16	103,103,103,103	0
85	OHX	5	3880	7/7	0.97	0.22	91,91,91,91	0
84	MG	1	3578	1/1	0.97	0.27	35,35,35,35	0
84	MG	1	3551	1/1	0.97	0.57	37,37,37,37	0
85	OHX	5	3889	7/7	0.97	0.25	72,72,72,72	0
85	OHX	5	3892	7/7	0.97	0.23	80,80,80,80	0
85	OHX	1	3967	7/7	0.97	0.35	94,94,94,94	0
85	OHX	5	3896	7/7	0.97	0.21	77,77,77,77	0
84	MG	6	1944	1/1	0.97	0.60	69,69,69,69	0
85	OHX	5	3901	7/7	0.97	0.19	110,110,110,110	0
85	OHX	5	3903	7/7	0.97	0.11	110,110,110,110	0
85	OHX	5	3904	7/7	0.97	0.20	76,76,76,76	0
85	OHX	5	3905	7/7	0.97	0.26	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	OHX	1	3970	7/7	0.97	0.31	94,94,94,94	0
85	OHX	1	3971	7/7	0.97	0.41	98,98,98,98	0
85	OHX	5	3911	7/7	0.97	0.27	80,80,80,80	0
85	OHX	5	3913	7/7	0.97	0.21	88,88,88,88	0
85	OHX	1	3972	7/7	0.97	0.31	77,77,77,77	0
85	OHX	1	3973	7/7	0.97	0.40	105,105,105,105	0
85	OHX	5	3922	7/7	0.97	0.16	97,97,97,97	0
85	OHX	5	3926	7/7	0.97	0.18	104,104,104,104	0
85	OHX	5	3930	7/7	0.97	0.37	75,75,75,75	0
84	MG	1	3683	1/1	0.97	0.36	34,34,34,34	0
85	OHX	5	3935	7/7	0.97	0.20	92,92,92,92	0
84	MG	5	3449	1/1	0.97	0.23	34,34,34,34	0
85	OHX	1	3977	7/7	0.97	0.29	98,98,98,98	0
85	OHX	2	2095	7/7	0.97	0.36	96,96,96,96	0
85	OHX	5	3941	7/7	0.97	0.28	90,90,90,90	0
85	OHX	1	3979	7/7	0.97	0.36	94,94,94,94	0
85	OHX	5	3944	7/7	0.97	0.36	74,74,74,74	0
84	MG	2	1931	1/1	0.97	0.54	65,65,65,65	0
85	OHX	5	3946	7/7	0.97	0.23	100,100,100,100	0
85	OHX	5	3947	7/7	0.97	0.36	79,79,79,79	0
85	OHX	5	3950	7/7	0.97	0.40	101,101,101,101	0
85	OHX	5	3951	7/7	0.97	0.27	92,92,92,92	0
85	OHX	5	3954	7/7	0.97	0.25	82,82,82,82	0
85	OHX	1	3982	7/7	0.97	0.32	107,107,107,107	0
85	OHX	5	3956	7/7	0.97	0.35	76,76,76,76	0
85	OHX	5	3957	7/7	0.97	0.28	84,84,84,84	0
85	OHX	5	3958	7/7	0.97	0.29	98,98,98,98	0
84	MG	1	3413	1/1	0.97	0.46	43,43,43,43	0
85	OHX	5	3960	7/7	0.97	0.32	105,105,105,105	0
85	OHX	1	3984	7/7	0.97	0.26	102,102,102,102	0
85	OHX	1	3985	7/7	0.97	0.41	97,97,97,97	0
85	OHX	1	3986	7/7	0.97	0.19	112,112,112,112	0
84	MG	1	3717	1/1	0.97	0.16	60,60,60,60	0
85	OHX	1	3988	7/7	0.97	0.32	104,104,104,104	0
85	OHX	1	3989	7/7	0.97	0.42	104,104,104,104	0
85	OHX	5	3970	7/7	0.97	0.37	90,90,90,90	0
85	OHX	1	3990	7/7	0.97	0.38	99,99,99,99	0
85	OHX	1	3991	7/7	0.97	0.28	119,119,119,119	0
85	OHX	5	3975	7/7	0.97	0.39	85,85,85,85	0
84	MG	1	3718	1/1	0.97	0.24	78,78,78,78	0
85	OHX	5	3977	7/7	0.97	0.42	70,70,70,70	0
84	MG	5	3454	1/1	0.97	0.40	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	OHX	1	3994	7/7	0.97	0.32	92,92,92,92	0
85	OHX	1	3995	7/7	0.97	0.12	86,86,86,86	0
85	OHX	1	3996	7/7	0.97	0.31	97,97,97,97	0
84	MG	1	3419	1/1	0.97	0.53	44,44,44,44	0
85	OHX	1	3998	7/7	0.97	0.42	102,102,102,102	0
85	OHX	5	3987	7/7	0.97	0.45	81,81,81,81	0
84	MG	6	1989	1/1	0.97	0.20	74,74,74,74	0
84	MG	2	1980	1/1	0.97	0.12	58,58,58,58	0
84	MG	1	3534	1/1	0.97	0.72	36,36,36,36	0
85	OHX	5	3992	7/7	0.97	0.39	97,97,97,97	0
85	OHX	5	3993	7/7	0.97	0.32	101,101,101,101	0
84	MG	5	3573	1/1	0.97	0.32	37,37,37,37	0
84	MG	n3	201	1/1	0.97	0.55	28,28,28,28	0
85	OHX	1	4008	7/7	0.97	0.19	82,82,82,82	0
85	OHX	5	3998	7/7	0.97	0.44	83,83,83,83	0
85	OHX	1	4010	7/7	0.97	0.45	104,104,104,104	0
84	MG	1	3636	1/1	0.97	0.27	46,46,46,46	0
85	OHX	5	4002	7/7	0.97	0.33	102,102,102,102	0
85	OHX	5	4003	7/7	0.97	0.25	86,86,86,86	0
85	OHX	5	4004	7/7	0.97	0.29	119,119,119,119	0
84	MG	1	3586	1/1	0.97	0.56	68,68,68,68	0
84	MG	1	3480	1/1	0.97	0.36	36,36,36,36	0
84	MG	5	3630	1/1	0.97	0.15	31,31,31,31	0
84	MG	1	3537	1/1	0.97	0.34	33,33,33,33	0
85	OHX	5	4010	7/7	0.97	0.38	75,75,75,75	0
84	MG	1	3519	1/1	0.97	0.77	38,38,38,38	0
84	MG	1	3695	1/1	0.97	0.28	40,40,40,40	0
85	OHX	1	4019	7/7	0.97	0.36	85,85,85,85	0
85	OHX	1	4020	7/7	0.97	0.39	118,118,118,118	0
85	OHX	1	4021	7/7	0.97	0.31	128,128,128,128	0
84	MG	o4	201	1/1	0.97	0.35	52,52,52,52	0
85	OHX	5	4021	7/7	0.97	0.38	82,82,82,82	0
84	MG	1	4041	1/1	0.97	0.30	41,41,41,41	0
85	OHX	1	4027	7/7	0.97	0.37	103,103,103,103	0
85	OHX	5	4026	7/7	0.97	0.37	105,105,105,105	0
85	OHX	5	4027	7/7	0.97	0.28	92,92,92,92	0
85	OHX	5	4028	7/7	0.97	0.32	86,86,86,86	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	6	1960	1/1	0.97	0.26	45,45,45,45	0
84	MG	1	3492	1/1	0.97	0.35	39,39,39,39	0
85	OHX	2	1993	7/7	0.97	0.14	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	OHX	2	1997	7/7	0.97	0.11	115,115,115,115	0
85	OHX	5	4037	7/7	0.97	0.28	89,89,89,89	0
85	OHX	5	4038	7/7	0.97	0.30	91,91,91,91	0
85	OHX	5	4039	7/7	0.97	0.40	105,105,105,105	0
85	OHX	5	4040	7/7	0.97	0.41	102,102,102,102	0
85	OHX	5	4041	7/7	0.97	0.44	96,96,96,96	0
85	OHX	1	4033	7/7	0.97	0.27	100,100,100,100	0
85	OHX	S8	301	7/7	0.97	0.26	124,124,124,124	0
84	MG	5	3468	1/1	0.97	0.49	51,51,51,51	0
85	OHX	5	4045	7/7	0.97	0.37	99,99,99,99	0
85	OHX	5	4046	7/7	0.97	0.35	75,75,75,75	0
85	OHX	C5	201	7/7	0.97	0.21	127,127,127,127	0
85	OHX	5	4048	7/7	0.97	0.28	104,104,104,104	0
84	MG	1	3591	1/1	0.97	0.15	44,44,44,44	0
85	OHX	SR	401	7/7	0.97	0.13	134,134,134,134	0
85	OHX	5	4052	7/7	0.97	0.38	94,94,94,94	0
85	OHX	3	215	7/7	0.97	0.18	98,98,98,98	0
85	OHX	1	3765	7/7	0.97	0.11	79,79,79,79	0
85	OHX	2	2005	7/7	0.97	0.13	94,94,94,94	0
85	OHX	1	3778	7/7	0.97	0.12	84,84,84,84	0
85	OHX	5	4057	7/7	0.97	0.34	96,96,96,96	0
85	OHX	4	221	7/7	0.97	0.32	88,88,88,88	0
85	OHX	1	3780	7/7	0.97	0.09	100,100,100,100	0
84	MG	5	3519	1/1	0.97	0.54	34,34,34,34	0
85	OHX	4	227	7/7	0.97	0.39	85,85,85,85	0
85	OHX	1	3795	7/7	0.97	0.13	83,83,83,83	0
84	MG	1	3566	1/1	0.97	0.37	37,37,37,37	0
85	OHX	5	4065	7/7	0.97	0.13	92,92,92,92	0
85	OHX	2	2014	7/7	0.97	0.20	89,89,89,89	0
85	OHX	1	3806	7/7	0.97	0.10	92,92,92,92	0
85	OHX	5	4069	7/7	0.97	0.11	129,129,129,129	0
85	OHX	1	3807	7/7	0.97	0.12	76,76,76,76	0
85	OHX	7	213	7/7	0.97	0.13	79,79,79,79	0
85	OHX	7	218	7/7	0.97	0.30	92,92,92,92	0
85	OHX	7	219	7/7	0.97	0.24	80,80,80,80	0
85	OHX	1	3809	7/7	0.97	0.09	107,107,107,107	0
84	MG	2	1977	1/1	0.97	0.27	75,75,75,75	0
85	OHX	8	212	7/7	0.97	0.10	91,91,91,91	0
85	OHX	8	215	7/7	0.97	0.15	94,94,94,94	0
85	OHX	8	217	7/7	0.97	0.20	101,101,101,101	0
85	OHX	8	218	7/7	0.97	0.29	79,79,79,79	0
85	OHX	8	219	7/7	0.97	0.29	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	OHX	1	3812	7/7	0.97	0.12	88,88,88,88	0
85	OHX	8	222	7/7	0.97	0.27	114,114,114,114	0
85	OHX	2	2017	7/7	0.97	0.15	89,89,89,89	0
85	OHX	8	224	7/7	0.97	0.45	94,94,94,94	0
85	OHX	13	407	7/7	0.97	0.28	78,78,78,78	0
85	OHX	1	3820	7/7	0.97	0.14	87,87,87,87	0
85	OHX	14	401	7/7	0.97	0.26	96,96,96,96	0
85	OHX	14	402	7/7	0.97	0.52	99,99,99,99	0
85	OHX	15	301	7/7	0.97	0.17	106,106,106,106	0
85	OHX	6	2036	7/7	0.97	0.10	110,110,110,110	0
85	OHX	19	202	7/7	0.97	0.23	92,92,92,92	0
85	OHX	6	2037	7/7	0.97	0.09	112,112,112,112	0
85	OHX	1	3822	7/7	0.97	0.11	95,95,95,95	0
85	OHX	6	2048	7/7	0.97	0.08	117,117,117,117	0
85	OHX	m7	204	7/7	0.97	0.40	84,84,84,84	0
85	OHX	o9	101	7/7	0.97	0.28	87,87,87,87	0
85	OHX	2	2018	7/7	0.97	0.12	106,106,106,106	0
85	OHX	6	2057	7/7	0.97	0.12	108,108,108,108	0
85	OHX	6	2058	7/7	0.97	0.17	99,99,99,99	0
85	OHX	2	2021	7/7	0.97	0.17	99,99,99,99	0
86	ZN	Q2	501	1/1	0.97	0.16	64,64,64,64	0
85	OHX	6	2066	7/7	0.97	0.17	83,83,83,83	0
84	MG	1	3522	1/1	0.97	0.34	32,32,32,32	0
85	OHX	6	2069	7/7	0.97	0.23	86,86,86,86	0
85	OHX	6	2074	7/7	0.97	0.14	106,106,106,106	0
84	MG	5	3524	1/1	0.97	0.66	34,34,34,34	0
85	OHX	6	2079	7/7	0.97	0.23	110,110,110,110	0
85	OHX	2	1990	7/7	0.98	0.09	95,95,95,95	0
85	OHX	6	2122	7/7	0.98	0.37	92,92,92,92	0
84	MG	1	3499	1/1	0.98	0.47	39,39,39,39	0
84	MG	5	3579	1/1	0.98	0.55	32,32,32,32	0
85	OHX	6	2125	7/7	0.98	0.27	87,87,87,87	0
85	OHX	1	3922	7/7	0.98	0.43	92,92,92,92	0
85	OHX	2	1995	7/7	0.98	0.09	91,91,91,91	0
85	OHX	1	3924	7/7	0.98	0.26	76,76,76,76	0
85	OHX	1	3925	7/7	0.98	0.10	116,116,116,116	0
85	OHX	1	3926	7/7	0.98	0.31	81,81,81,81	0
85	OHX	1	3927	7/7	0.98	0.29	92,92,92,92	0
84	MG	1	3540	1/1	0.98	0.45	35,35,35,35	0
85	OHX	2	1998	7/7	0.98	0.10	89,89,89,89	0
85	OHX	6	2134	7/7	0.98	0.29	112,112,112,112	0
85	OHX	2	1999	7/7	0.98	0.10	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	7	208	1/1	0.98	0.58	43,43,43,43	0
85	OHX	2	2002	7/7	0.98	0.08	84,84,84,84	0
85	OHX	6	2138	7/7	0.98	0.27	77,77,77,77	0
84	MG	5	3504	1/1	0.98	0.45	37,37,37,37	0
84	MG	6	1939	1/1	0.98	0.31	56,56,56,56	0
85	OHX	2	2007	7/7	0.98	0.14	94,94,94,94	0
84	MG	1	3410	1/1	0.98	0.45	35,35,35,35	0
85	OHX	2	2009	7/7	0.98	0.15	95,95,95,95	0
85	OHX	1	3939	7/7	0.98	0.32	94,94,94,94	0
84	MG	1	3555	1/1	0.98	0.16	35,35,35,35	0
85	OHX	2	2013	7/7	0.98	0.21	105,105,105,105	0
84	MG	5	3539	1/1	0.98	0.42	29,29,29,29	0
84	MG	6	1991	1/1	0.98	0.15	50,50,50,50	0
85	OHX	1	3944	7/7	0.98	0.18	100,100,100,100	0
85	OHX	2	2016	7/7	0.98	0.20	108,108,108,108	0
84	MG	2	1944	1/1	0.98	0.57	91,91,91,91	0
84	MG	5	3510	1/1	0.98	0.56	36,36,36,36	0
85	OHX	2	2020	7/7	0.98	0.09	103,103,103,103	0
84	MG	1	3557	1/1	0.98	0.70	37,37,37,37	0
85	OHX	1	3952	7/7	0.98	0.23	111,111,111,111	0
85	OHX	2	2022	7/7	0.98	0.12	107,107,107,107	0
85	OHX	1	3954	7/7	0.98	0.37	96,96,96,96	0
85	OHX	2	2023	7/7	0.98	0.22	90,90,90,90	0
85	OHX	1	3956	7/7	0.98	0.36	100,100,100,100	0
85	OHX	1	3959	7/7	0.98	0.28	84,84,84,84	0
85	OHX	2	2024	7/7	0.98	0.20	89,89,89,89	0
85	OHX	1	3961	7/7	0.98	0.23	104,104,104,104	0
84	MG	8	208	1/1	0.98	0.10	63,63,63,63	0
85	OHX	c8	201	7/7	0.98	0.15	117,117,117,117	0
85	OHX	1	3963	7/7	0.98	0.26	88,88,88,88	0
84	MG	1	3558	1/1	0.98	0.32	45,45,45,45	0
85	OHX	5	3770	7/7	0.98	0.13	63,63,63,63	0
85	OHX	5	3773	7/7	0.98	0.11	64,64,64,64	0
85	OHX	5	3775	7/7	0.98	0.11	60,60,60,60	0
85	OHX	5	3784	7/7	0.98	0.12	70,70,70,70	0
85	OHX	1	3965	7/7	0.98	0.20	109,109,109,109	0
85	OHX	5	3787	7/7	0.98	0.10	63,63,63,63	0
85	OHX	5	3788	7/7	0.98	0.08	78,78,78,78	0
84	MG	1	3716	1/1	0.98	0.10	33,33,33,33	0
85	OHX	5	3796	7/7	0.98	0.09	89,89,89,89	0
85	OHX	5	3799	7/7	0.98	0.16	82,82,82,82	0
85	OHX	5	3800	7/7	0.98	0.09	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	5	3546	1/1	0.98	0.67	39,39,39,39	0
85	OHX	5	3803	7/7	0.98	0.10	63,63,63,63	0
85	OHX	5	3804	7/7	0.98	0.11	63,63,63,63	0
85	OHX	5	3806	7/7	0.98	0.08	74,74,74,74	0
85	OHX	5	3807	7/7	0.98	0.10	74,74,74,74	0
85	OHX	5	3809	7/7	0.98	0.13	88,88,88,88	0
85	OHX	1	3968	7/7	0.98	0.28	86,86,86,86	0
85	OHX	5	3816	7/7	0.98	0.13	66,66,66,66	0
85	OHX	5	3817	7/7	0.98	0.12	67,67,67,67	0
85	OHX	2	2029	7/7	0.98	0.12	108,108,108,108	0
85	OHX	2	2030	7/7	0.98	0.20	103,103,103,103	0
85	OHX	5	3820	7/7	0.98	0.12	81,81,81,81	0
85	OHX	5	3821	7/7	0.98	0.10	74,74,74,74	0
85	OHX	5	3823	7/7	0.98	0.13	76,76,76,76	0
84	MG	1	3463	1/1	0.98	0.47	32,32,32,32	0
85	OHX	5	3827	7/7	0.98	0.20	76,76,76,76	0
85	OHX	5	3831	7/7	0.98	0.11	77,77,77,77	0
85	OHX	5	3834	7/7	0.98	0.14	79,79,79,79	0
85	OHX	5	3836	7/7	0.98	0.15	81,81,81,81	0
85	OHX	5	3837	7/7	0.98	0.26	72,72,72,72	0
85	OHX	C8	201	7/7	0.98	0.08	97,97,97,97	0
85	OHX	5	3840	7/7	0.98	0.20	73,73,73,73	0
85	OHX	2	2033	7/7	0.98	0.27	94,94,94,94	0
85	OHX	5	3845	7/7	0.98	0.11	87,87,87,87	0
85	OHX	5	3846	7/7	0.98	0.22	58,58,58,58	0
84	MG	1	3625	1/1	0.98	0.40	63,63,63,63	0
85	OHX	1	3975	7/7	0.98	0.34	85,85,85,85	0
85	OHX	1	3751	7/7	0.98	0.13	67,67,67,67	0
85	OHX	5	3853	7/7	0.98	0.10	83,83,83,83	0
85	OHX	5	3854	7/7	0.98	0.21	80,80,80,80	0
85	OHX	5	3855	7/7	0.98	0.23	83,83,83,83	0
85	OHX	5	3856	7/7	0.98	0.07	120,120,120,120	0
85	OHX	5	3857	7/7	0.98	0.20	71,71,71,71	0
85	OHX	5	3859	7/7	0.98	0.17	81,81,81,81	0
85	OHX	1	3755	7/7	0.98	0.12	67,67,67,67	0
85	OHX	1	3756	7/7	0.98	0.12	68,68,68,68	0
85	OHX	5	3866	7/7	0.98	0.19	87,87,87,87	0
85	OHX	5	3867	7/7	0.98	0.21	85,85,85,85	0
85	OHX	1	3757	7/7	0.98	0.11	70,70,70,70	0
85	OHX	1	3980	7/7	0.98	0.37	83,83,83,83	0
85	OHX	1	3764	7/7	0.98	0.15	64,64,64,64	0
85	OHX	5	3872	7/7	0.98	0.18	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3451	1/1	0.98	0.37	47,47,47,47	0
84	MG	1	3513	1/1	0.98	0.95	38,38,38,38	0
85	OHX	5	3875	7/7	0.98	0.10	112,112,112,112	0
85	OHX	5	3876	7/7	0.98	0.29	76,76,76,76	0
85	OHX	5	3877	7/7	0.98	0.19	80,80,80,80	0
85	OHX	1	3771	7/7	0.98	0.09	76,76,76,76	0
85	OHX	1	3773	7/7	0.98	0.08	73,73,73,73	0
85	OHX	1	3776	7/7	0.98	0.13	69,69,69,69	0
85	OHX	5	3883	7/7	0.98	0.19	91,91,91,91	0
85	OHX	1	3777	7/7	0.98	0.07	84,84,84,84	0
85	OHX	5	3885	7/7	0.98	0.26	92,92,92,92	0
85	OHX	2	2037	7/7	0.98	0.22	106,106,106,106	0
85	OHX	5	3887	7/7	0.98	0.23	72,72,72,72	0
84	MG	5	3552	1/1	0.98	0.57	36,36,36,36	0
85	OHX	5	3890	7/7	0.98	0.20	97,97,97,97	0
85	OHX	5	3891	7/7	0.98	0.22	84,84,84,84	0
85	OHX	1	3781	7/7	0.98	0.12	78,78,78,78	0
85	OHX	5	3893	7/7	0.98	0.15	111,111,111,111	0
85	OHX	5	3894	7/7	0.98	0.40	80,80,80,80	0
85	OHX	1	3783	7/7	0.98	0.11	70,70,70,70	0
85	OHX	1	3784	7/7	0.98	0.10	77,77,77,77	0
84	MG	6	1925	1/1	0.98	0.38	72,72,72,72	0
85	OHX	5	3899	7/7	0.98	0.25	80,80,80,80	0
85	OHX	5	3900	7/7	0.98	0.24	103,103,103,103	0
85	OHX	1	3789	7/7	0.98	0.10	88,88,88,88	0
85	OHX	5	3902	7/7	0.98	0.27	87,87,87,87	0
85	OHX	1	3791	7/7	0.98	0.11	73,73,73,73	0
85	OHX	1	3792	7/7	0.98	0.11	80,80,80,80	0
85	OHX	2	2041	7/7	0.98	0.10	119,119,119,119	0
85	OHX	1	3797	7/7	0.98	0.10	76,76,76,76	0
85	OHX	5	3907	7/7	0.98	0.17	116,116,116,116	0
85	OHX	5	3908	7/7	0.98	0.23	84,84,84,84	0
85	OHX	1	3999	7/7	0.98	0.25	82,82,82,82	0
85	OHX	5	3910	7/7	0.98	0.12	95,95,95,95	0
85	OHX	2	2042	7/7	0.98	0.15	110,110,110,110	0
85	OHX	5	3912	7/7	0.98	0.30	108,108,108,108	0
85	OHX	1	4001	7/7	0.98	0.25	108,108,108,108	0
85	OHX	2	2044	7/7	0.98	0.22	113,113,113,113	0
85	OHX	5	3915	7/7	0.98	0.25	91,91,91,91	0
85	OHX	5	3916	7/7	0.98	0.32	85,85,85,85	0
85	OHX	5	3917	7/7	0.98	0.23	86,86,86,86	0
85	OHX	5	3918	7/7	0.98	0.33	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	OHX	1	3804	7/7	0.98	0.10	88,88,88,88	0
85	OHX	1	4004	7/7	0.98	0.35	85,85,85,85	0
85	OHX	5	3923	7/7	0.98	0.20	85,85,85,85	0
85	OHX	5	3924	7/7	0.98	0.28	77,77,77,77	0
85	OHX	5	3925	7/7	0.98	0.22	81,81,81,81	0
85	OHX	1	3805	7/7	0.98	0.10	72,72,72,72	0
85	OHX	5	3927	7/7	0.98	0.23	87,87,87,87	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	5	3931	7/7	0.98	0.18	68,68,68,68	0
85	OHX	2	2046	7/7	0.98	0.16	105,105,105,105	0
85	OHX	5	3933	7/7	0.98	0.30	77,77,77,77	0
85	OHX	5	3934	7/7	0.98	0.26	91,91,91,91	0
84	MG	5	3554	1/1	0.98	0.42	29,29,29,29	0
85	OHX	5	3936	7/7	0.98	0.23	98,98,98,98	0
85	OHX	1	4011	7/7	0.98	0.32	100,100,100,100	0
85	OHX	2	2048	7/7	0.98	0.24	87,87,87,87	0
85	OHX	5	3939	7/7	0.98	0.26	83,83,83,83	0
84	MG	1	3628	1/1	0.98	0.72	50,50,50,50	0
85	OHX	2	2050	7/7	0.98	0.36	102,102,102,102	0
85	OHX	5	3942	7/7	0.98	0.25	98,98,98,98	0
85	OHX	1	3814	7/7	0.98	0.14	71,71,71,71	0
85	OHX	1	3816	7/7	0.98	0.12	84,84,84,84	0
85	OHX	1	3817	7/7	0.98	0.16	75,75,75,75	0
85	OHX	1	3819	7/7	0.98	0.09	90,90,90,90	0
85	OHX	2	2051	7/7	0.98	0.32	93,93,93,93	0
85	OHX	5	3948	7/7	0.98	0.31	92,92,92,92	0
84	MG	5	3556	1/1	0.98	0.41	36,36,36,36	0
84	MG	5	3557	1/1	0.98	0.68	42,42,42,42	0
85	OHX	5	3952	7/7	0.98	0.33	77,77,77,77	0
85	OHX	1	4022	7/7	0.98	0.41	77,77,77,77	0
84	MG	1	3579	1/1	0.98	0.42	40,40,40,40	0
85	OHX	1	3827	7/7	0.98	0.20	72,72,72,72	0
85	OHX	1	4025	7/7	0.98	0.44	101,101,101,101	0
85	OHX	1	4026	7/7	0.98	0.39	90,90,90,90	0
84	MG	6	1905	1/1	0.98	0.83	61,61,61,61	0
85	OHX	1	3829	7/7	0.98	0.15	82,82,82,82	0
85	OHX	1	3831	7/7	0.98	0.18	86,86,86,86	0
85	OHX	5	3962	7/7	0.98	0.23	111,111,111,111	0
85	OHX	1	3833	7/7	0.98	0.20	78,78,78,78	0
85	OHX	5	3964	7/7	0.98	0.34	106,106,106,106	0
85	OHX	1	3834	7/7	0.98	0.09	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	OHX	2	2056	7/7	0.98	0.09	127,127,127,127	0
85	OHX	1	3836	7/7	0.98	0.21	83,83,83,83	0
84	MG	5	3561	1/1	0.98	0.93	48,48,48,48	0
84	MG	5	3691	1/1	0.98	0.12	43,43,43,43	0
85	OHX	5	3971	7/7	0.98	0.23	94,94,94,94	0
85	OHX	1	3842	7/7	0.98	0.14	96,96,96,96	0
85	OHX	1	3843	7/7	0.98	0.23	79,79,79,79	0
85	OHX	5	3974	7/7	0.98	0.36	89,89,89,89	0
85	OHX	1	3844	7/7	0.98	0.19	71,71,71,71	0
85	OHX	3	210	7/7	0.98	0.09	77,77,77,77	0
85	OHX	3	212	7/7	0.98	0.11	81,81,81,81	0
85	OHX	3	213	7/7	0.98	0.18	97,97,97,97	0
85	OHX	5	3979	7/7	0.98	0.28	85,85,85,85	0
85	OHX	3	214	7/7	0.98	0.18	95,95,95,95	0
85	OHX	5	3981	7/7	0.98	0.28	97,97,97,97	0
85	OHX	1	3845	7/7	0.98	0.25	77,77,77,77	0
85	OHX	1	3846	7/7	0.98	0.19	97,97,97,97	0
85	OHX	3	217	7/7	0.98	0.31	85,85,85,85	0
85	OHX	5	3985	7/7	0.98	0.39	97,97,97,97	0
85	OHX	1	3847	7/7	0.98	0.21	91,91,91,91	0
85	OHX	1	3849	7/7	0.98	0.20	80,80,80,80	0
85	OHX	4	218	7/7	0.98	0.18	77,77,77,77	0
85	OHX	4	219	7/7	0.98	0.10	93,93,93,93	0
85	OHX	4	220	7/7	0.98	0.17	96,96,96,96	0
85	OHX	5	3991	7/7	0.98	0.23	87,87,87,87	0
85	OHX	1	3852	7/7	0.98	0.14	110,110,110,110	0
85	OHX	4	222	7/7	0.98	0.26	83,83,83,83	0
85	OHX	5	3994	7/7	0.98	0.30	97,97,97,97	0
85	OHX	1	3853	7/7	0.98	0.14	93,93,93,93	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	4	226	7/7	0.98	0.22	106,106,106,106	0
84	MG	5	3523	1/1	0.98	0.33	27,27,27,27	0
85	OHX	1	3857	7/7	0.98	0.21	79,79,79,79	0
85	OHX	2	2061	7/7	0.98	0.25	115,115,115,115	0
85	OHX	1	3859	7/7	0.98	0.16	119,119,119,119	0
85	OHX	1	3860	7/7	0.98	0.27	82,82,82,82	0
85	OHX	L3	403	7/7	0.98	0.22	86,86,86,86	0
85	OHX	5	4006	7/7	0.98	0.37	89,89,89,89	0
84	MG	1	3505	1/1	0.98	0.29	38,38,38,38	0
85	OHX	1	3863	7/7	0.98	0.16	95,95,95,95	0
85	OHX	M5	302	7/7	0.98	0.22	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	OHX	M7	205	7/7	0.98	0.30	101,101,101,101	0
85	OHX	5	4012	7/7	0.98	0.27	89,89,89,89	0
85	OHX	5	4013	7/7	0.98	0.41	96,96,96,96	0
84	MG	5	3565	1/1	0.98	0.54	49,49,49,49	0
85	OHX	5	4015	7/7	0.98	0.29	98,98,98,98	0
85	OHX	2	2064	7/7	0.98	0.20	92,92,92,92	0
85	OHX	O3	202	7/7	0.98	0.33	85,85,85,85	0
85	OHX	O7	104	7/7	0.98	0.09	77,77,77,77	0
85	OHX	O7	105	7/7	0.98	0.19	76,76,76,76	0
85	OHX	1	3866	7/7	0.98	0.26	91,91,91,91	0
85	OHX	6	2017	7/7	0.98	0.09	85,85,85,85	0
85	OHX	5	4022	7/7	0.98	0.38	94,94,94,94	0
85	OHX	1	3867	7/7	0.98	0.20	75,75,75,75	0
85	OHX	6	2028	7/7	0.98	0.09	89,89,89,89	0
85	OHX	5	4025	7/7	0.98	0.37	93,93,93,93	0
85	OHX	6	2029	7/7	0.98	0.08	110,110,110,110	0
85	OHX	6	2032	7/7	0.98	0.09	87,87,87,87	0
85	OHX	6	2033	7/7	0.98	0.13	74,74,74,74	0
85	OHX	1	3868	7/7	0.98	0.23	83,83,83,83	0
85	OHX	2	2065	7/7	0.98	0.21	104,104,104,104	0
85	OHX	6	2039	7/7	0.98	0.11	83,83,83,83	0
85	OHX	1	3870	7/7	0.98	0.22	97,97,97,97	0
85	OHX	6	2041	7/7	0.98	0.12	74,74,74,74	0
85	OHX	6	2042	7/7	0.98	0.13	100,100,100,100	0
85	OHX	5	4035	7/7	0.98	0.18	63,63,63,63	0
85	OHX	5	4036	7/7	0.98	0.22	82,82,82,82	0
85	OHX	6	2043	7/7	0.98	0.19	77,77,77,77	0
85	OHX	6	2046	7/7	0.98	0.10	95,95,95,95	0
85	OHX	6	2047	7/7	0.98	0.12	91,91,91,91	0
85	OHX	1	3872	7/7	0.98	0.18	98,98,98,98	0
85	OHX	6	2049	7/7	0.98	0.14	85,85,85,85	0
85	OHX	6	2051	7/7	0.98	0.12	93,93,93,93	0
85	OHX	6	2053	7/7	0.98	0.15	84,84,84,84	0
85	OHX	2	2066	7/7	0.98	0.20	93,93,93,93	0
85	OHX	6	2055	7/7	0.98	0.10	95,95,95,95	0
85	OHX	6	2056	7/7	0.98	0.13	82,82,82,82	0
85	OHX	1	3875	7/7	0.98	0.21	100,100,100,100	0
84	MG	1	3686	1/1	0.98	0.11	37,37,37,37	0
85	OHX	5	4049	7/7	0.98	0.33	85,85,85,85	0
85	OHX	6	2059	7/7	0.98	0.10	106,106,106,106	0
85	OHX	6	2060	7/7	0.98	0.12	138,138,138,138	0
85	OHX	6	2061	7/7	0.98	0.18	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	5	3568	1/1	0.98	0.56	35,35,35,35	0
85	OHX	6	2063	7/7	0.98	0.11	134,134,134,134	0
85	OHX	6	2064	7/7	0.98	0.07	141,141,141,141	0
85	OHX	6	2065	7/7	0.98	0.11	94,94,94,94	0
85	OHX	1	3880	7/7	0.98	0.23	89,89,89,89	0
85	OHX	6	2067	7/7	0.98	0.16	98,98,98,98	0
84	MG	5	3569	1/1	0.98	0.63	29,29,29,29	0
85	OHX	5	4060	7/7	0.98	0.30	125,125,125,125	0
85	OHX	1	3882	7/7	0.98	0.19	90,90,90,90	0
85	OHX	6	2070	7/7	0.98	0.28	98,98,98,98	0
85	OHX	6	2071	7/7	0.98	0.17	79,79,79,79	0
85	OHX	6	2072	7/7	0.98	0.23	92,92,92,92	0
84	MG	1	3453	1/1	0.98	0.39	33,33,33,33	0
85	OHX	6	2075	7/7	0.98	0.24	96,96,96,96	0
85	OHX	1	3886	7/7	0.98	0.22	101,101,101,101	0
85	OHX	2	2072	7/7	0.98	0.29	106,106,106,106	0
84	MG	5	4074	1/1	0.98	0.41	32,32,32,32	0
85	OHX	7	211	7/7	0.98	0.09	74,74,74,74	0
85	OHX	7	212	7/7	0.98	0.14	70,70,70,70	0
85	OHX	2	2074	7/7	0.98	0.24	101,101,101,101	0
85	OHX	7	214	7/7	0.98	0.15	71,71,71,71	0
85	OHX	7	217	7/7	0.98	0.15	95,95,95,95	0
85	OHX	6	2083	7/7	0.98	0.19	116,116,116,116	0
84	MG	5	3497	1/1	0.98	0.56	30,30,30,30	0
85	OHX	6	2085	7/7	0.98	0.24	78,78,78,78	0
85	OHX	6	2086	7/7	0.98	0.32	103,103,103,103	0
85	OHX	1	3891	7/7	0.98	0.22	81,81,81,81	0
85	OHX	8	213	7/7	0.98	0.18	83,83,83,83	0
85	OHX	8	214	7/7	0.98	0.13	102,102,102,102	0
84	MG	5	3528	1/1	0.98	0.26	36,36,36,36	0
85	OHX	8	216	7/7	0.98	0.31	86,86,86,86	0
85	OHX	1	3894	7/7	0.98	0.14	114,114,114,114	0
85	OHX	6	2090	7/7	0.98	0.23	115,115,115,115	0
85	OHX	1	3895	7/7	0.98	0.22	70,70,70,70	0
85	OHX	8	220	7/7	0.98	0.17	120,120,120,120	0
85	OHX	6	2092	7/7	0.98	0.17	96,96,96,96	0
85	OHX	1	3896	7/7	0.98	0.22	88,88,88,88	0
84	MG	1	3454	1/1	0.98	0.39	34,34,34,34	0
84	MG	6	1983	1/1	0.98	0.19	73,73,73,73	0
85	OHX	8	225	7/7	0.98	0.37	101,101,101,101	0
85	OHX	6	2096	7/7	0.98	0.21	100,100,100,100	0
85	OHX	6	2097	7/7	0.98	0.19	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	OHX	2	2079	7/7	0.98	0.23	115,115,115,115	0
85	OHX	1	3900	7/7	0.98	0.25	83,83,83,83	0
85	OHX	1	3901	7/7	0.98	0.19	106,106,106,106	0
85	OHX	6	2102	7/7	0.98	0.27	104,104,104,104	0
85	OHX	1	3902	7/7	0.98	0.26	88,88,88,88	0
85	OHX	6	2104	7/7	0.98	0.30	103,103,103,103	0
84	MG	6	1935	1/1	0.98	0.47	44,44,44,44	0
85	OHX	2	2081	7/7	0.98	0.28	109,109,109,109	0
85	OHX	m5	304	7/7	0.98	0.11	74,74,74,74	0
85	OHX	m5	305	7/7	0.98	0.18	94,94,94,94	0
84	MG	1	3550	1/1	0.98	0.26	40,40,40,40	0
85	OHX	n3	203	7/7	0.98	0.21	76,76,76,76	0
85	OHX	o7	502	7/7	0.98	0.13	79,79,79,79	0
85	OHX	1	3907	7/7	0.98	0.21	96,96,96,96	0
85	OHX	q2	502	7/7	0.98	0.16	61,61,61,61	0
85	OHX	2	2083	7/7	0.98	0.30	115,115,115,115	0
84	MG	7	203	1/1	0.98	0.38	58,58,58,58	0
86	ZN	D9	101	1/1	0.98	0.12	79,79,79,79	0
85	OHX	1	3911	7/7	0.98	0.23	103,103,103,103	0
84	MG	5	3706	1/1	0.98	0.23	37,37,37,37	0
85	OHX	6	2114	7/7	0.98	0.26	114,114,114,114	0
86	ZN	Q3	501	1/1	0.98	0.06	58,58,58,58	0
85	OHX	1	3913	7/7	0.98	0.27	70,70,70,70	0
85	OHX	2	1985	7/7	0.98	0.16	84,84,84,84	0
85	OHX	2	2087	7/7	0.98	0.26	119,119,119,119	0
85	OHX	2	2088	7/7	0.98	0.19	94,94,94,94	0
86	ZN	q0	201	1/1	0.98	0.10	36,36,36,36	0
85	OHX	2	1988	7/7	0.98	0.17	90,90,90,90	0
85	OHX	2	1989	7/7	0.98	0.08	92,92,92,92	0
85	OHX	1	3736	7/7	0.99	0.11	63,63,63,63	0
85	OHX	1	3821	7/7	0.99	0.15	77,77,77,77	0
85	OHX	6	2099	7/7	0.99	0.30	95,95,95,95	0
85	OHX	1	3738	7/7	0.99	0.08	56,56,56,56	0
85	OHX	1	3739	7/7	0.99	0.07	62,62,62,62	0
85	OHX	1	3824	7/7	0.99	0.09	56,56,56,56	0
85	OHX	1	3825	7/7	0.99	0.15	83,83,83,83	0
85	OHX	1	3740	7/7	0.99	0.13	60,60,60,60	0
85	OHX	1	3741	7/7	0.99	0.09	55,55,55,55	0
85	OHX	1	3742	7/7	0.99	0.11	65,65,65,65	0
85	OHX	1	3743	7/7	0.99	0.12	60,60,60,60	0
85	OHX	1	3830	7/7	0.99	0.11	86,86,86,86	0
85	OHX	1	3746	7/7	0.99	0.10	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	OHX	1	3832	7/7	0.99	0.19	75,75,75,75	0
85	OHX	6	2111	7/7	0.99	0.21	84,84,84,84	0
85	OHX	1	3747	7/7	0.99	0.14	64,64,64,64	0
85	OHX	1	3748	7/7	0.99	0.10	72,72,72,72	0
85	OHX	3	211	7/7	0.99	0.20	85,85,85,85	0
85	OHX	1	3749	7/7	0.99	0.11	67,67,67,67	0
85	OHX	1	3750	7/7	0.99	0.12	76,76,76,76	0
85	OHX	2	2038	7/7	0.99	0.24	93,93,93,93	0
85	OHX	5	3920	7/7	0.99	0.12	73,73,73,73	0
85	OHX	5	3921	7/7	0.99	0.24	95,95,95,95	0
85	OHX	1	3838	7/7	0.99	0.25	68,68,68,68	0
85	OHX	1	3938	7/7	0.99	0.24	92,92,92,92	0
85	OHX	1	3839	7/7	0.99	0.18	80,80,80,80	0
85	OHX	1	3753	7/7	0.99	0.09	67,67,67,67	0
85	OHX	1	3841	7/7	0.99	0.17	62,62,62,62	0
85	OHX	4	215	7/7	0.99	0.10	54,54,54,54	0
85	OHX	4	216	7/7	0.99	0.09	58,58,58,58	0
85	OHX	5	3929	7/7	0.99	0.18	76,76,76,76	0
85	OHX	4	217	7/7	0.99	0.08	68,68,68,68	0
85	OHX	2	2011	7/7	0.99	0.16	98,98,98,98	0
85	OHX	2	2069	7/7	0.99	0.15	112,112,112,112	0
85	OHX	2	1987	7/7	0.99	0.10	74,74,74,74	0
85	OHX	1	3758	7/7	0.99	0.05	67,67,67,67	0
85	OHX	1	3759	7/7	0.99	0.11	79,79,79,79	0
85	OHX	1	3760	7/7	0.99	0.09	68,68,68,68	0
85	OHX	1	3948	7/7	0.99	0.18	70,70,70,70	0
85	OHX	1	3848	7/7	0.99	0.15	90,90,90,90	0
85	OHX	1	3762	7/7	0.99	0.07	66,66,66,66	0
85	OHX	1	3951	7/7	0.99	0.29	81,81,81,81	0
85	OHX	1	3850	7/7	0.99	0.24	83,83,83,83	0
85	OHX	1	3851	7/7	0.99	0.23	82,82,82,82	0
85	OHX	1	3763	7/7	0.99	0.09	68,68,68,68	0
84	MG	1	3535	1/1	0.99	0.37	43,43,43,43	0
85	OHX	L3	402	7/7	0.99	0.27	86,86,86,86	0
85	OHX	1	3854	7/7	0.99	0.17	74,74,74,74	0
85	OHX	1	3957	7/7	0.99	0.32	111,111,111,111	0
85	OHX	1	3958	7/7	0.99	0.34	84,84,84,84	0
85	OHX	5	3949	7/7	0.99	0.18	63,63,63,63	0
84	MG	1	3562	1/1	0.99	0.56	48,48,48,48	0
85	OHX	M6	202	7/7	0.99	0.18	80,80,80,80	0
85	OHX	1	3766	7/7	0.99	0.08	76,76,76,76	0
85	OHX	5	3953	7/7	0.99	0.20	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	OHX	1	3767	7/7	0.99	0.12	69,69,69,69	0
85	OHX	N1	201	7/7	0.99	0.08	59,59,59,59	0
85	OHX	1	3768	7/7	0.99	0.06	83,83,83,83	0
85	OHX	N9	101	7/7	0.99	0.11	56,56,56,56	0
85	OHX	1	3769	7/7	0.99	0.07	63,63,63,63	0
85	OHX	2	2043	7/7	0.99	0.19	89,89,89,89	0
85	OHX	1	3861	7/7	0.99	0.14	67,67,67,67	0
84	MG	5	3560	1/1	0.99	0.47	35,35,35,35	0
85	OHX	Q2	503	7/7	0.99	0.20	59,59,59,59	0
85	OHX	6	2010	7/7	0.99	0.18	73,73,73,73	0
85	OHX	6	2011	7/7	0.99	0.09	61,61,61,61	0
85	OHX	5	3965	7/7	0.99	0.29	88,88,88,88	0
85	OHX	6	2012	7/7	0.99	0.10	67,67,67,67	0
85	OHX	6	2013	7/7	0.99	0.12	70,70,70,70	0
85	OHX	6	2015	7/7	0.99	0.11	75,75,75,75	0
85	OHX	6	2016	7/7	0.99	0.14	71,71,71,71	0
85	OHX	1	3772	7/7	0.99	0.06	74,74,74,74	0
85	OHX	6	2018	7/7	0.99	0.10	60,60,60,60	0
85	OHX	6	2019	7/7	0.99	0.13	77,77,77,77	0
85	OHX	6	2020	7/7	0.99	0.09	69,69,69,69	0
85	OHX	6	2021	7/7	0.99	0.09	74,74,74,74	0
85	OHX	5	3742	7/7	0.99	0.18	46,46,46,46	0
85	OHX	5	3746	7/7	0.99	0.16	54,54,54,54	0
85	OHX	5	3747	7/7	0.99	0.12	53,53,53,53	0
85	OHX	5	3748	7/7	0.99	0.10	55,55,55,55	0
85	OHX	5	3749	7/7	0.99	0.13	52,52,52,52	0
85	OHX	5	3750	7/7	0.99	0.11	54,54,54,54	0
85	OHX	5	3751	7/7	0.99	0.12	52,52,52,52	0
85	OHX	5	3753	7/7	0.99	0.16	68,68,68,68	0
85	OHX	5	3754	7/7	0.99	0.09	50,50,50,50	0
85	OHX	5	3755	7/7	0.99	0.09	50,50,50,50	0
85	OHX	5	3758	7/7	0.99	0.11	55,55,55,55	0
85	OHX	5	3759	7/7	0.99	0.08	62,62,62,62	0
85	OHX	5	3760	7/7	0.99	0.09	56,56,56,56	0
85	OHX	5	3761	7/7	0.99	0.08	55,55,55,55	0
85	OHX	5	3762	7/7	0.99	0.10	63,63,63,63	0
85	OHX	5	3764	7/7	0.99	0.06	57,57,57,57	0
85	OHX	5	3765	7/7	0.99	0.10	59,59,59,59	0
85	OHX	5	3767	7/7	0.99	0.11	63,63,63,63	0
85	OHX	5	3768	7/7	0.99	0.06	58,58,58,58	0
85	OHX	6	2022	7/7	0.99	0.09	87,87,87,87	0
85	OHX	5	3771	7/7	0.99	0.04	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	OHX	5	3772	7/7	0.99	0.05	61,61,61,61	0
85	OHX	6	2023	7/7	0.99	0.06	71,71,71,71	0
85	OHX	6	2024	7/7	0.99	0.07	71,71,71,71	0
85	OHX	5	3999	7/7	0.99	0.28	76,76,76,76	0
85	OHX	5	3776	7/7	0.99	0.10	86,86,86,86	0
85	OHX	5	3777	7/7	0.99	0.07	59,59,59,59	0
85	OHX	5	3778	7/7	0.99	0.06	64,64,64,64	0
85	OHX	5	3779	7/7	0.99	0.06	65,65,65,65	0
85	OHX	5	3780	7/7	0.99	0.05	59,59,59,59	0
85	OHX	5	3781	7/7	0.99	0.09	65,65,65,65	0
85	OHX	5	3782	7/7	0.99	0.10	76,76,76,76	0
85	OHX	5	3783	7/7	0.99	0.06	77,77,77,77	0
85	OHX	6	2025	7/7	0.99	0.09	73,73,73,73	0
85	OHX	5	3785	7/7	0.99	0.07	68,68,68,68	0
85	OHX	6	2026	7/7	0.99	0.07	71,71,71,71	0
85	OHX	5	4011	7/7	0.99	0.20	63,63,63,63	0
84	MG	6	1914	1/1	0.99	0.46	41,41,41,41	0
85	OHX	1	3774	7/7	0.99	0.06	74,74,74,74	0
85	OHX	5	3789	7/7	0.99	0.06	59,59,59,59	0
85	OHX	5	3790	7/7	0.99	0.08	58,58,58,58	0
85	OHX	5	3791	7/7	0.99	0.07	73,73,73,73	0
85	OHX	5	3792	7/7	0.99	0.06	81,81,81,81	0
85	OHX	5	3793	7/7	0.99	0.07	87,87,87,87	0
85	OHX	5	3794	7/7	0.99	0.08	69,69,69,69	0
85	OHX	1	3775	7/7	0.99	0.10	83,83,83,83	0
85	OHX	6	2030	7/7	0.99	0.19	74,74,74,74	0
85	OHX	5	3797	7/7	0.99	0.13	57,57,57,57	0
85	OHX	5	3798	7/7	0.99	0.08	80,80,80,80	0
85	OHX	6	2031	7/7	0.99	0.13	76,76,76,76	0
85	OHX	2	1992	7/7	0.99	0.10	89,89,89,89	0
85	OHX	5	3801	7/7	0.99	0.09	69,69,69,69	0
84	MG	6	1931	1/1	0.99	0.29	48,48,48,48	0
85	OHX	6	2034	7/7	0.99	0.07	91,91,91,91	0
85	OHX	6	2035	7/7	0.99	0.19	71,71,71,71	0
85	OHX	5	3805	7/7	0.99	0.09	73,73,73,73	0
85	OHX	2	2019	7/7	0.99	0.18	87,87,87,87	0
85	OHX	1	3779	7/7	0.99	0.08	71,71,71,71	0
85	OHX	5	3808	7/7	0.99	0.09	67,67,67,67	0
85	OHX	6	2038	7/7	0.99	0.11	71,71,71,71	0
85	OHX	1	3871	7/7	0.99	0.22	100,100,100,100	0
85	OHX	5	3811	7/7	0.99	0.11	73,73,73,73	0
85	OHX	5	3812	7/7	0.99	0.08	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	OHX	5	3813	7/7	0.99	0.09	81,81,81,81	0
85	OHX	5	3814	7/7	0.99	0.07	84,84,84,84	0
85	OHX	5	3815	7/7	0.99	0.11	68,68,68,68	0
85	OHX	2	1994	7/7	0.99	0.11	99,99,99,99	0
84	MG	1	3481	1/1	0.99	0.21	45,45,45,45	0
85	OHX	1	3874	7/7	0.99	0.20	91,91,91,91	0
85	OHX	1	3782	7/7	0.99	0.07	77,77,77,77	0
85	OHX	6	2044	7/7	0.99	0.11	81,81,81,81	0
85	OHX	6	2045	7/7	0.99	0.10	87,87,87,87	0
85	OHX	5	3822	7/7	0.99	0.17	64,64,64,64	0
85	OHX	1	3876	7/7	0.99	0.23	86,86,86,86	0
85	OHX	2	1996	7/7	0.99	0.10	83,83,83,83	0
85	OHX	5	3825	7/7	0.99	0.12	68,68,68,68	0
85	OHX	5	3826	7/7	0.99	0.10	62,62,62,62	0
85	OHX	1	3878	7/7	0.99	0.21	88,88,88,88	0
85	OHX	5	3828	7/7	0.99	0.19	73,73,73,73	0
85	OHX	5	3829	7/7	0.99	0.12	68,68,68,68	0
85	OHX	5	3830	7/7	0.99	0.14	64,64,64,64	0
84	MG	1	3576	1/1	0.99	0.57	28,28,28,28	0
85	OHX	5	3832	7/7	0.99	0.12	103,103,103,103	0
85	OHX	5	3833	7/7	0.99	0.07	61,61,61,61	0
85	OHX	6	2050	7/7	0.99	0.12	92,92,92,92	0
85	OHX	5	3835	7/7	0.99	0.13	73,73,73,73	0
85	OHX	1	3786	7/7	0.99	0.08	101,101,101,101	0
85	OHX	6	2052	7/7	0.99	0.09	110,110,110,110	0
85	OHX	5	3838	7/7	0.99	0.15	101,101,101,101	0
85	OHX	1	3787	7/7	0.99	0.07	73,73,73,73	0
84	MG	5	3577	1/1	0.99	0.50	45,45,45,45	0
85	OHX	5	4066	7/7	0.99	0.43	114,114,114,114	0
85	OHX	5	3841	7/7	0.99	0.08	97,97,97,97	0
85	OHX	5	3842	7/7	0.99	0.10	91,91,91,91	0
85	OHX	1	3883	7/7	0.99	0.19	106,106,106,106	0
85	OHX	5	3844	7/7	0.99	0.12	70,70,70,70	0
84	MG	1	3553	1/1	0.99	0.51	30,30,30,30	0
85	OHX	1	3885	7/7	0.99	0.22	78,78,78,78	0
85	OHX	5	3847	7/7	0.99	0.12	67,67,67,67	0
85	OHX	5	3848	7/7	0.99	0.20	80,80,80,80	0
85	OHX	7	215	7/7	0.99	0.09	82,82,82,82	0
85	OHX	7	216	7/7	0.99	0.13	87,87,87,87	0
85	OHX	1	3790	7/7	0.99	0.11	72,72,72,72	0
84	MG	1	3464	1/1	0.99	0.28	36,36,36,36	0
85	OHX	5	3851	7/7	0.99	0.08	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	OHX	2	2001	7/7	0.99	0.09	83,83,83,83	0
85	OHX	1	3793	7/7	0.99	0.06	89,89,89,89	0
85	OHX	8	211	7/7	0.99	0.08	55,55,55,55	0
85	OHX	1	3794	7/7	0.99	0.06	62,62,62,62	0
84	MG	5	3567	1/1	0.99	0.49	30,30,30,30	0
85	OHX	1	3796	7/7	0.99	0.07	79,79,79,79	0
85	OHX	1	3893	7/7	0.99	0.28	81,81,81,81	0
85	OHX	5	3858	7/7	0.99	0.21	82,82,82,82	0
84	MG	1	3483	1/1	0.99	0.31	45,45,45,45	0
85	OHX	1	3798	7/7	0.99	0.08	75,75,75,75	0
85	OHX	5	3861	7/7	0.99	0.06	103,103,103,103	0
85	OHX	5	3862	7/7	0.99	0.25	77,77,77,77	0
85	OHX	5	3863	7/7	0.99	0.22	86,86,86,86	0
85	OHX	2	2004	7/7	0.99	0.09	86,86,86,86	0
85	OHX	5	3865	7/7	0.99	0.11	87,87,87,87	0
85	OHX	2	2031	7/7	0.99	0.18	95,95,95,95	0
85	OHX	1	3801	7/7	0.99	0.11	81,81,81,81	0
85	OHX	13	406	7/7	0.99	0.14	79,79,79,79	0
85	OHX	5	3868	7/7	0.99	0.07	96,96,96,96	0
85	OHX	1	3802	7/7	0.99	0.13	75,75,75,75	0
85	OHX	1	3803	7/7	0.99	0.20	74,74,74,74	0
85	OHX	6	2073	7/7	0.99	0.28	86,86,86,86	0
85	OHX	1	4005	7/7	0.99	0.25	95,95,95,95	0
85	OHX	2	1983	7/7	0.99	0.11	75,75,75,75	0
85	OHX	6	2076	7/7	0.99	0.23	81,81,81,81	0
85	OHX	2	2006	7/7	0.99	0.12	113,113,113,113	0
85	OHX	6	2078	7/7	0.99	0.24	98,98,98,98	0
85	OHX	2	1984	7/7	0.99	0.11	78,78,78,78	0
85	OHX	1	4009	7/7	0.99	0.20	83,83,83,83	0
85	OHX	1	3904	7/7	0.99	0.16	82,82,82,82	0
85	OHX	6	2082	7/7	0.99	0.21	91,91,91,91	0
85	OHX	n3	202	7/7	0.99	0.08	72,72,72,72	0
85	OHX	5	3881	7/7	0.99	0.11	106,106,106,106	0
85	OHX	n9	102	7/7	0.99	0.14	59,59,59,59	0
85	OHX	o3	202	7/7	0.99	0.19	82,82,82,82	0
85	OHX	5	3882	7/7	0.99	0.26	67,67,67,67	0
84	MG	5	3547	1/1	0.99	0.53	33,33,33,33	0
85	OHX	1	3808	7/7	0.99	0.10	93,93,93,93	0
85	OHX	2	1986	7/7	0.99	0.10	81,81,81,81	0
85	OHX	1	3908	7/7	0.99	0.18	103,103,103,103	0
85	OHX	2	2010	7/7	0.99	0.17	88,88,88,88	0
85	OHX	5	3888	7/7	0.99	0.26	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	ZN	O7	101	1/1	0.99	0.07	42,42,42,42	0
85	OHX	1	3811	7/7	0.99	0.09	78,78,78,78	0
85	OHX	1	3730	7/7	0.99	0.18	55,55,55,55	0
85	OHX	1	3731	7/7	0.99	0.11	50,50,50,50	0
85	OHX	1	3732	7/7	0.99	0.13	57,57,57,57	0
85	OHX	1	3815	7/7	0.99	0.14	71,71,71,71	0
85	OHX	1	3733	7/7	0.99	0.10	47,47,47,47	0
85	OHX	1	3734	7/7	0.99	0.09	56,56,56,56	0
86	ZN	o7	501	1/1	0.99	0.07	45,45,45,45	0
85	OHX	1	3818	7/7	0.99	0.16	58,58,58,58	0
85	OHX	1	3735	7/7	0.99	0.11	54,54,54,54	0
86	ZN	q3	501	1/1	0.99	0.10	57,57,57,57	0
85	OHX	5	3898	7/7	0.99	0.17	80,80,80,80	0
85	OHX	1	3727	7/7	1.00	0.10	52,52,52,52	0
85	OHX	1	3728	7/7	1.00	0.10	44,44,44,44	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	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	3744	7/7	1.00	0.04	54,54,54,54	0
85	OHX	5	3774	7/7	1.00	0.11	53,53,53,53	0
85	OHX	5	3752	7/7	1.00	0.09	40,40,40,40	0
85	OHX	1	3761	7/7	1.00	0.06	60,60,60,60	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	3756	7/7	1.00	0.08	60,60,60,60	0
85	OHX	5	3757	7/7	1.00	0.10	58,58,58,58	0
85	OHX	1	3754	7/7	1.00	0.05	63,63,63,63	0
85	OHX	6	2009	7/7	1.00	0.12	57,57,57,57	0
85	OHX	1	3785	7/7	1.00	0.06	66,66,66,66	0
85	OHX	1	3726	7/7	1.00	0.13	43,43,43,43	0
85	OHX	5	3743	7/7	1.00	0.14	43,43,43,43	0
85	OHX	5	3763	7/7	1.00	0.09	61,61,61,61	0
85	OHX	5	3744	7/7	1.00	0.12	40,40,40,40	0
85	OHX	5	3745	7/7	1.00	0.10	43,43,43,43	0
85	OHX	5	3766	7/7	1.00	0.07	63,63,63,63	0

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

There are no such residues in this entry.