



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 5, 2020 – 08:54 am BST

PDB ID : 5DAT  
Title : Complex of yeast 80S ribosome with hypusine-containing eIF5A  
Authors : Melnikov, S.; Mailliot, J.; Shin, B.-S.; Rigger, L.; Yusupova, G.; Micura, R.;  
Dever, T.E.; Yusupov, M.  
Deposited on : 2015-08-20  
Resolution : 3.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

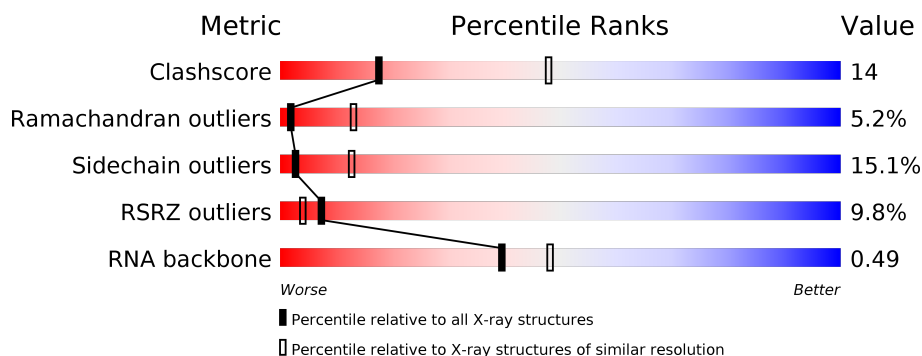
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)
RNA backbone	3102	1073 (3.50-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	
1	6	1800	
2	S0	251	
2	s0	251	
3	S1	254	
3	s1	254	

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Mol	Chain	Length	Quality of chain
4	S2	253	
4	s2	253	
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	124	
14	c2	124	
15	C3	150	
15	c3	150	
16	C4	136	

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Mol	Chain	Length	Quality of chain
16	c4	136	
17	C5	137	
17	c5	137	
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	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107	
27	d5	107	
28	D6	97	
28	d6	97	
29	D7	81	

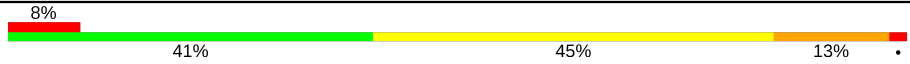

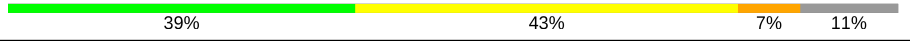

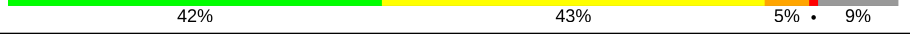
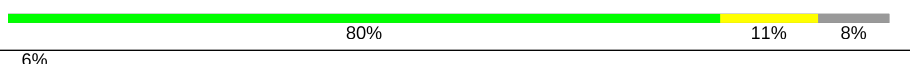
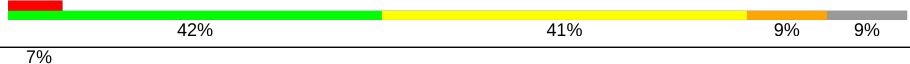

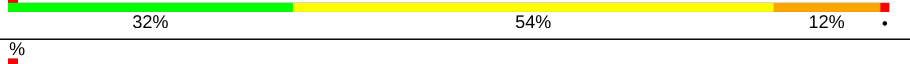


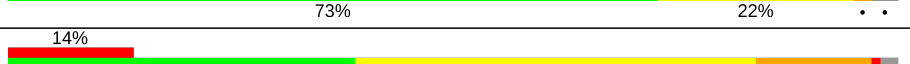

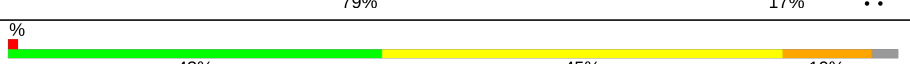

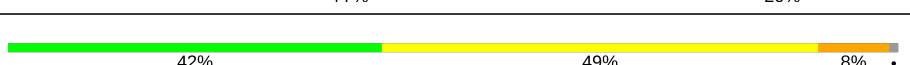
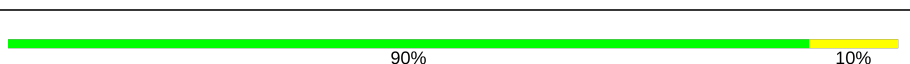
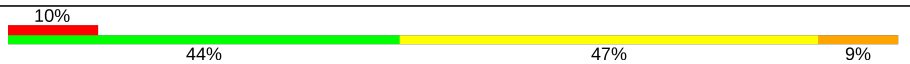



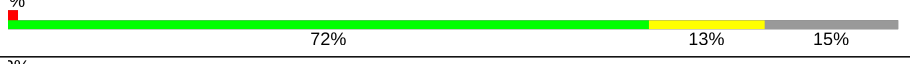



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Mol	Chain	Length	Quality of chain
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	62	
32	e0	62	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	

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Mol	Chain	Length	Quality of chain
42	L5	296	
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	204	
52	M6	198	
52	m6	198	
53	M7	183	
53	m7	183	
54	M8	185	
54	m8	185	

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

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

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Mol	Chain	Length	Quality of chain
80	d2	130	
81	m2	150	
82	m5	203	
83	p0	220	
84	p1	47	
84	p2	47	
85	f	157	
86	l1	213	

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
85	5CT	f	51	X	-	-	-
87	MG	1	3405	-	-	-	X
87	MG	1	3451	-	-	-	X
87	MG	1	3598	-	-	-	X
87	MG	1	3604	-	-	-	X
87	MG	1	3605	-	-	-	X
87	MG	1	3711	-	-	-	X
87	MG	2	1901	-	-	-	X
87	MG	2	1912	-	-	-	X
87	MG	2	1967	-	-	-	X
87	MG	5	3440	-	-	-	X
87	MG	5	3497	-	-	-	X
87	MG	5	3621	-	-	-	X
87	MG	5	3623	-	-	-	X
87	MG	5	3682	-	-	-	X
87	MG	5	3722	-	-	-	X
87	MG	5	3734	-	-	-	X
87	MG	5	3736	-	-	-	X
87	MG	5	3786	-	-	-	X
87	MG	6	1917	-	-	-	X
87	MG	6	1924	-	-	-	X
87	MG	6	1974	-	-	-	X
87	MG	6	1988	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	6	2007	-	-	-	X
87	MG	7	213	-	-	-	X
87	MG	M3	201	-	-	-	X
87	MG	M7	201	-	-	-	X
87	MG	M8	201	-	-	-	X
87	MG	O7	102	-	-	-	X
87	MG	S4	301	-	-	-	X
88	OHX	1	3851	-	-	X	-
88	OHX	1	3927	-	-	X	-
88	OHX	1	3939	-	-	X	-
88	OHX	1	3940	-	-	X	-
88	OHX	1	4001	-	-	X	-
88	OHX	1	4068	-	-	X	-
88	OHX	1	4077	-	-	X	-
88	OHX	2	2061	-	-	X	-
88	OHX	2	2092	-	-	X	-
88	OHX	2	2102	-	-	X	-
88	OHX	2	2133	-	-	X	-
88	OHX	2	2146	-	-	-	X
88	OHX	2	2150	-	-	X	-
88	OHX	5	3852	-	-	X	-
88	OHX	5	3900	-	-	X	-
88	OHX	5	3951	-	-	X	-
88	OHX	5	3961	-	-	X	-
88	OHX	5	4106	-	-	X	-
88	OHX	5	4126	-	-	X	-
88	OHX	5	4147	-	-	-	X
88	OHX	5	4157	-	-	X	-
88	OHX	6	2040	-	-	X	-
88	OHX	6	2067	-	-	X	-
88	OHX	6	2086	-	-	X	-
88	OHX	6	2096	-	-	X	-
88	OHX	6	2109	-	-	X	-
88	OHX	6	2126	-	-	X	-
88	OHX	6	2127	-	-	X	-
88	OHX	6	2142	-	-	X	-
88	OHX	6	2181	-	-	-	X
88	OHX	C3	201	-	-	X	-
88	OHX	L4	401	-	-	X	-

## 2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 414393 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	C0	96	Total	C	N	O	S	0	0	0
			772	499	126	145	2			
12	c0	96	Total	C	N	O	S	0	0	0
			761	490	125	144	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C1	155	Total	C	N	O	S	0	0	0
			1213	774	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	E0	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			
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
			2442	1544	418	472	8			

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			
36	5	3169	Total	C	N	O	P	0	0	0
			67780	30276	12216	22120	3168			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	l2	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	L3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
40	l3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	M5	204	Total	C	N	O	S	0	0	1
			1720	1077	361	281	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M5	170	LYS	-	insertion	UNP P05748

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	N2	100	Total	C	N	O	0	0	0
			796	516	131	149			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	n2	98	Total	C	N	O	0	0	0
			778	505	127	146			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 70 is a protein called 60S ribosomal protein L34-A (eL34).

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 80 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	d2	130	Total	C	N	O	S	0	0	1
			1021	650	188	180	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d2	47	TYR	-	insertion	UNP P0C0W1

- Molecule 81 is a protein called 60S ribosomal protein L12-A (uL11).

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

- Molecule 82 is a protein called 60S ribosomal protein L15-A.

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

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

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

- Molecule 84 is a protein called 60S ribosomal protein P1 alpha/P2 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
84	p1	47	Total	C	N	O		0	0	0
			235	141	47	47				
84	p2	46	Total	C	N	O		0	0	0
			230	138	46	46				

- Molecule 85 is a protein called Eukaryotic translation initiation factor 5A-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
85	f	148	Total	C	N	O	S	0	0	0
			1122	696	189	228	9			

- Molecule 86 is a protein called 60S ribosomal protein L1-A (uL1).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
86	l1	213	Total	C	N	O	0	0	0
			1063	637	213	213			

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	L7	3	Total	Mg	0	0
			3	3		
87	N9	1	Total	Mg	0	0
			1	1		
87	n8	3	Total	Mg	0	0
			3	3		
87	6	115	Total	Mg	0	0
			115	115		
87	Q0	1	Total	Mg	0	0
			1	1		
87	sM	1	Total	Mg	0	0
			1	1		
87	O4	1	Total	Mg	0	0
			1	1		
87	o9	1	Total	Mg	0	0
			1	1		
87	l3	1	Total	Mg	0	0
			1	1		
87	d6	1	Total	Mg	0	0
			1	1		
87	2	96	Total	Mg	0	0
			96	96		
87	d2	1	Total	Mg	0	0
			1	1		
87	m6	2	Total	Mg	0	0
			2	2		
87	f	3	Total	Mg	0	0
			3	3		
87	l7	1	Total	Mg	0	0
			1	1		
87	n0	2	Total	Mg	0	0
			2	2		
87	m3	1	Total	Mg	0	0
			1	1		
87	N6	1	Total	Mg	0	0
			1	1		

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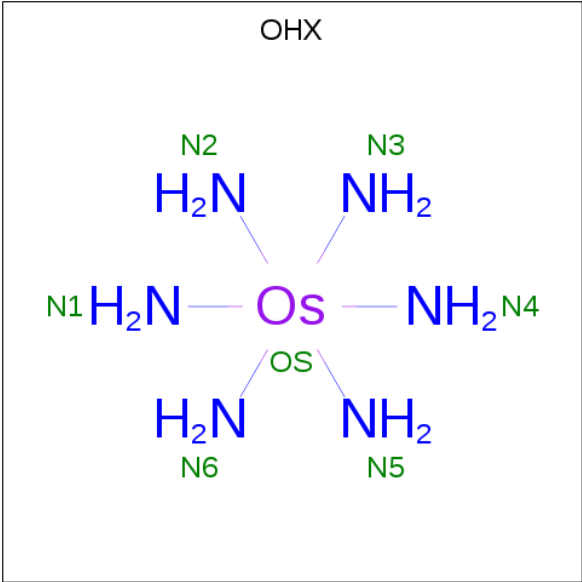
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	S9	1	Total 1	Mg 1	0	0
87	O3	2	Total 2	Mg 2	0	0
87	q0	1	Total 1	Mg 1	0	0
87	SM	1	Total 1	Mg 1	0	0
87	o4	1	Total 1	Mg 1	0	0
87	M0	1	Total 1	Mg 1	0	0
87	n6	1	Total 1	Mg 1	0	0
87	5	400	Total 400	Mg 400	0	0
87	O7	3	Total 3	Mg 3	0	0
87	n9	2	Total 2	Mg 2	0	0
87	1	362	Total 362	Mg 362	0	0
87	O2	1	Total 1	Mg 1	0	0
87	Q2	1	Total 1	Mg 1	0	0
87	M8	1	Total 1	Mg 1	0	0
87	D9	1	Total 1	Mg 1	0	0
87	d3	1	Total 1	Mg 1	0	0
87	M3	2	Total 2	Mg 2	0	0
87	N3	3	Total 3	Mg 3	0	0
87	N8	4	Total 4	Mg 4	0	0
87	4	20	Total 20	Mg 20	0	0
87	D4	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	S4	1	Total 1	Mg 1	0	0
87	L2	2	Total 2	Mg 2	0	0
87	l5	1	Total 1	Mg 1	0	0
87	m7	3	Total 3	Mg 3	0	0
87	M7	3	Total 3	Mg 3	0	0
87	L6	1	Total 1	Mg 1	0	0
87	s8	1	Total 1	Mg 1	0	0
87	o2	2	Total 2	Mg 2	0	0
87	c7	1	Total 1	Mg 1	0	0
87	7	16	Total 16	Mg 16	0	0
87	n3	1	Total 1	Mg 1	0	0
87	q1	1	Total 1	Mg 1	0	0
87	L3	3	Total 3	Mg 3	0	0
87	l2	3	Total 3	Mg 3	0	0
87	8	12	Total 12	Mg 12	0	0
87	m0	1	Total 1	Mg 1	0	0
87	M6	1	Total 1	Mg 1	0	0
87	N0	1	Total 1	Mg 1	0	0
87	3	9	Total 9	Mg 9	0	0

- Molecule 88 is osmium (III) hexammine (three-letter code: OHX) (formula: H<sub>12</sub>N<sub>6</sub>Os).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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			7	6	1		
88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
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			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
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			7	6	1		
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	1	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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			7	6	1		
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88	S1	1	Total	N	Os	0	0
			7	6	1		
88	S6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	S8	1	Total 7	N 6	Os 1	0	0
88	S9	1	Total 7	N 6	Os 1	1	0
88	C1	1	Total 7	N 6	Os 1	0	0
88	C3	1	Total 7	N 6	Os 1	0	0
88	C5	1	Total 7	N 6	Os 1	0	0
88	C8	1	Total 7	N 6	Os 1	1	0
88	D9	1	Total 7	N 6	Os 1	0	0
88	SR	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	1	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	2	0
88	1	1	Total 7	N 6	Os 1	2	0
88	1	1	Total 7	N 6	Os 1	1	0
88	1	1	Total 7	N 6	Os 1	1	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	1	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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			7	6	1		
88	1	1	Total	N	Os	1	0
			7	6	1		
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
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88	1	1	Total	N	Os	0	0
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			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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			7	6	1		
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	3	1	Total	N	Os	0	0
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88	3	1	Total	N	Os	0	0
			7	6	1		
88	3	1	Total	N	Os	0	0
			7	6	1		
88	3	1	Total	N	Os	0	0
			7	6	1		
88	3	1	Total	N	Os	0	0
			7	6	1		
88	3	1	Total	N	Os	0	0
			7	6	1		
88	3	1	Total	N	Os	0	0
			7	6	1		
88	3	1	Total	N	Os	0	0
			7	6	1		
88	3	1	Total	N	Os	0	0
			7	6	1		
88	3	1	Total	N	Os	0	0
			7	6	1		
88	4	1	Total	N	Os	1	0
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88	4	1	Total	N	Os	0	0
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88	4	1	Total	N	Os	0	0
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88	4	1	Total	N	Os	0	0
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88	4	1	Total	N	Os	0	0
			7	6	1		
88	4	1	Total	N	Os	0	0
			7	6	1		
88	4	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	4	1	Total 7	N 6	Os 1	0	0
88	4	1	Total 7	N 6	Os 1	0	0
88	4	1	Total 7	N 6	Os 1	1	0
88	4	1	Total 7	N 6	Os 1	1	0
88	4	1	Total 7	N 6	Os 1	0	0
88	4	1	Total 7	N 6	Os 1	0	0
88	4	1	Total 7	N 6	Os 1	0	0
88	4	1	Total 7	N 6	Os 1	0	0
88	4	1	Total 7	N 6	Os 1	0	0
88	L3	1	Total 7	N 6	Os 1	0	0
88	L4	1	Total 7	N 6	Os 1	0	0
88	L5	1	Total 7	N 6	Os 1	0	0
88	M0	1	Total 7	N 6	Os 1	0	0
88	M0	1	Total 7	N 6	Os 1	0	0
88	M5	1	Total 7	N 6	Os 1	0	0
88	M7	1	Total 7	N 6	Os 1	0	0
88	M7	1	Total 7	N 6	Os 1	0	0
88	M8	1	Total 7	N 6	Os 1	0	0
88	M9	1	Total 7	N 6	Os 1	0	0
88	N1	1	Total 7	N 6	Os 1	0	0
88	N8	1	Total 7	N 6	Os 1	0	0
88	N9	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	O3	1	Total 7	N 6	Os 1	0	0
88	O7	1	Total 7	N 6	Os 1	1	0
88	O7	1	Total 7	N 6	Os 1	0	0
88	O9	1	Total 7	N 6	Os 1	0	0
88	Q2	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	1	0
88	6	1	Total 7	N 6	Os 1	1	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	1	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
			7	6	1		
88	6	1	Total	N	Os	0	0
			7	6	1		
88	6	1	Total	N	Os	0	0
			7	6	1		
88	6	1	Total	N	Os	0	0
			7	6	1		
88	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
			7	6	1		
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88	6	1	Total	N	Os	0	0
			7	6	1		
88	6	1	Total	N	Os	0	0
			7	6	1		
88	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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			7	6	1		
88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
			7	6	1		
88	6	1	Total	N	Os	0	0
			7	6	1		
88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
			7	6	1		
88	6	1	Total	N	Os	1	0
			7	6	1		
88	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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			7	6	1		
88	6	1	Total	N	Os	0	0
			7	6	1		
88	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
			7	6	1		
88	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	s1	1	Total 7	N 6	Os 1	0	0
88	s4	1	Total 7	N 6	Os 1	0	0
88	s8	1	Total 7	N 6	Os 1	0	0
88	s9	1	Total 7	N 6	Os 1	0	0
88	c3	1	Total 7	N 6	Os 1	0	0
88	c5	1	Total 7	N 6	Os 1	0	0
88	c8	1	Total 7	N 6	Os 1	0	0
88	sR	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	1	0
88	5	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	2	0
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88	5	1	Total	N	Os	1	0
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88	5	1	Total	N	Os	1	0
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88	5	1	Total	N	Os	2	0
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88	5	1	Total	N	Os	1	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
88	5	1	Total	N	Os	1	0
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88	5	1	Total	N	Os	0	0
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			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
			7	6	1		
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	5	1	Total	N	Os	1	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	1	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	1	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	2	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	1	0
			7	6	1		
88	5	1	Total	N	Os	1	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	1	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	2	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	1	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	2	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	1	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	1	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	1	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	13	1	Total	N	Os	0	0
			7	6	1		
88	13	1	Total	N	Os	0	0
			7	6	1		
88	13	1	Total	N	Os	0	0
			7	6	1		
88	14	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	l4	1	Total	N	Os	0	0
			7	6	1		
88	l5	1	Total	N	Os	0	0
			7	6	1		
88	l5	1	Total	N	Os	0	0
			7	6	1		
88	l9	1	Total	N	Os	0	0
			7	6	1		
88	m0	1	Total	N	Os	0	0
			7	6	1		
88	m0	1	Total	N	Os	0	0
			7	6	1		
88	m0	1	Total	N	Os	0	0
			7	6	1		
88	m5	1	Total	N	Os	0	0
			7	6	1		
88	m7	1	Total	N	Os	0	0
			7	6	1		
88	m9	1	Total	N	Os	0	0
			7	6	1		
88	n3	1	Total	N	Os	0	0
			7	6	1		
88	n6	1	Total	N	Os	0	0
			7	6	1		
88	n9	1	Total	N	Os	0	0
			7	6	1		
88	o3	1	Total	N	Os	0	0
			7	6	1		
88	o7	1	Total	N	Os	0	0
			7	6	1		
88	o9	1	Total	N	Os	0	0
			7	6	1		
88	q1	1	Total	N	Os	1	0
			7	6	1		
88	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
89	q0	1	Total	Zn	0	0
			1	1		

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

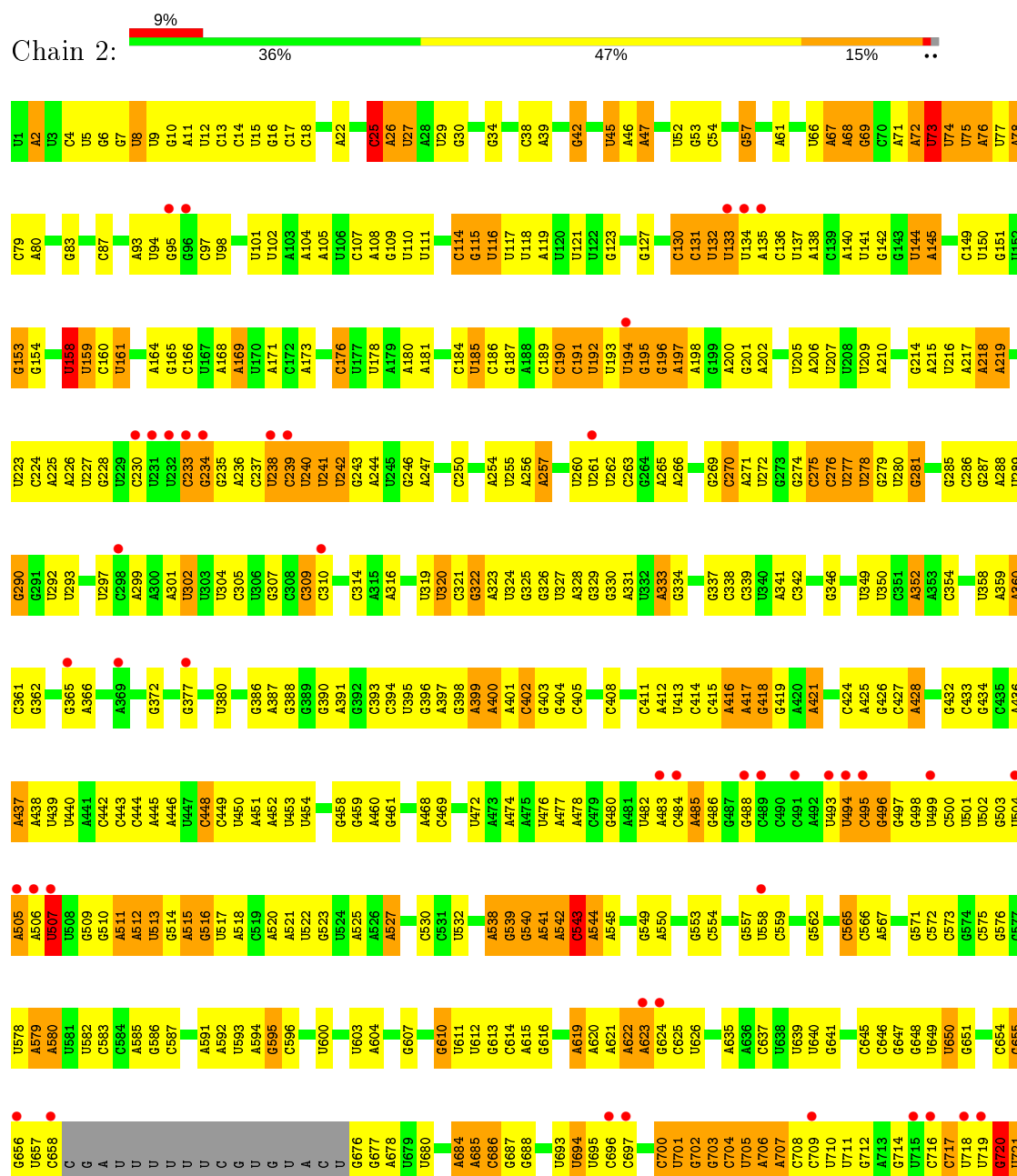
- Molecule 90 is water.

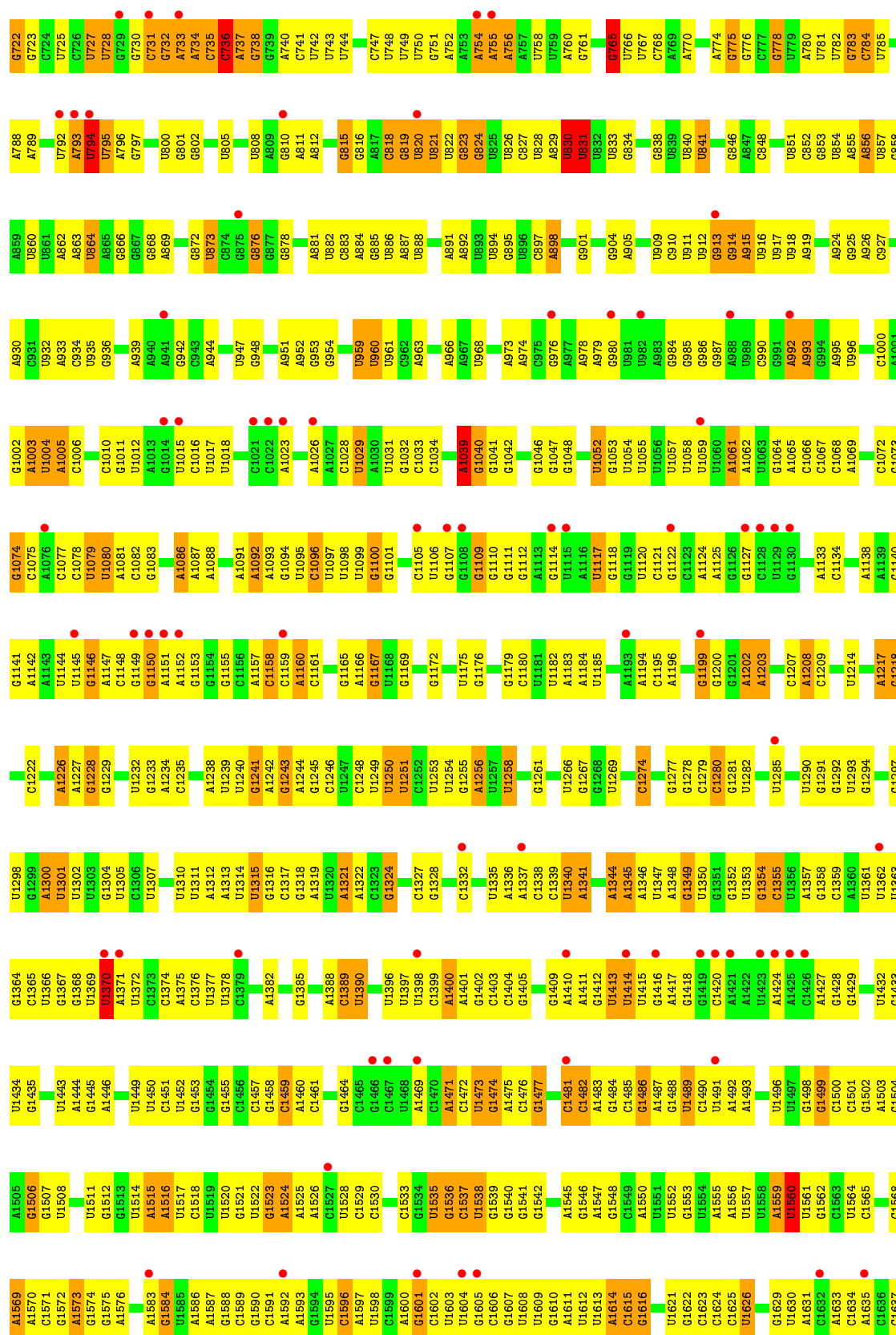
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
90	5	3	Total 3	O 3	0	0
90	f	9	Total 9	O 9	0	0

### 3 Residue-property plots

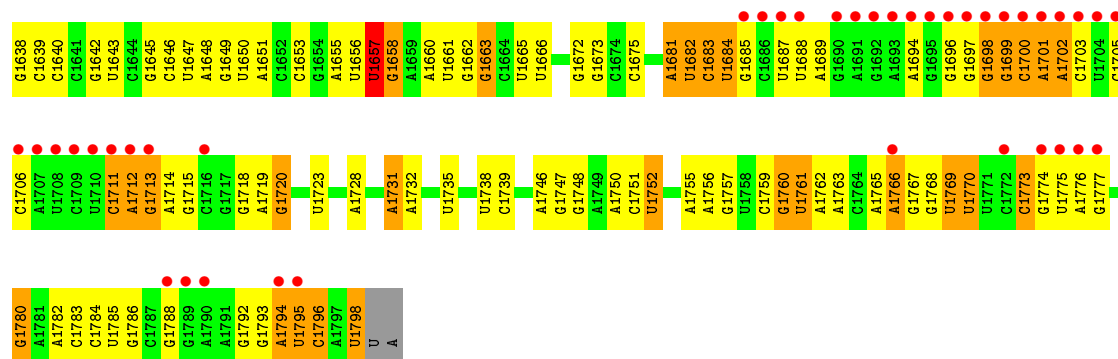
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: 18S ribosomal RNA



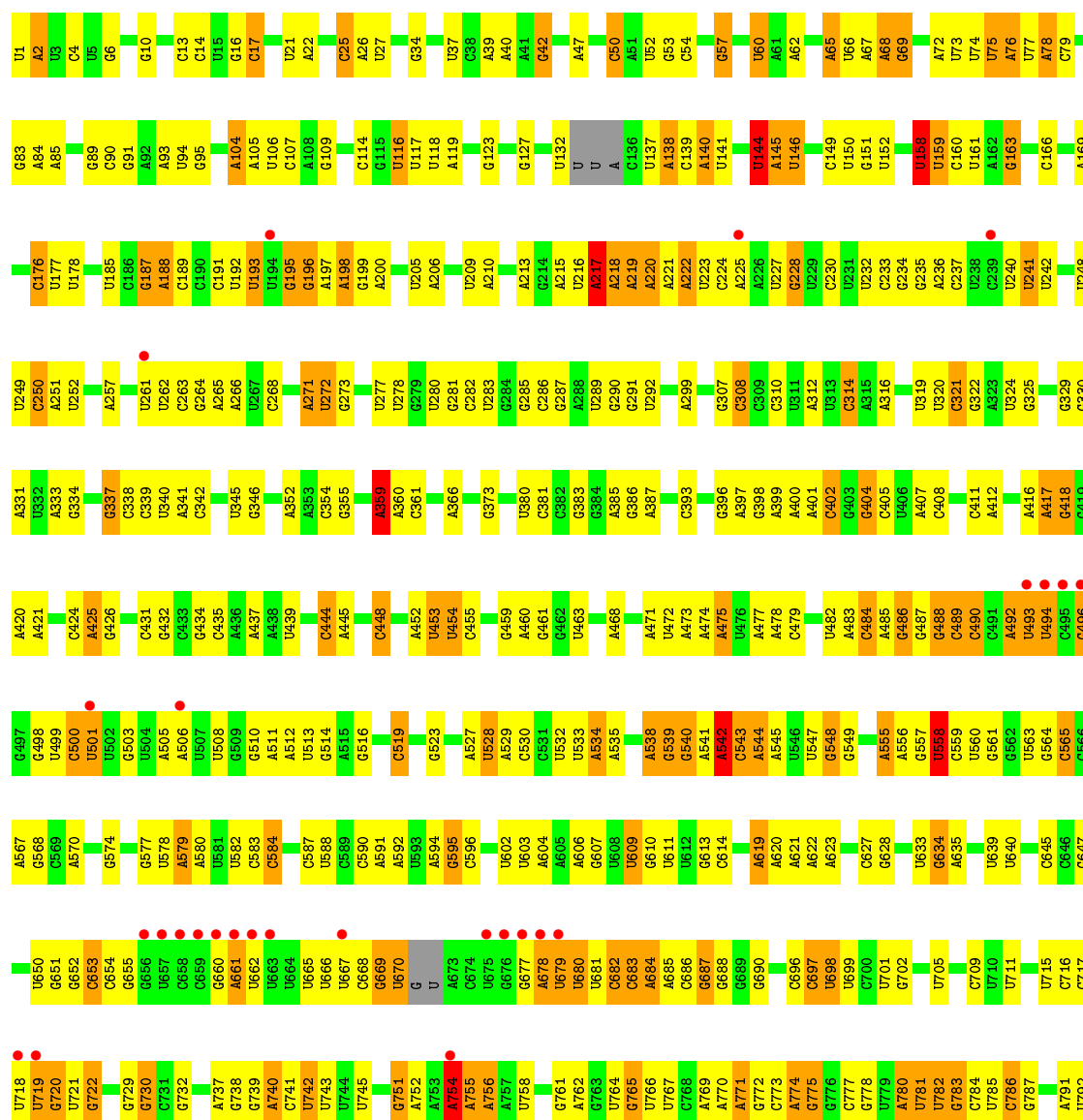




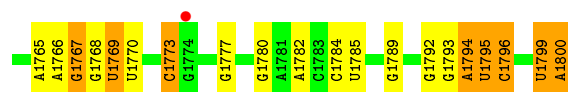


• Molecule 1: 18S ribosomal RNA

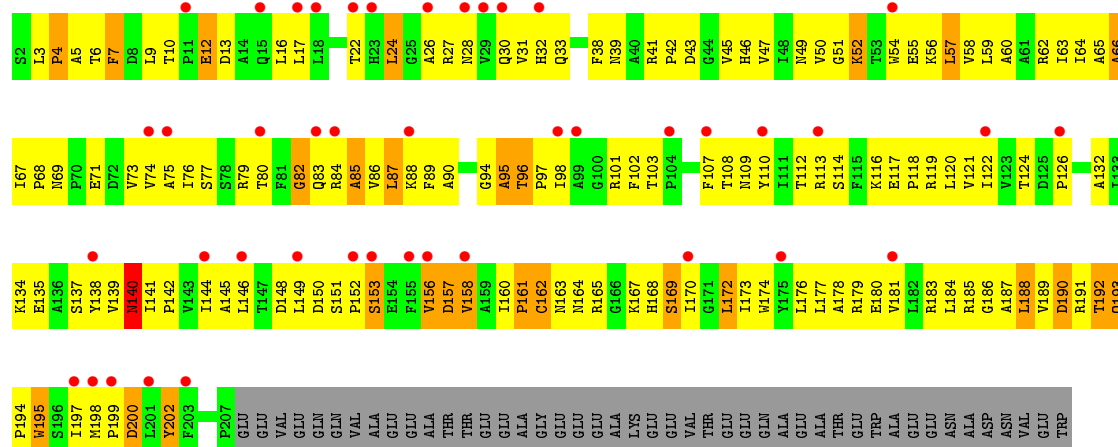
Chain 6: 5% 43% 43% 14%



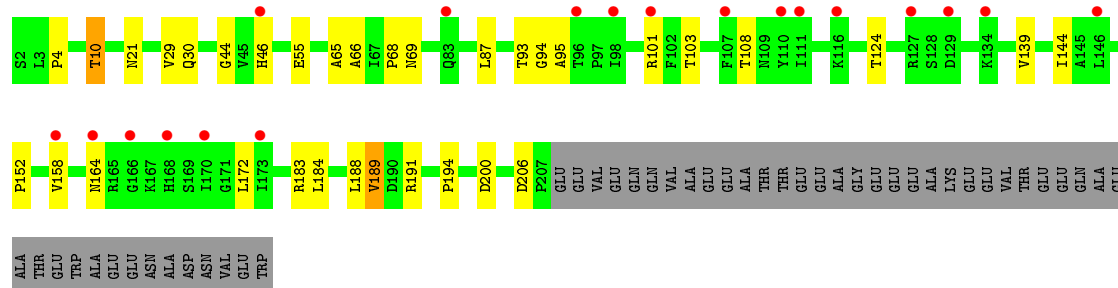
U1682	C1683	U1684	C1685	U1686	C1687	U1688	C1689	U1690	C1691	U1692	C1693	U1694	C1695	U1696	C1697	U1698	C1699	U1700	C1701	A1702	C1703	U1704	C1705	U1706	A1707	U1708	C1709	U1710	C1711	A1712	U1713	C1714	U1715	A1716	U1717	C1718	U1719	C1720	U1721	A1722	U1723	C1724	U1725	A1726	U1727	C1728	U1729	A1729	U1730	C1731	U1732	A1733	U1734	C1735	U1736	A1737	U1738	C1739	U1740	A1741	U1742	C1743	U1744	A1745	U1746	C1747	A1748	U1749	C1750	U1751	A1752	U1753	C1754	U1755	A1756	U1757	C1758	U1759	A1759	U1760	C1761	A1762																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
G1536	C1537	U1538	G1539	U1540	G1541	C1542	A1543	G1544	C1545	U1546	G1547	C1548	U1549	G1550	C1551	U1552	G1553	C1554	U1555	G1556	C1557	U1558	A1559	C1560	U1561	G1562	C1563	U1564	C1565	U1566	G1567	C1568	U1569	C1570	U1571	A1572	C1573	U1574	A1575	C1576	U1577	A1578	U1579	C1580	U1581	A1582	C1583	U1584	G1585	C1586	U1587	A1588	C1589	U1590	C1591	U1592	A1593	C1594	U1595	A1596	C1597	U1598	C1599	A1600	U1601	C1602	U1603																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
C1399	A1400	U1401	C1402	U1403	A1404	C1405	U1406	A1407	C1408	U1409	A1410	C1411	U1412	A1413	C1414	U1415	A1416	C1417	U1418	A1419	C1420	U1421	A1422	C1423	U1424	A1425	C1426	U1427	A1428	C1429	U1430	A1431	C1432	U1433	A1434	U1435	C1436	U1437	A1438	C1439	U1440	C1441	A1442	U1443	C1444	A1445	U1446	C1447	A1448	U1449	C1450	U1451	A1452	C1453	U1454	A1455	C1456	U1457	A1458	C1459	U1460	A1461	C1462	U1463	A1464	C1465	U1466	A1467	C1468	U1469	C1470																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
A1471	C1472	U1473	A1474	C1475	U1476	G1477	C1478	U1479	A1480	C1481	U1482	A1483	C1484	U1485	A1486	C1487	U1488	A1489	C1490	U1491	A1492	C1493	U1494	A1495	C1496	U1497	G1498	C1499	U1500	A1501	C1502	U1503	A1504	C1505	U1506	U1507	G1508	C1509	U1510	A1511	C1512	U1513	A1514	C1515	U1516	A1517	C1518	U1519	A1520	C1521	U1522	A1523	C1524	U1525	A1526	C1527	U1528	A1529	C1530	U1531	A1532	C1533	U1534	A1535																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
G1536	C1537	U1538	G1539	U1540	G1541	C1542	A1543	G1544	C1545	U1546	G1547	C1548	U1549	G1550	C1551	U1552	G1553	C1554	U1555	G1556	C1557	U1558	A1559	C1560	U1561	G1562	C1563	U1564	C1565	U1566	G1567	C1568	U1569	C1570	U1571	A1572	C1573	U1574	A1575	C1576	U1577	A1578	U1579	C1580	U1581	A1582	C1583	U1584	G1585	C1586	U1587	A1588	C1589	U1590	C1591	U1592	A1593	C1594	U1595	A1596	C1597	U1598	C1599	A1600	U1601	C1602	U1603																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
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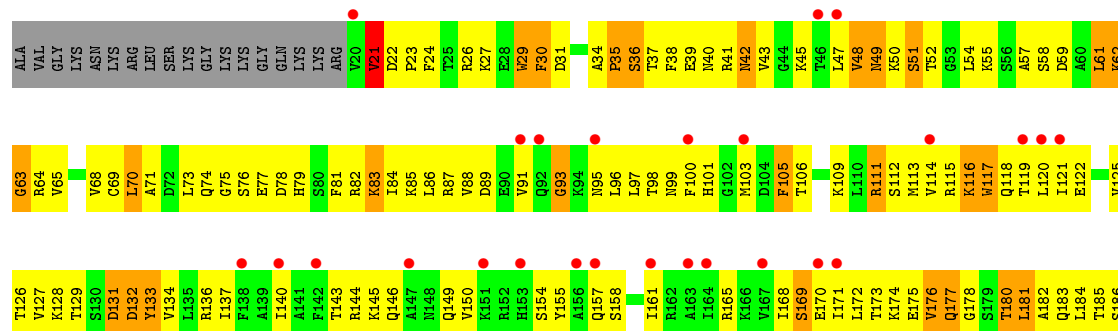
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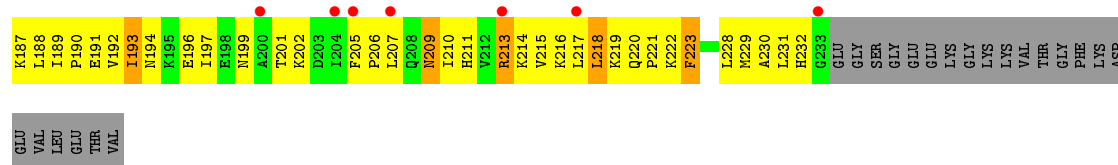


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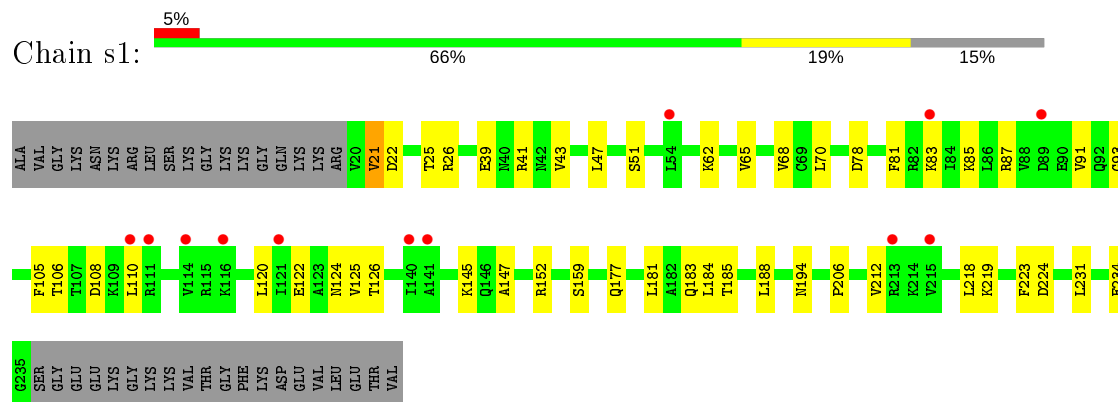


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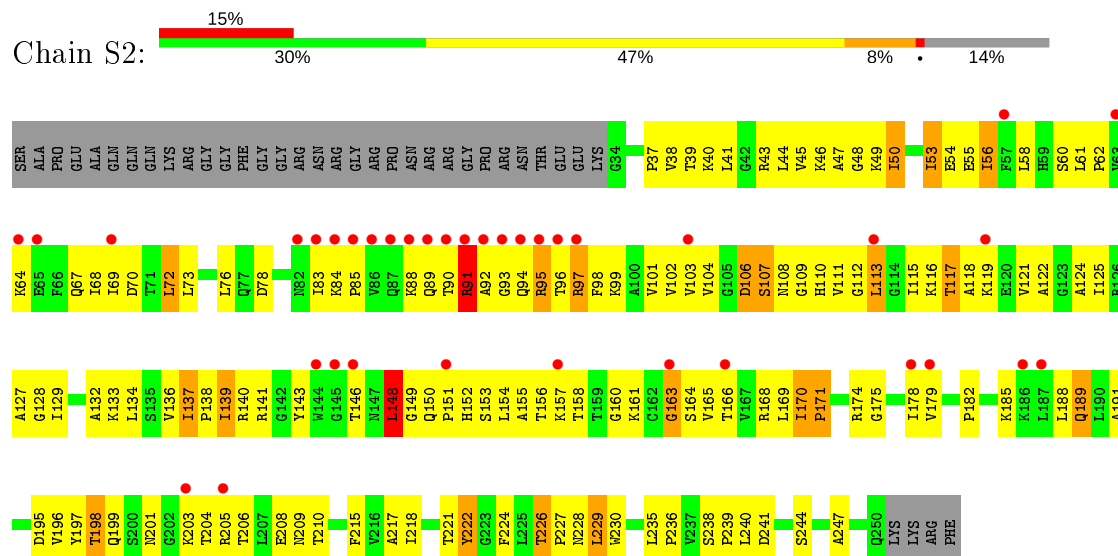




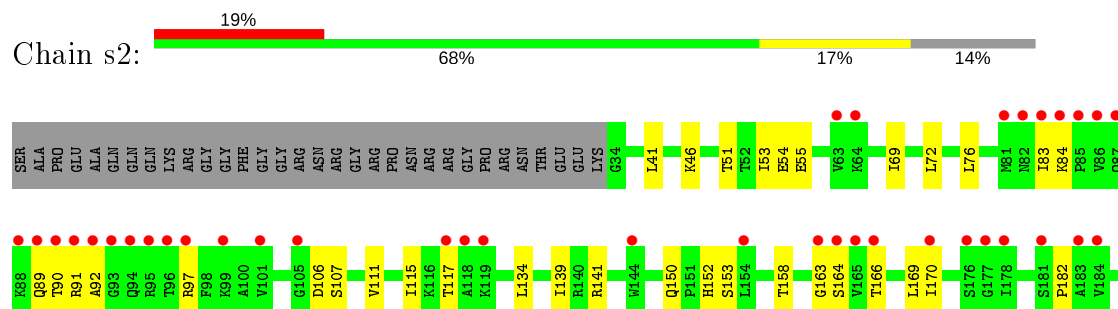
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• Molecule 4: 40S ribosomal protein S2

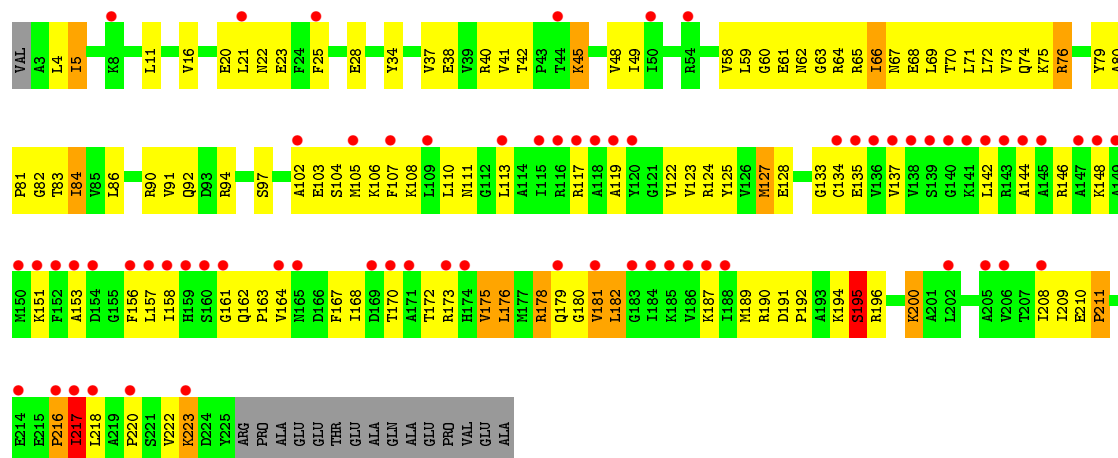


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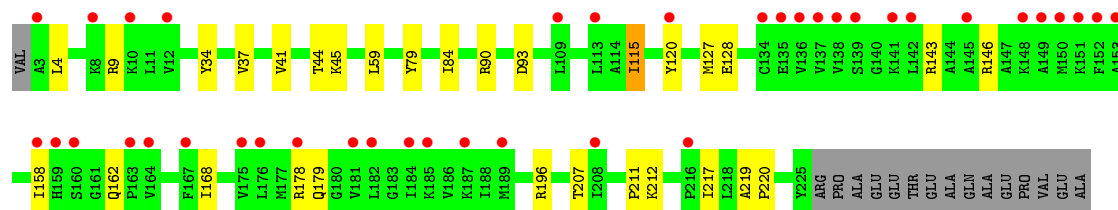
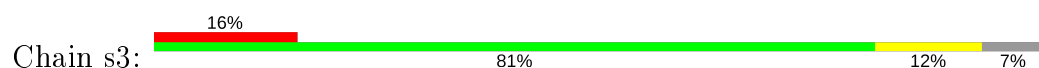




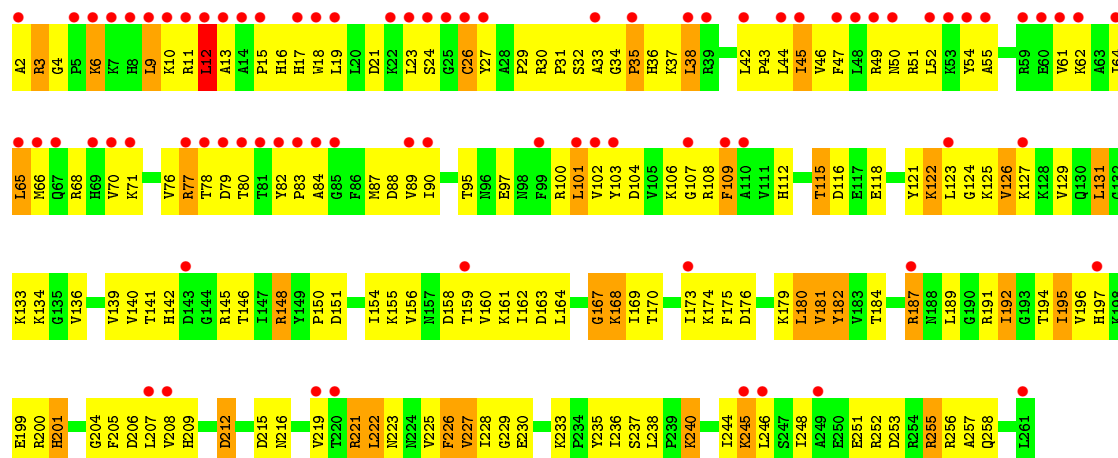
• Molecule 5: 40S ribosomal protein S3



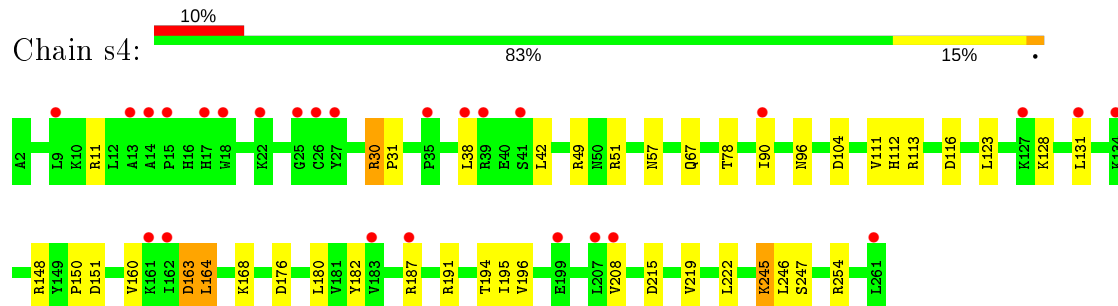
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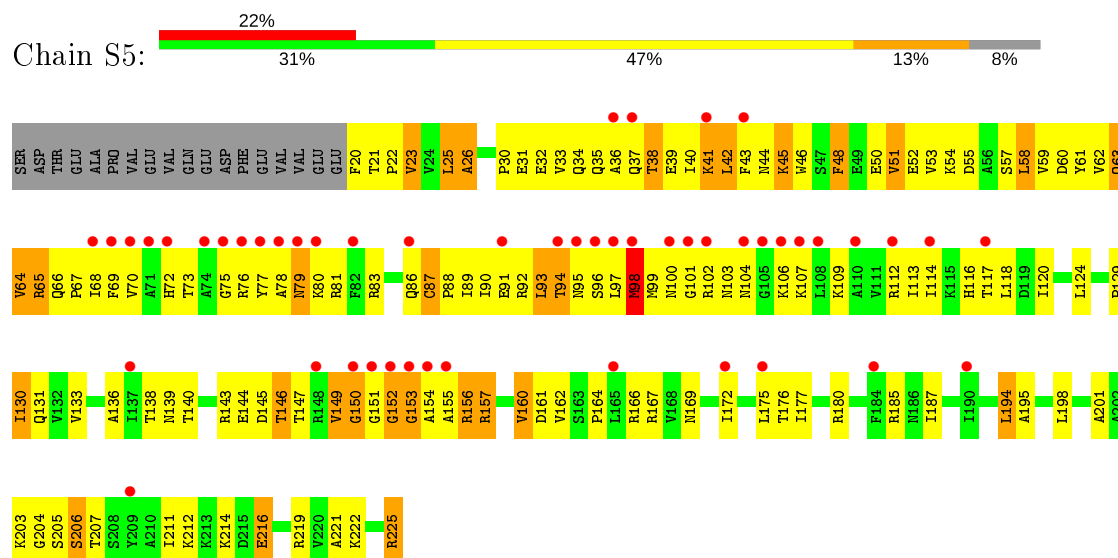
• Molecule 6: 40S ribosomal protein S4-A



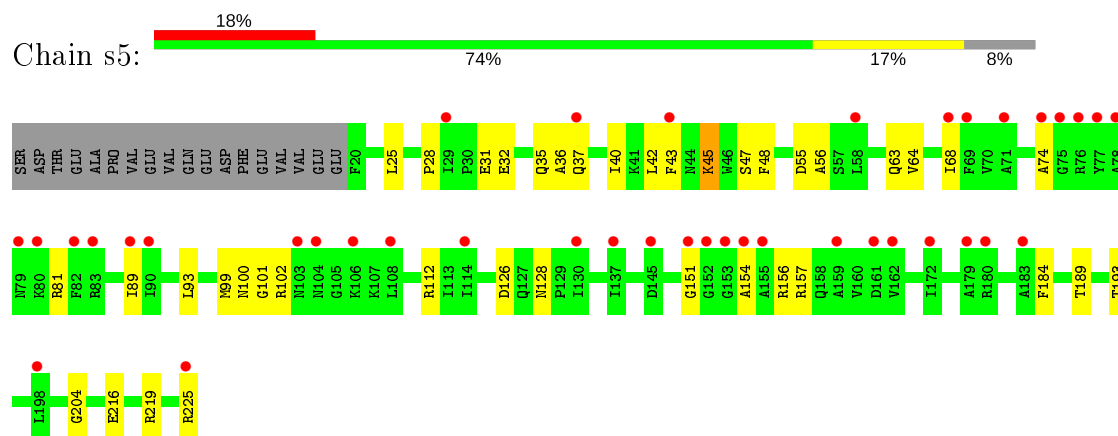
- Molecule 6: 40S ribosomal protein S4-A



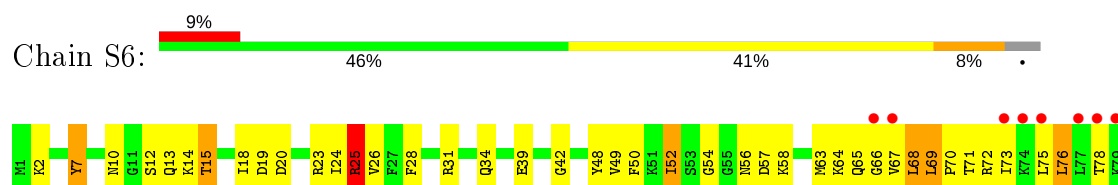
- Molecule 7: 40S ribosomal protein S5

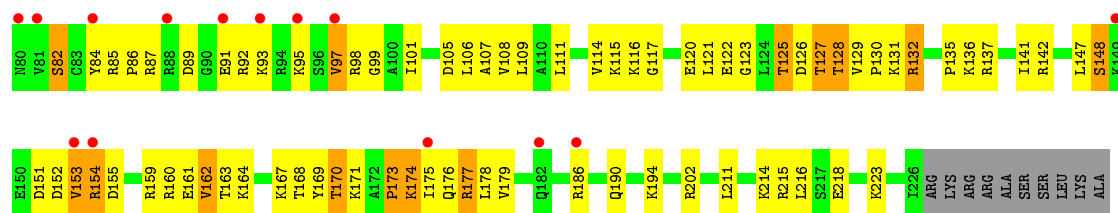


- Molecule 7: 40S ribosomal protein S5

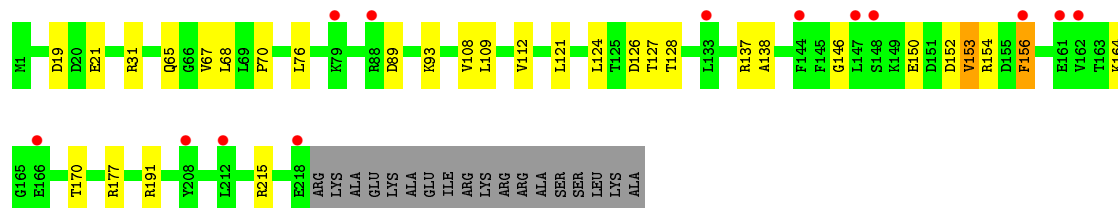
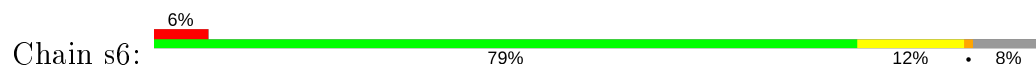


- Molecule 8: 40S ribosomal protein S6-A

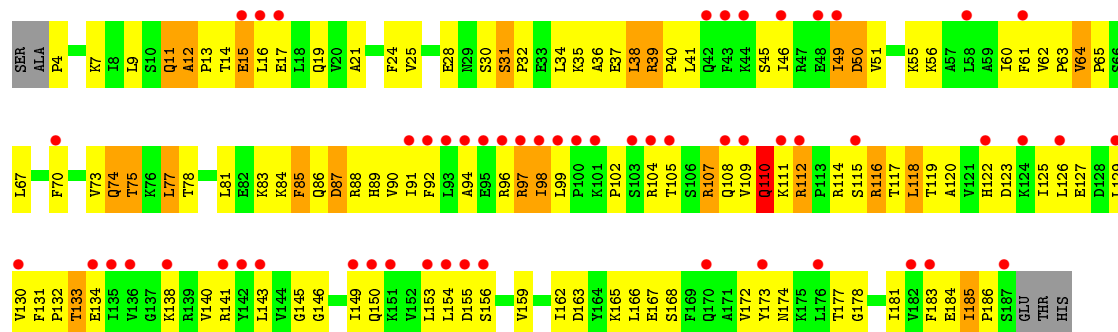




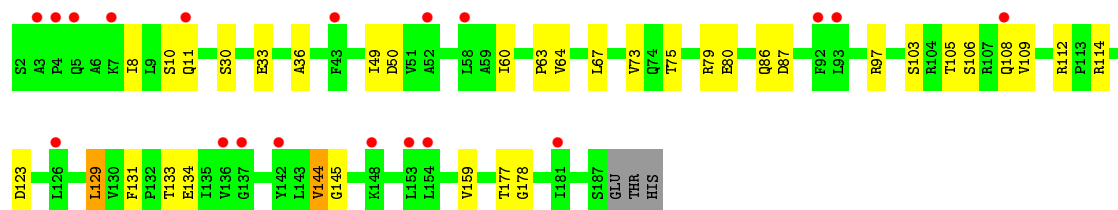
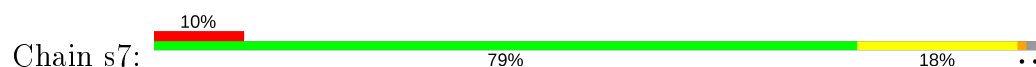
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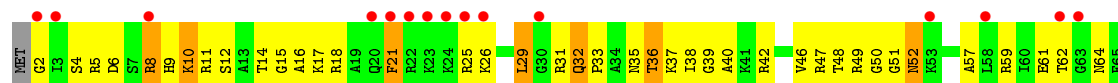
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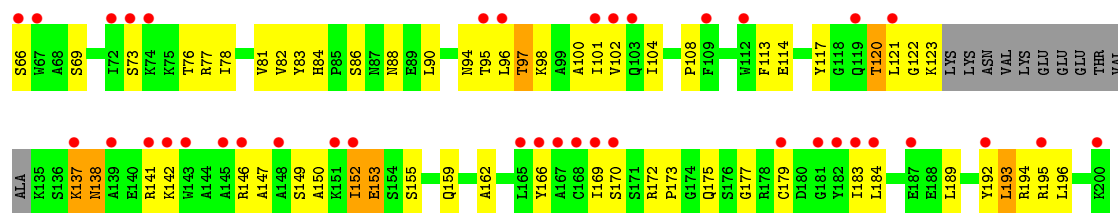


• Molecule 9: 40S ribosomal protein S7-A

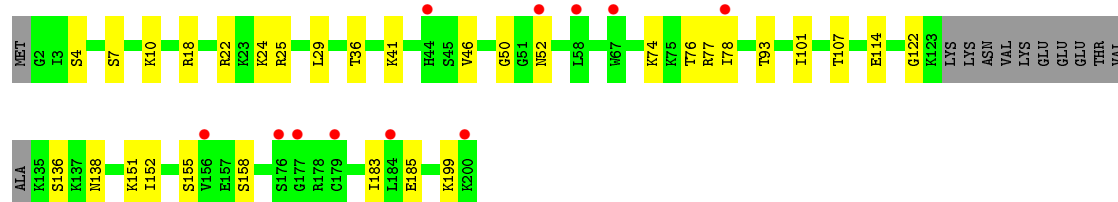
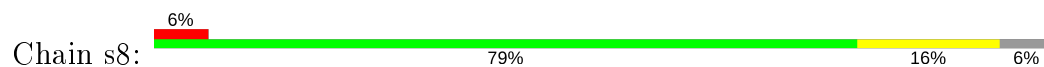


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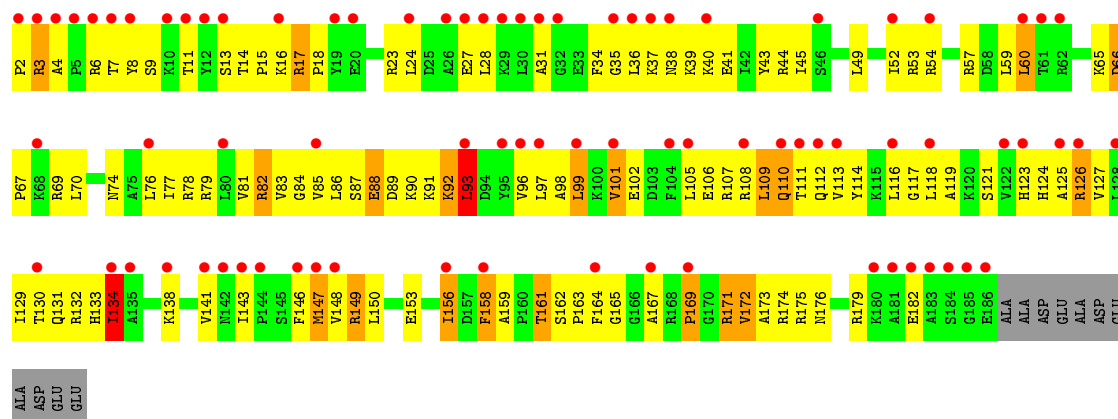




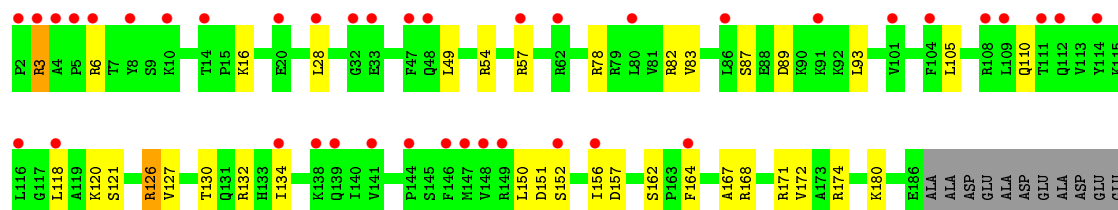
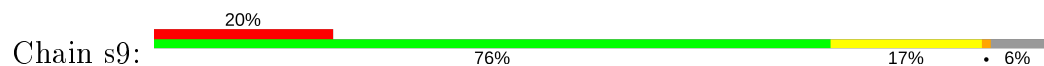
• Molecule 10: 40S ribosomal protein S8-A



• Molecule 11: 40S ribosomal protein S9-A



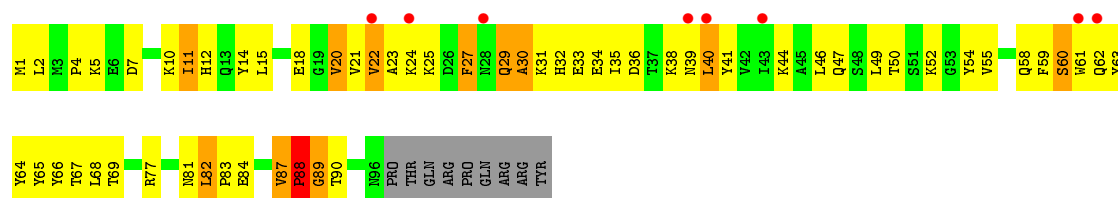
• Molecule 11: 40S ribosomal protein S9-A



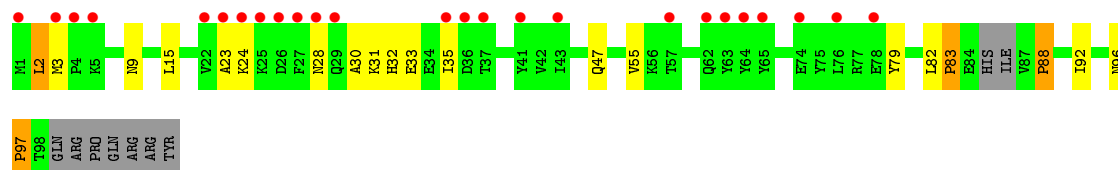
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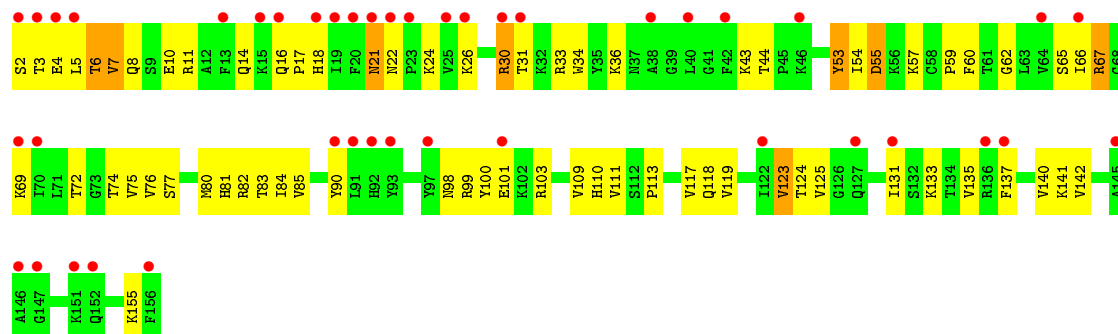




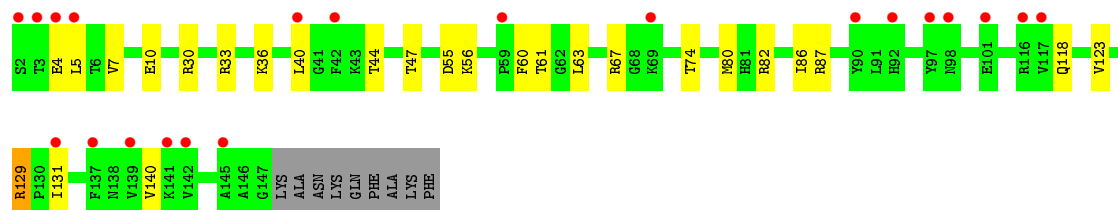
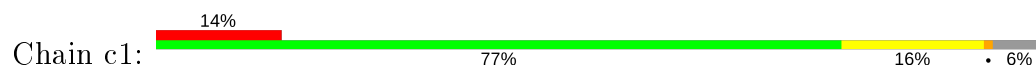
• Molecule 12: 40S ribosomal protein S10-A



• Molecule 13: 40S ribosomal protein S11-A



• Molecule 13: 40S ribosomal protein S11-A

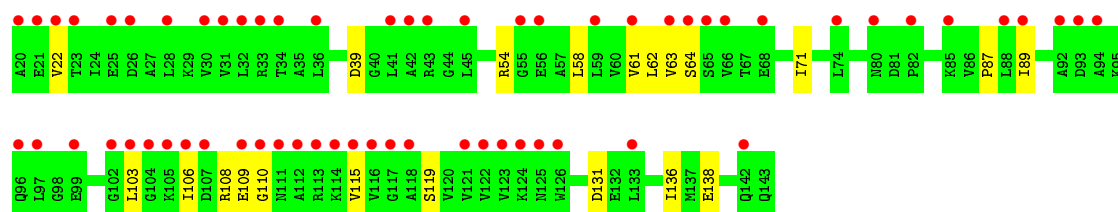
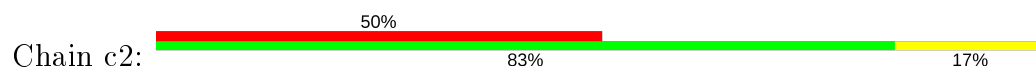


• Molecule 14: 40S ribosomal protein S12

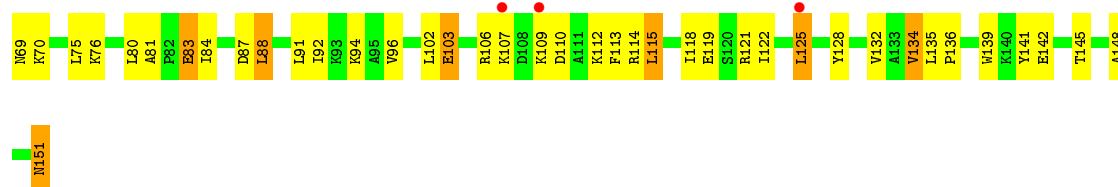
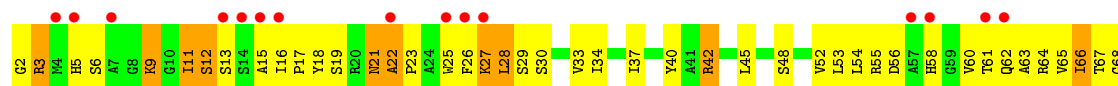
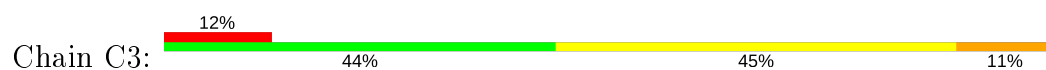




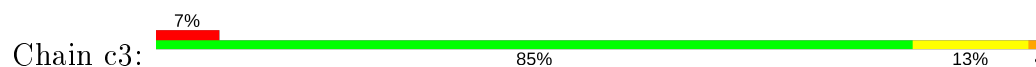
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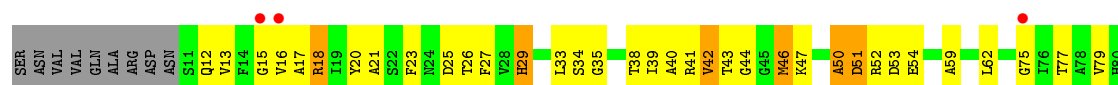
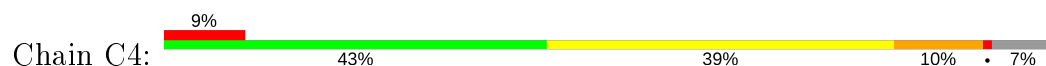
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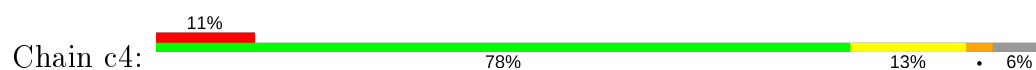
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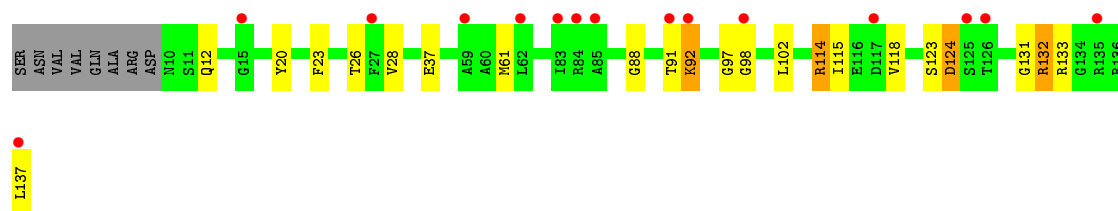


- Molecule 16: 40S ribosomal protein S14-A

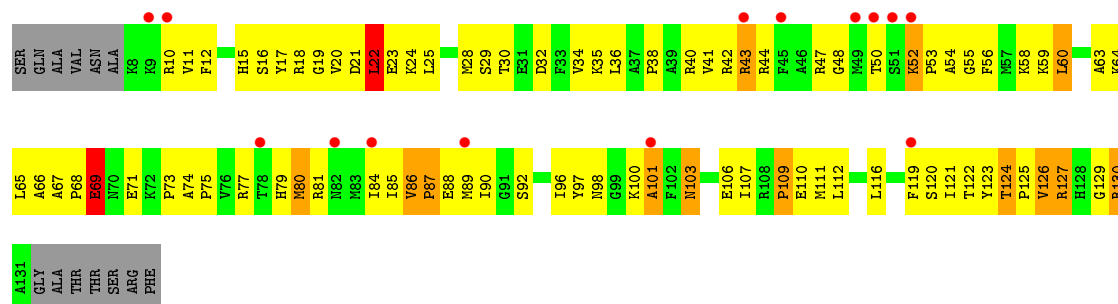


- Molecule 16: 40S ribosomal protein S14-A

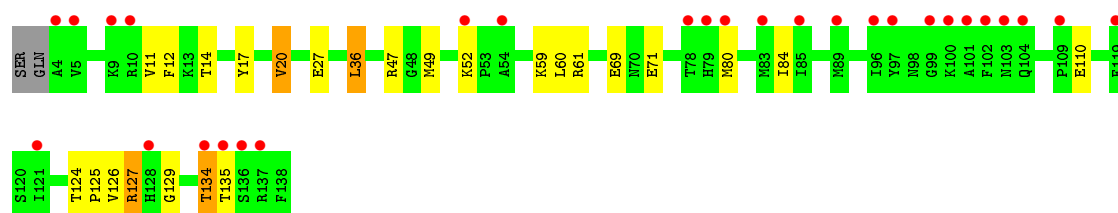
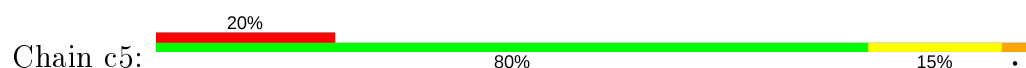




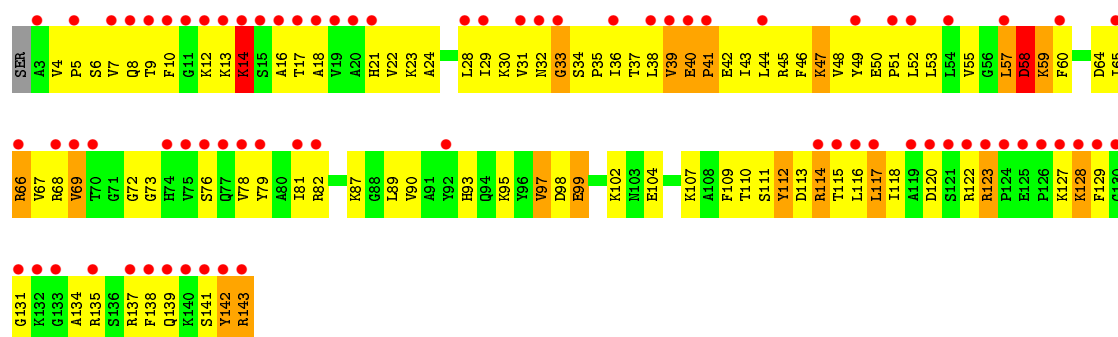
• Molecule 17: 40S ribosomal protein S15



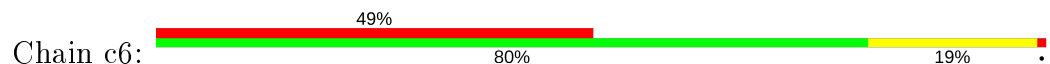
• Molecule 17: 40S ribosomal protein S15

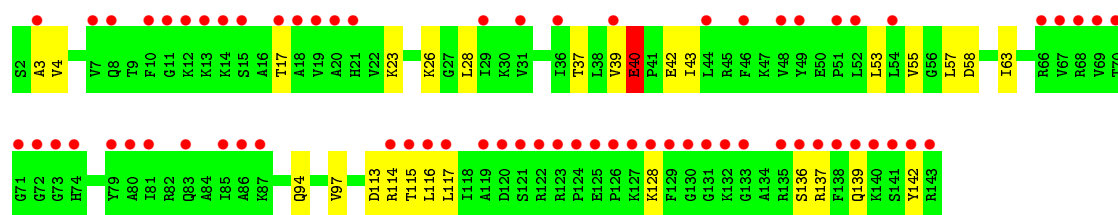


• Molecule 18: 40S ribosomal protein S16-A

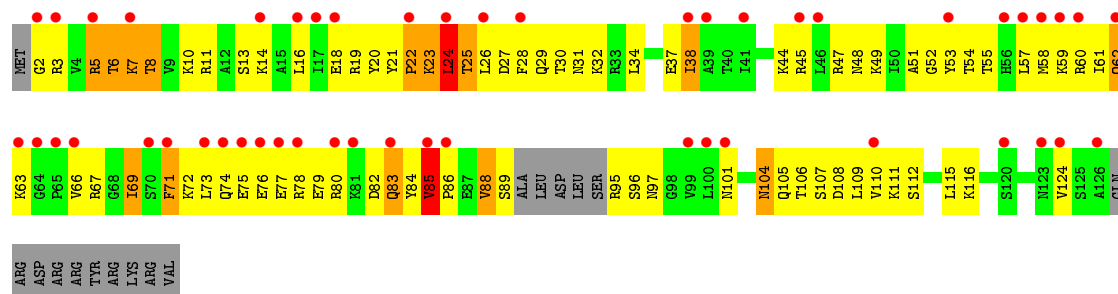


• Molecule 18: 40S ribosomal protein S16-A

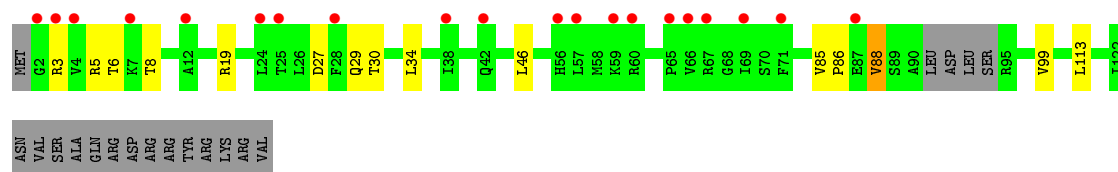
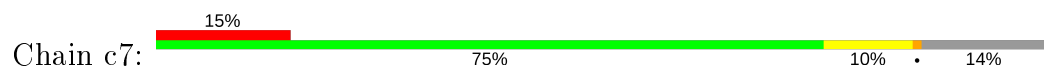




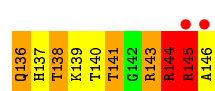
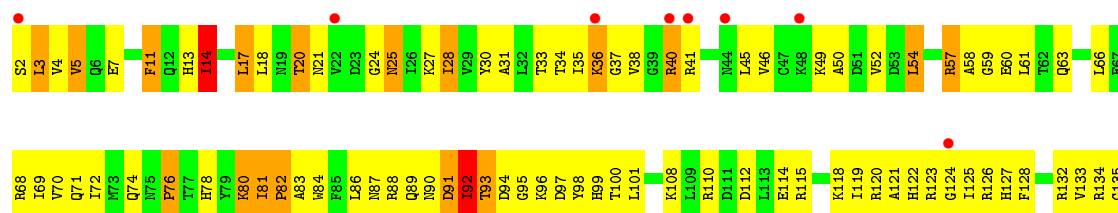
• Molecule 19: 40S ribosomal protein S17-A



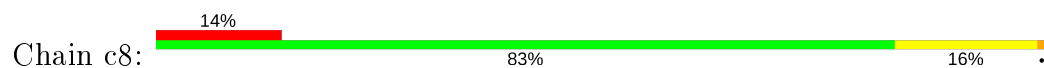
• Molecule 19: 40S ribosomal protein S17-A

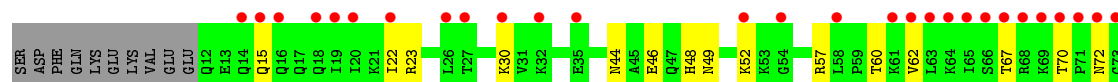


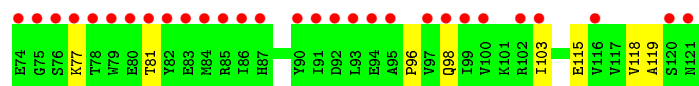
• Molecule 20: 40S ribosomal protein S18-A



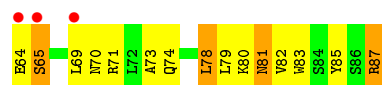
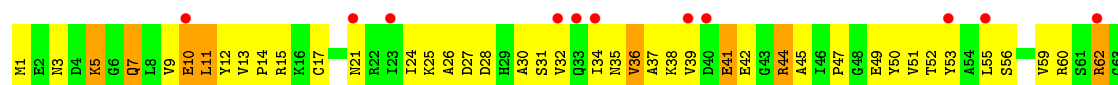
• Molecule 20: 40S ribosomal protein S18-A



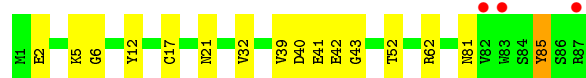
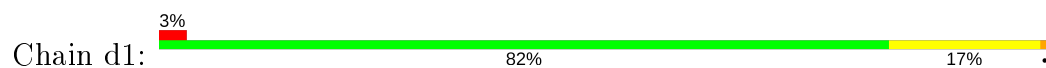




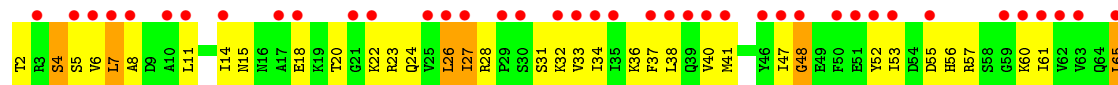
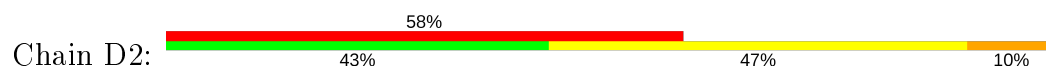
• Molecule 23: 40S ribosomal protein S21-A



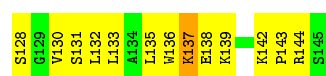
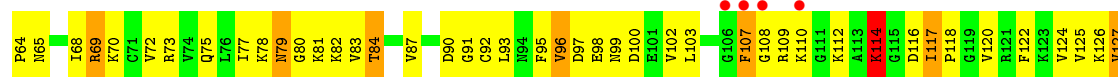
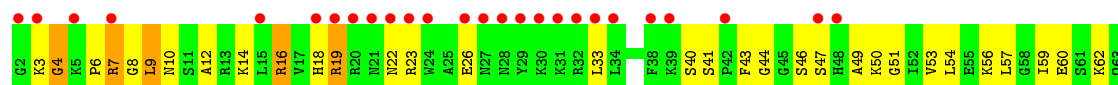
• Molecule 23: 40S ribosomal protein S21-A



• Molecule 24: 40S ribosomal protein S22-A

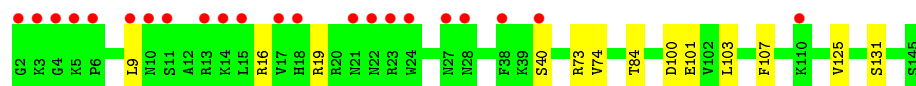


• Molecule 25: 40S ribosomal protein S23-A

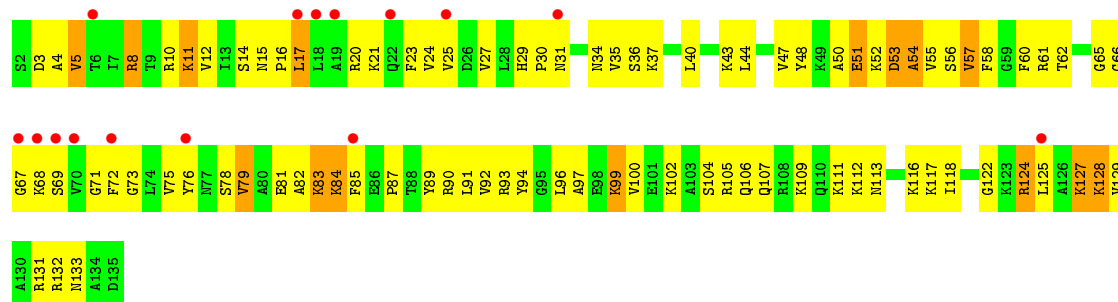


• Molecule 25: 40S ribosomal protein S23-A

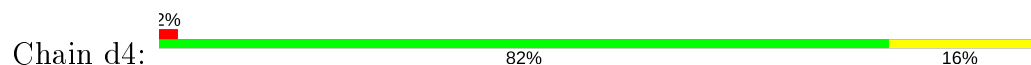




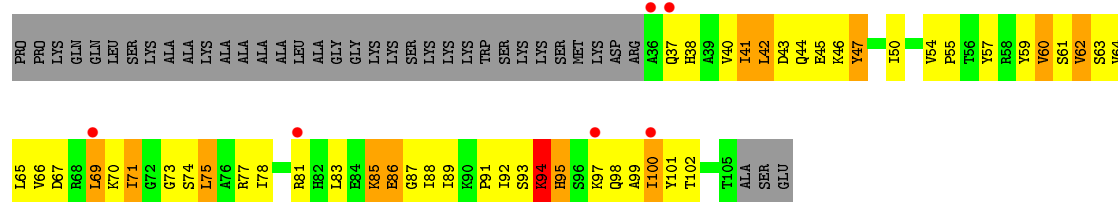
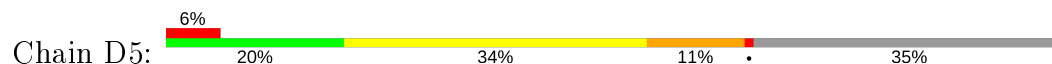
- Molecule 26: 40S ribosomal protein S24-A



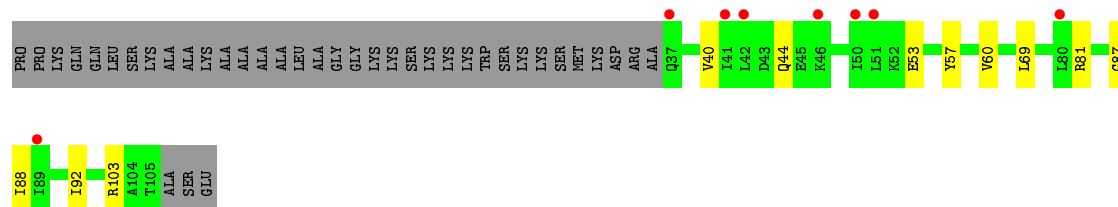
- Molecule 26: 40S ribosomal protein S24-A



- Molecule 27: 40S ribosomal protein S25-A

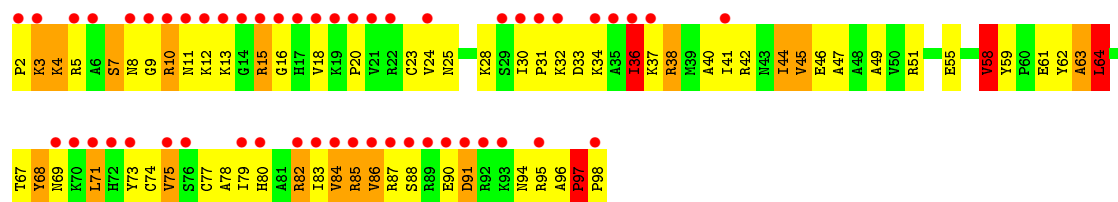


- Molecule 27: 40S ribosomal protein S25-A

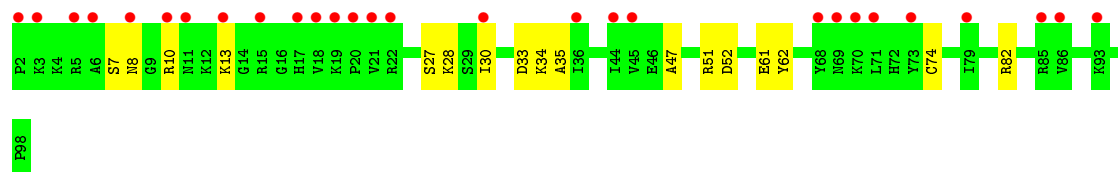
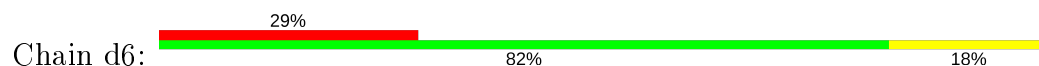


- Molecule 28: 40S ribosomal protein S26-B

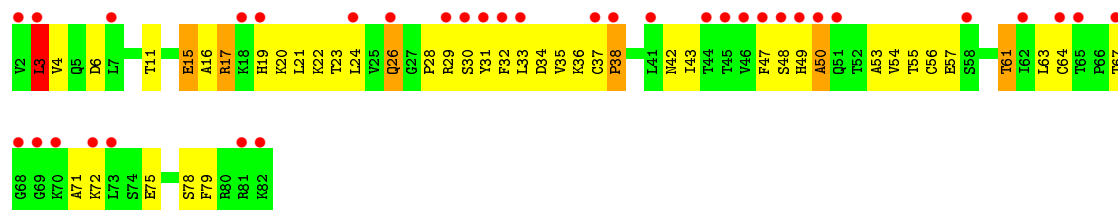
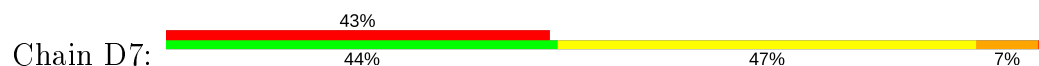




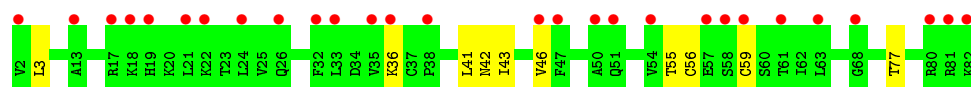
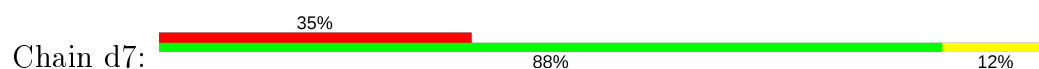
• Molecule 28: 40S ribosomal protein S26-B



• Molecule 29: 40S ribosomal protein S27-A



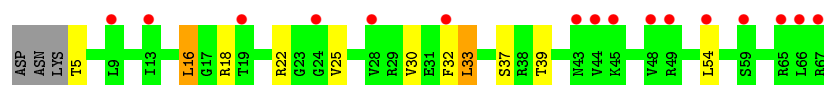
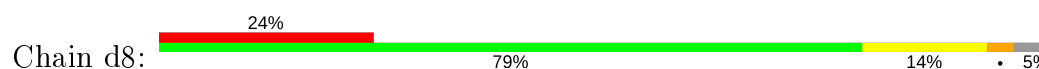
• Molecule 29: 40S ribosomal protein S27-A



• Molecule 30: 40S ribosomal protein S28-A

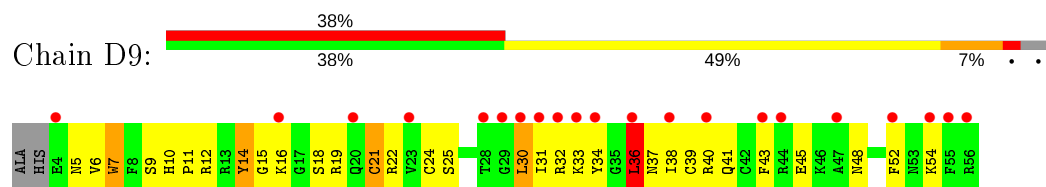


• Molecule 30: 40S ribosomal protein S28-A

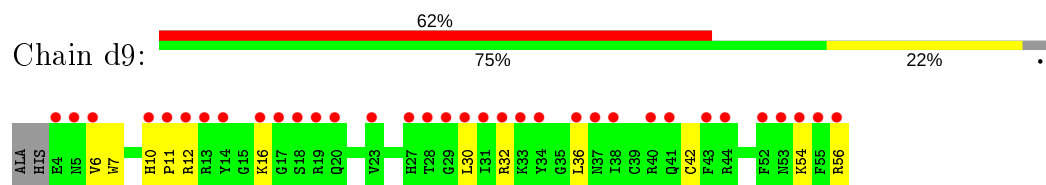




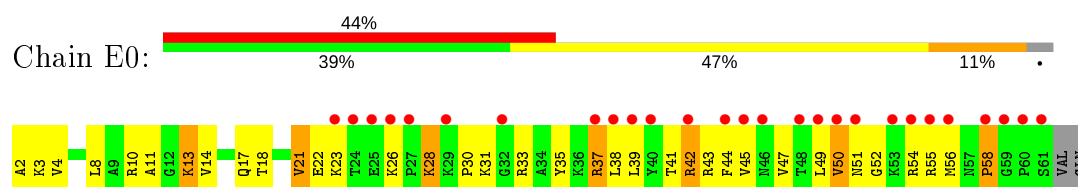
- Molecule 31: 40S ribosomal protein S29-A



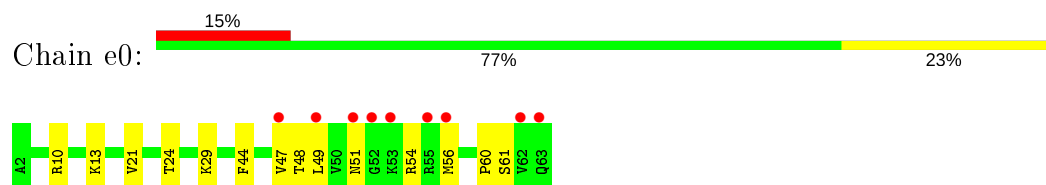
- Molecule 31: 40S ribosomal protein S29-A



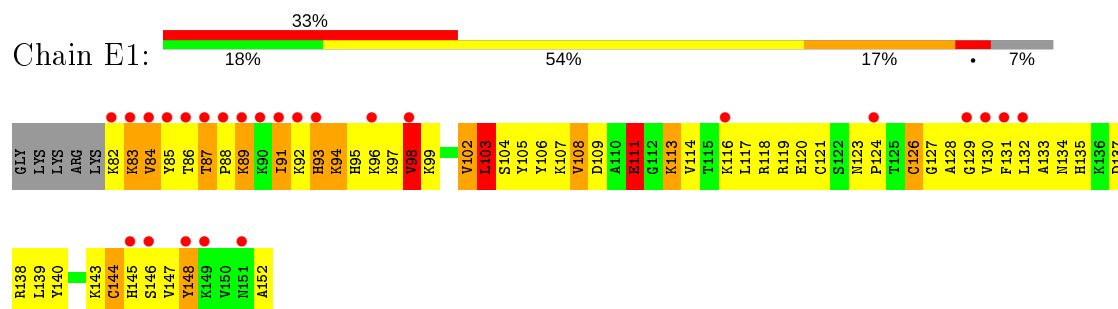
- Molecule 32: 40S ribosomal protein S30-A



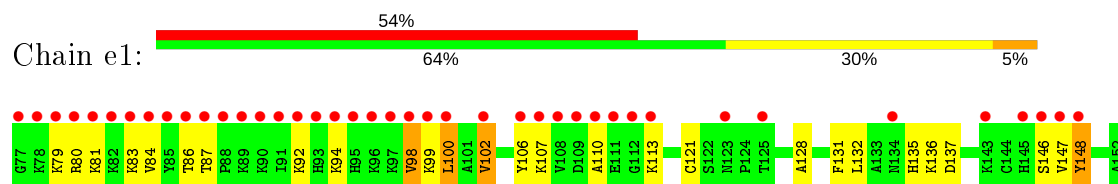
- Molecule 32: 40S ribosomal protein S30-A



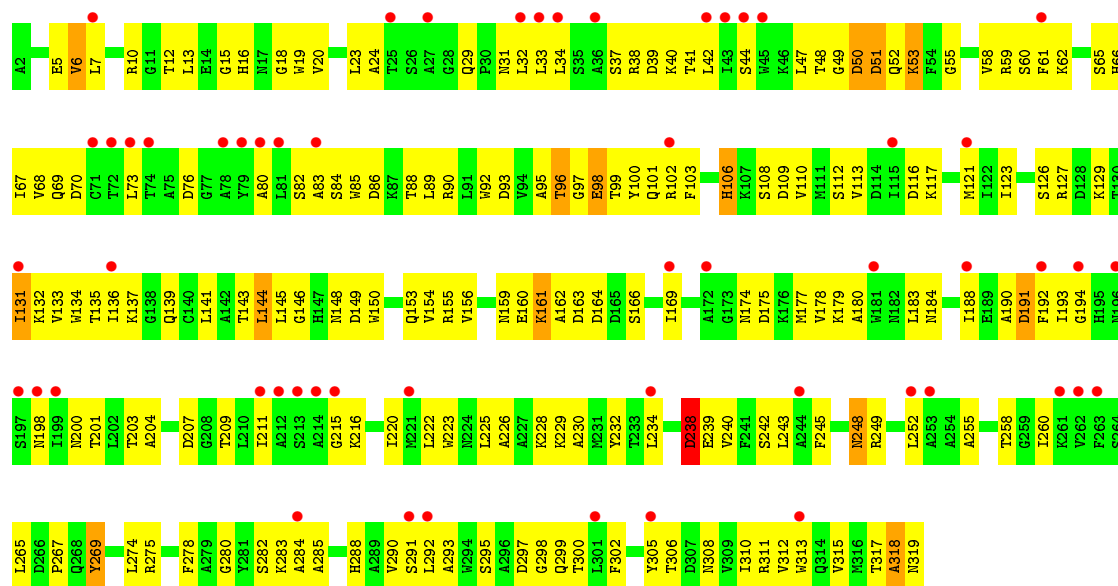
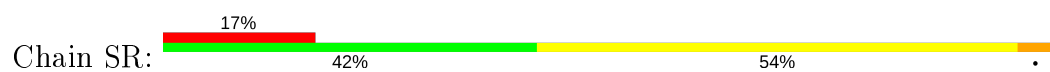
- Molecule 33: Ubiquitin-40S ribosomal protein S31



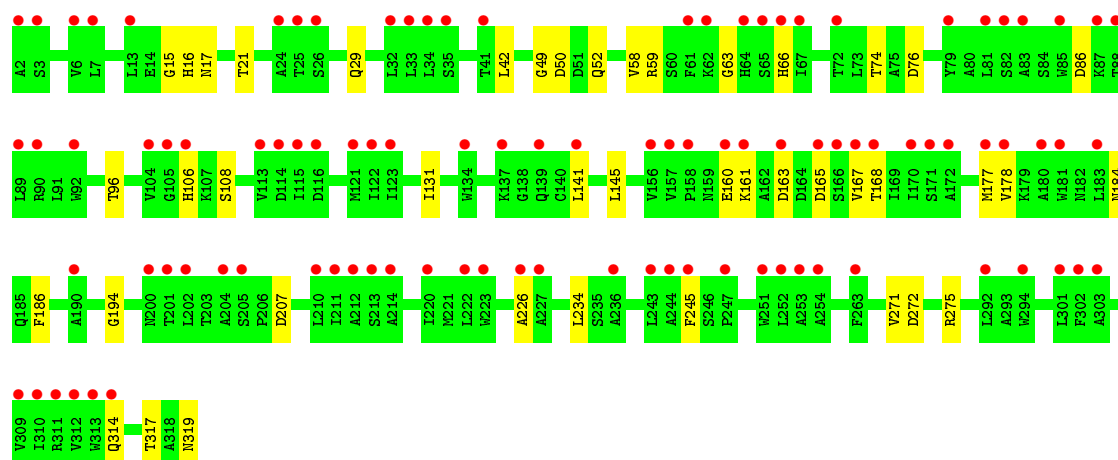
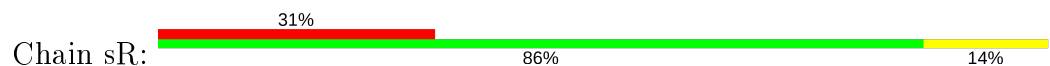
- Molecule 33: Ubiquitin-40S ribosomal protein S31



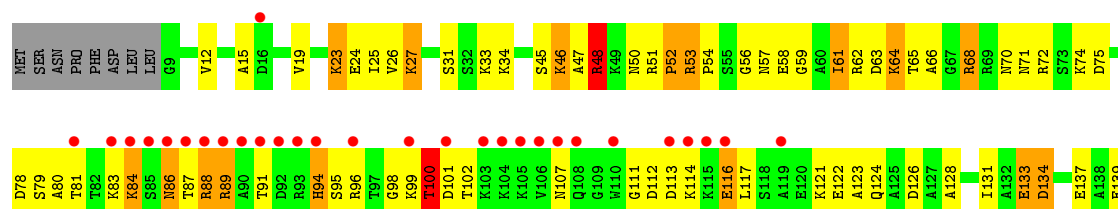
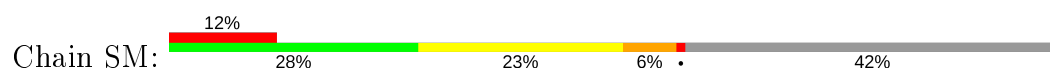
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



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



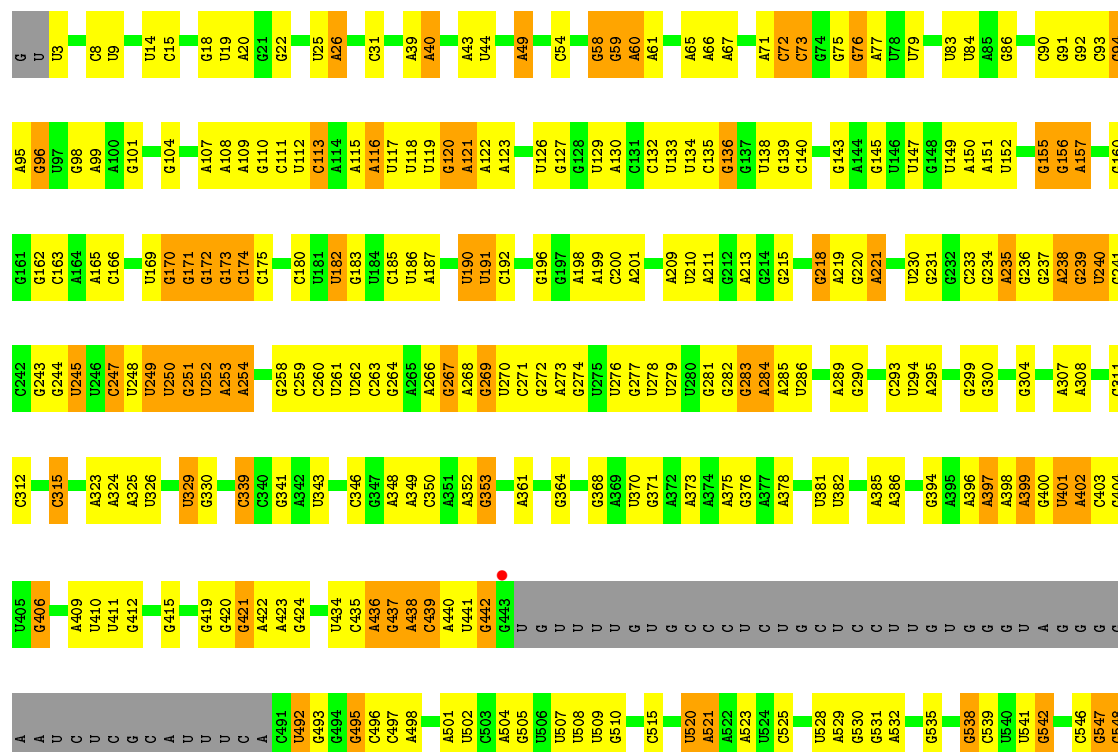
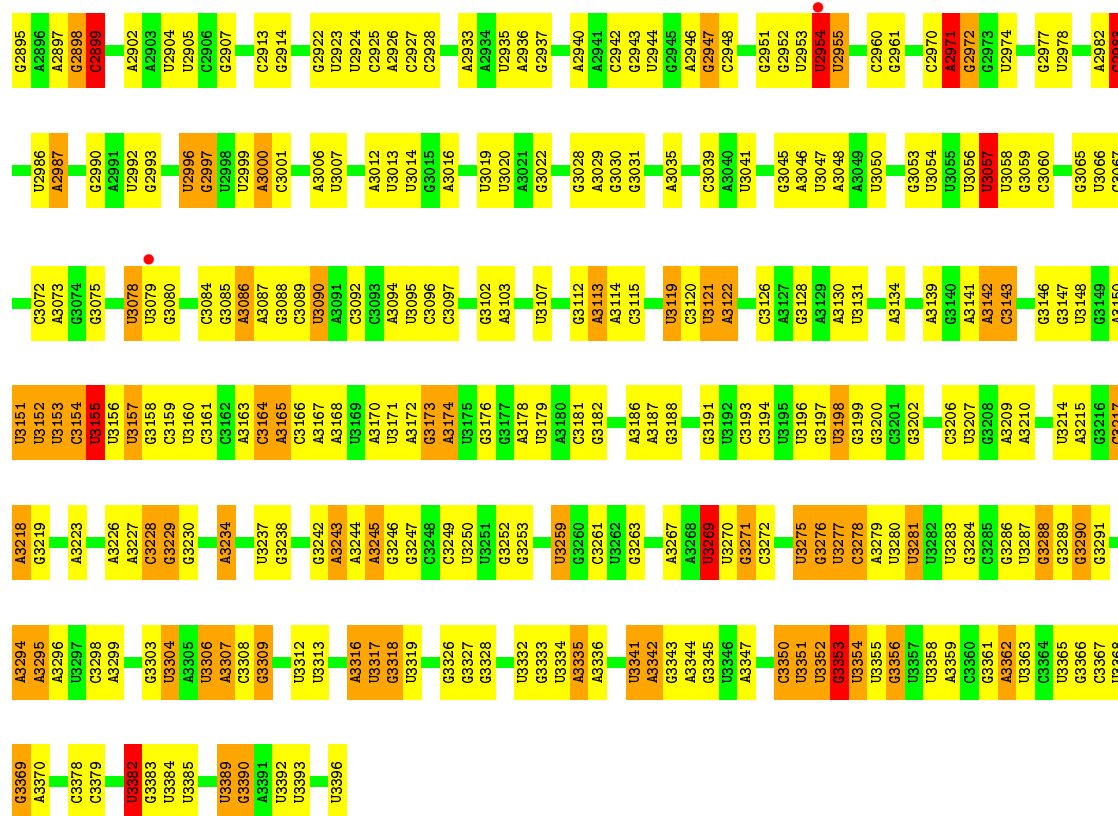
• Molecule 35: Suppressor protein STM1





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U1649	A1570	G1310	G1149	G1066	U995	U897	U814	G728	C641
G1650	A1571	G1311	U1151	U1070	A996	U898	A816	G736	U642
U1651	U1572	G1312	G1152	U1071	A997	U899	A817	A737	A645
U1654	U1573	G1313	A1153	G1072	A998	G900	C818	A738	U648
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G1655	A1489	G1317	A1163	U1074	G907	G907	A820	G740	G567
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U1659	G1493	G1320	A1163	U1082	G911	G911	G824	A744	U574
C1660	A1407	G1323	A1169	G1087	G912	G912	U828	C655	A578
A1667	G1408	G1327	A1170	A1093	A913	A913	U829	A566	G579
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U1682	A1506	G1333	A1180	U1098	U923	U923	G838	G760	C593
A1683	G1507	G1334	A1181	G1101	G924	G924	C839	G763	U594
A1683	C1508	G1335	A1182	A1102	G924	G924	C840	U764	G595
U1684	A1419	C1339	C1183	A1103	G934	G934	A841	A677	A598
G1685	U1425	G1340	C1183	G1104	U935	U935	G844	U678	C599
C1686	G1429	U1347	U1191	U1108	U936	U936	G844	U679	C599
U1687	U1430	G1348	C1192	U1109	A936	A936	G847	G600	U601
U1688	G1431	G1349	A1193	U1110	G937	G937	A847	U681	U602
U1689	G1432	G1349	A1193	U1111	C938	C938	A848	U682	A603
A1603	A1433	U1350	C1196	U1111	G1024	G1024	G853	G770	A604
G1604	G1434	U1351	A1197	U1114	A1025	A1025	A771	G772	G604
A1605	A1435	G1352	A1200	G1115	U1028	U1028	G857	U772	G609
C1609	U1436	G1353	C1201	G1116	A1030	A1030	G857	U773	G610
A1613	G1437	G1354	A1202	G1117	U1033	U1033	G860	U776	A611
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U1620	U1444	G1364	U1210	U1124	A1040	A1040	G876	C694	A619
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G1640	G1382	G1383	G1228	A1143	A1057	A1057	A801	A716	G635
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A1642	A1477	U1305	A1231	U1145	A1062	A1062	U889	G718	C637
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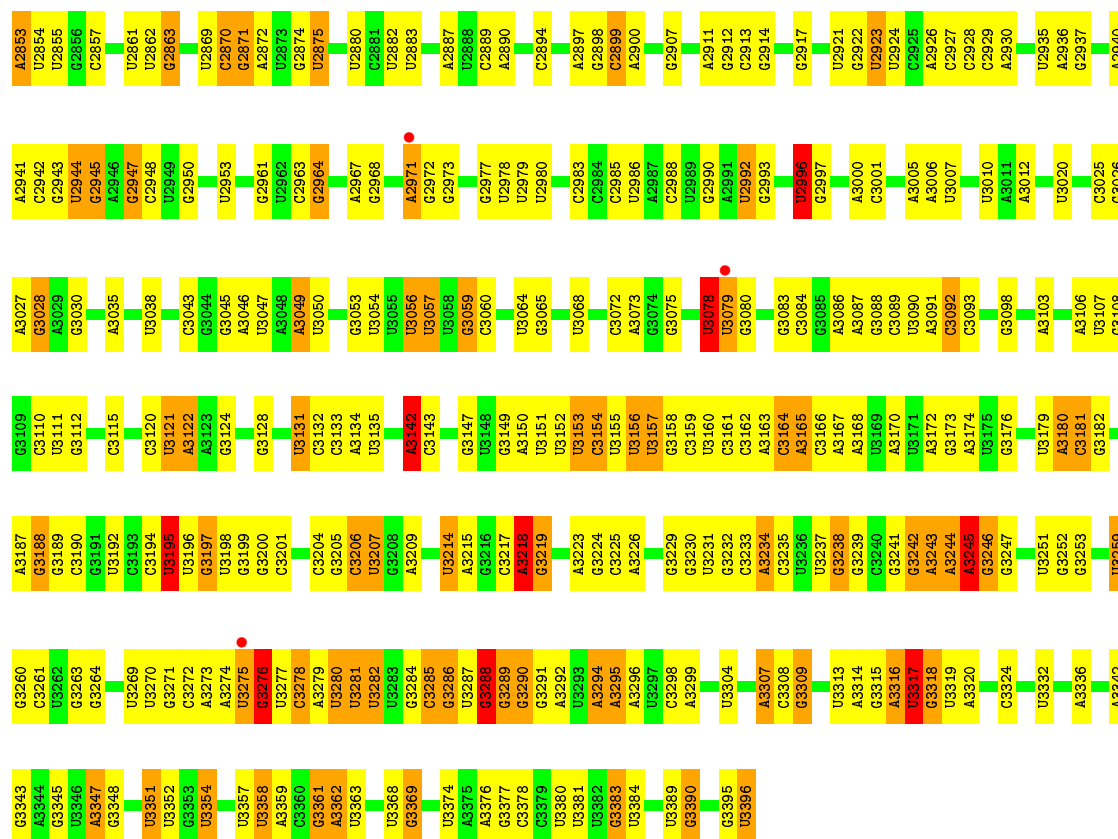




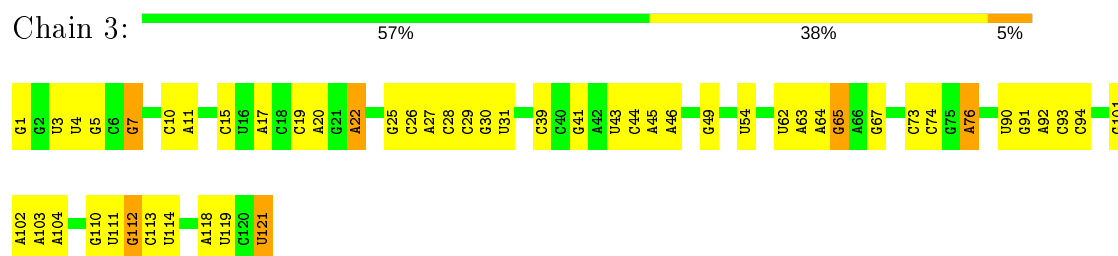
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G1661	A1498	C1498	G1409	G1320	C1239	C1238	G1144	A1062	G979	A896	G799	A715	G639	U553
G1662	C1499	G1321	G1412	G1322	A1240	C1241	G1145	A1064	A880	U897	G805	A716	U640	A554
G1674	A1503	G1323	G1413	G1324	G1242	G1243	G1152	A1065	U891	U898	A806	C717	C641	U555
G1675	A1506	U1325	G1414	U1324	A1244	G1243	G1153	A1066	G902	U899	U811	G718	U642	U556
A1676	G1507	G1329	G1418	U1329	A1245	A1244	A1153	C1069	G901	G901	U812	A645	U643	U557
A1677	C1508	A1330	A1419	A1330	G1246	A1246	C1155	U1070	G902	G902	G644	A646	U644	U558
U1682	G1508	U1331	C1420	U1331	G1249	G1249	C1156	U1071	A904	A904	A817	A647	U645	A559
U1686	G1514	C1335	C1423	C1335	G1256	G1256	G1157	G1072	G993	G993	G728	G646	C646	C562
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A1619	G1541	A1351	G1440	A1351	U1265	U1265	U1181	U1088	G1013	U922	G838	G750	U664	C593
U1716	G1542	A1352	U1441	A1352	G1266	G1266	U1182	G1089	G1014	G923	G839	A751	U667	U594
G1717	U1543	U1353	A1446	U1353	A1273	A1273	C1183	G1093	U1015	G924	C840	G758	G667	G595
G1718	G1547	A1354	G1447	A1354	C1274	C1274	C1184	U1094	C1016	A926	G668	C596	G668	C596
U1721	C1548	U1355	G1450	A1355	A1275	A1275	C1185	U1095	C1017	C927	U672	A598	U669	G597
G1723	U1549	G1356	A1453	U1356	C1276	C1276	C1189	U1096	G1018	A936	G845	G763	U673	C599
A1625	C1550	G1357	A1454	G1357	C1277	C1277	A1190	G1097	G1019	G937	A847	C765	G674	U601
U1626	U1554	U1360	U1455	U1360	G1280	G1280	U1191	A1098	G1020	U942	A848	U766	C675	A602
G1627	U1555	G1361	U1456	U1361	G1281	G1281	C1192	U1100	U1022	U943	C849	U767	G676	A603
C1628	C1556	G1362	A1456	G1362	C1292	C1292	C1196	A1103	C1023	U944	U850	G770	A677	G604
U1629	U1557	G1365	G1466	G1365	U1293	U1293	A1197	G1101	A1025	C945	U871	A771	U679	A607
C1631	G1560	A1366	U1470	A1366	G1294	G1294	C1199	A1102	G1024	U946	U872	U772	U680	A608
A1632	U1561	G1367	U1471	G1367	G1295	G1295	A1200	G1104	A1026	G947	G857	G773	U681	G609
C1633	C1562	U1368	U1472	U1368	C1298	C1298	C1201	U1108	U1028	C948	G860	U773	U682	G610
G1634	G1563	A1369	C1478	A1369	U1299	U1299	A1204	U1109	G1029	C949	C861	U777	U683	A611
G1635	U1564	G1373	U1479	G1373	G1300	G1300	A1205	U1110	A1030	G953	G869	U777	G684	U612
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A1643	U1566	G1381	A1481	G1381	A1302	A1302	G1116	U1116	U1039	U955	G781	U782	G686	A619
C1644	A1567	G1382	U1482	G1382	A1305	A1305	G1117	U1117	U1041	U956	G873	U783	U687	U620
U1645	U1568	G1383	G1483	G1383	U1306	U1306	U1208	G1115	U1039	C957	A784	A783	A621	A621
G1646	U1570	U1384	U1484	U1384	G1307	G1307	G1209	G1116	U1041	U958	G878	U785	C695	U623
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A1648	U1572	A1386	G1486	A1386	U1309	U1309	G1222	U1120	U1041	U959	U880	A787	A697	U628
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G1650	U1574	U1388	G1488	U1388	G1313	G1313	U1224	U1122	A1047	A962	C881	C788	U698	A630
A1654	A1575	G1389	U1491	G1389	G1314	G1314	A1231	U1123	A1047	G963	A882	A789	G701	U630
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A1656	U1577	A1393	G1493	A1393	U1315	U1315	G1234	U1128	U1050	A970	A888	U794	C634	C634

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C2772	A2694	A2595	C2772	A2384	A2296	A2214	C2129	U	G1935	A1842	A1760
C2773	A2695	A2596	C2773	A2385	U2297		A2131	A	U1938	C1846	
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	G2706	C2539	C2539	G2400		G2234	G2155	G	G1952	C1774	
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	U2715	C2545	C2545	G2406	A2320	G2247		U	G	U1782	
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C2812	U2721	C2551	C2551	A2413	U2336	G2253		C	G		
A2813	U2722	U2552	U2552	G2414	C2337	U2254	A2172	U	G	U1880	
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	C2735	C2565	C2565	U2427	U2350		G2185	U	U	G1902	
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C2826	G2745	C2567	C2567	A2430	C2352	G2271	G2187	C	A	G1906	
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A2837	G2751	G2573	G2573	A2441	A2361	C2277	G2194	A	U	C1917	
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G2847	G2761	U2582	U2582	U2450	G2370	U2285	A2207	C	U		
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	A2763	G2584	G2584	U2452	A2372	C2287	U2209	C	C		
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C2849	G2765	G2586	G2586	G2454	A2374	C2289	G2211	C	G	U1931	
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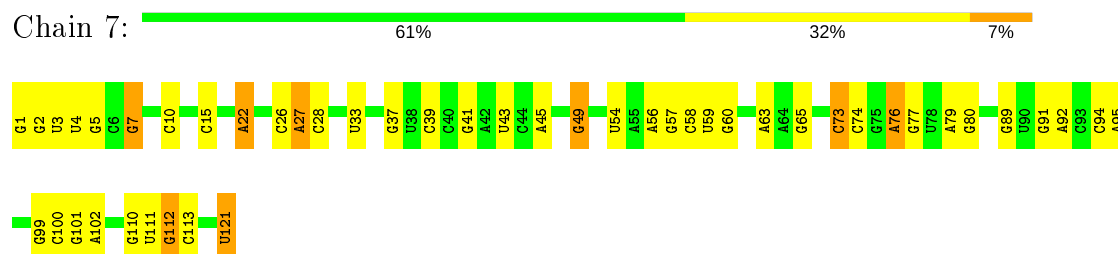




- Molecule 37: 5S ribosomal RNA

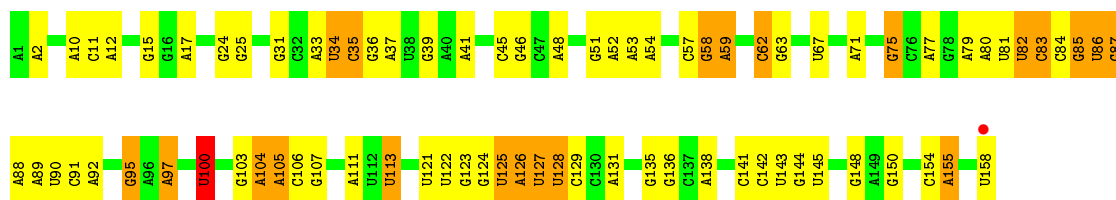


- Molecule 37: 5S ribosomal RNA



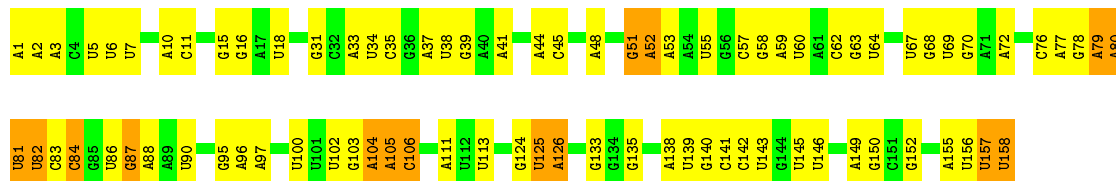
- Molecule 38: 5.8S ribosomal RNA





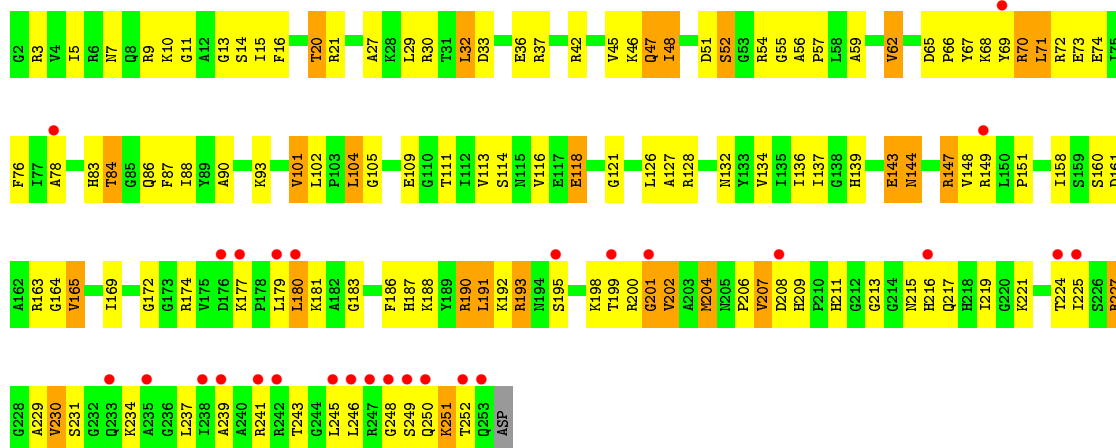
• Molecule 38: 5.8S ribosomal RNA

Chain 8: 48% 42% 9%



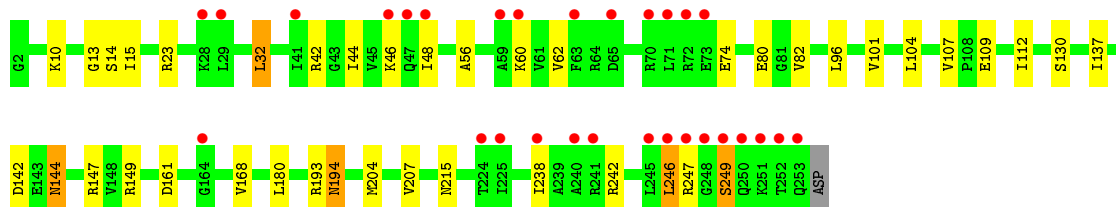
• Molecule 39: 60S ribosomal protein L2-A

Chain L2: 11% 47% 42% 11%



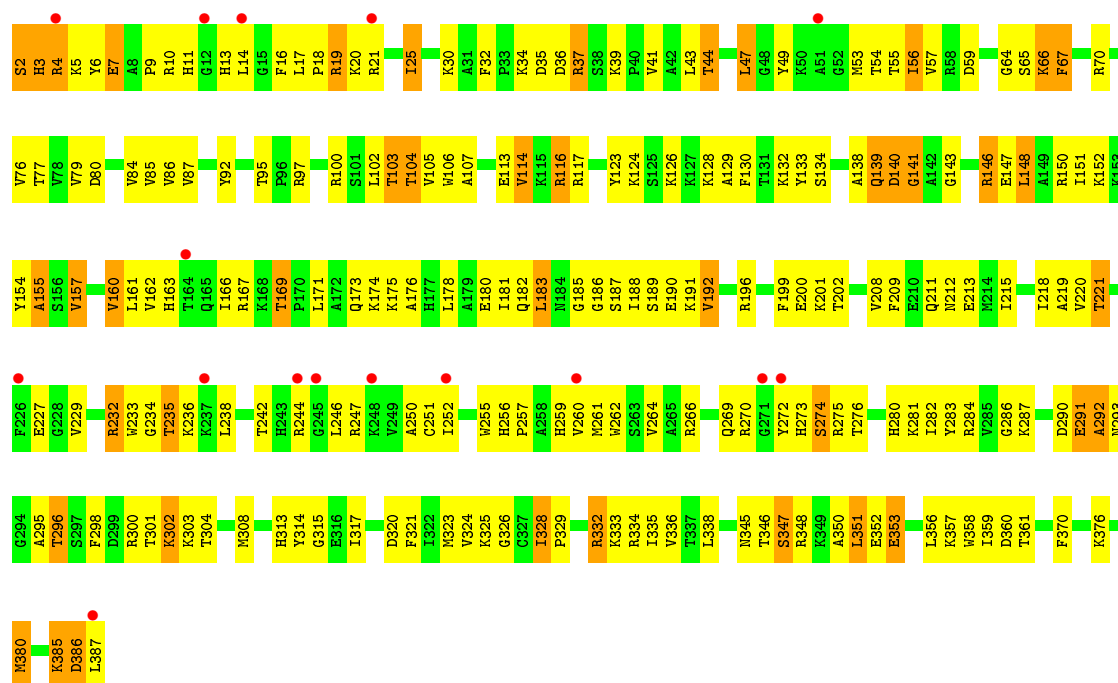
• Molecule 39: 60S ribosomal protein L2-A

Chain L2: 11% 83% 14%

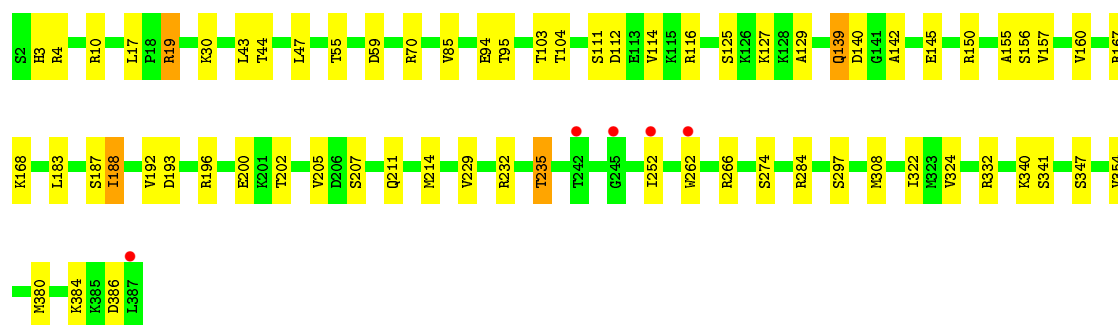
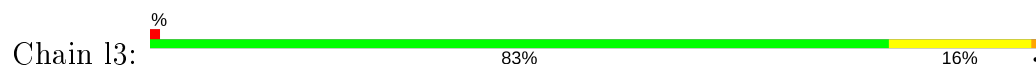


• Molecule 40: 60S ribosomal protein L3

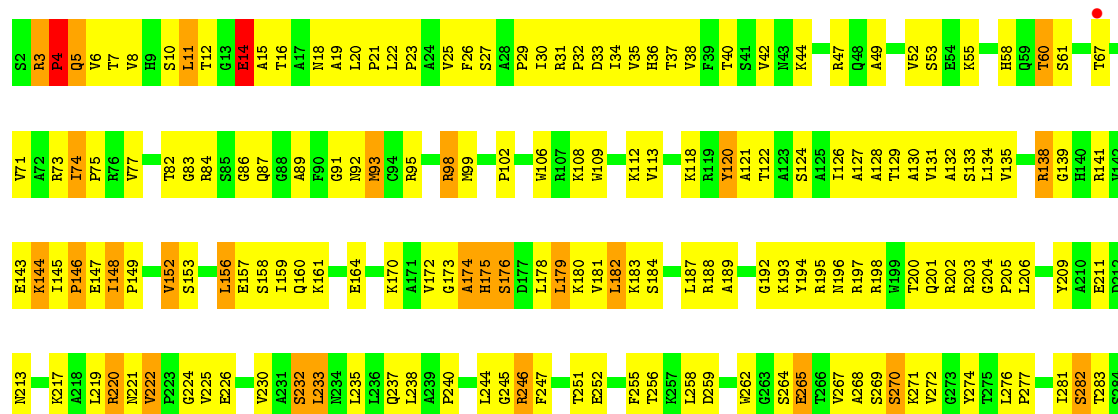
Chain L3: 4% 44% 45% 11%

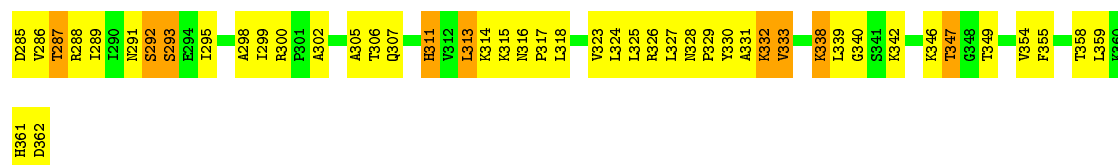


- Molecule 40: 60S ribosomal protein L3



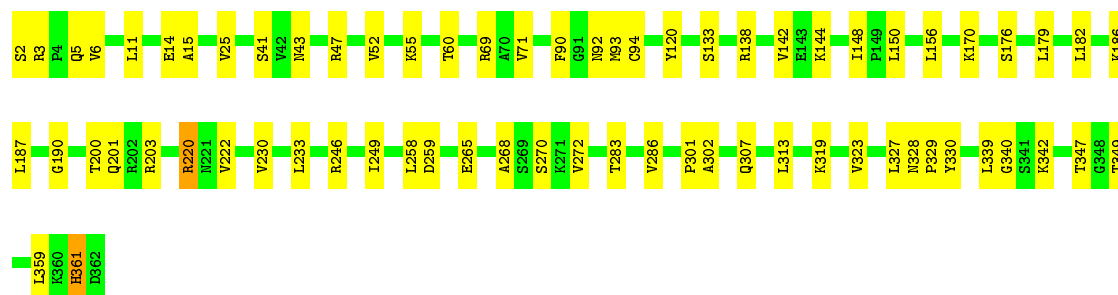
- Molecule 41: 60S ribosomal protein L4-A





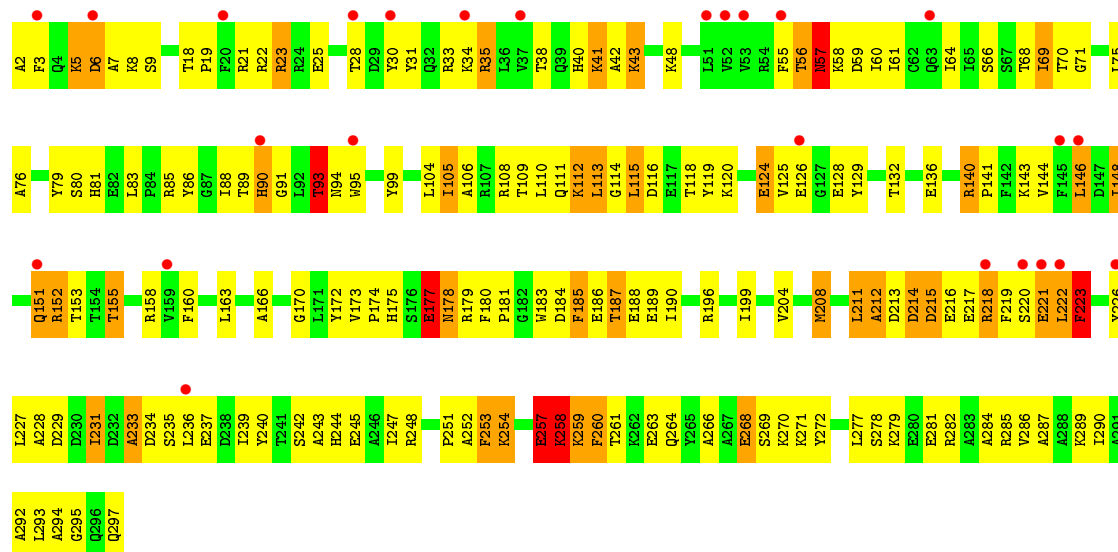
- Molecule 41: 60S ribosomal protein L4-A

Chain 14: 81% 19%



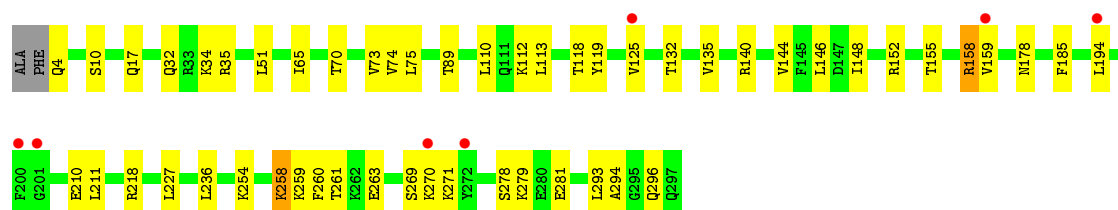
- Molecule 42: 60S ribosomal protein L5

Chain L5: 8% 41% 45% 13%

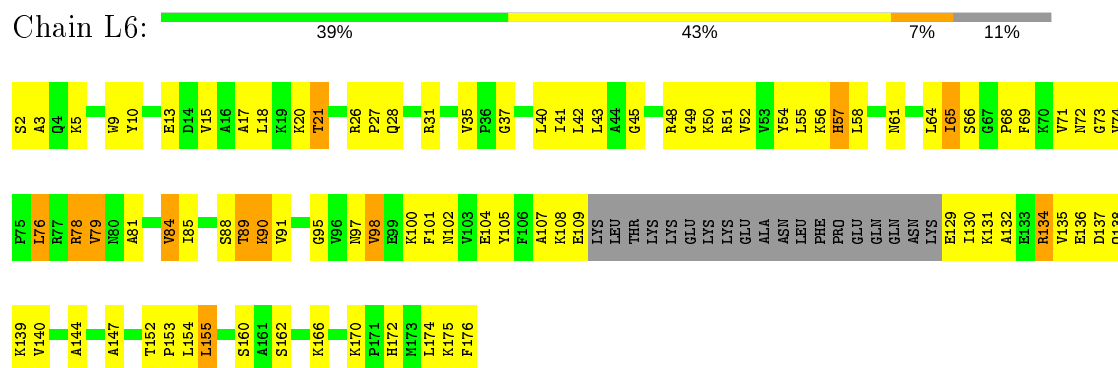


- Molecule 42: 60S ribosomal protein L5

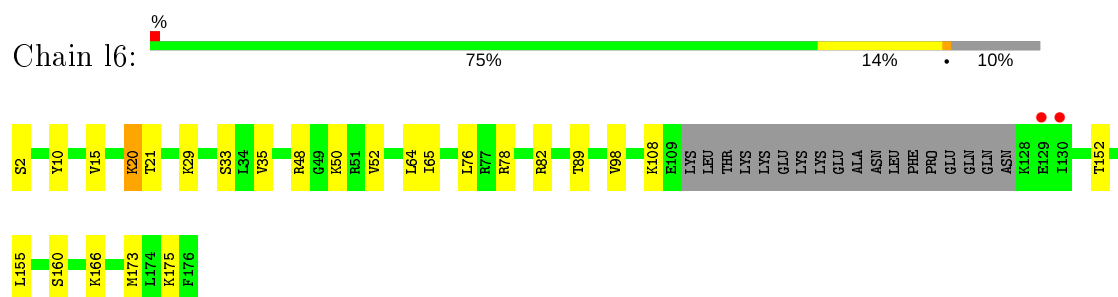
Chain L5: 2% 82% 17%



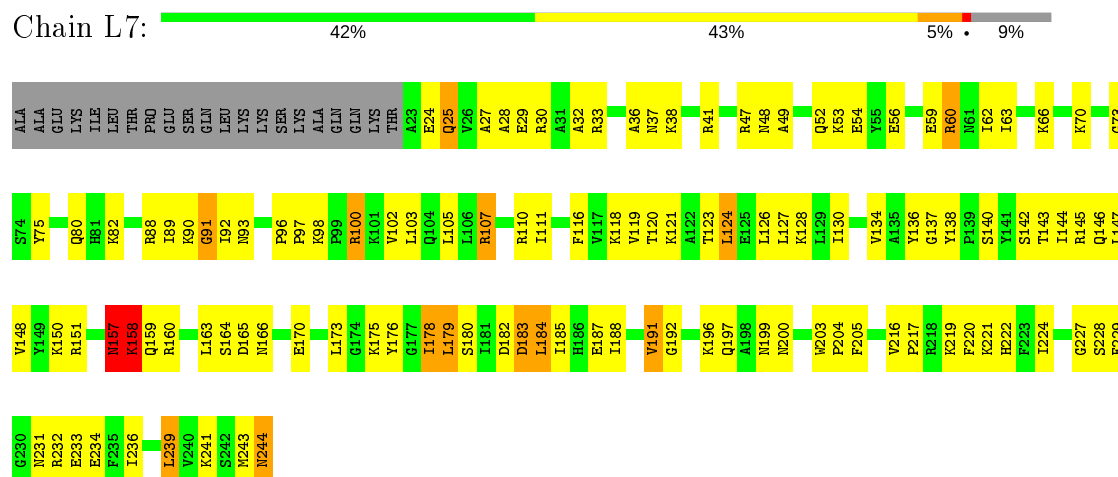
- Molecule 43: 60S ribosomal protein L6-A



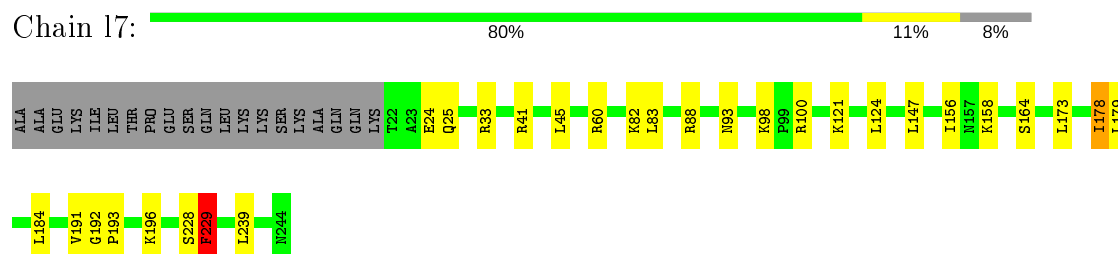
- Molecule 43: 60S ribosomal protein L6-A



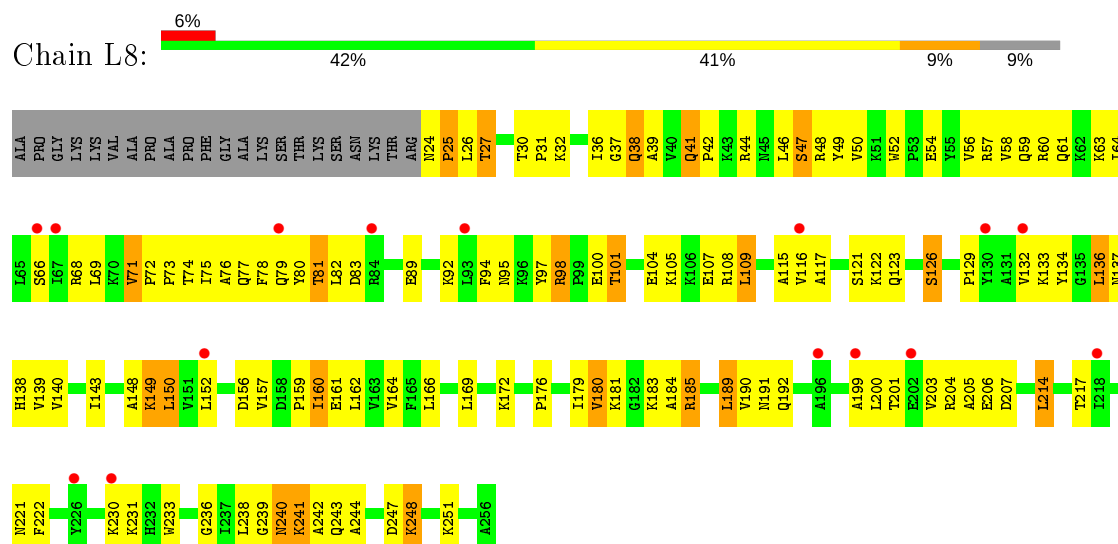
- Molecule 44: 60S ribosomal protein L7-A



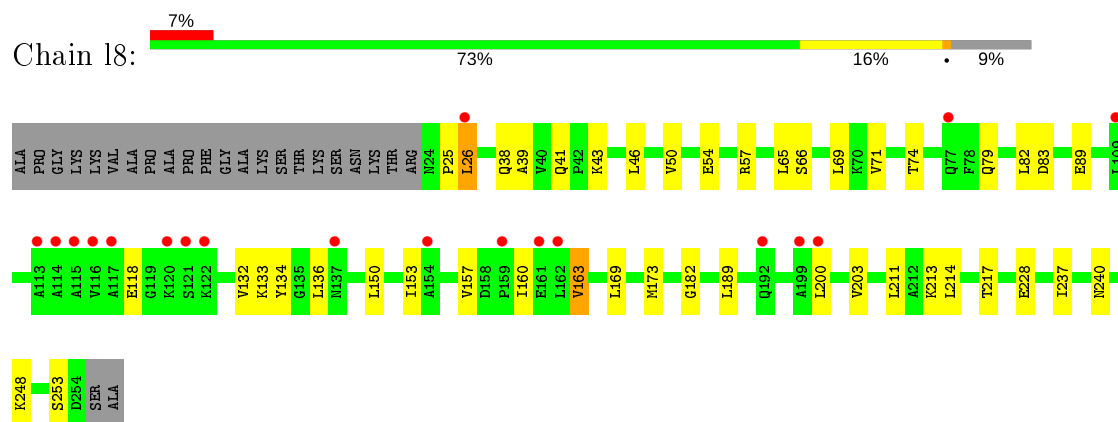
- Molecule 44: 60S ribosomal protein L7-A



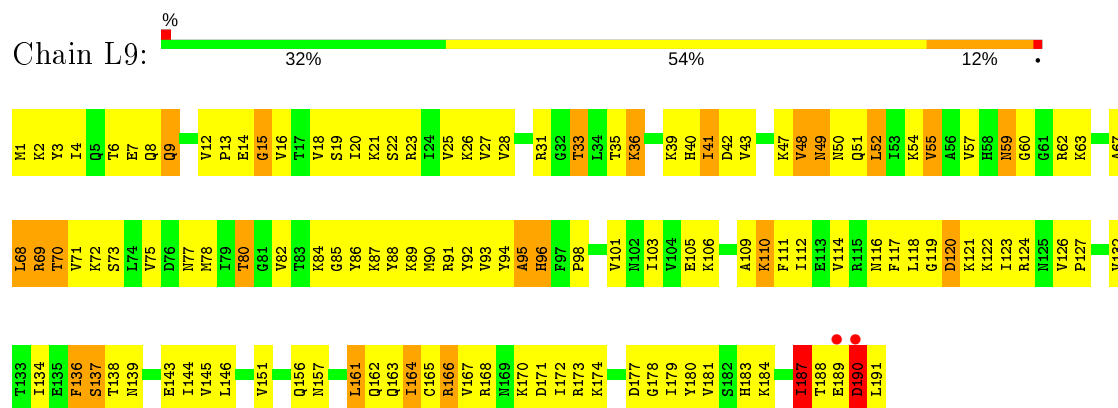
- Molecule 45: 60S ribosomal protein L8-A



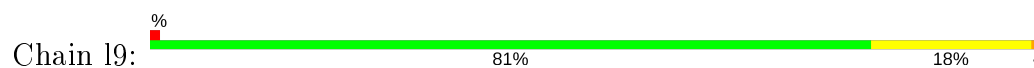
- Molecule 45: 60S ribosomal protein L8-A

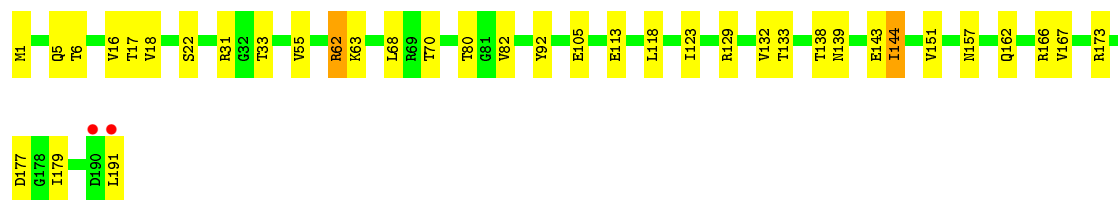


- Molecule 46: 60S ribosomal protein L9-A



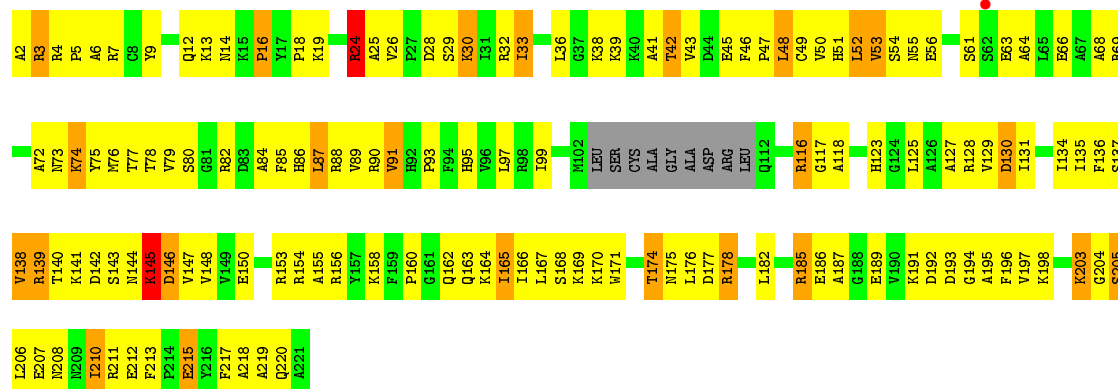
- Molecule 46: 60S ribosomal protein L9-A





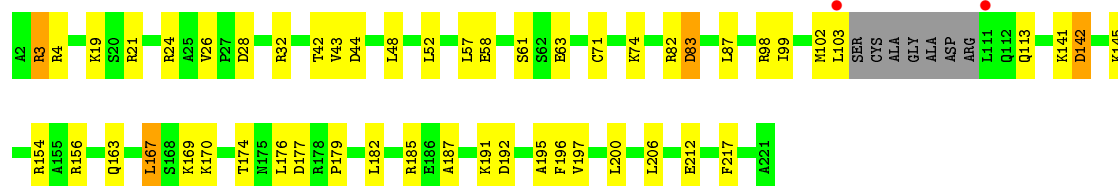
• Molecule 47: 60S ribosomal protein L10

Chain M0: 31% 53% 11% . .



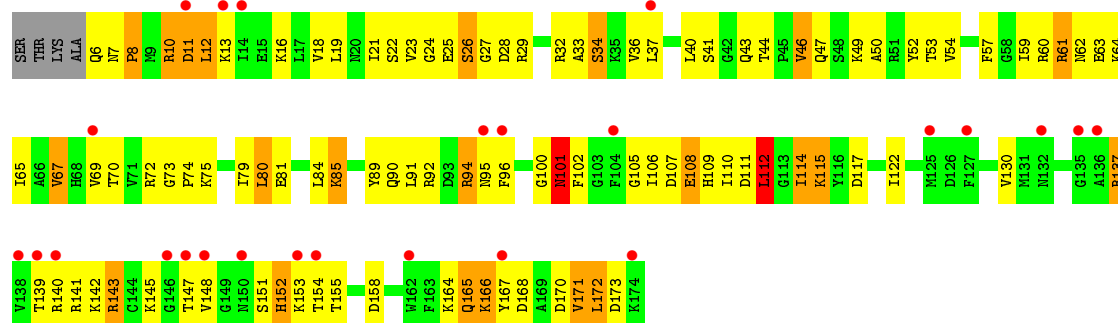
• Molecule 47: 60S ribosomal protein L10

Chain m0: % 73% 22% . .

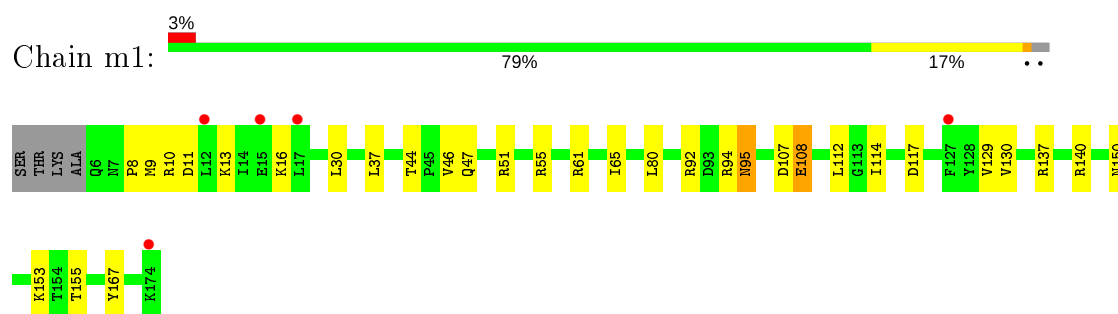


• Molecule 48: 60S ribosomal protein L11-B

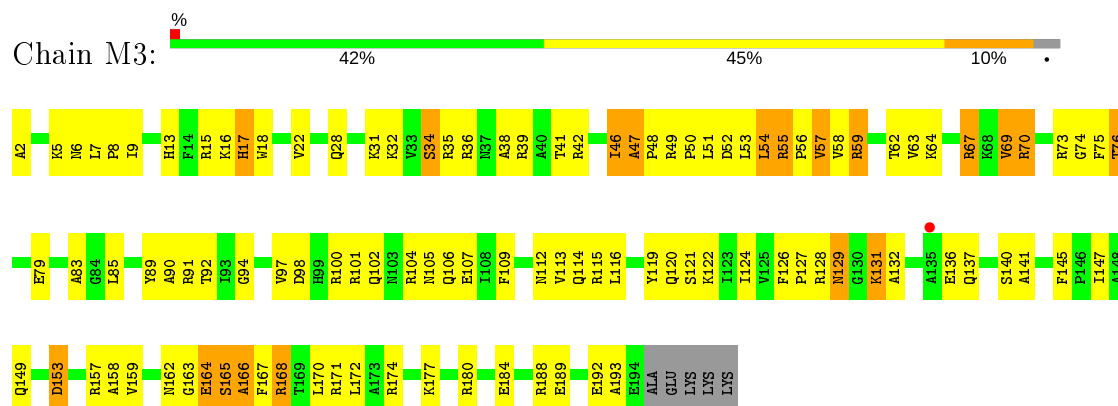
Chain M1: 14% 39% 45% 13% . .



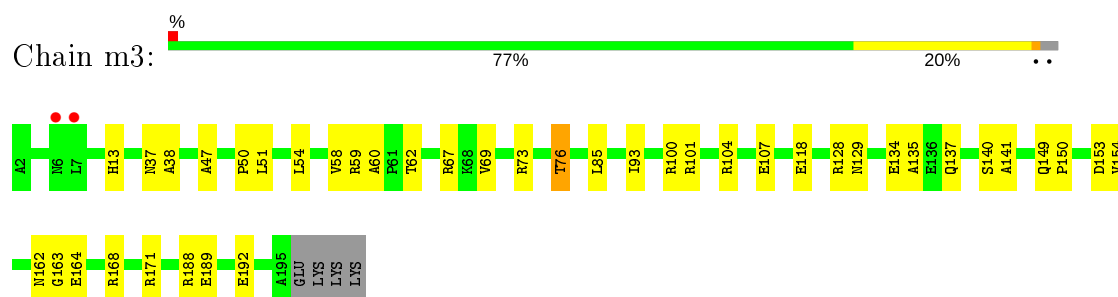
• Molecule 48: 60S ribosomal protein L11-B



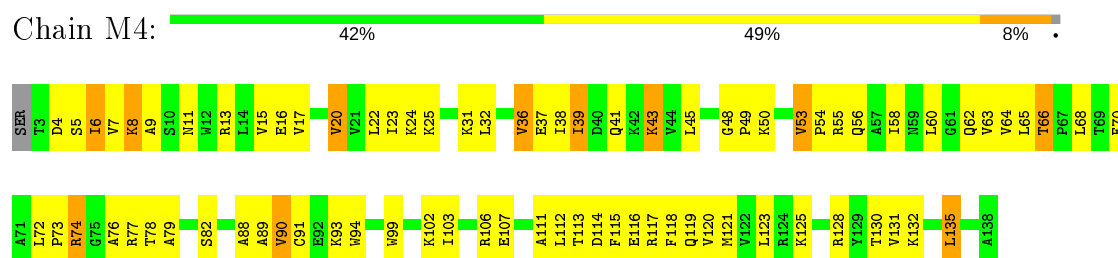
- Molecule 49: 60S ribosomal protein L13-A



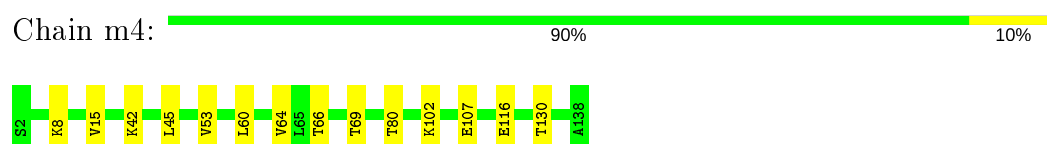
- Molecule 49: 60S ribosomal protein L13-A



- Molecule 50: 60S ribosomal protein L14-A

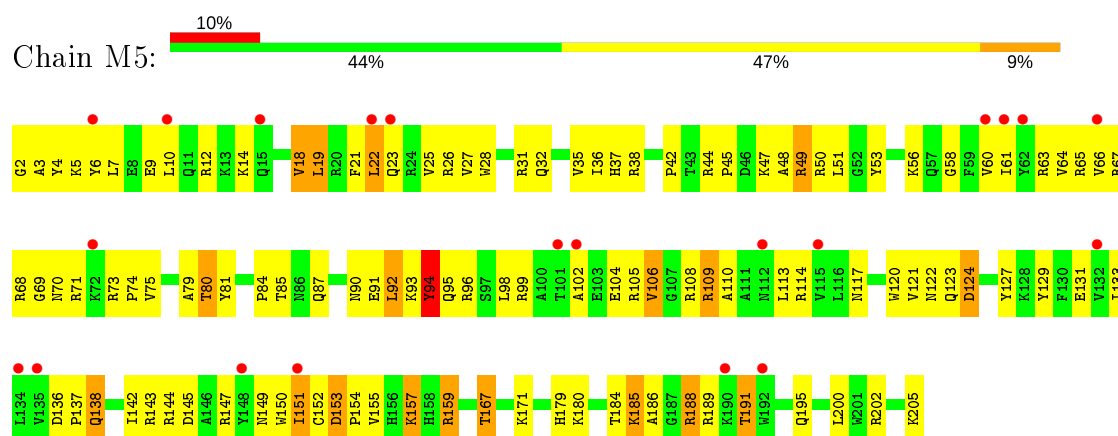


- Molecule 50: 60S ribosomal protein L14-A

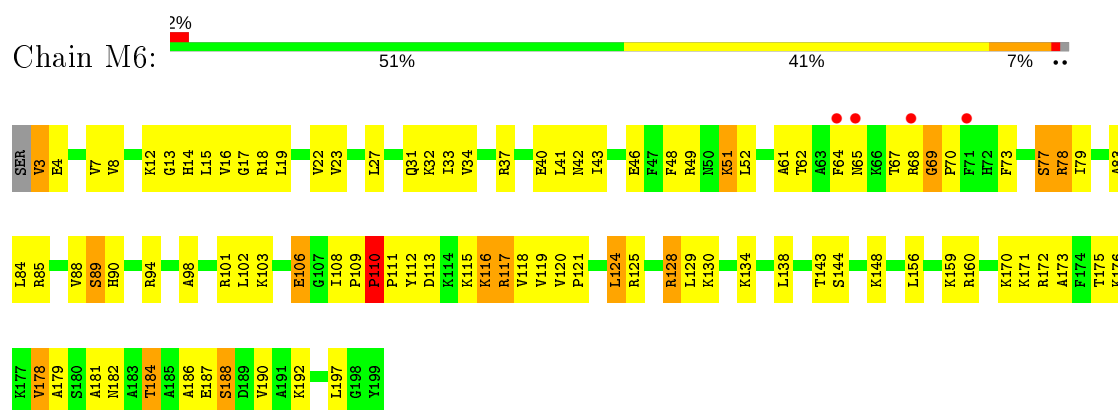




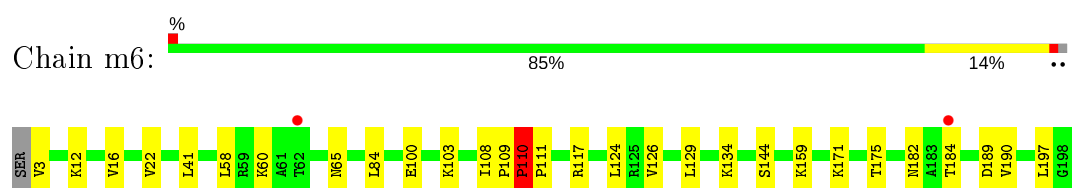
- Molecule 51: 60S ribosomal protein L15-A



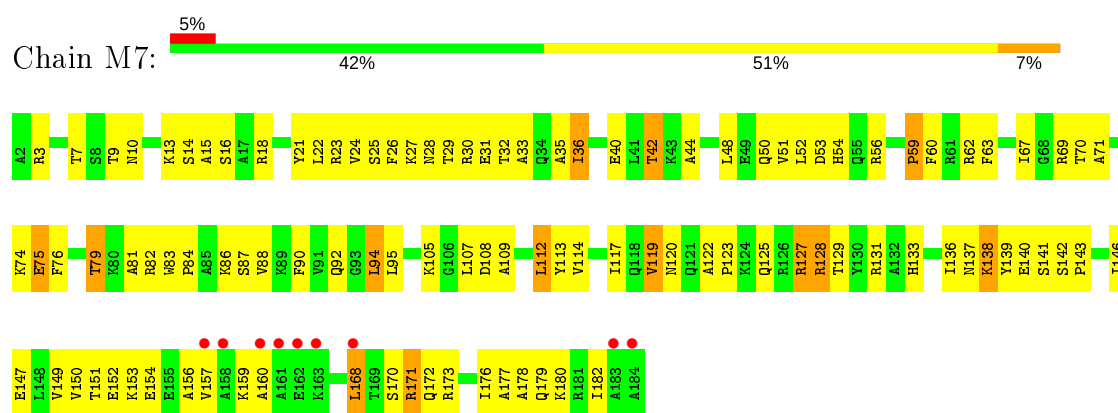
- Molecule 52: 60S ribosomal protein L16-A



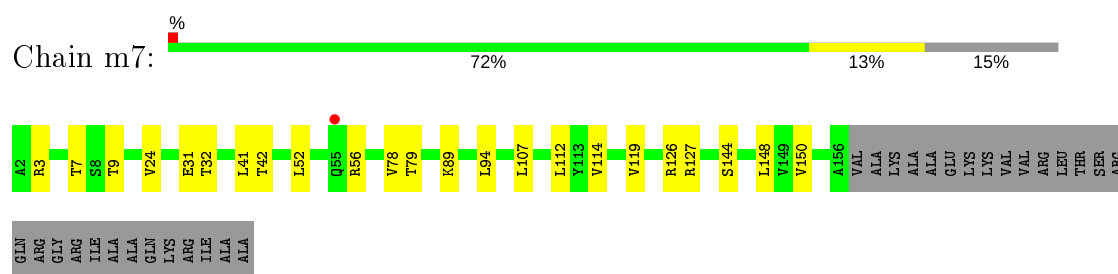
- Molecule 52: 60S ribosomal protein L16-A



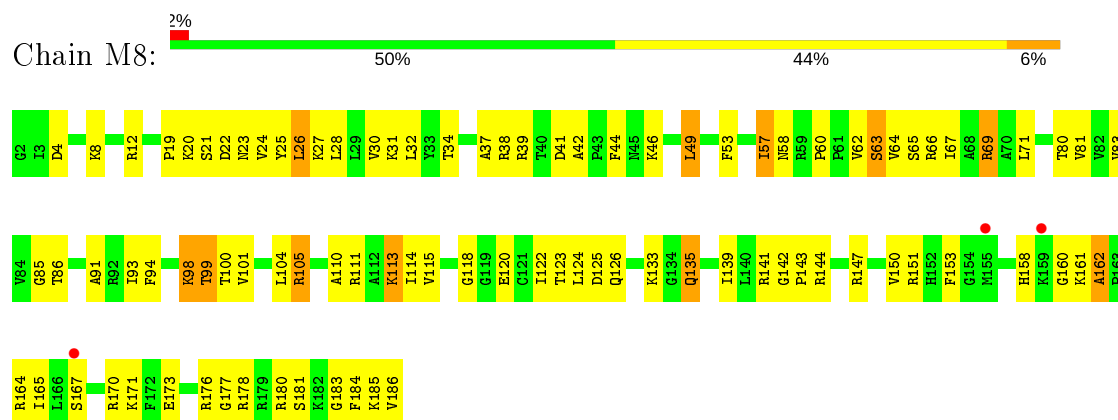
- Molecule 53: 60S ribosomal protein L17-A



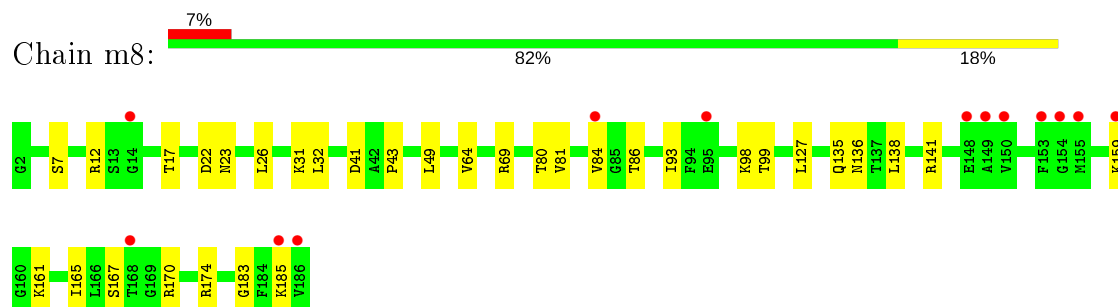
- Molecule 53: 60S ribosomal protein L17-A



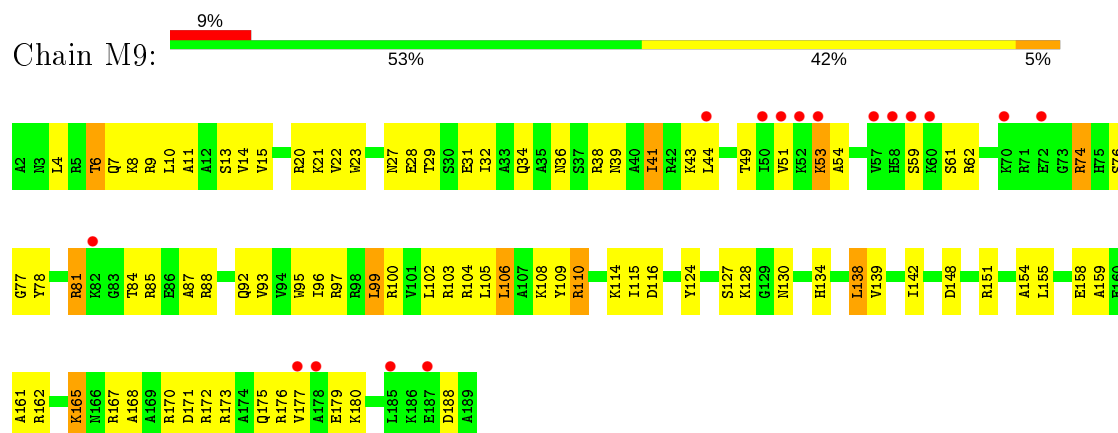
- Molecule 54: 60S ribosomal protein L18-A



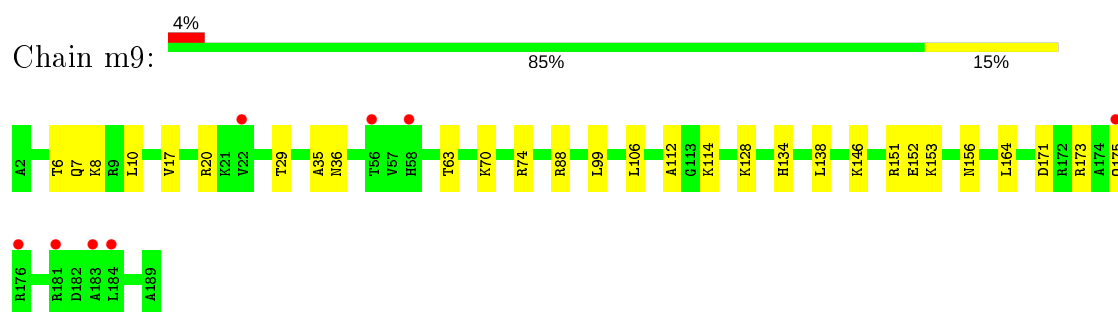
- Molecule 54: 60S ribosomal protein L18-A



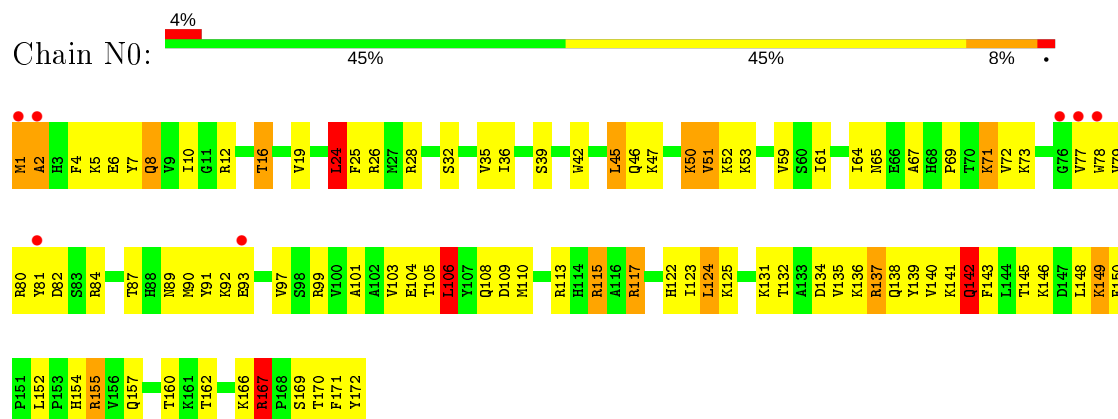
- Molecule 55: 60S ribosomal protein L19-A



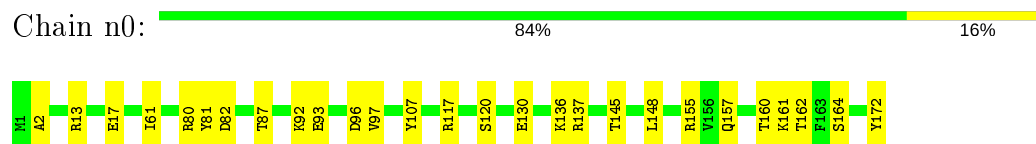
- Molecule 55: 60S ribosomal protein L19-A



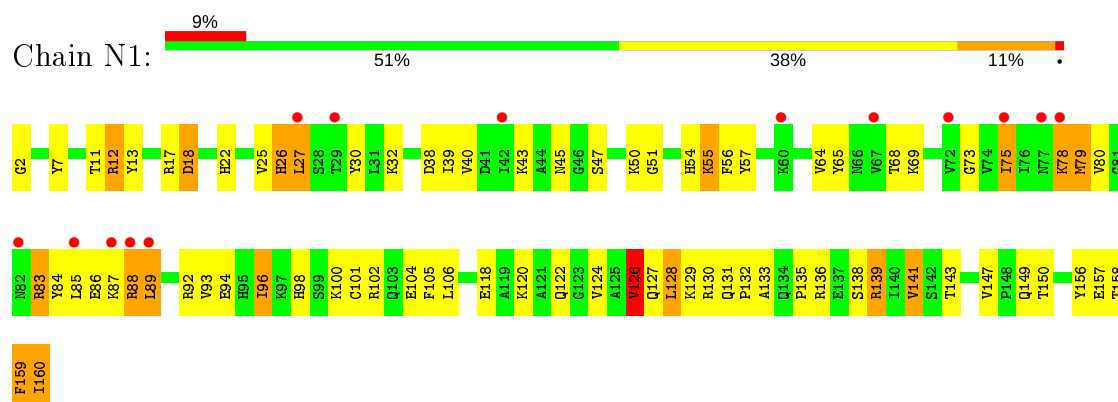
- Molecule 56: 60S ribosomal protein L20-A



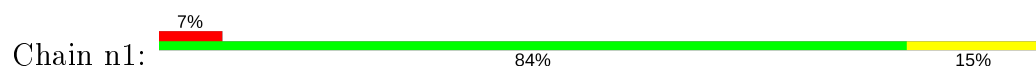
- Molecule 56: 60S ribosomal protein L20-A

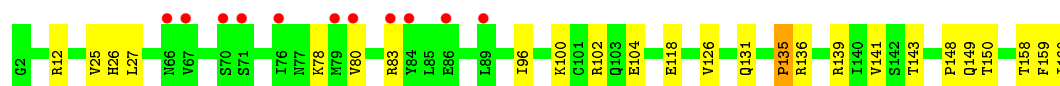


- Molecule 57: 60S ribosomal protein L21-A



- Molecule 57: 60S ribosomal protein L21-A

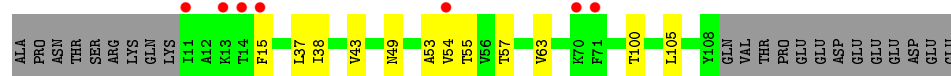
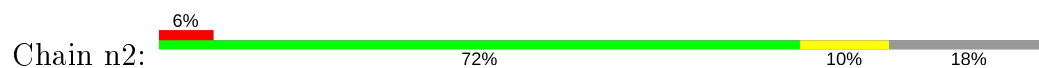




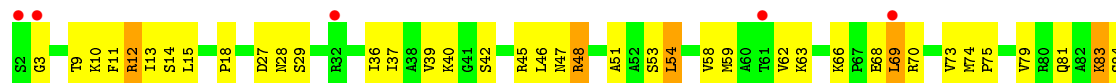
- Molecule 58: 60S ribosomal protein L22-A



- Molecule 58: 60S ribosomal protein L22-A



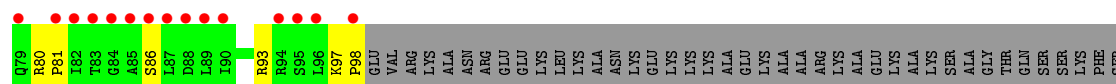
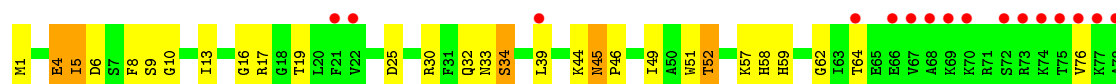
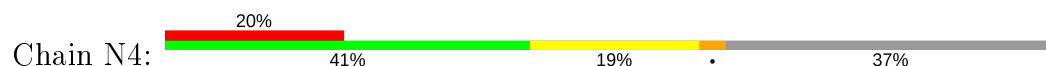
- Molecule 59: 60S ribosomal protein L23-A



- Molecule 59: 60S ribosomal protein L23-A



- Molecule 60: 60S ribosomal protein L24-A



LYS  
GLN  
GLN  
ALA  
GLY  
GLY  
ALA  
PHE  
GLN  
LYS  
VAL  
ALA  
ALA  
THR  
SER  
ARG

• Molecule 60: 60S ribosomal protein L24-A

Chain n4: 9% 77% 10% 13%

M1 I5 T19 D25 S26 L39 Q42 L54 I63 T64 E65 E66 E67 A68 K69 S72 V76 A85 S95 L96 K97 K98 P98 V100 R101 K102 R105 E106 G132 T133 Q134 S135

ALA  
ALA  
THR  
SER  
ARG

• Molecule 61: 60S ribosomal protein L25

Chain N5: 3% 31% 44% 11% 14%

ALA PRO SER ALA LYS THR ALA LYS LYS LYS VAL VAL VAL LYS GLY THR ASN GLY LYS K22 A23 L24 K25 V26 R27 T28 T31 F32 R33 L34 F35 K36 T37 L38 K39 L40 A41 R42 K45 Y46 A47 S48 A50 V51 P52 H53 Y54 R55 L57 D58 S59 I63 E64 Q65

P66 I67 T68 S69 E70 T71 A72 K73 R74 K75 V76 R80 T81 L82 W83 F84 Q85 V86 K92 Y93 Q94 I95 K100 E101 L102 Y103 E104 V105 D106 Y107 L108 K109 V110 R111 T112 L113 V114 R115 P116 M117 G118 T119 K120 K121 A122 Y123 V124 R125 L126 D129 Y130 D131 A132 L133 D134 I135

A136 N137 N138 I139 I142

• Molecule 61: 60S ribosomal protein L25

Chain n5: 2% 65% 19% 15%

ALA PRO SER ALA LYS THR ALA LYS LYS LYS VAL VAL VAL LYS GLY THR ASN GLY LYS LYS A23 L24 K25 V26 R27 T28 S29 R33 K36 T37 L38 K39 L40 P44 K46 Y46 A47 S48 M50 R56 L57 I63 E64 Q65 T71 K89 L102 D106 V107 L108

R115 R125 I135 A136 N137 N138 I142


• Molecule 62: 60S ribosomal protein L26-A

Chain N6: 3% 39% 49% 10%

A2 K3 Q4 S5 L6 D7 V8 S9 S10 D11 R12 R13 R16 Y19 F20 F21 T21 A22 P23 Q26 R27 R28 V29 L30 K37 E38 L39 R40 A41 Q42 Y43 G44 I45 L48 P49 I50 R51 R52 D53 D54 E55 V56 L57 V58 V59 R60 K69 I70 V73 Y74 R75 L76 K77 F78

A79 W80 Q81 W82 D83 T86 R87 E88 R89 R90 R91 G92 V95 P96 I97 N98 L99 H100 P101 S102 K103 L104 V105 I106 T107 K108 L109 D112 K113 L114 R115 K116 A117 L118 L119 Q120 K121 K122 G123 G124 K125 L126 E127

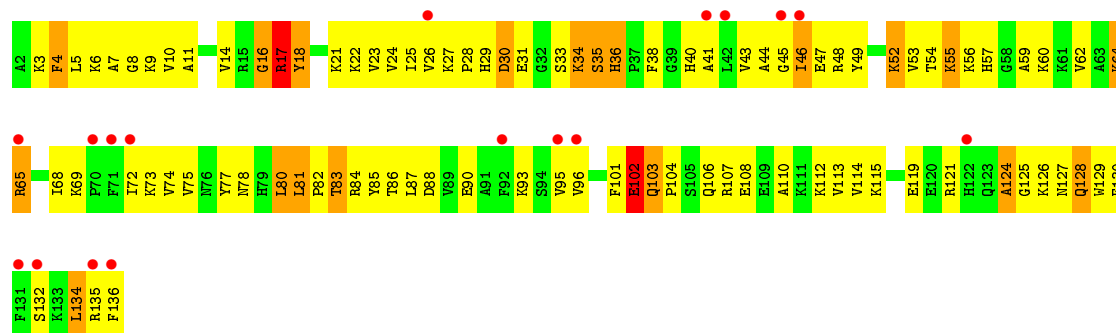
• Molecule 62: 60S ribosomal protein L26-A

Chain n6:  82% 18%




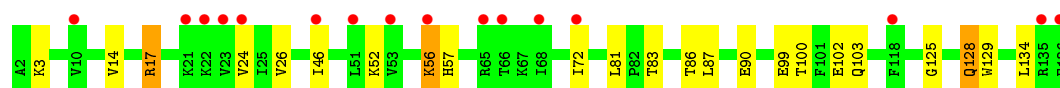
- Molecule 63: 60S ribosomal protein L27-A

Chain N7:  13% 30% 55% 14%



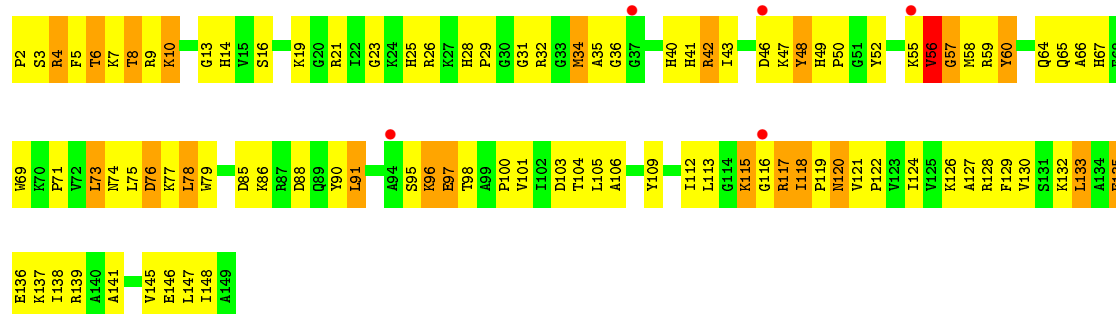
- Molecule 63: 60S ribosomal protein L27-A

Chain n7:  12% 83% 15%




- Molecule 64: 60S ribosomal protein L28

Chain N8:  3% 34% 51% 14%

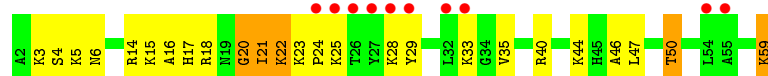


- Molecule 64: 60S ribosomal protein L28

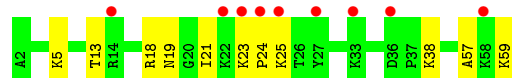
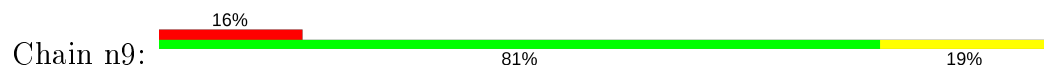
Chain n8:  5% 82% 17%



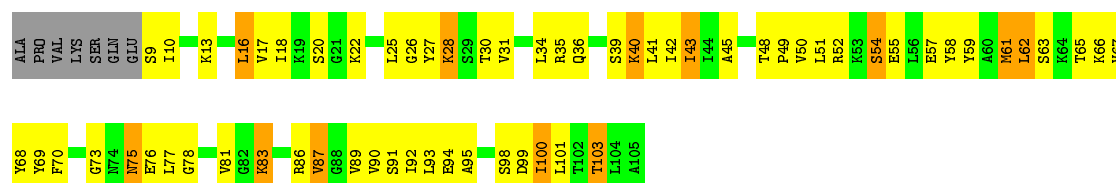
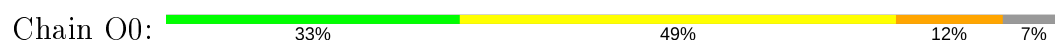
- Molecule 65: 60S ribosomal protein L29



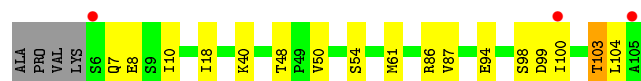
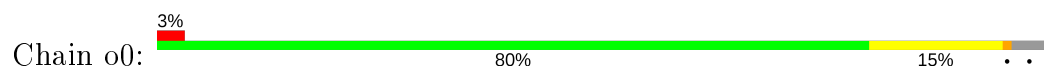
- Molecule 65: 60S ribosomal protein L29



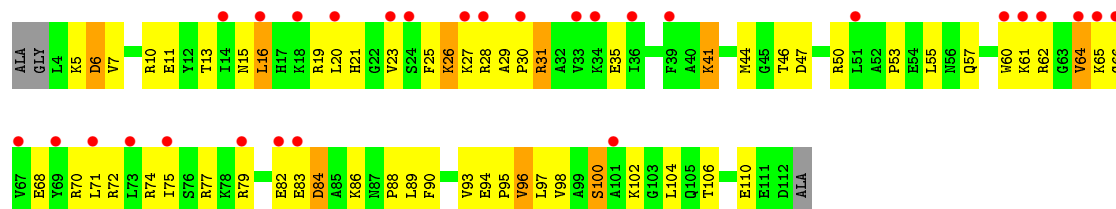
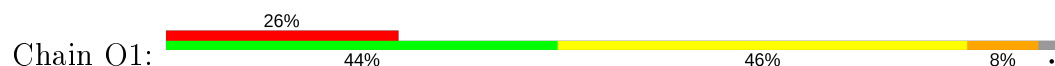
- Molecule 66: 60S ribosomal protein L30



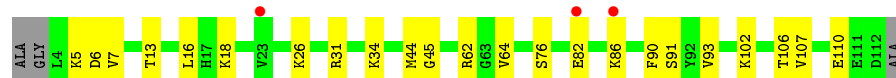
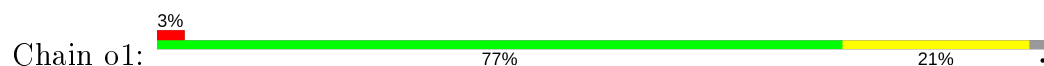
- Molecule 66: 60S ribosomal protein L30



- Molecule 67: 60S ribosomal protein L31-A

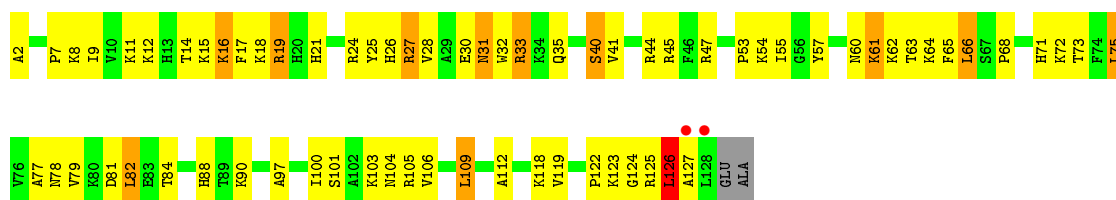


- Molecule 67: 60S ribosomal protein L31-A




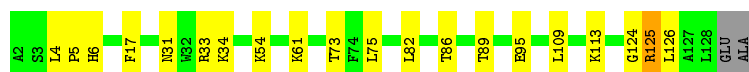
- Molecule 68: 60S ribosomal protein L32

Chain O2: 



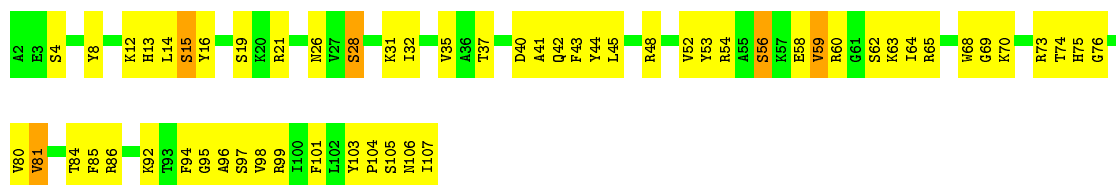
- Molecule 68: 60S ribosomal protein L32

Chain o2: 




- Molecule 69: 60S ribosomal protein L33-A

Chain O3: 




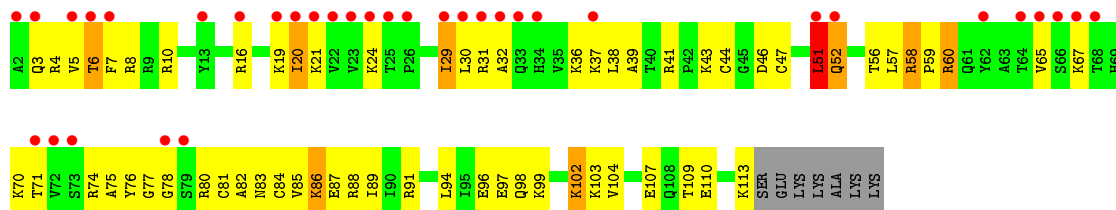
- Molecule 69: 60S ribosomal protein L33-A

Chain o3: 




- Molecule 70: 60S ribosomal protein L34-A (eL34)

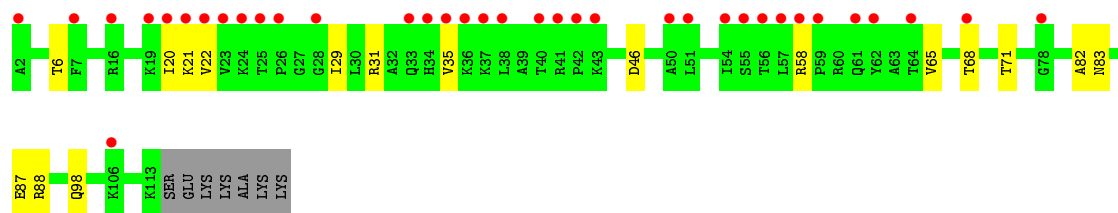
Chain O4: 



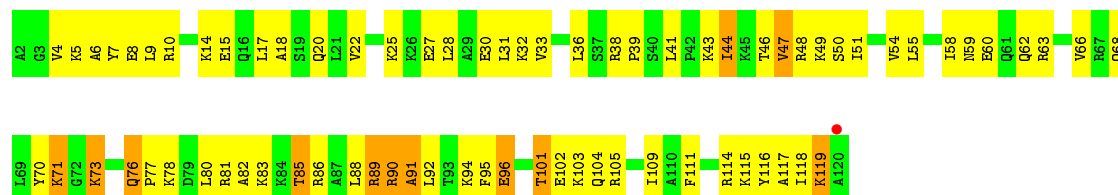
- Molecule 70: 60S ribosomal protein L34-A (eL34)

Chain o4: 

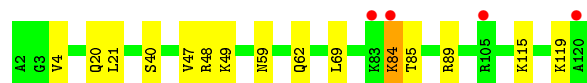
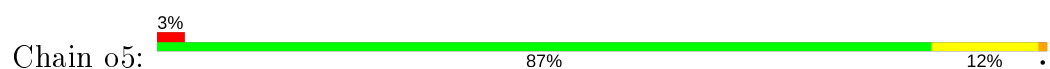




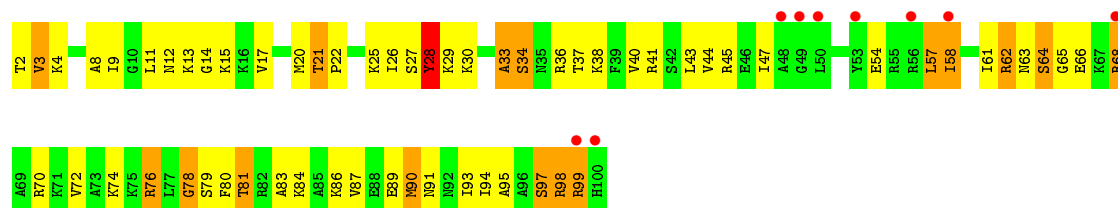
- Molecule 71: 60S ribosomal protein L35-A



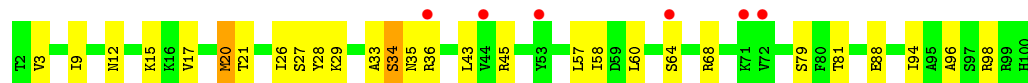
- Molecule 71: 60S ribosomal protein L35-A



- Molecule 72: 60S ribosomal protein L36-A

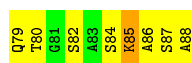


- Molecule 72: 60S ribosomal protein L36-A

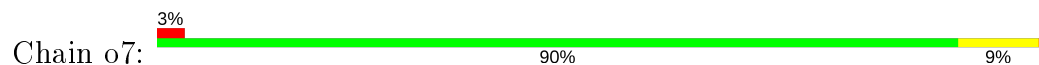


- Molecule 73: 60S ribosomal protein L37-A

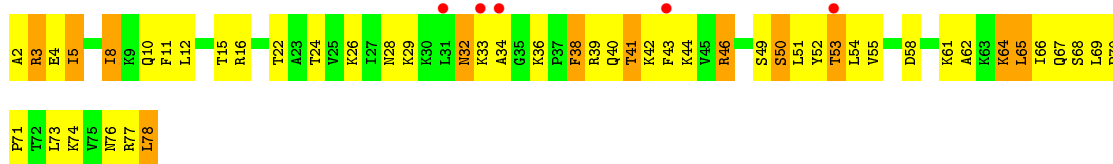




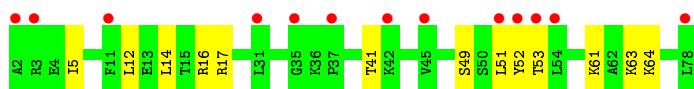
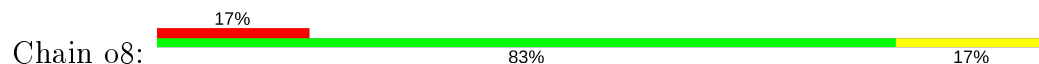
- Molecule 73: 60S ribosomal protein L37-A



- Molecule 74: 60S ribosomal protein L38



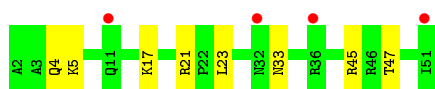
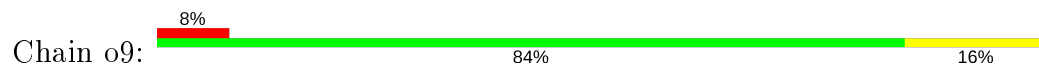
- Molecule 74: 60S ribosomal protein L38



- Molecule 75: 60S ribosomal protein L39




- Molecule 75: 60S ribosomal protein L39



- Molecule 76: Ubiquitin-60S ribosomal protein L40



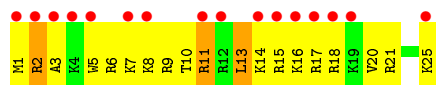
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:  85% 13% .



- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:  24% 64% 12%



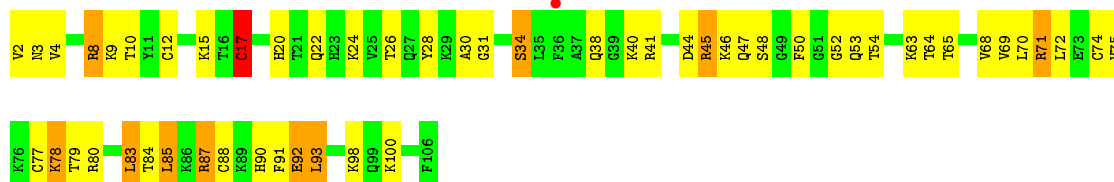
- Molecule 77: 60S ribosomal protein L41-A

Chain q1:  12% 68% 32%




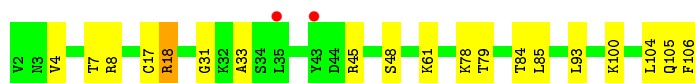
- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:  49% 41% 10%



- Molecule 78: 60S ribosomal protein L42-A

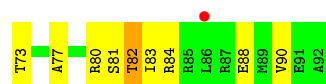
Chain q2:  2% 82% 17%



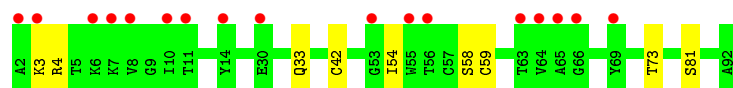
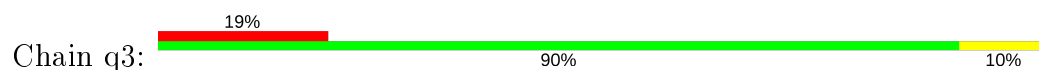
- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:  7% 44% 47% 9%

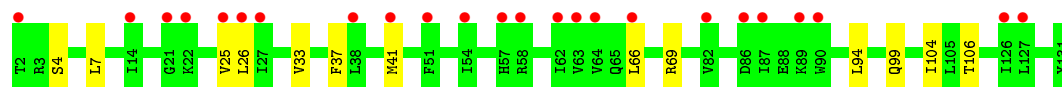
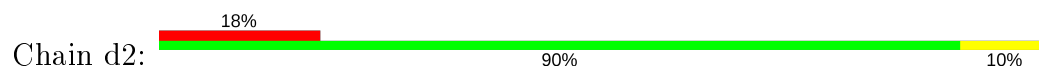




- Molecule 79: 60S ribosomal protein L43-A



- Molecule 80: 40S ribosomal protein S22-A

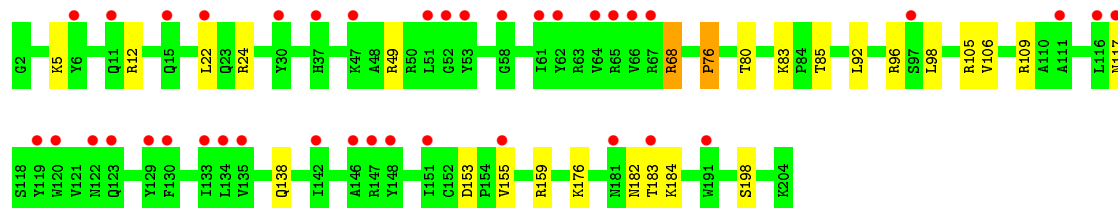
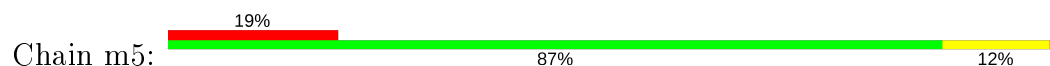


- Molecule 81: 60S ribosomal protein L12-A (uL11)

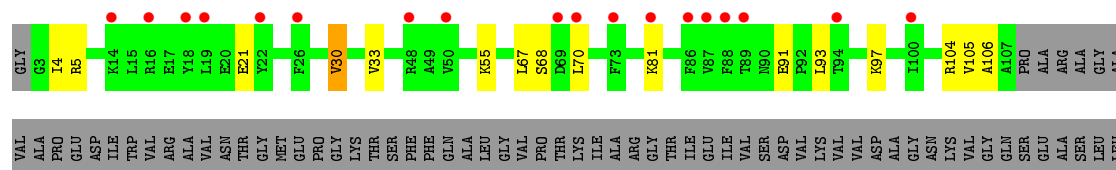


There are no outlier residues recorded for this chain.

- Molecule 82: 60S ribosomal protein L15-A



- Molecule 83: 60S acidic ribosomal protein P0



- Molecule 84: 60S ribosomal protein P1 alpha/P2 beta

Chain p1:  100%

There are no outlier residues recorded for this chain.

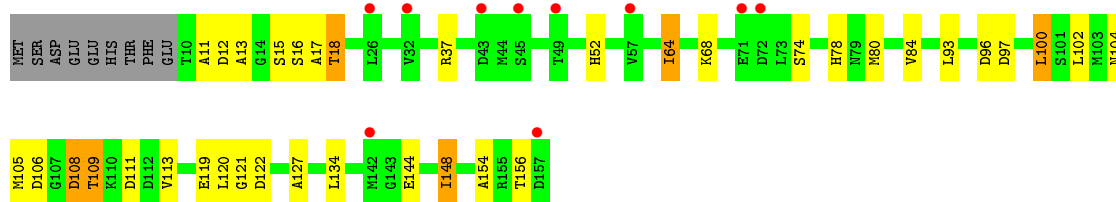
- Molecule 84: 60S ribosomal protein P1 alpha/P2 beta

Chain p2:  98%



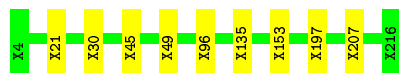
- Molecule 85: Eukaryotic translation initiation factor 5A-1

Chain f:  6% 71% 20% 6%



- Molecule 86: 60S ribosomal protein L1-A (uL1)

Chain l1:  96%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	435.63Å 286.45Å 303.41Å 90.00° 98.85° 90.00°	Depositor
Resolution (Å)	189.16 – 3.15 194.90 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (189.16-3.15) 99.8 (194.90-3.15)	Depositor EDS
$R_{merge}$	0.98	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.204 , 0.252 0.207 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.9	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 69.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	414393	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 5CT, OHX, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	2	0.43	0/42467	0.94	50/66169 (0.1%)
1	6	0.50	0/42790	0.98	58/66673 (0.1%)
2	S0	0.30	0/1617	0.51	0/2215
2	s0	0.33	0/1623	0.56	0/2222
3	S1	0.28	0/1735	0.52	0/2335
3	s1	0.35	0/1748	0.55	0/2352
4	S2	0.33	0/1665	0.53	0/2263
4	s2	0.38	0/1665	0.61	0/2263
5	S3	0.32	0/1759	0.52	0/2368
5	s3	0.31	0/1759	0.49	0/2368
6	S4	0.32	0/2109	0.56	0/2839
6	s4	0.36	0/2109	0.58	0/2839
7	S5	0.29	0/1629	0.51	0/2202
7	s5	0.30	0/1629	0.51	0/2202
8	S6	0.34	0/1823	0.50	0/2439
8	s6	0.37	0/1779	0.55	0/2379
9	S7	0.31	0/1506	0.54	0/2028
9	s7	0.32	0/1516	0.56	0/2043
10	S8	0.35	0/1514	0.53	0/2021
10	s8	0.38	0/1514	0.54	0/2021
11	S9	0.31	0/1519	0.52	0/2035
11	s9	0.36	0/1519	0.52	0/2035
12	C0	0.31	0/789	0.53	1/1067 (0.1%)
12	c0	0.29	0/776	0.58	3/1047 (0.3%)
13	C1	0.36	0/1239	0.53	0/1673
13	c1	0.40	0/1194	0.55	0/1610
14	C2	0.29	0/898	0.52	1/1220 (0.1%)
14	c2	0.26	0/898	0.50	0/1220
15	C3	0.34	0/1215	0.55	0/1638
15	c3	0.37	0/1215	0.52	0/1638
16	C4	0.28	0/901	0.55	0/1217
16	c4	0.34	0/960	0.58	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	C5	0.32	0/998	0.56	0/1341
17	c5	0.36	0/1060	0.56	1/1426 (0.1%)
18	C6	0.32	0/1125	0.58	1/1510 (0.1%)
18	c6	0.34	0/1131	0.55	0/1518
19	C7	0.35	0/935	0.55	0/1254
19	c7	0.32	0/914	0.52	0/1224
20	C8	0.32	0/1211	0.54	0/1628
20	c8	0.34	0/1211	0.53	0/1628
21	C9	0.32	0/1130	0.52	0/1517
21	c9	0.31	0/1130	0.52	0/1517
22	D0	0.33	0/865	0.53	0/1169
22	d0	0.33	0/892	0.53	0/1205
23	D1	0.32	0/693	0.51	0/935
23	d1	0.36	0/693	0.55	0/935
24	D2	0.33	0/1038	0.60	1/1395 (0.1%)
25	D3	0.39	0/1139	0.58	0/1518
25	d3	0.42	0/1139	0.60	0/1518
26	D4	0.34	0/1087	0.50	0/1449
26	d4	0.36	0/1087	0.57	0/1449
27	D5	0.28	0/571	0.52	0/768
27	d5	0.29	0/566	0.52	0/761
28	D6	0.34	0/782	0.58	0/1047
28	d6	0.42	0/782	0.57	0/1047
29	D7	0.31	0/620	0.52	0/838
29	d7	0.32	0/620	0.54	0/838
30	D8	0.28	0/499	0.49	0/670
30	d8	0.32	0/499	0.53	0/670
31	D9	0.33	0/452	0.57	1/600 (0.2%)
31	d9	0.36	0/452	0.53	0/600
32	E0	0.29	0/483	0.49	0/643
32	e0	0.37	0/499	0.61	0/665
33	E1	0.32	0/577	0.60	0/770
33	e1	0.32	0/619	0.61	0/822
34	SR	0.29	0/2490	0.50	0/3389
34	sR	0.28	0/2495	0.48	0/3395
35	SM	0.35	0/1113	0.58	2/1502 (0.1%)
35	sM	0.37	0/682	0.52	0/921
36	1	0.66	11/75394 (0.0%)	1.10	227/117545 (0.2%)
36	5	0.69	7/75865 (0.0%)	1.12	209/118275 (0.2%)
37	3	0.55	0/2883	0.97	2/4491 (0.0%)
37	7	0.67	1/2883 (0.0%)	1.08	6/4491 (0.1%)
38	4	0.61	0/3746	1.06	2/5832 (0.0%)
38	8	0.61	0/3746	1.04	3/5832 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	L2	0.43	0/1948	0.62	0/2617
39	l2	0.46	0/1946	0.65	1/2614 (0.0%)
40	L3	0.46	0/3146	0.61	0/4228
40	l3	0.51	0/3146	0.63	0/4228
41	L4	0.47	0/2800	0.67	2/3790 (0.1%)
41	l4	0.47	1/2800 (0.0%)	0.66	2/3790 (0.1%)
42	L5	0.39	0/2425	0.57	0/3271
42	l5	0.46	0/2408	0.59	0/3248
43	L6	0.45	0/1260	0.58	0/1694
43	l6	0.49	0/1269	0.61	0/1705
44	L7	0.48	0/1821	0.63	0/2451
44	l7	0.51	0/1828	0.66	2/2461 (0.1%)
45	L8	0.37	0/1836	0.56	0/2481
45	l8	0.36	0/1795	0.55	0/2429
46	L9	0.45	0/1539	0.60	0/2073
46	l9	0.49	0/1539	0.62	0/2073
47	M0	0.48	0/1741	0.62	1/2335 (0.0%)
47	m0	0.50	0/1758	0.69	2/2358 (0.1%)
48	M1	0.36	0/1374	0.57	1/1842 (0.1%)
48	m1	0.43	0/1374	0.60	0/1842
49	M3	0.44	0/1568	0.59	0/2106
49	m3	0.44	0/1573	0.63	0/2113
50	M4	0.46	0/1068	0.58	0/1438
50	m4	0.48	0/1074	0.59	0/1446
51	M5	0.47	0/1755	0.64	0/2350
52	M6	0.53	0/1585	0.65	1/2128 (0.0%)
52	m6	0.60	0/1585	0.69	1/2128 (0.0%)
53	M7	0.48	0/1443	0.61	0/1944
53	m7	0.57	0/1250	0.65	0/1683
54	M8	0.45	0/1465	0.64	0/1965
54	m8	0.47	0/1465	0.66	0/1965
55	M9	0.33	0/1538	0.50	0/2050
55	m9	0.41	0/1538	0.53	0/2050
56	N0	0.47	0/1481	0.65	2/1990 (0.1%)
56	n0	0.52	0/1481	0.64	0/1990
57	N1	0.46	0/1300	0.58	0/1743
57	n1	0.51	0/1300	0.59	0/1743
58	N2	0.31	0/812	0.52	0/1099
58	n2	0.37	0/794	0.57	0/1076
59	N3	0.47	0/1018	0.61	0/1369
59	n3	0.53	0/1018	0.64	0/1369
60	N4	0.37	0/712	0.52	0/958
60	n4	0.42	0/1052	0.55	0/1398

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
61	N5	0.43	0/979	0.60	0/1321
61	n5	0.43	0/974	0.60	0/1314
62	N6	0.47	0/1004	0.67	2/1341 (0.1%)
62	n6	0.43	0/1004	0.63	0/1341
63	N7	0.35	0/1118	0.56	0/1497
63	n7	0.35	0/1118	0.53	0/1497
64	N8	0.46	0/1204	0.66	0/1612
64	n8	0.49	0/1204	0.67	0/1612
65	N9	0.44	0/473	0.58	0/629
65	n9	0.50	0/473	0.69	0/629
66	O0	0.32	0/751	0.51	0/1008
66	o0	0.34	0/775	0.52	0/1040
67	O1	0.43	0/890	0.54	0/1196
67	o1	0.47	0/897	0.65	0/1205
68	O2	0.50	0/1041	0.63	0/1394
68	o2	0.54	0/1041	0.65	0/1394
69	O3	0.52	0/868	0.61	0/1168
69	o3	0.55	0/868	0.65	0/1168
70	O4	0.38	0/890	0.57	1/1189 (0.1%)
70	o4	0.41	0/890	0.60	0/1189
71	O5	0.44	0/978	0.61	0/1301
71	o5	0.39	0/974	0.56	0/1297
72	O6	0.41	0/778	0.61	0/1034
72	o6	0.42	0/777	0.59	0/1033
73	O7	0.48	0/696	0.68	0/923
73	o7	0.47	0/696	0.70	1/923 (0.1%)
74	O8	0.36	0/618	0.53	0/826
74	o8	0.36	0/614	0.56	0/822
75	O9	0.48	0/443	0.69	0/588
75	o9	0.52	0/443	0.62	0/588
76	Q0	0.45	0/423	0.66	0/562
76	q0	0.52	0/423	0.64	0/562
77	Q1	0.40	0/234	0.67	0/300
77	q1	0.51	0/234	0.66	0/300
78	Q2	0.58	1/860 (0.1%)	0.64	0/1136
78	q2	0.63	1/860 (0.1%)	0.70	1/1136 (0.1%)
79	Q3	0.42	0/701	0.59	0/934
79	q3	0.49	0/701	0.60	0/934
80	d2	0.37	0/1035	0.62	1/1388 (0.1%)
82	m5	0.43	0/1757	0.60	0/2354
83	p0	0.30	0/1092	0.48	0/1474
85	f	0.40	0/1121	0.64	0/1508
All	All	0.53	22/432423 (0.0%)	0.91	589/634777 (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
12	c0	0	1
16	c4	0	1
18	c6	0	1
19	C7	0	1
20	C8	0	1
27	D5	0	1
28	D6	0	2
44	L7	0	1
44	l7	0	1
52	M6	0	2
52	m6	0	1
64	n8	0	2
65	N9	0	1
85	f	1	0
86	l1	0	13
All	All	1	29

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	q2	17	CYS	CB-SG	11.44	2.01	1.82
78	Q2	17	CYS	CB-SG	10.39	2.00	1.82
36	1	2954	U	C2-N3	9.03	1.44	1.37
36	5	1152	G	N9-C4	-8.08	1.31	1.38
36	1	2808	A	N3-C4	7.52	1.39	1.34

The worst 5 of 589 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-16.35	116.19	126.00
36	5	1152	G	N3-C4-C5	16.30	136.75	128.60
36	5	1152	G	C2-N3-C4	-13.10	105.35	111.90
36	5	2199	G	N1-C6-O6	12.73	127.54	119.90
36	5	2403	G	N1-C6-O6	10.83	126.40	119.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
85	f	51	5CT	C2

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	C7	85	VAL	Peptide
20	C8	81	ILE	Peptide
27	D5	94	LYS	Peptide
28	D6	10	ARG	Peptide
28	D6	97	PRO	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37970	0	19106	944	0
1	6	38260	0	19251	794	0
2	S0	1577	0	1567	152	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	125	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	140	0
4	s2	1635	0	1723	0	0
5	S3	1734	0	1816	107	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	160	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	140	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	108	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	112	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	107	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	134	0
11	s9	1494	0	1573	0	0
12	C0	772	0	727	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	c0	761	0	697	0	0
13	C1	1213	0	1257	61	0
13	c1	1168	0	1233	0	0
14	C2	890	0	887	67	0
14	c2	890	0	887	0	0
15	C3	1192	0	1255	82	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	69	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	89	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	93	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	90	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	111	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	94	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	79	0
22	d0	882	0	939	0	0
23	D1	684	0	672	69	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	62	0
25	D3	1121	0	1196	76	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	95	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	38	0
27	d5	558	0	598	0	0
28	D6	769	0	814	86	0
28	d6	769	0	814	0	0
29	D7	610	0	630	42	0
29	d7	610	0	631	0	0
30	D8	497	0	535	42	0
30	d8	497	0	535	0	0
31	D9	442	0	427	35	0
31	d9	442	0	428	0	0
32	E0	475	0	525	39	0
32	e0	491	0	542	0	0
33	E1	566	0	602	58	0
33	e1	608	0	657	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	SR	2437	0	2386	146	0
34	sR	2442	0	2392	0	0
35	SM	1104	0	1002	65	0
35	sM	679	0	615	0	0
36	1	67355	0	33847	1247	0
36	5	67780	0	34064	1259	0
37	3	2579	0	1304	46	0
37	7	2579	0	1304	37	0
38	4	3353	0	1695	65	0
38	8	3353	0	1695	64	0
39	L2	1914	0	1981	125	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	193	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	206	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	165	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	77	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	112	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	112	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	133	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1736	136	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	86	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	122	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	69	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1778	113	0
52	M6	1555	0	1659	97	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	93	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	87	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	m9	1521	0	1617	0	0
56	N0	1445	0	1486	93	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	90	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	38	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	53	0
59	n3	1003	0	1047	0	0
60	N4	699	0	640	27	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	75	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	65	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	97	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	111	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	30	0
65	n9	462	0	491	0	0
66	O0	743	0	797	54	0
66	o0	767	0	816	0	0
67	O1	876	0	912	44	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	65	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	49	0
69	o3	850	0	880	0	0
70	O4	880	0	945	69	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	68	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	73	0
72	o6	770	0	846	0	0
73	O7	681	0	683	44	0
73	o7	681	0	683	0	0
74	O8	612	0	682	50	0
74	o8	608	0	671	0	0
75	O9	436	0	475	53	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
76	q0	417	0	455	0	0
77	Q1	233	0	284	23	0
77	q1	233	0	284	0	0
78	Q2	847	0	914	54	0
78	q2	847	0	914	0	0
79	Q3	694	0	734	41	0
79	q3	694	0	734	0	0
80	d2	1021	0	1057	0	0
81	m2	750	0	178	0	0
82	m5	1720	0	1779	0	0
83	p0	1077	0	1041	0	0
84	p1	235	0	53	0	0
84	p2	230	0	53	0	0
85	f	1122	0	1115	0	0
86	l1	1063	0	203	0	0
87	1	362	0	0	0	0
87	2	96	0	0	0	0
87	3	9	0	0	0	0
87	4	20	0	0	0	0
87	5	400	0	0	0	0
87	6	115	0	0	0	0
87	7	16	0	0	0	0
87	8	12	0	0	0	0
87	D4	1	0	0	0	0
87	D9	1	0	0	0	0
87	L2	2	0	0	0	0
87	L3	3	0	0	0	0
87	L6	1	0	0	0	0
87	L7	3	0	0	0	0
87	M0	1	0	0	0	0
87	M3	2	0	0	0	0
87	M6	1	0	0	0	0
87	M7	3	0	0	0	0
87	M8	1	0	0	0	0
87	N0	1	0	0	0	0
87	N3	3	0	0	0	0
87	N6	1	0	0	0	0
87	N8	4	0	0	0	0
87	N9	1	0	0	0	0
87	O2	1	0	0	0	0
87	O3	2	0	0	0	0
87	O4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	O7	3	0	0	0	0
87	Q0	1	0	0	0	0
87	Q2	1	0	0	0	0
87	S4	1	0	0	0	0
87	S9	1	0	0	0	0
87	SM	1	0	0	0	0
87	c7	1	0	0	0	0
87	d2	1	0	0	0	0
87	d3	1	0	0	0	0
87	d6	1	0	0	0	0
87	f	3	0	0	0	0
87	l2	3	0	0	0	0
87	l3	1	0	0	0	0
87	l5	1	0	0	0	0
87	l7	1	0	0	0	0
87	m0	1	0	0	0	0
87	m3	1	0	0	0	0
87	m6	2	0	0	0	0
87	m7	3	0	0	0	0
87	n0	2	0	0	0	0
87	n3	1	0	0	0	0
87	n6	1	0	0	0	0
87	n8	3	0	0	0	0
87	n9	2	0	0	0	0
87	o2	2	0	0	0	0
87	o4	1	0	0	0	0
87	o9	1	0	0	0	0
87	q0	1	0	0	0	0
87	q1	1	0	0	0	0
87	s8	1	0	0	0	0
87	sM	1	0	0	0	0
88	1	2457	0	0	243	0
88	2	1113	0	0	141	0
88	3	77	0	0	3	0
88	4	112	0	0	9	0
88	5	2562	0	0	262	0
88	6	1211	0	0	121	0
88	7	84	0	0	4	0
88	8	140	0	0	14	0
88	C1	7	0	0	0	0
88	C3	7	0	0	5	0
88	C5	7	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	C8	7	0	0	0	0
88	D9	7	0	0	1	0
88	L3	7	0	0	3	0
88	L4	7	0	0	4	0
88	L5	7	0	0	1	0
88	M0	14	0	0	4	0
88	M5	7	0	0	1	0
88	M7	14	0	0	3	0
88	M8	7	0	0	0	0
88	M9	7	0	0	2	0
88	N1	7	0	0	1	0
88	N8	7	0	0	0	0
88	N9	7	0	0	1	0
88	O3	7	0	0	1	0
88	O7	14	0	0	4	0
88	O9	7	0	0	1	0
88	Q2	7	0	0	1	0
88	S1	7	0	0	3	0
88	S6	7	0	0	3	0
88	S8	7	0	0	2	0
88	S9	7	0	0	1	0
88	SR	7	0	0	3	0
88	c3	7	0	0	0	0
88	c5	7	0	0	0	0
88	c8	7	0	0	0	0
88	l3	21	0	0	0	0
88	l4	14	0	0	0	0
88	l5	14	0	0	0	0
88	l9	7	0	0	0	0
88	m0	21	0	0	0	0
88	m5	7	0	0	0	0
88	m7	7	0	0	0	0
88	m9	7	0	0	0	0
88	n3	7	0	0	0	0
88	n6	7	0	0	0	0
88	n9	7	0	0	0	0
88	o3	7	0	0	0	0
88	o7	7	0	0	0	0
88	o9	7	0	0	0	0
88	q1	7	0	0	0	0
88	q2	7	0	0	0	0
88	s1	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	s4	7	0	0	0	0
88	s8	7	0	0	0	0
88	s9	7	0	0	0	0
88	sR	7	0	0	0	0
89	D6	1	0	0	0	0
89	D7	1	0	0	0	0
89	D9	1	0	0	0	0
89	E1	1	0	0	0	0
89	O7	1	0	0	0	0
89	Q0	1	0	0	0	0
89	Q2	1	0	0	0	0
89	Q3	1	0	0	0	0
89	d6	1	0	0	0	0
89	d7	1	0	0	0	0
89	d9	1	0	0	0	0
89	e1	1	0	0	0	0
89	o7	1	0	0	0	0
89	q0	1	0	0	0	0
89	q2	1	0	0	0	0
89	q3	1	0	0	0	0
90	5	3	0	0	0	0
90	f	9	0	0	0	0
All	All	414393	0	299160	9284	0

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

The worst 5 of 9284 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:Q2:17:CYS:SG	78:Q2:17:CYS:CB	1.99	1.49
40:L3:41:VAL:HA	40:L3:185:GLY:HA3	1.64	1.04
36:1:2820:A:H5''	36:1:2821:C:OP2	1.62	0.99
36:1:1481:A:O2'	36:1:1858:A:N3	1.96	0.97
24:D2:2:THR:N	1:6:1034:C:HO2'	337.95	0.97

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	156 (76%)	29 (14%)	19 (9%)	0	3
2	s0	204/251 (81%)	159 (78%)	28 (14%)	17 (8%)	1	4
3	S1	212/254 (84%)	153 (72%)	34 (16%)	25 (12%)	0	1
3	s1	214/254 (84%)	172 (80%)	29 (14%)	13 (6%)	1	10
4	S2	215/253 (85%)	173 (80%)	33 (15%)	9 (4%)	3	17
4	s2	215/253 (85%)	176 (82%)	31 (14%)	8 (4%)	3	19
5	S3	221/239 (92%)	189 (86%)	24 (11%)	8 (4%)	3	20
5	s3	221/239 (92%)	180 (81%)	30 (14%)	11 (5%)	2	14
6	S4	258/260 (99%)	207 (80%)	35 (14%)	16 (6%)	1	9
6	s4	258/260 (99%)	211 (82%)	30 (12%)	17 (7%)	1	8
7	S5	204/224 (91%)	158 (78%)	32 (16%)	14 (7%)	1	7
7	s5	204/224 (91%)	157 (77%)	29 (14%)	18 (9%)	1	3
8	S6	224/236 (95%)	193 (86%)	22 (10%)	9 (4%)	3	18
8	s6	216/236 (92%)	188 (87%)	19 (9%)	9 (4%)	3	17
9	S7	182/189 (96%)	139 (76%)	28 (15%)	15 (8%)	1	4
9	s7	184/189 (97%)	147 (80%)	20 (11%)	17 (9%)	1	3
10	S8	184/200 (92%)	160 (87%)	16 (9%)	8 (4%)	2	17
10	s8	184/200 (92%)	154 (84%)	21 (11%)	9 (5%)	2	14
11	S9	183/196 (93%)	145 (79%)	28 (15%)	10 (6%)	2	12
11	s9	183/196 (93%)	150 (82%)	23 (13%)	10 (6%)	2	12
12	C0	94/105 (90%)	74 (79%)	13 (14%)	7 (7%)	1	6
12	c0	92/105 (88%)	60 (65%)	17 (18%)	15 (16%)	0	0
13	C1	153/155 (99%)	119 (78%)	27 (18%)	7 (5%)	2	15
13	c1	144/155 (93%)	120 (83%)	19 (13%)	5 (4%)	3	21
14	C2	122/124 (98%)	74 (61%)	33 (27%)	15 (12%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	c2	122/124 (98%)	76 (62%)	33 (27%)	13 (11%)	0	2
15	C3	148/150 (99%)	127 (86%)	17 (12%)	4 (3%)	5	27
15	c3	148/150 (99%)	118 (80%)	23 (16%)	7 (5%)	2	15
16	C4	125/136 (92%)	86 (69%)	25 (20%)	14 (11%)	0	2
16	c4	126/136 (93%)	98 (78%)	17 (14%)	11 (9%)	1	4
17	C5	122/137 (89%)	89 (73%)	20 (16%)	13 (11%)	0	2
17	c5	133/137 (97%)	99 (74%)	20 (15%)	14 (10%)	0	2
18	C6	139/142 (98%)	114 (82%)	13 (9%)	12 (9%)	1	4
18	c6	140/142 (99%)	117 (84%)	14 (10%)	9 (6%)	1	9
19	C7	116/136 (85%)	89 (77%)	16 (14%)	11 (10%)	0	3
19	c7	113/136 (83%)	87 (77%)	21 (19%)	5 (4%)	2	16
20	C8	143/145 (99%)	110 (77%)	24 (17%)	9 (6%)	1	9
20	c8	143/145 (99%)	110 (77%)	26 (18%)	7 (5%)	2	14
21	C9	141/143 (99%)	113 (80%)	22 (16%)	6 (4%)	2	17
21	c9	141/143 (99%)	121 (86%)	14 (10%)	6 (4%)	2	17
22	D0	105/120 (88%)	88 (84%)	15 (14%)	2 (2%)	8	36
22	d0	108/120 (90%)	89 (82%)	13 (12%)	6 (6%)	2	12
23	D1	85/87 (98%)	65 (76%)	14 (16%)	6 (7%)	1	6
23	d1	85/87 (98%)	66 (78%)	13 (15%)	6 (7%)	1	6
24	D2	127/129 (98%)	106 (84%)	18 (14%)	3 (2%)	6	30
25	D3	142/144 (99%)	116 (82%)	15 (11%)	11 (8%)	1	5
25	d3	142/144 (99%)	128 (90%)	12 (8%)	2 (1%)	11	43
26	D4	132/134 (98%)	112 (85%)	11 (8%)	9 (7%)	1	7
26	d4	132/134 (98%)	109 (83%)	14 (11%)	9 (7%)	1	7
27	D5	68/107 (64%)	49 (72%)	12 (18%)	7 (10%)	0	2
27	d5	67/107 (63%)	52 (78%)	12 (18%)	3 (4%)	2	16
28	D6	95/97 (98%)	57 (60%)	21 (22%)	17 (18%)	0	0
28	d6	95/97 (98%)	68 (72%)	19 (20%)	8 (8%)	1	4
29	D7	79/81 (98%)	66 (84%)	5 (6%)	8 (10%)	0	2
29	d7	79/81 (98%)	60 (76%)	18 (23%)	1 (1%)	12	44
30	D8	61/66 (92%)	53 (87%)	6 (10%)	2 (3%)	4	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	d8	61/66 (92%)	45 (74%)	12 (20%)	4 (7%)	1	8
31	D9	51/55 (93%)	41 (80%)	8 (16%)	2 (4%)	3	19
31	d9	51/55 (93%)	40 (78%)	8 (16%)	3 (6%)	1	11
32	E0	58/62 (94%)	43 (74%)	11 (19%)	4 (7%)	1	7
32	e0	60/62 (97%)	45 (75%)	10 (17%)	5 (8%)	1	4
33	E1	69/76 (91%)	35 (51%)	20 (29%)	14 (20%)	0	0
33	e1	74/76 (97%)	40 (54%)	14 (19%)	20 (27%)	0	0
34	SR	316/318 (99%)	263 (83%)	40 (13%)	13 (4%)	3	18
34	sR	316/318 (99%)	257 (81%)	43 (14%)	16 (5%)	2	13
35	SM	155/273 (57%)	107 (69%)	27 (17%)	21 (14%)	0	1
35	sM	98/273 (36%)	60 (61%)	22 (22%)	16 (16%)	0	0
39	L2	250/253 (99%)	221 (88%)	20 (8%)	9 (4%)	3	20
39	l2	250/253 (99%)	216 (86%)	24 (10%)	10 (4%)	3	18
40	L3	384/386 (100%)	329 (86%)	41 (11%)	14 (4%)	3	20
40	l3	384/386 (100%)	344 (90%)	30 (8%)	10 (3%)	5	28
41	L4	359/361 (99%)	303 (84%)	37 (10%)	19 (5%)	2	13
41	l4	359/361 (99%)	301 (84%)	40 (11%)	18 (5%)	2	14
42	L5	294/296 (99%)	239 (81%)	32 (11%)	23 (8%)	1	5
42	l5	292/296 (99%)	263 (90%)	19 (6%)	10 (3%)	3	21
43	L6	152/175 (87%)	132 (87%)	17 (11%)	3 (2%)	7	34
43	l6	153/175 (87%)	134 (88%)	16 (10%)	3 (2%)	7	34
44	L7	220/243 (90%)	199 (90%)	13 (6%)	8 (4%)	3	20
44	l7	221/243 (91%)	208 (94%)	8 (4%)	5 (2%)	6	31
45	L8	231/255 (91%)	188 (81%)	35 (15%)	8 (4%)	3	21
45	l8	229/255 (90%)	186 (81%)	30 (13%)	13 (6%)	1	12
46	L9	189/191 (99%)	161 (85%)	19 (10%)	9 (5%)	2	15
46	l9	189/191 (99%)	168 (89%)	18 (10%)	3 (2%)	9	40
47	M0	207/220 (94%)	172 (83%)	28 (14%)	7 (3%)	3	21
47	m0	209/220 (95%)	173 (83%)	19 (9%)	17 (8%)	1	4
48	M1	167/173 (96%)	125 (75%)	27 (16%)	15 (9%)	1	3
48	m1	167/173 (96%)	142 (85%)	18 (11%)	7 (4%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	M3	191/198 (96%)	161 (84%)	20 (10%)	10 (5%)	2	13
49	m3	192/198 (97%)	155 (81%)	19 (10%)	18 (9%)	0	3
50	M4	134/137 (98%)	119 (89%)	12 (9%)	3 (2%)	6	32
50	m4	135/137 (98%)	125 (93%)	8 (6%)	2 (2%)	10	41
51	M5	199/204 (98%)	174 (87%)	20 (10%)	5 (2%)	5	29
52	M6	195/198 (98%)	173 (89%)	18 (9%)	4 (2%)	7	33
52	m6	195/198 (98%)	177 (91%)	13 (7%)	5 (3%)	5	28
53	M7	181/183 (99%)	156 (86%)	20 (11%)	5 (3%)	5	26
53	m7	153/183 (84%)	139 (91%)	13 (8%)	1 (1%)	22	59
54	M8	183/185 (99%)	165 (90%)	13 (7%)	5 (3%)	5	27
54	m8	183/185 (99%)	157 (86%)	20 (11%)	6 (3%)	4	22
55	M9	186/188 (99%)	160 (86%)	23 (12%)	3 (2%)	9	40
55	m9	186/188 (99%)	167 (90%)	15 (8%)	4 (2%)	6	32
56	N0	170/172 (99%)	154 (91%)	11 (6%)	5 (3%)	4	25
56	n0	170/172 (99%)	158 (93%)	10 (6%)	2 (1%)	13	46
57	N1	157/159 (99%)	141 (90%)	13 (8%)	3 (2%)	8	36
57	n1	157/159 (99%)	130 (83%)	24 (15%)	3 (2%)	8	36
58	N2	98/120 (82%)	74 (76%)	16 (16%)	8 (8%)	1	4
58	n2	96/120 (80%)	79 (82%)	14 (15%)	3 (3%)	4	23
59	N3	134/136 (98%)	120 (90%)	11 (8%)	3 (2%)	6	32
59	n3	134/136 (98%)	124 (92%)	9 (7%)	1 (1%)	22	59
60	N4	96/155 (62%)	72 (75%)	19 (20%)	5 (5%)	2	13
60	n4	133/155 (86%)	108 (81%)	18 (14%)	7 (5%)	2	13
61	N5	119/141 (84%)	107 (90%)	9 (8%)	3 (2%)	5	29
61	n5	118/141 (84%)	99 (84%)	9 (8%)	10 (8%)	1	4
62	N6	124/126 (98%)	108 (87%)	14 (11%)	2 (2%)	9	40
62	n6	124/126 (98%)	110 (89%)	9 (7%)	5 (4%)	3	18
63	N7	133/135 (98%)	103 (77%)	16 (12%)	14 (10%)	0	2
63	n7	133/135 (98%)	103 (77%)	22 (16%)	8 (6%)	1	10
64	N8	146/148 (99%)	121 (83%)	18 (12%)	7 (5%)	2	15
64	n8	146/148 (99%)	121 (83%)	19 (13%)	6 (4%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
65	N9	56/58 (97%)	45 (80%)	9 (16%)	2 (4%)	3	20
65	n9	56/58 (97%)	40 (71%)	11 (20%)	5 (9%)	1	3
66	O0	95/104 (91%)	84 (88%)	11 (12%)	0	100	100
66	o0	98/104 (94%)	84 (86%)	8 (8%)	6 (6%)	1	10
67	O1	107/112 (96%)	96 (90%)	5 (5%)	6 (6%)	2	12
67	o1	107/112 (96%)	82 (77%)	20 (19%)	5 (5%)	2	15
68	O2	125/129 (97%)	113 (90%)	9 (7%)	3 (2%)	6	30
68	o2	125/129 (97%)	109 (87%)	11 (9%)	5 (4%)	3	18
69	O3	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
69	o3	104/106 (98%)	92 (88%)	11 (11%)	1 (1%)	15	51
70	O4	110/119 (92%)	99 (90%)	11 (10%)	0	100	100
70	o4	110/119 (92%)	94 (86%)	15 (14%)	1 (1%)	17	53
71	O5	117/119 (98%)	97 (83%)	18 (15%)	2 (2%)	9	38
71	o5	117/119 (98%)	104 (89%)	10 (8%)	3 (3%)	5	28
72	O6	97/99 (98%)	77 (79%)	11 (11%)	9 (9%)	0	3
72	o6	97/99 (98%)	79 (81%)	10 (10%)	8 (8%)	1	4
73	O7	85/87 (98%)	71 (84%)	12 (14%)	2 (2%)	6	30
73	o7	85/87 (98%)	71 (84%)	13 (15%)	1 (1%)	13	46
74	O8	75/77 (97%)	65 (87%)	8 (11%)	2 (3%)	5	27
74	o8	75/77 (97%)	61 (81%)	11 (15%)	3 (4%)	3	18
75	O9	48/50 (96%)	42 (88%)	5 (10%)	1 (2%)	7	33
75	o9	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
76	Q0	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	7	34
76	q0	50/52 (96%)	44 (88%)	5 (10%)	1 (2%)	7	34
77	Q1	23/25 (92%)	23 (100%)	0	0	100	100
77	q1	23/25 (92%)	21 (91%)	1 (4%)	1 (4%)	2	17
78	Q2	103/105 (98%)	84 (82%)	16 (16%)	3 (3%)	4	25
78	q2	103/105 (98%)	90 (87%)	8 (8%)	5 (5%)	2	14
79	Q3	89/91 (98%)	77 (86%)	9 (10%)	3 (3%)	3	21
79	q3	89/91 (98%)	79 (89%)	9 (10%)	1 (1%)	14	48
80	d2	125/130 (96%)	114 (91%)	10 (8%)	1 (1%)	19	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
82	m5	201/203 (99%)	178 (89%)	19 (10%)	4 (2%)	7	34
83	p0	139/220 (63%)	112 (81%)	20 (14%)	7 (5%)	2	14
85	f	145/157 (92%)	96 (66%)	29 (20%)	20 (14%)	0	1
All	All	22474/24167 (93%)	18605 (83%)	2710 (12%)	1159 (5%)	2	13

5 of 1159 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	158	VAL
2	S0	191	ARG
2	S0	192	THR
2	S0	202	TYR

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/209 (78%)	139 (85%)	25 (15%)	3	12
2	s0	165/209 (79%)	146 (88%)	19 (12%)	5	22
3	S1	191/223 (86%)	167 (87%)	24 (13%)	4	19
3	s1	192/223 (86%)	156 (81%)	36 (19%)	1	7
4	S2	176/204 (86%)	151 (86%)	25 (14%)	3	14
4	s2	176/204 (86%)	140 (80%)	36 (20%)	1	5
5	S3	182/194 (94%)	155 (85%)	27 (15%)	3	13
5	s3	182/194 (94%)	162 (89%)	20 (11%)	6	24
6	S4	221/221 (100%)	190 (86%)	31 (14%)	3	15
6	s4	221/221 (100%)	191 (86%)	30 (14%)	3	16
7	S5	173/190 (91%)	146 (84%)	27 (16%)	2	11
7	s5	173/190 (91%)	150 (87%)	23 (13%)	4	17
8	S6	188/201 (94%)	164 (87%)	24 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	s6	187/201 (93%)	163 (87%)	24 (13%)	4	18
9	S7	165/169 (98%)	141 (86%)	24 (14%)	3	14
9	s7	165/169 (98%)	144 (87%)	21 (13%)	4	19
10	S8	150/161 (93%)	136 (91%)	14 (9%)	9	31
10	s8	150/161 (93%)	128 (85%)	22 (15%)	3	13
11	S9	158/165 (96%)	136 (86%)	22 (14%)	3	15
11	s9	158/165 (96%)	130 (82%)	28 (18%)	2	8
12	C0	77/98 (79%)	69 (90%)	8 (10%)	7	26
12	c0	73/98 (74%)	67 (92%)	6 (8%)	11	38
13	C1	129/136 (95%)	122 (95%)	7 (5%)	22	55
13	c1	129/136 (95%)	107 (83%)	22 (17%)	2	9
14	C2	88/100 (88%)	79 (90%)	9 (10%)	7	27
14	c2	88/100 (88%)	80 (91%)	8 (9%)	9	32
15	C3	127/127 (100%)	107 (84%)	20 (16%)	2	11
15	c3	127/127 (100%)	108 (85%)	19 (15%)	3	13
16	C4	81/104 (78%)	68 (84%)	13 (16%)	2	10
16	c4	97/104 (93%)	83 (86%)	14 (14%)	3	14
17	C5	101/113 (89%)	87 (86%)	14 (14%)	3	15
17	c5	103/113 (91%)	89 (86%)	14 (14%)	3	16
18	C6	117/118 (99%)	101 (86%)	16 (14%)	3	16
18	c6	118/118 (100%)	98 (83%)	20 (17%)	2	9
19	C7	94/124 (76%)	77 (82%)	17 (18%)	1	8
19	c7	92/124 (74%)	81 (88%)	11 (12%)	5	21
20	C8	128/128 (100%)	105 (82%)	23 (18%)	1	8
20	c8	128/128 (100%)	108 (84%)	20 (16%)	2	11
21	C9	115/115 (100%)	101 (88%)	14 (12%)	5	20
21	c9	115/115 (100%)	98 (85%)	17 (15%)	3	13
22	D0	100/113 (88%)	87 (87%)	13 (13%)	4	18
22	d0	103/113 (91%)	86 (84%)	17 (16%)	2	10
23	D1	74/74 (100%)	64 (86%)	10 (14%)	4	17
23	d1	74/74 (100%)	63 (85%)	11 (15%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	D2	110/110 (100%)	92 (84%)	18 (16%)	2	10
25	D3	119/119 (100%)	103 (87%)	16 (13%)	4	17
25	d3	119/119 (100%)	108 (91%)	11 (9%)	9	31
26	D4	112/112 (100%)	101 (90%)	11 (10%)	8	28
26	d4	112/112 (100%)	95 (85%)	17 (15%)	3	12
27	D5	61/88 (69%)	48 (79%)	13 (21%)	1	5
27	d5	61/88 (69%)	53 (87%)	8 (13%)	4	18
28	D6	83/83 (100%)	70 (84%)	13 (16%)	2	11
28	d6	83/83 (100%)	74 (89%)	9 (11%)	6	25
29	D7	70/70 (100%)	64 (91%)	6 (9%)	10	35
29	d7	70/70 (100%)	61 (87%)	9 (13%)	4	18
30	D8	56/59 (95%)	49 (88%)	7 (12%)	4	19
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%)	38 (81%)	9 (19%)	1	7
32	E0	51/53 (96%)	45 (88%)	6 (12%)	5	21
32	e0	53/53 (100%)	44 (83%)	9 (17%)	2	9
33	E1	62/66 (94%)	51 (82%)	11 (18%)	2	8
33	e1	66/66 (100%)	55 (83%)	11 (17%)	2	9
34	SR	259/261 (99%)	239 (92%)	20 (8%)	13	41
34	sR	260/261 (100%)	233 (90%)	27 (10%)	7	26
35	SM	97/228 (42%)	73 (75%)	24 (25%)	0	2
35	sM	54/228 (24%)	48 (89%)	6 (11%)	6	24
39	L2	193/195 (99%)	163 (84%)	30 (16%)	2	11
39	l2	192/195 (98%)	157 (82%)	35 (18%)	1	8
40	L3	319/322 (99%)	263 (82%)	56 (18%)	2	9
40	l3	320/322 (99%)	259 (81%)	61 (19%)	1	7
41	L4	288/288 (100%)	241 (84%)	47 (16%)	2	10
41	l4	288/288 (100%)	238 (83%)	50 (17%)	2	9
42	L5	244/244 (100%)	196 (80%)	48 (20%)	1	6
42	l5	243/244 (100%)	199 (82%)	44 (18%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	L6	134/152 (88%)	113 (84%)	21 (16%)	2	11
43	l6	135/152 (89%)	112 (83%)	23 (17%)	2	9
44	L7	186/204 (91%)	166 (89%)	20 (11%)	6	25
44	l7	187/204 (92%)	162 (87%)	25 (13%)	4	17
45	L8	187/207 (90%)	155 (83%)	32 (17%)	2	9
45	l8	177/207 (86%)	144 (81%)	33 (19%)	1	8
46	L9	171/171 (100%)	143 (84%)	28 (16%)	2	10
46	l9	171/171 (100%)	135 (79%)	36 (21%)	1	5
47	M0	177/186 (95%)	148 (84%)	29 (16%)	2	10
47	m0	179/186 (96%)	142 (79%)	37 (21%)	1	5
48	M1	147/150 (98%)	121 (82%)	26 (18%)	2	8
48	m1	147/150 (98%)	120 (82%)	27 (18%)	1	8
49	M3	154/158 (98%)	136 (88%)	18 (12%)	5	22
49	m3	154/158 (98%)	130 (84%)	24 (16%)	2	11
50	M4	107/108 (99%)	87 (81%)	20 (19%)	1	8
50	m4	108/108 (100%)	96 (89%)	12 (11%)	6	24
51	M5	175/176 (99%)	149 (85%)	26 (15%)	3	13
52	M6	160/161 (99%)	143 (89%)	17 (11%)	6	25
52	m6	160/161 (99%)	136 (85%)	24 (15%)	3	13
53	M7	140/145 (97%)	121 (86%)	19 (14%)	3	16
53	m7	125/145 (86%)	103 (82%)	22 (18%)	2	9
54	M8	150/150 (100%)	133 (89%)	17 (11%)	6	23
54	m8	150/150 (100%)	123 (82%)	27 (18%)	1	8
55	M9	153/153 (100%)	137 (90%)	16 (10%)	7	26
55	m9	153/153 (100%)	128 (84%)	25 (16%)	2	10
56	N0	156/156 (100%)	126 (81%)	30 (19%)	1	7
56	n0	156/156 (100%)	131 (84%)	25 (16%)	2	10
57	N1	136/136 (100%)	113 (83%)	23 (17%)	2	9
57	n1	136/136 (100%)	113 (83%)	23 (17%)	2	9
58	N2	87/106 (82%)	78 (90%)	9 (10%)	7	26
58	n2	85/106 (80%)	76 (89%)	9 (11%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	N3	104/104 (100%)	91 (88%)	13 (12%)	4	19
59	n3	104/104 (100%)	97 (93%)	7 (7%)	16	47
60	N4	57/129 (44%)	50 (88%)	7 (12%)	4	20
60	n4	100/129 (78%)	90 (90%)	10 (10%)	7	28
61	N5	104/117 (89%)	82 (79%)	22 (21%)	1	5
61	n5	104/117 (89%)	83 (80%)	21 (20%)	1	6
62	N6	109/109 (100%)	90 (83%)	19 (17%)	2	9
62	n6	109/109 (100%)	91 (84%)	18 (16%)	2	10
63	N7	115/115 (100%)	97 (84%)	18 (16%)	2	11
63	n7	115/115 (100%)	97 (84%)	18 (16%)	2	11
64	N8	118/118 (100%)	102 (86%)	16 (14%)	3	16
64	n8	118/118 (100%)	97 (82%)	21 (18%)	2	8
65	N9	46/46 (100%)	41 (89%)	5 (11%)	6	24
65	n9	46/46 (100%)	40 (87%)	6 (13%)	4	18
66	O0	81/87 (93%)	65 (80%)	16 (20%)	1	6
66	o0	84/87 (97%)	72 (86%)	12 (14%)	3	14
67	O1	92/96 (96%)	76 (83%)	16 (17%)	2	9
67	o1	94/96 (98%)	76 (81%)	18 (19%)	1	7
68	O2	109/110 (99%)	90 (83%)	19 (17%)	2	9
68	o2	109/110 (99%)	93 (85%)	16 (15%)	3	13
69	O3	90/90 (100%)	78 (87%)	12 (13%)	4	17
69	o3	90/90 (100%)	78 (87%)	12 (13%)	4	17
70	O4	95/101 (94%)	80 (84%)	15 (16%)	2	11
70	o4	95/101 (94%)	79 (83%)	16 (17%)	2	9
71	O5	104/104 (100%)	88 (85%)	16 (15%)	2	12
71	o5	103/104 (99%)	90 (87%)	13 (13%)	4	19
72	O6	81/81 (100%)	70 (86%)	11 (14%)	3	16
72	o6	80/81 (99%)	58 (72%)	22 (28%)	0	1
73	O7	70/70 (100%)	58 (83%)	12 (17%)	2	9
73	o7	70/70 (100%)	62 (89%)	8 (11%)	5	23
74	O8	68/68 (100%)	53 (78%)	15 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	o8	67/68 (98%)	57 (85%)	10 (15%)	3	13
75	O9	45/45 (100%)	36 (80%)	9 (20%)	1	6
75	o9	45/45 (100%)	37 (82%)	8 (18%)	2	8
76	Q0	47/47 (100%)	39 (83%)	8 (17%)	2	9
76	q0	47/47 (100%)	39 (83%)	8 (17%)	2	9
77	Q1	23/23 (100%)	20 (87%)	3 (13%)	4	18
77	q1	23/23 (100%)	16 (70%)	7 (30%)	0	1
78	Q2	90/90 (100%)	75 (83%)	15 (17%)	2	9
78	q2	90/90 (100%)	76 (84%)	14 (16%)	2	11
79	Q3	71/71 (100%)	58 (82%)	13 (18%)	1	8
79	q3	71/71 (100%)	63 (89%)	8 (11%)	6	23
80	d2	110/111 (99%)	99 (90%)	11 (10%)	7	28
82	m5	175/175 (100%)	151 (86%)	24 (14%)	3	16
83	p0	105/186 (56%)	94 (90%)	11 (10%)	7	26
85	f	123/132 (93%)	100 (81%)	23 (19%)	1	8
All	All	18849/20264 (93%)	16010 (85%)	2839 (15%)	3	13

5 of 2839 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
71	O5	102	GLU
10	s8	36	THR
64	n8	123	VAL
74	O8	67	GLN
4	s2	97	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
74	O8	32	ASN
6	s4	142	HIS
63	n7	127	ASN
3	s1	209	ASN
9	s7	71	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1776/1800 (98%)	448 (25%)	41 (2%)
1	6	1791/1800 (99%)	444 (24%)	32 (1%)
36	1	3145/3396 (92%)	646 (20%)	55 (1%)
36	5	3163/3396 (93%)	632 (19%)	59 (1%)
37	3	120/121 (99%)	10 (8%)	0
37	7	120/121 (99%)	17 (14%)	1 (0%)
38	4	157/158 (99%)	35 (22%)	4 (2%)
38	8	157/158 (99%)	32 (20%)	0
All	All	10429/10950 (95%)	2264 (21%)	192 (1%)

5 of 2264 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	8	U
1	2	25	C
1	2	26	A

5 of 192 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	3056	U
1	6	542	A
36	5	2586	G
36	1	3228	C
38	4	85	G

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	5CT	f	51	85	13,14,15	2.24	4 (30%)	9,15,17	2.12	3 (33%)

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
85	5CT	f	51	85	1/1/2/4	7/13/14/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	f	51	5CT	O1-C2	-6.40	1.24	1.43
85	f	51	5CT	C1-NZ	-3.09	1.41	1.47
85	f	51	5CT	C1-C2	2.24	1.57	1.52
85	f	51	5CT	CB-CA	2.16	1.56	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	f	51	5CT	C3-C2-C1	3.86	120.96	112.16
85	f	51	5CT	O1-C2-C1	3.31	120.64	109.32
85	f	51	5CT	O1-C2-C3	3.21	118.39	109.21

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
85	f	51	5CT	C2

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	f	51	5CT	C2-C3-C4-N1
85	f	51	5CT	CG-CD-CE-NZ
85	f	51	5CT	NZ-C1-C2-C3
85	f	51	5CT	CE-CD-CG-CB
85	f	51	5CT	CD-CE-NZ-C1

There are no ring outliers.

No monomer is involved in short contacts.



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2290 ligands modelled in this entry, 1124 are monoatomic - leaving 1166 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	$\# Z  > 2$
88	OHX	5	3842	-	0,6,6	0.00	-	-		
88	OHX	1	4020	-	0,6,6	0.00	-	-		
88	OHX	5	3817	-	0,6,6	0.00	-	-		
88	OHX	1	3965	-	0,6,6	0.00	-	-		
88	OHX	5	4051	-	0,6,6	0.00	-	-		
88	OHX	1	4099	-	0,6,6	0.00	-	-		
88	OHX	1	3787	-	0,6,6	0.00	-	-		
88	OHX	2	2035	-	0,6,6	0.00	-	-		
88	OHX	2	2065	-	0,6,6	0.00	-	-		
88	OHX	6	2090	-	0,6,6	0.00	-	-		
88	OHX	2	2013	-	0,6,6	0.00	-	-		
88	OHX	1	3911	-	0,6,6	0.00	-	-		
88	OHX	1	4000	-	0,6,6	0.00	-	-		
88	OHX	5	3815	-	0,6,6	0.00	-	-		
88	OHX	6	2123	-	0,6,6	0.00	-	-		
88	OHX	1	3809	-	0,6,6	0.00	-	-		
88	OHX	6	2118	-	0,6,6	0.00	-	-		
88	OHX	1	3783	-	0,6,6	0.00	-	-		
88	OHX	3	211	-	0,6,6	0.00	-	-		
88	OHX	1	3878	-	0,6,6	0.00	-	-		
88	OHX	1	3938	-	0,6,6	0.00	-	-		
88	OHX	5	3892	-	0,6,6	0.00	-	-		
88	OHX	1	3863	-	0,6,6	0.00	-	-		
88	OHX	1	3879	-	0,6,6	0.00	-	-		
88	OHX	6	2184	-	0,6,6	0.00	-	-		
88	OHX	6	2046	-	0,6,6	0.00	-	-		
88	OHX	6	2137	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	1	3986	-	0,6,6	0.00	-	-		
88	OHX	1	3844	-	0,6,6	0.00	-	-		
88	OHX	5	4000	-	0,6,6	0.00	-	-		
88	OHX	1	3837	-	0,6,6	0.00	-	-		
88	OHX	1	4075	-	0,6,6	0.00	-	-		
88	OHX	1	3930	-	0,6,6	0.00	-	-		
88	OHX	5	4093	-	0,6,6	0.00	-	-		
88	OHX	q1	702	-	0,6,6	0.00	-	-		
88	OHX	2	2002	-	0,6,6	0.00	-	-		
88	OHX	6	2133	-	0,6,6	0.00	-	-		
88	OHX	4	232	-	0,6,6	0.00	-	-		
88	OHX	6	2078	-	0,6,6	0.00	-	-		
88	OHX	M7	205	-	0,6,6	0.00	-	-		
88	OHX	S9	202	-	0,6,6	0.00	-	-		
88	OHX	n3	202	-	0,6,6	0.00	-	-		
88	OHX	5	4064	-	0,6,6	0.00	-	-		
88	OHX	1	3954	-	0,6,6	0.00	-	-		
88	OHX	1	3757	-	0,6,6	0.00	-	-		
88	OHX	6	2111	-	0,6,6	0.00	-	-		
88	OHX	1	3820	-	0,6,6	0.00	-	-		
88	OHX	M8	202	-	0,6,6	0.00	-	-		
88	OHX	2	2071	-	0,6,6	0.00	-	-		
88	OHX	1	3854	-	0,6,6	0.00	-	-		
88	OHX	5	3862	-	0,6,6	0.00	-	-		
88	OHX	2	2139	-	0,6,6	0.00	-	-		
88	OHX	1	3990	-	0,6,6	0.00	-	-		
88	OHX	1	3922	-	0,6,6	0.00	-	-		
88	OHX	1	3928	-	0,6,6	0.00	-	-		
88	OHX	1	3927	-	0,6,6	0.00	-	-		
88	OHX	1	3847	-	0,6,6	0.00	-	-		
88	OHX	5	4157	-	0,6,6	0.00	-	-		
88	OHX	2	2034	-	0,6,6	0.00	-	-		
88	OHX	6	2100	-	0,6,6	0.00	-	-		
88	OHX	5	3860	-	0,6,6	0.00	-	-		
88	OHX	5	3937	-	0,6,6	0.00	-	-		
88	OHX	1	3978	-	0,6,6	0.00	-	-		
88	OHX	5	4117	-	0,6,6	0.00	-	-		
88	OHX	6	2129	-	0,6,6	0.00	-	-		
88	OHX	5	3810	-	0,6,6	0.00	-	-		
88	OHX	5	4134	-	0,6,6	0.00	-	-		
88	OHX	4	221	-	0,6,6	0.00	-	-		
88	OHX	6	2051	-	0,6,6	0.00	-	-		
88	OHX	1	3786	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	6	2126	-	0,6,6	0.00	-	-		
88	OHX	C5	201	-	0,6,6	0.00	-	-		
88	OHX	6	2130	-	0,6,6	0.00	-	-		
88	OHX	6	2043	-	0,6,6	0.00	-	-		
88	OHX	5	4150	-	0,6,6	0.00	-	-		
88	OHX	5	3964	-	0,6,6	0.00	-	-		
88	OHX	5	4021	-	0,6,6	0.00	-	-		
88	OHX	1	3981	-	0,6,6	0.00	-	-		
88	OHX	5	3856	-	0,6,6	0.00	-	-		
88	OHX	8	219	-	0,6,6	0.00	-	-		
88	OHX	6	2088	-	0,6,6	0.00	-	-		
88	OHX	1	3950	-	0,6,6	0.00	-	-		
88	OHX	1	3796	-	0,6,6	0.00	-	-		
88	OHX	5	3870	-	0,6,6	0.00	-	-		
88	OHX	1	3766	-	0,6,6	0.00	-	-		
88	OHX	5	3844	-	0,6,6	0.00	-	-		
88	OHX	n6	202	-	0,6,6	0.00	-	-		
88	OHX	S1	301	-	0,6,6	0.00	-	-		
88	OHX	3	216	-	0,6,6	0.00	-	-		
88	OHX	1	3969	-	0,6,6	0.00	-	-		
88	OHX	1	3900	-	0,6,6	0.00	-	-		
88	OHX	1	3983	-	0,6,6	0.00	-	-		
88	OHX	1	3982	-	0,6,6	0.00	-	-		
88	OHX	8	217	-	0,6,6	0.00	-	-		
88	OHX	6	2033	-	0,6,6	0.00	-	-		
88	OHX	1	3818	-	0,6,6	0.00	-	-		
88	OHX	5	4063	-	0,6,6	0.00	-	-		
88	OHX	1	3958	-	0,6,6	0.00	-	-		
88	OHX	5	4148	-	0,6,6	0.00	-	-		
88	OHX	5	3846	-	0,6,6	0.00	-	-		
88	OHX	3	210	-	0,6,6	0.00	-	-		
88	OHX	5	4091	-	0,6,6	0.00	-	-		
88	OHX	6	2018	-	0,6,6	0.00	-	-		
88	OHX	5	4113	-	0,6,6	0.00	-	-		
88	OHX	2	2102	1	0,6,6	0.00	-	-		
88	OHX	6	2183	-	0,6,6	0.00	-	-		
88	OHX	1	3831	-	0,6,6	0.00	-	-		
88	OHX	5	3900	-	0,6,6	0.00	-	-		
88	OHX	1	3865	-	0,6,6	0.00	-	-		
88	OHX	5	3905	-	0,6,6	0.00	-	-		
88	OHX	D9	103	-	0,6,6	0.00	-	-		
88	OHX	5	4036	-	0,6,6	0.00	-	-		
88	OHX	2	2058	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	O7	105	73	0,6,6	0.00	-	-		
88	OHX	2	2055	-	0,6,6	0.00	-	-		
88	OHX	7	227	-	0,6,6	0.00	-	-		
88	OHX	5	3981	-	0,6,6	0.00	-	-		
88	OHX	1	3860	-	0,6,6	0.00	-	-		
88	OHX	5	3940	-	0,6,6	0.00	-	-		
88	OHX	1	3764	-	0,6,6	0.00	-	-		
88	OHX	2	2119	-	0,6,6	0.00	-	-		
88	OHX	5	4073	-	0,6,6	0.00	-	-		
88	OHX	1	3822	-	0,6,6	0.00	-	-		
88	OHX	2	2140	-	0,6,6	0.00	-	-		
88	OHX	2	2099	-	0,6,6	0.00	-	-		
88	OHX	5	4103	-	0,6,6	0.00	-	-		
88	OHX	5	4078	-	0,6,6	0.00	-	-		
88	OHX	1	4039	-	0,6,6	0.00	-	-		
88	OHX	5	3976	-	0,6,6	0.00	-	-		
88	OHX	5	3902	-	0,6,6	0.00	-	-		
88	OHX	5	3893	-	0,6,6	0.00	-	-		
88	OHX	1	4008	-	0,6,6	0.00	-	-		
88	OHX	L5	301	-	0,6,6	0.00	-	-		
88	OHX	6	2141	-	0,6,6	0.00	-	-		
88	OHX	C8	201	-	0,6,6	0.00	-	-		
88	OHX	6	2128	-	0,6,6	0.00	-	-		
88	OHX	6	2039	-	0,6,6	0.00	-	-		
88	OHX	1	3908	-	0,6,6	0.00	-	-		
88	OHX	1	3770	-	0,6,6	0.00	-	-		
88	OHX	5	4074	-	0,6,6	0.00	-	-		
88	OHX	5	3891	-	0,6,6	0.00	-	-		
88	OHX	5	3866	-	0,6,6	0.00	-	-		
88	OHX	5	3816	-	0,6,6	0.00	-	-		
88	OHX	1	4015	-	0,6,6	0.00	-	-		
88	OHX	1	4068	-	0,6,6	0.00	-	-		
88	OHX	1	3896	-	0,6,6	0.00	-	-		
88	OHX	2	2029	-	0,6,6	0.00	-	-		
88	OHX	2	2107	-	0,6,6	0.00	-	-		
88	OHX	5	3971	-	0,6,6	0.00	-	-		
88	OHX	6	2094	-	0,6,6	0.00	-	-		
88	OHX	2	2070	-	0,6,6	0.00	-	-		
88	OHX	5	4061	-	0,6,6	0.00	-	-		
88	OHX	5	4094	-	0,6,6	0.00	-	-		
88	OHX	1	4049	-	0,6,6	0.00	-	-		
88	OHX	2	2096	-	0,6,6	0.00	-	-		
88	OHX	5	4070	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	1	3834	-	0,6,6	0.00	-	-		
88	OHX	2	2050	-	0,6,6	0.00	-	-		
88	OHX	5	4102	-	0,6,6	0.00	-	-		
88	OHX	2	2030	-	0,6,6	0.00	-	-		
88	OHX	1	3998	-	0,6,6	0.00	-	-		
88	OHX	6	2164	-	0,6,6	0.00	-	-		
88	OHX	1	3761	-	0,6,6	0.00	-	-		
88	OHX	2	2144	-	0,6,6	0.00	-	-		
88	OHX	5	4095	-	0,6,6	0.00	-	-		
88	OHX	6	2016	-	0,6,6	0.00	-	-		
88	OHX	1	3962	-	0,6,6	0.00	-	-		
88	OHX	5	3936	-	0,6,6	0.00	-	-		
88	OHX	1	4059	-	0,6,6	0.00	-	-		
88	OHX	6	2031	-	0,6,6	0.00	-	-		
88	OHX	6	2074	-	0,6,6	0.00	-	-		
88	OHX	1	4076	-	0,6,6	0.00	-	-		
88	OHX	6	2112	-	0,6,6	0.00	-	-		
88	OHX	2	2056	-	0,6,6	0.00	-	-		
88	OHX	1	3883	-	0,6,6	0.00	-	-		
88	OHX	1	3970	-	0,6,6	0.00	-	-		
88	OHX	2	2047	-	0,6,6	0.00	-	-		
88	OHX	1	4066	-	0,6,6	0.00	-	-		
88	OHX	1	4057	-	0,6,6	0.00	-	-		
88	OHX	5	3969	-	0,6,6	0.00	-	-		
88	OHX	2	2011	-	0,6,6	0.00	-	-		
88	OHX	2	2076	-	0,6,6	0.00	-	-		
88	OHX	6	2138	-	0,6,6	0.00	-	-		
88	OHX	1	3992	-	0,6,6	0.00	-	-		
88	OHX	1	3918	-	0,6,6	0.00	-	-		
88	OHX	o9	102	-	0,6,6	0.00	-	-		
88	OHX	1	3839	-	0,6,6	0.00	-	-		
88	OHX	2	2009	-	0,6,6	0.00	-	-		
88	OHX	1	3929	-	0,6,6	0.00	-	-		
88	OHX	2	2026	-	0,6,6	0.00	-	-		
88	OHX	1	3903	-	0,6,6	0.00	-	-		
88	OHX	2	2087	-	0,6,6	0.00	-	-		
88	OHX	1	3949	-	0,6,6	0.00	-	-		
88	OHX	1	4054	-	0,6,6	0.00	-	-		
88	OHX	6	2053	-	0,6,6	0.00	-	-		
88	OHX	1	3816	-	0,6,6	0.00	-	-		
88	OHX	m5	301	-	0,6,6	0.00	-	-		
88	OHX	5	4053	-	0,6,6	0.00	-	-		
88	OHX	6	2149	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	2	2015	-	0,6,6	0.00	-	-		
88	OHX	6	2073	-	0,6,6	0.00	-	-		
88	OHX	1	3758	-	0,6,6	0.00	-	-		
88	OHX	6	2084	-	0,6,6	0.00	-	-		
88	OHX	1	4089	-	0,6,6	0.00	-	-		
88	OHX	5	4128	-	0,6,6	0.00	-	-		
88	OHX	5	3872	-	0,6,6	0.00	-	-		
88	OHX	1	3971	-	0,6,6	0.00	-	-		
88	OHX	5	3918	-	0,6,6	0.00	-	-		
88	OHX	1	3840	-	0,6,6	0.00	-	-		
88	OHX	5	3889	-	0,6,6	0.00	-	-		
88	OHX	1	4011	-	0,6,6	0.00	-	-		
88	OHX	2	2127	-	0,6,6	0.00	-	-		
88	OHX	5	4089	-	0,6,6	0.00	-	-		
88	OHX	M5	301	-	0,6,6	0.00	-	-		
88	OHX	6	2171	-	0,6,6	0.00	-	-		
88	OHX	6	2153	-	0,6,6	0.00	-	-		
88	OHX	5	4106	-	0,6,6	0.00	-	-		
88	OHX	6	2079	-	0,6,6	0.00	-	-		
88	OHX	2	2074	-	0,6,6	0.00	-	-		
88	OHX	7	226	-	0,6,6	0.00	-	-		
88	OHX	5	3854	-	0,6,6	0.00	-	-		
88	OHX	2	2036	-	0,6,6	0.00	-	-		
88	OHX	1	4003	-	0,6,6	0.00	-	-		
88	OHX	5	4046	-	0,6,6	0.00	-	-		
88	OHX	1	4047	-	0,6,6	0.00	-	-		
88	OHX	5	4020	-	0,6,6	0.00	-	-		
88	OHX	5	3952	-	0,6,6	0.00	-	-		
88	OHX	1	3804	-	0,6,6	0.00	-	-		
88	OHX	5	4066	-	0,6,6	0.00	-	-		
88	OHX	2	2138	-	0,6,6	0.00	-	-		
88	OHX	6	2096	-	0,6,6	0.00	-	-		
88	OHX	6	2165	-	0,6,6	0.00	-	-		
88	OHX	5	4114	-	0,6,6	0.00	-	-		
88	OHX	5	4098	-	0,6,6	0.00	-	-		
88	OHX	1	4073	-	0,6,6	0.00	-	-		
88	OHX	1	3848	-	0,6,6	0.00	-	-		
88	OHX	1	3989	-	0,6,6	0.00	-	-		
88	OHX	5	4145	-	0,6,6	0.00	-	-		
88	OHX	6	2059	-	0,6,6	0.00	-	-		
88	OHX	1	3857	-	0,6,6	0.00	-	-		
88	OHX	2	2052	-	0,6,6	0.00	-	-		
88	OHX	8	214	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	6	2095	-	0,6,6	0.00	-	-		
88	OHX	6	2081	-	0,6,6	0.00	-	-		
88	OHX	1	4029	-	0,6,6	0.00	-	-		
88	OHX	2	2021	-	0,6,6	0.00	-	-		
88	OHX	2	1994	-	0,6,6	0.00	-	-		
88	OHX	7	217	-	0,6,6	0.00	-	-		
88	OHX	N1	201	-	0,6,6	0.00	-	-		
88	OHX	5	3850	-	0,6,6	0.00	-	-		
88	OHX	1	3836	-	0,6,6	0.00	-	-		
88	OHX	5	3966	-	0,6,6	0.00	-	-		
88	OHX	1	3932	-	0,6,6	0.00	-	-		
88	OHX	5	4077	-	0,6,6	0.00	-	-		
88	OHX	6	2185	-	0,6,6	0.00	-	-		
88	OHX	5	3988	-	0,6,6	0.00	-	-		
88	OHX	1	3943	-	0,6,6	0.00	-	-		
88	OHX	5	3863	-	0,6,6	0.00	-	-		
88	OHX	1	3886	-	0,6,6	0.00	-	-		
88	OHX	5	4037	-	0,6,6	0.00	-	-		
88	OHX	1	4104	-	0,6,6	0.00	-	-		
88	OHX	1	3901	-	0,6,6	0.00	-	-		
88	OHX	2	2023	-	0,6,6	0.00	-	-		
88	OHX	5	4121	-	0,6,6	0.00	-	-		
88	OHX	5	3886	-	0,6,6	0.00	-	-		
88	OHX	5	3929	-	0,6,6	0.00	-	-		
88	OHX	l3	404	-	0,6,6	0.00	-	-		
88	OHX	6	2148	-	0,6,6	0.00	-	-		
88	OHX	5	3859	-	0,6,6	0.00	-	-		
88	OHX	1	3944	-	0,6,6	0.00	-	-		
88	OHX	1	4042	-	0,6,6	0.00	-	-		
88	OHX	5	4104	-	0,6,6	0.00	-	-		
88	OHX	5	3910	-	0,6,6	0.00	-	-		
88	OHX	1	3907	-	0,6,6	0.00	-	-		
88	OHX	2	2033	-	0,6,6	0.00	-	-		
88	OHX	5	3995	-	0,6,6	0.00	-	-		
88	OHX	5	4097	-	0,6,6	0.00	-	-		
88	OHX	6	2050	-	0,6,6	0.00	-	-		
88	OHX	8	216	-	0,6,6	0.00	-	-		
88	OHX	5	4092	-	0,6,6	0.00	-	-		
88	OHX	1	3993	-	0,6,6	0.00	-	-		
88	OHX	1	4063	-	0,6,6	0.00	-	-		
88	OHX	5	4133	-	0,6,6	0.00	-	-		
88	OHX	5	3965	-	0,6,6	0.00	-	-		
88	OHX	2	2054	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	5	3992	-	0,6,6	0.00	-	-		
88	OHX	5	4007	-	0,6,6	0.00	-	-		
88	OHX	5	3970	-	0,6,6	0.00	-	-		
88	OHX	1	4094	-	0,6,6	0.00	-	-		
88	OHX	6	2089	-	0,6,6	0.00	-	-		
88	OHX	1	3821	-	0,6,6	0.00	-	-		
88	OHX	1	4061	-	0,6,6	0.00	-	-		
88	OHX	1	3843	-	0,6,6	0.00	-	-		
88	OHX	1	3859	-	0,6,6	0.00	-	-		
88	OHX	1	3984	-	0,6,6	0.00	-	-		
88	OHX	1	3862	-	0,6,6	0.00	-	-		
88	OHX	1	3991	-	0,6,6	0.00	-	-		
88	OHX	1	4088	-	0,6,6	0.00	-	-		
88	OHX	5	4033	-	0,6,6	0.00	-	-		
88	OHX	1	3920	-	0,6,6	0.00	-	-		
88	OHX	5	3848	-	0,6,6	0.00	-	-		
88	OHX	2	2093	-	0,6,6	0.00	-	-		
88	OHX	5	4022	-	0,6,6	0.00	-	-		
88	OHX	6	2017	-	0,6,6	0.00	-	-		
88	OHX	1	3931	-	0,6,6	0.00	-	-		
88	OHX	2	2135	-	0,6,6	0.00	-	-		
88	OHX	5	3960	-	0,6,6	0.00	-	-		
88	OHX	1	3828	-	0,6,6	0.00	-	-		
88	OHX	8	221	-	0,6,6	0.00	-	-		
88	OHX	1	3794	-	0,6,6	0.00	-	-		
88	OHX	5	3926	-	0,6,6	0.00	-	-		
88	OHX	5	3822	-	0,6,6	0.00	-	-		
88	OHX	1	3914	-	0,6,6	0.00	-	-		
88	OHX	2	2079	-	0,6,6	0.00	-	-		
88	OHX	1	4024	-	0,6,6	0.00	-	-		
88	OHX	1	3810	-	0,6,6	0.00	-	-		
88	OHX	2	2104	-	0,6,6	0.00	-	-		
88	OHX	5	3962	-	0,6,6	0.00	-	-		
88	OHX	5	4058	-	0,6,6	0.00	-	-		
88	OHX	5	4124	-	0,6,6	0.00	-	-		
88	OHX	5	3805	-	0,6,6	0.00	-	-		
88	OHX	sR	401	-	0,6,6	0.00	-	-		
88	OHX	1	3775	-	0,6,6	0.00	-	-		
88	OHX	4	223	-	0,6,6	0.00	-	-		
88	OHX	1	3781	-	0,6,6	0.00	-	-		
88	OHX	6	2065	-	0,6,6	0.00	-	-		
88	OHX	2	2143	-	0,6,6	0.00	-	-		
88	OHX	6	2147	-	0,6,6	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	2	2120	-	0,6,6	0.00	-	-		
88	OHX	1	3769	-	0,6,6	0.00	-	-		
88	OHX	5	3849	-	0,6,6	0.00	-	-		
88	OHX	5	4025	-	0,6,6	0.00	-	-		
88	OHX	2	2098	-	0,6,6	0.00	-	-		
88	OHX	1	3923	-	0,6,6	0.00	-	-		
88	OHX	5	3993	-	0,6,6	0.00	-	-		
88	OHX	5	3998	-	0,6,6	0.00	-	-		
88	OHX	1	3780	-	0,6,6	0.00	-	-		
88	OHX	6	2097	-	0,6,6	0.00	-	-		
88	OHX	5	3823	-	0,6,6	0.00	-	-		
88	OHX	1	4006	-	0,6,6	0.00	-	-		
88	OHX	6	2162	-	0,6,6	0.00	-	-		
88	OHX	5	3954	-	0,6,6	0.00	-	-		
88	OHX	6	2101	-	0,6,6	0.00	-	-		
88	OHX	5	4029	-	0,6,6	0.00	-	-		
88	OHX	1	4064	-	0,6,6	0.00	-	-		
88	OHX	2	2062	-	0,6,6	0.00	-	-		
88	OHX	7	221	-	0,6,6	0.00	-	-		
88	OHX	1	3921	-	0,6,6	0.00	-	-		
88	OHX	1	3909	-	0,6,6	0.00	-	-		
88	OHX	1	3880	-	0,6,6	0.00	-	-		
88	OHX	6	2049	-	0,6,6	0.00	-	-		
88	OHX	2	2118	-	0,6,6	0.00	-	-		
88	OHX	5	4111	-	0,6,6	0.00	-	-		
88	OHX	5	3879	-	0,6,6	0.00	-	-		
88	OHX	5	4135	-	0,6,6	0.00	-	-		
88	OHX	2	2064	-	0,6,6	0.00	-	-		
88	OHX	8	228	-	0,6,6	0.00	-	-		
88	OHX	6	2115	-	0,6,6	0.00	-	-		
88	OHX	2	2083	-	0,6,6	0.00	-	-		
88	OHX	2	2077	-	0,6,6	0.00	-	-		
88	OHX	5	4076	-	0,6,6	0.00	-	-		
88	OHX	2	2133	-	0,6,6	0.00	-	-		
88	OHX	1	4038	-	0,6,6	0.00	-	-		
88	OHX	2	2016	-	0,6,6	0.00	-	-		
88	OHX	2	2075	-	0,6,6	0.00	-	-		
88	OHX	1	4048	-	0,6,6	0.00	-	-		
88	OHX	4	226	-	0,6,6	0.00	-	-		
88	OHX	1	3917	-	0,6,6	0.00	-	-		
88	OHX	5	3901	-	0,6,6	0.00	-	-		
88	OHX	1	3795	-	0,6,6	0.00	-	-		
88	OHX	5	3833	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	5	4107	-	0,6,6	0.00	-	-		
88	OHX	6	2140	-	0,6,6	0.00	-	-		
88	OHX	1	3987	-	0,6,6	0.00	-	-		
88	OHX	1	3817	-	0,6,6	0.00	-	-		
88	OHX	5	4032	-	0,6,6	0.00	-	-		
88	OHX	1	3850	-	0,6,6	0.00	-	-		
88	OHX	5	3798	-	0,6,6	0.00	-	-		
88	OHX	5	3946	-	0,6,6	0.00	-	-		
88	OHX	6	2134	-	0,6,6	0.00	-	-		
88	OHX	6	2082	-	0,6,6	0.00	-	-		
88	OHX	5	4101	-	0,6,6	0.00	-	-		
88	OHX	5	3959	-	0,6,6	0.00	-	-		
88	OHX	6	2019	-	0,6,6	0.00	-	-		
88	OHX	1	3957	-	0,6,6	0.00	-	-		
88	OHX	5	3907	-	0,6,6	0.00	-	-		
88	OHX	1	4051	-	0,6,6	0.00	-	-		
88	OHX	6	2105	-	0,6,6	0.00	-	-		
88	OHX	1	3768	-	0,6,6	0.00	-	-		
88	OHX	5	4065	-	0,6,6	0.00	-	-		
88	OHX	2	2122	-	0,6,6	0.00	-	-		
88	OHX	5	3986	-	0,6,6	0.00	-	-		
88	OHX	6	2040	-	0,6,6	0.00	-	-		
88	OHX	5	4084	-	0,6,6	0.00	-	-		
88	OHX	5	3983	-	0,6,6	0.00	-	-		
88	OHX	5	4155	-	0,6,6	0.00	-	-		
88	OHX	5	3824	-	0,6,6	0.00	-	-		
88	OHX	6	2023	-	0,6,6	0.00	-	-		
88	OHX	1	3972	-	0,6,6	0.00	-	-		
88	OHX	5	4042	-	0,6,6	0.00	-	-		
88	OHX	5	3841	-	0,6,6	0.00	-	-		
88	OHX	1	3892	-	0,6,6	0.00	-	-		
88	OHX	5	4072	-	0,6,6	0.00	-	-		
88	OHX	2	2145	-	0,6,6	0.00	-	-		
88	OHX	7	222	-	0,6,6	0.00	-	-		
88	OHX	2	2003	-	0,6,6	0.00	-	-		
88	OHX	2	2046	-	0,6,6	0.00	-	-		
88	OHX	1	4071	-	0,6,6	0.00	-	-		
88	OHX	5	3922	-	0,6,6	0.00	-	-		
88	OHX	2	2019	-	0,6,6	0.00	-	-		
88	OHX	5	4008	-	0,6,6	0.00	-	-		
88	OHX	1	3773	-	0,6,6	0.00	-	-		
88	OHX	1	3942	-	0,6,6	0.00	-	-		
88	OHX	m9	201	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	6	2072	-	0,6,6	0.00	-	-		
88	OHX	1	4012	-	0,6,6	0.00	-	-		
88	OHX	1	4032	-	0,6,6	0.00	-	-		
88	OHX	5	4086	-	0,6,6	0.00	-	-		
88	OHX	5	4151	-	0,6,6	0.00	-	-		
88	OHX	5	3806	-	0,6,6	0.00	-	-		
88	OHX	5	4112	-	0,6,6	0.00	-	-		
88	OHX	6	2021	-	0,6,6	0.00	-	-		
88	OHX	5	3999	-	0,6,6	0.00	-	-		
88	OHX	1	3945	-	0,6,6	0.00	-	-		
88	OHX	2	2024	-	0,6,6	0.00	-	-		
88	OHX	5	3890	-	0,6,6	0.00	-	-		
88	OHX	1	4083	-	0,6,6	0.00	-	-		
88	OHX	1	4062	-	0,6,6	0.00	-	-		
88	OHX	5	3820	-	0,6,6	0.00	-	-		
88	OHX	6	2108	-	0,6,6	0.00	-	-		
88	OHX	m0	302	-	0,6,6	0.00	-	-		
88	OHX	5	3912	-	0,6,6	0.00	-	-		
88	OHX	1	3842	-	0,6,6	0.00	-	-		
88	OHX	6	2156	-	0,6,6	0.00	-	-		
88	OHX	1	4035	-	0,6,6	0.00	-	-		
88	OHX	2	1995	-	0,6,6	0.00	-	-		
88	OHX	5	3897	-	0,6,6	0.00	-	-		
88	OHX	2	2051	-	0,6,6	0.00	-	-		
88	OHX	5	3947	-	0,6,6	0.00	-	-		
88	OHX	5	3953	-	0,6,6	0.00	-	-		
88	OHX	1	3815	-	0,6,6	0.00	-	-		
88	OHX	5	3831	-	0,6,6	0.00	-	-		
88	OHX	5	3874	-	0,6,6	0.00	-	-		
88	OHX	1	3964	-	0,6,6	0.00	-	-		
88	OHX	5	4152	-	0,6,6	0.00	-	-		
88	OHX	1	3941	-	0,6,6	0.00	-	-		
88	OHX	2	2095	-	0,6,6	0.00	-	-		
88	OHX	5	3997	-	0,6,6	0.00	-	-		
88	OHX	6	2060	-	0,6,6	0.00	-	-		
88	OHX	6	2121	-	0,6,6	0.00	-	-		
88	OHX	1	3985	-	0,6,6	0.00	-	-		
88	OHX	6	2058	-	0,6,6	0.00	-	-		
88	OHX	1	3953	-	0,6,6	0.00	-	-		
88	OHX	2	2059	-	0,6,6	0.00	-	-		
88	OHX	5	3847	-	0,6,6	0.00	-	-		
88	OHX	2	2057	-	0,6,6	0.00	-	-		
88	OHX	5	3956	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	1	3919	-	0,6,6	0.00	-	-		
88	OHX	1	4052	-	0,6,6	0.00	-	-		
88	OHX	5	3972	-	0,6,6	0.00	-	-		
88	OHX	15	302	-	0,6,6	0.00	-	-		
88	OHX	1	3881	-	0,6,6	0.00	-	-		
88	OHX	6	2145	-	0,6,6	0.00	-	-		
88	OHX	2	2148	-	0,6,6	0.00	-	-		
88	OHX	2	2132	-	0,6,6	0.00	-	-		
88	OHX	O3	203	-	0,6,6	0.00	-	-		
88	OHX	1	3875	-	0,6,6	0.00	-	-		
88	OHX	5	3982	-	0,6,6	0.00	-	-		
88	OHX	1	3819	-	0,6,6	0.00	-	-		
88	OHX	6	2135	-	0,6,6	0.00	-	-		
88	OHX	1	3902	-	0,6,6	0.00	-	-		
88	OHX	1	4081	-	0,6,6	0.00	-	-		
88	OHX	c3	201	-	0,6,6	0.00	-	-		
88	OHX	5	4110	-	0,6,6	0.00	-	-		
88	OHX	4	235	-	0,6,6	0.00	-	-		
88	OHX	1	3895	-	0,6,6	0.00	-	-		
88	OHX	1	3904	-	0,6,6	0.00	-	-		
88	OHX	1	3994	-	0,6,6	0.00	-	-		
88	OHX	S6	301	-	0,6,6	0.00	-	-		
88	OHX	2	2089	-	0,6,6	0.00	-	-		
88	OHX	5	4052	-	0,6,6	0.00	-	-		
88	OHX	2	2078	-	0,6,6	0.00	-	-		
88	OHX	2	2073	-	0,6,6	0.00	-	-		
88	OHX	1	3852	-	0,6,6	0.00	-	-		
88	OHX	5	3943	-	0,6,6	0.00	-	-		
88	OHX	6	2047	-	0,6,6	0.00	-	-		
88	OHX	8	225	-	0,6,6	0.00	-	-		
88	OHX	5	3915	-	0,6,6	0.00	-	-		
88	OHX	6	2013	-	0,6,6	0.00	-	-		
88	OHX	5	3803	-	0,6,6	0.00	-	-		
88	OHX	6	2098	-	0,6,6	0.00	-	-		
88	OHX	1	3826	-	0,6,6	0.00	-	-		
88	OHX	1	4053	-	0,6,6	0.00	-	-		
88	OHX	6	2113	-	0,6,6	0.00	-	-		
88	OHX	5	3958	-	0,6,6	0.00	-	-		
88	OHX	5	3830	-	0,6,6	0.00	-	-		
88	OHX	5	3818	-	0,6,6	0.00	-	-		
88	OHX	2	2028	-	0,6,6	0.00	-	-		
88	OHX	6	2022	-	0,6,6	0.00	-	-		
88	OHX	6	2077	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	1	3825	-	0,6,6	0.00	-	-		
88	OHX	6	2067	1	0,6,6	0.00	-	-		
88	OHX	5	3857	-	0,6,6	0.00	-	-		
88	OHX	1	4098	-	0,6,6	0.00	-	-		
88	OHX	5	3858	-	0,6,6	0.00	-	-		
88	OHX	2	2039	-	0,6,6	0.00	-	-		
88	OHX	5	3935	-	0,6,6	0.00	-	-		
88	OHX	5	4047	-	0,6,6	0.00	-	-		
88	OHX	5	4129	-	0,6,6	0.00	-	-		
88	OHX	m0	304	-	0,6,6	0.00	-	-		
88	OHX	l3	402	-	0,6,6	0.00	-	-		
88	OHX	1	3777	-	0,6,6	0.00	-	-		
88	OHX	1	3812	-	0,6,6	0.00	-	-		
88	OHX	6	2176	-	0,6,6	0.00	-	-		
88	OHX	2	2137	-	0,6,6	0.00	-	-		
88	OHX	5	3979	-	0,6,6	0.00	-	-		
88	OHX	2	2041	-	0,6,6	0.00	-	-		
88	OHX	6	2102	-	0,6,6	0.00	-	-		
88	OHX	5	4067	-	0,6,6	0.00	-	-		
88	OHX	1	3915	-	0,6,6	0.00	-	-		
88	OHX	1	4046	-	0,6,6	0.00	-	-		
88	OHX	2	2022	-	0,6,6	0.00	-	-		
88	OHX	1	3940	-	0,6,6	0.00	-	-		
88	OHX	s4	301	-	0,6,6	0.00	-	-		
88	OHX	6	2152	-	0,6,6	0.00	-	-		
88	OHX	6	2117	-	0,6,6	0.00	-	-		
88	OHX	1	3789	-	0,6,6	0.00	-	-		
88	OHX	6	2151	-	0,6,6	0.00	-	-		
88	OHX	5	3795	-	0,6,6	0.00	-	-		
88	OHX	2	2067	-	0,6,6	0.00	-	-		
88	OHX	1	3784	-	0,6,6	0.00	-	-		
88	OHX	6	2066	-	0,6,6	0.00	-	-		
88	OHX	5	4048	-	0,6,6	0.00	-	-		
88	OHX	1	3951	-	0,6,6	0.00	-	-		
88	OHX	1	4070	-	0,6,6	0.00	-	-		
88	OHX	6	2182	-	0,6,6	0.00	-	-		
88	OHX	5	3839	-	0,6,6	0.00	-	-		
88	OHX	5	4158	-	0,6,6	0.00	-	-		
88	OHX	6	2157	-	0,6,6	0.00	-	-		
88	OHX	2	2115	-	0,6,6	0.00	-	-		
88	OHX	5	4085	-	0,6,6	0.00	-	-		
88	OHX	1	3997	-	0,6,6	0.00	-	-		
88	OHX	6	2161	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	1	3946	-	0,6,6	0.00	-	-		
88	OHX	5	4131	-	0,6,6	0.00	-	-		
88	OHX	2	2063	-	0,6,6	0.00	-	-		
88	OHX	5	3968	-	0,6,6	0.00	-	-		
88	OHX	5	4014	-	0,6,6	0.00	-	-		
88	OHX	5	3827	-	0,6,6	0.00	-	-		
88	OHX	4	224	-	0,6,6	0.00	-	-		
88	OHX	2	2017	-	0,6,6	0.00	-	-		
88	OHX	1	3973	-	0,6,6	0.00	-	-		
88	OHX	5	4118	-	0,6,6	0.00	-	-		
88	OHX	2	2134	-	0,6,6	0.00	-	-		
88	OHX	6	2169	-	0,6,6	0.00	-	-		
88	OHX	c5	800	-	0,6,6	0.00	-	-		
88	OHX	6	2180	-	0,6,6	0.00	-	-		
88	OHX	1	4017	-	0,6,6	0.00	-	-		
88	OHX	5	4024	-	0,6,6	0.00	-	-		
88	OHX	N9	102	-	0,6,6	0.00	-	-		
88	OHX	1	4087	-	0,6,6	0.00	-	-		
88	OHX	6	2136	-	0,6,6	0.00	-	-		
88	OHX	1	4074	-	0,6,6	0.00	-	-		
88	OHX	1	3995	-	0,6,6	0.00	-	-		
88	OHX	6	2167	-	0,6,6	0.00	-	-		
88	OHX	6	2179	-	0,6,6	0.00	-	-		
88	OHX	6	2075	-	0,6,6	0.00	-	-		
88	OHX	1	3797	-	0,6,6	0.00	-	-		
88	OHX	5	3797	-	0,6,6	0.00	-	-		
88	OHX	2	2150	-	0,6,6	0.00	-	-		
88	OHX	2	2042	-	0,6,6	0.00	-	-		
88	OHX	5	3994	-	0,6,6	0.00	-	-		
88	OHX	6	2026	-	0,6,6	0.00	-	-		
88	OHX	5	3945	-	0,6,6	0.00	-	-		
88	OHX	5	3895	-	0,6,6	0.00	-	-		
88	OHX	6	2144	-	0,6,6	0.00	-	-		
88	OHX	6	2175	-	0,6,6	0.00	-	-		
88	OHX	6	2029	-	0,6,6	0.00	-	-		
88	OHX	1	3888	-	0,6,6	0.00	-	-		
88	OHX	5	3852	36	0,6,6	0.00	-	-		
88	OHX	1	3936	-	0,6,6	0.00	-	-		
88	OHX	6	2155	-	0,6,6	0.00	-	-		
88	OHX	1	4034	-	0,6,6	0.00	-	-		
88	OHX	1	3829	-	0,6,6	0.00	-	-		
88	OHX	1	3910	-	0,6,6	0.00	-	-		
88	OHX	5	3885	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	C1	201	-	0,6,6	0.00	-	-		
88	OHX	6	2159	-	0,6,6	0.00	-	-		
88	OHX	6	2024	-	0,6,6	0.00	-	-		
88	OHX	7	220	-	0,6,6	0.00	-	-		
88	OHX	6	2025	-	0,6,6	0.00	-	-		
88	OHX	5	4006	-	0,6,6	0.00	-	-		
88	OHX	1	3765	-	0,6,6	0.00	-	-		
88	OHX	5	4115	-	0,6,6	0.00	-	-		
88	OHX	1	3977	-	0,6,6	0.00	-	-		
88	OHX	2	2108	-	0,6,6	0.00	-	-		
88	OHX	2	2103	-	0,6,6	0.00	-	-		
88	OHX	5	3814	-	0,6,6	0.00	-	-		
88	OHX	2	2004	-	0,6,6	0.00	-	-		
88	OHX	1	3845	-	0,6,6	0.00	-	-		
88	OHX	1	3887	-	0,6,6	0.00	-	-		
88	OHX	6	2174	-	0,6,6	0.00	-	-		
88	OHX	5	3864	-	0,6,6	0.00	-	-		
88	OHX	2	2117	-	0,6,6	0.00	-	-		
88	OHX	5	3906	-	0,6,6	0.00	-	-		
88	OHX	1	3763	-	0,6,6	0.00	-	-		
88	OHX	5	4159	-	0,6,6	0.00	-	-		
88	OHX	1	3778	-	0,6,6	0.00	-	-		
88	OHX	6	2139	-	0,6,6	0.00	-	-		
88	OHX	5	4081	-	0,6,6	0.00	-	-		
88	OHX	1	3899	-	0,6,6	0.00	-	-		
88	OHX	5	3923	-	0,6,6	0.00	-	-		
88	OHX	3	218	-	0,6,6	0.00	-	-		
88	OHX	1	3890	-	0,6,6	0.00	-	-		
88	OHX	5	3808	-	0,6,6	0.00	-	-		
88	OHX	6	2028	-	0,6,6	0.00	-	-		
88	OHX	4	233	-	0,6,6	0.00	-	-		
88	OHX	1	3897	-	0,6,6	0.00	-	-		
88	OHX	1	3759	-	0,6,6	0.00	-	-		
88	OHX	1	3803	-	0,6,6	0.00	-	-		
88	OHX	1	3806	-	0,6,6	0.00	-	-		
88	OHX	2	2105	-	0,6,6	0.00	-	-		
88	OHX	1	3774	-	0,6,6	0.00	-	-		
88	OHX	5	3908	-	0,6,6	0.00	-	-		
88	OHX	1	4018	-	0,6,6	0.00	-	-		
88	OHX	1	3874	-	0,6,6	0.00	-	-		
88	OHX	1	4097	-	0,6,6	0.00	-	-		
88	OHX	7	218	-	0,6,6	0.00	-	-		
88	OHX	1	3858	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	5	4005	-	0,6,6	0.00	-	-		
88	OHX	1	4028	-	0,6,6	0.00	-	-		
88	OHX	1	3851	-	0,6,6	0.00	-	-		
88	OHX	2	2005	-	0,6,6	0.00	-	-		
88	OHX	5	3875	-	0,6,6	0.00	-	-		
88	OHX	1	4019	-	0,6,6	0.00	-	-		
88	OHX	5	3978	-	0,6,6	0.00	-	-		
88	OHX	1	4069	-	0,6,6	0.00	-	-		
88	OHX	2	2068	-	0,6,6	0.00	-	-		
88	OHX	1	4100	-	0,6,6	0.00	-	-		
88	OHX	8	232	-	0,6,6	0.00	-	-		
88	OHX	2	2048	-	0,6,6	0.00	-	-		
88	OHX	1	4041	-	0,6,6	0.00	-	-		
88	OHX	5	3938	-	0,6,6	0.00	-	-		
88	OHX	1	3906	-	0,6,6	0.00	-	-		
88	OHX	5	3855	-	0,6,6	0.00	-	-		
88	OHX	1	3947	-	0,6,6	0.00	-	-		
88	OHX	2	2152	-	0,6,6	0.00	-	-		
88	OHX	5	3934	-	0,6,6	0.00	-	-		
88	OHX	5	3975	-	0,6,6	0.00	-	-		
88	OHX	1	4037	-	0,6,6	0.00	-	-		
88	OHX	5	3894	-	0,6,6	0.00	-	-		
88	OHX	2	2040	-	0,6,6	0.00	-	-		
88	OHX	2	2121	-	0,6,6	0.00	-	-		
88	OHX	1	3832	-	0,6,6	0.00	-	-		
88	OHX	6	2086	-	0,6,6	0.00	-	-		
88	OHX	6	2076	-	0,6,6	0.00	-	-		
88	OHX	1	3790	-	0,6,6	0.00	-	-		
88	OHX	5	4016	-	0,6,6	0.00	-	-		
88	OHX	2	2114	-	0,6,6	0.00	-	-		
88	OHX	1	3968	-	0,6,6	0.00	-	-		
88	OHX	4	234	-	0,6,6	0.00	-	-		
88	OHX	1	3976	-	0,6,6	0.00	-	-		
88	OHX	6	2061	-	0,6,6	0.00	-	-		
88	OHX	2	2123	-	0,6,6	0.00	-	-		
88	OHX	5	3832	-	0,6,6	0.00	-	-		
88	OHX	5	3985	-	0,6,6	0.00	-	-		
88	OHX	6	2070	-	0,6,6	0.00	-	-		
88	OHX	5	3950	-	0,6,6	0.00	-	-		
88	OHX	5	3861	-	0,6,6	0.00	-	-		
88	OHX	5	3825	-	0,6,6	0.00	-	-		
88	OHX	5	3802	-	0,6,6	0.00	-	-		
88	OHX	5	4100	-	0,6,6	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	5	4083	-	0,6,6	0.00	-	-		
88	OHX	5	4004	-	0,6,6	0.00	-	-		
88	OHX	1	3811	-	0,6,6	0.00	-	-		
88	OHX	1	3956	-	0,6,6	0.00	-	-		
88	OHX	5	3878	-	0,6,6	0.00	-	-		
88	OHX	2	2142	-	0,6,6	0.00	-	-		
88	OHX	n9	103	-	0,6,6	0.00	-	-		
88	OHX	2	2147	-	0,6,6	0.00	-	-		
88	OHX	M7	204	-	0,6,6	0.00	-	-		
88	OHX	2	2010	-	0,6,6	0.00	-	-		
88	OHX	5	3881	-	0,6,6	0.00	-	-		
88	OHX	2	2014	-	0,6,6	0.00	-	-		
88	OHX	1	3877	-	0,6,6	0.00	-	-		
88	OHX	L3	404	-	0,6,6	0.00	-	-		
88	OHX	2	1997	-	0,6,6	0.00	-	-		
88	OHX	5	3840	-	0,6,6	0.00	-	-		
88	OHX	5	4054	-	0,6,6	0.00	-	-		
88	OHX	6	2071	-	0,6,6	0.00	-	-		
88	OHX	5	3801	-	0,6,6	0.00	-	-		
88	OHX	5	3903	-	0,6,6	0.00	-	-		
88	OHX	6	2160	-	0,6,6	0.00	-	-		
88	OHX	5	3804	-	0,6,6	0.00	-	-		
88	OHX	1	3939	-	0,6,6	0.00	-	-		
88	OHX	1	3952	-	0,6,6	0.00	-	-		
88	OHX	5	4079	-	0,6,6	0.00	-	-		
88	OHX	1	3776	-	0,6,6	0.00	-	-		
88	OHX	1	3889	-	0,6,6	0.00	-	-		
88	OHX	6	2092	-	0,6,6	0.00	-	-		
88	OHX	5	4031	-	0,6,6	0.00	-	-		
88	OHX	5	3939	-	0,6,6	0.00	-	-		
88	OHX	1	3793	-	0,6,6	0.00	-	-		
88	OHX	6	2104	-	0,6,6	0.00	-	-		
88	OHX	1	4007	-	0,6,6	0.00	-	-		
88	OHX	5	4030	-	0,6,6	0.00	-	-		
88	OHX	5	4130	-	0,6,6	0.00	-	-		
88	OHX	5	3914	-	0,6,6	0.00	-	-		
88	OHX	Q2	503	-	0,6,6	0.00	-	-		
88	OHX	1	4014	-	0,6,6	0.00	-	-		
88	OHX	5	4017	-	0,6,6	0.00	-	-		
88	OHX	5	3882	-	0,6,6	0.00	-	-		
88	OHX	6	2052	-	0,6,6	0.00	-	-		
88	OHX	5	3904	-	0,6,6	0.00	-	-		
88	OHX	5	4137	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	5	4126	36	0,6,6	0.00	-	-		
88	OHX	O9	101	-	0,6,6	0.00	-	-		
88	OHX	2	2037	-	0,6,6	0.00	-	-		
88	OHX	5	3813	-	0,6,6	0.00	-	-		
88	OHX	2	2088	-	0,6,6	0.00	-	-		
88	OHX	8	229	-	0,6,6	0.00	-	-		
88	OHX	5	4096	-	0,6,6	0.00	-	-		
88	OHX	6	2030	-	0,6,6	0.00	-	-		
88	OHX	6	2158	-	0,6,6	0.00	-	-		
88	OHX	4	220	-	0,6,6	0.00	-	-		
88	OHX	1	3999	-	0,6,6	0.00	-	-		
88	OHX	6	2038	-	0,6,6	0.00	-	-		
88	OHX	5	4002	-	0,6,6	0.00	-	-		
88	OHX	5	4088	-	0,6,6	0.00	-	-		
88	OHX	1	3830	-	0,6,6	0.00	-	-		
88	OHX	5	4060	-	0,6,6	0.00	-	-		
88	OHX	5	3989	-	0,6,6	0.00	-	-		
88	OHX	6	2041	-	0,6,6	0.00	-	-		
88	OHX	6	2032	-	0,6,6	0.00	-	-		
88	OHX	1	3926	-	0,6,6	0.00	-	-		
88	OHX	6	2154	-	0,6,6	0.00	-	-		
88	OHX	1	3760	-	0,6,6	0.00	-	-		
88	OHX	1	3872	-	0,6,6	0.00	-	-		
88	OHX	5	4045	-	0,6,6	0.00	-	-		
88	OHX	1	3838	-	0,6,6	0.00	-	-		
88	OHX	1	3835	-	0,6,6	0.00	-	-		
88	OHX	6	2054	-	0,6,6	0.00	-	-		
88	OHX	1	4025	-	0,6,6	0.00	-	-		
88	OHX	1	3785	-	0,6,6	0.00	-	-		
88	OHX	3	214	-	0,6,6	0.00	-	-		
88	OHX	5	3869	-	0,6,6	0.00	-	-		
88	OHX	6	2177	-	0,6,6	0.00	-	-		
88	OHX	1	4106	-	0,6,6	0.00	-	-		
88	OHX	1	4050	-	0,6,6	0.00	-	-		
88	OHX	5	4043	-	0,6,6	0.00	-	-		
88	OHX	2	2125	-	0,6,6	0.00	-	-		
88	OHX	8	220	-	0,6,6	0.00	-	-		
88	OHX	5	3884	-	0,6,6	0.00	-	-		
88	OHX	6	2034	-	0,6,6	0.00	-	-		
88	OHX	1	4036	-	0,6,6	0.00	-	-		
88	OHX	5	3898	-	0,6,6	0.00	-	-		
88	OHX	1	3979	-	0,6,6	0.00	-	-		
88	OHX	1	3855	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	1	4091	-	0,6,6	0.00	-	-		
88	OHX	6	2015	-	0,6,6	0.00	-	-		
88	OHX	2	2085	-	0,6,6	0.00	-	-		
88	OHX	2	2069	-	0,6,6	0.00	-	-		
88	OHX	5	4142	-	0,6,6	0.00	-	-		
88	OHX	5	3917	-	0,6,6	0.00	-	-		
88	OHX	5	3944	-	0,6,6	0.00	-	-		
88	OHX	5	3991	-	0,6,6	0.00	-	-		
88	OHX	6	2106	-	0,6,6	0.00	-	-		
88	OHX	5	4153	-	0,6,6	0.00	-	-		
88	OHX	2	2053	-	0,6,6	0.00	-	-		
88	OHX	6	2143	-	0,6,6	0.00	-	-		
88	OHX	5	4059	-	0,6,6	0.00	-	-		
88	OHX	5	4056	-	0,6,6	0.00	-	-		
88	OHX	3	213	-	0,6,6	0.00	-	-		
88	OHX	1	3960	-	0,6,6	0.00	-	-		
88	OHX	6	2170	-	0,6,6	0.00	-	-		
88	OHX	1	4055	-	0,6,6	0.00	-	-		
88	OHX	6	2063	-	0,6,6	0.00	-	-		
88	OHX	1	4072	-	0,6,6	0.00	-	-		
88	OHX	1	3853	-	0,6,6	0.00	-	-		
88	OHX	5	4013	-	0,6,6	0.00	-	-		
88	OHX	1	4043	-	0,6,6	0.00	-	-		
88	OHX	2	2149	-	0,6,6	0.00	-	-		
88	OHX	5	3963	-	0,6,6	0.00	-	-		
88	OHX	2	1999	-	0,6,6	0.00	-	-		
88	OHX	5	3977	-	0,6,6	0.00	-	-		
88	OHX	1	4058	-	0,6,6	0.00	-	-		
88	OHX	L4	401	-	0,6,6	0.00	-	-		
88	OHX	5	4120	-	0,6,6	0.00	-	-		
88	OHX	6	2085	-	0,6,6	0.00	-	-		
88	OHX	5	3933	-	0,6,6	0.00	-	-		
88	OHX	5	3835	-	0,6,6	0.00	-	-		
88	OHX	5	3843	-	0,6,6	0.00	-	-		
88	OHX	1	4107	-	0,6,6	0.00	-	-		
88	OHX	6	2124	-	0,6,6	0.00	-	-		
88	OHX	3	219	-	0,6,6	0.00	-	-		
88	OHX	5	4068	36	0,6,6	0.00	-	-		
88	OHX	2	2113	-	0,6,6	0.00	-	-		
88	OHX	5	3932	-	0,6,6	0.00	-	-		
88	OHX	6	2122	-	0,6,6	0.00	-	-		
88	OHX	1	3823	-	0,6,6	0.00	-	-		
88	OHX	6	2172	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	6	2173	-	0,6,6	0.00	-	-		
88	OHX	4	231	-	0,6,6	0.00	-	-		
88	OHX	1	4096	-	0,6,6	0.00	-	-		
88	OHX	8	231	-	0,6,6	0.00	-	-		
88	OHX	2	2126	-	0,6,6	0.00	-	-		
88	OHX	1	3824	-	0,6,6	0.00	-	-		
88	OHX	1	3813	-	0,6,6	0.00	-	-		
88	OHX	8	226	-	0,6,6	0.00	-	-		
88	OHX	1	3959	-	0,6,6	0.00	-	-		
88	OHX	5	4139	-	0,6,6	0.00	-	-		
88	OHX	6	2181	-	0,6,6	0.00	-	-		
88	OHX	5	4026	-	0,6,6	0.00	-	-		
88	OHX	1	4102	-	0,6,6	0.00	-	-		
88	OHX	6	2132	-	0,6,6	0.00	-	-		
88	OHX	2	2131	-	0,6,6	0.00	-	-		
88	OHX	1	4105	-	0,6,6	0.00	-	-		
88	OHX	5	4023	-	0,6,6	0.00	-	-		
88	OHX	1	3870	-	0,6,6	0.00	-	-		
88	OHX	2	2130	-	0,6,6	0.00	-	-		
88	OHX	2	2061	-	0,6,6	0.00	-	-		
88	OHX	5	3794	-	0,6,6	0.00	-	-		
88	OHX	N8	205	-	0,6,6	0.00	-	-		
88	OHX	C3	201	-	0,6,6	0.00	-	-		
88	OHX	6	2127	-	0,6,6	0.00	-	-		
88	OHX	1	3885	-	0,6,6	0.00	-	-		
88	OHX	5	3829	-	0,6,6	0.00	-	-		
88	OHX	5	3949	-	0,6,6	0.00	-	-		
88	OHX	1	3782	-	0,6,6	0.00	-	-		
88	OHX	5	3899	-	0,6,6	0.00	-	-		
88	OHX	1	4093	-	0,6,6	0.00	-	-		
88	OHX	2	2000	-	0,6,6	0.00	-	-		
88	OHX	6	2150	-	0,6,6	0.00	-	-		
88	OHX	1	3762	-	0,6,6	0.00	-	-		
88	OHX	1	3868	-	0,6,6	0.00	-	-		
88	OHX	2	2109	-	0,6,6	0.00	-	-		
88	OHX	c8	201	-	0,6,6	0.00	-	-		
88	OHX	8	224	-	0,6,6	0.00	-	-		
88	OHX	4	225	-	0,6,6	0.00	-	-		
88	OHX	1	3924	-	0,6,6	0.00	-	-		
88	OHX	5	3974	-	0,6,6	0.00	-	-		
88	OHX	6	2131	-	0,6,6	0.00	-	-		
88	OHX	1	4016	-	0,6,6	0.00	-	-		
88	OHX	5	4044	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	1	4080	-	0,6,6	0.00	-	-		
88	OHX	5	4136	-	0,6,6	0.00	-	-		
88	OHX	2	2080	-	0,6,6	0.00	-	-		
88	OHX	2	2110	-	0,6,6	0.00	-	-		
88	OHX	5	3821	-	0,6,6	0.00	-	-		
88	OHX	2	2031	-	0,6,6	0.00	-	-		
88	OHX	5	3951	-	0,6,6	0.00	-	-		
88	OHX	1	3893	-	0,6,6	0.00	-	-		
88	OHX	5	3877	-	0,6,6	0.00	-	-		
88	OHX	6	2142	-	0,6,6	0.00	-	-		
88	OHX	5	3811	-	0,6,6	0.00	-	-		
88	OHX	2	2066	-	0,6,6	0.00	-	-		
88	OHX	1	3805	-	0,6,6	0.00	-	-		
88	OHX	1	3866	-	0,6,6	0.00	-	-		
88	OHX	5	3948	-	0,6,6	0.00	-	-		
88	OHX	6	2057	-	0,6,6	0.00	-	-		
88	OHX	5	3919	-	0,6,6	0.00	-	-		
88	OHX	5	3925	-	0,6,6	0.00	-	-		
88	OHX	6	2027	-	0,6,6	0.00	-	-		
88	OHX	2	2097	-	0,6,6	0.00	-	-		
88	OHX	2	1998	-	0,6,6	0.00	-	-		
88	OHX	2	2044	-	0,6,6	0.00	-	-		
88	OHX	5	4010	-	0,6,6	0.00	-	-		
88	OHX	1	3876	-	0,6,6	0.00	-	-		
88	OHX	2	2128	-	0,6,6	0.00	-	-		
88	OHX	1	3791	-	0,6,6	0.00	-	-		
88	OHX	8	213	-	0,6,6	0.00	-	-		
88	OHX	1	4095	-	0,6,6	0.00	-	-		
88	OHX	2	2101	-	0,6,6	0.00	-	-		
88	OHX	5	3838	-	0,6,6	0.00	-	-		
88	OHX	8	222	-	0,6,6	0.00	-	-		
88	OHX	6	2068	-	0,6,6	0.00	-	-		
88	OHX	5	4057	-	0,6,6	0.00	-	-		
88	OHX	6	2119	-	0,6,6	0.00	-	-		
88	OHX	5	4040	-	0,6,6	0.00	-	-		
88	OHX	6	2146	-	0,6,6	0.00	-	-		
88	OHX	1	3937	-	0,6,6	0.00	-	-		
88	OHX	5	4009	-	0,6,6	0.00	-	-		
88	OHX	1	3867	-	0,6,6	0.00	-	-		
88	OHX	6	2103	-	0,6,6	0.00	-	-		
88	OHX	5	4041	-	0,6,6	0.00	-	-		
88	OHX	2	2027	-	0,6,6	0.00	-	-		
88	OHX	5	4154	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	1	4060	-	0,6,6	0.00	-	-		
88	OHX	1	4082	-	0,6,6	0.00	-	-		
88	OHX	o7	502	-	0,6,6	0.00	-	-		
88	OHX	5	3873	-	0,6,6	0.00	-	-		
88	OHX	5	3928	-	0,6,6	0.00	-	-		
88	OHX	5	3920	-	0,6,6	0.00	-	-		
88	OHX	5	4028	-	0,6,6	0.00	-	-		
88	OHX	1	3891	-	0,6,6	0.00	-	-		
88	OHX	5	3921	-	0,6,6	0.00	-	-		
88	OHX	5	4082	-	0,6,6	0.00	-	-		
88	OHX	6	2163	-	0,6,6	0.00	-	-		
88	OHX	5	4141	-	0,6,6	0.00	-	-		
88	OHX	5	4015	-	0,6,6	0.00	-	-		
88	OHX	5	4001	-	0,6,6	0.00	-	-		
88	OHX	1	3799	-	0,6,6	0.00	-	-		
88	OHX	1	4010	-	0,6,6	0.00	-	-		
88	OHX	2	2007	-	0,6,6	0.00	-	-		
88	OHX	4	227	-	0,6,6	0.00	-	-		
88	OHX	l5	303	-	0,6,6	0.00	-	-		
88	OHX	1	3788	-	0,6,6	0.00	-	-		
88	OHX	5	4109	-	0,6,6	0.00	-	-		
88	OHX	1	4056	-	0,6,6	0.00	-	-		
88	OHX	6	2107	-	0,6,6	0.00	-	-		
88	OHX	6	2109	-	0,6,6	0.00	-	-		
88	OHX	1	4022	-	0,6,6	0.00	-	-		
88	OHX	5	4069	-	0,6,6	0.00	-	-		
88	OHX	5	4144	-	0,6,6	0.00	-	-		
88	OHX	6	2014	-	0,6,6	0.00	-	-		
88	OHX	2	2025	-	0,6,6	0.00	-	-		
88	OHX	o3	201	-	0,6,6	0.00	-	-		
88	OHX	5	3887	-	0,6,6	0.00	-	-		
88	OHX	5	3867	-	0,6,6	0.00	-	-		
88	OHX	1	3913	-	0,6,6	0.00	-	-		
88	OHX	6	2069	-	0,6,6	0.00	-	-		
88	OHX	1	3934	-	0,6,6	0.00	-	-		
88	OHX	5	4156	-	0,6,6	0.00	-	-		
88	OHX	5	4119	-	0,6,6	0.00	-	-		
88	OHX	4	228	-	0,6,6	0.00	-	-		
88	OHX	5	3851	-	0,6,6	0.00	-	-		
88	OHX	5	3930	-	0,6,6	0.00	-	-		
88	OHX	5	3924	-	0,6,6	0.00	-	-		
88	OHX	q2	502	-	0,6,6	0.00	-	-		
88	OHX	O7	106	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	8	230	-	0,6,6	0.00	-	-		
88	OHX	6	2168	-	0,6,6	0.00	-	-		
88	OHX	2	1996	-	0,6,6	0.00	-	-		
88	OHX	5	4116	-	0,6,6	0.00	-	-		
88	OHX	6	2116	-	0,6,6	0.00	-	-		
88	OHX	1	3898	-	0,6,6	0.00	-	-		
88	OHX	s1	301	-	0,6,6	0.00	-	-		
88	OHX	2	2111	-	0,6,6	0.00	-	-		
88	OHX	5	4012	-	0,6,6	0.00	-	-		
88	OHX	2	2151	-	0,6,6	0.00	-	-		
88	OHX	1	4078	-	0,6,6	0.00	-	-		
88	OHX	6	2120	-	0,6,6	0.00	-	-		
88	OHX	5	3876	-	0,6,6	0.00	-	-		
88	OHX	2	2092	-	0,6,6	0.00	-	-		
88	OHX	1	4009	-	0,6,6	0.00	-	-		
88	OHX	6	2035	-	0,6,6	0.00	-	-		
88	OHX	2	2038	-	0,6,6	0.00	-	-		
88	OHX	5	4147	-	0,6,6	0.00	-	-		
88	OHX	6	2044	-	0,6,6	0.00	-	-		
88	OHX	1	4031	-	0,6,6	0.00	-	-		
88	OHX	1	3767	-	0,6,6	0.00	-	-		
88	OHX	1	4004	-	0,6,6	0.00	-	-		
88	OHX	2	2091	-	0,6,6	0.00	-	-		
88	OHX	5	4138	-	0,6,6	0.00	-	-		
88	OHX	6	2037	-	0,6,6	0.00	-	-		
88	OHX	6	2036	-	0,6,6	0.00	-	-		
88	OHX	5	4149	-	0,6,6	0.00	-	-		
88	OHX	1	4001	-	0,6,6	0.00	-	-		
88	OHX	5	3796	-	0,6,6	0.00	-	-		
88	OHX	1	3801	-	0,6,6	0.00	-	-		
88	OHX	1	4103	-	0,6,6	0.00	-	-		
88	OHX	1	3861	-	0,6,6	0.00	-	-		
88	OHX	2	2001	-	0,6,6	0.00	-	-		
88	OHX	1	4092	-	0,6,6	0.00	-	-		
88	OHX	6	2087	-	0,6,6	0.00	-	-		
88	OHX	5	3837	-	0,6,6	0.00	-	-		
88	OHX	1	3841	-	0,6,6	0.00	-	-		
88	OHX	6	2178	-	0,6,6	0.00	-	-		
88	OHX	1	3967	-	0,6,6	0.00	-	-		
88	OHX	1	3935	-	0,6,6	0.00	-	-		
88	OHX	5	4125	-	0,6,6	0.00	-	-		
88	OHX	5	3880	-	0,6,6	0.00	-	-		
88	OHX	1	4040	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	2	2020	-	0,6,6	0.00	-	-		
88	OHX	2	2081	-	0,6,6	0.00	-	-		
88	OHX	2	2043	-	0,6,6	0.00	-	-		
88	OHX	5	3865	-	0,6,6	0.00	-	-		
88	OHX	4	222	-	0,6,6	0.00	-	-		
88	OHX	5	3973	-	0,6,6	0.00	-	-		
88	OHX	1	3884	-	0,6,6	0.00	-	-		
88	OHX	s9	201	-	0,6,6	0.00	-	-		
88	OHX	M0	302	-	0,6,6	0.00	-	-		
88	OHX	1	4026	-	0,6,6	0.00	-	-		
88	OHX	5	4132	-	0,6,6	0.00	-	-		
88	OHX	1	4101	-	0,6,6	0.00	-	-		
88	OHX	M9	201	-	0,6,6	0.00	-	-		
88	OHX	1	3871	-	0,6,6	0.00	-	-		
88	OHX	5	4055	-	0,6,6	0.00	-	-		
88	OHX	2	2112	-	0,6,6	0.00	-	-		
88	OHX	5	4087	-	0,6,6	0.00	-	-		
88	OHX	1	3827	-	0,6,6	0.00	-	-		
88	OHX	2	2018	-	0,6,6	0.00	-	-		
88	OHX	1	3779	-	0,6,6	0.00	-	-		
88	OHX	2	2060	-	0,6,6	0.00	-	-		
88	OHX	5	3984	-	0,6,6	0.00	-	-		
88	OHX	1	3846	-	0,6,6	0.00	-	-		
88	OHX	3	212	-	0,6,6	0.00	-	-		
88	OHX	1	3772	-	0,6,6	0.00	-	-		
88	OHX	2	2100	-	0,6,6	0.00	-	-		
88	OHX	6	2099	-	0,6,6	0.00	-	-		
88	OHX	1	4085	-	0,6,6	0.00	-	-		
88	OHX	1	3925	-	0,6,6	0.00	-	-		
88	OHX	1	3975	-	0,6,6	0.00	-	-		
88	OHX	1	4044	-	0,6,6	0.00	-	-		
88	OHX	5	4099	-	0,6,6	0.00	-	-		
88	OHX	1	3996	-	0,6,6	0.00	-	-		
88	OHX	6	2125	-	0,6,6	0.00	-	-		
88	OHX	3	209	-	0,6,6	0.00	-	-		
88	OHX	1	3974	-	0,6,6	0.00	-	-		
88	OHX	7	225	-	0,6,6	0.00	-	-		
88	OHX	5	4090	-	0,6,6	0.00	-	-		
88	OHX	5	3836	-	0,6,6	0.00	-	-		
88	OHX	1	4030	-	0,6,6	0.00	-	-		
88	OHX	5	4080	-	0,6,6	0.00	-	-		
88	OHX	5	3909	-	0,6,6	0.00	-	-		
88	OHX	5	3990	-	0,6,6	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	5	3955	-	0,6,6	0.00	-	-		
88	OHX	1	4067	-	0,6,6	0.00	-	-		
88	OHX	19	201	-	0,6,6	0.00	-	-		
88	OHX	2	2106	-	0,6,6	0.00	-	-		
88	OHX	5	4019	-	0,6,6	0.00	-	-		
88	OHX	1	3948	-	0,6,6	0.00	-	-		
88	OHX	m0	303	-	0,6,6	0.00	-	-		
88	OHX	1	4021	-	0,6,6	0.00	-	-		
88	OHX	2	2012	-	0,6,6	0.00	-	-		
88	OHX	1	3802	-	0,6,6	0.00	-	-		
88	OHX	1	3933	-	0,6,6	0.00	-	-		
88	OHX	7	219	-	0,6,6	0.00	-	-		
88	OHX	1	3873	-	0,6,6	0.00	-	-		
88	OHX	5	4018	-	0,6,6	0.00	-	-		
88	OHX	2	2116	-	0,6,6	0.00	-	-		
88	OHX	1	3814	-	0,6,6	0.00	-	-		
88	OHX	1	4027	-	0,6,6	0.00	-	-		
88	OHX	6	2055	-	0,6,6	0.00	-	-		
88	OHX	5	3883	-	0,6,6	0.00	-	-		
88	OHX	5	3871	-	0,6,6	0.00	-	-		
88	OHX	2	2090	-	0,6,6	0.00	-	-		
88	OHX	1	3963	-	0,6,6	0.00	-	-		
88	OHX	5	4038	-	0,6,6	0.00	-	-		
88	OHX	5	4123	-	0,6,6	0.00	-	-		
88	OHX	5	4140	-	0,6,6	0.00	-	-		
88	OHX	5	3980	-	0,6,6	0.00	-	-		
88	OHX	1	3869	-	0,6,6	0.00	-	-		
88	OHX	5	3911	-	0,6,6	0.00	-	-		
88	OHX	8	223	-	0,6,6	0.00	-	-		
88	OHX	6	2083	-	0,6,6	0.00	-	-		
88	OHX	5	3807	-	0,6,6	0.00	-	-		
88	OHX	5	4105	-	0,6,6	0.00	-	-		
88	OHX	5	3828	-	0,6,6	0.00	-	-		
88	OHX	5	3868	-	0,6,6	0.00	-	-		
88	OHX	5	4034	-	0,6,6	0.00	-	-		
88	OHX	5	4122	-	0,6,6	0.00	-	-		
88	OHX	5	3812	-	0,6,6	0.00	-	-		
88	OHX	2	2006	-	0,6,6	0.00	-	-		
88	OHX	1	3849	-	0,6,6	0.00	-	-		
88	OHX	l3	403	-	0,6,6	0.00	-	-		
88	OHX	5	3809	-	0,6,6	0.00	-	-		
88	OHX	14	401	-	0,6,6	0.00	-	-		
88	OHX	1	3980	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	5	3799	-	0,6,6	0.00	-	-		
88	OHX	5	3927	-	0,6,6	0.00	-	-		
88	OHX	6	2064	-	0,6,6	0.00	-	-		
88	OHX	8	215	-	0,6,6	0.00	-	-		
88	OHX	6	2110	-	0,6,6	0.00	-	-		
88	OHX	5	4146	-	0,6,6	0.00	-	-		
88	OHX	5	4011	-	0,6,6	0.00	-	-		
88	OHX	5	3845	-	0,6,6	0.00	-	-		
88	OHX	4	229	-	0,6,6	0.00	-	-		
88	OHX	5	3931	-	0,6,6	0.00	-	-		
88	OHX	2	2086	-	0,6,6	0.00	-	-		
88	OHX	5	3853	-	0,6,6	0.00	-	-		
88	OHX	6	2056	-	0,6,6	0.00	-	-		
88	OHX	5	3941	-	0,6,6	0.00	-	-		
88	OHX	5	4062	-	0,6,6	0.00	-	-		
88	OHX	1	3894	-	0,6,6	0.00	-	-		
88	OHX	5	4049	-	0,6,6	0.00	-	-		
88	OHX	6	2114	-	0,6,6	0.00	-	-		
88	OHX	1	3807	-	0,6,6	0.00	-	-		
88	OHX	1	3808	-	0,6,6	0.00	-	-		
88	OHX	6	2045	-	0,6,6	0.00	-	-		
88	OHX	5	3896	-	0,6,6	0.00	-	-		
88	OHX	1	3833	-	0,6,6	0.00	-	-		
88	OHX	6	2020	-	0,6,6	0.00	-	-		
88	OHX	5	3826	-	0,6,6	0.00	-	-		
88	OHX	5	4035	-	0,6,6	0.00	-	-		
88	OHX	6	2062	-	0,6,6	0.00	-	-		
88	OHX	5	3819	-	0,6,6	0.00	-	-		
88	OHX	2	2008	-	0,6,6	0.00	-	-		
88	OHX	5	4071	-	0,6,6	0.00	-	-		
88	OHX	5	4050	-	0,6,6	0.00	-	-		
88	OHX	1	4033	-	0,6,6	0.00	-	-		
88	OHX	1	3800	-	0,6,6	0.00	-	-		
88	OHX	1	4005	-	0,6,6	0.00	-	-		
88	OHX	5	3800	-	0,6,6	0.00	-	-		
88	OHX	6	2091	-	0,6,6	0.00	-	-		
88	OHX	1	4002	-	0,6,6	0.00	-	-		
88	OHX	6	2080	-	0,6,6	0.00	-	-		
88	OHX	5	4039	-	0,6,6	0.00	-	-		
88	OHX	1	4045	-	0,6,6	0.00	-	-		
88	OHX	6	2093	-	0,6,6	0.00	-	-		
88	OHX	3	217	-	0,6,6	0.00	-	-		
88	OHX	1	3771	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	5	4108	-	0,6,6	0.00	-	-		
88	OHX	5	3888	-	0,6,6	0.00	-	-		
88	OHX	1	3864	-	0,6,6	0.00	-	-		
88	OHX	1	3955	-	0,6,6	0.00	-	-		
88	OHX	1	3966	-	0,6,6	0.00	-	-		
88	OHX	7	216	-	0,6,6	0.00	-	-		
88	OHX	6	2042	-	0,6,6	0.00	-	-		
88	OHX	1	4084	-	0,6,6	0.00	-	-		
88	OHX	5	3957	-	0,6,6	0.00	-	-		
88	OHX	2	2049	-	0,6,6	0.00	-	-		
88	OHX	5	4143	-	0,6,6	0.00	-	-		
88	OHX	1	3912	-	0,6,6	0.00	-	-		
88	OHX	m7	204	-	0,6,6	0.00	-	-		
88	OHX	4	230	-	0,6,6	0.00	-	-		
88	OHX	5	3961	-	0,6,6	0.00	-	-		
88	OHX	1	4065	-	0,6,6	0.00	-	-		
88	OHX	1	3988	-	0,6,6	0.00	-	-		
88	OHX	1	3792	-	0,6,6	0.00	-	-		
88	OHX	5	3942	-	0,6,6	0.00	-	-		
88	OHX	5	4027	-	0,6,6	0.00	-	-		
88	OHX	1	3882	-	0,6,6	0.00	-	-		
88	OHX	1	4090	-	0,6,6	0.00	-	-		
88	OHX	8	218	-	0,6,6	0.00	-	-		
88	OHX	5	3834	-	0,6,6	0.00	-	-		
88	OHX	5	3987	-	0,6,6	0.00	-	-		
88	OHX	1	4077	-	0,6,6	0.00	-	-		
88	OHX	2	2129	-	0,6,6	0.00	-	-		
88	OHX	8	227	-	0,6,6	0.00	-	-		
88	OHX	S8	301	-	0,6,6	0.00	-	-		
88	OHX	5	4003	-	0,6,6	0.00	-	-		
88	OHX	s8	302	-	0,6,6	0.00	-	-		
88	OHX	5	4127	-	0,6,6	0.00	-	-		
88	OHX	1	4013	-	0,6,6	0.00	-	-		
88	OHX	M0	303	-	0,6,6	0.00	-	-		
88	OHX	6	2048	-	0,6,6	0.00	-	-		
88	OHX	5	3967	-	0,6,6	0.00	-	-		
88	OHX	14	402	-	0,6,6	0.00	-	-		
88	OHX	1	3916	-	0,6,6	0.00	-	-		
88	OHX	2	2146	-	0,6,6	0.00	-	-		
88	OHX	1	4023	-	0,6,6	0.00	-	-		
88	OHX	2	2136	-	0,6,6	0.00	-	-		
88	OHX	7	223	-	0,6,6	0.00	-	-		
88	OHX	2	2084	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	1	3961	-	0,6,6	0.00	-	-		
88	OHX	2	2124	-	0,6,6	0.00	-	-		
88	OHX	1	3905	-	0,6,6	0.00	-	-		
88	OHX	5	3996	-	0,6,6	0.00	-	-		
88	OHX	6	2166	-	0,6,6	0.00	-	-		
88	OHX	2	2045	-	0,6,6	0.00	-	-		
88	OHX	2	2141	-	0,6,6	0.00	-	-		
88	OHX	1	3856	-	0,6,6	0.00	-	-		
88	OHX	1	4086	-	0,6,6	0.00	-	-		
88	OHX	2	2094	-	0,6,6	0.00	-	-		
88	OHX	5	4075	-	0,6,6	0.00	-	-		
88	OHX	SR	401	-	0,6,6	0.00	-	-		
88	OHX	3	215	-	0,6,6	0.00	-	-		
88	OHX	2	2082	-	0,6,6	0.00	-	-		
88	OHX	2	2072	-	0,6,6	0.00	-	-		
88	OHX	7	224	-	0,6,6	0.00	-	-		
88	OHX	1	4079	-	0,6,6	0.00	-	-		
88	OHX	2	2032	-	0,6,6	0.00	-	-		
88	OHX	1	3798	-	0,6,6	0.00	-	-		
88	OHX	5	3913	-	0,6,6	0.00	-	-		
88	OHX	5	3916	-	0,6,6	0.00	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

582 monomers are involved in 844 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	1	4020	OHX	3	0
88	1	3965	OHX	1	0
88	5	4051	OHX	1	0
88	1	4099	OHX	1	0
88	2	2013	OHX	1	0
88	1	3783	OHX	1	0
88	3	211	OHX	1	0
88	1	3938	OHX	1	0
88	1	3879	OHX	1	0
88	6	2184	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	6	2137	OHX	1	0
88	1	3844	OHX	1	0
88	5	4000	OHX	3	0
88	1	4075	OHX	1	0
88	1	3930	OHX	1	0
88	2	2002	OHX	1	0
88	M7	205	OHX	2	0
88	S9	202	OHX	1	0
88	5	4064	OHX	1	0
88	2	2071	OHX	2	0
88	1	3990	OHX	1	0
88	1	3928	OHX	1	0
88	1	3927	OHX	5	0
88	1	3847	OHX	1	0
88	5	4157	OHX	4	0
88	2	2034	OHX	1	0
88	5	3860	OHX	2	0
88	5	3937	OHX	2	0
88	5	3810	OHX	1	0
88	5	4134	OHX	1	0
88	4	221	OHX	2	0
88	6	2051	OHX	1	0
88	6	2126	OHX	4	0
88	C5	201	OHX	2	0
88	5	4150	OHX	1	0
88	5	4021	OHX	2	0
88	8	219	OHX	1	0
88	1	3950	OHX	2	0
88	5	3870	OHX	1	0
88	1	3766	OHX	1	0
88	S1	301	OHX	3	0
88	1	3969	OHX	1	0
88	1	3983	OHX	2	0
88	1	3982	OHX	1	0
88	6	2033	OHX	1	0
88	1	3818	OHX	1	0
88	5	4091	OHX	1	0
88	2	2102	OHX	4	0
88	5	3900	OHX	6	0
88	5	3905	OHX	2	0
88	D9	103	OHX	1	0
88	5	4036	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	2	2058	OHX	1	0
88	O7	105	OHX	3	0
88	2	2055	OHX	2	0
88	1	3860	OHX	1	0
88	5	3940	OHX	1	0
88	1	3764	OHX	1	0
88	2	2119	OHX	2	0
88	5	4078	OHX	1	0
88	1	4039	OHX	1	0
88	5	3976	OHX	3	0
88	L5	301	OHX	1	0
88	6	2141	OHX	1	0
88	1	3770	OHX	1	0
88	5	4074	OHX	1	0
88	5	3891	OHX	1	0
88	1	4068	OHX	6	0
88	2	2029	OHX	1	0
88	2	2107	OHX	1	0
88	5	3971	OHX	1	0
88	5	4094	OHX	1	0
88	5	4102	OHX	1	0
88	2	2030	OHX	1	0
88	1	3998	OHX	1	0
88	6	2164	OHX	1	0
88	5	4095	OHX	1	0
88	6	2016	OHX	1	0
88	1	3962	OHX	1	0
88	6	2074	OHX	2	0
88	2	2056	OHX	1	0
88	1	3970	OHX	1	0
88	2	2011	OHX	1	0
88	2	2076	OHX	1	0
88	2	2009	OHX	2	0
88	1	3903	OHX	2	0
88	2	2087	OHX	1	0
88	1	3949	OHX	1	0
88	6	2053	OHX	1	0
88	5	4053	OHX	2	0
88	2	2015	OHX	1	0
88	1	3758	OHX	1	0
88	6	2084	OHX	1	0
88	1	4089	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	1	3971	OHX	1	0
88	5	3918	OHX	1	0
88	1	4011	OHX	1	0
88	2	2127	OHX	1	0
88	5	4089	OHX	1	0
88	M5	301	OHX	1	0
88	6	2153	OHX	1	0
88	5	4106	OHX	5	0
88	6	2079	OHX	1	0
88	2	2074	OHX	3	0
88	5	3854	OHX	1	0
88	2	2036	OHX	1	0
88	1	4003	OHX	1	0
88	5	3952	OHX	1	0
88	1	3804	OHX	2	0
88	2	2138	OHX	3	0
88	6	2096	OHX	4	0
88	2	2052	OHX	1	0
88	8	214	OHX	1	0
88	6	2095	OHX	1	0
88	6	2081	OHX	2	0
88	2	2021	OHX	1	0
88	2	1994	OHX	2	0
88	N1	201	OHX	1	0
88	1	3836	OHX	2	0
88	5	3966	OHX	1	0
88	5	3988	OHX	1	0
88	1	3943	OHX	1	0
88	5	3863	OHX	1	0
88	1	3886	OHX	1	0
88	1	4104	OHX	1	0
88	2	2023	OHX	1	0
88	5	4121	OHX	2	0
88	5	3886	OHX	1	0
88	6	2148	OHX	1	0
88	5	3859	OHX	1	0
88	1	4042	OHX	1	0
88	2	2033	OHX	1	0
88	5	3995	OHX	2	0
88	6	2050	OHX	1	0
88	8	216	OHX	1	0
88	5	4092	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	1	3993	OHX	1	0
88	1	4063	OHX	3	0
88	5	3970	OHX	3	0
88	6	2089	OHX	1	0
88	1	3821	OHX	2	0
88	1	3984	OHX	1	0
88	1	3862	OHX	2	0
88	1	3991	OHX	1	0
88	1	3920	OHX	2	0
88	5	3848	OHX	1	0
88	5	4022	OHX	1	0
88	2	2135	OHX	1	0
88	8	221	OHX	1	0
88	5	3926	OHX	1	0
88	5	3822	OHX	1	0
88	2	2079	OHX	3	0
88	1	3810	OHX	1	0
88	2	2104	OHX	3	0
88	5	3962	OHX	2	0
88	5	4058	OHX	1	0
88	5	4124	OHX	2	0
88	5	3805	OHX	1	0
88	1	3775	OHX	2	0
88	4	223	OHX	1	0
88	1	3781	OHX	1	0
88	2	2143	OHX	1	0
88	5	4025	OHX	1	0
88	2	2098	OHX	1	0
88	1	3923	OHX	2	0
88	5	3998	OHX	1	0
88	6	2097	OHX	1	0
88	5	3823	OHX	2	0
88	1	4006	OHX	2	0
88	6	2101	OHX	1	0
88	1	4064	OHX	2	0
88	2	2062	OHX	1	0
88	7	221	OHX	1	0
88	1	3909	OHX	1	0
88	1	3880	OHX	1	0
88	5	4111	OHX	1	0
88	2	2064	OHX	2	0
88	2	2133	OHX	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	1	4038	OHX	1	0
88	2	2016	OHX	1	0
88	2	2075	OHX	2	0
88	1	3795	OHX	1	0
88	5	3833	OHX	1	0
88	5	4107	OHX	3	0
88	6	2140	OHX	1	0
88	5	4032	OHX	2	0
88	1	3850	OHX	1	0
88	5	3946	OHX	1	0
88	6	2134	OHX	2	0
88	5	3959	OHX	1	0
88	1	3957	OHX	1	0
88	1	4051	OHX	1	0
88	1	3768	OHX	1	0
88	5	4065	OHX	1	0
88	2	2122	OHX	1	0
88	6	2040	OHX	4	0
88	5	4084	OHX	1	0
88	5	4042	OHX	1	0
88	1	3892	OHX	2	0
88	5	4072	OHX	1	0
88	2	2003	OHX	1	0
88	1	4071	OHX	1	0
88	1	3773	OHX	2	0
88	1	3942	OHX	2	0
88	1	4012	OHX	1	0
88	1	4032	OHX	2	0
88	5	3806	OHX	1	0
88	5	4112	OHX	2	0
88	2	2024	OHX	2	0
88	5	3890	OHX	1	0
88	1	4062	OHX	1	0
88	5	3912	OHX	1	0
88	6	2156	OHX	2	0
88	1	4035	OHX	1	0
88	5	3947	OHX	1	0
88	5	3831	OHX	1	0
88	1	3964	OHX	1	0
88	5	4152	OHX	1	0
88	5	3997	OHX	2	0
88	6	2060	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	6	2121	OHX	2	0
88	1	3985	OHX	2	0
88	1	3953	OHX	2	0
88	5	3847	OHX	1	0
88	5	3972	OHX	1	0
88	6	2145	OHX	1	0
88	2	2148	OHX	1	0
88	2	2132	OHX	1	0
88	O3	203	OHX	1	0
88	1	3875	OHX	2	0
88	5	3982	OHX	1	0
88	1	3819	OHX	2	0
88	6	2135	OHX	1	0
88	1	3902	OHX	1	0
88	5	4110	OHX	1	0
88	4	235	OHX	1	0
88	1	3904	OHX	2	0
88	S6	301	OHX	3	0
88	5	4052	OHX	1	0
88	1	3852	OHX	2	0
88	5	3943	OHX	1	0
88	8	225	OHX	1	0
88	5	3803	OHX	1	0
88	1	3826	OHX	1	0
88	1	4053	OHX	1	0
88	5	3818	OHX	1	0
88	2	2028	OHX	1	0
88	6	2022	OHX	1	0
88	1	3825	OHX	3	0
88	6	2067	OHX	4	0
88	5	3858	OHX	1	0
88	5	3935	OHX	2	0
88	5	4047	OHX	1	0
88	2	2137	OHX	1	0
88	5	3979	OHX	1	0
88	2	2041	OHX	1	0
88	6	2102	OHX	1	0
88	5	4067	OHX	1	0
88	1	3915	OHX	1	0
88	1	4046	OHX	2	0
88	2	2022	OHX	1	0
88	1	3940	OHX	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	6	2152	OHX	2	0
88	6	2151	OHX	1	0
88	5	3795	OHX	1	0
88	2	2067	OHX	1	0
88	6	2066	OHX	1	0
88	5	4048	OHX	1	0
88	1	3951	OHX	3	0
88	1	4070	OHX	1	0
88	6	2182	OHX	1	0
88	5	3839	OHX	1	0
88	5	4085	OHX	1	0
88	1	3946	OHX	1	0
88	5	3968	OHX	1	0
88	4	224	OHX	1	0
88	2	2017	OHX	2	0
88	5	4118	OHX	1	0
88	2	2134	OHX	1	0
88	6	2169	OHX	1	0
88	1	4017	OHX	1	0
88	5	4024	OHX	2	0
88	N9	102	OHX	1	0
88	6	2136	OHX	2	0
88	1	3995	OHX	1	0
88	6	2179	OHX	1	0
88	6	2075	OHX	1	0
88	5	3797	OHX	2	0
88	2	2150	OHX	5	0
88	2	2042	OHX	1	0
88	5	3994	OHX	1	0
88	5	3945	OHX	2	0
88	6	2144	OHX	1	0
88	6	2175	OHX	2	0
88	6	2029	OHX	1	0
88	1	3888	OHX	2	0
88	5	3852	OHX	4	0
88	1	3936	OHX	1	0
88	1	3829	OHX	1	0
88	5	3885	OHX	2	0
88	6	2159	OHX	2	0
88	6	2025	OHX	1	0
88	2	2108	OHX	1	0
88	5	3814	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	1	3845	OHX	1	0
88	6	2174	OHX	3	0
88	5	3864	OHX	1	0
88	2	2117	OHX	2	0
88	5	4159	OHX	1	0
88	1	3778	OHX	1	0
88	6	2139	OHX	1	0
88	5	4081	OHX	2	0
88	1	3899	OHX	1	0
88	5	3923	OHX	1	0
88	3	218	OHX	1	0
88	6	2028	OHX	1	0
88	1	3897	OHX	2	0
88	1	3806	OHX	1	0
88	2	2105	OHX	1	0
88	1	3874	OHX	1	0
88	1	4097	OHX	1	0
88	7	218	OHX	1	0
88	5	4005	OHX	1	0
88	1	4028	OHX	1	0
88	1	3851	OHX	6	0
88	2	2005	OHX	2	0
88	5	3978	OHX	1	0
88	1	4069	OHX	2	0
88	2	2068	OHX	2	0
88	1	4100	OHX	2	0
88	5	3855	OHX	2	0
88	5	3934	OHX	1	0
88	5	3975	OHX	3	0
88	1	4037	OHX	1	0
88	2	2040	OHX	1	0
88	6	2086	OHX	4	0
88	6	2076	OHX	1	0
88	5	4016	OHX	1	0
88	5	3832	OHX	1	0
88	6	2070	OHX	1	0
88	5	3950	OHX	2	0
88	5	3861	OHX	2	0
88	5	4083	OHX	1	0
88	5	4004	OHX	1	0
88	2	2142	OHX	1	0
88	2	2147	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	M7	204	OHX	1	0
88	2	2010	OHX	2	0
88	5	3881	OHX	2	0
88	L3	404	OHX	3	0
88	2	1997	OHX	2	0
88	5	3840	OHX	1	0
88	6	2160	OHX	2	0
88	5	3804	OHX	1	0
88	1	3939	OHX	4	0
88	1	3952	OHX	1	0
88	5	4079	OHX	1	0
88	1	3776	OHX	2	0
88	6	2092	OHX	1	0
88	5	3939	OHX	1	0
88	6	2104	OHX	2	0
88	5	4130	OHX	1	0
88	Q2	503	OHX	1	0
88	5	3904	OHX	1	0
88	5	4137	OHX	3	0
88	5	4126	OHX	6	0
88	O9	101	OHX	1	0
88	2	2037	OHX	1	0
88	5	3813	OHX	1	0
88	8	229	OHX	1	0
88	5	4096	OHX	1	0
88	1	3999	OHX	1	0
88	6	2038	OHX	1	0
88	5	4088	OHX	2	0
88	6	2032	OHX	1	0
88	1	4025	OHX	1	0
88	3	214	OHX	1	0
88	6	2177	OHX	1	0
88	1	4050	OHX	2	0
88	2	2125	OHX	1	0
88	8	220	OHX	1	0
88	5	3884	OHX	1	0
88	1	4036	OHX	1	0
88	5	3898	OHX	1	0
88	1	3979	OHX	2	0
88	1	3855	OHX	1	0
88	5	4142	OHX	1	0
88	6	2106	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	5	4153	OHX	1	0
88	2	2053	OHX	1	0
88	5	4059	OHX	2	0
88	6	2170	OHX	1	0
88	1	4055	OHX	2	0
88	6	2063	OHX	3	0
88	1	4072	OHX	1	0
88	5	4013	OHX	2	0
88	2	1999	OHX	1	0
88	L4	401	OHX	4	0
88	6	2085	OHX	2	0
88	5	3933	OHX	2	0
88	5	3843	OHX	1	0
88	1	4107	OHX	2	0
88	5	4068	OHX	3	0
88	2	2113	OHX	1	0
88	1	3823	OHX	1	0
88	6	2173	OHX	1	0
88	4	231	OHX	1	0
88	1	4096	OHX	1	0
88	8	231	OHX	1	0
88	2	2126	OHX	2	0
88	1	3813	OHX	1	0
88	5	4139	OHX	1	0
88	1	4102	OHX	1	0
88	2	2131	OHX	1	0
88	1	3870	OHX	2	0
88	2	2130	OHX	1	0
88	2	2061	OHX	8	0
88	C3	201	OHX	5	0
88	6	2127	OHX	4	0
88	5	3829	OHX	1	0
88	5	3949	OHX	1	0
88	1	3782	OHX	2	0
88	5	3899	OHX	1	0
88	1	3762	OHX	2	0
88	1	3868	OHX	1	0
88	4	225	OHX	1	0
88	1	4016	OHX	2	0
88	1	4080	OHX	2	0
88	2	2031	OHX	1	0
88	5	3951	OHX	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	1	3893	OHX	1	0
88	6	2142	OHX	4	0
88	1	3805	OHX	1	0
88	5	3948	OHX	1	0
88	5	3925	OHX	1	0
88	6	2027	OHX	1	0
88	2	2097	OHX	1	0
88	2	2044	OHX	2	0
88	1	3876	OHX	3	0
88	2	2101	OHX	1	0
88	5	3838	OHX	1	0
88	8	222	OHX	2	0
88	5	4040	OHX	3	0
88	6	2146	OHX	1	0
88	1	3937	OHX	2	0
88	5	4041	OHX	1	0
88	5	4154	OHX	1	0
88	1	4060	OHX	2	0
88	5	3873	OHX	1	0
88	5	3928	OHX	2	0
88	5	3920	OHX	1	0
88	5	3921	OHX	2	0
88	5	4082	OHX	2	0
88	5	4001	OHX	1	0
88	1	4010	OHX	1	0
88	2	2007	OHX	1	0
88	1	3788	OHX	1	0
88	1	4056	OHX	1	0
88	6	2109	OHX	4	0
88	6	2014	OHX	1	0
88	1	3913	OHX	1	0
88	6	2069	OHX	2	0
88	5	4156	OHX	1	0
88	4	228	OHX	1	0
88	5	3851	OHX	3	0
88	5	3930	OHX	3	0
88	O7	106	OHX	1	0
88	8	230	OHX	1	0
88	2	1996	OHX	1	0
88	6	2116	OHX	1	0
88	1	3898	OHX	1	0
88	2	2111	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	5	3876	OHX	2	0
88	2	2092	OHX	4	0
88	1	4009	OHX	1	0
88	6	2044	OHX	1	0
88	1	3767	OHX	1	0
88	2	2091	OHX	1	0
88	5	4138	OHX	1	0
88	6	2037	OHX	1	0
88	6	2036	OHX	1	0
88	5	4149	OHX	1	0
88	1	4001	OHX	6	0
88	5	3796	OHX	2	0
88	1	3801	OHX	1	0
88	1	4103	OHX	1	0
88	6	2087	OHX	1	0
88	1	3841	OHX	1	0
88	1	3935	OHX	2	0
88	1	4040	OHX	2	0
88	2	2020	OHX	1	0
88	4	222	OHX	1	0
88	1	3884	OHX	1	0
88	M0	302	OHX	1	0
88	5	4132	OHX	1	0
88	1	4101	OHX	1	0
88	M9	201	OHX	2	0
88	1	3871	OHX	2	0
88	5	4055	OHX	2	0
88	1	3779	OHX	1	0
88	2	2100	OHX	1	0
88	1	3975	OHX	1	0
88	5	4099	OHX	2	0
88	3	209	OHX	1	0
88	7	225	OHX	1	0
88	5	3836	OHX	1	0
88	5	4080	OHX	2	0
88	5	3990	OHX	1	0
88	5	3955	OHX	1	0
88	1	3802	OHX	1	0
88	7	219	OHX	1	0
88	1	3873	OHX	1	0
88	5	4018	OHX	1	0
88	2	2116	OHX	1	0

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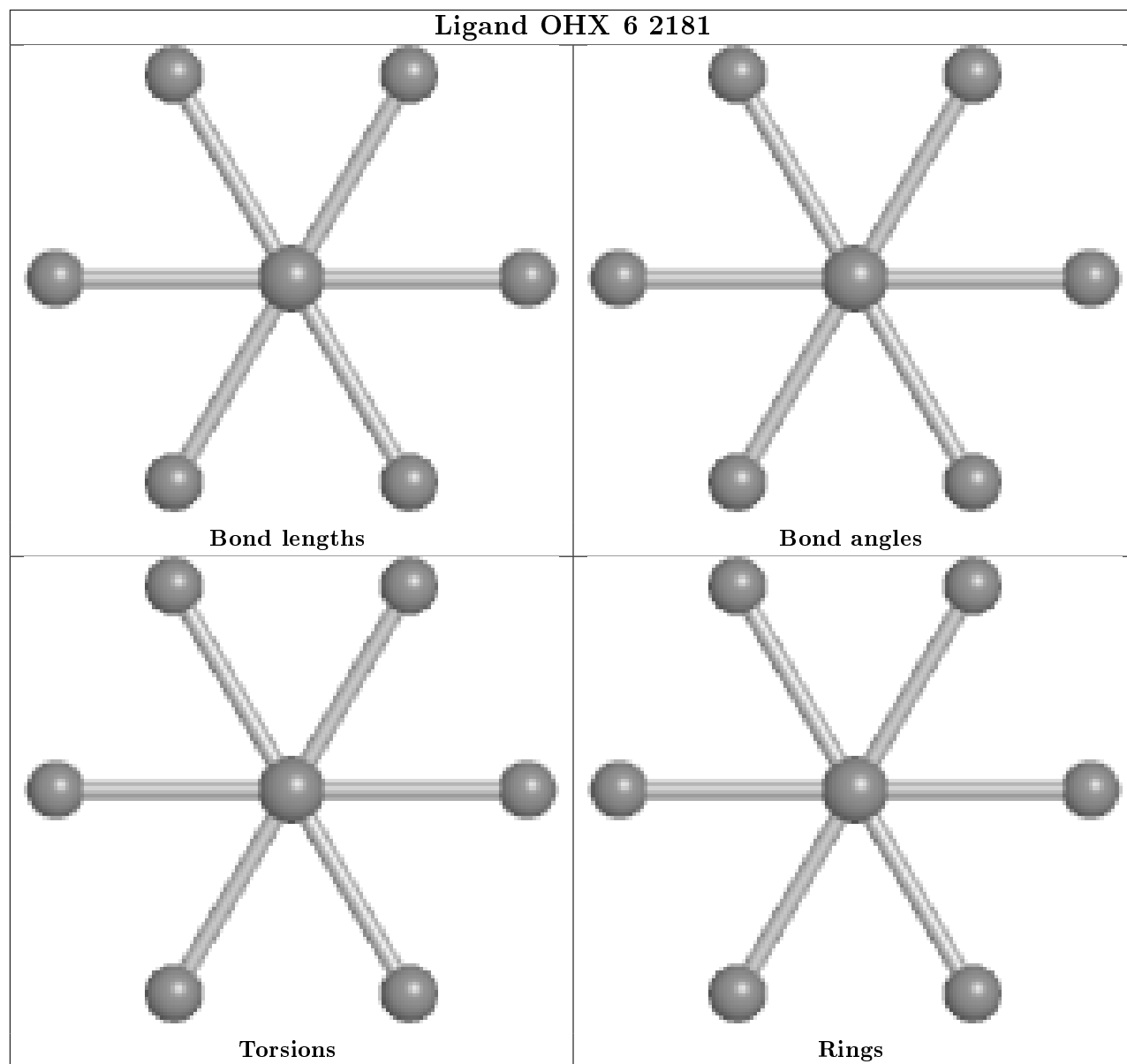
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	1	3814	OHX	1	0
88	6	2055	OHX	1	0
88	2	2090	OHX	1	0
88	5	4038	OHX	1	0
88	5	4140	OHX	1	0
88	5	3911	OHX	2	0
88	8	223	OHX	1	0
88	5	3807	OHX	2	0
88	5	3828	OHX	1	0
88	5	3868	OHX	1	0
88	5	4034	OHX	1	0
88	2	2006	OHX	1	0
88	1	3849	OHX	1	0
88	5	3809	OHX	2	0
88	1	3980	OHX	2	0
88	5	3799	OHX	2	0
88	6	2064	OHX	1	0
88	8	215	OHX	1	0
88	6	2110	OHX	1	0
88	5	3845	OHX	1	0
88	5	3931	OHX	1	0
88	2	2086	OHX	2	0
88	5	3853	OHX	1	0
88	5	3941	OHX	1	0
88	1	3894	OHX	1	0
88	1	3808	OHX	1	0
88	6	2045	OHX	2	0
88	5	3896	OHX	1	0
88	1	3833	OHX	1	0
88	6	2020	OHX	1	0
88	2	2008	OHX	2	0
88	5	4071	OHX	2	0
88	1	4033	OHX	1	0
88	6	2091	OHX	1	0
88	1	4002	OHX	1	0
88	1	4045	OHX	2	0
88	5	4108	OHX	1	0
88	1	3864	OHX	1	0
88	1	3955	OHX	1	0
88	1	4084	OHX	1	0
88	2	2049	OHX	1	0
88	5	4143	OHX	1	0

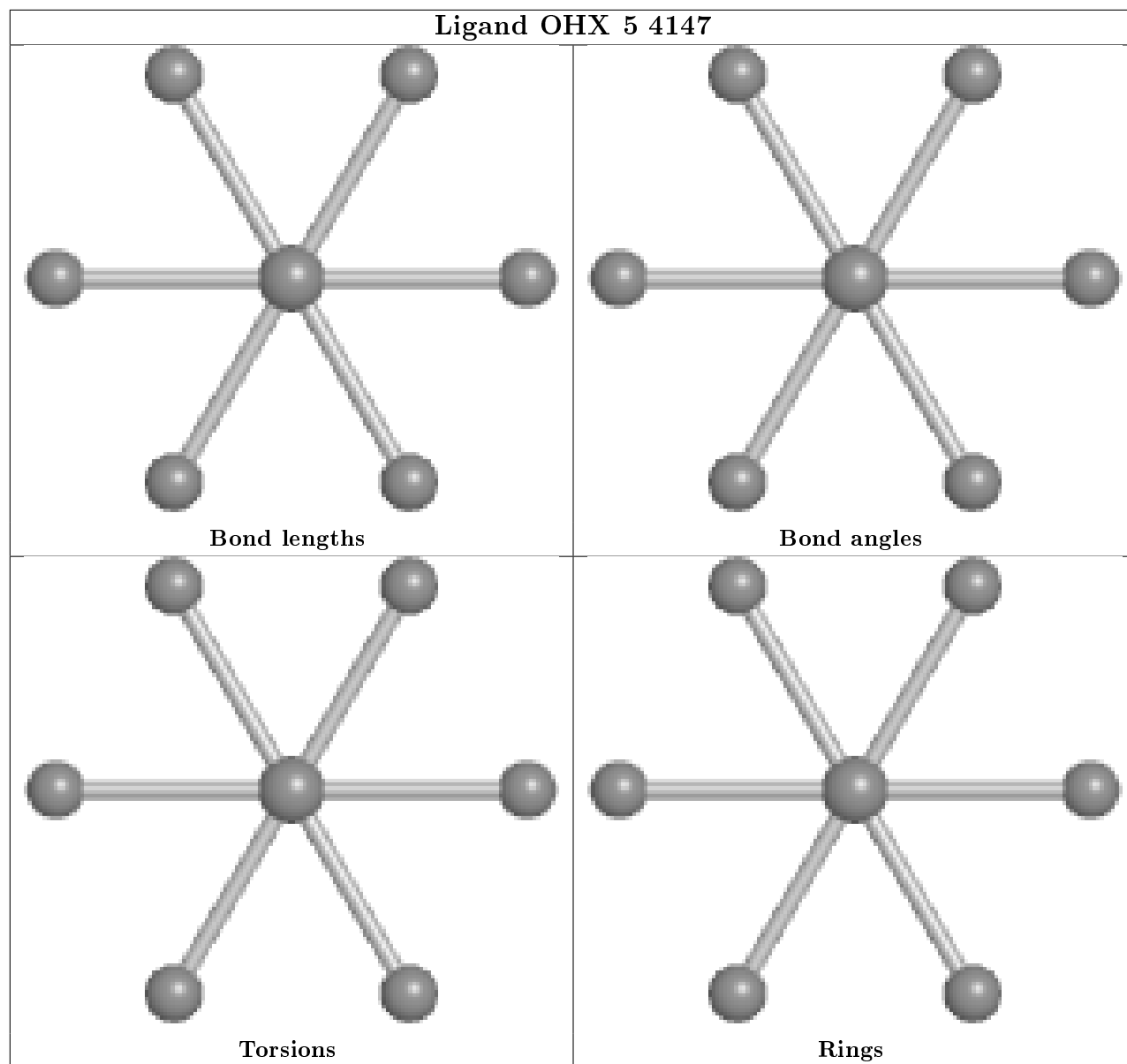
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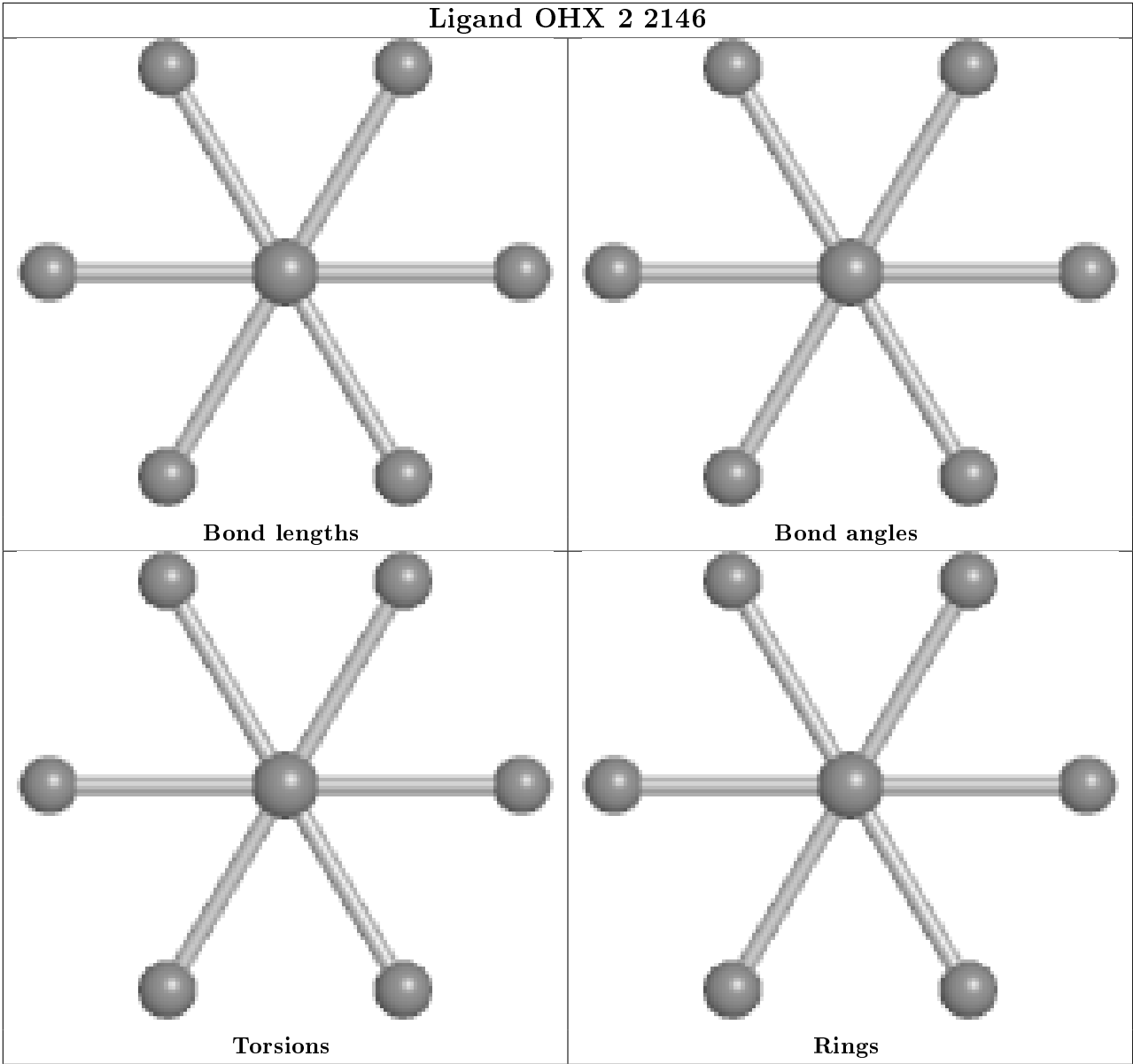
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	5	3961	OHX	4	0
88	1	4065	OHX	1	0
88	1	3792	OHX	1	0
88	1	3882	OHX	2	0
88	1	4090	OHX	2	0
88	5	3834	OHX	1	0
88	5	3987	OHX	3	0
88	1	4077	OHX	4	0
88	2	2129	OHX	3	0
88	8	227	OHX	1	0
88	S8	301	OHX	2	0
88	5	4003	OHX	2	0
88	M0	303	OHX	3	0
88	5	3967	OHX	1	0
88	1	4023	OHX	1	0
88	1	3961	OHX	1	0
88	5	3996	OHX	2	0
88	6	2166	OHX	1	0
88	2	2045	OHX	1	0
88	1	4086	OHX	1	0
88	5	4075	OHX	1	0
88	SR	401	OHX	3	0
88	2	2082	OHX	3	0
88	7	224	OHX	1	0
88	5	3913	OHX	1	0
88	5	3916	OHX	2	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
86	l1	46
1	2	2
81	m2	2

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Mol	Chain	Number of breaks
36	5	1

The worst 5 of 51 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1716:C	O3'	1717:G	P	5.68
1	l1	132:UNK	C	133:UNK	N	4.51
1	m2	23:UNK	C	28:UNK	N	4.14
1	l1	81:UNK	C	82:UNK	N	3.84
1	5	2437:G	O3'	2438:A	P	3.63

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.76	159 (8%) 9 5	57, 96, 178, 219	0
1	6	1795/1800 (99%)	0.51	86 (4%) 30 17	44, 84, 166, 211	0
2	S0	206/251 (82%)	1.12	43 (20%) 1 0	100, 115, 126, 138	0
2	s0	206/251 (82%)	0.62	19 (9%) 9 5	81, 98, 114, 118	0
3	S1	214/254 (84%)	0.80	33 (15%) 2 1	104, 134, 156, 161	0
3	s1	216/254 (85%)	0.49	12 (5%) 24 13	77, 91, 111, 123	0
4	S2	217/253 (85%)	0.91	37 (17%) 1 1	81, 93, 109, 115	0
4	s2	217/253 (85%)	1.13	48 (22%) 0 0	65, 81, 96, 112	0
5	S3	223/239 (93%)	1.34	68 (30%) 0 0	84, 97, 119, 130	0
5	s3	223/239 (93%)	0.80	39 (17%) 1 1	80, 109, 133, 136	0
6	S4	260/260 (100%)	1.33	80 (30%) 0 0	71, 96, 106, 121	0
6	s4	260/260 (100%)	0.71	26 (10%) 7 4	59, 86, 100, 121	0
7	S5	206/224 (91%)	1.11	50 (24%) 0 0	103, 122, 131, 135	0
7	s5	206/224 (91%)	0.93	40 (19%) 1 0	83, 106, 121, 129	0
8	S6	226/236 (95%)	0.49	22 (9%) 7 4	72, 102, 122, 133	0
8	s6	218/236 (92%)	0.48	13 (5%) 21 11	60, 90, 110, 121	0
9	S7	184/189 (97%)	1.31	56 (30%) 0 0	98, 122, 142, 148	0
9	s7	186/189 (98%)	0.67	19 (10%) 6 3	79, 107, 134, 139	0
10	S8	188/200 (94%)	1.47	54 (28%) 0 0	67, 83, 116, 129	0
10	s8	188/200 (94%)	0.71	11 (5%) 22 12	56, 74, 119, 135	0
11	S9	185/196 (94%)	1.94	80 (43%) 0 0	86, 103, 129, 145	0
11	s9	185/196 (94%)	1.22	40 (21%) 0 0	72, 90, 120, 138	0
12	C0	96/105 (91%)	0.33	8 (8%) 11 6	89, 110, 128, 138	0
12	c0	96/105 (91%)	1.13	25 (26%) 0 0	101, 132, 145, 150	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
13	C1	155/155 (100%)	1.51	42 (27%)	0	0	71, 82, 114, 129	0
13	c1	146/155 (94%)	1.22	21 (14%)	2	1	59, 71, 99, 122	0
14	C2	124/124 (100%)	0.72	14 (11%)	5	3	135, 143, 151, 154	0
14	c2	124/124 (100%)	2.28	62 (50%)	0	0	172, 187, 200, 208	0
15	C3	150/150 (100%)	0.64	18 (12%)	4	2	77, 91, 111, 115	0
15	c3	150/150 (100%)	0.65	11 (7%)	15	8	64, 80, 95, 100	0
16	C4	127/136 (93%)	0.38	12 (9%)	8	4	78, 131, 145, 150	0
16	c4	128/136 (94%)	0.78	15 (11%)	4	2	58, 92, 102, 108	0
17	C5	124/137 (90%)	0.71	14 (11%)	5	3	84, 100, 116, 128	0
17	c5	135/137 (98%)	1.18	28 (20%)	1	0	76, 101, 113, 119	0
18	C6	141/142 (99%)	2.41	75 (53%)	0	0	89, 110, 115, 118	0
18	c6	142/142 (100%)	2.19	69 (48%)	0	0	75, 99, 113, 127	0
19	C7	120/136 (88%)	1.75	49 (40%)	0	0	96, 110, 133, 135	0
19	c7	117/136 (86%)	0.89	20 (17%)	1	1	83, 98, 116, 118	0
20	C8	145/145 (100%)	0.47	10 (6%)	16	9	83, 109, 130, 138	0
20	c8	145/145 (100%)	0.70	20 (13%)	2	1	82, 97, 120, 130	0
21	C9	143/143 (100%)	1.99	70 (48%)	0	0	94, 108, 119, 126	0
21	c9	143/143 (100%)	1.09	25 (17%)	1	1	78, 93, 110, 119	0
22	D0	107/120 (89%)	2.13	47 (43%)	0	0	82, 112, 129, 132	0
22	d0	110/120 (91%)	2.22	57 (51%)	0	0	79, 110, 138, 141	0
23	D1	87/87 (100%)	0.84	14 (16%)	1	1	96, 104, 120, 127	0
23	d1	87/87 (100%)	0.33	3 (3%)	45	28	78, 87, 109, 119	0
24	D2	129/129 (100%)	2.44	75 (58%)	0	0	80, 93, 99, 108	0
25	D3	144/144 (100%)	1.04	30 (20%)	1	0	67, 73, 81, 95	0
25	d3	144/144 (100%)	0.71	22 (15%)	2	1	54, 61, 72, 82	0
26	D4	134/134 (100%)	0.62	15 (11%)	5	3	80, 104, 115, 122	0
26	d4	134/134 (100%)	0.17	3 (2%)	62	47	68, 91, 103, 109	0
27	D5	70/107 (65%)	0.51	6 (8%)	10	5	119, 133, 139, 141	0
27	d5	69/107 (64%)	0.90	8 (11%)	4	2	97, 117, 127, 130	0
28	D6	97/97 (100%)	2.04	52 (53%)	0	0	82, 95, 140, 144	0
28	d6	97/97 (100%)	1.43	28 (28%)	0	0	62, 74, 105, 112	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
29	D7	81/81 (100%)	1.90	35 (43%) 0 0	95, 109, 134, 140	0
29	d7	81/81 (100%)	1.69	28 (34%) 0 0	79, 93, 127, 132	0
30	D8	63/66 (95%)	0.83	13 (20%) 1 0	111, 126, 137, 141	0
30	d8	63/66 (95%)	1.17	16 (25%) 0 0	98, 113, 124, 135	0
31	D9	53/55 (96%)	1.69	21 (39%) 0 0	83, 87, 103, 110	0
31	d9	53/55 (96%)	2.93	34 (64%) 0 0	77, 88, 125, 139	0
32	E0	60/62 (96%)	2.27	27 (45%) 0 0	74, 101, 125, 127	0
32	e0	62/62 (100%)	0.68	9 (14%) 2 1	62, 89, 112, 115	0
33	E1	71/76 (93%)	1.56	25 (35%) 0 0	103, 132, 143, 147	0
33	e1	76/76 (100%)	2.81	41 (53%) 0 0	108, 162, 178, 183	0
34	SR	318/318 (100%)	1.01	55 (17%) 1 1	106, 117, 131, 147	0
34	sR	318/318 (100%)	1.44	99 (31%) 0 0	106, 124, 137, 148	0
35	SM	159/273 (58%)	0.90	33 (20%) 1 0	58, 94, 141, 144	0
35	sM	104/273 (38%)	0.36	7 (6%) 17 9	50, 106, 179, 186	0
36	1	3149/3396 (92%)	0.33	37 (1%) 79 68	35, 57, 128, 216	0
36	5	3169/3396 (93%)	0.38	40 (1%) 77 66	33, 53, 126, 187	0
37	3	121/121 (100%)	0.18	0 100 100	41, 72, 85, 91	0
37	7	121/121 (100%)	0.21	0 100 100	39, 58, 68, 77	0
38	4	158/158 (100%)	0.19	1 (0%) 89 84	43, 58, 94, 137	0
38	8	158/158 (100%)	0.21	0 100 100	43, 59, 94, 128	0
39	L2	252/253 (99%)	0.90	28 (11%) 5 3	44, 61, 76, 85	0
39	l2	252/253 (99%)	1.03	29 (11%) 4 2	40, 56, 73, 80	0
40	L3	386/386 (100%)	0.39	16 (4%) 37 22	40, 59, 72, 87	0
40	l3	386/386 (100%)	0.21	5 (1%) 77 66	34, 48, 62, 78	0
41	L4	361/361 (100%)	0.03	1 (0%) 94 92	38, 53, 69, 74	0
41	l4	361/361 (100%)	0.04	0 100 100	39, 55, 72, 84	0
42	L5	296/296 (100%)	0.66	25 (8%) 11 5	55, 79, 95, 114	0
42	l5	294/296 (99%)	0.38	7 (2%) 59 43	46, 62, 87, 102	0
43	L6	156/175 (89%)	0.09	0 100 100	47, 54, 70, 83	0
43	l6	157/175 (89%)	0.11	2 (1%) 77 66	48, 56, 76, 87	0
44	L7	222/243 (91%)	0.08	0 100 100	38, 48, 76, 105	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	l7	223/243 (91%)	0.04	0 100 100	38, 47, 77, 109	0
45	L8	233/255 (91%)	0.61	15 (6%) 19 10	67, 81, 110, 120	0
45	l8	231/255 (90%)	0.58	19 (8%) 11 6	69, 82, 109, 118	0
46	L9	191/191 (100%)	0.15	2 (1%) 82 73	54, 65, 77, 87	0
46	l9	191/191 (100%)	0.11	2 (1%) 82 73	43, 55, 71, 81	0
47	M0	211/220 (95%)	0.24	1 (0%) 91 86	41, 55, 88, 106	0
47	m0	213/220 (96%)	0.28	2 (0%) 84 75	39, 56, 80, 97	0
48	M1	169/173 (97%)	0.87	25 (14%) 2 1	63, 81, 93, 100	0
48	m1	169/173 (97%)	0.42	5 (2%) 50 33	51, 65, 76, 83	0
49	M3	193/198 (97%)	0.29	1 (0%) 91 86	38, 63, 100, 123	0
49	m3	194/198 (97%)	0.18	2 (1%) 82 73	39, 66, 96, 120	0
50	M4	136/137 (99%)	-0.02	0 100 100	49, 56, 68, 78	0
50	m4	137/137 (100%)	-0.07	0 100 100	45, 52, 66, 80	0
51	M5	204/204 (100%)	1.00	21 (10%) 6 3	40, 54, 66, 70	0
52	M6	197/198 (99%)	0.34	4 (2%) 65 50	39, 44, 64, 67	20 (10%)
52	m6	197/198 (99%)	0.29	2 (1%) 82 73	34, 40, 63, 65	18 (9%)
53	M7	183/183 (100%)	0.58	9 (4%) 29 16	43, 50, 97, 121	0
53	m7	155/183 (84%)	0.33	1 (0%) 89 84	37, 45, 59, 88	0
54	M8	185/185 (100%)	0.37	3 (1%) 72 59	41, 54, 69, 90	0
54	m8	185/185 (100%)	0.60	13 (7%) 16 8	40, 55, 64, 69	0
55	M9	188/188 (100%)	0.42	16 (8%) 10 5	60, 74, 144, 150	0
55	m9	188/188 (100%)	0.32	8 (4%) 35 21	49, 62, 125, 137	0
56	N0	172/172 (100%)	0.41	7 (4%) 37 22	46, 54, 65, 73	0
56	n0	172/172 (100%)	0.06	0 100 100	41, 48, 61, 70	0
57	N1	159/159 (100%)	0.70	14 (8%) 10 5	41, 54, 96, 103	0
57	n1	159/159 (100%)	0.65	11 (6%) 16 9	38, 48, 82, 89	0
58	N2	100/120 (83%)	0.41	7 (7%) 16 8	89, 104, 117, 121	0
58	n2	98/120 (81%)	0.67	7 (7%) 16 8	73, 85, 93, 97	0
59	N3	136/136 (100%)	0.55	7 (5%) 28 15	46, 56, 68, 76	0
59	n3	136/136 (100%)	0.54	2 (1%) 73 61	35, 45, 56, 60	0
60	N4	98/155 (63%)	2.10	31 (31%) 0 0	57, 69, 134, 146	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
60	n4	135/155 (87%)	0.77	14 (10%) 6 3	45, 93, 120, 132	0
61	N5	121/141 (85%)	0.47	4 (3%) 46 29	55, 66, 82, 107	0
61	n5	120/141 (85%)	0.27	3 (2%) 57 42	53, 66, 81, 93	0
62	N6	126/126 (100%)	0.49	4 (3%) 47 30	46, 60, 71, 77	0
62	n6	126/126 (100%)	0.45	0 100 100	49, 63, 75, 82	0
63	N7	135/135 (100%)	0.97	17 (12%) 3 2	81, 93, 105, 113	0
63	n7	135/135 (100%)	0.70	16 (11%) 4 2	74, 88, 99, 104	0
64	N8	148/148 (100%)	0.47	5 (3%) 45 28	35, 56, 78, 89	0
64	n8	148/148 (100%)	0.65	7 (4%) 31 17	35, 55, 76, 80	0
65	N9	58/58 (100%)	1.10	10 (17%) 1 1	37, 60, 96, 109	0
65	n9	58/58 (100%)	0.83	9 (15%) 2 1	37, 56, 77, 87	0
66	O0	97/104 (93%)	-0.25	0 100 100	81, 89, 107, 111	0
66	o0	100/104 (96%)	-0.04	3 (3%) 50 33	72, 80, 100, 109	0
67	O1	109/112 (97%)	1.23	29 (26%) 0 0	57, 69, 91, 98	0
67	o1	109/112 (97%)	0.66	3 (2%) 53 36	45, 57, 88, 104	0
68	O2	127/129 (98%)	0.28	2 (1%) 72 59	36, 48, 61, 74	0
68	o2	127/129 (98%)	0.22	0 100 100	34, 51, 64, 70	0
69	O3	106/106 (100%)	0.31	0 100 100	39, 45, 64, 74	0
69	o3	106/106 (100%)	0.53	3 (2%) 53 36	38, 45, 69, 77	0
70	O4	112/119 (94%)	1.29	35 (31%) 0 0	55, 71, 106, 113	0
70	o4	112/119 (94%)	1.43	36 (32%) 0 0	48, 66, 102, 107	0
71	O5	119/119 (100%)	0.03	1 (0%) 86 78	51, 68, 76, 81	0
71	o5	119/119 (100%)	0.19	4 (3%) 45 28	55, 68, 83, 92	0
72	O6	99/99 (100%)	0.49	9 (9%) 9 5	59, 69, 97, 110	0
72	o6	99/99 (100%)	0.76	6 (6%) 21 11	63, 71, 88, 106	0
73	O7	87/87 (100%)	0.59	2 (2%) 60 46	42, 48, 66, 85	0
73	o7	87/87 (100%)	0.72	3 (3%) 45 28	39, 47, 73, 92	0
74	O8	77/77 (100%)	0.42	5 (6%) 18 10	77, 90, 107, 112	0
74	o8	77/77 (100%)	0.88	13 (16%) 1 1	73, 86, 99, 101	0
75	O9	50/50 (100%)	0.74	3 (6%) 21 11	49, 55, 58, 58	0
75	o9	50/50 (100%)	0.97	4 (8%) 12 6	47, 52, 60, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
76	Q0	52/52 (100%)	0.58	2 (3%) 40 25	46, 52, 67, 73	0
76	q0	52/52 (100%)	0.31	0 100 100	39, 45, 55, 58	0
77	Q1	25/25 (100%)	2.42	16 (64%) 0 0	58, 64, 68, 69	0
77	q1	25/25 (100%)	1.29	3 (12%) 4 2	50, 53, 56, 57	0
78	Q2	105/105 (100%)	0.26	1 (0%) 82 73	42, 56, 75, 99	0
78	q2	105/105 (100%)	0.17	2 (1%) 66 53	41, 54, 69, 107	0
79	Q3	91/91 (100%)	0.67	6 (6%) 18 10	51, 64, 78, 86	0
79	q3	91/91 (100%)	1.12	17 (18%) 1 0	44, 56, 72, 82	0
80	d2	130/130 (100%)	1.21	24 (18%) 1 0	63, 75, 82, 91	0
81	m2	0/150	-	-	-	-
82	m5	203/203 (100%)	1.31	39 (19%) 1 0	41, 56, 68, 73	0
83	p0	143/220 (65%)	0.99	28 (19%) 1 0	103, 124, 217, 227	0
84	p1	0/47	-	-	-	-
84	p2	0/47	-	-	-	-
85	f	147/157 (93%)	0.42	10 (6%) 17 9	48, 81, 147, 150	4 (2%)
86	l1	0/213	-	-	-	-
All	All	33262/35574 (93%)	0.66	3272 (9%) 7 4	33, 73, 133, 227	42 (0%)

The worst 5 of 3272 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2	1694	A	15.4
1	2	1693	A	14.8
60	N4	86	SER	14.5
60	N4	75	THR	14.4
1	2	1708	U	14.1

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

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
85	5CT	f	51	15/16	0.89	0.49	46,46,46,46	15

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
87	MG	2	1967	1/1	0.26	0.47	130,130,130,130	0
87	MG	2	1925	1/1	0.29	0.32	99,99,99,99	0
87	MG	2	1954	1/1	0.33	0.26	82,82,82,82	0
87	MG	2	1973	1/1	0.41	0.34	107,107,107,107	0
87	MG	1	3717	1/1	0.43	0.26	61,61,61,61	0
87	MG	2	1901	1/1	0.52	0.40	87,87,87,87	0
87	MG	6	1924	1/1	0.53	0.61	84,84,84,84	0
87	MG	2	1963	1/1	0.54	0.31	95,95,95,95	0
87	MG	1	3605	1/1	0.54	0.46	55,55,55,55	0
87	MG	1	3427	1/1	0.56	0.32	53,53,53,53	0
87	MG	6	1988	1/1	0.56	0.78	61,61,61,61	0
87	MG	N3	202	1/1	0.57	0.19	65,65,65,65	0
87	MG	5	3621	1/1	0.57	0.55	99,99,99,99	0
87	MG	5	3749	1/1	0.58	0.27	70,70,70,70	0
87	MG	M3	201	1/1	0.59	0.44	97,97,97,97	0
87	MG	5	3531	1/1	0.60	0.24	48,48,48,48	0
87	MG	M8	201	1/1	0.60	0.42	51,51,51,51	0
87	MG	4	217	1/1	0.61	0.26	60,60,60,60	0
87	MG	2	1975	1/1	0.61	0.17	74,74,74,74	0
87	MG	5	3785	1/1	0.61	0.28	52,52,52,52	0
87	MG	2	1949	1/1	0.61	0.31	90,90,90,90	0
87	MG	6	1917	1/1	0.62	0.45	78,78,78,78	0
87	MG	1	3451	1/1	0.62	0.46	64,64,64,64	0
87	MG	1	3718	1/1	0.62	0.38	108,108,108,108	0
87	MG	8	212	1/1	0.62	0.31	67,67,67,67	0
87	MG	5	3682	1/1	0.63	0.53	50,50,50,50	0
87	MG	1	3719	1/1	0.66	0.29	58,58,58,58	0
87	MG	S4	301	1/1	0.66	2.12	88,88,88,88	0
87	MG	5	3701	1/1	0.67	0.26	48,48,48,48	0
87	MG	2	1912	1/1	0.68	0.47	88,88,88,88	0
87	MG	5	3569	1/1	0.68	0.37	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	3675	1/1	0.69	0.36	65,65,65,65	0
87	MG	5	3757	1/1	0.69	0.23	59,59,59,59	0
87	MG	3	208	1/1	0.69	0.27	67,67,67,67	0
88	OHX	3	219	7/7	0.69	0.33	78,78,78,78	5
87	MG	6	2007	1/1	0.69	0.56	100,100,100,100	0
87	MG	2	1970	1/1	0.70	0.20	91,91,91,91	0
87	MG	1	3604	1/1	0.70	0.64	90,90,90,90	0
87	MG	1	3662	1/1	0.70	0.28	43,43,43,43	0
88	OHX	6	2185	7/7	0.70	0.28	75,75,75,75	4
87	MG	1	3597	1/1	0.70	0.14	68,68,68,68	0
87	MG	5	3402	1/1	0.70	0.33	47,47,47,47	0
87	MG	5	3739	1/1	0.70	0.35	63,63,63,63	0
87	MG	5	3623	1/1	0.70	0.65	95,95,95,95	0
87	MG	2	1941	1/1	0.71	0.15	81,81,81,81	0
87	MG	6	1991	1/1	0.71	0.29	65,65,65,65	0
87	MG	1	3407	1/1	0.71	0.19	52,52,52,52	0
87	MG	1	3660	1/1	0.71	0.20	52,52,52,52	0
88	OHX	6	2181	7/7	0.72	0.79	92,92,92,92	5
87	MG	2	1942	1/1	0.72	0.29	77,77,77,77	0
87	MG	5	3641	1/1	0.72	0.23	39,39,39,39	0
88	OHX	1	3966	7/7	0.73	0.29	55,55,55,55	2
87	MG	M7	201	1/1	0.73	0.45	73,73,73,73	0
87	MG	5	3467	1/1	0.73	0.23	125,125,125,125	0
87	MG	5	3648	1/1	0.73	0.26	55,55,55,55	0
87	MG	5	3668	1/1	0.73	0.29	64,64,64,64	0
88	OHX	5	4138	7/7	0.73	0.26	138,138,138,138	6
87	MG	5	3755	1/1	0.73	0.17	64,64,64,64	0
87	MG	2	1909	1/1	0.74	0.33	84,84,84,84	0
89	ZN	D7	101	1/1	0.74	0.33	152,152,152,152	0
87	MG	6	1915	1/1	0.74	0.27	82,82,82,82	0
87	MG	5	3706	1/1	0.74	0.39	69,69,69,69	0
88	OHX	5	4147	7/7	0.74	0.45	52,52,52,52	5
87	MG	1	3679	1/1	0.74	0.30	45,45,45,45	0
87	MG	6	1979	1/1	0.74	0.19	54,54,54,54	0
87	MG	5	3734	1/1	0.74	0.69	93,93,93,93	0
87	MG	1	3670	1/1	0.74	0.37	44,44,44,44	0
87	MG	5	3775	1/1	0.74	0.21	63,63,63,63	0
87	MG	6	1914	1/1	0.74	0.23	78,78,78,78	0
87	MG	s8	301	1/1	0.74	0.31	63,63,63,63	0
87	MG	5	3736	1/1	0.74	0.42	80,80,80,80	0
87	MG	5	3722	1/1	0.75	0.71	46,46,46,46	1
88	OHX	5	4091	7/7	0.75	0.38	34,34,34,34	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	6	1973	1/1	0.75	0.38	102,102,102,102	0
88	OHX	1	4101	7/7	0.75	0.26	85,85,85,85	6
87	MG	o2	202	1/1	0.75	0.17	52,52,52,52	0
87	MG	1	3700	1/1	0.75	0.22	63,63,63,63	0
88	OHX	5	4137	7/7	0.75	0.28	96,96,96,96	6
87	MG	2	1976	1/1	0.75	0.18	75,75,75,75	0
87	MG	1	3680	1/1	0.75	0.31	66,66,66,66	0
87	MG	5	3440	1/1	0.75	0.50	81,81,81,81	0
87	MG	6	1974	1/1	0.76	0.53	94,94,94,94	0
87	MG	5	3416	1/1	0.76	0.12	49,49,49,49	0
87	MG	5	3684	1/1	0.76	0.17	75,75,75,75	0
87	MG	1	3468	1/1	0.76	0.17	48,48,48,48	0
87	MG	5	3786	1/1	0.76	0.49	90,90,90,90	0
87	MG	1	3413	1/1	0.76	0.18	66,66,66,66	0
87	MG	5	3768	1/1	0.76	0.29	62,62,62,62	0
87	MG	1	3406	1/1	0.76	0.23	48,48,48,48	0
87	MG	6	1989	1/1	0.76	0.26	81,81,81,81	0
87	MG	5	3502	1/1	0.76	0.28	44,44,44,44	0
87	MG	N8	203	1/1	0.77	0.23	52,52,52,52	0
87	MG	2	1930	1/1	0.77	0.17	76,76,76,76	0
87	MG	1	3681	1/1	0.77	0.30	54,54,54,54	0
87	MG	1	4110	1/1	0.77	0.15	73,73,73,73	0
87	MG	1	3484	1/1	0.77	0.37	81,81,81,81	0
88	OHX	1	4050	7/7	0.77	0.27	106,106,106,106	5
87	MG	1	3405	1/1	0.77	0.70	118,118,118,118	0
87	MG	4	218	1/1	0.77	0.28	41,41,41,41	0
87	MG	6	2012	1/1	0.77	0.14	72,72,72,72	0
87	MG	6	1912	1/1	0.77	0.26	59,59,59,59	0
87	MG	1	3598	1/1	0.77	0.40	70,70,70,70	0
87	MG	6	1961	1/1	0.77	0.19	68,68,68,68	0
87	MG	c7	201	1/1	0.77	0.32	78,78,78,78	0
87	MG	1	3711	1/1	0.77	0.72	59,59,59,59	1
87	MG	1	3747	1/1	0.77	0.35	55,55,55,55	0
87	MG	f	1003	1/1	0.78	0.20	50,50,50,50	0
87	MG	1	3635	1/1	0.78	0.31	61,61,61,61	0
87	MG	7	213	1/1	0.78	0.48	60,60,60,60	0
87	MG	1	3721	1/1	0.78	0.18	60,60,60,60	0
87	MG	6	1945	1/1	0.78	0.36	66,66,66,66	0
87	MG	6	1998	1/1	0.78	0.20	55,55,55,55	0
87	MG	O7	102	1/1	0.78	0.56	67,67,67,67	0
88	OHX	2	2135	7/7	0.78	0.25	194,194,194,194	7
87	MG	1	3621	1/1	0.78	0.21	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	3691	1/1	0.78	0.30	52,52,52,52	0
87	MG	5	3790	1/1	0.78	0.27	70,70,70,70	0
87	MG	2	1959	1/1	0.78	0.37	84,84,84,84	0
87	MG	1	3530	1/1	0.79	0.38	63,63,63,63	0
87	MG	o4	201	1/1	0.79	0.26	50,50,50,50	0
88	OHX	2	2147	7/7	0.79	0.30	102,102,102,102	6
87	MG	2	1979	1/1	0.79	0.18	68,68,68,68	0
87	MG	5	3737	1/1	0.79	0.16	51,51,51,51	0
87	MG	2	1960	1/1	0.79	0.37	75,75,75,75	0
87	MG	2	1906	1/1	0.79	0.17	67,67,67,67	0
87	MG	2	1944	1/1	0.79	0.24	80,80,80,80	0
87	MG	5	3432	1/1	0.79	0.21	46,46,46,46	0
87	MG	2	1919	1/1	0.79	0.27	70,70,70,70	0
88	OHX	1	4097	7/7	0.79	0.31	74,74,74,74	5
87	MG	1	3666	1/1	0.79	0.25	66,66,66,66	0
87	MG	1	3613	1/1	0.79	0.35	60,60,60,60	0
87	MG	5	3789	1/1	0.79	0.23	59,59,59,59	0
87	MG	2	1980	1/1	0.79	0.26	89,89,89,89	0
87	MG	5	3702	1/1	0.80	0.26	62,62,62,62	0
88	OHX	2	2149	7/7	0.80	0.21	134,134,134,134	6
87	MG	5	3464	1/1	0.80	0.35	118,118,118,118	0
87	MG	5	3497	1/1	0.80	0.68	48,48,48,48	1
87	MG	5	3742	1/1	0.80	0.35	61,61,61,61	0
87	MG	5	3657	1/1	0.80	0.21	42,42,42,42	0
87	MG	5	3412	1/1	0.80	0.28	37,37,37,37	0
87	MG	1	3443	1/1	0.80	0.36	36,36,36,36	0
88	OHX	5	4142	7/7	0.80	0.52	37,37,37,37	6
87	MG	6	1951	1/1	0.80	0.45	74,74,74,74	0
87	MG	N0	201	1/1	0.80	0.24	51,51,51,51	0
87	MG	1	3609	1/1	0.80	0.24	44,44,44,44	0
87	MG	1	3723	1/1	0.80	0.21	70,70,70,70	0
87	MG	5	3639	1/1	0.80	0.41	69,69,69,69	0
87	MG	8	210	1/1	0.80	0.10	86,86,86,86	0
87	MG	5	3421	1/1	0.80	0.39	63,63,63,63	0
87	MG	1	3726	1/1	0.80	0.22	60,60,60,60	0
87	MG	d3	201	1/1	0.80	0.20	60,60,60,60	0
87	MG	1	3421	1/1	0.80	0.30	44,44,44,44	0
87	MG	1	3696	1/1	0.80	0.23	62,62,62,62	0
88	OHX	2	2146	7/7	0.80	0.44	82,82,82,82	5
87	MG	5	3625	1/1	0.80	0.31	52,52,52,52	0
87	MG	S9	201	1/1	0.80	0.35	99,99,99,99	0
88	OHX	1	3869	7/7	0.80	0.37	56,56,56,56	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	6	1969	1/1	0.81	0.23	73,73,73,73	0
87	MG	5	3490	1/1	0.81	0.15	51,51,51,51	0
87	MG	5	3735	1/1	0.81	0.23	49,49,49,49	1
87	MG	Q2	502	1/1	0.81	0.20	72,72,72,72	0
88	OHX	M7	204	7/7	0.81	0.56	43,43,43,43	4
87	MG	6	1985	1/1	0.81	0.16	90,90,90,90	0
87	MG	5	3683	1/1	0.81	0.23	41,41,41,41	0
87	MG	1	3423	1/1	0.81	0.26	49,49,49,49	0
89	ZN	e1	501	1/1	0.81	0.06	168,168,168,168	0
87	MG	6	2005	1/1	0.81	0.64	72,72,72,72	0
88	OHX	5	4132	7/7	0.81	0.28	72,72,72,72	5
87	MG	2	1902	1/1	0.81	0.24	59,59,59,59	0
87	MG	N9	101	1/1	0.81	0.25	33,33,33,33	0
88	OHX	6	2167	7/7	0.81	0.36	48,48,48,48	2
87	MG	1	3418	1/1	0.81	0.49	78,78,78,78	0
87	MG	L6	201	1/1	0.81	0.26	53,53,53,53	0
87	MG	6	1959	1/1	0.81	0.22	80,80,80,80	0
87	MG	1	3450	1/1	0.81	0.32	62,62,62,62	0
88	OHX	8	230	7/7	0.81	0.33	65,65,65,65	5
87	MG	5	3486	1/1	0.81	0.25	45,45,45,45	0
88	OHX	m7	204	7/7	0.81	0.42	50,50,50,50	4
87	MG	6	2188	1/1	0.81	0.06	81,81,81,81	0
87	MG	5	3601	1/1	0.81	0.21	55,55,55,55	0
87	MG	m6	202	1/1	0.81	0.30	52,52,52,52	0
87	MG	1	3463	1/1	0.81	0.27	51,51,51,51	0
87	MG	6	1936	1/1	0.81	0.20	59,59,59,59	0
87	MG	5	3548	1/1	0.81	0.36	45,45,45,45	0
87	MG	2	1926	1/1	0.81	0.33	61,61,61,61	0
87	MG	1	3704	1/1	0.81	0.21	53,53,53,53	0
88	OHX	2	2137	7/7	0.81	0.13	148,148,148,148	6
88	OHX	1	4069	7/7	0.82	0.36	51,51,51,51	3
87	MG	5	3670	1/1	0.82	1.34	36,36,36,36	1
87	MG	2	1905	1/1	0.82	0.19	65,65,65,65	0
87	MG	4	203	1/1	0.82	0.40	52,52,52,52	0
87	MG	4	216	1/1	0.82	0.17	65,65,65,65	0
88	OHX	5	4136	7/7	0.82	0.36	85,85,85,85	6
88	OHX	2	2126	7/7	0.82	0.26	111,111,111,111	5
88	OHX	1	4072	7/7	0.82	0.24	68,68,68,68	5
88	OHX	5	4159	7/7	0.82	0.17	162,162,162,162	7
87	MG	6	1967	1/1	0.82	0.21	64,64,64,64	0
87	MG	5	3792	1/1	0.82	0.33	44,44,44,44	1
87	MG	5	3476	1/1	0.82	0.15	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	6	1908	1/1	0.82	0.30	58,58,58,58	0
87	MG	5	3459	1/1	0.82	0.17	43,43,43,43	0
88	OHX	5	4019	7/7	0.82	0.36	60,60,60,60	5
88	OHX	2	2152	7/7	0.82	0.18	104,104,104,104	5
87	MG	5	3731	1/1	0.82	0.47	44,44,44,44	0
87	MG	1	3708	1/1	0.82	0.25	50,50,50,50	0
87	MG	1	3431	1/1	0.82	0.12	52,52,52,52	0
87	MG	6	1995	1/1	0.82	0.45	67,67,67,67	0
87	MG	5	3499	1/1	0.82	0.22	50,50,50,50	0
87	MG	8	207	1/1	0.82	0.19	50,50,50,50	0
87	MG	6	1919	1/1	0.82	0.13	66,66,66,66	0
87	MG	n0	201	1/1	0.83	0.24	45,45,45,45	0
87	MG	5	3666	1/1	0.83	0.23	39,39,39,39	0
87	MG	5	3644	1/1	0.83	0.29	43,43,43,43	0
88	OHX	6	2137	7/7	0.83	0.33	85,85,85,85	5
87	MG	5	3552	1/1	0.83	0.39	46,46,46,46	0
87	MG	5	3664	1/1	0.83	0.21	44,44,44,44	0
87	MG	2	1971	1/1	0.83	0.19	64,64,64,64	0
87	MG	7	207	1/1	0.83	0.37	40,40,40,40	0
87	MG	2	2155	1/1	0.83	0.27	83,83,83,83	0
88	OHX	1	4100	7/7	0.83	0.29	71,71,71,71	3
87	MG	6	2011	1/1	0.83	0.26	79,79,79,79	0
87	MG	5	3446	1/1	0.83	0.33	43,43,43,43	0
88	OHX	1	4030	7/7	0.83	0.23	73,73,73,73	3
87	MG	6	1932	1/1	0.83	0.20	60,60,60,60	0
87	MG	5	3619	1/1	0.83	0.30	53,53,53,53	0
87	MG	1	3750	1/1	0.83	0.28	55,55,55,55	0
87	MG	5	3419	1/1	0.83	0.30	51,51,51,51	0
87	MG	5	3710	1/1	0.83	0.31	46,46,46,46	0
87	MG	2	1981	1/1	0.83	0.32	60,60,60,60	0
88	OHX	2	2144	7/7	0.83	0.38	97,97,97,97	6
87	MG	1	3617	1/1	0.83	0.55	44,44,44,44	0
88	OHX	5	4100	7/7	0.83	0.72	50,50,50,50	4
87	MG	1	3618	1/1	0.83	0.28	53,53,53,53	0
88	OHX	8	229	7/7	0.83	0.28	49,49,49,49	4
87	MG	5	3454	1/1	0.83	0.40	48,48,48,48	0
88	OHX	5	4151	7/7	0.83	0.36	60,60,60,60	6
87	MG	1	3562	1/1	0.83	0.23	49,49,49,49	0
88	OHX	5	4099	7/7	0.83	0.24	75,75,75,75	5
87	MG	2	1918	1/1	0.83	0.26	65,65,65,65	0
87	MG	M7	203	1/1	0.83	0.23	44,44,44,44	0
87	MG	6	2010	1/1	0.83	0.19	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	6	1962	1/1	0.83	0.27	95,95,95,95	0
87	MG	2	1965	1/1	0.83	0.16	81,81,81,81	0
87	MG	6	1984	1/1	0.83	0.40	72,72,72,72	0
87	MG	4	214	1/1	0.83	0.27	71,71,71,71	0
88	OHX	1	4067	7/7	0.83	0.30	104,104,104,104	4
87	MG	5	3754	1/1	0.83	0.33	49,49,49,49	0
88	OHX	5	4088	7/7	0.83	0.55	41,41,41,41	6
88	OHX	2	2117	7/7	0.83	0.20	95,95,95,95	5
88	OHX	5	4153	7/7	0.83	0.32	50,50,50,50	6
88	OHX	2	2129	7/7	0.83	0.14	118,118,118,118	6
87	MG	1	3685	1/1	0.84	0.28	50,50,50,50	0
87	MG	1	3524	1/1	0.84	0.56	62,62,62,62	0
87	MG	1	3665	1/1	0.84	0.28	63,63,63,63	0
87	MG	5	3767	1/1	0.84	0.49	40,40,40,40	0
87	MG	7	214	1/1	0.84	0.29	66,66,66,66	0
87	MG	4	201	1/1	0.84	0.51	62,62,62,62	0
87	MG	1	3536	1/1	0.84	0.32	43,43,43,43	0
88	OHX	2	2114	7/7	0.84	0.37	99,99,99,99	4
87	MG	2	1993	1/1	0.84	0.11	76,76,76,76	0
87	MG	6	1993	1/1	0.84	0.27	56,56,56,56	0
88	OHX	1	4041	7/7	0.84	0.23	200,200,200,200	7
87	MG	5	3615	1/1	0.84	0.17	35,35,35,35	0
88	OHX	1	4027	7/7	0.84	0.33	50,50,50,50	4
87	MG	5	3616	1/1	0.84	0.26	63,63,63,63	0
89	ZN	d7	101	1/1	0.84	0.32	142,142,142,142	0
88	OHX	1	4061	7/7	0.84	0.31	53,53,53,53	3
87	MG	l5	301	1/1	0.84	0.36	56,56,56,56	0
87	MG	5	3680	1/1	0.84	0.21	41,41,41,41	0
88	OHX	6	2164	7/7	0.84	0.38	81,81,81,81	5
88	OHX	2	2139	7/7	0.84	0.29	164,164,164,164	7
87	MG	1	3420	1/1	0.84	0.19	39,39,39,39	0
87	MG	5	3718	1/1	0.84	0.28	59,59,59,59	0
87	MG	5	3676	1/1	0.84	0.29	62,62,62,62	0
88	OHX	6	2146	7/7	0.84	0.35	53,53,53,53	3
87	MG	5	3418	1/1	0.84	0.13	41,41,41,41	0
88	OHX	6	2180	7/7	0.84	0.13	137,137,137,137	6
87	MG	1	3678	1/1	0.84	0.34	69,69,69,69	0
88	OHX	1	4082	7/7	0.84	0.39	44,44,44,44	4
88	OHX	2	2124	7/7	0.84	0.51	88,88,88,88	7
87	MG	5	3728	1/1	0.84	0.22	47,47,47,47	0
87	MG	5	3636	1/1	0.84	0.11	54,54,54,54	0
87	MG	1	3697	1/1	0.84	0.45	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	n0	202	1/1	0.84	0.33	48,48,48,48	0
87	MG	6	1986	1/1	0.84	0.07	63,63,63,63	0
87	MG	5	3700	1/1	0.84	0.21	53,53,53,53	0
87	MG	5	3667	1/1	0.84	0.36	54,54,54,54	0
88	OHX	5	4103	7/7	0.84	0.24	63,63,63,63	7
87	MG	1	3614	1/1	0.84	0.26	55,55,55,55	0
88	OHX	S6	301	7/7	0.85	0.20	105,105,105,105	5
87	MG	1	3736	1/1	0.85	0.25	54,54,54,54	0
87	MG	5	3427	1/1	0.85	0.22	40,40,40,40	0
88	OHX	5	4158	7/7	0.85	0.19	49,49,49,49	1
87	MG	1	3532	1/1	0.85	0.29	43,43,43,43	0
87	MG	5	3708	1/1	0.85	0.32	46,46,46,46	0
87	MG	1	3745	1/1	0.85	0.23	47,47,47,47	0
87	MG	2	1922	1/1	0.85	0.20	60,60,60,60	0
87	MG	1	3659	1/1	0.85	0.34	86,86,86,86	0
88	OHX	l5	303	7/7	0.85	0.27	94,94,94,94	6
87	MG	6	1921	1/1	0.85	0.22	71,71,71,71	0
87	MG	3	206	1/1	0.85	0.19	66,66,66,66	0
87	MG	N8	204	1/1	0.85	0.20	56,56,56,56	0
87	MG	2	1990	1/1	0.85	0.27	74,74,74,74	0
87	MG	1	3644	1/1	0.85	0.21	51,51,51,51	0
88	OHX	m9	201	7/7	0.85	0.21	61,61,61,61	4
88	OHX	5	4111	7/7	0.85	0.29	77,77,77,77	6
87	MG	1	3448	1/1	0.85	0.33	54,54,54,54	0
88	OHX	m0	304	7/7	0.85	0.34	44,44,44,44	5
87	MG	N8	201	1/1	0.85	0.32	57,57,57,57	0
87	MG	5	3693	1/1	0.85	0.26	47,47,47,47	0
88	OHX	2	2108	7/7	0.85	0.23	83,83,83,83	3
88	OHX	6	2165	7/7	0.85	0.22	119,119,119,119	7
87	MG	6	1920	1/1	0.85	0.23	53,53,53,53	0
87	MG	1	3637	1/1	0.85	0.27	47,47,47,47	0
87	MG	1	3459	1/1	0.85	0.40	52,52,52,52	0
87	MG	2	1978	1/1	0.85	0.24	58,58,58,58	0
88	OHX	1	3865	7/7	0.85	0.42	46,46,46,46	4
87	MG	1	3486	1/1	0.85	0.25	49,49,49,49	0
87	MG	1	3677	1/1	0.85	0.20	49,49,49,49	0
87	MG	1	3742	1/1	0.85	0.18	68,68,68,68	0
87	MG	1	3709	1/1	0.85	0.63	44,44,44,44	0
87	MG	5	3730	1/1	0.85	0.28	44,44,44,44	0
87	MG	1	3619	1/1	0.85	0.22	49,49,49,49	0
87	MG	5	3481	1/1	0.85	0.60	48,48,48,48	0
87	MG	5	3451	1/1	0.85	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4166	1/1	0.85	0.32	68,68,68,68	0
87	MG	5	3536	1/1	0.85	0.50	36,36,36,36	0
88	OHX	2	2074	7/7	0.85	0.15	179,179,179,179	7
87	MG	2	1966	1/1	0.85	0.16	90,90,90,90	0
88	OHX	1	4102	7/7	0.85	0.30	58,58,58,58	2
87	MG	1	3694	1/1	0.85	0.35	81,81,81,81	0
87	MG	6	1926	1/1	0.85	0.21	57,57,57,57	0
87	MG	1	3402	1/1	0.85	0.39	53,53,53,53	0
88	OHX	1	4060	7/7	0.85	0.30	61,61,61,61	4
88	OHX	5	4104	7/7	0.85	0.32	54,54,54,54	3
87	MG	5	3671	1/1	0.86	0.17	44,44,44,44	0
87	MG	1	3683	1/1	0.86	0.33	46,46,46,46	0
88	OHX	2	2121	7/7	0.86	0.41	60,60,60,60	5
87	MG	1	3535	1/1	0.86	0.49	44,44,44,44	0
88	OHX	1	4084	7/7	0.86	0.36	47,47,47,47	4
87	MG	5	3721	1/1	0.86	0.21	54,54,54,54	0
87	MG	12	302	1/1	0.86	0.24	50,50,50,50	0
87	MG	1	3563	1/1	0.86	0.47	40,40,40,40	0
87	MG	1	4113	1/1	0.86	1.27	55,55,55,55	1
87	MG	6	1933	1/1	0.86	0.21	90,90,90,90	0
87	MG	5	3538	1/1	0.86	0.27	45,45,45,45	0
88	OHX	1	4070	7/7	0.86	0.22	71,71,71,71	4
87	MG	2	1933	1/1	0.86	0.23	84,84,84,84	0
87	MG	4	207	1/1	0.86	0.17	37,37,37,37	0
87	MG	1	3716	1/1	0.86	0.32	44,44,44,44	0
87	MG	1	3751	1/1	0.86	0.26	61,61,61,61	0
87	MG	O3	201	1/1	0.86	0.94	44,44,44,44	1
87	MG	1	3462	1/1	0.86	0.38	50,50,50,50	0
88	OHX	2	2039	7/7	0.86	0.22	133,133,133,133	5
88	OHX	6	2133	7/7	0.86	0.14	148,148,148,148	7
88	OHX	M9	201	7/7	0.86	0.15	75,75,75,75	3
87	MG	5	3705	1/1	0.86	0.24	50,50,50,50	0
87	MG	2	1969	1/1	0.86	0.11	93,93,93,93	0
87	MG	8	202	1/1	0.86	0.28	44,44,44,44	0
87	MG	1	3638	1/1	0.86	0.40	69,69,69,69	0
87	MG	1	3749	1/1	0.86	0.20	48,48,48,48	0
87	MG	5	3547	1/1	0.86	0.40	51,51,51,51	0
87	MG	2	1903	1/1	0.86	0.14	59,59,59,59	0
87	MG	5	3626	1/1	0.86	0.24	53,53,53,53	0
87	MG	1	3746	1/1	0.86	0.30	56,56,56,56	0
87	MG	L2	302	1/1	0.86	0.19	44,44,44,44	0
88	OHX	6	2182	7/7	0.86	0.21	152,152,152,152	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	3770	1/1	0.86	0.30	40,40,40,40	0
87	MG	2	1904	1/1	0.86	0.53	75,75,75,75	0
88	OHX	5	4082	7/7	0.86	0.22	99,99,99,99	5
87	MG	o2	201	1/1	0.86	0.26	37,37,37,37	0
87	MG	2	1962	1/1	0.86	0.20	66,66,66,66	0
87	MG	5	3653	1/1	0.86	0.20	37,37,37,37	0
87	MG	5	3673	1/1	0.86	0.11	48,48,48,48	1
87	MG	1	3661	1/1	0.86	0.33	46,46,46,46	0
88	OHX	5	4090	7/7	0.86	0.23	83,83,83,83	4
87	MG	4	212	1/1	0.86	0.19	54,54,54,54	0
87	MG	1	3674	1/1	0.86	0.64	75,75,75,75	0
87	MG	5	3672	1/1	0.86	0.19	48,48,48,48	0
88	OHX	1	4011	7/7	0.86	0.26	117,117,117,117	4
87	MG	1	3449	1/1	0.86	0.29	42,42,42,42	0
87	MG	2	1950	1/1	0.86	0.30	99,99,99,99	0
87	MG	1	3738	1/1	0.86	0.29	62,62,62,62	0
88	OHX	2	2150	7/7	0.86	0.11	140,140,140,140	7
87	MG	5	3783	1/1	0.86	0.30	70,70,70,70	0
87	MG	1	3596	1/1	0.86	0.31	64,64,64,64	0
87	MG	5	3607	1/1	0.86	0.25	52,52,52,52	0
87	MG	5	3545	1/1	0.86	0.33	44,44,44,44	0
87	MG	5	3485	1/1	0.87	0.47	73,73,73,73	0
87	MG	1	3642	1/1	0.87	0.25	37,37,37,37	0
88	OHX	M8	202	7/7	0.87	0.26	49,49,49,49	2
87	MG	5	3488	1/1	0.87	0.40	34,34,34,34	0
88	OHX	5	3795	7/7	0.87	0.35	38,38,38,38	1
88	OHX	2	2133	7/7	0.87	0.18	108,108,108,108	6
88	OHX	5	4131	7/7	0.87	0.32	59,59,59,59	2
87	MG	1	3741	1/1	0.87	0.30	46,46,46,46	0
87	MG	2	1992	1/1	0.87	0.16	86,86,86,86	0
87	MG	1	3629	1/1	0.87	0.24	52,52,52,52	0
87	MG	5	3719	1/1	0.87	0.11	60,60,60,60	0
87	MG	2	1946	1/1	0.87	0.34	66,66,66,66	0
87	MG	5	3577	1/1	0.87	0.49	39,39,39,39	0
87	MG	6	1925	1/1	0.87	0.33	52,52,52,52	0
87	MG	1	3646	1/1	0.87	0.40	41,41,41,41	0
87	MG	5	3645	1/1	0.87	0.27	48,48,48,48	0
87	MG	5	3685	1/1	0.87	0.25	44,44,44,44	0
87	MG	1	3690	1/1	0.87	0.15	46,46,46,46	0
87	MG	1	3671	1/1	0.87	0.14	47,47,47,47	0
88	OHX	2	2128	7/7	0.87	0.33	62,62,62,62	3
87	MG	5	3627	1/1	0.87	0.22	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	2	2119	7/7	0.87	0.23	84,84,84,84	3
87	MG	6	1980	1/1	0.87	0.28	83,83,83,83	0
88	OHX	1	4056	7/7	0.87	0.27	74,74,74,74	4
88	OHX	1	4051	7/7	0.87	0.26	59,59,59,59	4
87	MG	5	3780	1/1	0.87	0.39	43,43,43,43	0
87	MG	3	203	1/1	0.87	0.30	38,38,38,38	0
88	OHX	1	4086	7/7	0.87	0.34	136,136,136,136	7
87	MG	5	3608	1/1	0.87	0.12	47,47,47,47	0
87	MG	6	2000	1/1	0.87	0.26	47,47,47,47	0
87	MG	7	208	1/1	0.87	0.34	55,55,55,55	0
87	MG	5	3725	1/1	0.87	0.27	53,53,53,53	0
87	MG	6	1997	1/1	0.87	0.40	122,122,122,122	0
87	MG	5	3724	1/1	0.87	0.24	44,44,44,44	0
87	MG	2	1986	1/1	0.87	0.15	99,99,99,99	0
87	MG	1	3699	1/1	0.87	0.20	48,48,48,48	0
87	MG	1	3615	1/1	0.87	0.12	67,67,67,67	0
87	MG	M3	202	1/1	0.87	0.20	44,44,44,44	0
88	OHX	C5	201	7/7	0.87	0.20	116,116,116,116	5
87	MG	5	3738	1/1	0.87	0.19	51,51,51,51	0
87	MG	4	219	1/1	0.87	0.35	58,58,58,58	0
87	MG	5	3605	1/1	0.87	0.32	56,56,56,56	0
87	MG	5	3597	1/1	0.87	0.17	48,48,48,48	0
88	OHX	5	4061	7/7	0.87	0.23	61,61,61,61	1
87	MG	1	3528	1/1	0.87	0.30	40,40,40,40	0
87	MG	8	204	1/1	0.87	0.27	52,52,52,52	0
88	OHX	5	4130	7/7	0.87	0.26	54,54,54,54	5
87	MG	5	3542	1/1	0.87	0.26	38,38,38,38	0
87	MG	1	3515	1/1	0.87	0.18	54,54,54,54	0
87	MG	1	3647	1/1	0.87	0.21	58,58,58,58	0
87	MG	L3	402	1/1	0.87	0.31	58,58,58,58	0
87	MG	5	3551	1/1	0.87	0.20	46,46,46,46	0
87	MG	2	1913	1/1	0.87	0.29	69,69,69,69	0
88	OHX	1	3975	7/7	0.87	0.33	59,59,59,59	5
87	MG	2	1989	1/1	0.87	0.27	103,103,103,103	0
88	OHX	6	2115	7/7	0.87	0.24	70,70,70,70	4
87	MG	5	3563	1/1	0.87	0.42	45,45,45,45	0
88	OHX	5	3996	7/7	0.87	0.29	116,116,116,116	3
87	MG	SM	301	1/1	0.87	0.30	58,58,58,58	0
87	MG	5	3484	1/1	0.87	0.14	48,48,48,48	0
87	MG	1	3710	1/1	0.87	0.19	45,45,45,45	0
87	MG	5	3589	1/1	0.87	0.37	33,33,33,33	0
87	MG	O4	201	1/1	0.87	0.19	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	3751	1/1	0.87	0.47	51,51,51,51	0
87	MG	1	3641	1/1	0.87	0.51	58,58,58,58	0
88	OHX	5	4093	7/7	0.87	0.32	80,80,80,80	6
87	MG	6	1964	1/1	0.87	0.30	75,75,75,75	0
87	MG	5	3692	1/1	0.88	0.18	59,59,59,59	0
87	MG	5	3756	1/1	0.88	0.42	39,39,39,39	0
87	MG	1	3729	1/1	0.88	0.15	55,55,55,55	0
88	OHX	5	4134	7/7	0.88	0.24	50,50,50,50	6
87	MG	6	1999	1/1	0.88	0.29	57,57,57,57	0
88	OHX	5	4070	7/7	0.88	0.26	69,69,69,69	3
88	OHX	1	4020	7/7	0.88	0.32	46,46,46,46	4
87	MG	2	2153	1/1	0.88	0.17	77,77,77,77	0
88	OHX	6	2102	7/7	0.88	0.29	69,69,69,69	3
87	MG	N6	201	1/1	0.88	0.33	64,64,64,64	0
87	MG	5	3564	1/1	0.88	0.38	33,33,33,33	0
88	OHX	M0	303	7/7	0.88	0.19	97,97,97,97	7
88	OHX	4	235	7/7	0.88	0.28	59,59,59,59	3
88	OHX	5	4095	7/7	0.88	0.28	60,60,60,60	4
87	MG	2	1937	1/1	0.88	0.25	66,66,66,66	0
87	MG	6	1994	1/1	0.88	0.75	57,57,57,57	1
87	MG	D9	102	1/1	0.88	0.22	90,90,90,90	0
87	MG	1	3655	1/1	0.88	0.20	44,44,44,44	0
87	MG	1	3713	1/1	0.88	0.44	72,72,72,72	0
88	OHX	6	2136	7/7	0.88	0.20	165,165,165,165	7
88	OHX	1	3990	7/7	0.88	0.25	80,80,80,80	4
87	MG	2	1934	1/1	0.88	0.37	93,93,93,93	0
88	OHX	5	4155	7/7	0.88	0.24	58,58,58,58	4
87	MG	5	3745	1/1	0.88	0.22	39,39,39,39	0
87	MG	1	3519	1/1	0.88	0.33	55,55,55,55	0
87	MG	6	1942	1/1	0.88	0.37	78,78,78,78	0
88	OHX	6	2134	7/7	0.88	0.18	88,88,88,88	6
87	MG	1	3714	1/1	0.88	0.26	46,46,46,46	0
88	OHX	1	4103	7/7	0.88	0.34	46,46,46,46	4
88	OHX	1	3846	7/7	0.88	0.37	43,43,43,43	3
87	MG	5	3642	1/1	0.88	0.45	54,54,54,54	0
88	OHX	1	4104	7/7	0.88	0.27	56,56,56,56	5
87	MG	1	3703	1/1	0.88	0.21	59,59,59,59	0
88	OHX	2	2127	7/7	0.88	0.15	146,146,146,146	6
88	OHX	S9	202	7/7	0.88	0.50	87,87,87,87	5
87	MG	q0	202	1/1	0.88	0.41	50,50,50,50	0
87	MG	1	3411	1/1	0.88	0.24	46,46,46,46	0
87	MG	1	3473	1/1	0.88	0.36	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	3652	1/1	0.88	0.27	46,46,46,46	0
87	MG	1	3593	1/1	0.88	0.22	48,48,48,48	0
88	OHX	6	2109	7/7	0.88	0.20	100,100,100,100	5
87	MG	2	1945	1/1	0.88	0.38	90,90,90,90	0
87	MG	5	3449	1/1	0.88	0.26	37,37,37,37	0
88	OHX	6	2140	7/7	0.88	0.19	119,119,119,119	7
88	OHX	5	3909	7/7	0.88	0.32	54,54,54,54	3
88	OHX	1	4073	7/7	0.88	0.21	55,55,55,55	2
88	OHX	4	230	7/7	0.88	0.30	47,47,47,47	3
88	OHX	5	3923	7/7	0.88	0.38	37,37,37,37	4
87	MG	7	209	1/1	0.88	0.15	59,59,59,59	0
88	OHX	5	4152	7/7	0.88	0.35	50,50,50,50	3
88	OHX	1	4094	7/7	0.88	0.32	60,60,60,60	3
88	OHX	5	4041	7/7	0.88	0.29	47,47,47,47	3
87	MG	1	3416	1/1	0.88	0.39	42,42,42,42	0
88	OHX	6	2170	7/7	0.88	0.25	76,76,76,76	6
87	MG	2	1957	1/1	0.88	0.14	74,74,74,74	0
87	MG	1	3417	1/1	0.88	0.26	50,50,50,50	0
88	OHX	1	4088	7/7	0.88	0.28	58,58,58,58	7
88	OHX	6	2160	7/7	0.88	0.18	98,98,98,98	7
88	OHX	2	2145	7/7	0.88	0.19	88,88,88,88	3
87	MG	1	3702	1/1	0.88	0.45	42,42,42,42	0
88	OHX	1	4085	7/7	0.88	0.31	42,42,42,42	3
87	MG	2	2154	1/1	0.88	0.21	105,105,105,105	0
87	MG	1	3419	1/1	0.88	0.32	47,47,47,47	0
88	OHX	1	4038	7/7	0.88	0.27	83,83,83,83	4
87	MG	1	3754	1/1	0.88	0.22	39,39,39,39	0
87	MG	5	3408	1/1	0.88	0.31	48,48,48,48	0
87	MG	1	3689	1/1	0.88	0.24	55,55,55,55	0
87	MG	1	3446	1/1	0.88	0.31	53,53,53,53	0
87	MG	1	3691	1/1	0.88	0.30	65,65,65,65	0
87	MG	5	4160	1/1	0.88	0.29	39,39,39,39	0
88	OHX	5	4089	7/7	0.88	0.37	67,67,67,67	5
87	MG	7	211	1/1	0.88	0.26	52,52,52,52	0
87	MG	5	3665	1/1	0.88	0.48	39,39,39,39	1
88	OHX	2	2151	7/7	0.88	0.28	109,109,109,109	6
87	MG	2	1987	1/1	0.88	0.36	96,96,96,96	0
88	OHX	5	4139	7/7	0.88	0.29	58,58,58,58	5
87	MG	1	3494	1/1	0.88	0.57	51,51,51,51	0
88	OHX	1	3956	7/7	0.88	0.28	65,65,65,65	3
87	MG	5	3674	1/1	0.88	0.29	50,50,50,50	0
87	MG	5	3595	1/1	0.89	0.41	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	1	4015	7/7	0.89	0.28	52,52,52,52	4
87	MG	5	3465	1/1	0.89	0.30	36,36,36,36	0
88	OHX	1	3965	7/7	0.89	0.24	64,64,64,64	5
88	OHX	2	2107	7/7	0.89	0.15	108,108,108,108	4
87	MG	7	206	1/1	0.89	0.52	54,54,54,54	0
88	OHX	6	2176	7/7	0.89	0.32	63,63,63,63	4
88	OHX	6	2071	7/7	0.89	0.37	57,57,57,57	3
88	OHX	6	2127	7/7	0.89	0.21	98,98,98,98	5
87	MG	1	3622	1/1	0.89	0.21	44,44,44,44	0
88	OHX	15	302	7/7	0.89	0.23	105,105,105,105	5
87	MG	1	3458	1/1	0.89	0.41	43,43,43,43	0
87	MG	5	3643	1/1	0.89	0.12	60,60,60,60	0
88	OHX	6	2117	7/7	0.89	0.24	94,94,94,94	5
88	OHX	1	3976	7/7	0.89	0.28	83,83,83,83	4
88	OHX	6	2144	7/7	0.89	0.19	139,139,139,139	7
87	MG	5	4161	1/1	0.89	0.14	39,39,39,39	0
88	OHX	2	2142	7/7	0.89	0.43	101,101,101,101	6
87	MG	5	3748	1/1	0.89	0.12	45,45,45,45	0
88	OHX	5	4129	7/7	0.89	0.26	58,58,58,58	3
87	MG	1	3599	1/1	0.89	0.26	61,61,61,61	0
88	OHX	1	4099	7/7	0.89	0.26	72,72,72,72	6
87	MG	5	3637	1/1	0.89	0.32	57,57,57,57	0
87	MG	1	3568	1/1	0.89	0.45	40,40,40,40	0
87	MG	5	3726	1/1	0.89	0.24	47,47,47,47	0
88	OHX	L5	301	7/7	0.89	0.38	81,81,81,81	7
87	MG	5	3599	1/1	0.89	0.20	42,42,42,42	0
87	MG	1	3439	1/1	0.89	0.43	55,55,55,55	0
87	MG	5	3594	1/1	0.89	0.42	36,36,36,36	0
88	OHX	5	3993	7/7	0.89	0.30	58,58,58,58	3
88	OHX	6	2175	7/7	0.89	0.23	57,57,57,57	5
88	OHX	5	4154	7/7	0.89	0.28	42,42,42,42	3
87	MG	2	1974	1/1	0.89	0.24	71,71,71,71	0
88	OHX	1	4064	7/7	0.89	0.23	62,62,62,62	5
88	OHX	O9	101	7/7	0.89	0.41	47,47,47,47	4
87	MG	5	3462	1/1	0.89	0.16	39,39,39,39	0
87	MG	L3	403	1/1	0.89	0.11	52,52,52,52	0
87	MG	M6	201	1/1	0.89	0.21	47,47,47,47	0
87	MG	5	3781	1/1	0.89	0.64	56,56,56,56	0
87	MG	1	3712	1/1	0.89	0.27	40,40,40,40	0
88	OHX	6	2173	7/7	0.89	0.17	88,88,88,88	6
87	MG	1	3591	1/1	0.89	0.29	52,52,52,52	0
88	OHX	1	3989	7/7	0.89	0.27	78,78,78,78	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	3617	1/1	0.89	0.29	35,35,35,35	0
87	MG	7	212	1/1	0.89	0.52	70,70,70,70	0
87	MG	2	1911	1/1	0.89	0.26	65,65,65,65	0
87	MG	1	3412	1/1	0.89	0.29	46,46,46,46	0
87	MG	1	3456	1/1	0.89	0.38	33,33,33,33	0
87	MG	5	3444	1/1	0.89	0.49	55,55,55,55	0
88	OHX	5	4124	7/7	0.89	0.12	163,163,163,163	7
87	MG	5	3546	1/1	0.89	0.31	56,56,56,56	0
87	MG	5	3763	1/1	0.89	0.18	41,41,41,41	0
88	OHX	5	4156	7/7	0.89	0.25	78,78,78,78	7
87	MG	1	3654	1/1	0.89	0.22	56,56,56,56	0
87	MG	N3	203	1/1	0.89	0.18	55,55,55,55	0
87	MG	5	3793	1/1	0.89	0.30	49,49,49,49	0
88	OHX	o9	102	7/7	0.89	0.34	47,47,47,47	5
87	MG	5	3450	1/1	0.89	0.34	48,48,48,48	0
88	OHX	1	4031	7/7	0.89	0.21	116,116,116,116	3
87	MG	1	3552	1/1	0.89	0.41	52,52,52,52	0
87	MG	5	3466	1/1	0.89	0.24	44,44,44,44	0
87	MG	5	3669	1/1	0.89	0.25	76,76,76,76	0
88	OHX	l3	404	7/7	0.89	0.24	71,71,71,71	3
87	MG	L7	302	1/1	0.89	0.22	47,47,47,47	0
88	OHX	1	3899	7/7	0.89	0.44	50,50,50,50	5
87	MG	1	3664	1/1	0.89	0.19	60,60,60,60	0
87	MG	1	3730	1/1	0.89	0.19	72,72,72,72	0
87	MG	4	211	1/1	0.89	0.36	66,66,66,66	0
87	MG	5	3610	1/1	0.89	0.51	45,45,45,45	0
88	OHX	6	2151	7/7	0.89	0.22	58,58,58,58	4
88	OHX	5	4149	7/7	0.89	0.19	101,101,101,101	7
87	MG	1	3437	1/1	0.89	0.18	51,51,51,51	0
88	OHX	5	3915	7/7	0.89	0.26	127,127,127,127	5
87	MG	d6	102	1/1	0.89	0.73	65,65,65,65	0
87	MG	5	3443	1/1	0.89	0.17	46,46,46,46	0
88	OHX	5	4071	7/7	0.89	0.31	42,42,42,42	4
88	OHX	6	2110	7/7	0.89	0.26	65,65,65,65	3
87	MG	2	1915	1/1	0.89	0.25	78,78,78,78	0
87	MG	5	3426	1/1	0.89	0.27	65,65,65,65	0
88	OHX	2	2065	7/7	0.89	0.24	117,117,117,117	3
87	MG	8	211	1/1	0.89	0.23	56,56,56,56	0
88	OHX	sR	401	7/7	0.90	0.23	125,125,125,125	5
88	OHX	5	4117	7/7	0.90	0.34	36,36,36,36	2
88	OHX	7	226	7/7	0.90	0.35	61,61,61,61	4
87	MG	1	3475	1/1	0.90	0.25	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	6	2129	7/7	0.90	0.22	58,58,58,58	3
87	MG	6	1930	1/1	0.90	0.10	63,63,63,63	0
88	OHX	1	4105	7/7	0.90	0.17	98,98,98,98	3
88	OHX	5	4098	7/7	0.90	0.18	74,74,74,74	6
88	OHX	O7	105	7/7	0.90	0.33	76,76,76,76	4
88	OHX	2	2052	7/7	0.90	0.18	94,94,94,94	3
88	OHX	C3	201	7/7	0.90	0.26	94,94,94,94	3
87	MG	1	3627	1/1	0.90	0.28	44,44,44,44	0
88	OHX	5	4025	7/7	0.90	0.23	133,133,133,133	6
88	OHX	1	3950	7/7	0.90	0.31	99,99,99,99	5
87	MG	5	3651	1/1	0.90	0.37	45,45,45,45	0
87	MG	1	3506	1/1	0.90	0.30	51,51,51,51	0
87	MG	5	3699	1/1	0.90	0.25	35,35,35,35	0
87	MG	m6	201	1/1	0.90	0.36	42,42,42,42	0
87	MG	2	1953	1/1	0.90	0.33	65,65,65,65	0
88	OHX	1	4076	7/7	0.90	0.83	48,48,48,48	3
88	OHX	1	4055	7/7	0.90	0.30	71,71,71,71	5
87	MG	6	1905	1/1	0.90	0.18	67,67,67,67	0
88	OHX	1	4002	7/7	0.90	0.25	55,55,55,55	2
87	MG	1	3500	1/1	0.90	0.43	40,40,40,40	0
88	OHX	1	4090	7/7	0.90	0.24	46,46,46,46	4
87	MG	5	3760	1/1	0.90	0.31	48,48,48,48	0
87	MG	6	1928	1/1	0.90	0.24	70,70,70,70	0
88	OHX	5	4081	7/7	0.90	0.53	72,72,72,72	4
87	MG	1	3625	1/1	0.90	0.20	56,56,56,56	0
87	MG	1	3698	1/1	0.90	0.41	57,57,57,57	0
87	MG	2	1977	1/1	0.90	0.24	83,83,83,83	0
87	MG	1	3436	1/1	0.90	0.24	40,40,40,40	0
87	MG	5	3761	1/1	0.90	1.13	41,41,41,41	1
88	OHX	5	4079	7/7	0.90	0.25	45,45,45,45	3
87	MG	6	1992	1/1	0.90	0.26	84,84,84,84	0
87	MG	6	1937	1/1	0.90	0.24	71,71,71,71	0
88	OHX	6	2152	7/7	0.90	0.29	87,87,87,87	5
88	OHX	1	4079	7/7	0.90	0.20	120,120,120,120	7
88	OHX	6	2111	7/7	0.90	0.29	94,94,94,94	7
88	OHX	5	4028	7/7	0.90	0.35	39,39,39,39	3
88	OHX	6	2158	7/7	0.90	0.25	70,70,70,70	1
87	MG	n9	102	1/1	0.90	0.61	41,41,41,41	0
88	OHX	1	4001	7/7	0.90	0.17	200,200,200,200	7
88	OHX	5	4125	7/7	0.90	0.25	51,51,51,51	3
87	MG	5	3677	1/1	0.90	0.15	69,69,69,69	0
88	OHX	c5	800	7/7	0.90	0.26	117,117,117,117	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	3692	1/1	0.90	0.36	58,58,58,58	1
87	MG	2	1938	1/1	0.90	0.21	67,67,67,67	0
88	OHX	1	4040	7/7	0.90	0.20	59,59,59,59	2
87	MG	5	3632	1/1	0.90	0.29	51,51,51,51	0
87	MG	6	2002	1/1	0.90	0.21	55,55,55,55	0
88	OHX	8	224	7/7	0.90	0.28	46,46,46,46	4
87	MG	5	3690	1/1	0.90	0.51	68,68,68,68	0
87	MG	1	3748	1/1	0.90	0.30	45,45,45,45	0
88	OHX	6	2161	7/7	0.90	0.17	133,133,133,133	7
87	MG	L2	301	1/1	0.90	0.15	43,43,43,43	0
88	OHX	1	4022	7/7	0.90	0.32	50,50,50,50	4
87	MG	5	3777	1/1	0.90	0.13	67,67,67,67	0
88	OHX	1	3924	7/7	0.90	0.32	64,64,64,64	4
88	OHX	5	4044	7/7	0.90	0.26	54,54,54,54	3
88	OHX	1	4080	7/7	0.90	0.22	60,60,60,60	5
87	MG	1	3546	1/1	0.90	0.18	48,48,48,48	0
88	OHX	2	2062	7/7	0.90	0.22	93,93,93,93	4
88	OHX	6	2088	7/7	0.90	0.26	107,107,107,107	3
88	OHX	1	4081	7/7	0.90	0.34	61,61,61,61	5
87	MG	2	1931	1/1	0.90	0.33	70,70,70,70	0
88	OHX	1	4043	7/7	0.90	0.18	125,125,125,125	6
88	OHX	5	4122	7/7	0.90	0.40	55,55,55,55	4
87	MG	5	3662	1/1	0.90	0.12	55,55,55,55	0
87	MG	n8	203	1/1	0.90	0.20	45,45,45,45	0
88	OHX	1	4018	7/7	0.90	0.30	42,42,42,42	1
87	MG	4	210	1/1	0.90	0.35	61,61,61,61	0
88	OHX	5	4037	7/7	0.90	0.25	62,62,62,62	6
87	MG	2	1923	1/1	0.90	0.15	89,89,89,89	0
88	OHX	1	3984	7/7	0.90	0.30	72,72,72,72	4
87	MG	5	3773	1/1	0.90	0.53	40,40,40,40	0
87	MG	5	3477	1/1	0.90	0.22	76,76,76,76	0
87	MG	5	4163	1/1	0.90	0.25	34,34,34,34	0
87	MG	5	3550	1/1	0.90	0.31	37,37,37,37	0
88	OHX	2	2096	7/7	0.91	0.21	100,100,100,100	4
88	OHX	6	2169	7/7	0.91	0.16	61,61,61,61	5
87	MG	5	3688	1/1	0.91	0.14	66,66,66,66	0
87	MG	O3	202	1/1	0.91	0.26	40,40,40,40	0
87	MG	1	3587	1/1	0.91	0.09	63,63,63,63	0
88	OHX	5	4118	7/7	0.91	0.24	67,67,67,67	5
87	MG	5	3468	1/1	0.91	0.35	49,49,49,49	0
88	OHX	1	4059	7/7	0.91	0.24	65,65,65,65	4
88	OHX	5	3962	7/7	0.91	0.28	61,61,61,61	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	6	2118	7/7	0.91	0.25	62,62,62,62	3
87	MG	5	3482	1/1	0.91	0.44	30,30,30,30	0
87	MG	6	1949	1/1	0.91	0.28	80,80,80,80	0
87	MG	5	3618	1/1	0.91	0.20	56,56,56,56	0
88	OHX	2	2057	7/7	0.91	0.20	96,96,96,96	3
87	MG	6	1975	1/1	0.91	0.25	58,58,58,58	0
87	MG	8	209	1/1	0.91	0.34	50,50,50,50	0
87	MG	1	3581	1/1	0.91	0.22	42,42,42,42	0
87	MG	5	3678	1/1	0.91	0.22	52,52,52,52	0
87	MG	4	204	1/1	0.91	0.43	48,48,48,48	0
88	OHX	5	4036	7/7	0.91	0.24	47,47,47,47	3
87	MG	d2	201	1/1	0.91	0.19	71,71,71,71	0
88	OHX	5	4116	7/7	0.91	0.22	47,47,47,47	3
88	OHX	5	4092	7/7	0.91	0.25	64,64,64,64	5
88	OHX	5	4157	7/7	0.91	0.28	85,85,85,85	5
88	OHX	4	234	7/7	0.91	0.30	64,64,64,64	5
87	MG	O7	103	1/1	0.91	0.84	55,55,55,55	1
87	MG	5	3479	1/1	0.91	0.24	54,54,54,54	0
87	MG	1	3752	1/1	0.91	0.13	51,51,51,51	0
88	OHX	1	4062	7/7	0.91	0.30	39,39,39,39	3
87	MG	5	3524	1/1	0.91	0.35	35,35,35,35	0
88	OHX	1	4006	7/7	0.91	0.23	68,68,68,68	4
88	OHX	1	4057	7/7	0.91	0.25	77,77,77,77	3
87	MG	5	3423	1/1	0.91	0.20	38,38,38,38	0
88	OHX	N8	205	7/7	0.91	0.20	105,105,105,105	7
87	MG	5	3631	1/1	0.91	0.15	50,50,50,50	0
87	MG	6	2186	1/1	0.91	0.20	67,67,67,67	0
88	OHX	2	2141	7/7	0.91	0.44	78,78,78,78	5
88	OHX	2	2143	7/7	0.91	0.63	61,61,61,61	5
87	MG	5	3663	1/1	0.91	0.43	84,84,84,84	0
88	OHX	5	4054	7/7	0.91	0.26	46,46,46,46	2
87	MG	5	3575	1/1	0.91	0.48	42,42,42,42	0
87	MG	6	1966	1/1	0.91	0.18	83,83,83,83	0
88	OHX	3	218	7/7	0.91	0.28	49,49,49,49	4
88	OHX	1	4074	7/7	0.91	0.20	156,156,156,156	7
88	OHX	5	4102	7/7	0.91	0.21	53,53,53,53	5
87	MG	5	3463	1/1	0.91	0.25	56,56,56,56	0
88	OHX	5	4127	7/7	0.91	0.30	45,45,45,45	5
88	OHX	2	2094	7/7	0.91	0.23	79,79,79,79	5
87	MG	5	3420	1/1	0.91	0.15	35,35,35,35	0
87	MG	1	3470	1/1	0.91	0.30	47,47,47,47	0
87	MG	2	1924	1/1	0.91	0.15	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	5	4128	7/7	0.91	0.18	99,99,99,99	4
87	MG	1	3483	1/1	0.91	0.28	39,39,39,39	0
87	MG	6	2003	1/1	0.91	0.68	51,51,51,51	0
88	OHX	1	4039	7/7	0.91	0.23	76,76,76,76	5
88	OHX	1	4042	7/7	0.91	0.36	52,52,52,52	5
87	MG	D4	201	1/1	0.91	0.33	69,69,69,69	0
87	MG	M7	202	1/1	0.91	0.36	41,41,41,41	0
88	OHX	2	2051	7/7	0.91	0.17	136,136,136,136	4
87	MG	5	3604	1/1	0.91	0.21	39,39,39,39	0
87	MG	5	3558	1/1	0.91	0.33	37,37,37,37	0
88	OHX	2	2064	7/7	0.91	0.29	79,79,79,79	3
87	MG	1	3616	1/1	0.91	0.23	44,44,44,44	0
89	ZN	q2	501	1/1	0.91	0.08	79,79,79,79	0
88	OHX	6	2168	7/7	0.91	0.25	72,72,72,72	3
87	MG	5	3713	1/1	0.91	0.39	55,55,55,55	0
87	MG	7	205	1/1	0.91	0.52	34,34,34,34	0
88	OHX	D9	103	7/7	0.91	0.24	89,89,89,89	5
87	MG	1	3545	1/1	0.91	0.29	42,42,42,42	0
87	MG	1	3429	1/1	0.91	0.17	42,42,42,42	0
88	OHX	6	2120	7/7	0.91	0.23	84,84,84,84	5
87	MG	1	3445	1/1	0.91	0.30	46,46,46,46	0
87	MG	1	3753	1/1	0.91	0.28	64,64,64,64	0
87	MG	1	3537	1/1	0.91	0.36	36,36,36,36	0
87	MG	5	3712	1/1	0.91	0.19	40,40,40,40	0
88	OHX	2	2100	7/7	0.91	0.23	70,70,70,70	5
88	OHX	1	4032	7/7	0.91	0.23	56,56,56,56	5
88	OHX	3	216	7/7	0.91	0.31	62,62,62,62	3
87	MG	6	2009	1/1	0.91	0.43	73,73,73,73	0
88	OHX	8	227	7/7	0.91	0.27	56,56,56,56	4
88	OHX	14	402	7/7	0.91	0.27	52,52,52,52	5
87	MG	1	3529	1/1	0.91	0.17	49,49,49,49	0
88	OHX	1	4089	7/7	0.91	0.34	63,63,63,63	3
88	OHX	2	2106	7/7	0.91	0.17	108,108,108,108	5
87	MG	5	3609	1/1	0.91	0.24	38,38,38,38	0
87	MG	2	1988	1/1	0.91	0.20	66,66,66,66	0
88	OHX	8	225	7/7	0.91	0.29	70,70,70,70	5
88	OHX	6	2177	7/7	0.91	0.26	68,68,68,68	5
87	MG	5	3495	1/1	0.91	0.20	34,34,34,34	0
88	OHX	1	4075	7/7	0.91	0.34	74,74,74,74	5
87	MG	1	3403	1/1	0.91	0.17	43,43,43,43	0
87	MG	1	3464	1/1	0.91	0.24	39,39,39,39	0
88	OHX	5	4034	7/7	0.91	0.22	72,72,72,72	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	3467	1/1	0.91	0.27	54,54,54,54	0
88	OHX	2	2087	7/7	0.91	0.23	100,100,100,100	6
87	MG	1	3557	1/1	0.91	0.36	33,33,33,33	0
88	OHX	1	4098	7/7	0.91	0.44	45,45,45,45	5
89	ZN	E1	501	1/1	0.91	0.12	132,132,132,132	0
88	OHX	1	4033	7/7	0.91	0.34	52,52,52,52	5
87	MG	5	3457	1/1	0.91	0.29	34,34,34,34	0
88	OHX	6	2155	7/7	0.91	0.14	108,108,108,108	5
88	OHX	5	4146	7/7	0.91	0.26	39,39,39,39	2
87	MG	1	3428	1/1	0.91	0.24	52,52,52,52	0
88	OHX	6	2124	7/7	0.91	0.42	81,81,81,81	4
87	MG	1	3701	1/1	0.91	0.29	35,35,35,35	0
88	OHX	5	4150	7/7	0.91	0.38	41,41,41,41	6
88	OHX	6	2166	7/7	0.91	0.40	65,65,65,65	5
88	OHX	5	4121	7/7	0.91	0.20	145,145,145,145	7
87	MG	5	3567	1/1	0.92	0.30	38,38,38,38	0
87	MG	5	3655	1/1	0.92	0.19	42,42,42,42	0
88	OHX	2	2115	7/7	0.92	0.17	103,103,103,103	5
87	MG	1	3586	1/1	0.92	0.23	51,51,51,51	0
88	OHX	5	3898	7/7	0.92	0.29	70,70,70,70	5
88	OHX	5	4133	7/7	0.92	0.27	38,38,38,38	4
87	MG	5	3686	1/1	0.92	0.15	40,40,40,40	0
88	OHX	4	233	7/7	0.92	0.33	63,63,63,63	2
87	MG	5	3612	1/1	0.92	0.24	38,38,38,38	0
87	MG	5	3475	1/1	0.92	0.31	34,34,34,34	0
88	OHX	5	4145	7/7	0.92	0.29	47,47,47,47	4
88	OHX	2	2123	7/7	0.92	0.18	94,94,94,94	4
88	OHX	1	3947	7/7	0.92	0.24	92,92,92,92	5
87	MG	6	1990	1/1	0.92	0.34	72,72,72,72	0
87	MG	5	3774	1/1	0.92	0.18	50,50,50,50	0
88	OHX	6	2086	7/7	0.92	0.37	68,68,68,68	5
87	MG	6	1904	1/1	0.92	0.27	82,82,82,82	0
87	MG	5	3716	1/1	0.92	0.18	40,40,40,40	0
88	OHX	6	2130	7/7	0.92	0.23	61,61,61,61	3
88	OHX	1	4096	7/7	0.92	0.26	52,52,52,52	3
87	MG	1	3724	1/1	0.92	0.12	86,86,86,86	0
88	OHX	1	4066	7/7	0.92	0.23	37,37,37,37	3
88	OHX	6	2106	7/7	0.92	0.18	80,80,80,80	3
87	MG	1	3645	1/1	0.92	0.32	57,57,57,57	0
88	OHX	5	4144	7/7	0.92	0.32	49,49,49,49	5
88	OHX	5	4140	7/7	0.92	0.26	52,52,52,52	5
88	OHX	5	4135	7/7	0.92	0.23	68,68,68,68	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	7	228	1/1	0.92	0.27	38,38,38,38	0
88	OHX	1	4095	7/7	0.92	0.26	45,45,45,45	3
88	OHX	2	2140	7/7	0.92	0.52	65,65,65,65	4
87	MG	5	3442	1/1	0.92	0.27	36,36,36,36	0
87	MG	5	3791	1/1	0.92	0.26	42,42,42,42	0
88	OHX	1	4065	7/7	0.92	0.28	98,98,98,98	7
88	OHX	2	2099	7/7	0.92	0.20	99,99,99,99	4
87	MG	5	3746	1/1	0.92	0.17	59,59,59,59	0
88	OHX	6	2128	7/7	0.92	0.39	56,56,56,56	3
87	MG	5	3778	1/1	0.92	0.24	64,64,64,64	0
88	OHX	6	2184	7/7	0.92	0.10	115,115,115,115	6
87	MG	5	3439	1/1	0.92	0.31	46,46,46,46	0
87	MG	5	3487	1/1	0.92	0.20	52,52,52,52	0
88	OHX	c3	201	7/7	0.92	0.19	89,89,89,89	3
88	OHX	M7	205	7/7	0.92	0.30	57,57,57,57	5
88	OHX	1	4025	7/7	0.92	0.30	42,42,42,42	3
88	OHX	6	2179	7/7	0.92	0.18	99,99,99,99	4
87	MG	5	3709	1/1	0.92	0.40	56,56,56,56	0
87	MG	1	3460	1/1	0.92	0.23	59,59,59,59	0
87	MG	6	2187	1/1	0.92	0.15	93,93,93,93	0
88	OHX	2	2118	7/7	0.92	0.34	82,82,82,82	5
88	OHX	2	2053	7/7	0.92	0.19	120,120,120,120	5
88	OHX	6	2172	7/7	0.92	0.31	73,73,73,73	6
88	OHX	6	2159	7/7	0.92	0.10	135,135,135,135	6
87	MG	5	3458	1/1	0.92	0.31	39,39,39,39	0
87	MG	5	3759	1/1	0.92	0.23	44,44,44,44	0
87	MG	6	1907	1/1	0.92	0.16	76,76,76,76	0
88	OHX	5	4052	7/7	0.92	0.20	58,58,58,58	5
87	MG	q1	701	1/1	0.92	0.16	52,52,52,52	0
87	MG	1	3527	1/1	0.92	0.33	40,40,40,40	0
88	OHX	5	4066	7/7	0.92	0.27	53,53,53,53	3
88	OHX	6	2138	7/7	0.92	0.61	62,62,62,62	5
87	MG	5	3493	1/1	0.92	0.20	38,38,38,38	0
88	OHX	2	2061	7/7	0.92	0.27	63,63,63,63	4
88	OHX	1	4071	7/7	0.92	0.26	40,40,40,40	4
87	MG	1	3438	1/1	0.92	0.31	36,36,36,36	0
87	MG	1	3634	1/1	0.92	0.32	60,60,60,60	0
88	OHX	2	2095	7/7	0.92	0.18	70,70,70,70	5
88	OHX	1	4029	7/7	0.92	0.22	51,51,51,51	3
87	MG	6	1983	1/1	0.92	0.17	60,60,60,60	0
87	MG	5	3741	1/1	0.92	0.21	39,39,39,39	0
87	MG	6	1940	1/1	0.92	0.28	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	3694	1/1	0.92	0.23	45,45,45,45	0
87	MG	5	3406	1/1	0.92	0.18	47,47,47,47	0
87	MG	1	3531	1/1	0.92	0.40	52,52,52,52	0
87	MG	5	3628	1/1	0.92	0.20	42,42,42,42	0
88	OHX	2	2088	7/7	0.92	0.23	99,99,99,99	3
87	MG	1	3663	1/1	0.92	0.24	52,52,52,52	0
87	MG	1	3569	1/1	0.92	0.50	35,35,35,35	0
87	MG	1	3705	1/1	0.92	0.23	48,48,48,48	0
87	MG	1	4108	1/1	0.92	0.17	41,41,41,41	0
87	MG	1	3603	1/1	0.92	0.24	45,45,45,45	0
87	MG	1	3611	1/1	0.92	0.37	59,59,59,59	0
87	MG	5	3624	1/1	0.92	0.34	41,41,41,41	0
88	OHX	5	4119	7/7	0.92	0.30	51,51,51,51	4
87	MG	5	3733	1/1	0.92	0.44	39,39,39,39	0
87	MG	6	1952	1/1	0.92	0.33	58,58,58,58	0
88	OHX	5	4110	7/7	0.92	0.28	54,54,54,54	5
88	OHX	1	4034	7/7	0.92	0.38	50,50,50,50	5
88	OHX	2	2078	7/7	0.92	0.21	77,77,77,77	5
88	OHX	6	2094	7/7	0.92	0.17	106,106,106,106	5
87	MG	5	3523	1/1	0.92	0.25	38,38,38,38	0
87	MG	8	205	1/1	0.92	0.22	45,45,45,45	0
88	OHX	5	3918	7/7	0.92	0.41	46,46,46,46	3
88	OHX	6	2092	7/7	0.92	0.28	61,61,61,61	3
87	MG	2	1952	1/1	0.92	0.16	71,71,71,71	0
88	OHX	5	4035	7/7	0.92	0.30	42,42,42,42	4
87	MG	5	3764	1/1	0.92	0.45	110,110,110,110	0
87	MG	5	3506	1/1	0.92	0.35	34,34,34,34	0
88	OHX	5	4086	7/7	0.92	0.23	45,45,45,45	4
87	MG	5	3447	1/1	0.92	0.26	46,46,46,46	0
88	OHX	6	2156	7/7	0.92	0.21	62,62,62,62	4
87	MG	o9	101	1/1	0.92	0.40	53,53,53,53	0
87	MG	1	3682	1/1	0.92	0.39	50,50,50,50	0
88	OHX	2	2116	7/7	0.92	0.17	146,146,146,146	7
87	MG	1	3631	1/1	0.92	0.39	79,79,79,79	0
87	MG	5	3711	1/1	0.92	0.41	63,63,63,63	0
87	MG	5	3779	1/1	0.92	0.26	51,51,51,51	0
88	OHX	5	3990	7/7	0.92	0.28	80,80,80,80	3
88	OHX	6	2150	7/7	0.92	0.26	66,66,66,66	1
87	MG	5	3660	1/1	0.92	0.15	50,50,50,50	0
87	MG	1	3461	1/1	0.92	0.26	46,46,46,46	0
87	MG	1	3561	1/1	0.92	0.42	46,46,46,46	0
87	MG	5	3554	1/1	0.92	0.35	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	3717	1/1	0.92	0.24	44,44,44,44	0
88	OHX	5	4062	7/7	0.92	0.24	50,50,50,50	5
88	OHX	5	4076	7/7	0.92	0.21	38,38,38,38	2
87	MG	5	3557	1/1	0.92	0.20	49,49,49,49	0
87	MG	5	3504	1/1	0.92	0.41	36,36,36,36	0
87	MG	1	3481	1/1	0.92	0.27	40,40,40,40	0
88	OHX	1	4054	7/7	0.92	0.23	43,43,43,43	3
88	OHX	1	3915	7/7	0.92	0.23	72,72,72,72	3
88	OHX	5	3991	7/7	0.92	0.32	96,96,96,96	4
87	MG	1	3454	1/1	0.92	0.27	43,43,43,43	0
87	MG	5	3729	1/1	0.92	0.17	51,51,51,51	0
88	OHX	1	4046	7/7	0.92	0.17	105,105,105,105	5
87	MG	8	208	1/1	0.92	0.35	46,46,46,46	0
87	MG	5	3681	1/1	0.92	0.14	130,130,130,130	0
87	MG	6	1934	1/1	0.93	0.52	79,79,79,79	0
87	MG	6	1943	1/1	0.93	0.51	51,51,51,51	0
87	MG	1	3538	1/1	0.93	0.42	46,46,46,46	0
87	MG	5	3492	1/1	0.93	0.30	46,46,46,46	0
87	MG	2	1940	1/1	0.93	0.18	72,72,72,72	0
88	OHX	2	2134	7/7	0.93	0.18	85,85,85,85	4
88	OHX	5	3967	7/7	0.93	0.28	45,45,45,45	2
87	MG	7	204	1/1	0.93	0.42	46,46,46,46	0
87	MG	2	1983	1/1	0.93	0.20	71,71,71,71	0
87	MG	1	3658	1/1	0.93	0.28	43,43,43,43	0
88	OHX	S8	301	7/7	0.93	0.16	109,109,109,109	6
88	OHX	1	3908	7/7	0.93	0.26	80,80,80,80	2
88	OHX	1	4106	7/7	0.93	0.52	60,60,60,60	4
87	MG	2	1948	1/1	0.93	0.19	66,66,66,66	0
88	OHX	5	4049	7/7	0.93	0.30	40,40,40,40	2
87	MG	5	3658	1/1	0.93	0.19	39,39,39,39	0
87	MG	5	3766	1/1	0.93	0.24	33,33,33,33	0
87	MG	5	3600	1/1	0.93	0.31	45,45,45,45	0
87	MG	5	3620	1/1	0.93	0.40	44,44,44,44	0
88	OHX	6	2142	7/7	0.93	0.29	68,68,68,68	5
87	MG	2	1935	1/1	0.93	0.43	67,67,67,67	0
87	MG	5	3404	1/1	0.93	0.38	35,35,35,35	0
87	MG	n6	201	1/1	0.93	0.29	59,59,59,59	0
88	OHX	5	4050	7/7	0.93	0.21	39,39,39,39	4
87	MG	5	3537	1/1	0.93	0.35	42,42,42,42	0
87	MG	6	1996	1/1	0.93	0.36	60,60,60,60	0
88	OHX	6	2153	7/7	0.93	0.21	75,75,75,75	3
87	MG	2	1936	1/1	0.93	0.26	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	2	2120	7/7	0.93	0.15	123,123,123,123	5
87	MG	4	202	1/1	0.93	0.41	53,53,53,53	0
87	MG	2	1955	1/1	0.93	0.37	78,78,78,78	0
88	OHX	1	4087	7/7	0.93	0.22	45,45,45,45	4
87	MG	5	3772	1/1	0.93	0.14	65,65,65,65	0
87	MG	5	3566	1/1	0.93	0.29	40,40,40,40	0
87	MG	2	1972	1/1	0.93	0.23	91,91,91,91	0
88	OHX	7	227	7/7	0.93	0.22	59,59,59,59	3
88	OHX	2	2136	7/7	0.93	0.27	72,72,72,72	5
87	MG	5	3650	1/1	0.93	0.47	43,43,43,43	0
88	OHX	2	2013	7/7	0.93	0.22	105,105,105,105	3
88	OHX	5	4143	7/7	0.93	0.14	116,116,116,116	5
87	MG	5	3704	1/1	0.93	0.42	44,44,44,44	0
87	MG	6	1957	1/1	0.93	0.52	65,65,65,65	0
88	OHX	5	4031	7/7	0.93	0.47	60,60,60,60	5
87	MG	1	3521	1/1	0.93	0.51	43,43,43,43	0
88	OHX	5	4003	7/7	0.93	0.26	41,41,41,41	2
88	OHX	1	3859	7/7	0.93	0.32	82,82,82,82	5
87	MG	2	1908	1/1	0.93	0.18	84,84,84,84	0
88	OHX	5	4045	7/7	0.93	0.22	56,56,56,56	4
88	OHX	2	2060	7/7	0.93	0.19	73,73,73,73	1
87	MG	1	3496	1/1	0.93	0.26	40,40,40,40	0
88	OHX	6	2171	7/7	0.93	0.14	131,131,131,131	7
88	OHX	1	4024	7/7	0.93	0.21	61,61,61,61	1
88	OHX	1	4091	7/7	0.93	0.40	44,44,44,44	5
88	OHX	6	2154	7/7	0.93	0.30	69,69,69,69	5
88	OHX	6	2147	7/7	0.93	0.29	82,82,82,82	5
88	OHX	6	2077	7/7	0.93	0.24	87,87,87,87	4
87	MG	5	3646	1/1	0.93	0.24	38,38,38,38	0
88	OHX	5	3977	7/7	0.93	0.26	41,41,41,41	5
87	MG	1	3582	1/1	0.93	0.20	38,38,38,38	0
87	MG	5	3517	1/1	0.93	0.24	42,42,42,42	0
87	MG	5	3438	1/1	0.93	0.41	48,48,48,48	0
88	OHX	1	4007	7/7	0.93	0.29	40,40,40,40	4
88	OHX	2	2082	7/7	0.93	0.22	86,86,86,86	5
88	OHX	5	4123	7/7	0.93	0.22	47,47,47,47	3
88	OHX	2	2131	7/7	0.93	0.35	86,86,86,86	6
88	OHX	1	4016	7/7	0.93	0.18	63,63,63,63	3
87	MG	1	3559	1/1	0.93	0.36	33,33,33,33	0
88	OHX	5	4101	7/7	0.93	0.28	54,54,54,54	5
88	OHX	5	3988	7/7	0.93	0.28	54,54,54,54	2
88	OHX	2	2046	7/7	0.93	0.25	98,98,98,98	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	2	2122	7/7	0.93	0.21	83,83,83,83	3
87	MG	1	3620	1/1	0.93	0.32	39,39,39,39	0
87	MG	1	3592	1/1	0.93	0.33	47,47,47,47	0
88	OHX	5	3992	7/7	0.93	0.31	41,41,41,41	4
87	MG	1	3707	1/1	0.93	1.14	45,45,45,45	1
87	MG	8	203	1/1	0.93	0.14	52,52,52,52	0
88	OHX	2	2101	7/7	0.93	0.19	100,100,100,100	5
87	MG	5	3687	1/1	0.93	0.25	47,47,47,47	0
87	MG	n9	101	1/1	0.93	0.21	32,32,32,32	0
87	MG	5	3534	1/1	0.93	0.32	41,41,41,41	0
88	OHX	5	4064	7/7	0.93	0.37	38,38,38,38	3
87	MG	6	1978	1/1	0.93	0.17	88,88,88,88	0
87	MG	2	1968	1/1	0.93	0.16	89,89,89,89	0
88	OHX	5	4069	7/7	0.93	0.32	143,143,143,143	7
88	OHX	6	2126	7/7	0.93	0.19	74,74,74,74	5
88	OHX	1	3967	7/7	0.93	0.32	37,37,37,37	4
88	OHX	1	3985	7/7	0.93	0.19	114,114,114,114	4
87	MG	1	3564	1/1	0.93	0.47	47,47,47,47	0
87	MG	O7	104	1/1	0.93	2.40	43,43,43,43	1
88	OHX	1	3923	7/7	0.93	0.34	36,36,36,36	2
88	OHX	6	2090	7/7	0.93	0.27	84,84,84,84	6
88	OHX	5	4113	7/7	0.93	0.40	53,53,53,53	3
87	MG	5	3478	1/1	0.93	0.37	58,58,58,58	0
88	OHX	2	2102	7/7	0.93	0.13	161,161,161,161	7
88	OHX	5	3983	7/7	0.93	0.26	42,42,42,42	3
87	MG	5	3638	1/1	0.93	0.28	41,41,41,41	0
87	MG	N8	202	1/1	0.93	0.33	44,44,44,44	0
87	MG	3	205	1/1	0.93	0.50	60,60,60,60	0
87	MG	1	3567	1/1	0.93	0.44	48,48,48,48	0
88	OHX	6	2145	7/7	0.93	0.31	88,88,88,88	6
87	MG	5	3401	1/1	0.93	0.19	42,42,42,42	0
88	OHX	5	4055	7/7	0.93	0.26	44,44,44,44	3
87	MG	5	3675	1/1	0.93	0.25	42,42,42,42	0
88	OHX	5	4078	7/7	0.93	0.29	38,38,38,38	5
88	OHX	2	2148	7/7	0.93	0.54	67,67,67,67	4
88	OHX	6	2162	7/7	0.93	0.20	87,87,87,87	4
88	OHX	5	4047	7/7	0.93	0.22	52,52,52,52	3
87	MG	5	3622	1/1	0.93	0.30	38,38,38,38	0
88	OHX	5	4083	7/7	0.93	0.26	74,74,74,74	5
87	MG	1	3733	1/1	0.93	1.15	37,37,37,37	1
88	OHX	19	201	7/7	0.93	0.28	65,65,65,65	2
88	OHX	2	2090	7/7	0.93	0.18	84,84,84,84	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	3	207	1/1	0.93	0.27	68,68,68,68	0
88	OHX	8	228	7/7	0.93	0.27	67,67,67,67	3
88	OHX	8	223	7/7	0.93	0.29	95,95,95,95	3
87	MG	5	3415	1/1	0.93	0.55	55,55,55,55	0
88	OHX	2	2132	7/7	0.93	0.24	81,81,81,81	5
88	OHX	1	4009	7/7	0.93	0.29	42,42,42,42	3
87	MG	5	3661	1/1	0.93	0.34	43,43,43,43	0
88	OHX	6	2139	7/7	0.93	0.21	91,91,91,91	4
88	OHX	5	4011	7/7	0.93	0.28	56,56,56,56	1
88	OHX	5	3933	7/7	0.93	0.25	64,64,64,64	3
87	MG	1	3737	1/1	0.93	0.16	53,53,53,53	0
87	MG	5	3720	1/1	0.93	0.33	42,42,42,42	0
87	MG	7	201	1/1	0.93	0.36	51,51,51,51	0
87	MG	1	3688	1/1	0.93	0.26	39,39,39,39	0
88	OHX	1	3999	7/7	0.93	0.25	55,55,55,55	5
87	MG	6	1948	1/1	0.93	0.20	55,55,55,55	0
87	MG	5	3453	1/1	0.93	0.24	38,38,38,38	0
87	MG	1	3693	1/1	0.93	0.29	53,53,53,53	0
87	MG	2	1910	1/1	0.93	0.30	65,65,65,65	0
87	MG	1	3504	1/1	0.93	0.24	42,42,42,42	0
87	MG	1	3511	1/1	0.93	0.32	36,36,36,36	0
88	OHX	2	2130	7/7	0.93	0.18	103,103,103,103	7
88	OHX	5	4042	7/7	0.93	0.26	47,47,47,47	3
88	OHX	1	4077	7/7	0.93	0.20	56,56,56,56	5
87	MG	1	3404	1/1	0.93	0.21	60,60,60,60	0
87	MG	5	3434	1/1	0.93	0.31	44,44,44,44	0
88	OHX	s9	201	7/7	0.93	0.36	73,73,73,73	5
88	OHX	3	215	7/7	0.93	0.20	80,80,80,80	2
87	MG	n8	201	1/1	0.93	0.20	34,34,34,34	0
87	MG	5	3602	1/1	0.94	0.28	35,35,35,35	0
88	OHX	6	2065	7/7	0.94	0.22	141,141,141,141	6
87	MG	5	3452	1/1	0.94	0.26	35,35,35,35	0
87	MG	1	3401	1/1	0.94	0.44	46,46,46,46	0
88	OHX	2	2111	7/7	0.94	0.26	73,73,73,73	5
87	MG	6	1938	1/1	0.94	0.49	98,98,98,98	0
87	MG	5	3703	1/1	0.94	0.38	48,48,48,48	0
88	OHX	1	3997	7/7	0.94	0.33	49,49,49,49	2
87	MG	6	1913	1/1	0.94	0.26	44,44,44,44	0
87	MG	2	1932	1/1	0.94	0.15	78,78,78,78	0
88	OHX	1	4093	7/7	0.94	0.37	42,42,42,42	5
87	MG	1	3715	1/1	0.94	0.18	49,49,49,49	0
87	MG	5	3732	1/1	0.94	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	3539	1/1	0.94	0.34	29,29,29,29	0
88	OHX	5	4074	7/7	0.94	0.32	53,53,53,53	4
87	MG	6	1982	1/1	0.94	0.31	61,61,61,61	0
88	OHX	2	2070	7/7	0.94	0.27	100,100,100,100	5
87	MG	5	3762	1/1	0.94	0.98	45,45,45,45	1
88	OHX	1	4092	7/7	0.94	0.20	49,49,49,49	4
87	MG	1	3555	1/1	0.94	0.28	45,45,45,45	0
88	OHX	6	2113	7/7	0.94	0.17	66,66,66,66	2
87	MG	1	3424	1/1	0.94	0.12	61,61,61,61	0
87	MG	1	3492	1/1	0.94	0.32	39,39,39,39	0
88	OHX	2	2056	7/7	0.94	0.14	108,108,108,108	5
87	MG	17	301	1/1	0.94	0.18	46,46,46,46	0
88	OHX	6	2123	7/7	0.94	0.21	70,70,70,70	4
87	MG	1	3426	1/1	0.94	0.42	45,45,45,45	0
88	OHX	1	3972	7/7	0.94	0.28	53,53,53,53	2
87	MG	1	3739	1/1	0.94	0.41	45,45,45,45	0
88	OHX	2	2113	7/7	0.94	0.16	99,99,99,99	4
87	MG	5	3707	1/1	0.94	0.13	44,44,44,44	0
87	MG	1	3610	1/1	0.94	0.20	39,39,39,39	1
87	MG	1	3740	1/1	0.94	0.29	62,62,62,62	0
88	OHX	s4	301	7/7	0.94	0.20	82,82,82,82	2
88	OHX	8	231	7/7	0.94	0.20	62,62,62,62	3
88	OHX	1	4049	7/7	0.94	0.19	99,99,99,99	3
87	MG	5	3521	1/1	0.94	0.34	45,45,45,45	0
87	MG	5	3753	1/1	0.94	0.18	42,42,42,42	0
87	MG	1	3482	1/1	0.94	0.29	51,51,51,51	0
87	MG	1	3673	1/1	0.94	0.61	61,61,61,61	0
88	OHX	5	3950	7/7	0.94	0.28	40,40,40,40	4
87	MG	5	3723	1/1	0.94	0.60	55,55,55,55	0
88	OHX	6	2149	7/7	0.94	0.26	49,49,49,49	4
87	MG	1	3534	1/1	0.94	0.34	40,40,40,40	0
87	MG	1	3608	1/1	0.94	0.14	49,49,49,49	0
87	MG	6	1902	1/1	0.94	0.12	59,59,59,59	0
87	MG	5	3456	1/1	0.94	0.19	40,40,40,40	0
87	MG	5	3528	1/1	0.94	0.24	34,34,34,34	0
88	OHX	2	2110	7/7	0.94	0.35	61,61,61,61	5
88	OHX	3	217	7/7	0.94	0.23	78,78,78,78	5
88	OHX	5	3998	7/7	0.94	0.33	101,101,101,101	4
88	OHX	4	232	7/7	0.94	0.24	45,45,45,45	4
88	OHX	1	3853	7/7	0.94	0.37	70,70,70,70	1
87	MG	1	3632	1/1	0.94	0.30	41,41,41,41	0
87	MG	5	3747	1/1	0.94	0.24	46,46,46,46	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	3469	1/1	0.94	0.35	63,63,63,63	0
87	MG	6	1981	1/1	0.94	0.16	85,85,85,85	0
87	MG	1	3755	1/1	0.94	0.28	53,53,53,53	0
87	MG	5	3647	1/1	0.94	0.23	41,41,41,41	0
88	OHX	1	4053	7/7	0.94	0.29	51,51,51,51	4
87	MG	5	3592	1/1	0.94	0.39	45,45,45,45	0
87	MG	2	1943	1/1	0.94	0.29	78,78,78,78	0
87	MG	1	3589	1/1	0.94	0.17	53,53,53,53	0
88	OHX	5	4097	7/7	0.94	0.21	132,132,132,132	5
87	MG	1	3472	1/1	0.94	0.36	58,58,58,58	0
88	OHX	6	2080	7/7	0.94	0.25	76,76,76,76	2
88	OHX	6	2084	7/7	0.94	0.22	98,98,98,98	5
88	OHX	5	4033	7/7	0.94	0.31	37,37,37,37	5
88	OHX	1	4013	7/7	0.94	0.22	60,60,60,60	3
88	OHX	1	3939	7/7	0.94	0.23	76,76,76,76	4
88	OHX	5	3994	7/7	0.94	0.26	45,45,45,45	3
88	OHX	5	4053	7/7	0.94	0.24	67,67,67,67	4
87	MG	2	1917	1/1	0.94	0.17	65,65,65,65	0
87	MG	1	3465	1/1	0.94	0.40	30,30,30,30	0
88	OHX	5	4057	7/7	0.94	0.26	73,73,73,73	6
88	OHX	6	2119	7/7	0.94	0.19	62,62,62,62	2
87	MG	2	1956	1/1	0.94	0.55	90,90,90,90	0
87	MG	5	3758	1/1	0.94	0.43	58,58,58,58	0
87	MG	6	1947	1/1	0.94	0.21	58,58,58,58	0
88	OHX	6	2178	7/7	0.94	0.16	97,97,97,97	5
88	OHX	1	3948	7/7	0.94	0.24	73,73,73,73	3
87	MG	1	3520	1/1	0.94	0.39	53,53,53,53	0
87	MG	1	3517	1/1	0.94	0.45	40,40,40,40	0
88	OHX	5	3961	7/7	0.94	0.21	56,56,56,56	3
87	MG	6	1923	1/1	0.94	0.34	82,82,82,82	0
88	OHX	5	4012	7/7	0.94	0.23	49,49,49,49	3
87	MG	Q0	202	1/1	0.94	0.76	56,56,56,56	0
87	MG	sM	301	1/1	0.94	0.19	50,50,50,50	0
87	MG	3	204	1/1	0.94	0.43	37,37,37,37	0
88	OHX	1	4036	7/7	0.94	0.28	70,70,70,70	3
87	MG	1	3722	1/1	0.94	0.35	56,56,56,56	0
87	MG	1	3565	1/1	0.94	0.17	50,50,50,50	0
88	OHX	6	2087	7/7	0.94	0.18	100,100,100,100	5
87	MG	5	3424	1/1	0.94	0.23	51,51,51,51	0
88	OHX	1	3900	7/7	0.94	0.20	51,51,51,51	3
88	OHX	1	3935	7/7	0.94	0.23	55,55,55,55	2
88	OHX	s8	302	7/7	0.94	0.24	108,108,108,108	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	1	4047	7/7	0.94	0.25	48,48,48,48	3
88	OHX	5	4030	7/7	0.94	0.31	48,48,48,48	1
88	OHX	5	4114	7/7	0.94	0.27	47,47,47,47	4
87	MG	1	3756	1/1	0.94	0.16	54,54,54,54	0
87	MG	1	3573	1/1	0.94	0.38	53,53,53,53	0
87	MG	1	3501	1/1	0.94	0.32	47,47,47,47	0
87	MG	1	3430	1/1	0.94	0.12	50,50,50,50	0
87	MG	1	3539	1/1	0.94	0.30	45,45,45,45	0
87	MG	2	1951	1/1	0.94	0.21	106,106,106,106	0
88	OHX	1	3953	7/7	0.94	0.26	131,131,131,131	7
88	OHX	5	3796	7/7	0.94	0.28	52,52,52,52	2
88	OHX	5	4039	7/7	0.94	0.23	55,55,55,55	3
87	MG	5	3611	1/1	0.94	0.29	46,46,46,46	0
88	OHX	5	4108	7/7	0.94	0.26	64,64,64,64	4
88	OHX	2	2109	7/7	0.94	0.25	73,73,73,73	4
87	MG	1	3457	1/1	0.94	0.33	32,32,32,32	0
87	MG	1	3649	1/1	0.94	0.42	45,45,45,45	0
88	OHX	6	2183	7/7	0.94	0.15	101,101,101,101	6
87	MG	5	3530	1/1	0.94	0.32	46,46,46,46	0
88	OHX	1	4019	7/7	0.94	0.21	65,65,65,65	2
88	OHX	2	2047	7/7	0.94	0.20	88,88,88,88	5
87	MG	5	3784	1/1	0.94	0.28	41,41,41,41	0
88	OHX	2	2014	7/7	0.94	0.28	75,75,75,75	4
87	MG	2	1907	1/1	0.94	0.36	65,65,65,65	0
88	OHX	1	4037	7/7	0.94	0.20	60,60,60,60	6
87	MG	5	3437	1/1	0.94	0.30	33,33,33,33	0
87	MG	1	3672	1/1	0.94	0.23	68,68,68,68	0
88	OHX	1	3856	7/7	0.94	0.28	45,45,45,45	4
88	OHX	5	4075	7/7	0.94	0.21	49,49,49,49	3
88	OHX	SR	401	7/7	0.94	0.14	133,133,133,133	5
87	MG	1	3731	1/1	0.94	0.51	47,47,47,47	1
88	OHX	6	2064	7/7	0.94	0.28	97,97,97,97	3
88	OHX	1	3907	7/7	0.94	0.30	69,69,69,69	3
88	OHX	5	4022	7/7	0.94	0.22	96,96,96,96	6
87	MG	5	3525	1/1	0.94	0.24	46,46,46,46	0
88	OHX	2	2035	7/7	0.94	0.21	100,100,100,100	6
88	OHX	6	2163	7/7	0.94	0.20	62,62,62,62	7
87	MG	5	3425	1/1	0.94	0.38	37,37,37,37	0
87	MG	6	1953	1/1	0.94	0.43	51,51,51,51	0
88	OHX	1	3904	7/7	0.94	0.22	55,55,55,55	3
87	MG	2	1939	1/1	0.94	0.18	79,79,79,79	0
88	OHX	1	3912	7/7	0.94	0.30	112,112,112,112	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	1	4063	7/7	0.94	0.26	55,55,55,55	4
88	OHX	5	3959	7/7	0.94	0.29	78,78,78,78	2
88	OHX	1	3838	7/7	0.94	0.28	78,78,78,78	3
88	OHX	1	3964	7/7	0.94	0.24	54,54,54,54	4
88	OHX	1	4078	7/7	0.94	0.27	45,45,45,45	6
88	OHX	6	2107	7/7	0.94	0.18	114,114,114,114	7
87	MG	5	3430	1/1	0.94	0.13	41,41,41,41	0
88	OHX	6	2043	7/7	0.94	0.20	91,91,91,91	4
88	OHX	5	4058	7/7	0.94	0.23	50,50,50,50	4
88	OHX	1	3995	7/7	0.94	0.18	98,98,98,98	7
88	OHX	2	2105	7/7	0.95	0.16	106,106,106,106	4
88	OHX	2	2092	7/7	0.95	0.22	113,113,113,113	5
88	OHX	2	2138	7/7	0.95	0.36	72,72,72,72	6
88	OHX	2	2075	7/7	0.95	0.22	60,60,60,60	4
87	MG	L7	303	1/1	0.95	0.14	51,51,51,51	0
88	OHX	4	223	7/7	0.95	0.27	67,67,67,67	3
87	MG	5	3787	1/1	0.95	0.15	42,42,42,42	0
87	MG	6	1910	1/1	0.95	0.21	59,59,59,59	0
87	MG	5	3634	1/1	0.95	0.24	47,47,47,47	0
88	OHX	8	214	7/7	0.95	0.30	80,80,80,80	4
88	OHX	1	3903	7/7	0.95	0.27	52,52,52,52	3
88	OHX	1	4005	7/7	0.95	0.29	60,60,60,60	5
88	OHX	8	226	7/7	0.95	0.23	92,92,92,92	5
88	OHX	2	2002	7/7	0.95	0.23	109,109,109,109	4
87	MG	1	3657	1/1	0.95	0.33	50,50,50,50	0
87	MG	6	1965	1/1	0.95	0.31	63,63,63,63	0
88	OHX	2	2071	7/7	0.95	0.25	104,104,104,104	5
88	OHX	5	4016	7/7	0.95	0.26	78,78,78,78	3
87	MG	5	3782	1/1	0.95	0.28	52,52,52,52	0
87	MG	1	3547	1/1	0.95	0.47	38,38,38,38	0
87	MG	1	3728	1/1	0.95	0.26	75,75,75,75	0
87	MG	5	3697	1/1	0.95	0.38	40,40,40,40	0
88	OHX	1	4083	7/7	0.95	0.22	90,90,90,90	4
87	MG	m3	201	1/1	0.95	0.19	40,40,40,40	0
88	OHX	5	3920	7/7	0.95	0.33	48,48,48,48	2
87	MG	5	3553	1/1	0.95	0.32	36,36,36,36	0
87	MG	5	3750	1/1	0.95	0.14	47,47,47,47	0
87	MG	1	3695	1/1	0.95	0.46	59,59,59,59	0
87	MG	5	3491	1/1	0.95	0.23	46,46,46,46	0
87	MG	5	3470	1/1	0.95	0.25	49,49,49,49	0
87	MG	5	3579	1/1	0.95	0.35	32,32,32,32	0
87	MG	5	3436	1/1	0.95	0.24	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	1	3971	7/7	0.95	0.28	61,61,61,61	3
87	MG	1	3499	1/1	0.95	0.31	40,40,40,40	0
88	OHX	2	2104	7/7	0.95	0.23	106,106,106,106	7
88	OHX	5	4018	7/7	0.95	0.28	87,87,87,87	4
87	MG	1	3478	1/1	0.95	0.24	39,39,39,39	0
87	MG	5	4162	1/1	0.95	1.68	36,36,36,36	1
88	OHX	2	2048	7/7	0.95	0.18	97,97,97,97	3
88	OHX	5	3904	7/7	0.95	0.30	67,67,67,67	3
88	OHX	1	4035	7/7	0.95	0.20	64,64,64,64	4
87	MG	1	3566	1/1	0.95	0.45	53,53,53,53	0
88	OHX	1	3893	7/7	0.95	0.20	131,131,131,131	5
87	MG	1	3490	1/1	0.95	0.38	40,40,40,40	0
88	OHX	5	4120	7/7	0.95	0.28	38,38,38,38	3
87	MG	5	3776	1/1	0.95	0.19	49,49,49,49	0
88	OHX	1	4058	7/7	0.95	0.13	106,106,106,106	6
88	OHX	5	3840	7/7	0.95	0.33	65,65,65,65	2
88	OHX	1	3969	7/7	0.95	0.26	64,64,64,64	4
88	OHX	5	4094	7/7	0.95	0.19	64,64,64,64	5
88	OHX	1	3831	7/7	0.95	0.29	85,85,85,85	3
88	OHX	1	3949	7/7	0.95	0.22	37,37,37,37	2
88	OHX	5	3997	7/7	0.95	0.24	42,42,42,42	3
88	OHX	5	3932	7/7	0.95	0.36	88,88,88,88	3
87	MG	6	1956	1/1	0.95	0.34	61,61,61,61	0
88	OHX	6	2143	7/7	0.95	0.16	74,74,74,74	5
88	OHX	1	3914	7/7	0.95	0.26	70,70,70,70	4
87	MG	5	3414	1/1	0.95	0.36	34,34,34,34	0
88	OHX	5	4059	7/7	0.95	0.27	40,40,40,40	2
88	OHX	1	4044	7/7	0.95	0.23	62,62,62,62	4
88	OHX	5	3912	7/7	0.95	0.27	43,43,43,43	4
88	OHX	2	2020	7/7	0.95	0.23	73,73,73,73	4
87	MG	2	1928	1/1	0.95	0.32	74,74,74,74	0
88	OHX	5	4148	7/7	0.95	0.17	45,45,45,45	6
88	OHX	5	3966	7/7	0.95	0.25	55,55,55,55	4
88	OHX	1	3906	7/7	0.95	0.19	59,59,59,59	2
87	MG	5	3410	1/1	0.95	0.29	37,37,37,37	0
87	MG	1	3636	1/1	0.95	0.32	58,58,58,58	0
88	OHX	6	2068	7/7	0.95	0.22	99,99,99,99	3
87	MG	5	3585	1/1	0.95	0.48	38,38,38,38	0
87	MG	5	3752	1/1	0.95	0.37	41,41,41,41	1
87	MG	5	3659	1/1	0.95	0.27	49,49,49,49	0
87	MG	1	3434	1/1	0.95	0.25	59,59,59,59	0
87	MG	5	3727	1/1	0.95	0.36	46,46,46,46	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	5	4084	7/7	0.95	0.20	48,48,48,48	5
88	OHX	5	3939	7/7	0.95	0.33	46,46,46,46	3
88	OHX	6	2125	7/7	0.95	0.16	76,76,76,76	2
87	MG	1	3526	1/1	0.95	0.29	38,38,38,38	0
88	OHX	4	231	7/7	0.95	0.19	56,56,56,56	3
88	OHX	1	3892	7/7	0.95	0.23	149,149,149,149	5
88	OHX	q1	702	7/7	0.95	0.20	48,48,48,48	3
88	OHX	1	4010	7/7	0.95	0.36	50,50,50,50	6
88	OHX	6	2097	7/7	0.95	0.18	97,97,97,97	3
88	OHX	1	3870	7/7	0.95	0.25	43,43,43,43	3
88	OHX	7	225	7/7	0.95	0.25	43,43,43,43	4
87	MG	6	1972	1/1	0.95	0.10	60,60,60,60	0
88	OHX	5	3989	7/7	0.95	0.26	48,48,48,48	3
88	OHX	1	3982	7/7	0.95	0.20	50,50,50,50	2
88	OHX	2	2112	7/7	0.95	0.15	103,103,103,103	6
88	OHX	c8	201	7/7	0.95	0.22	94,94,94,94	5
88	OHX	5	3905	7/7	0.95	0.27	118,118,118,118	3
88	OHX	5	4005	7/7	0.95	0.20	78,78,78,78	6
87	MG	1	3502	1/1	0.95	0.28	38,38,38,38	0
87	MG	5	3403	1/1	0.95	0.40	41,41,41,41	0
87	MG	1	3493	1/1	0.95	0.40	30,30,30,30	0
87	MG	5	3606	1/1	0.95	0.15	40,40,40,40	0
87	MG	5	3635	1/1	0.95	0.26	42,42,42,42	0
88	OHX	2	2085	7/7	0.95	0.19	83,83,83,83	3
87	MG	5	3409	1/1	0.95	0.31	41,41,41,41	0
88	OHX	5	3931	7/7	0.95	0.27	55,55,55,55	3
88	OHX	5	3981	7/7	0.95	0.18	60,60,60,60	5
88	OHX	5	3958	7/7	0.95	0.26	52,52,52,52	2
87	MG	4	215	1/1	0.95	0.94	51,51,51,51	1
88	OHX	2	2068	7/7	0.95	0.17	144,144,144,144	6
88	OHX	1	3993	7/7	0.95	0.26	53,53,53,53	2
88	OHX	1	3938	7/7	0.95	0.26	53,53,53,53	3
88	OHX	2	2010	7/7	0.95	0.27	86,86,86,86	5
88	OHX	5	3924	7/7	0.95	0.27	45,45,45,45	4
88	OHX	1	3991	7/7	0.95	0.40	88,88,88,88	5
88	OHX	1	4017	7/7	0.95	0.32	50,50,50,50	5
88	OHX	6	2141	7/7	0.95	0.15	87,87,87,87	5
88	OHX	5	4046	7/7	0.95	0.23	46,46,46,46	2
88	OHX	8	219	7/7	0.95	0.25	59,59,59,59	2
87	MG	6	1958	1/1	0.95	0.47	51,51,51,51	0
87	MG	6	1987	1/1	0.95	0.30	58,58,58,58	0
87	MG	1	3570	1/1	0.95	0.40	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	3735	1/1	0.95	1.81	38,38,38,38	0
88	OHX	1	4012	7/7	0.95	0.28	41,41,41,41	4
87	MG	1	3706	1/1	0.95	0.27	36,36,36,36	0
88	OHX	1	3843	7/7	0.95	0.25	111,111,111,111	1
88	OHX	1	3962	7/7	0.95	0.24	42,42,42,42	3
87	MG	O2	201	1/1	0.95	0.65	36,36,36,36	1
88	OHX	2	2083	7/7	0.95	0.17	100,100,100,100	6
88	OHX	6	2099	7/7	0.95	0.19	64,64,64,64	5
87	MG	N3	201	1/1	0.95	0.32	39,39,39,39	0
87	MG	1	3727	1/1	0.95	0.36	46,46,46,46	0
88	OHX	5	4063	7/7	0.95	0.21	54,54,54,54	2
88	OHX	5	4115	7/7	0.95	0.21	92,92,92,92	2
87	MG	1	3676	1/1	0.95	0.72	49,49,49,49	0
87	MG	5	3471	1/1	0.95	0.31	59,59,59,59	0
87	MG	5	3555	1/1	0.95	0.32	36,36,36,36	0
87	MG	1	3628	1/1	0.95	0.32	51,51,51,51	0
87	MG	5	3522	1/1	0.95	0.48	45,45,45,45	0
88	OHX	1	3926	7/7	0.95	0.26	50,50,50,50	3
88	OHX	5	4080	7/7	0.95	0.19	111,111,111,111	4
88	OHX	2	2091	7/7	0.95	0.15	85,85,85,85	4
88	OHX	5	3871	7/7	0.95	0.39	42,42,42,42	3
88	OHX	6	2066	7/7	0.95	0.19	161,161,161,161	6
88	OHX	1	4021	7/7	0.95	0.19	48,48,48,48	5
88	OHX	5	4112	7/7	0.95	0.18	57,57,57,57	3
88	OHX	1	3951	7/7	0.95	0.24	41,41,41,41	3
88	OHX	5	3999	7/7	0.95	0.26	53,53,53,53	1
88	OHX	m0	302	7/7	0.95	0.27	97,97,97,97	4
87	MG	1	3684	1/1	0.95	0.15	57,57,57,57	0
87	MG	1	3512	1/1	0.95	0.45	37,37,37,37	0
87	MG	5	3519	1/1	0.95	0.34	32,32,32,32	0
88	OHX	5	3930	7/7	0.95	0.23	49,49,49,49	3
88	OHX	1	3980	7/7	0.95	0.15	182,182,182,182	7
88	OHX	1	3890	7/7	0.95	0.16	106,106,106,106	5
87	MG	m7	203	1/1	0.95	0.30	35,35,35,35	0
87	MG	6	1963	1/1	0.95	0.19	89,89,89,89	0
87	MG	1	3607	1/1	0.95	0.19	45,45,45,45	0
87	MG	6	1946	1/1	0.95	0.30	48,48,48,48	0
88	OHX	6	2073	7/7	0.95	0.24	68,68,68,68	5
87	MG	6	1918	1/1	0.95	0.35	48,48,48,48	0
88	OHX	5	4105	7/7	0.95	0.26	44,44,44,44	5
87	MG	3	201	1/1	0.95	0.37	71,71,71,71	0
87	MG	n8	202	1/1	0.95	0.27	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	3602	1/1	0.95	0.25	43,43,43,43	0
87	MG	7	202	1/1	0.95	0.43	26,26,26,26	0
87	MG	1	3656	1/1	0.95	0.35	44,44,44,44	0
88	OHX	1	3994	7/7	0.95	0.22	47,47,47,47	2
87	MG	1	3571	1/1	0.95	0.40	48,48,48,48	0
87	MG	5	3743	1/1	0.95	0.23	45,45,45,45	0
87	MG	2	1920	1/1	0.95	0.27	61,61,61,61	0
87	MG	1	3624	1/1	0.95	0.26	38,38,38,38	0
88	OHX	M0	302	7/7	0.95	0.30	50,50,50,50	4
87	MG	2	1958	1/1	0.95	0.11	70,70,70,70	0
87	MG	5	3695	1/1	0.95	0.21	39,39,39,39	0
87	MG	5	3788	1/1	0.95	0.61	40,40,40,40	0
87	MG	1	3612	1/1	0.95	0.11	58,58,58,58	0
88	OHX	5	4027	7/7	0.95	0.20	45,45,45,45	4
87	MG	1	3720	1/1	0.95	0.17	48,48,48,48	0
88	OHX	5	4106	7/7	0.95	0.25	52,52,52,52	3
87	MG	5	3411	1/1	0.95	0.24	37,37,37,37	0
88	OHX	5	4013	7/7	0.95	0.23	67,67,67,67	4
87	MG	5	3581	1/1	0.95	0.48	28,28,28,28	0
88	OHX	7	224	7/7	0.95	0.27	51,51,51,51	4
87	MG	5	3461	1/1	0.95	0.51	48,48,48,48	0
88	OHX	6	2098	7/7	0.95	0.21	75,75,75,75	4
88	OHX	1	4023	7/7	0.95	0.22	69,69,69,69	6
87	MG	5	3474	1/1	0.95	0.17	39,39,39,39	0
87	MG	1	3518	1/1	0.95	0.47	41,41,41,41	0
88	OHX	5	4015	7/7	0.95	0.23	66,66,66,66	4
87	MG	1	3415	1/1	0.95	0.47	57,57,57,57	0
88	OHX	2	2072	7/7	0.95	0.20	104,104,104,104	5
88	OHX	1	3958	7/7	0.96	0.25	47,47,47,47	4
88	OHX	1	4014	7/7	0.96	0.22	53,53,53,53	3
87	MG	1	3441	1/1	0.96	0.29	56,56,56,56	0
88	OHX	5	4067	7/7	0.96	0.17	41,41,41,41	4
87	MG	1	3725	1/1	0.96	0.26	43,43,43,43	0
87	MG	1	3548	1/1	0.96	0.40	35,35,35,35	0
87	MG	l3	401	1/1	0.96	0.44	31,31,31,31	0
88	OHX	6	2075	7/7	0.96	0.19	71,71,71,71	2
87	MG	5	3489	1/1	0.96	0.33	40,40,40,40	0
87	MG	6	2001	1/1	0.96	0.81	51,51,51,51	0
88	OHX	5	4077	7/7	0.96	0.28	53,53,53,53	5
88	OHX	6	2135	7/7	0.96	0.11	88,88,88,88	5
88	OHX	2	2023	7/7	0.96	0.29	111,111,111,111	2
88	OHX	5	3894	7/7	0.96	0.26	56,56,56,56	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4165	1/1	0.96	1.10	39,39,39,39	1
88	OHX	1	3952	7/7	0.96	0.22	46,46,46,46	5
88	OHX	8	222	7/7	0.96	0.23	59,59,59,59	3
88	OHX	2	2073	7/7	0.96	0.21	64,64,64,64	4
88	OHX	6	2029	7/7	0.96	0.31	67,67,67,67	5
88	OHX	2	2037	7/7	0.96	0.24	102,102,102,102	3
87	MG	1	3668	1/1	0.96	0.21	51,51,51,51	0
87	MG	1	3452	1/1	0.96	0.31	36,36,36,36	0
88	OHX	1	3873	7/7	0.96	0.27	50,50,50,50	2
88	OHX	6	2148	7/7	0.96	0.15	93,93,93,93	5
88	OHX	5	3934	7/7	0.96	0.28	98,98,98,98	2
87	MG	5	3529	1/1	0.96	0.50	28,28,28,28	0
87	MG	1	3556	1/1	0.96	0.37	29,29,29,29	0
88	OHX	1	3910	7/7	0.96	0.20	75,75,75,75	3
88	OHX	5	3858	7/7	0.96	0.31	45,45,45,45	4
88	OHX	5	4000	7/7	0.96	0.26	48,48,48,48	4
88	OHX	1	3839	7/7	0.96	0.27	55,55,55,55	3
87	MG	1	3630	1/1	0.96	0.13	40,40,40,40	0
88	OHX	5	3995	7/7	0.96	0.28	68,68,68,68	5
88	OHX	5	3927	7/7	0.96	0.22	48,48,48,48	2
88	OHX	1	3897	7/7	0.96	0.21	51,51,51,51	5
88	OHX	8	220	7/7	0.96	0.25	75,75,75,75	3
87	MG	5	3590	1/1	0.96	0.39	37,37,37,37	0
87	MG	5	3494	1/1	0.96	0.25	35,35,35,35	0
87	MG	1	3588	1/1	0.96	0.28	55,55,55,55	0
88	OHX	7	223	7/7	0.96	0.29	65,65,65,65	1
88	OHX	6	2070	7/7	0.96	0.19	86,86,86,86	3
88	OHX	1	3979	7/7	0.96	0.20	69,69,69,69	3
87	MG	5	3586	1/1	0.96	0.38	31,31,31,31	0
88	OHX	1	3937	7/7	0.96	0.21	54,54,54,54	4
87	MG	1	3651	1/1	0.96	0.19	58,58,58,58	0
88	OHX	1	4107	7/7	0.96	0.23	151,151,151,151	6
88	OHX	2	2069	7/7	0.96	0.13	122,122,122,122	3
88	OHX	1	3981	7/7	0.96	0.24	49,49,49,49	3
88	OHX	1	3802	7/7	0.96	0.35	66,66,66,66	3
88	OHX	6	2061	7/7	0.96	0.21	84,84,84,84	2
87	MG	5	3540	1/1	0.96	0.40	36,36,36,36	0
88	OHX	5	4008	7/7	0.96	0.28	40,40,40,40	3
87	MG	1	3523	1/1	0.96	0.42	33,33,33,33	0
87	MG	5	3570	1/1	0.96	0.30	38,38,38,38	0
87	MG	1	3480	1/1	0.96	0.17	55,55,55,55	0
87	MG	5	3483	1/1	0.96	0.16	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	3474	1/1	0.96	0.32	43,43,43,43	0
88	OHX	1	3911	7/7	0.96	0.22	64,64,64,64	4
87	MG	6	1927	1/1	0.96	0.28	54,54,54,54	0
87	MG	5	3518	1/1	0.96	0.41	31,31,31,31	0
88	OHX	5	4073	7/7	0.96	0.20	47,47,47,47	2
87	MG	5	3744	1/1	0.96	0.11	42,42,42,42	0
88	OHX	L4	401	7/7	0.96	0.31	61,61,61,61	6
87	MG	2	1947	1/1	0.96	0.20	98,98,98,98	0
88	OHX	5	3965	7/7	0.96	0.34	61,61,61,61	3
88	OHX	5	4002	7/7	0.96	0.27	63,63,63,63	4
87	MG	5	3630	1/1	0.96	0.27	55,55,55,55	0
88	OHX	6	2112	7/7	0.96	0.22	69,69,69,69	3
88	OHX	6	2083	7/7	0.96	0.32	85,85,85,85	7
87	MG	1	3408	1/1	0.96	0.31	38,38,38,38	0
87	MG	5	3431	1/1	0.96	0.43	44,44,44,44	0
87	MG	6	1929	1/1	0.96	0.29	68,68,68,68	0
87	MG	1	3732	1/1	0.96	0.40	37,37,37,37	0
87	MG	6	1935	1/1	0.96	0.35	50,50,50,50	0
87	MG	5	3533	1/1	0.96	0.30	54,54,54,54	0
87	MG	1	3687	1/1	0.96	0.47	41,41,41,41	1
87	MG	1	3442	1/1	0.96	0.33	45,45,45,45	0
87	MG	5	3513	1/1	0.96	0.30	48,48,48,48	0
88	OHX	6	2044	7/7	0.96	0.25	51,51,51,51	3
88	OHX	2	2050	7/7	0.96	0.21	77,77,77,77	3
88	OHX	2	2026	7/7	0.96	0.18	99,99,99,99	3
87	MG	5	3572	1/1	0.96	0.46	32,32,32,32	0
87	MG	4	205	1/1	0.96	0.28	40,40,40,40	0
88	OHX	5	4056	7/7	0.96	0.23	49,49,49,49	5
88	OHX	1	3889	7/7	0.96	0.20	49,49,49,49	3
87	MG	6	2008	1/1	0.96	0.26	83,83,83,83	0
88	OHX	6	2051	7/7	0.96	0.26	123,123,123,123	5
87	MG	5	3507	1/1	0.96	0.45	37,37,37,37	0
88	OHX	1	3875	7/7	0.96	0.21	86,86,86,86	3
87	MG	1	3560	1/1	0.96	0.60	35,35,35,35	0
88	OHX	5	4068	7/7	0.96	0.32	38,38,38,38	4
88	OHX	5	3963	7/7	0.96	0.33	64,64,64,64	2
88	OHX	1	4048	7/7	0.96	0.17	52,52,52,52	3
88	OHX	1	3954	7/7	0.96	0.25	54,54,54,54	3
88	OHX	1	4004	7/7	0.96	0.26	59,59,59,59	4
88	OHX	1	3963	7/7	0.96	0.19	58,58,58,58	3
87	MG	1	3491	1/1	0.96	0.27	44,44,44,44	0
88	OHX	5	3872	7/7	0.96	0.33	71,71,71,71	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	1	3820	7/7	0.96	0.28	86,86,86,86	3
87	MG	1	3595	1/1	0.96	0.35	45,45,45,45	0
87	MG	5	3510	1/1	0.96	0.36	35,35,35,35	0
87	MG	1	4109	1/1	0.96	0.20	56,56,56,56	0
88	OHX	5	4017	7/7	0.96	0.21	69,69,69,69	4
87	MG	2	1991	1/1	0.96	0.13	76,76,76,76	0
87	MG	5	3696	1/1	0.96	0.11	56,56,56,56	0
88	OHX	8	218	7/7	0.96	0.27	73,73,73,73	2
88	OHX	1	3978	7/7	0.96	0.19	74,74,74,74	5
87	MG	5	3469	1/1	0.96	0.28	38,38,38,38	0
87	MG	5	3679	1/1	0.96	0.14	50,50,50,50	0
87	MG	1	3669	1/1	0.96	0.25	38,38,38,38	0
87	MG	5	3576	1/1	0.96	0.22	35,35,35,35	0
88	OHX	2	2081	7/7	0.96	0.23	78,78,78,78	6
88	OHX	1	3977	7/7	0.96	0.21	51,51,51,51	3
88	OHX	6	2131	7/7	0.96	0.26	53,53,53,53	4
87	MG	6	1911	1/1	0.96	0.23	91,91,91,91	0
88	OHX	2	2103	7/7	0.96	0.27	77,77,77,77	3
87	MG	5	3512	1/1	0.96	0.12	40,40,40,40	0
88	OHX	1	3988	7/7	0.96	0.27	68,68,68,68	3
87	MG	M0	301	1/1	0.96	0.29	42,42,42,42	0
87	MG	1	3444	1/1	0.96	0.22	44,44,44,44	0
87	MG	1	3455	1/1	0.96	0.40	32,32,32,32	0
87	MG	2	1927	1/1	0.96	0.29	95,95,95,95	0
88	OHX	2	2031	7/7	0.96	0.17	102,102,102,102	1
87	MG	1	3495	1/1	0.96	0.31	40,40,40,40	0
87	MG	6	1903	1/1	0.96	0.15	53,53,53,53	0
88	OHX	2	2007	7/7	0.96	0.19	136,136,136,136	6
88	OHX	2	2024	7/7	0.96	0.16	98,98,98,98	6
87	MG	1	3590	1/1	0.96	0.39	70,70,70,70	0
87	MG	5	3689	1/1	0.96	1.08	39,39,39,39	1
88	OHX	2	2038	7/7	0.96	0.18	110,110,110,110	3
88	OHX	6	2093	7/7	0.96	0.21	47,47,47,47	2
88	OHX	6	2105	7/7	0.96	0.16	83,83,83,83	2
87	MG	1	3509	1/1	0.96	0.16	39,39,39,39	0
87	MG	5	3527	1/1	0.96	0.27	39,39,39,39	0
87	MG	1	3542	1/1	0.96	0.31	36,36,36,36	0
87	MG	6	1939	1/1	0.96	0.14	57,57,57,57	0
88	OHX	6	2095	7/7	0.96	0.24	104,104,104,104	3
87	MG	2	1961	1/1	0.96	0.17	101,101,101,101	0
88	OHX	6	2103	7/7	0.96	0.27	90,90,90,90	7
88	OHX	5	4109	7/7	0.96	0.34	68,68,68,68	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	3614	1/1	0.96	0.20	44,44,44,44	0
87	MG	7	210	1/1	0.96	0.32	49,49,49,49	0
88	OHX	5	3986	7/7	0.96	0.21	46,46,46,46	3
88	OHX	5	4141	7/7	0.96	0.23	74,74,74,74	3
88	OHX	5	3953	7/7	0.96	0.25	101,101,101,101	2
87	MG	1	3623	1/1	0.96	0.37	48,48,48,48	0
87	MG	L3	401	1/1	0.96	0.19	41,41,41,41	0
87	MG	1	3477	1/1	0.96	0.16	41,41,41,41	0
88	OHX	1	4008	7/7	0.96	0.25	53,53,53,53	6
88	OHX	5	4021	7/7	0.96	0.21	41,41,41,41	5
87	MG	1	3488	1/1	0.96	0.33	46,46,46,46	0
87	MG	1	3513	1/1	0.96	0.26	50,50,50,50	0
88	OHX	6	2052	7/7	0.96	0.26	73,73,73,73	2
88	OHX	1	3919	7/7	0.96	0.17	96,96,96,96	3
87	MG	5	3769	1/1	0.96	0.94	43,43,43,43	1
87	MG	1	3553	1/1	0.96	0.28	41,41,41,41	0
87	MG	5	3771	1/1	0.96	0.17	38,38,38,38	0
88	OHX	4	228	7/7	0.96	0.26	96,96,96,96	3
88	OHX	2	2067	7/7	0.96	0.19	124,124,124,124	5
87	MG	5	3543	1/1	0.96	0.24	41,41,41,41	0
88	OHX	2	2058	7/7	0.96	0.22	61,61,61,61	3
88	OHX	1	3916	7/7	0.96	0.23	45,45,45,45	2
88	OHX	2	2036	7/7	0.96	0.25	75,75,75,75	5
88	OHX	8	232	7/7	0.96	0.15	48,48,48,48	3
88	OHX	1	4068	7/7	0.96	0.27	50,50,50,50	6
88	OHX	1	4026	7/7	0.96	0.21	51,51,51,51	2
88	OHX	5	4065	7/7	0.96	0.25	82,82,82,82	3
88	OHX	5	4087	7/7	0.96	0.30	45,45,45,45	6
87	MG	1	3626	1/1	0.96	0.19	43,43,43,43	0
87	MG	5	4164	1/1	0.96	0.36	55,55,55,55	0
88	OHX	1	3942	7/7	0.96	0.17	87,87,87,87	3
87	MG	5	3428	1/1	0.96	0.13	34,34,34,34	0
88	OHX	1	3827	7/7	0.96	0.24	73,73,73,73	1
87	MG	1	3435	1/1	0.96	0.46	35,35,35,35	0
87	MG	5	3505	1/1	0.96	0.23	52,52,52,52	0
87	MG	5	3560	1/1	0.96	0.43	34,34,34,34	0
87	MG	1	3601	1/1	0.96	0.37	47,47,47,47	0
87	MG	6	1950	1/1	0.96	0.18	76,76,76,76	0
87	MG	5	3448	1/1	0.96	0.33	34,34,34,34	0
88	OHX	1	3933	7/7	0.96	0.26	53,53,53,53	4
88	OHX	6	2100	7/7	0.96	0.18	65,65,65,65	4
87	MG	2	1984	1/1	0.96	0.31	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	3600	1/1	0.96	0.28	48,48,48,48	0
87	MG	1	3744	1/1	0.96	0.36	34,34,34,34	0
87	MG	8	201	1/1	0.96	0.15	51,51,51,51	0
87	MG	1	3433	1/1	0.96	0.28	37,37,37,37	0
88	OHX	2	2044	7/7	0.96	0.16	130,130,130,130	7
88	OHX	5	3853	7/7	0.96	0.29	69,69,69,69	2
88	OHX	14	401	7/7	0.96	0.34	69,69,69,69	5
87	MG	1	3516	1/1	0.96	0.36	36,36,36,36	0
87	MG	5	3544	1/1	0.96	0.40	54,54,54,54	0
87	MG	2	1985	1/1	0.96	0.18	81,81,81,81	0
88	OHX	5	3956	7/7	0.96	0.28	81,81,81,81	3
87	MG	5	3526	1/1	0.96	0.40	35,35,35,35	0
87	MG	5	3740	1/1	0.96	0.33	34,34,34,34	0
88	OHX	2	2097	7/7	0.96	0.21	88,88,88,88	4
87	MG	6	1916	1/1	0.96	0.16	71,71,71,71	0
87	MG	1	3549	1/1	0.96	0.27	39,39,39,39	0
87	MG	5	3503	1/1	0.96	0.09	47,47,47,47	0
87	MG	1	3525	1/1	0.96	0.33	35,35,35,35	0
88	OHX	1	3998	7/7	0.96	0.20	67,67,67,67	3
87	MG	m7	201	1/1	0.96	0.40	40,40,40,40	0
88	OHX	5	3954	7/7	0.96	0.23	73,73,73,73	3
88	OHX	6	2157	7/7	0.96	0.28	51,51,51,51	3
87	MG	5	3596	1/1	0.96	0.18	46,46,46,46	0
87	MG	5	3407	1/1	0.96	0.32	36,36,36,36	0
87	MG	5	3500	1/1	0.96	0.30	41,41,41,41	0
87	MG	1	3633	1/1	0.96	0.25	52,52,52,52	0
88	OHX	5	4085	7/7	0.96	0.24	66,66,66,66	3
87	MG	5	3587	1/1	0.96	0.40	39,39,39,39	0
88	OHX	1	3961	7/7	0.96	0.24	41,41,41,41	4
89	ZN	D9	101	1/1	0.96	0.11	86,86,86,86	0
87	MG	6	1944	1/1	0.96	0.26	70,70,70,70	0
88	OHX	1	3932	7/7	0.96	0.19	87,87,87,87	2
88	OHX	2	2125	7/7	0.96	0.09	113,113,113,113	4
88	OHX	1	3884	7/7	0.96	0.25	54,54,54,54	3
87	MG	1	3476	1/1	0.97	0.21	43,43,43,43	0
87	MG	7	203	1/1	0.97	0.39	57,57,57,57	0
88	OHX	6	2076	7/7	0.97	0.19	54,54,54,54	5
88	OHX	1	3943	7/7	0.97	0.18	89,89,89,89	3
88	OHX	1	3946	7/7	0.97	0.19	56,56,56,56	3
88	OHX	5	3940	7/7	0.97	0.23	42,42,42,42	2
87	MG	1	3574	1/1	0.97	0.18	41,41,41,41	0
88	OHX	5	3838	7/7	0.97	0.36	62,62,62,62	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	1	3973	7/7	0.97	0.26	52,52,52,52	3
87	MG	m7	202	1/1	0.97	0.29	37,37,37,37	0
87	MG	6	1901	1/1	0.97	0.25	55,55,55,55	0
88	OHX	1	3816	7/7	0.97	0.28	66,66,66,66	5
88	OHX	5	3861	7/7	0.97	0.27	55,55,55,55	2
88	OHX	5	4126	7/7	0.97	0.24	53,53,53,53	6
88	OHX	1	3944	7/7	0.97	0.20	44,44,44,44	1
87	MG	5	3603	1/1	0.97	0.24	38,38,38,38	0
88	OHX	1	3909	7/7	0.97	0.19	68,68,68,68	3
87	MG	5	3574	1/1	0.97	0.37	41,41,41,41	0
88	OHX	5	3985	7/7	0.97	0.23	46,46,46,46	4
88	OHX	2	2033	7/7	0.97	0.15	91,91,91,91	7
88	OHX	1	3898	7/7	0.97	0.30	80,80,80,80	5
88	OHX	6	2121	7/7	0.97	0.16	89,89,89,89	5
88	OHX	2	2027	7/7	0.97	0.15	94,94,94,94	5
87	MG	1	3432	1/1	0.97	0.14	51,51,51,51	0
88	OHX	2	2054	7/7	0.97	0.15	104,104,104,104	5
88	OHX	5	3928	7/7	0.97	0.22	101,101,101,101	3
88	OHX	5	3970	7/7	0.97	0.20	57,57,57,57	3
88	OHX	5	3864	7/7	0.97	0.25	87,87,87,87	3
88	OHX	6	2082	7/7	0.97	0.17	93,93,93,93	4
87	MG	1	3594	1/1	0.97	0.42	50,50,50,50	0
88	OHX	2	2089	7/7	0.97	0.18	88,88,88,88	3
87	MG	1	3522	1/1	0.97	0.21	48,48,48,48	0
87	MG	1	3505	1/1	0.97	0.42	36,36,36,36	0
88	OHX	5	3873	7/7	0.97	0.27	65,65,65,65	3
88	OHX	5	3978	7/7	0.97	0.20	45,45,45,45	3
87	MG	m0	301	1/1	0.97	0.22	45,45,45,45	0
88	OHX	5	4001	7/7	0.97	0.21	40,40,40,40	3
87	MG	1	3734	1/1	0.97	0.16	35,35,35,35	0
87	MG	1	3639	1/1	0.97	0.17	58,58,58,58	0
88	OHX	m0	303	7/7	0.97	0.26	49,49,49,49	1
88	OHX	1	3868	7/7	0.97	0.27	68,68,68,68	3
88	OHX	5	3856	7/7	0.97	0.28	60,60,60,60	2
88	OHX	2	2042	7/7	0.97	0.16	100,100,100,100	4
88	OHX	5	3975	7/7	0.97	0.22	70,70,70,70	2
87	MG	6	2004	1/1	0.97	0.15	90,90,90,90	0
88	OHX	S1	301	7/7	0.97	0.18	117,117,117,117	3
88	OHX	8	221	7/7	0.97	0.24	42,42,42,42	4
87	MG	6	1955	1/1	0.97	0.36	64,64,64,64	0
88	OHX	5	3976	7/7	0.97	0.24	50,50,50,50	4
87	MG	1	3498	1/1	0.97	0.42	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	5	4107	7/7	0.97	0.27	48,48,48,48	5
87	MG	L7	301	1/1	0.97	0.24	41,41,41,41	0
87	MG	6	1970	1/1	0.97	0.22	52,52,52,52	0
88	OHX	2	2028	7/7	0.97	0.21	74,74,74,74	4
88	OHX	1	4028	7/7	0.97	0.30	70,70,70,70	4
88	OHX	1	3877	7/7	0.97	0.25	44,44,44,44	1
88	OHX	5	4038	7/7	0.97	0.25	65,65,65,65	4
88	OHX	6	2079	7/7	0.97	0.22	52,52,52,52	4
88	OHX	1	3960	7/7	0.97	0.26	110,110,110,110	2
88	OHX	5	4043	7/7	0.97	0.23	46,46,46,46	5
88	OHX	1	3934	7/7	0.97	0.16	65,65,65,65	3
88	OHX	L3	404	7/7	0.97	0.19	68,68,68,68	2
88	OHX	5	3886	7/7	0.97	0.29	66,66,66,66	3
88	OHX	1	3891	7/7	0.97	0.18	63,63,63,63	3
87	MG	1	3584	1/1	0.97	0.36	43,43,43,43	0
88	OHX	5	3944	7/7	0.97	0.24	50,50,50,50	4
88	OHX	1	3922	7/7	0.97	0.26	74,74,74,74	4
88	OHX	5	3946	7/7	0.97	0.23	100,100,100,100	3
88	OHX	6	2039	7/7	0.97	0.17	123,123,123,123	3
87	MG	1	3414	1/1	0.97	0.21	45,45,45,45	0
88	OHX	6	2104	7/7	0.97	0.16	83,83,83,83	5
88	OHX	2	2079	7/7	0.97	0.15	122,122,122,122	6
88	OHX	1	3896	7/7	0.97	0.17	57,57,57,57	4
88	OHX	1	3824	7/7	0.97	0.27	57,57,57,57	2
88	OHX	2	1999	7/7	0.97	0.22	104,104,104,104	2
87	MG	5	3573	1/1	0.97	0.48	41,41,41,41	0
88	OHX	5	4096	7/7	0.97	0.24	55,55,55,55	4
88	OHX	5	3971	7/7	0.97	0.17	43,43,43,43	2
87	MG	5	3516	1/1	0.97	0.41	36,36,36,36	0
87	MG	5	3765	1/1	0.97	0.15	47,47,47,47	0
87	MG	5	3473	1/1	0.97	0.48	59,59,59,59	0
88	OHX	q2	502	7/7	0.97	0.23	46,46,46,46	3
88	OHX	5	3964	7/7	0.97	0.24	53,53,53,53	5
88	OHX	6	2063	7/7	0.97	0.18	138,138,138,138	4
88	OHX	5	4032	7/7	0.97	0.30	51,51,51,51	3
89	ZN	Q2	501	1/1	0.97	0.07	79,79,79,79	0
88	OHX	1	3812	7/7	0.97	0.30	100,100,100,100	3
88	OHX	3	211	7/7	0.97	0.34	55,55,55,55	2
87	MG	5	3509	1/1	0.97	0.25	43,43,43,43	0
87	MG	5	3640	1/1	0.97	0.23	38,38,38,38	0
88	OHX	5	4026	7/7	0.97	0.20	68,68,68,68	6
87	MG	3	220	1/1	0.97	0.34	49,49,49,49	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
89	ZN	d6	101	1/1	0.97	0.11	71,71,71,71	0
88	OHX	5	4023	7/7	0.97	0.19	97,97,97,97	5
88	OHX	5	3979	7/7	0.97	0.35	84,84,84,84	3
87	MG	1	4112	1/1	0.97	0.81	35,35,35,35	1
87	MG	5	3501	1/1	0.97	0.33	33,33,33,33	0
87	MG	1	3648	1/1	0.97	0.15	46,46,46,46	0
88	OHX	6	2101	7/7	0.97	0.15	88,88,88,88	3
88	OHX	5	3980	7/7	0.97	0.28	54,54,54,54	3
88	OHX	6	2060	7/7	0.97	0.21	96,96,96,96	3
87	MG	2	1929	1/1	0.97	0.20	75,75,75,75	0
88	OHX	1	3845	7/7	0.97	0.22	70,70,70,70	2
88	OHX	2	2019	7/7	0.97	0.24	93,93,93,93	3
88	OHX	5	4060	7/7	0.97	0.25	38,38,38,38	4
88	OHX	6	2174	7/7	0.97	0.17	86,86,86,86	6
88	OHX	5	3936	7/7	0.97	0.20	51,51,51,51	1
88	OHX	2	2040	7/7	0.97	0.23	68,68,68,68	4
87	MG	1	3425	1/1	0.97	0.33	48,48,48,48	0
88	OHX	6	2074	7/7	0.97	0.19	71,71,71,71	2
88	OHX	1	3931	7/7	0.97	0.28	53,53,53,53	4
88	OHX	6	2057	7/7	0.97	0.21	65,65,65,65	2
87	MG	5	3613	1/1	0.97	0.26	45,45,45,45	0
88	OHX	6	2122	7/7	0.97	0.20	64,64,64,64	3
88	OHX	1	3876	7/7	0.97	0.20	56,56,56,56	4
88	OHX	1	3880	7/7	0.97	0.24	62,62,62,62	4
87	MG	2	1964	1/1	0.97	0.22	69,69,69,69	0
88	OHX	1	3941	7/7	0.97	0.26	46,46,46,46	3
88	OHX	6	2049	7/7	0.97	0.25	95,95,95,95	2
88	OHX	5	4040	7/7	0.97	0.24	40,40,40,40	4
88	OHX	2	2080	7/7	0.97	0.17	107,107,107,107	7
88	OHX	5	4009	7/7	0.97	0.26	41,41,41,41	3
88	OHX	1	3829	7/7	0.97	0.24	60,60,60,60	2
88	OHX	5	4010	7/7	0.97	0.26	62,62,62,62	4
88	OHX	6	2059	7/7	0.97	0.23	67,67,67,67	4
88	OHX	5	3879	7/7	0.97	0.23	61,61,61,61	3
88	OHX	8	217	7/7	0.97	0.26	85,85,85,85	3
87	MG	1	3575	1/1	0.97	0.37	35,35,35,35	0
87	MG	1	3643	1/1	0.97	0.32	35,35,35,35	0
88	OHX	2	2059	7/7	0.97	0.14	90,90,90,90	1
87	MG	1	3440	1/1	0.97	0.24	52,52,52,52	0
88	OHX	6	2069	7/7	0.97	0.20	74,74,74,74	4
87	MG	1	3447	1/1	0.97	0.24	41,41,41,41	0
88	OHX	1	4003	7/7	0.97	0.18	57,57,57,57	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	O7	106	7/7	0.97	0.25	55,55,55,55	3
87	MG	5	3405	1/1	0.97	0.40	34,34,34,34	0
88	OHX	3	213	7/7	0.97	0.17	76,76,76,76	4
88	OHX	4	222	7/7	0.97	0.24	57,57,57,57	3
88	OHX	4	227	7/7	0.97	0.22	42,42,42,42	3
88	OHX	2	2041	7/7	0.97	0.15	110,110,110,110	5
88	OHX	1	3810	7/7	0.97	0.28	89,89,89,89	4
88	OHX	5	3926	7/7	0.97	0.28	41,41,41,41	5
88	OHX	6	2116	7/7	0.97	0.18	62,62,62,62	3
88	OHX	5	4029	7/7	0.97	0.24	49,49,49,49	4
87	MG	1	3572	1/1	0.97	0.31	44,44,44,44	0
88	OHX	5	3929	7/7	0.97	0.26	42,42,42,42	4
88	OHX	1	3807	7/7	0.97	0.26	86,86,86,86	3
88	OHX	6	2035	7/7	0.97	0.21	82,82,82,82	3
87	MG	1	3514	1/1	0.97	0.35	35,35,35,35	0
87	MG	6	1977	1/1	0.97	0.09	70,70,70,70	0
88	OHX	5	3899	7/7	0.97	0.26	72,72,72,72	2
87	MG	5	3698	1/1	0.97	0.27	65,65,65,65	0
88	OHX	5	3910	7/7	0.97	0.19	64,64,64,64	4
88	OHX	6	2032	7/7	0.97	0.22	131,131,131,131	3
88	OHX	2	2045	7/7	0.97	0.34	65,65,65,65	4
88	OHX	2	2076	7/7	0.97	0.14	78,78,78,78	2
87	MG	1	3543	1/1	0.97	0.26	36,36,36,36	0
88	OHX	2	2001	7/7	0.97	0.19	104,104,104,104	2
87	MG	5	3422	1/1	0.97	0.25	40,40,40,40	0
88	OHX	5	3973	7/7	0.97	0.22	153,153,153,153	7
87	MG	5	3532	1/1	0.97	0.40	37,37,37,37	0
87	MG	5	3656	1/1	0.97	0.35	42,42,42,42	0
87	MG	5	3714	1/1	0.97	0.80	39,39,39,39	1
87	MG	5	3515	1/1	0.97	0.10	42,42,42,42	0
87	MG	f	1002	1/1	0.97	0.22	58,58,58,58	0
88	OHX	2	2025	7/7	0.97	0.21	74,74,74,74	4
88	OHX	5	3947	7/7	0.97	0.24	53,53,53,53	5
87	MG	5	3508	1/1	0.97	0.40	34,34,34,34	0
87	MG	5	3556	1/1	0.97	0.35	33,33,33,33	0
87	MG	2	1921	1/1	0.97	0.27	69,69,69,69	0
87	MG	1	3583	1/1	0.97	0.25	42,42,42,42	0
87	MG	12	303	1/1	0.97	0.49	45,45,45,45	0
88	OHX	5	4048	7/7	0.97	0.21	41,41,41,41	5
88	OHX	1	3957	7/7	0.97	0.19	48,48,48,48	3
88	OHX	1	3917	7/7	0.97	0.23	52,52,52,52	5
88	OHX	4	229	7/7	0.97	0.21	92,92,92,92	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	6	1960	1/1	0.97	0.18	52,52,52,52	0
88	OHX	1	3974	7/7	0.97	0.16	61,61,61,61	5
87	MG	6	1976	1/1	0.97	0.27	54,54,54,54	0
87	MG	1	3508	1/1	0.97	0.35	37,37,37,37	0
88	OHX	5	3955	7/7	0.97	0.20	42,42,42,42	2
87	MG	1	3503	1/1	0.97	0.48	34,34,34,34	0
88	OHX	1	3888	7/7	0.97	0.26	45,45,45,45	3
88	OHX	1	3894	7/7	0.97	0.19	49,49,49,49	4
88	OHX	3	214	7/7	0.97	0.21	77,77,77,77	4
88	OHX	1	3809	7/7	0.97	0.28	77,77,77,77	3
88	OHX	M5	301	7/7	0.97	0.20	66,66,66,66	4
87	MG	1	3686	1/1	0.97	0.64	47,47,47,47	1
87	MG	5	3652	1/1	0.97	0.29	44,44,44,44	0
87	MG	5	3549	1/1	0.97	0.37	56,56,56,56	0
88	OHX	6	2091	7/7	0.97	0.20	90,90,90,90	5
87	MG	1	3487	1/1	0.97	0.35	35,35,35,35	0
87	MG	6	1909	1/1	0.97	0.21	109,109,109,109	0
88	OHX	5	3897	7/7	0.97	0.22	76,76,76,76	2
88	OHX	1	3945	7/7	0.97	0.18	52,52,52,52	1
87	MG	1	3533	1/1	0.97	0.30	50,50,50,50	0
88	OHX	1	3992	7/7	0.97	0.31	82,82,82,82	5
88	OHX	5	4024	7/7	0.97	0.32	74,74,74,74	5
88	OHX	2	2086	7/7	0.97	0.21	94,94,94,94	4
88	OHX	5	3854	7/7	0.97	0.29	80,80,80,80	3
88	OHX	1	3881	7/7	0.97	0.30	60,60,60,60	1
88	OHX	5	4020	7/7	0.97	0.30	40,40,40,40	2
88	OHX	5	4006	7/7	0.97	0.21	49,49,49,49	2
87	MG	5	3433	1/1	0.97	0.18	60,60,60,60	0
87	MG	5	3571	1/1	0.97	0.41	39,39,39,39	0
88	OHX	1	4000	7/7	0.97	0.28	104,104,104,104	5
87	MG	1	3453	1/1	0.97	0.25	51,51,51,51	0
87	MG	5	3598	1/1	0.97	0.11	50,50,50,50	0
88	OHX	1	3886	7/7	0.97	0.22	124,124,124,124	4
88	OHX	1	4045	7/7	0.97	0.19	45,45,45,45	4
87	MG	5	3580	1/1	0.97	0.47	44,44,44,44	0
88	OHX	6	2050	7/7	0.97	0.21	87,87,87,87	3
88	OHX	1	3861	7/7	0.97	0.32	99,99,99,99	3
88	OHX	5	3957	7/7	0.97	0.25	38,38,38,38	2
87	MG	5	3633	1/1	0.97	0.30	43,43,43,43	0
88	OHX	1	3787	7/7	0.97	0.28	70,70,70,70	3
87	MG	1	3410	1/1	0.97	0.38	55,55,55,55	0
88	OHX	6	2072	7/7	0.97	0.18	70,70,70,70	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	1	3927	7/7	0.97	0.26	48,48,48,48	4
88	OHX	5	3943	7/7	0.97	0.21	69,69,69,69	2
87	MG	1	3497	1/1	0.97	0.42	34,34,34,34	0
87	MG	5	3584	1/1	0.97	0.33	31,31,31,31	0
88	OHX	7	218	7/7	0.97	0.30	56,56,56,56	2
88	OHX	5	3948	7/7	0.97	0.22	50,50,50,50	3
87	MG	6	1941	1/1	0.97	0.43	47,47,47,47	0
87	MG	4	208	1/1	0.97	0.33	49,49,49,49	0
87	MG	5	3715	1/1	0.97	0.33	39,39,39,39	0
88	OHX	2	2084	7/7	0.97	0.17	87,87,87,87	3
87	MG	5	3561	1/1	0.97	0.40	35,35,35,35	0
88	OHX	1	3905	7/7	0.97	0.26	52,52,52,52	2
88	OHX	5	3901	7/7	0.97	0.29	67,67,67,67	2
88	OHX	5	3938	7/7	0.97	0.26	41,41,41,41	4
88	OHX	5	3972	7/7	0.97	0.22	60,60,60,60	4
88	OHX	1	3968	7/7	0.97	0.30	72,72,72,72	3
87	MG	1	3551	1/1	0.97	0.24	32,32,32,32	0
87	MG	1	3650	1/1	0.98	0.14	55,55,55,55	0
88	OHX	1	3832	7/7	0.98	0.31	88,88,88,88	3
88	OHX	2	2034	7/7	0.98	0.17	79,79,79,79	5
88	OHX	1	3930	7/7	0.98	0.24	42,42,42,42	4
87	MG	1	3541	1/1	0.98	0.42	39,39,39,39	0
88	OHX	o3	201	7/7	0.98	0.22	49,49,49,49	3
88	OHX	5	3892	7/7	0.98	0.24	45,45,45,45	3
87	MG	1	3466	1/1	0.98	0.24	42,42,42,42	0
87	MG	4	236	1/1	0.98	0.55	56,56,56,56	0
88	OHX	1	3862	7/7	0.98	0.23	54,54,54,54	4
87	MG	5	3520	1/1	0.98	0.57	39,39,39,39	0
88	OHX	5	3868	7/7	0.98	0.21	77,77,77,77	4
87	MG	1	3640	1/1	0.98	0.50	66,66,66,66	0
87	MG	7	215	1/1	0.98	1.07	54,54,54,54	1
88	OHX	5	3960	7/7	0.98	0.25	108,108,108,108	4
88	OHX	1	3929	7/7	0.98	0.28	116,116,116,116	5
88	OHX	5	3844	7/7	0.98	0.25	47,47,47,47	1
87	MG	5	3591	1/1	0.98	0.31	45,45,45,45	0
87	MG	5	3511	1/1	0.98	0.42	31,31,31,31	0
88	OHX	1	3860	7/7	0.98	0.24	40,40,40,40	2
87	MG	n3	201	1/1	0.98	0.40	31,31,31,31	0
88	OHX	1	3858	7/7	0.98	0.20	61,61,61,61	3
88	OHX	3	210	7/7	0.98	0.23	48,48,48,48	3
88	OHX	5	3875	7/7	0.98	0.28	53,53,53,53	3
88	OHX	5	3903	7/7	0.98	0.19	55,55,55,55	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	1	3959	7/7	0.98	0.21	51,51,51,51	2
87	MG	2	1914	1/1	0.98	0.21	77,77,77,77	0
88	OHX	6	2096	7/7	0.98	0.14	86,86,86,86	5
87	MG	5	3417	1/1	0.98	0.26	38,38,38,38	0
87	MG	1	3489	1/1	0.98	0.23	44,44,44,44	0
88	OHX	2	1996	7/7	0.98	0.21	99,99,99,99	2
88	OHX	1	3867	7/7	0.98	0.23	84,84,84,84	3
88	OHX	5	3852	7/7	0.98	0.20	75,75,75,75	2
87	MG	6	1931	1/1	0.98	0.32	54,54,54,54	0
87	MG	5	3455	1/1	0.98	0.17	45,45,45,45	0
88	OHX	2	2098	7/7	0.98	0.17	70,70,70,70	3
87	MG	5	3654	1/1	0.98	0.28	33,33,33,33	0
87	MG	5	3649	1/1	0.98	0.17	47,47,47,47	0
88	OHX	C1	201	7/7	0.98	0.19	97,97,97,97	5
88	OHX	1	3872	7/7	0.98	0.23	47,47,47,47	2
87	MG	6	1906	1/1	0.98	0.43	51,51,51,51	0
87	MG	1	3577	1/1	0.98	0.48	27,27,27,27	0
88	OHX	5	3911	7/7	0.98	0.28	137,137,137,137	3
88	OHX	1	3879	7/7	0.98	0.19	82,82,82,82	3
88	OHX	1	3920	7/7	0.98	0.22	44,44,44,44	4
88	OHX	5	3937	7/7	0.98	0.20	136,136,136,136	1
88	OHX	1	3864	7/7	0.98	0.20	65,65,65,65	2
87	MG	2	1982	1/1	0.98	0.07	75,75,75,75	0
88	OHX	s1	301	7/7	0.98	0.21	91,91,91,91	2
87	MG	5	3629	1/1	0.98	0.27	43,43,43,43	0
87	MG	1	3580	1/1	0.98	0.52	27,27,27,27	0
88	OHX	1	3902	7/7	0.98	0.23	51,51,51,51	1
88	OHX	2	2018	7/7	0.98	0.19	83,83,83,83	3
88	OHX	2	2030	7/7	0.98	0.19	71,71,71,71	4
88	OHX	2	2008	7/7	0.98	0.20	89,89,89,89	3
88	OHX	5	4004	7/7	0.98	0.23	49,49,49,49	2
87	MG	1	3667	1/1	0.98	0.64	38,38,38,38	1
87	MG	1	3422	1/1	0.98	0.35	58,58,58,58	0
88	OHX	C8	201	7/7	0.98	0.25	106,106,106,106	3
88	OHX	8	216	7/7	0.98	0.20	60,60,60,60	4
88	OHX	5	3850	7/7	0.98	0.30	72,72,72,72	1
88	OHX	5	3941	7/7	0.98	0.17	60,60,60,60	1
88	OHX	6	2017	7/7	0.98	0.23	79,79,79,79	5
87	MG	1	3471	1/1	0.98	0.20	36,36,36,36	0
88	OHX	1	3830	7/7	0.98	0.26	57,57,57,57	1
88	OHX	7	216	7/7	0.98	0.33	71,71,71,71	2
88	OHX	6	2081	7/7	0.98	0.16	74,74,74,74	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	6	2089	7/7	0.98	0.20	58,58,58,58	3
88	OHX	1	3803	7/7	0.98	0.26	60,60,60,60	3
88	OHX	1	3847	7/7	0.98	0.25	42,42,42,42	2
88	OHX	6	2053	7/7	0.98	0.20	86,86,86,86	5
88	OHX	1	3885	7/7	0.98	0.18	51,51,51,51	3
88	OHX	6	2046	7/7	0.98	0.21	60,60,60,60	3
88	OHX	5	3829	7/7	0.98	0.24	56,56,56,56	2
88	OHX	5	3826	7/7	0.98	0.28	47,47,47,47	3
88	OHX	5	3908	7/7	0.98	0.24	58,58,58,58	2
88	OHX	5	3949	7/7	0.98	0.24	50,50,50,50	4
88	OHX	6	2036	7/7	0.98	0.20	58,58,58,58	2
87	MG	1	3579	1/1	0.98	0.42	38,38,38,38	0
87	MG	6	2006	1/1	0.98	0.51	83,83,83,83	0
87	MG	1	3576	1/1	0.98	0.39	31,31,31,31	0
88	OHX	2	2049	7/7	0.98	0.20	78,78,78,78	6
88	OHX	6	2031	7/7	0.98	0.23	81,81,81,81	3
88	OHX	1	3987	7/7	0.98	0.26	65,65,65,65	5
87	MG	5	3498	1/1	0.98	0.28	64,64,64,64	0
87	MG	8	206	1/1	0.98	0.21	58,58,58,58	0
88	OHX	5	3922	7/7	0.98	0.27	59,59,59,59	3
88	OHX	6	2108	7/7	0.98	0.20	91,91,91,91	5
88	OHX	5	3877	7/7	0.98	0.26	54,54,54,54	3
88	OHX	5	3925	7/7	0.98	0.23	46,46,46,46	4
88	OHX	5	3942	7/7	0.98	0.24	46,46,46,46	3
88	OHX	n3	202	7/7	0.98	0.21	63,63,63,63	3
88	OHX	1	3970	7/7	0.98	0.19	53,53,53,53	4
88	OHX	5	3921	7/7	0.98	0.22	83,83,83,83	3
87	MG	4	213	1/1	0.98	0.38	49,49,49,49	0
88	OHX	5	3974	7/7	0.98	0.23	49,49,49,49	3
88	OHX	2	2029	7/7	0.98	0.15	103,103,103,103	4
88	OHX	7	222	7/7	0.98	0.31	66,66,66,66	2
88	OHX	6	2062	7/7	0.98	0.18	114,114,114,114	4
87	MG	5	3480	1/1	0.98	0.32	44,44,44,44	0
88	OHX	1	3955	7/7	0.98	0.28	100,100,100,100	2
88	OHX	5	4072	7/7	0.98	0.22	42,42,42,42	4
88	OHX	1	3918	7/7	0.98	0.30	70,70,70,70	3
87	MG	5	3559	1/1	0.98	0.46	31,31,31,31	0
88	OHX	2	2000	7/7	0.98	0.18	102,102,102,102	3
87	MG	5	3541	1/1	0.98	0.47	38,38,38,38	0
87	MG	1	3558	1/1	0.98	0.18	38,38,38,38	0
88	OHX	1	3913	7/7	0.98	0.19	55,55,55,55	2
87	MG	5	3496	1/1	0.98	0.29	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	2	2066	7/7	0.98	0.13	139,139,139,139	6
87	MG	1	3479	1/1	0.98	0.24	54,54,54,54	0
88	OHX	5	3885	7/7	0.98	0.24	42,42,42,42	3
88	OHX	1	3901	7/7	0.98	0.19	63,63,63,63	5
88	OHX	1	4052	7/7	0.98	0.21	58,58,58,58	2
87	MG	5	3472	1/1	0.98	0.20	44,44,44,44	0
88	OHX	1	3842	7/7	0.98	0.28	109,109,109,109	3
88	OHX	5	3902	7/7	0.98	0.19	39,39,39,39	3
88	OHX	Q2	503	7/7	0.98	0.22	45,45,45,45	2
87	MG	6	1954	1/1	0.98	0.34	51,51,51,51	0
88	OHX	2	2032	7/7	0.98	0.17	92,92,92,92	4
88	OHX	5	3916	7/7	0.98	0.23	90,90,90,90	5
87	MG	2	1916	1/1	0.98	0.17	60,60,60,60	0
88	OHX	1	3871	7/7	0.98	0.21	50,50,50,50	4
88	OHX	6	2114	7/7	0.98	0.28	65,65,65,65	2
88	OHX	5	4051	7/7	0.98	0.17	51,51,51,51	2
88	OHX	6	2037	7/7	0.98	0.18	95,95,95,95	3
88	OHX	5	3847	7/7	0.98	0.33	87,87,87,87	3
88	OHX	1	3825	7/7	0.98	0.27	90,90,90,90	3
88	OHX	5	3914	7/7	0.98	0.21	54,54,54,54	4
88	OHX	6	2085	7/7	0.98	0.17	69,69,69,69	2
88	OHX	5	3835	7/7	0.98	0.24	55,55,55,55	3
87	MG	1	3550	1/1	0.98	0.32	32,32,32,32	0
88	OHX	O3	203	7/7	0.98	0.23	47,47,47,47	3
87	MG	1	4111	1/1	0.98	0.31	44,44,44,44	1
88	OHX	5	3857	7/7	0.98	0.24	52,52,52,52	3
88	OHX	5	3935	7/7	0.98	0.21	45,45,45,45	3
87	MG	5	3583	1/1	0.98	0.45	28,28,28,28	0
88	OHX	1	3837	7/7	0.98	0.28	64,64,64,64	3
88	OHX	5	3987	7/7	0.98	0.17	69,69,69,69	5
88	OHX	1	3887	7/7	0.98	0.21	63,63,63,63	1
88	OHX	5	3982	7/7	0.98	0.22	43,43,43,43	3
87	MG	5	3514	1/1	0.98	0.43	36,36,36,36	0
88	OHX	5	3851	7/7	0.98	0.22	41,41,41,41	3
88	OHX	1	3852	7/7	0.98	0.21	79,79,79,79	2
88	OHX	2	2093	7/7	0.98	0.17	91,91,91,91	7
88	OHX	6	2047	7/7	0.98	0.20	68,68,68,68	4
88	OHX	5	3824	7/7	0.98	0.25	62,62,62,62	2
88	OHX	5	4007	7/7	0.98	0.23	35,35,35,35	3
88	OHX	6	2132	7/7	0.98	0.15	61,61,61,61	5
88	OHX	1	3925	7/7	0.98	0.20	56,56,56,56	7
88	OHX	5	3874	7/7	0.98	0.25	62,62,62,62	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	3507	1/1	0.98	0.41	36,36,36,36	0
88	OHX	5	3893	7/7	0.98	0.20	76,76,76,76	4
88	OHX	4	226	7/7	0.98	0.20	75,75,75,75	1
87	MG	1	3510	1/1	0.98	0.27	36,36,36,36	0
87	MG	1	3409	1/1	0.98	0.36	37,37,37,37	0
88	OHX	4	225	7/7	0.98	0.19	57,57,57,57	3
88	OHX	5	3951	7/7	0.98	0.26	49,49,49,49	3
88	OHX	5	3883	7/7	0.98	0.23	54,54,54,54	4
87	MG	5	3582	1/1	0.98	0.46	34,34,34,34	0
88	OHX	1	3940	7/7	0.98	0.26	47,47,47,47	4
88	OHX	2	2021	7/7	0.98	0.18	71,71,71,71	4
87	MG	1	3485	1/1	0.98	0.41	32,32,32,32	0
88	OHX	1	3996	7/7	0.98	0.23	55,55,55,55	5
89	ZN	d9	101	1/1	0.98	0.14	89,89,89,89	0
88	OHX	1	3840	7/7	0.98	0.15	90,90,90,90	5
88	OHX	l3	402	7/7	0.98	0.22	50,50,50,50	2
87	MG	3	202	1/1	0.98	0.47	54,54,54,54	0
88	OHX	1	3921	7/7	0.98	0.21	73,73,73,73	3
88	OHX	2	2022	7/7	0.98	0.18	78,78,78,78	2
88	OHX	5	3842	7/7	0.98	0.30	77,77,77,77	3
88	OHX	1	3866	7/7	0.98	0.23	53,53,53,53	3
87	MG	5	3435	1/1	0.98	0.26	39,39,39,39	0
88	OHX	1	3821	7/7	0.98	0.23	83,83,83,83	3
87	MG	1	3606	1/1	0.98	0.25	44,44,44,44	0
88	OHX	5	3848	7/7	0.98	0.24	58,58,58,58	3
88	OHX	8	215	7/7	0.98	0.23	59,59,59,59	2
87	MG	6	1971	1/1	0.98	0.22	56,56,56,56	0
88	OHX	5	3945	7/7	0.98	0.19	59,59,59,59	5
88	OHX	5	3845	7/7	0.98	0.28	79,79,79,79	4
88	OHX	5	3866	7/7	0.98	0.25	61,61,61,61	2
87	MG	5	3588	1/1	0.98	0.29	37,37,37,37	0
88	OHX	1	3791	7/7	0.98	0.27	58,58,58,58	3
88	OHX	1	3808	7/7	0.98	0.24	52,52,52,52	1
88	OHX	1	3936	7/7	0.98	0.21	103,103,103,103	3
88	OHX	5	3907	7/7	0.98	0.26	41,41,41,41	2
87	MG	5	3535	1/1	0.98	0.31	41,41,41,41	0
87	MG	l2	301	1/1	0.98	0.12	40,40,40,40	0
88	OHX	1	3800	7/7	0.98	0.28	91,91,91,91	3
87	MG	5	3568	1/1	0.98	0.38	33,33,33,33	0
88	OHX	5	3969	7/7	0.98	0.25	54,54,54,54	4
88	OHX	2	2077	7/7	0.98	0.19	73,73,73,73	3
87	MG	6	1922	1/1	0.98	0.36	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	5	3968	7/7	0.98	0.19	58,58,58,58	3
88	OHX	1	3799	7/7	0.98	0.25	61,61,61,61	1
88	OHX	4	224	7/7	0.98	0.23	81,81,81,81	4
87	MG	4	206	1/1	0.98	0.38	40,40,40,40	0
88	OHX	5	3900	7/7	0.98	0.20	39,39,39,39	3
88	OHX	1	3806	7/7	0.98	0.24	73,73,73,73	2
88	OHX	5	3887	7/7	0.98	0.31	87,87,87,87	3
88	OHX	2	2063	7/7	0.98	0.15	80,80,80,80	4
88	OHX	6	2078	7/7	0.98	0.18	66,66,66,66	2
88	OHX	2	2005	7/7	0.98	0.19	90,90,90,90	3
88	OHX	1	3855	7/7	0.98	0.24	102,102,102,102	4
88	OHX	6	2058	7/7	0.98	0.21	77,77,77,77	3
87	MG	1	3585	1/1	0.98	0.28	45,45,45,45	0
87	MG	5	3565	1/1	0.98	0.30	34,34,34,34	0
88	OHX	1	3878	7/7	0.98	0.20	46,46,46,46	4
88	OHX	1	3874	7/7	0.98	0.25	43,43,43,43	3
88	OHX	n6	202	7/7	0.98	0.20	89,89,89,89	5
88	OHX	1	3814	7/7	0.98	0.24	76,76,76,76	5
88	OHX	1	3986	7/7	0.98	0.20	41,41,41,41	2
88	OHX	2	2017	7/7	0.98	0.17	118,118,118,118	5
88	OHX	7	220	7/7	0.98	0.22	43,43,43,43	3
88	OHX	1	3801	7/7	0.99	0.22	55,55,55,55	2
87	MG	1	3544	1/1	0.99	0.10	58,58,58,58	0
88	OHX	6	2041	7/7	0.99	0.22	61,61,61,61	2
88	OHX	1	3760	7/7	0.99	0.26	64,64,64,64	3
88	OHX	7	221	7/7	0.99	0.27	67,67,67,67	2
88	OHX	5	3814	7/7	0.99	0.23	54,54,54,54	4
88	OHX	1	3983	7/7	0.99	0.21	52,52,52,52	4
88	OHX	6	2048	7/7	0.99	0.21	64,64,64,64	2
88	OHX	1	3815	7/7	0.99	0.30	51,51,51,51	3
88	OHX	5	3906	7/7	0.99	0.23	40,40,40,40	2
87	MG	5	3593	1/1	0.99	0.53	28,28,28,28	0
88	OHX	5	3822	7/7	0.99	0.23	49,49,49,49	1
88	OHX	1	3795	7/7	0.99	0.22	51,51,51,51	3
88	OHX	5	3919	7/7	0.99	0.16	53,53,53,53	1
88	OHX	5	3815	7/7	0.99	0.22	56,56,56,56	3
88	OHX	1	3882	7/7	0.99	0.21	65,65,65,65	5
88	OHX	5	3888	7/7	0.99	0.24	51,51,51,51	1
88	OHX	2	2016	7/7	0.99	0.17	87,87,87,87	4
88	OHX	1	3844	7/7	0.99	0.20	56,56,56,56	3
88	OHX	1	3818	7/7	0.99	0.20	106,106,106,106	3
88	OHX	6	2045	7/7	0.99	0.15	87,87,87,87	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	1	3833	7/7	0.99	0.20	61,61,61,61	3
88	OHX	6	2026	7/7	0.99	0.22	69,69,69,69	2
88	OHX	5	3917	7/7	0.99	0.20	41,41,41,41	2
88	OHX	5	3833	7/7	0.99	0.23	52,52,52,52	2
88	OHX	1	3835	7/7	0.99	0.20	60,60,60,60	3
88	OHX	1	3798	7/7	0.99	0.21	71,71,71,71	1
88	OHX	6	2025	7/7	0.99	0.21	98,98,98,98	2
88	OHX	1	3928	7/7	0.99	0.20	52,52,52,52	3
88	OHX	2	2043	7/7	0.99	0.20	80,80,80,80	3
88	OHX	1	3822	7/7	0.99	0.23	46,46,46,46	2
88	OHX	1	3826	7/7	0.99	0.24	52,52,52,52	2
88	OHX	1	3813	7/7	0.99	0.22	54,54,54,54	1
88	OHX	6	2034	7/7	0.99	0.20	70,70,70,70	3
88	OHX	7	219	7/7	0.99	0.26	44,44,44,44	2
88	OHX	2	2004	7/7	0.99	0.20	112,112,112,112	3
87	MG	5	3429	1/1	0.99	0.44	30,30,30,30	0
88	OHX	5	3867	7/7	0.99	0.22	75,75,75,75	1
88	OHX	8	213	7/7	0.99	0.24	58,58,58,58	2
88	OHX	5	3837	7/7	0.99	0.31	74,74,74,74	2
88	OHX	1	3768	7/7	0.99	0.20	63,63,63,63	5
88	OHX	1	3763	7/7	0.99	0.27	72,72,72,72	2
88	OHX	6	2042	7/7	0.99	0.17	66,66,66,66	2
87	MG	6	1968	1/1	0.99	0.23	55,55,55,55	0
88	OHX	1	3819	7/7	0.99	0.20	68,68,68,68	3
88	OHX	5	3880	7/7	0.99	0.23	45,45,45,45	2
88	OHX	1	3836	7/7	0.99	0.30	78,78,78,78	3
88	OHX	2	2015	7/7	0.99	0.18	81,81,81,81	1
88	OHX	6	2019	7/7	0.99	0.18	87,87,87,87	2
88	OHX	1	3770	7/7	0.99	0.21	71,71,71,71	2
88	OHX	5	3799	7/7	0.99	0.24	54,54,54,54	2
88	OHX	1	3781	7/7	0.99	0.25	92,92,92,92	4
88	OHX	5	3841	7/7	0.99	0.26	51,51,51,51	1
88	OHX	5	3821	7/7	0.99	0.23	69,69,69,69	1
88	OHX	6	2018	7/7	0.99	0.24	64,64,64,64	3
88	OHX	6	2020	7/7	0.99	0.23	77,77,77,77	3
88	OHX	5	3811	7/7	0.99	0.26	59,59,59,59	1
88	OHX	1	3805	7/7	0.99	0.24	60,60,60,60	3
88	OHX	5	3827	7/7	0.99	0.22	40,40,40,40	3
88	OHX	5	3876	7/7	0.99	0.22	54,54,54,54	1
88	OHX	6	2022	7/7	0.99	0.19	66,66,66,66	3
88	OHX	2	1998	7/7	0.99	0.19	73,73,73,73	3
88	OHX	2	2003	7/7	0.99	0.17	98,98,98,98	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	5	3913	7/7	0.99	0.19	55,55,55,55	3
88	OHX	5	3806	7/7	0.99	0.22	58,58,58,58	1
88	OHX	6	2021	7/7	0.99	0.22	95,95,95,95	3
88	OHX	1	3767	7/7	0.99	0.22	68,68,68,68	3
88	OHX	1	3778	7/7	0.99	0.22	69,69,69,69	2
87	MG	5	3445	1/1	0.99	0.32	38,38,38,38	0
88	OHX	1	3895	7/7	0.99	0.21	50,50,50,50	3
88	OHX	n9	103	7/7	0.99	0.24	59,59,59,59	3
88	OHX	N9	102	7/7	0.99	0.23	63,63,63,63	1
88	OHX	l3	403	7/7	0.99	0.19	47,47,47,47	2
88	OHX	1	3841	7/7	0.99	0.21	48,48,48,48	2
88	OHX	1	3788	7/7	0.99	0.27	67,67,67,67	3
88	OHX	1	3764	7/7	0.99	0.22	54,54,54,54	3
88	OHX	5	3896	7/7	0.99	0.30	106,106,106,106	1
88	OHX	5	3859	7/7	0.99	0.20	58,58,58,58	1
88	OHX	5	3865	7/7	0.99	0.21	49,49,49,49	2
88	OHX	2	1997	7/7	0.99	0.18	89,89,89,89	2
88	OHX	5	3804	7/7	0.99	0.24	56,56,56,56	1
88	OHX	1	3883	7/7	0.99	0.19	48,48,48,48	5
88	OHX	5	3816	7/7	0.99	0.24	69,69,69,69	1
88	OHX	1	3776	7/7	0.99	0.20	72,72,72,72	1
88	OHX	6	2028	7/7	0.99	0.23	67,67,67,67	2
88	OHX	5	3891	7/7	0.99	0.20	60,60,60,60	3
88	OHX	5	3830	7/7	0.99	0.25	95,95,95,95	2
88	OHX	1	3766	7/7	0.99	0.24	55,55,55,55	1
87	MG	1	3554	1/1	0.99	0.52	30,30,30,30	0
88	OHX	5	3984	7/7	0.99	0.21	42,42,42,42	3
88	OHX	7	217	7/7	0.99	0.22	61,61,61,61	5
88	OHX	o7	502	7/7	0.99	0.20	57,57,57,57	1
88	OHX	1	3848	7/7	0.99	0.18	45,45,45,45	2
88	OHX	1	3834	7/7	0.99	0.20	47,47,47,47	2
88	OHX	6	2027	7/7	0.99	0.24	77,77,77,77	1
88	OHX	1	3851	7/7	0.99	0.22	42,42,42,42	4
88	OHX	3	212	7/7	0.99	0.28	76,76,76,76	2
88	OHX	1	3761	7/7	0.99	0.26	66,66,66,66	2
87	MG	1	3540	1/1	0.99	0.25	35,35,35,35	0
88	OHX	1	3817	7/7	0.99	0.20	50,50,50,50	4
88	OHX	6	2055	7/7	0.99	0.14	110,110,110,110	2
89	ZN	o7	501	1/1	0.99	0.17	48,48,48,48	0
88	OHX	5	3825	7/7	0.99	0.22	62,62,62,62	3
88	OHX	1	3777	7/7	0.99	0.22	74,74,74,74	3
88	OHX	5	3862	7/7	0.99	0.21	47,47,47,47	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	1	3854	7/7	0.99	0.22	53,53,53,53	3
88	OHX	2	2011	7/7	0.99	0.20	80,80,80,80	2
87	MG	f	1001	1/1	0.99	0.41	42,42,42,42	0
89	ZN	q3	501	1/1	0.99	0.18	63,63,63,63	0
88	OHX	1	3790	7/7	0.99	0.24	77,77,77,77	3
87	MG	1	3743	1/1	0.99	0.15	49,49,49,49	0
88	OHX	6	2040	7/7	0.99	0.18	130,130,130,130	5
88	OHX	2	1995	7/7	0.99	0.21	90,90,90,90	2
87	MG	5	3413	1/1	0.99	0.24	41,41,41,41	0
88	OHX	6	2024	7/7	0.99	0.20	83,83,83,83	2
87	MG	1	3653	1/1	0.99	0.25	57,57,57,57	1
88	OHX	N1	201	7/7	0.99	0.23	56,56,56,56	2
88	OHX	1	3796	7/7	0.99	0.31	77,77,77,77	3
88	OHX	1	3779	7/7	0.99	0.21	82,82,82,82	2
88	OHX	1	3863	7/7	0.99	0.23	69,69,69,69	4
88	OHX	1	3772	7/7	0.99	0.26	51,51,51,51	2
88	OHX	4	221	7/7	0.99	0.23	64,64,64,64	3
87	MG	5	3578	1/1	0.99	0.41	38,38,38,38	0
88	OHX	5	3889	7/7	0.99	0.22	47,47,47,47	3
88	OHX	1	3797	7/7	0.99	0.22	55,55,55,55	2
88	OHX	3	209	7/7	0.99	0.28	68,68,68,68	3
88	OHX	m5	301	7/7	0.99	0.17	72,72,72,72	3
88	OHX	5	3863	7/7	0.99	0.23	89,89,89,89	2
88	OHX	5	3836	7/7	0.99	0.19	78,78,78,78	3
88	OHX	6	2023	7/7	0.99	0.21	73,73,73,73	2
89	ZN	Q0	201	1/1	0.99	0.18	49,49,49,49	0
87	MG	1	3578	1/1	0.99	0.43	34,34,34,34	0
88	OHX	2	2055	7/7	0.99	0.15	83,83,83,83	5
88	OHX	1	3789	7/7	0.99	0.20	70,70,70,70	3
88	OHX	2	2012	7/7	0.99	0.21	80,80,80,80	5
88	OHX	5	3860	7/7	0.99	0.20	73,73,73,73	2
88	OHX	1	3774	7/7	0.99	0.22	63,63,63,63	4
88	OHX	1	3857	7/7	0.99	0.22	38,38,38,38	3
88	OHX	1	3758	7/7	0.99	0.24	61,61,61,61	1
88	OHX	5	3882	7/7	0.99	0.21	56,56,56,56	4
88	OHX	5	3952	7/7	0.99	0.21	45,45,45,45	3
88	OHX	1	3804	7/7	0.99	0.23	74,74,74,74	3
88	OHX	5	3846	7/7	0.99	0.27	88,88,88,88	1
89	ZN	q0	201	1/1	0.99	0.21	45,45,45,45	0
88	OHX	5	3805	7/7	0.99	0.23	63,63,63,63	2
88	OHX	1	3849	7/7	0.99	0.18	65,65,65,65	2
88	OHX	5	3813	7/7	0.99	0.21	63,63,63,63	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	1	3771	7/7	0.99	0.26	68,68,68,68	2
89	ZN	D6	500	1/1	0.99	0.12	89,89,89,89	0
88	OHX	5	3855	7/7	0.99	0.20	59,59,59,59	4
88	OHX	1	3775	7/7	0.99	0.23	49,49,49,49	3
88	OHX	1	3773	7/7	0.99	0.23	63,63,63,63	3
88	OHX	5	3812	7/7	0.99	0.25	58,58,58,58	1
88	OHX	2	2006	7/7	0.99	0.17	72,72,72,72	4
87	MG	5	3562	1/1	0.99	0.28	31,31,31,31	0
88	OHX	6	2054	7/7	0.99	0.21	89,89,89,89	2
88	OHX	1	3786	7/7	0.99	0.23	46,46,46,46	2
88	OHX	5	3831	7/7	0.99	0.24	54,54,54,54	2
88	OHX	6	2056	7/7	0.99	0.18	75,75,75,75	3
88	OHX	6	2015	7/7	0.99	0.19	73,73,73,73	2
87	MG	5	3441	1/1	0.99	0.34	35,35,35,35	0
88	OHX	2	2009	7/7	0.99	0.17	86,86,86,86	5
87	MG	5	3460	1/1	0.99	0.38	34,34,34,34	0
88	OHX	5	3843	7/7	0.99	0.21	47,47,47,47	3
88	OHX	6	2067	7/7	0.99	0.19	157,157,157,157	5
88	OHX	1	3811	7/7	0.99	0.26	58,58,58,58	3
88	OHX	1	3793	7/7	0.99	0.25	62,62,62,62	1
88	OHX	5	3878	7/7	0.99	0.23	44,44,44,44	2
88	OHX	1	3794	7/7	0.99	0.23	65,65,65,65	3
89	ZN	O7	101	1/1	0.99	0.15	49,49,49,49	0
88	OHX	1	3823	7/7	0.99	0.21	57,57,57,57	2
88	OHX	1	3782	7/7	0.99	0.25	67,67,67,67	3
88	OHX	5	3839	7/7	0.99	0.23	53,53,53,53	2
88	OHX	6	2033	7/7	0.99	0.19	60,60,60,60	5
88	OHX	1	3828	7/7	0.99	0.19	65,65,65,65	2
88	OHX	5	3890	7/7	0.99	0.19	56,56,56,56	3
88	OHX	1	3762	7/7	0.99	0.23	59,59,59,59	2
88	OHX	5	3870	7/7	0.99	0.21	48,48,48,48	3
88	OHX	5	3884	7/7	0.99	0.28	53,53,53,53	3
88	OHX	1	3765	7/7	0.99	0.23	59,59,59,59	2
88	OHX	1	3850	7/7	0.99	0.19	57,57,57,57	3
88	OHX	6	2038	7/7	0.99	0.19	63,63,63,63	5
87	MG	4	209	1/1	0.99	0.23	58,58,58,58	0
88	OHX	6	2016	7/7	0.99	0.22	83,83,83,83	4
88	OHX	5	4014	7/7	0.99	0.13	72,72,72,72	4
88	OHX	5	3895	7/7	0.99	0.20	47,47,47,47	3
88	OHX	1	3785	7/7	0.99	0.24	49,49,49,49	3
88	OHX	5	3869	7/7	0.99	0.20	45,45,45,45	3
88	OHX	5	3849	7/7	0.99	0.21	127,127,127,127	2

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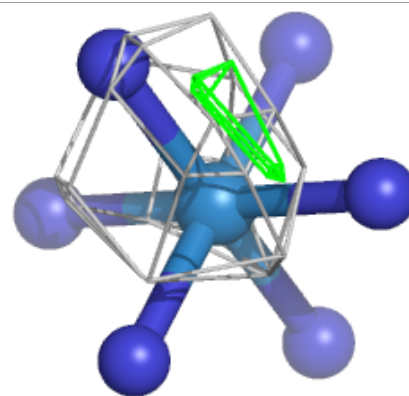
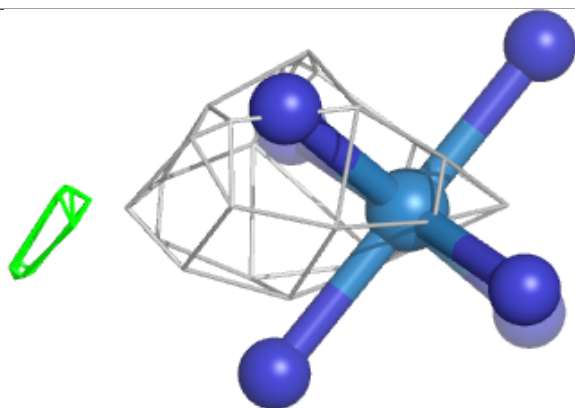
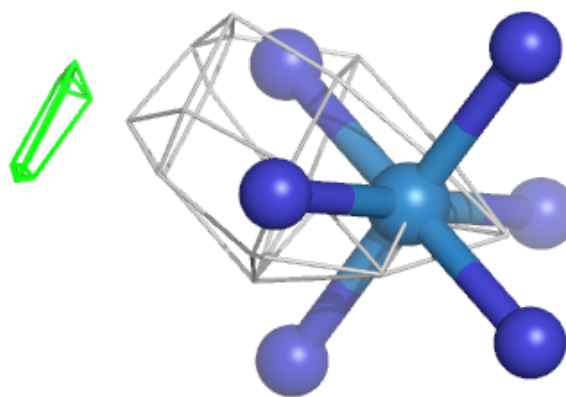
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
88	OHX	6	2014	7/7	0.99	0.19	85,85,85,85	2
88	OHX	4	220	7/7	0.99	0.24	60,60,60,60	3
88	OHX	1	3780	7/7	0.99	0.25	72,72,72,72	2
89	ZN	Q3	501	1/1	0.99	0.14	74,74,74,74	0
88	OHX	6	2030	7/7	0.99	0.20	60,60,60,60	1
88	OHX	5	3818	7/7	1.00	0.23	63,63,63,63	3
88	OHX	5	3802	7/7	1.00	0.23	62,62,62,62	3
88	OHX	5	3807	7/7	1.00	0.22	49,49,49,49	2
88	OHX	1	3792	7/7	1.00	0.21	54,54,54,54	2
88	OHX	5	3823	7/7	1.00	0.23	43,43,43,43	1
88	OHX	5	3828	7/7	1.00	0.20	49,49,49,49	2
88	OHX	5	3800	7/7	1.00	0.24	57,57,57,57	4
88	OHX	5	3819	7/7	1.00	0.21	65,65,65,65	2
88	OHX	1	3784	7/7	1.00	0.23	74,74,74,74	2
88	OHX	5	3834	7/7	1.00	0.21	52,52,52,52	5
88	OHX	5	3809	7/7	1.00	0.22	54,54,54,54	2
88	OHX	1	3759	7/7	1.00	0.24	55,55,55,55	2
88	OHX	5	3801	7/7	1.00	0.27	63,63,63,63	2
88	OHX	1	3769	7/7	1.00	0.22	64,64,64,64	4
88	OHX	5	3794	7/7	1.00	0.22	50,50,50,50	3
88	OHX	5	3808	7/7	1.00	0.26	71,71,71,71	2
88	OHX	5	3820	7/7	1.00	0.20	65,65,65,65	4
88	OHX	5	3797	7/7	1.00	0.25	55,55,55,55	3
88	OHX	2	1994	7/7	1.00	0.21	85,85,85,85	0
88	OHX	5	3798	7/7	1.00	0.25	58,58,58,58	2
88	OHX	5	3810	7/7	1.00	0.22	69,69,69,69	0
88	OHX	5	3803	7/7	1.00	0.20	60,60,60,60	2
88	OHX	5	3817	7/7	1.00	0.20	66,66,66,66	1
88	OHX	1	3757	7/7	1.00	0.24	56,56,56,56	1
88	OHX	1	3783	7/7	1.00	0.21	57,57,57,57	2
88	OHX	5	3832	7/7	1.00	0.20	55,55,55,55	2
88	OHX	5	3881	7/7	1.00	0.19	51,51,51,51	1
88	OHX	6	2013	7/7	1.00	0.21	69,69,69,69	1

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

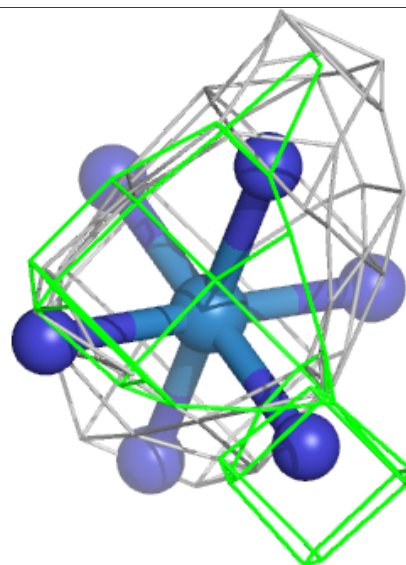
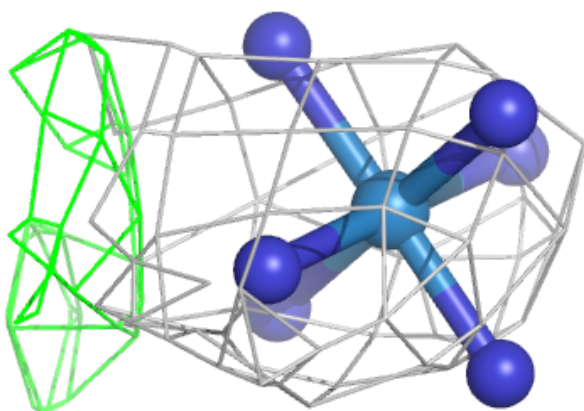
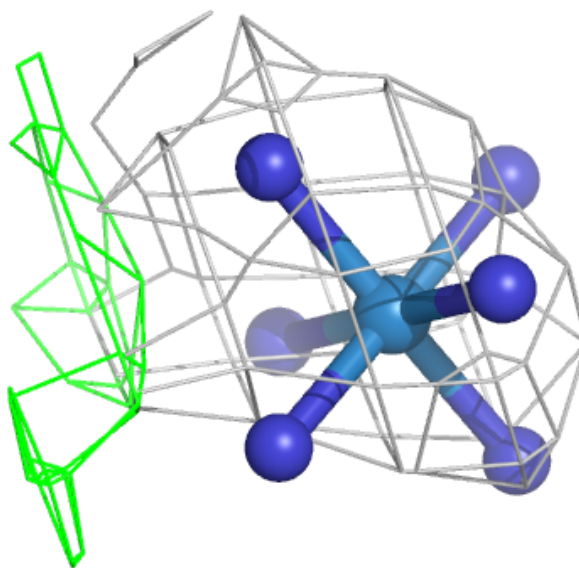
**Electron density around OHX 6 2181:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



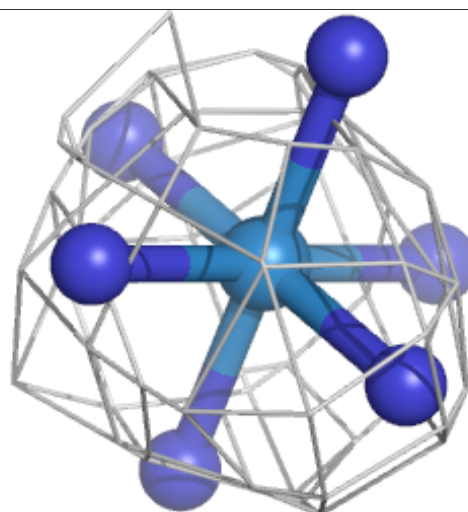
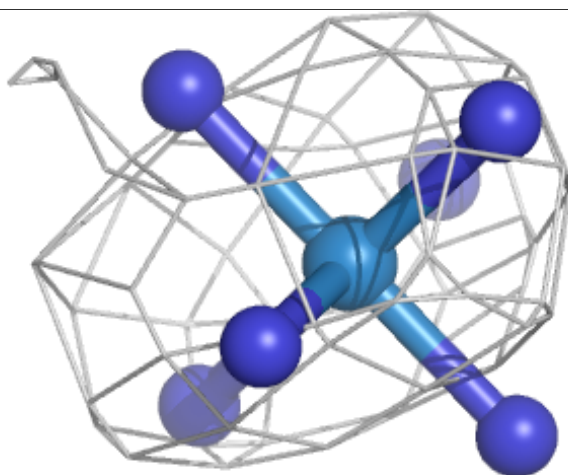
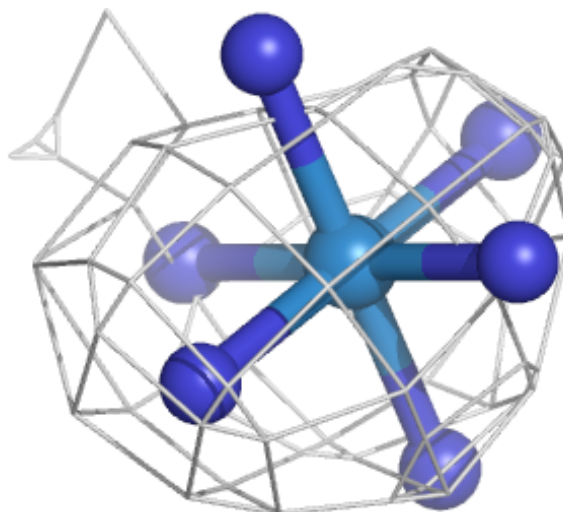
**Electron density around OHX 5 4147:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around OHX 2 2146:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.