



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 09:25 AM UTC

PDB ID : 5DGE / pdb_00005dge
Title : Coping with proline stalling: structural basis of hypusine-induced protein synthesis by the eukaryotic ribosome
Authors : Melnikov, S.; Mailliot, J.; Shin, B.-S.; Rigger, L.; Yusupova, G.; Micura, R.; Dever, T.E.; Yusupov, M.
Deposited on : 2015-08-27
Resolution : 3.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

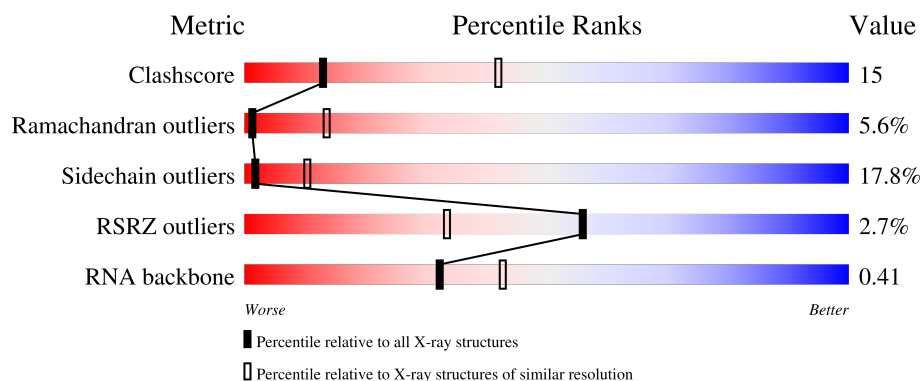
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)
RNA backbone	3983	1186 (3.92-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	

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Mol	Chain	Length	Quality of chain
3	S1	254	
3	s1	254	
4	S2	253	
4	s2	253	
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	

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

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Mol	Chain	Length	Quality of chain
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	63	
32	e0	63	
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	

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

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

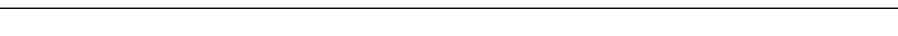
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Mol	Chain	Length	Quality of chain
65	n9	58	
66	O0	104	
66	o0	104	
67	O1	112	
67	o1	112	
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	121	
70	o4	121	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	

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Mol	Chain	Length	Quality of chain
78	Q2	105	
78	q2	105	
79	Q3	91	
79	q3	91	
80	m2	165	
81	p0	311	
82	p1	106	
82	p2	106	
83	f	157	
84	B	3	
84	C	3	

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
83	5CT	f	51	X	-	-	X
85	MG	1	3560	-	-	-	X
85	MG	1	3595	-	-	-	X
85	MG	1	3635	-	-	-	X
85	MG	2	1907	-	-	-	X
85	MG	2	1911	-	-	-	X
85	MG	2	1912	-	-	-	X
85	MG	2	1922	-	-	-	X
85	MG	2	1928	-	-	-	X
85	MG	2	1932	-	-	-	X
85	MG	2	1933	-	-	-	X
85	MG	2	1949	-	-	-	X
85	MG	2	1951	-	-	-	X
85	MG	2	1974	-	-	-	X
85	MG	5	3628	-	-	-	X
85	MG	6	1901	-	-	-	X
85	MG	6	1937	-	-	-	X
85	MG	6	1943	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	6	1974	-	-	-	X
85	MG	M7	201	-	-	-	X
86	OHX	1	3854	-	-	X	-
86	OHX	1	3889	-	-	X	-
86	OHX	1	3940	-	-	X	-
86	OHX	1	4071	-	-	X	-
86	OHX	1	4082	-	-	X	-
86	OHX	1	4085	-	-	X	-
86	OHX	2	2058	-	-	X	-
86	OHX	2	2099	-	-	X	-
86	OHX	2	2131	-	-	X	-
86	OHX	5	3915	-	-	X	-
86	OHX	5	3918	-	-	X	-
86	OHX	5	3955	-	-	X	-
86	OHX	5	4001	-	-	X	-
86	OHX	5	4002	-	-	X	-
86	OHX	5	4084	-	-	X	-
86	OHX	6	2067	-	-	X	-
86	OHX	6	2124	-	-	X	-
86	OHX	C5	201	-	-	X	-
86	OHX	M0	304	-	-	X	-
86	OHX	O7	104	-	-	X	-
86	OHX	c5	202	-	-	X	-
86	OHX	o7	502	-	-	X	-

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 413121 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		0	0	0
			1481	951	265	265				
9	s7	186	Total	C	N	O		0	0	0
			1491	957	267	267				

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

- 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				

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
			2436	1541	418	469	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	sR	318	Total	C	N	O	S	0	0	0
			2441	1544	418	471	8			

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
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
			1764	1131	316	314	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L8	119	ALA	GLY	conflict	UNP P17076
l8	119	ALA	GLY	conflict	UNP P17076

- 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-A.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M1	3	THR	ALA	conflict	UNP P0C0W9
m1	3	THR	ALA	conflict	UNP P0C0W9

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	O0	97	Total	C	N	O	S	0	0	0
			742	479	124	138	1			
66	o0	100	Total	C	N	O	S	0	0	0
			766	492	128	145	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	Q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			
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 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
80	m2	150	Total	C	N	O	0	0	0
			739	439	150	150			

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

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

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

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

- Molecule 83 is a protein called Eukaryotic translation initiation factor 5A-1.

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

- Molecule 84 is a RNA chain called DNA (5'-R(*CP*CP*(NA))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
84	B	3	Total	C	N	O	P	0	0	0
			59	28	12	17	2			
84	C	3	Total	C	N	O	P	0	0	0
			62	28	12	19	3			

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	2	90	Total	Mg	0	0
			90	90		
85	S2	1	Total	Mg	0	0
			1	1		
85	D3	1	Total	Mg	0	0
			1	1		
85	SM	1	Total	Mg	0	0
			1	1		
85	1	361	Total	Mg	0	0
			361	361		
85	3	8	Total	Mg	0	0
			8	8		
85	4	15	Total	Mg	0	0
			15	15		
85	L2	2	Total	Mg	0	0
			2	2		
85	L3	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L6	1	Total 1	Mg 1	0	0
85	L7	3	Total 3	Mg 3	0	0
85	M0	2	Total 2	Mg 2	0	0
85	M5	2	Total 2	Mg 2	0	0
85	M6	3	Total 3	Mg 3	0	0
85	M7	4	Total 4	Mg 4	0	0
85	M9	1	Total 1	Mg 1	0	0
85	N3	1	Total 1	Mg 1	0	0
85	N6	1	Total 1	Mg 1	0	0
85	N8	3	Total 3	Mg 3	0	0
85	O4	1	Total 1	Mg 1	0	0
85	O7	2	Total 2	Mg 2	0	0
85	Q2	1	Total 1	Mg 1	0	0
85	6	111	Total 111	Mg 111	0	0
85	s4	1	Total 1	Mg 1	0	0
85	s8	2	Total 2	Mg 2	0	0
85	c8	2	Total 2	Mg 2	0	0
85	c9	1	Total 1	Mg 1	0	0
85	d2	1	Total 1	Mg 1	0	0
85	d3	1	Total 1	Mg 1	0	0
85	d6	1	Total 1	Mg 1	0	0

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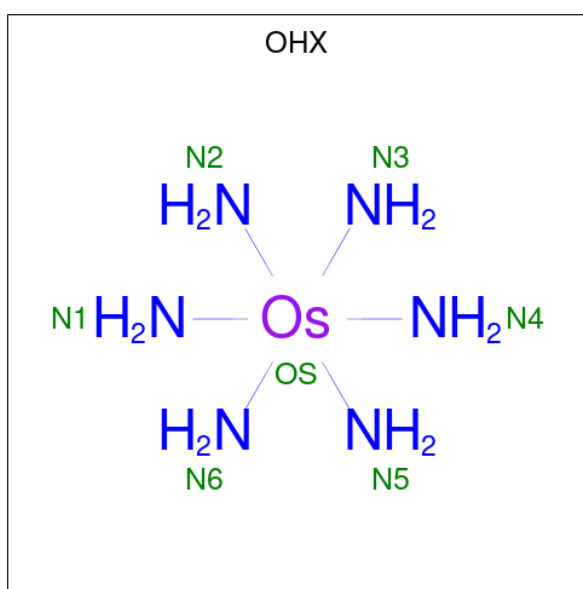
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	5	415	Total 415	Mg 415	0	0
85	7	13	Total 13	Mg 13	0	0
85	8	10	Total 10	Mg 10	0	0
85	l2	2	Total 2	Mg 2	0	0
85	l3	2	Total 2	Mg 2	0	0
85	l4	1	Total 1	Mg 1	0	0
85	l5	1	Total 1	Mg 1	0	0
85	l7	2	Total 2	Mg 2	0	0
85	m0	1	Total 1	Mg 1	0	0
85	m3	1	Total 1	Mg 1	0	0
85	m5	3	Total 3	Mg 3	0	0
85	m7	3	Total 3	Mg 3	0	0
85	n0	1	Total 1	Mg 1	0	0
85	n3	1	Total 1	Mg 1	0	0
85	n6	1	Total 1	Mg 1	0	0
85	n8	2	Total 2	Mg 2	0	0
85	o2	1	Total 1	Mg 1	0	0
85	o3	1	Total 1	Mg 1	0	0
85	o4	1	Total 1	Mg 1	0	0
85	q1	1	Total 1	Mg 1	0	0
85	q2	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	q3	1	Total	Mg	0	0
			1	1		
85	f	1	Total	Mg	0	0
			1	1		
85	B	1	Total	Mg	0	0
			1	1		
85	C	1	Total	Mg	0	0
			1	1		

- Molecule 86 is osmium (III) hexammine (CCD ID: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	S1	1	Total 7	N 6	Os 1	0	0
86	S6	1	Total 7	N 6	Os 1	0	0
86	S8	1	Total 7	N 6	Os 1	0	0
86	S9	1	Total 7	N 6	Os 1	0	0
86	C3	1	Total 7	N 6	Os 1	0	0
86	C5	1	Total 7	N 6	Os 1	0	0
86	C8	1	Total 7	N 6	Os 1	0	0
86	D9	1	Total 7	N 6	Os 1	0	0
86	SR	1	Total 7	N 6	Os 1	0	0
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86	1	1	Total 7	N 6	Os 1	1	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	1	0

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	3	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	4	1	Total	N	Os	0	0
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			7	6	1		
86	L3	1	Total	N	Os	0	0
			7	6	1		
86	L3	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	L3	1	Total 7	N 6	Os 1	0	0
86	L4	1	Total 7	N 6	Os 1	0	0
86	L5	1	Total 7	N 6	Os 1	0	0
86	M0	1	Total 7	N 6	Os 1	0	0
86	M0	1	Total 7	N 6	Os 1	0	0
86	M5	1	Total 7	N 6	Os 1	0	0
86	M5	1	Total 7	N 6	Os 1	0	0
86	M6	1	Total 7	N 6	Os 1	0	0
86	M7	1	Total 7	N 6	Os 1	0	0
86	M8	1	Total 7	N 6	Os 1	0	0
86	M9	1	Total 7	N 6	Os 1	0	0
86	N8	1	Total 7	N 6	Os 1	0	0
86	N9	1	Total 7	N 6	Os 1	0	0
86	O1	1	Total 7	N 6	Os 1	0	0
86	O3	1	Total 7	N 6	Os 1	0	0
86	O4	1	Total 7	N 6	Os 1	0	0
86	O7	1	Total 7	N 6	Os 1	0	0
86	O9	1	Total 7	N 6	Os 1	0	0
86	Q2	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	2	0
86	6	1	Total 7	N 6	Os 1	1	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	1	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
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			7	6	1		
86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	s1	1	Total 7	N 6	Os 1	0	0
86	s4	1	Total 7	N 6	Os 1	0	0
86	s8	1	Total 7	N 6	Os 1	0	0
86	s9	1	Total 7	N 6	Os 1	0	0
86	c3	1	Total 7	N 6	Os 1	0	0
86	c5	1	Total 7	N 6	Os 1	0	0
86	c5	1	Total 7	N 6	Os 1	0	0
86	c8	1	Total 7	N 6	Os 1	0	0
86	d4	1	Total 7	N 6	Os 1	0	0
86	d9	1	Total 7	N 6	Os 1	0	0
86	sR	1	Total 7	N 6	Os 1	0	0
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86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	l3	1	Total 7	N 6	Os 1	0	0
86	l3	1	Total 7	N 6	Os 1	0	0
86	l4	1	Total 7	N 6	Os 1	0	0
86	l4	1	Total 7	N 6	Os 1	0	0
86	l5	1	Total 7	N 6	Os 1	0	0
86	l5	1	Total 7	N 6	Os 1	1	0
86	l9	1	Total 7	N 6	Os 1	0	0
86	m0	1	Total 7	N 6	Os 1	0	0
86	m0	1	Total 7	N 6	Os 1	0	0
86	m1	1	Total 7	N 6	Os 1	0	0
86	m4	1	Total 7	N 6	Os 1	0	0
86	m5	1	Total 7	N 6	Os 1	0	0
86	m5	1	Total 7	N 6	Os 1	0	0
86	m5	1	Total 7	N 6	Os 1	0	0
86	m6	1	Total 7	N 6	Os 1	0	0
86	m7	1	Total 7	N 6	Os 1	0	0
86	m8	1	Total 7	N 6	Os 1	0	0
86	m9	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	o6	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

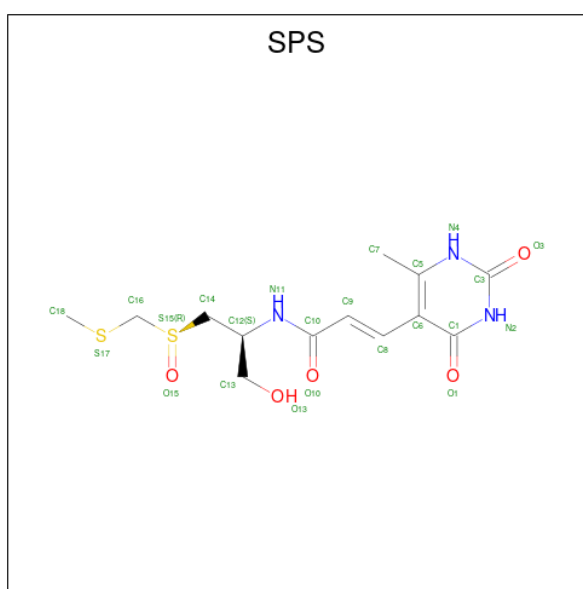
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	D6	1	Total	Zn	0	0
			1	1		
87	D7	1	Total	Zn	0	0
			1	1		
87	D9	1	Total	Zn	0	0
			1	1		
87	E1	1	Total	Zn	0	0
			1	1		
87	O7	1	Total	Zn	0	0
			1	1		
87	Q0	1	Total	Zn	0	0
			1	1		
87	Q2	1	Total	Zn	0	0
			1	1		
87	Q3	1	Total	Zn	0	0
			1	1		
87	d6	1	Total	Zn	0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

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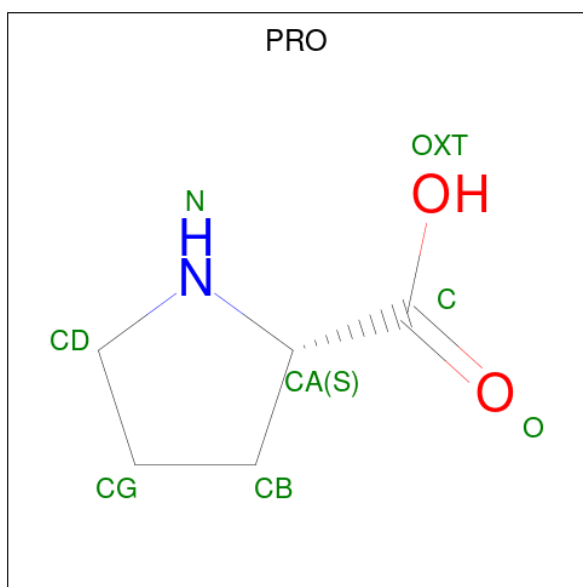
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	o7	1	Total	Zn	0	0
			1	1		
87	q0	1	Total	Zn	0	0
			1	1		
87	q2	1	Total	Zn	0	0
			1	1		
87	q3	1	Total	Zn	0	0
			1	1		

- Molecule 88 is SPARSOMYCIN (CCD ID: SPS) (formula: $C_{13}H_{19}N_3O_5S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
88	1	1	Total	C	N	O	S	0	0
			23	13	3	5	2		
88	5	1	Total	C	N	O	S	0	0
			23	13	3	5	2		

- Molecule 89 is PROLINE (CCD ID: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
89	1	1	Total	C	N	O	0	0
			7	5	1	1		
89	5	1	Total	C	N	O	0	0
			7	5	1	1		
89	B	1	Total	C	N	O	0	0
			7	5	1	1		
89	C	1	Total	C	N	O	0	0
			7	5	1	1		

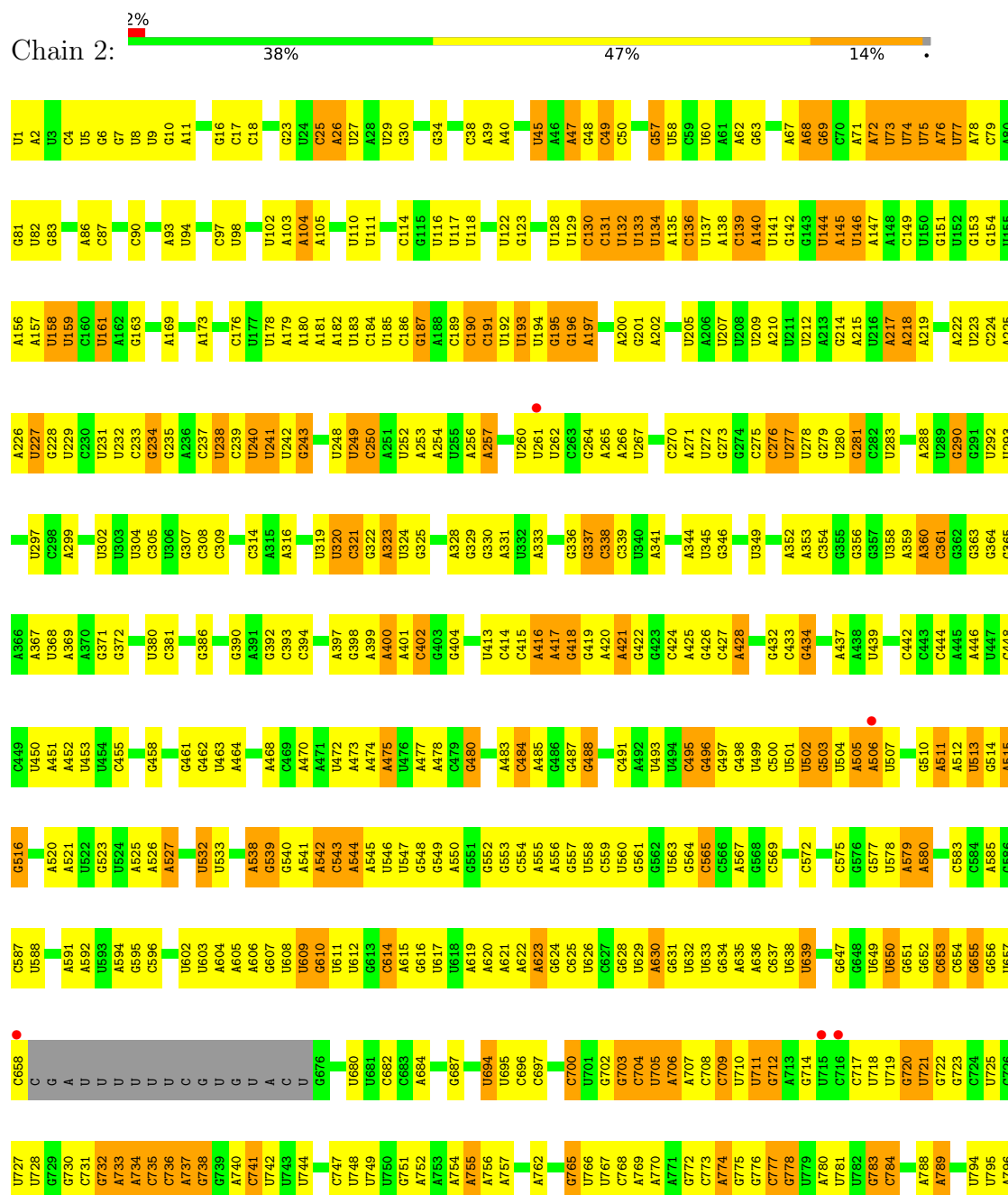
- Molecule 90 is water.

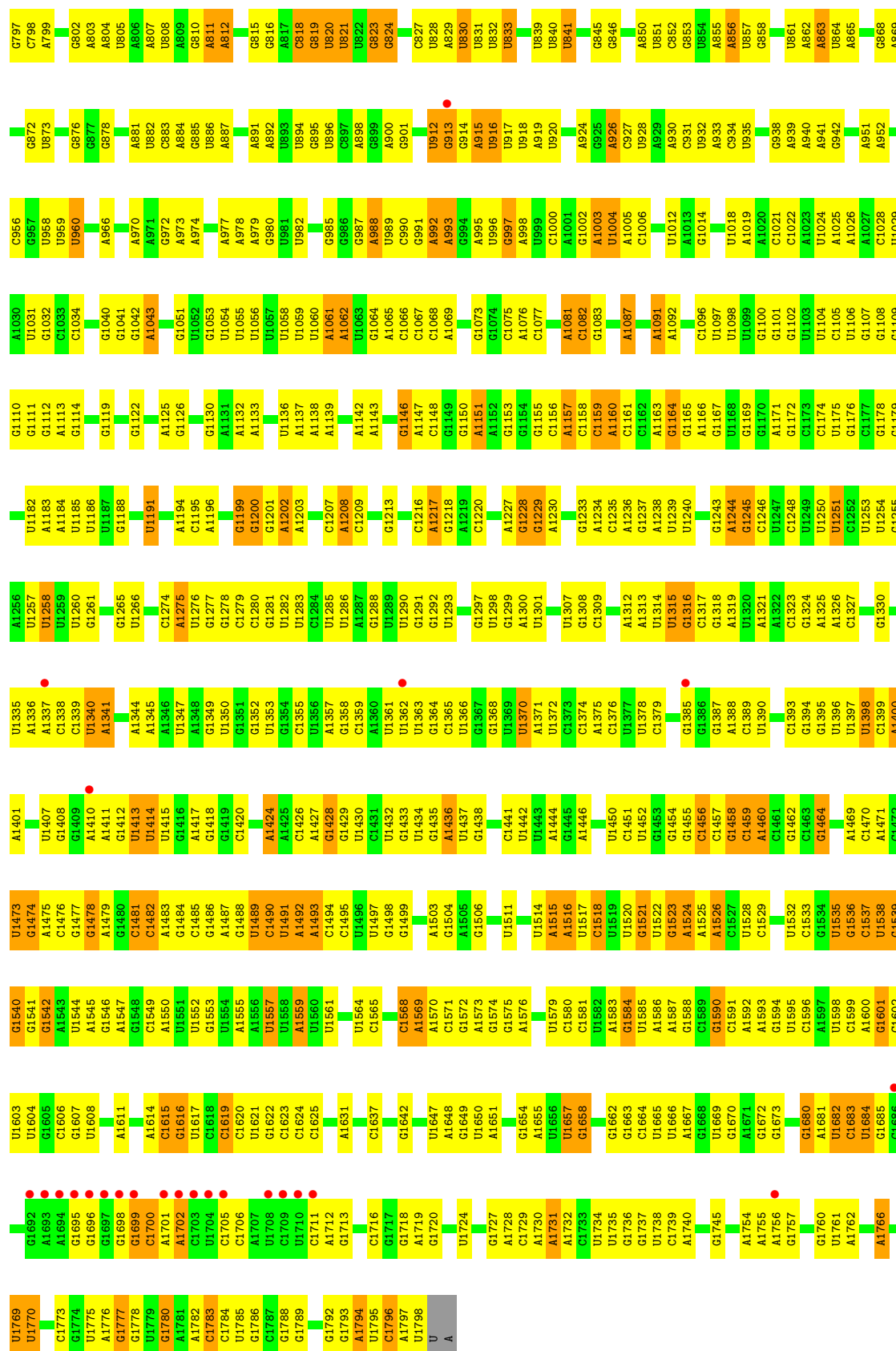
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
90	5	6	Total	O	0	0
			6	6		
90	f	6	Total	O	0	0
			6	6		

3 Residue-property plots

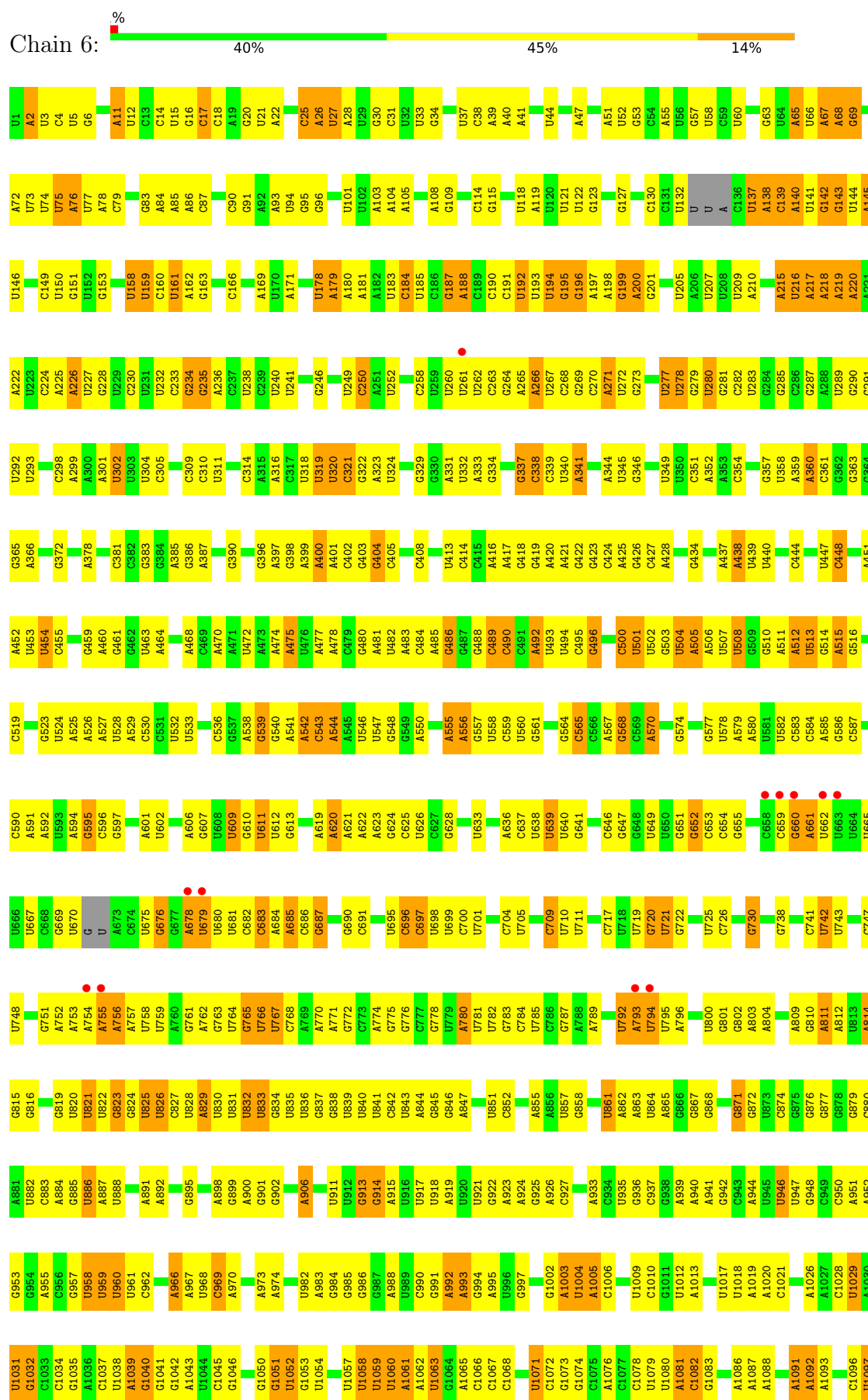
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 18S ribosomal RNA

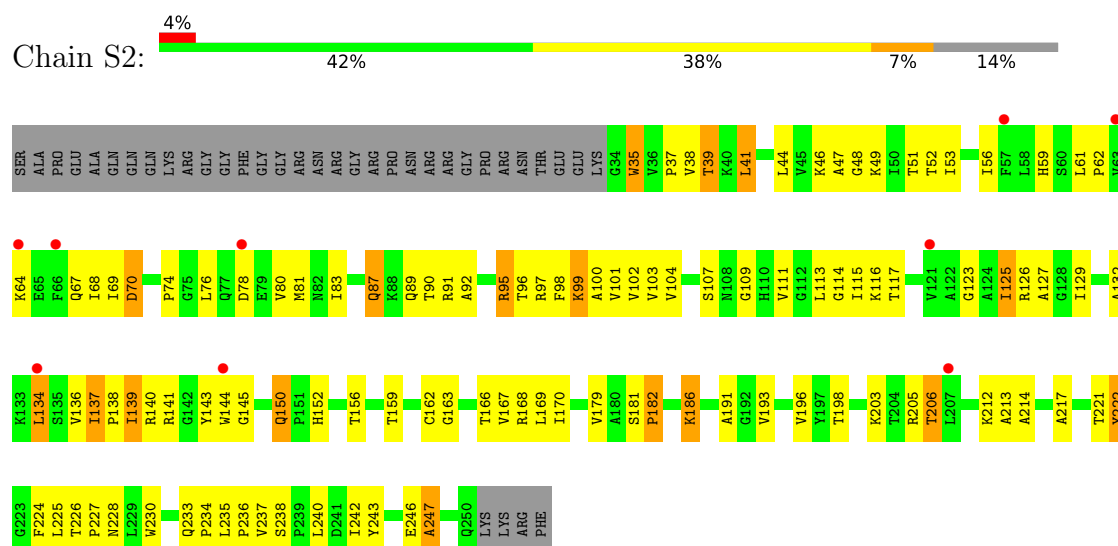




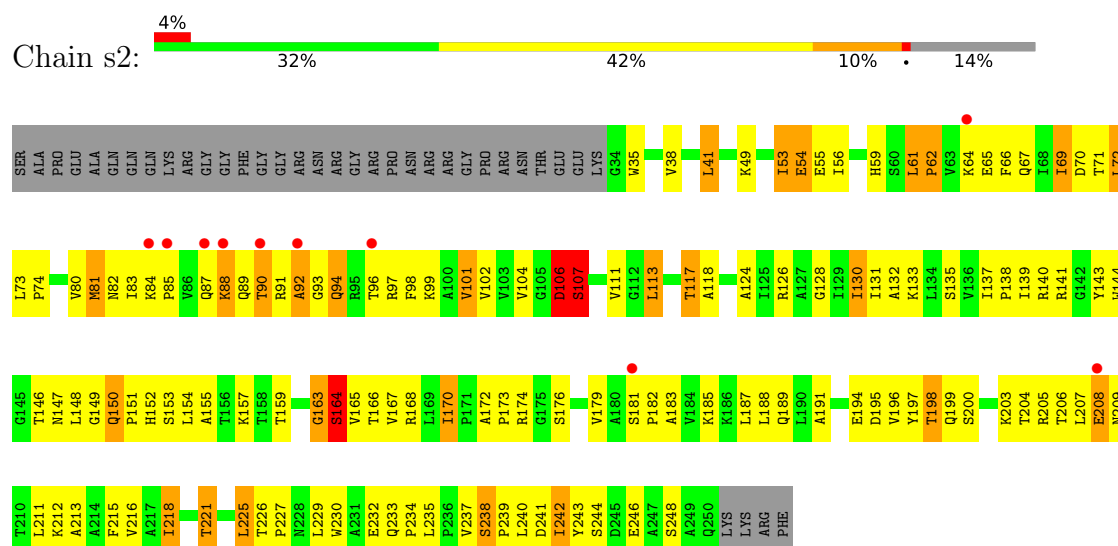
- Molecule 1: 18S ribosomal RNA



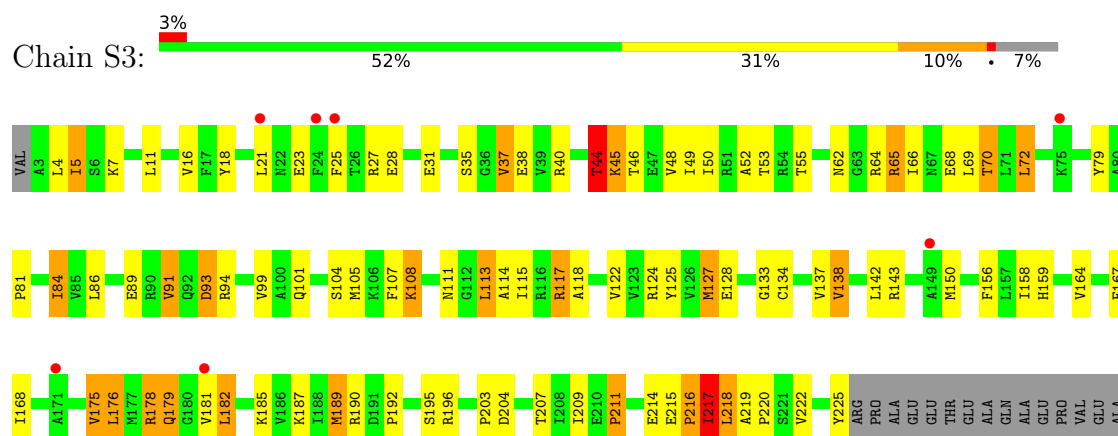
- Molecule 4: 40S ribosomal protein S2



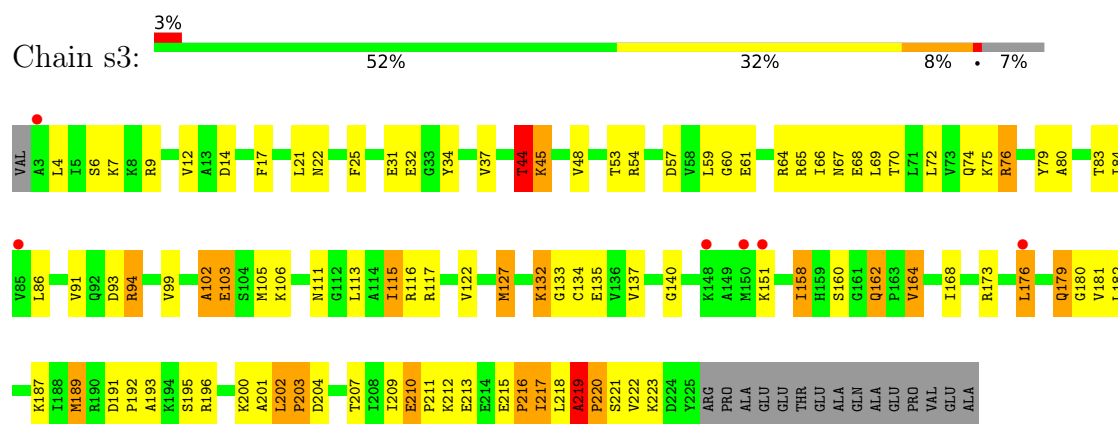
- Molecule 4: 40S ribosomal protein S2



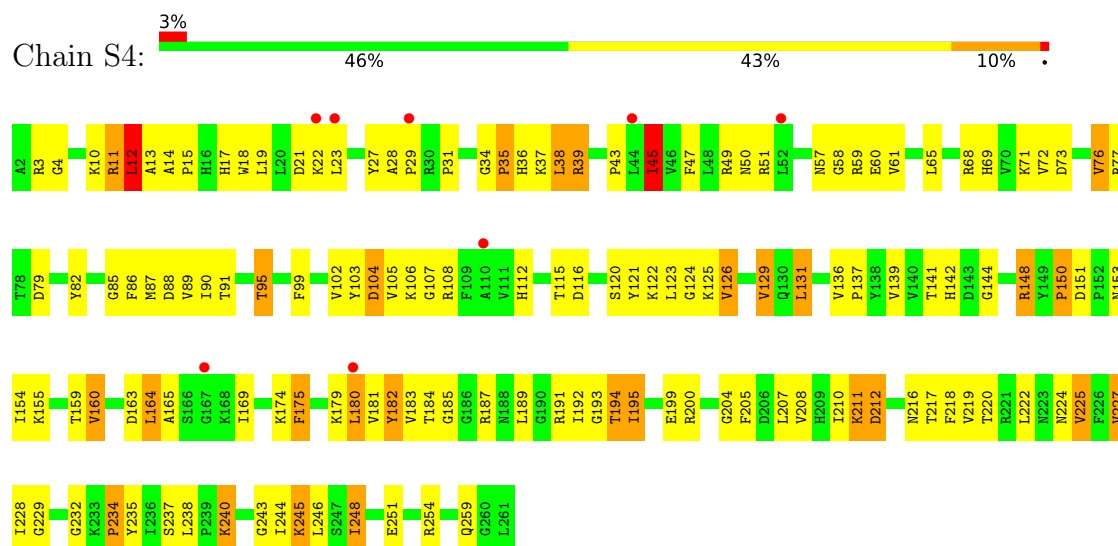
- Molecule 5: 40S ribosomal protein S3



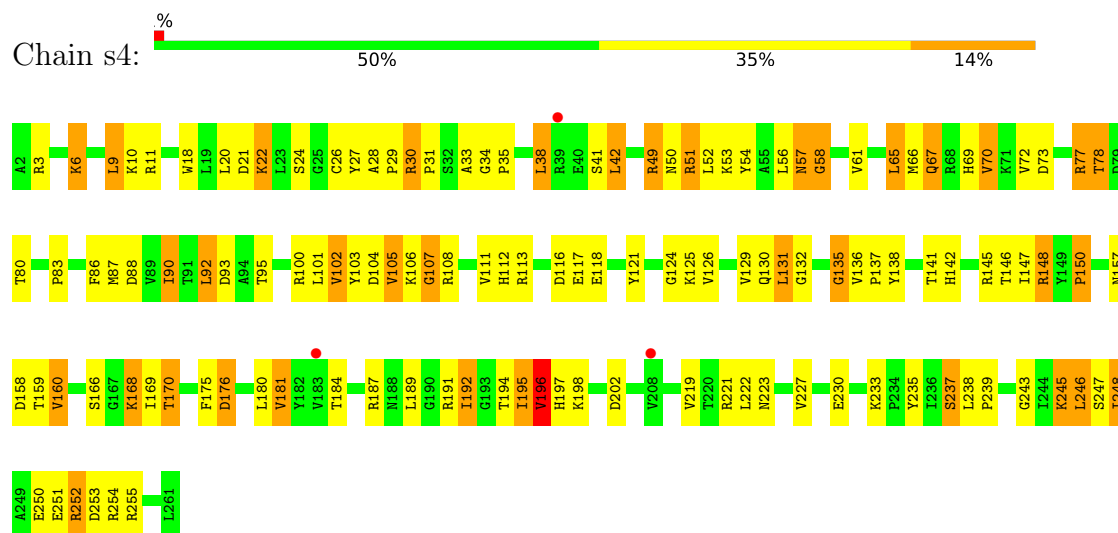
- Molecule 5: 40S ribosomal protein S3



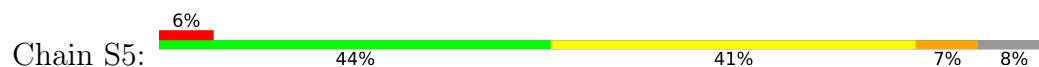
• Molecule 6: 40S ribosomal protein S4-A

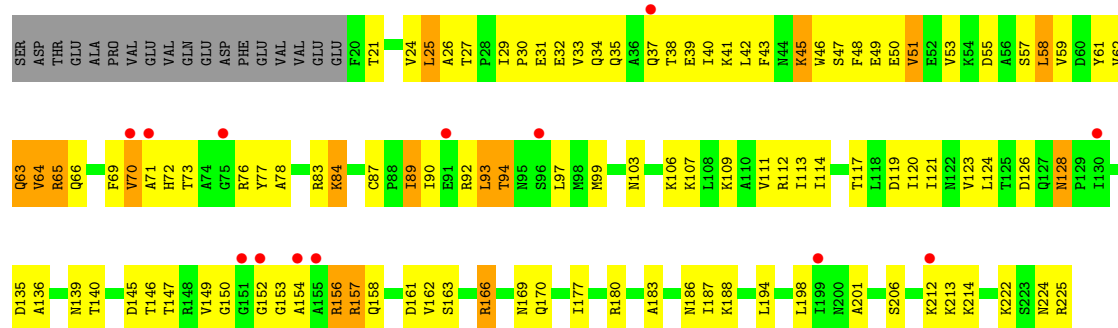


• Molecule 6: 40S ribosomal protein S4-A

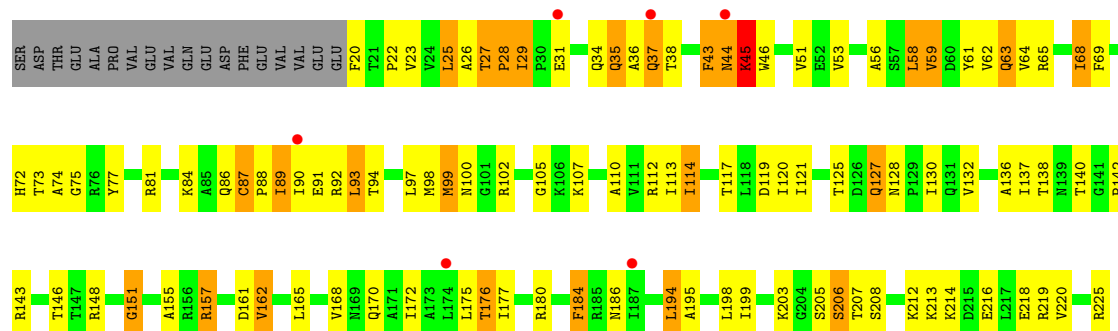


• Molecule 7: 40S ribosomal protein S5

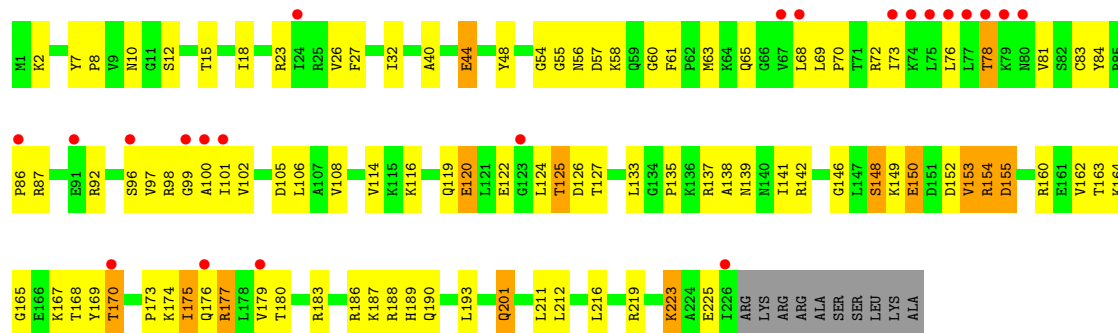




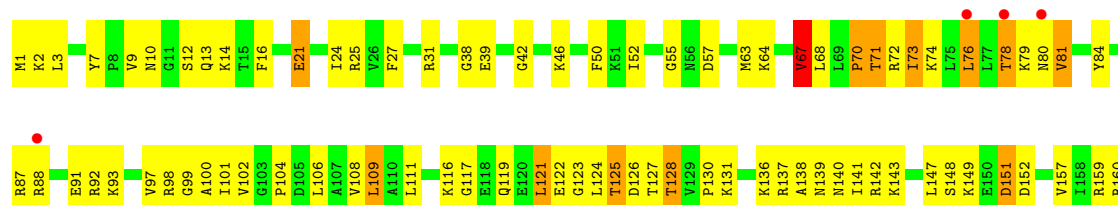
• Molecule 7: 40S ribosomal protein S5

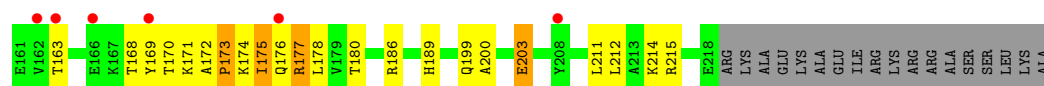


• Molecule 8: 40S ribosomal protein S6-A

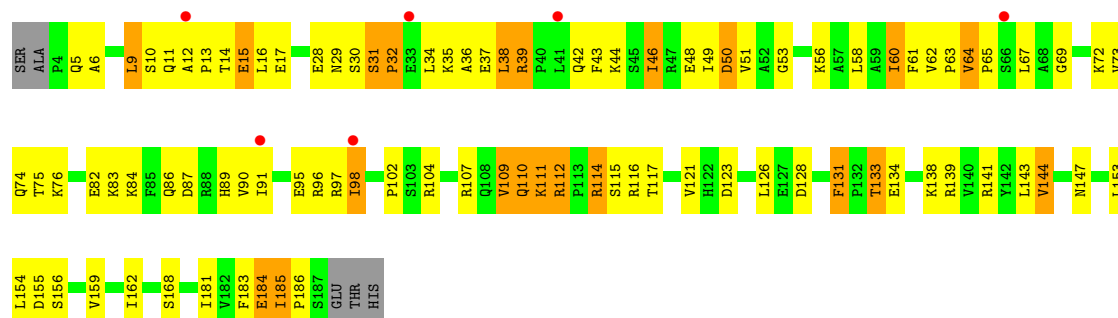


• Molecule 8: 40S ribosomal protein S6-A

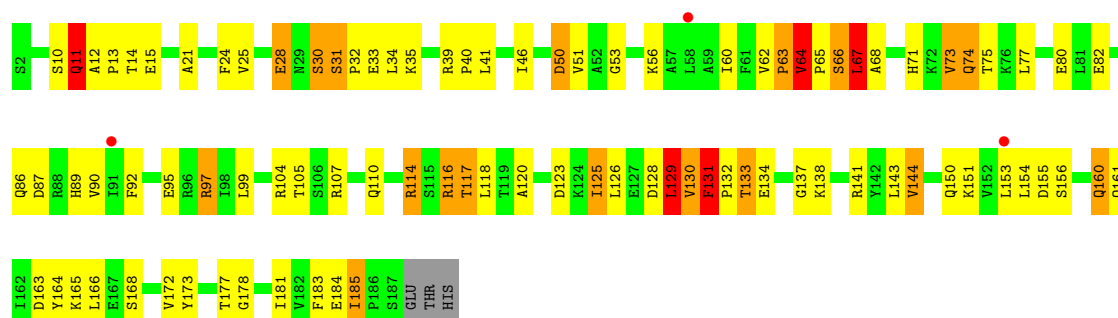




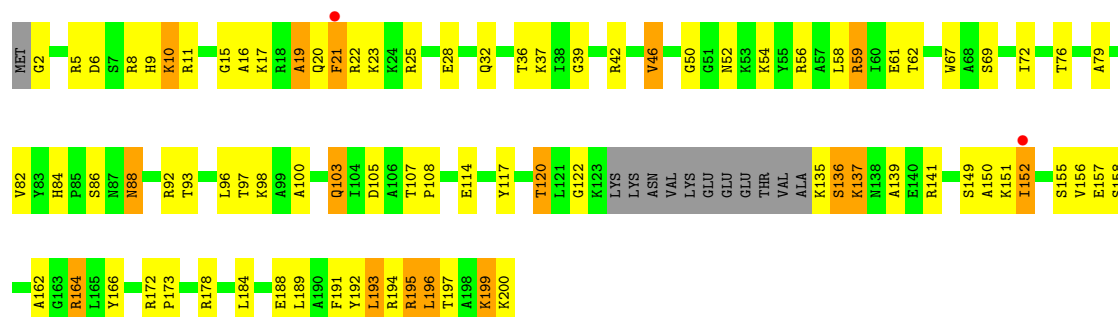
• Molecule 9: 40S ribosomal protein S7-A



• Molecule 9: 40S ribosomal protein S7-A

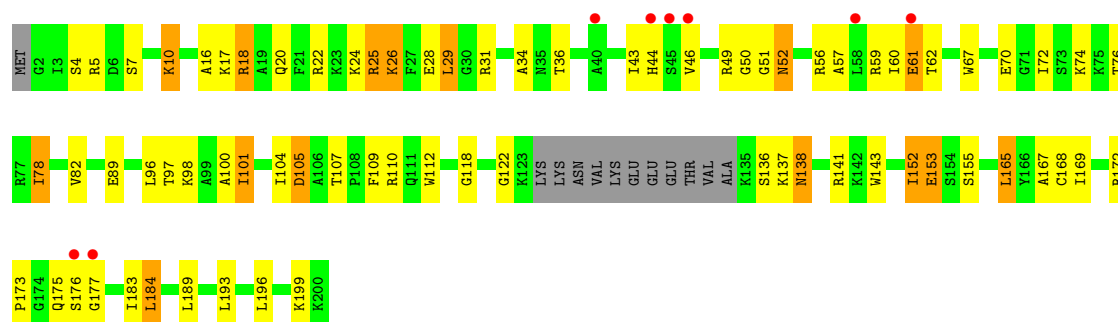


• Molecule 10: 40S ribosomal protein S8-A

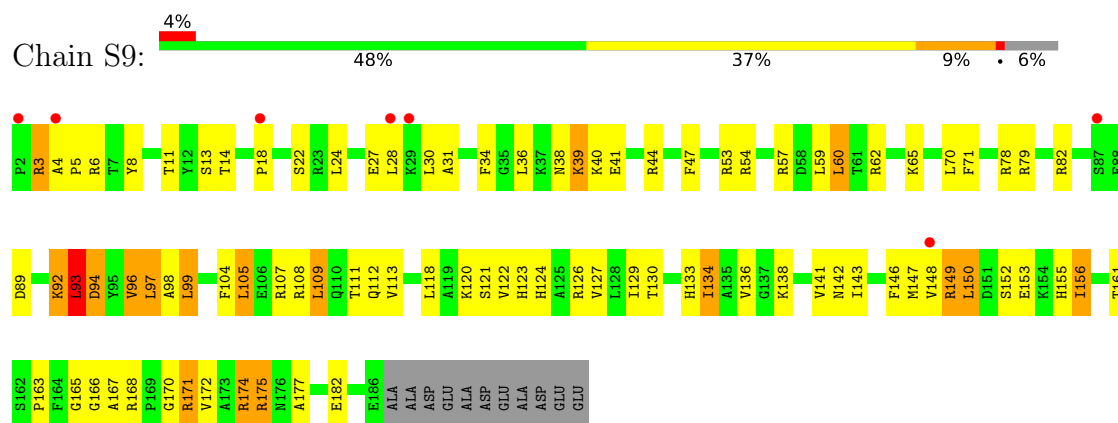


• Molecule 10: 40S ribosomal protein S8-A

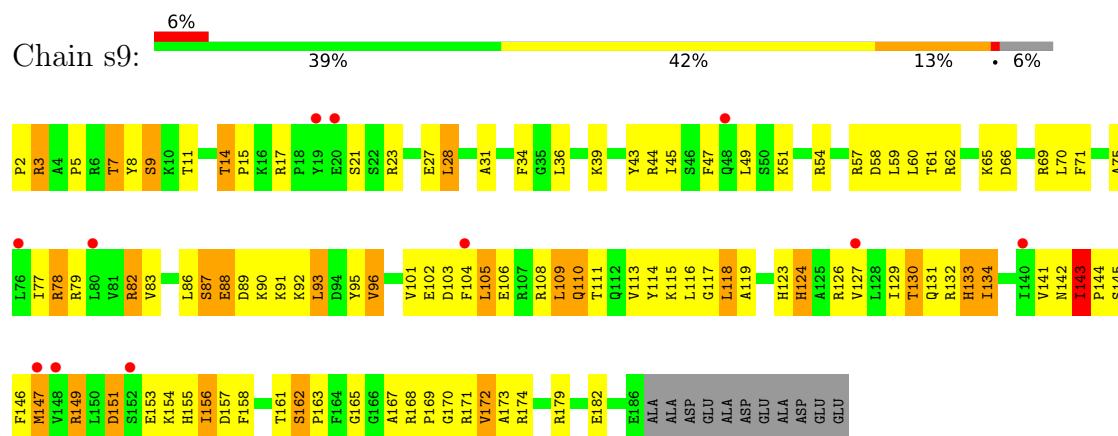




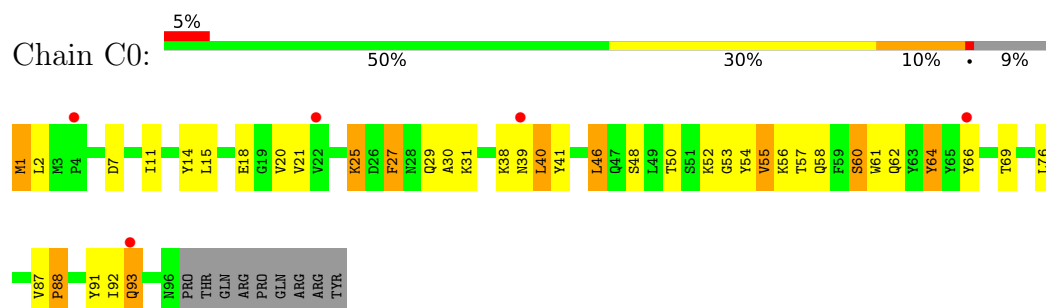
- Molecule 11: 40S ribosomal protein S9-A



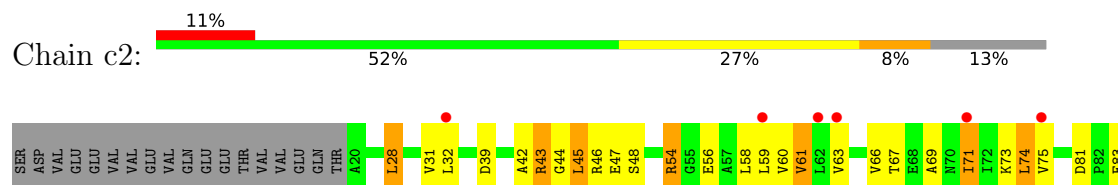
- Molecule 11: 40S ribosomal protein S9-A



- Molecule 12: 40S ribosomal protein S10-A

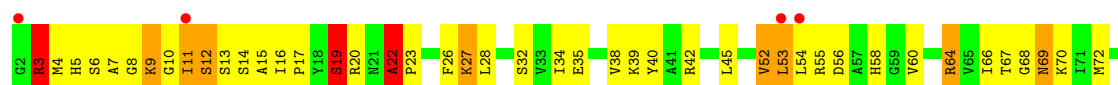


- Molecule 12: 40S ribosomal protein S10-A





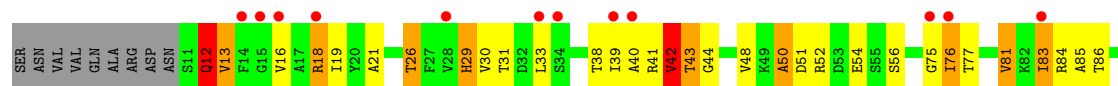
- Molecule 15: 40S ribosomal protein S13



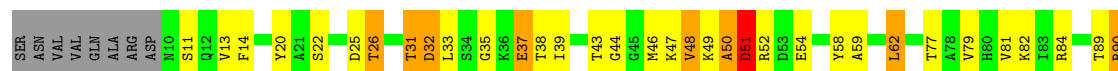
- Molecule 15: 40S ribosomal protein S13



- Molecule 16: 40S ribosomal protein S14-A

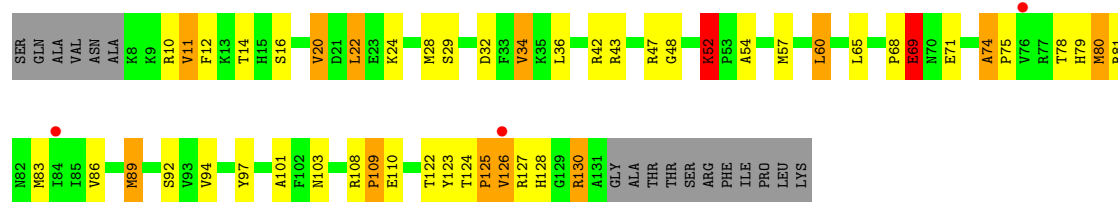


- Molecule 16: 40S ribosomal protein S14-A

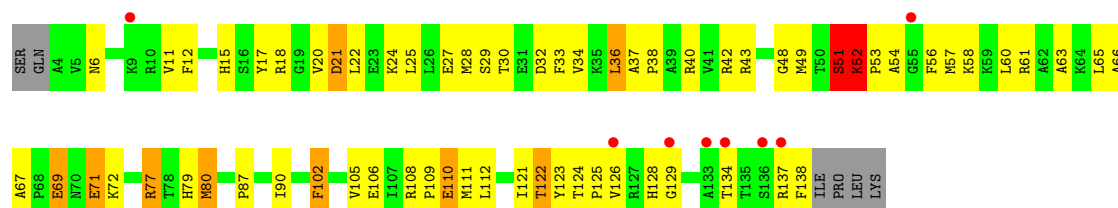


- Molecule 17: 40S ribosomal protein S15

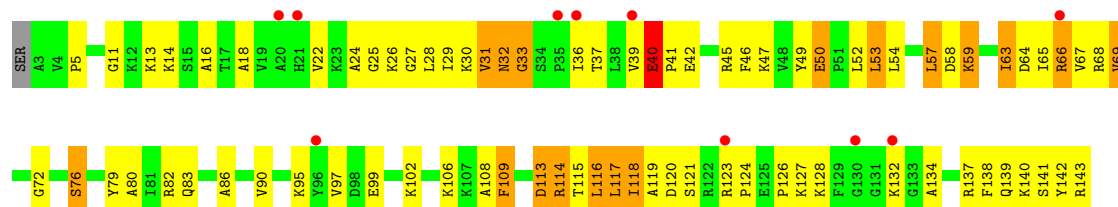
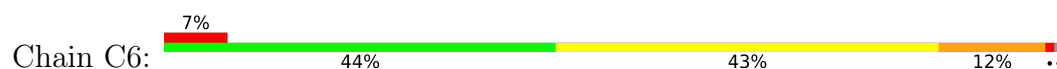




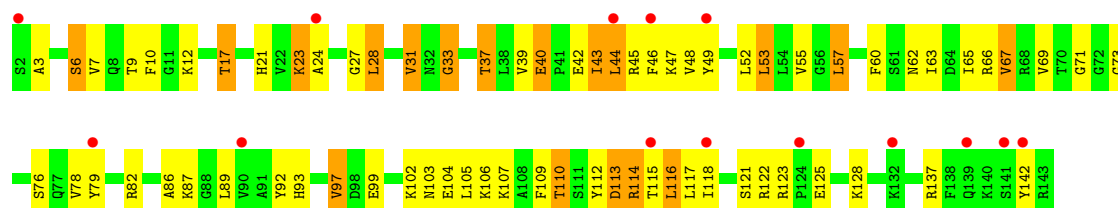
• Molecule 17: 40S ribosomal protein S15



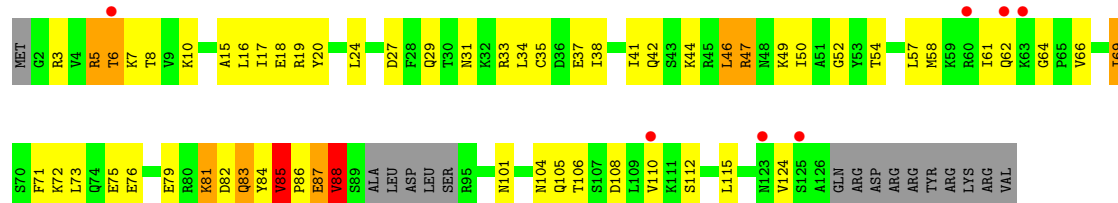
• Molecule 18: 40S ribosomal protein S16-A



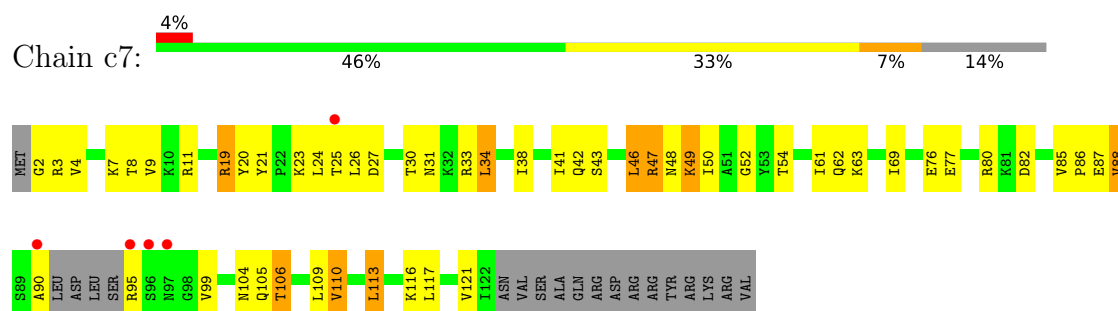
• Molecule 18: 40S ribosomal protein S16-A



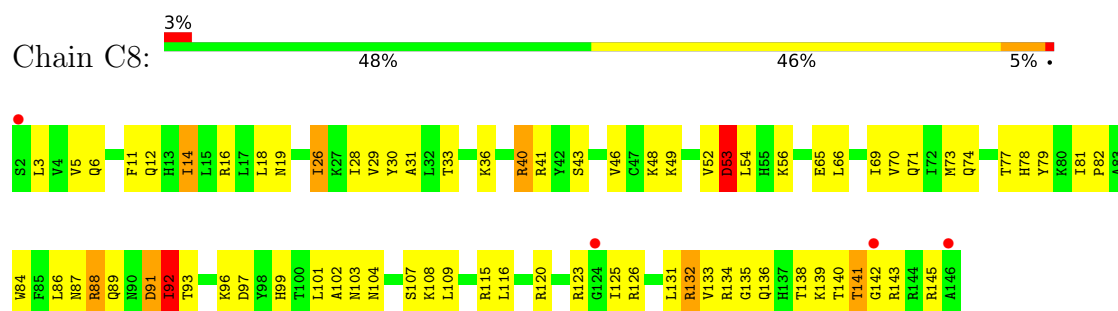
• Molecule 19: 40S ribosomal protein S17-A



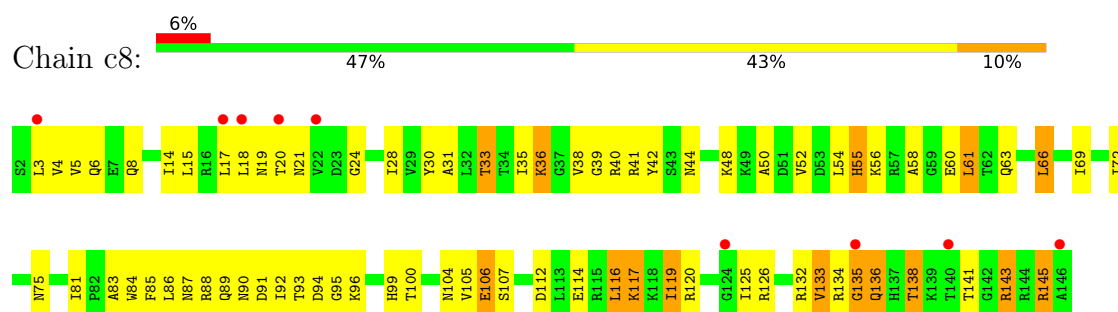
- Molecule 19: 40S ribosomal protein S17-A



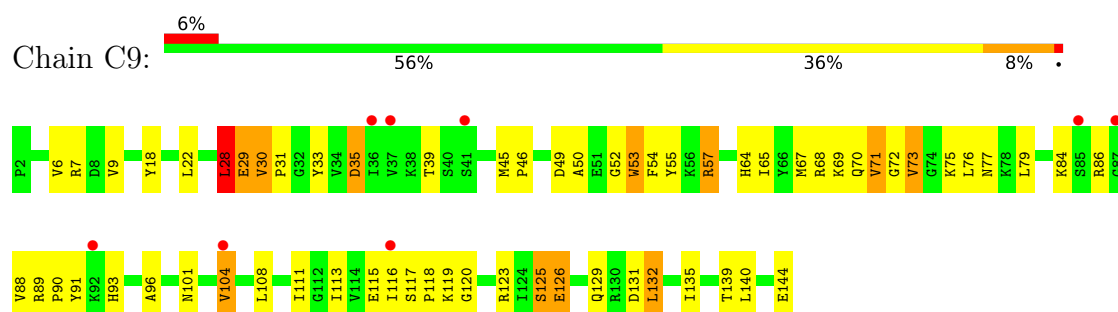
- Molecule 20: 40S ribosomal protein S18-A



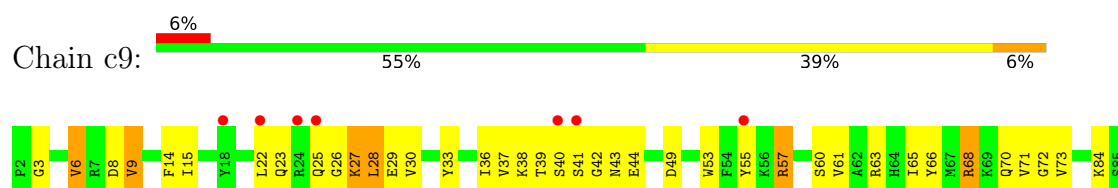
- Molecule 20: 40S ribosomal protein S18-A



- Molecule 21: 40S ribosomal protein S19-A

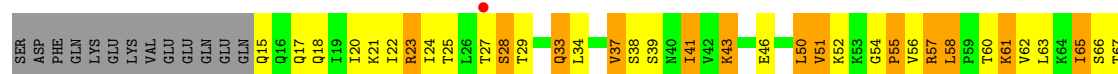


- Molecule 21: 40S ribosomal protein S19-A

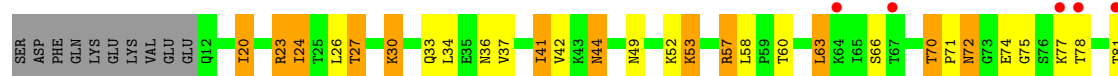




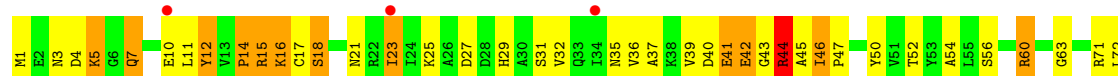
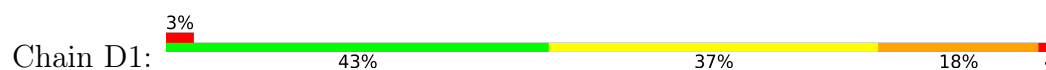
- Molecule 22: 40S ribosomal protein S20



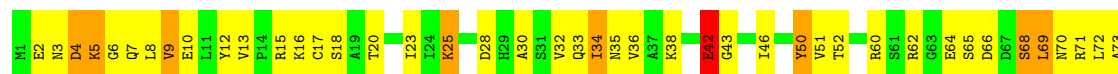
- Molecule 22: 40S ribosomal protein S20



- Molecule 23: 40S ribosomal protein S21-A

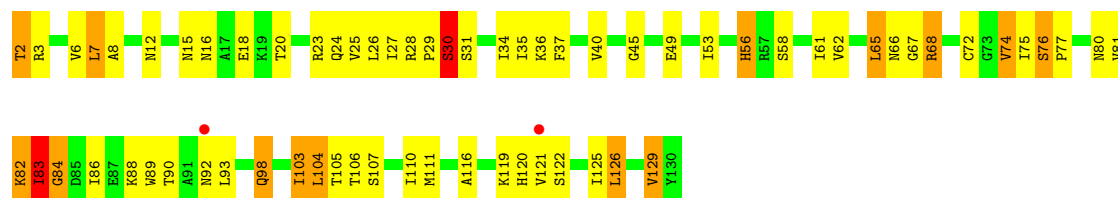


- Molecule 23: 40S ribosomal protein S21-A



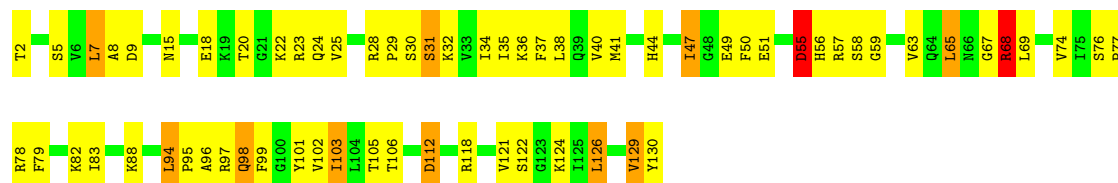
- Molecule 24: 40S ribosomal protein S22-A





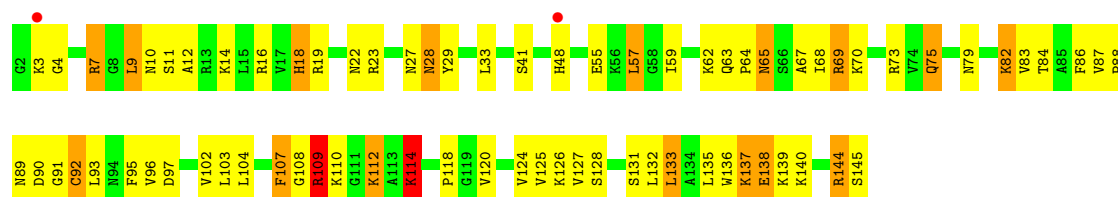
• Molecule 24: 40S ribosomal protein S22-A

Chain d2: 49% 42% 8% .



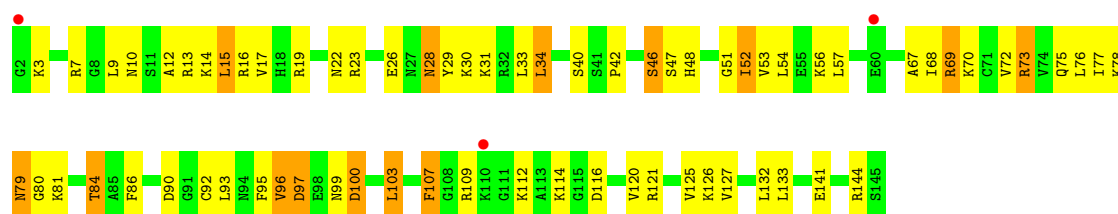
• Molecule 25: 40S ribosomal protein S23-A

Chain D3: 49% 39% 11% .



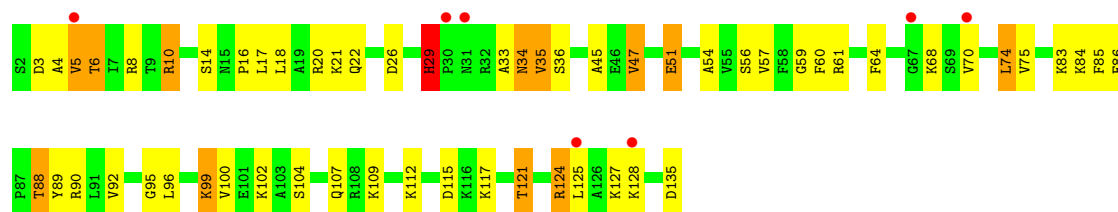
• Molecule 25: 40S ribosomal protein S23-A

Chain d3: 2% 52% 38% 10%

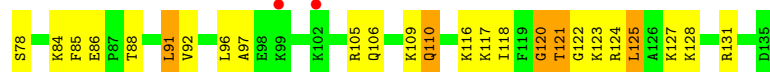
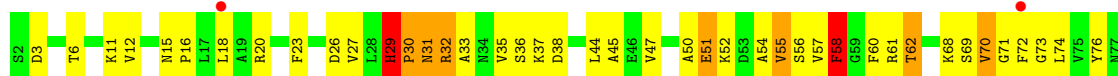


• Molecule 26: 40S ribosomal protein S24-A

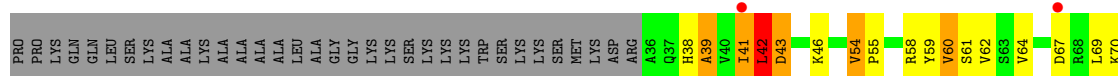
Chain D4: 5% 57% 34% 9% .



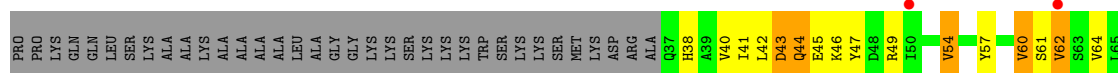
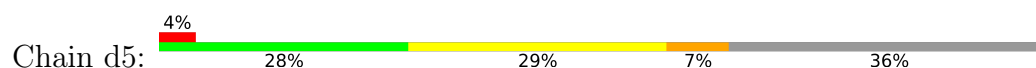
• Molecule 26: 40S ribosomal protein S24-A



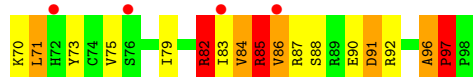
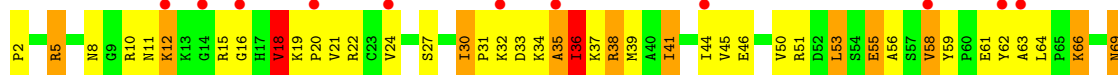
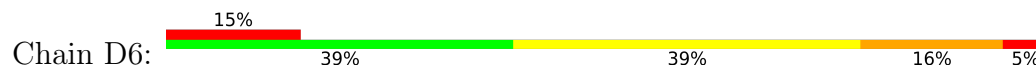
• Molecule 27: 40S ribosomal protein S25-A



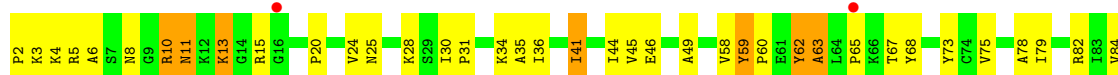
• Molecule 27: 40S ribosomal protein S25-A



• Molecule 28: 40S ribosomal protein S26-A



• Molecule 28: 40S ribosomal protein S26-A

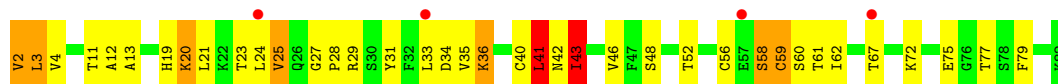




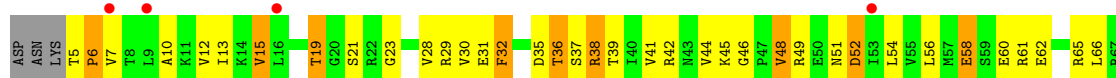
- Molecule 29: 40S ribosomal protein S27-A



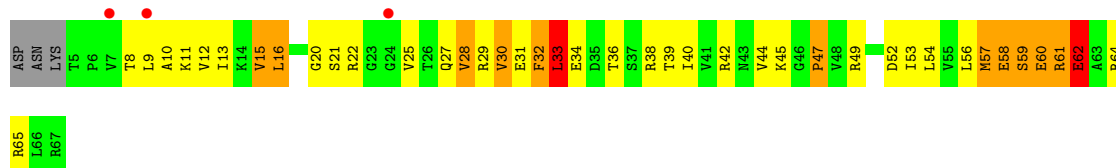
- Molecule 29: 40S ribosomal protein S27-A



- Molecule 30: 40S ribosomal protein S28-A



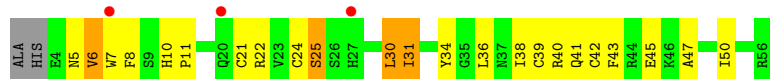
- Molecule 30: 40S ribosomal protein S28-A



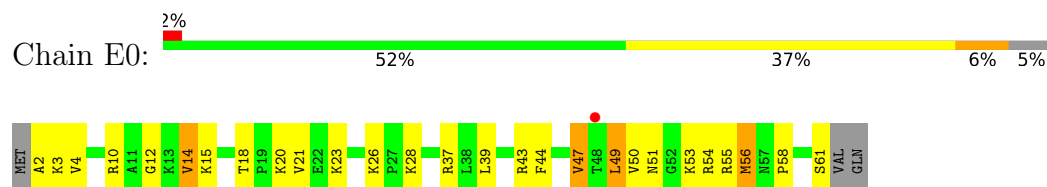
- Molecule 31: 40S ribosomal protein S29-A



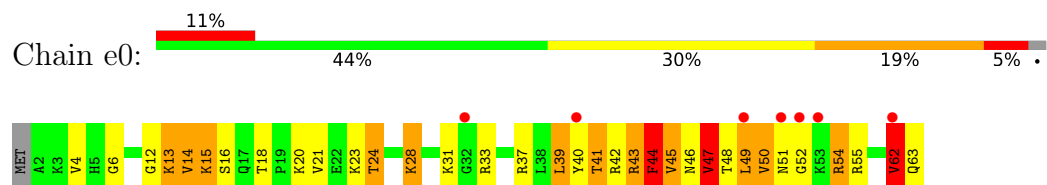
- Molecule 31: 40S ribosomal protein S29-A



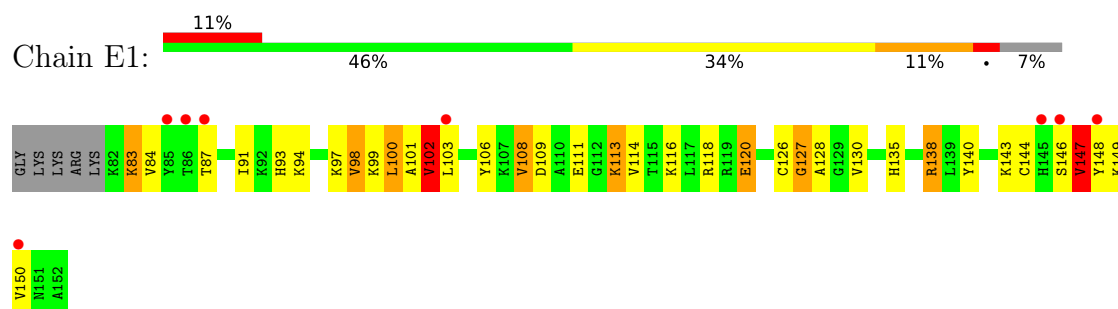
- Molecule 32: 40S ribosomal protein S30-A



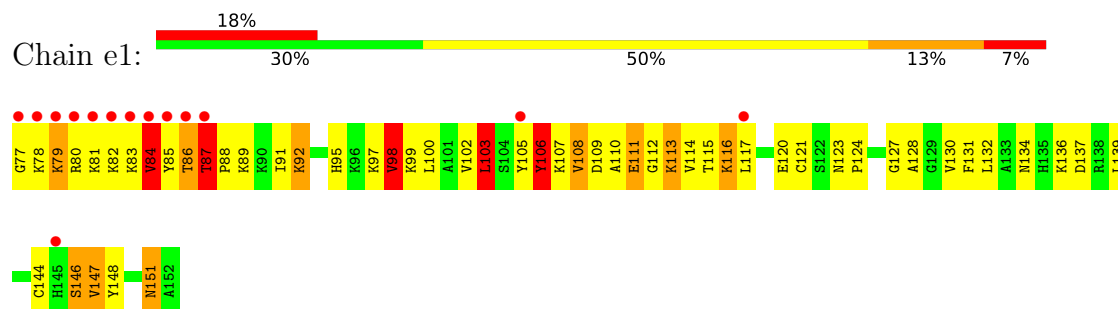
- Molecule 32: 40S ribosomal protein S30-A



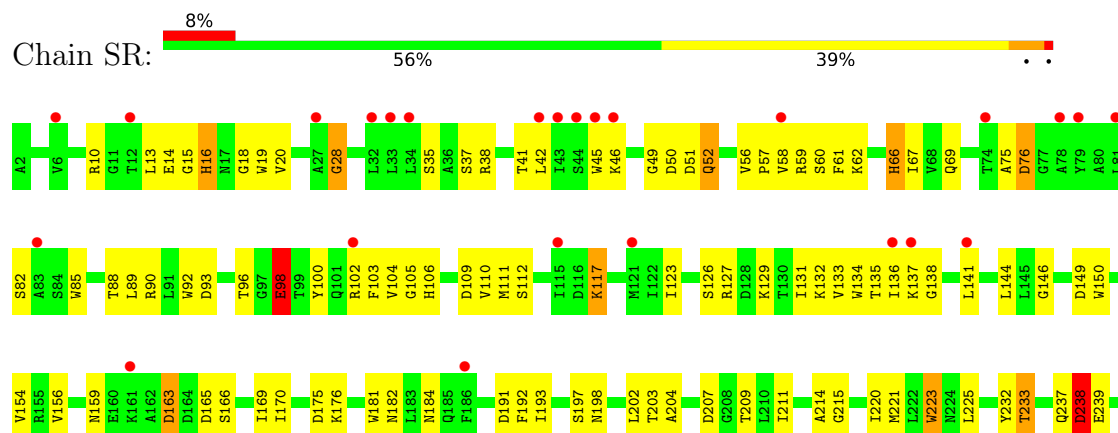
- Molecule 33: Ubiquitin-40S ribosomal protein S31



- Molecule 33: Ubiquitin-40S ribosomal protein S31

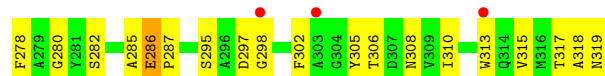
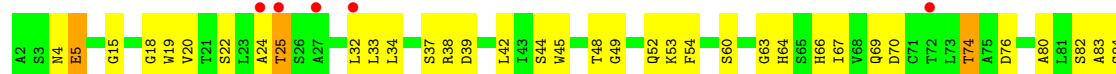


- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

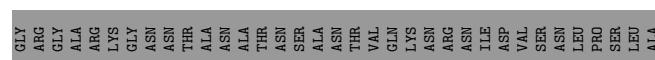
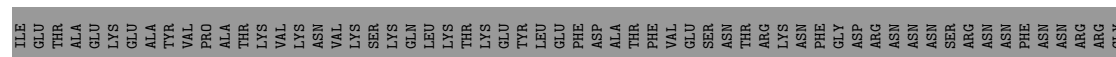
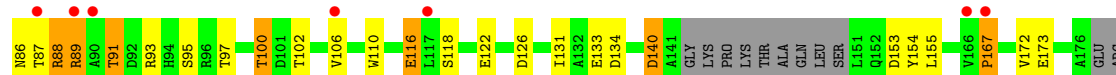
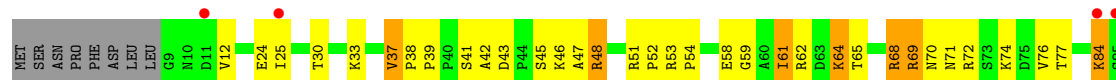
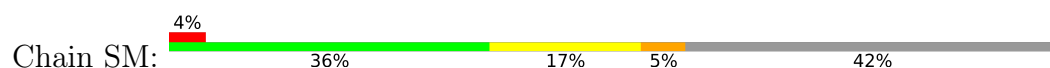




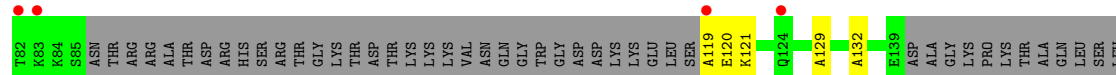
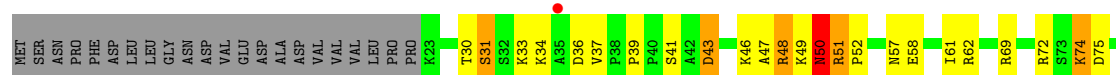
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



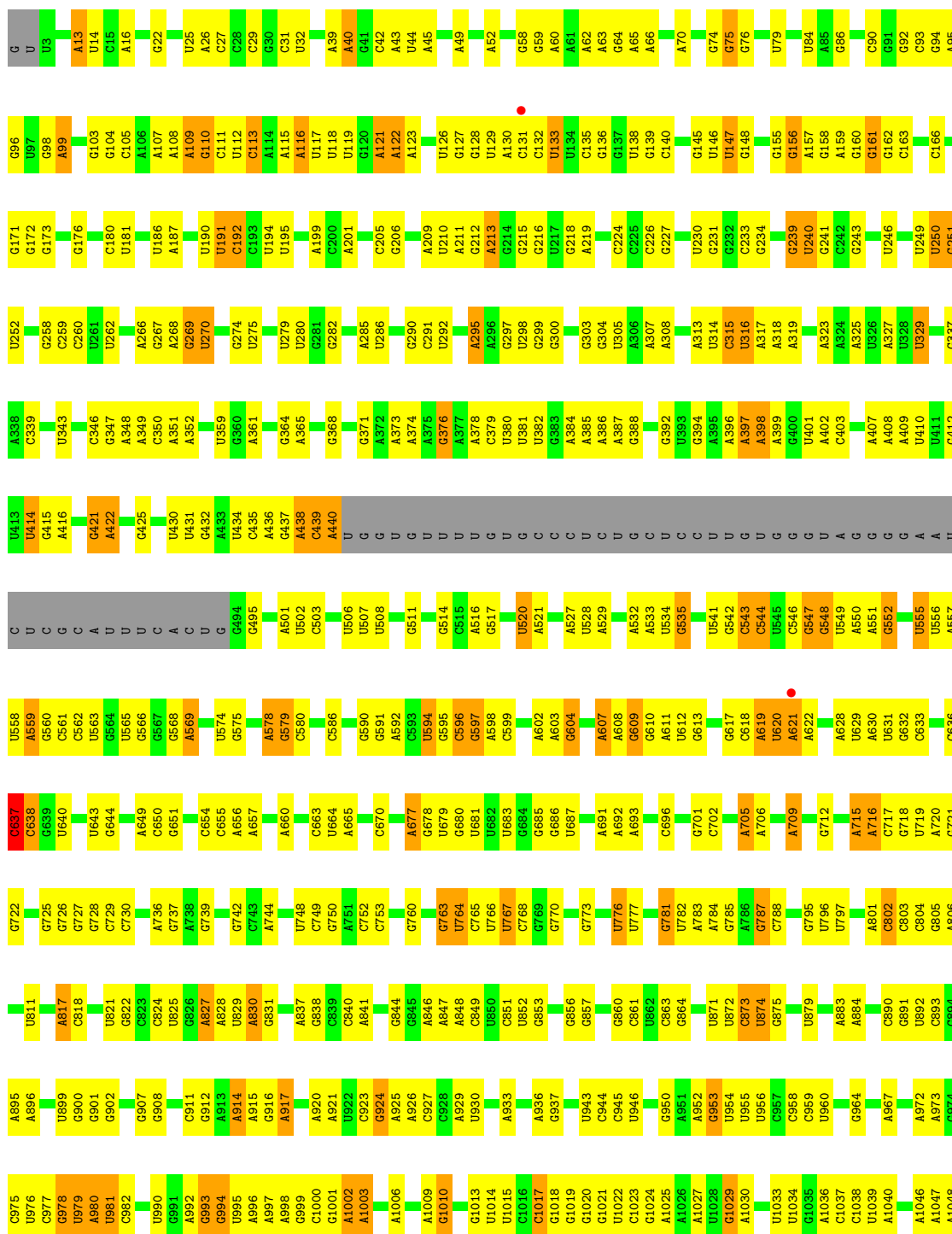
• Molecule 35: Suppressor protein STM1



• Molecule 35: Suppressor protein STM1

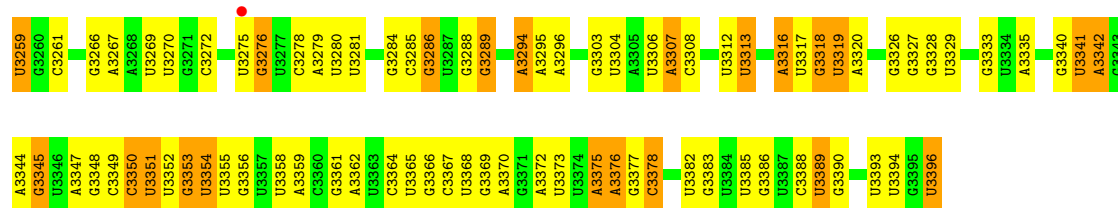


- Molecule 36: 25S ribosomal RNA

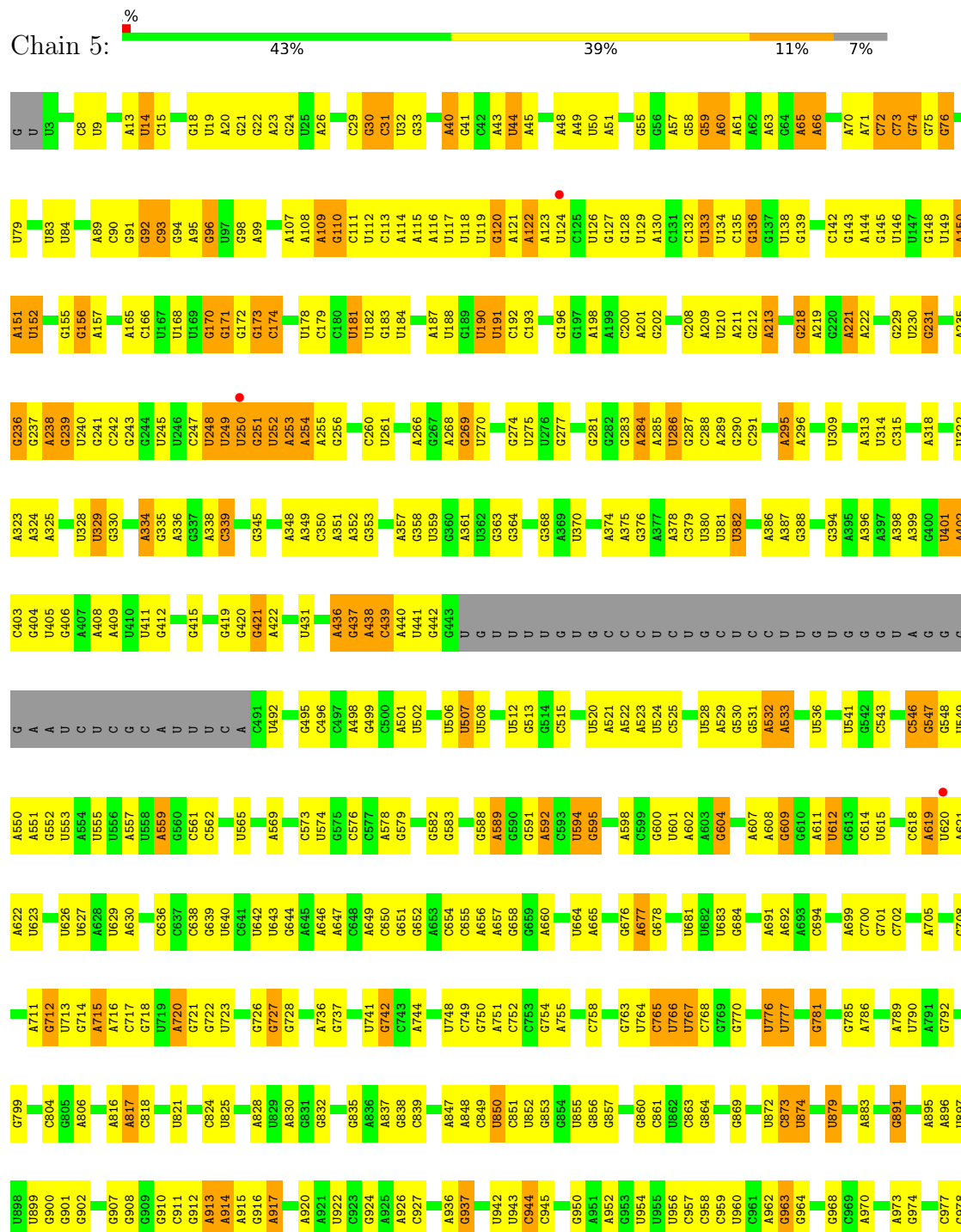




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G3115	A2971	G3043	C2884	A2802	U2883	A2802	U2723	U2655	A2562	U	U2433	A2356	A2271	U2203
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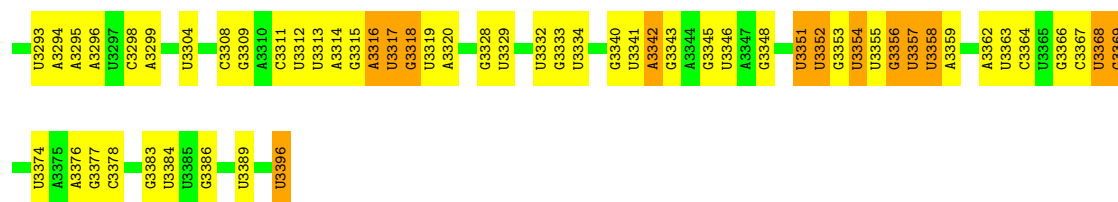


• Molecule 36: 25S ribosomal RNA

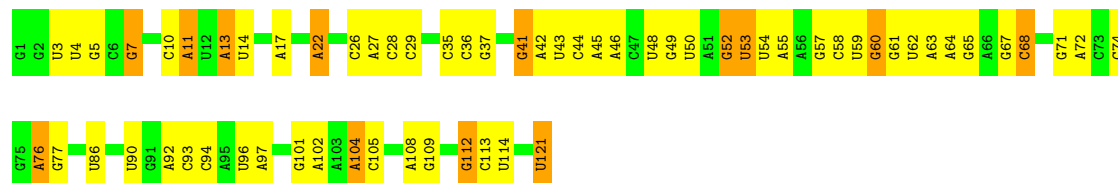


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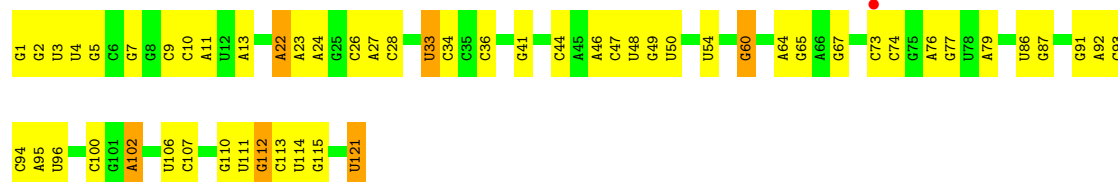
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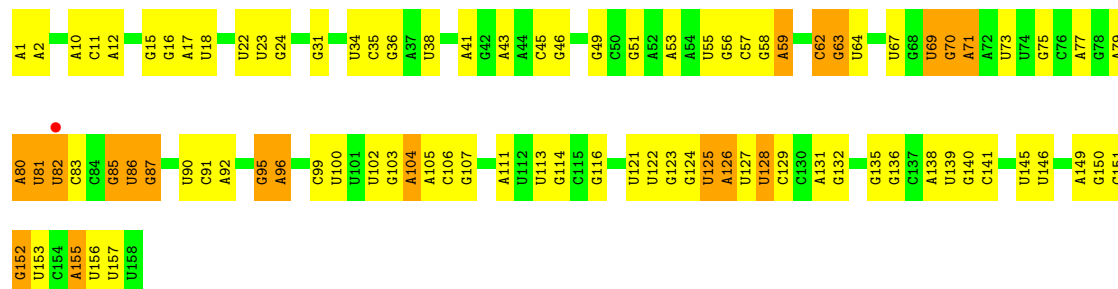
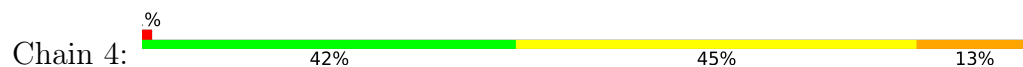
• Molecule 37: 5S ribosomal RNA



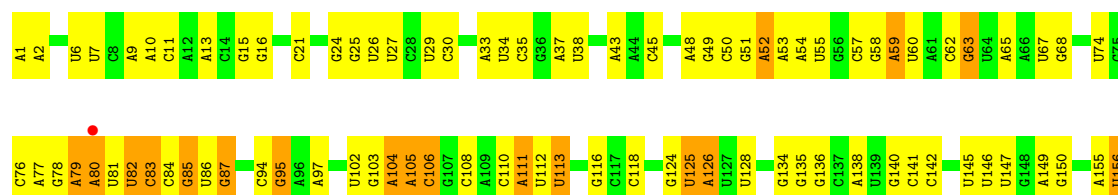
• Molecule 37: 5S ribosomal RNA



• Molecule 38: 5.8S ribosomal RNA

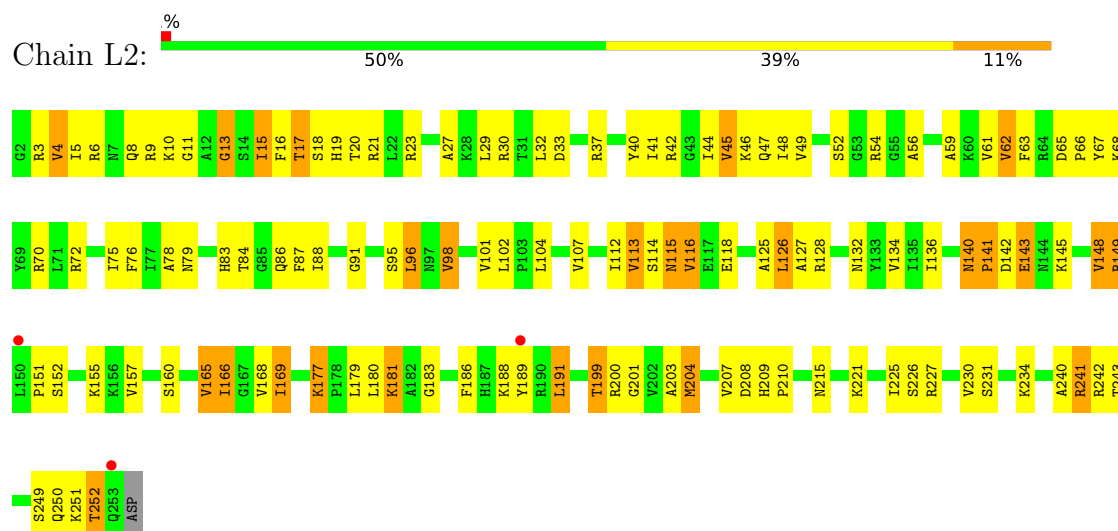


• Molecule 38: 5.8S ribosomal RNA

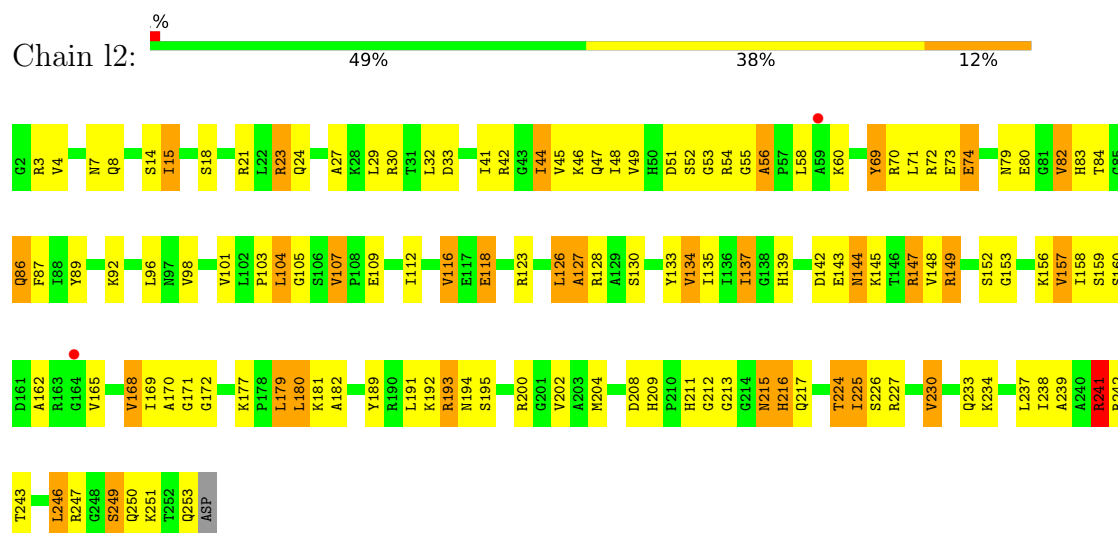


U157
U158

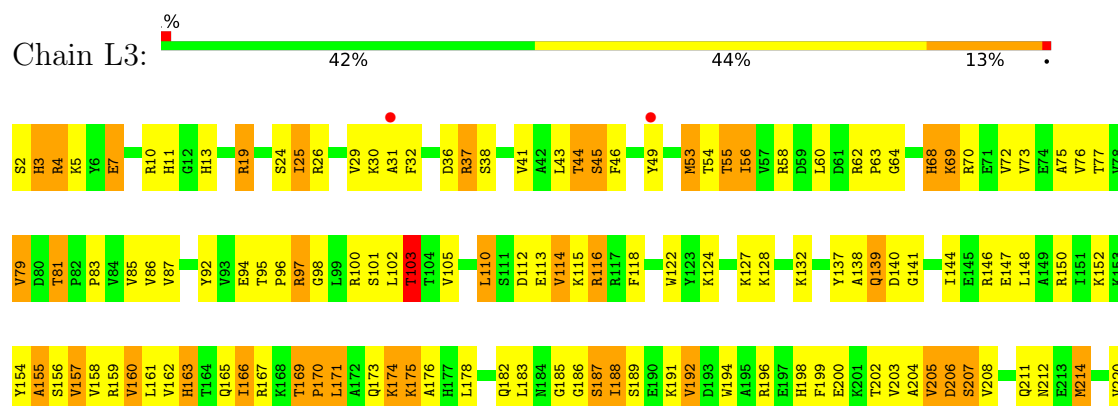
- Molecule 39: 60S ribosomal protein L2-A

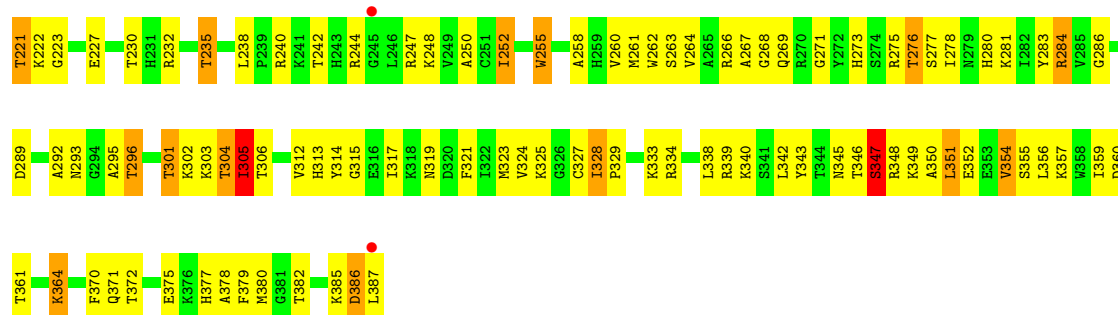


- Molecule 39: 60S ribosomal protein L2-A

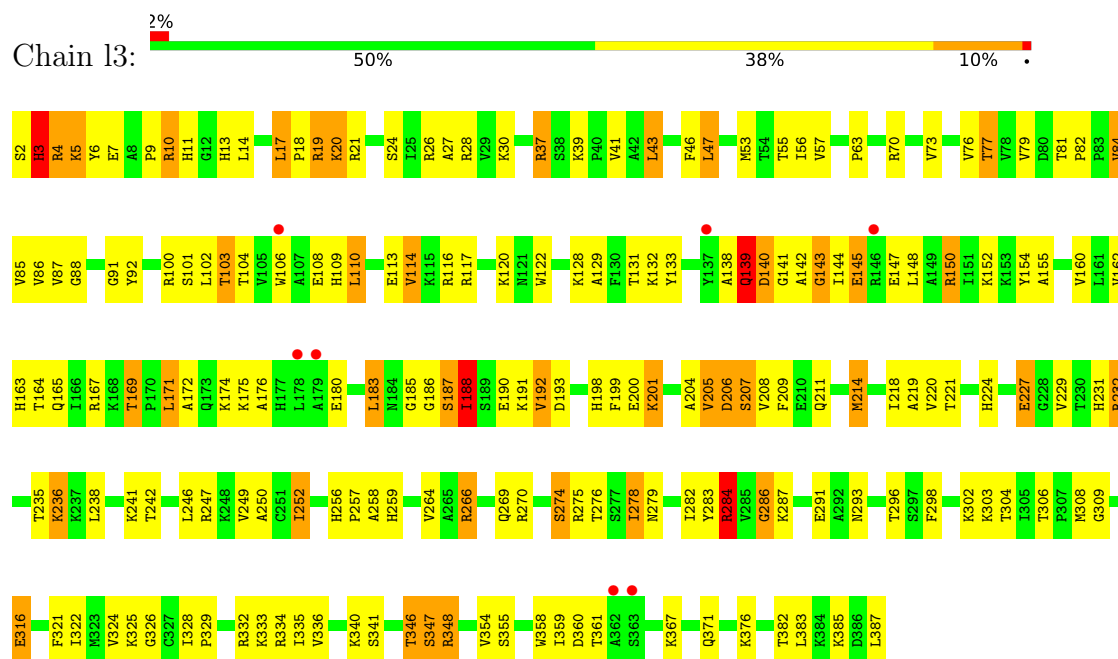


- Molecule 40: 60S ribosomal protein L3

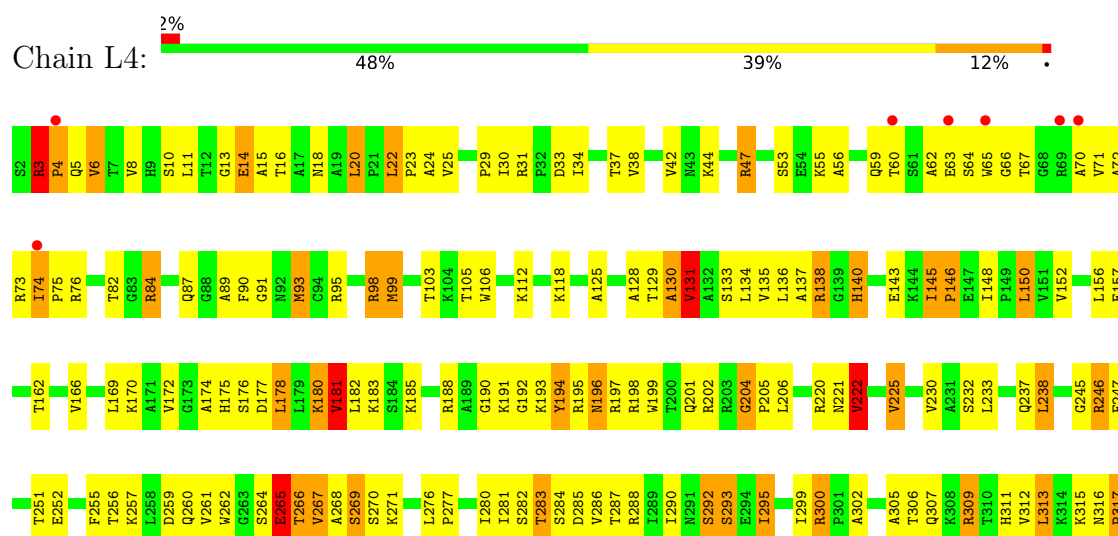


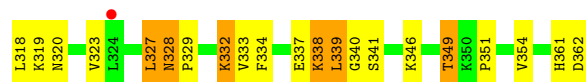


• Molecule 40: 60S ribosomal protein L3

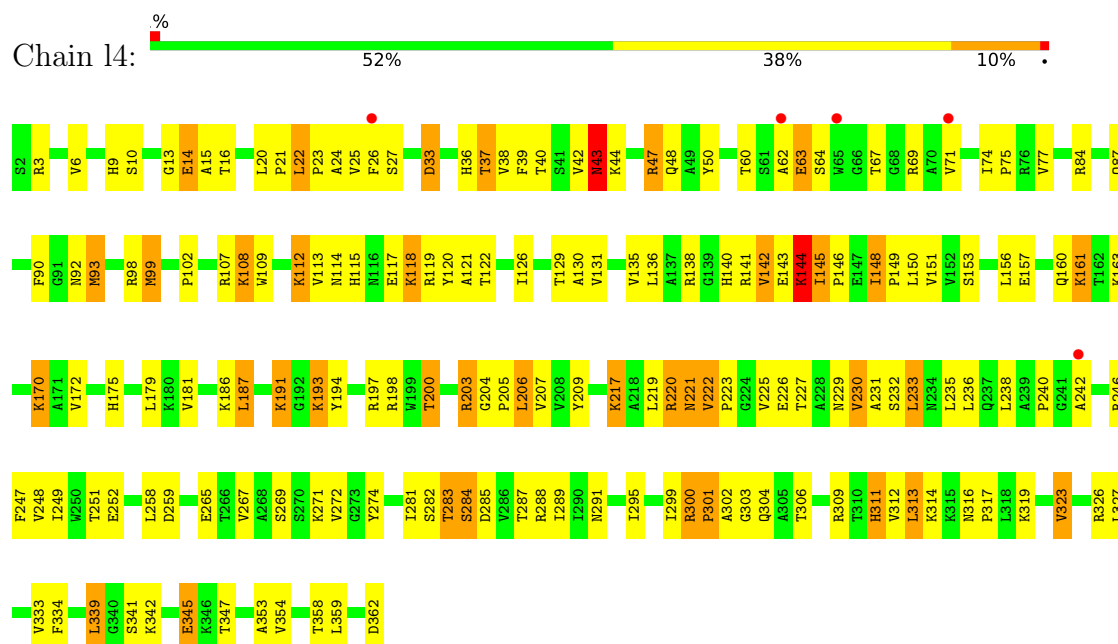


• Molecule 41: 60S ribosomal protein L4-A

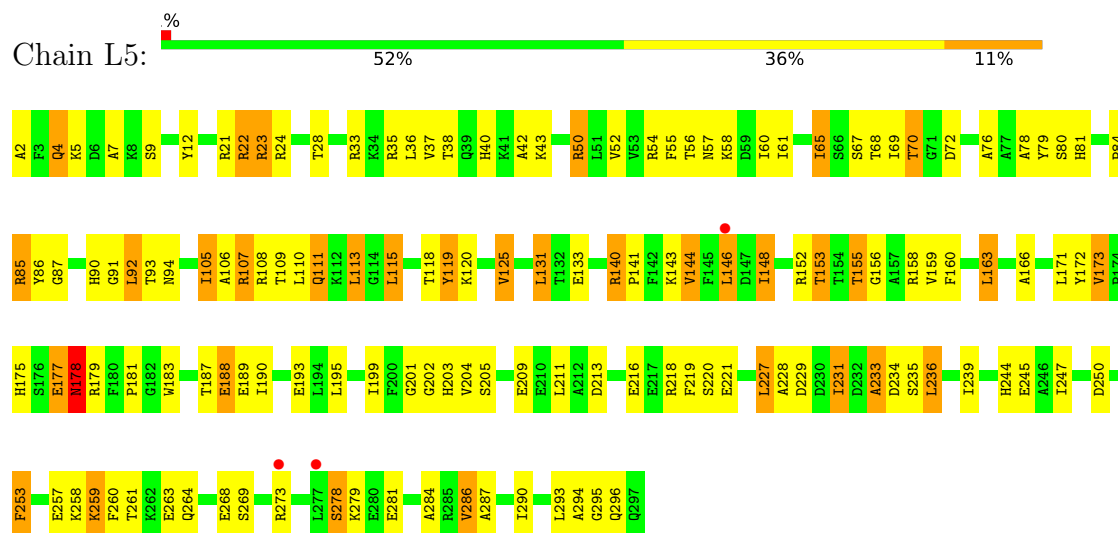




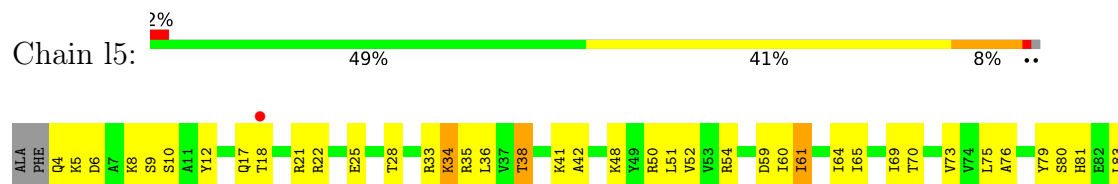
• Molecule 41: 60S ribosomal protein L4-A



• Molecule 42: 60S ribosomal protein L5



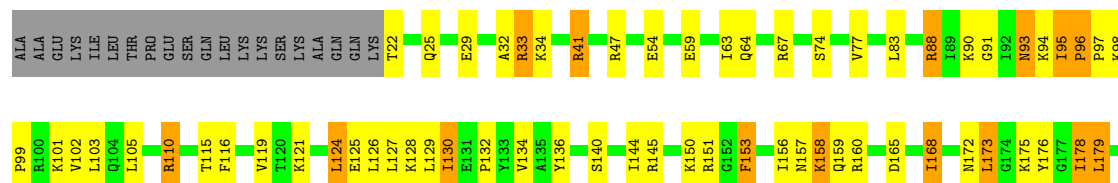
• Molecule 42: 60S ribosomal protein L5





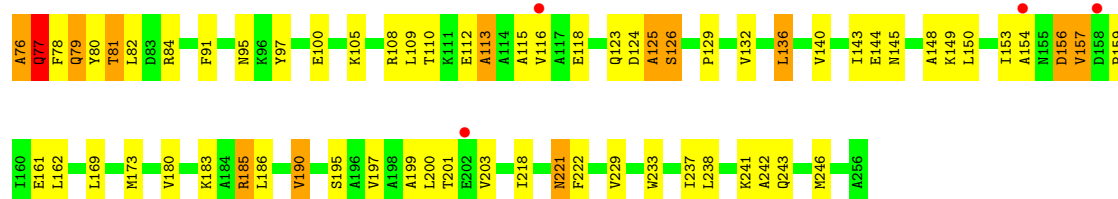
• Molecule 44: 60S ribosomal protein L7-A

Chain 17: 51% 33% 7% 8%



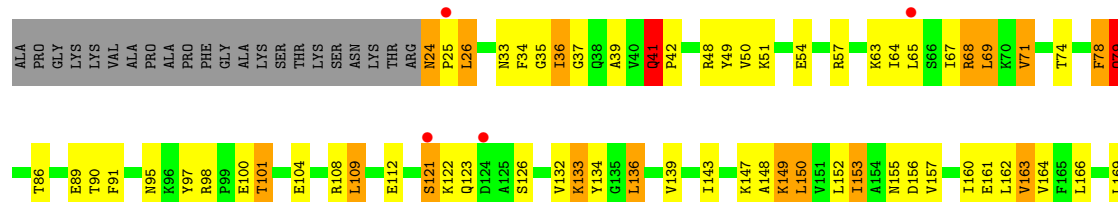
• Molecule 45: 60S ribosomal protein L8-A

Chain L8: 3% 56% 29% 5% 9%

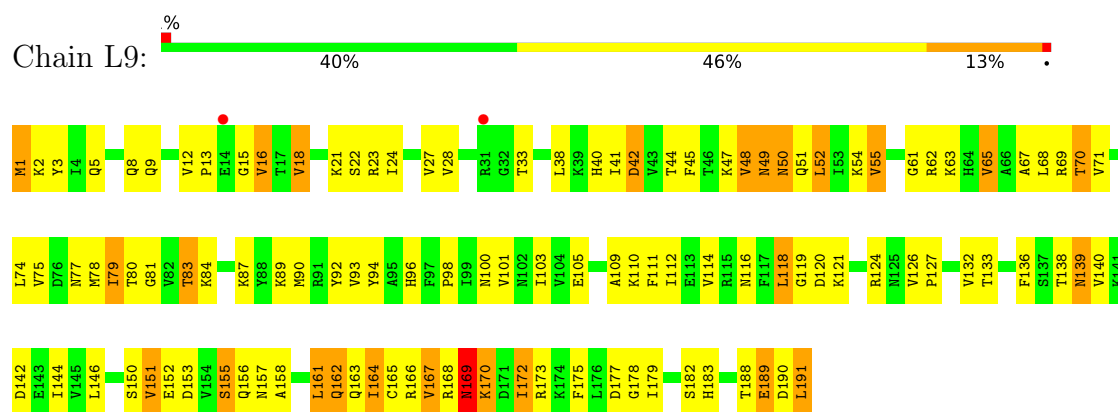


• Molecule 45: 60S ribosomal protein L8-A

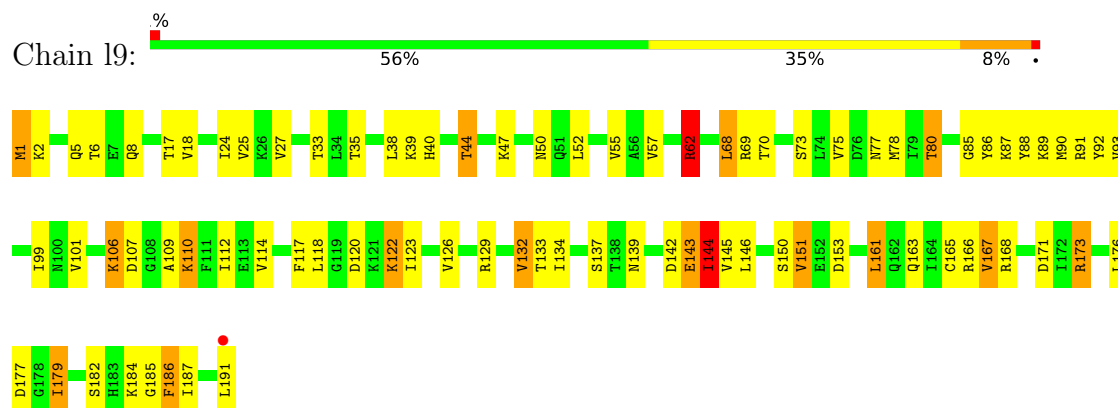
Chain l8: 2% 53% 29% 7% 9%



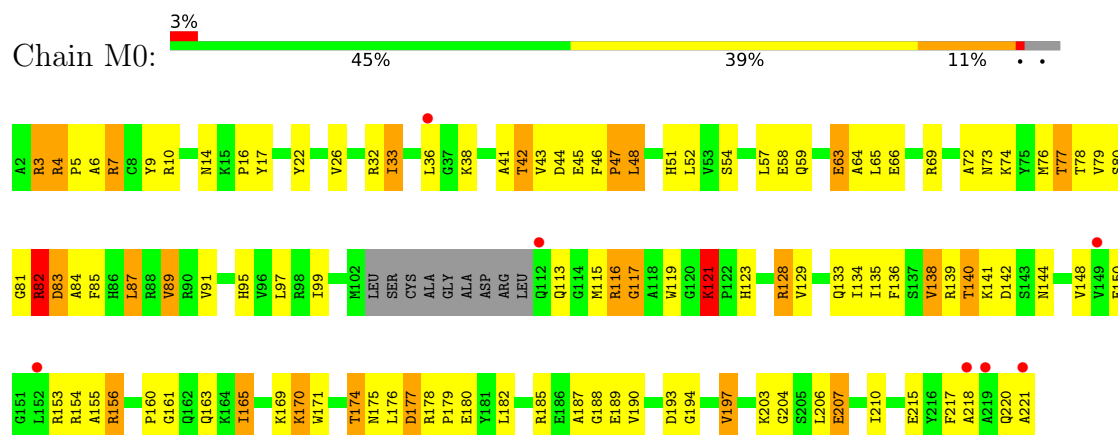
• Molecule 46: 60S ribosomal protein L9-A



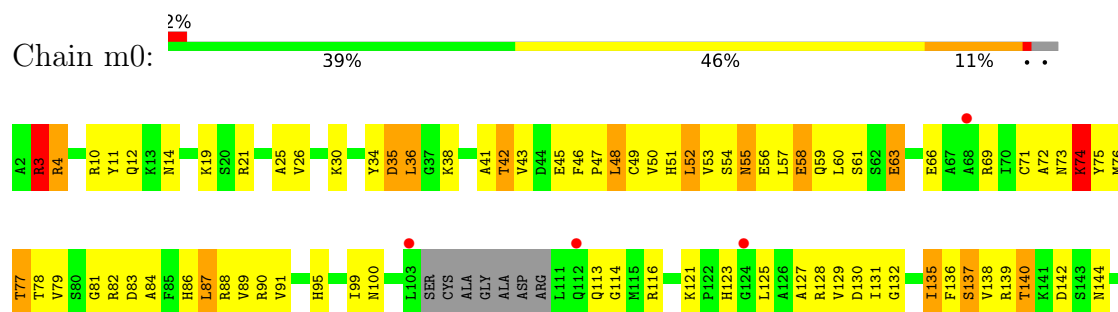
• Molecule 46: 60S ribosomal protein L9-A

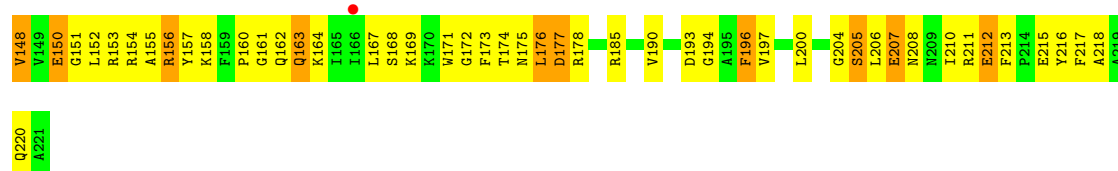


• Molecule 47: 60S ribosomal protein L10

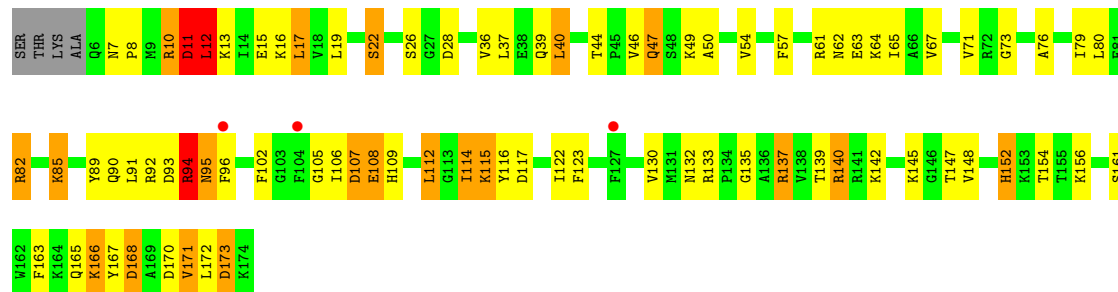


• Molecule 47: 60S ribosomal protein L10

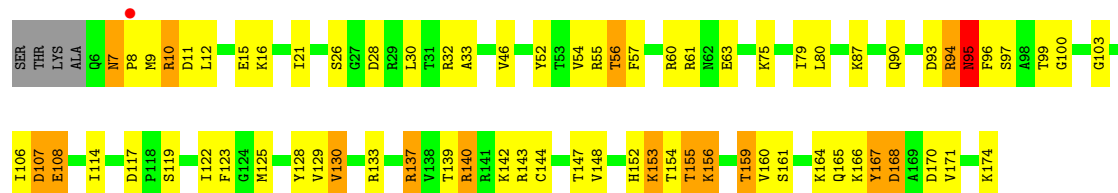




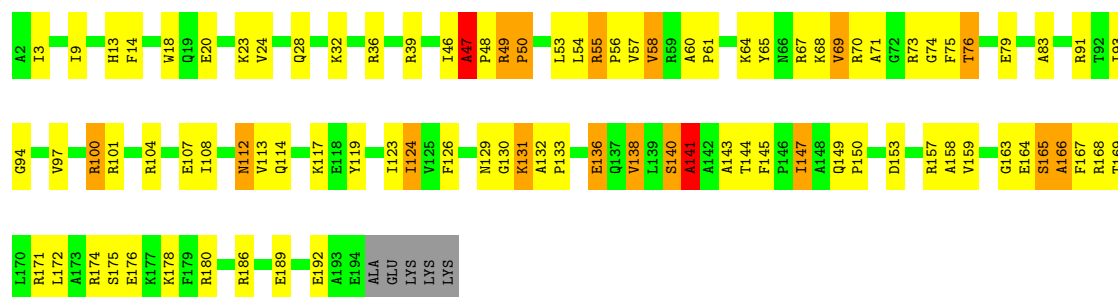
• Molecule 48: 60S ribosomal protein L11-A



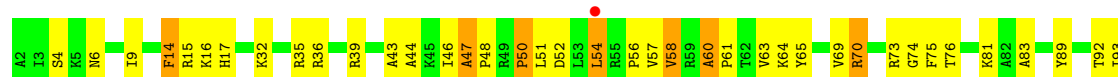
• Molecule 48: 60S ribosomal protein L11-A

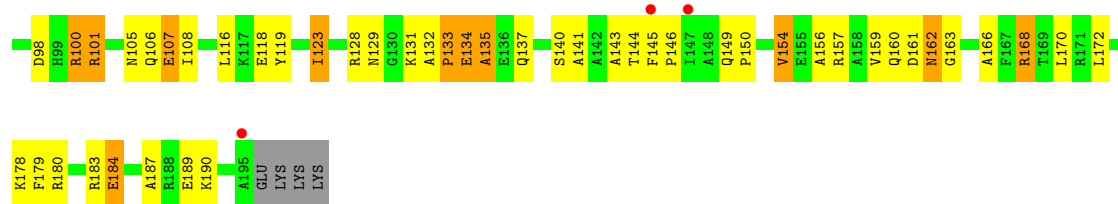


• Molecule 49: 60S ribosomal protein L13-A



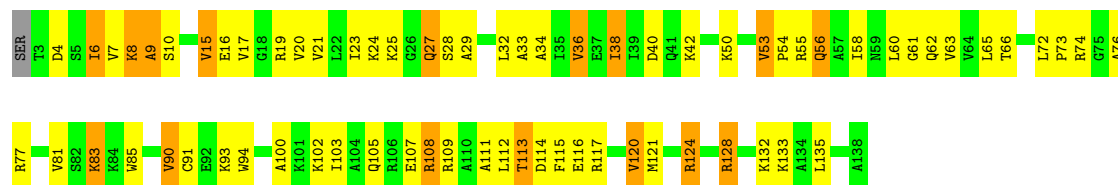
• Molecule 49: 60S ribosomal protein L13-A





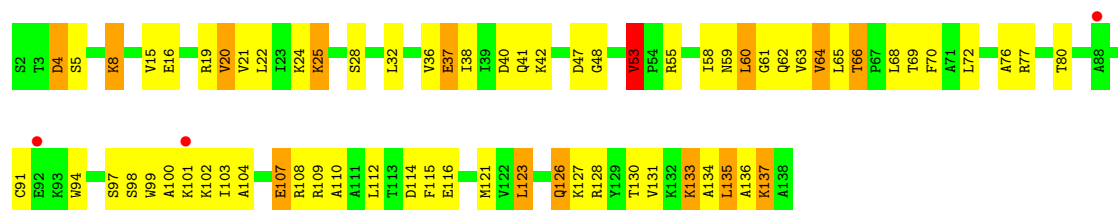
• Molecule 50: 60S ribosomal protein L14-A

Chain M4: 48% 39% 12%



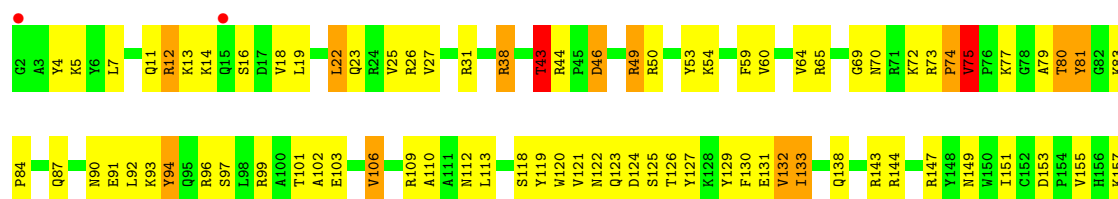
• Molecule 50: 60S ribosomal protein L14-A

Chain m4: 2% 50% 39% 10%



• Molecule 51: 60S ribosomal protein L15-A

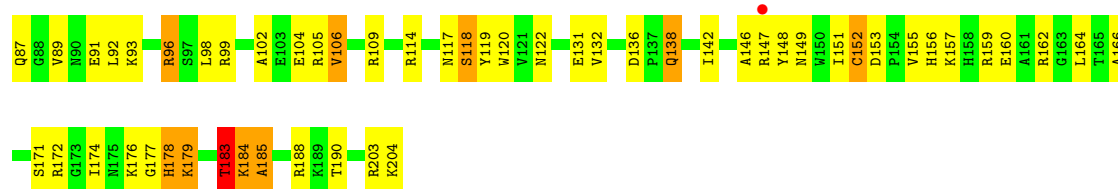
Chain M5: % 50% 42% 7%



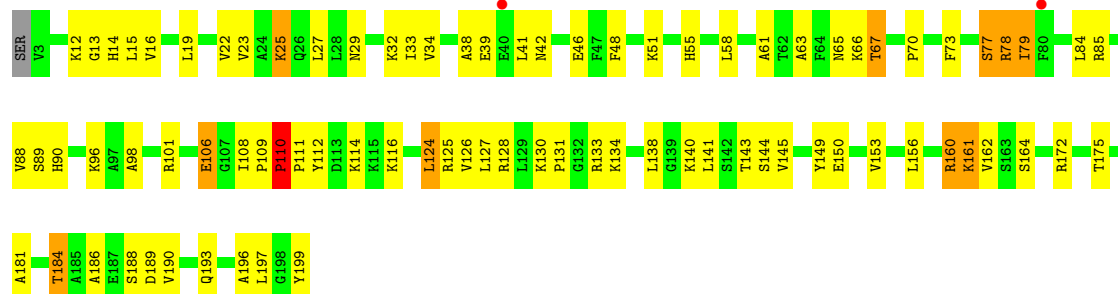
• Molecule 51: 60S ribosomal protein L15-A

Chain m5: % 55% 37% 7%

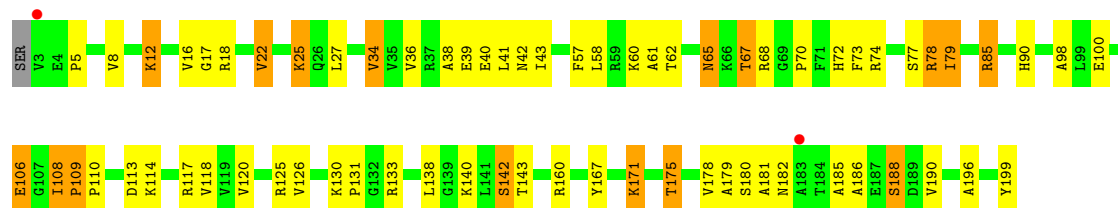




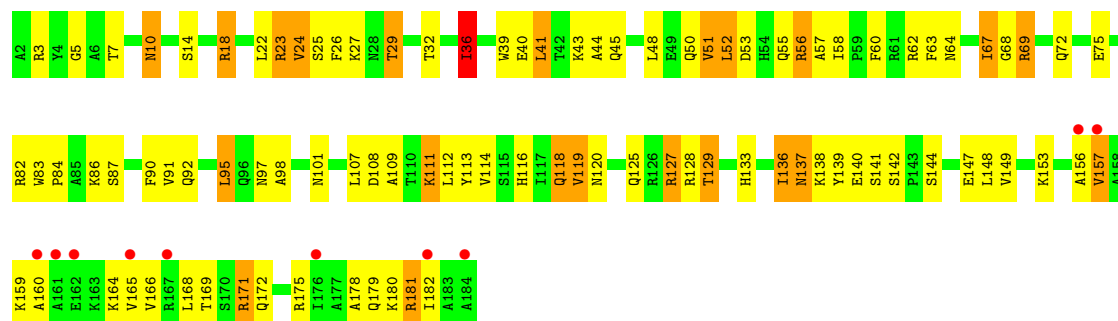
• Molecule 52: 60S ribosomal protein L16-A



• Molecule 52: 60S ribosomal protein L16-A

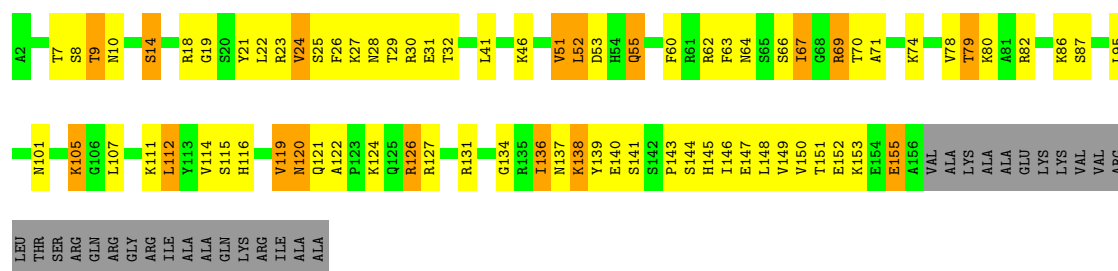


• Molecule 53: 60S ribosomal protein L17-A

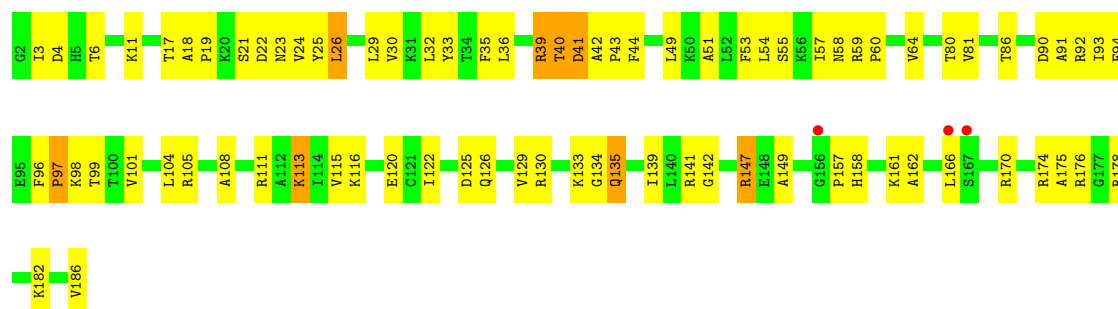


• Molecule 53: 60S ribosomal protein L17-A

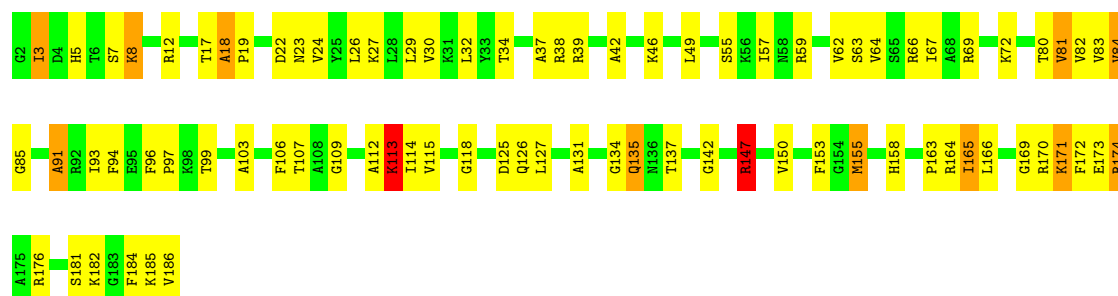




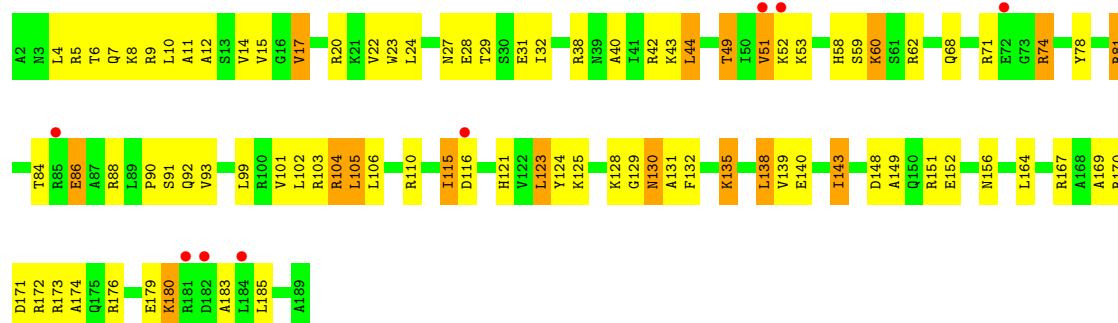
• Molecule 54: 60S ribosomal protein L18-A



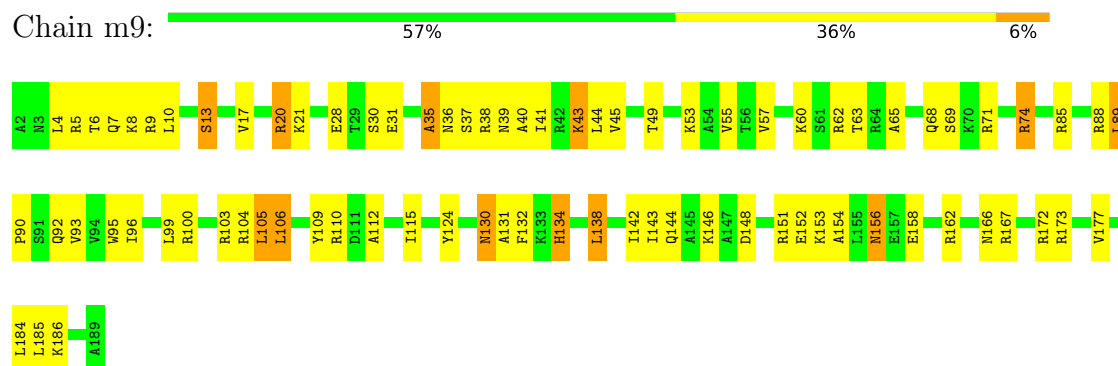
• Molecule 54: 60S ribosomal protein L18-A



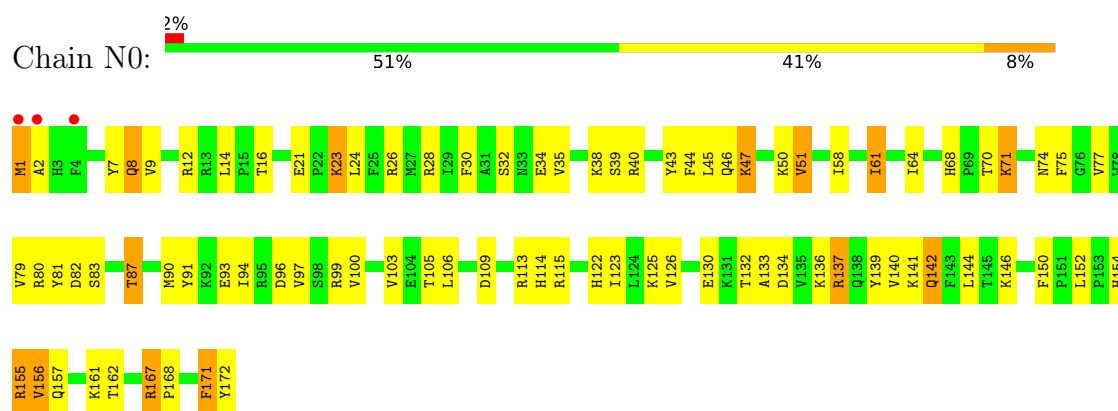
• Molecule 55: 60S ribosomal protein L19-A



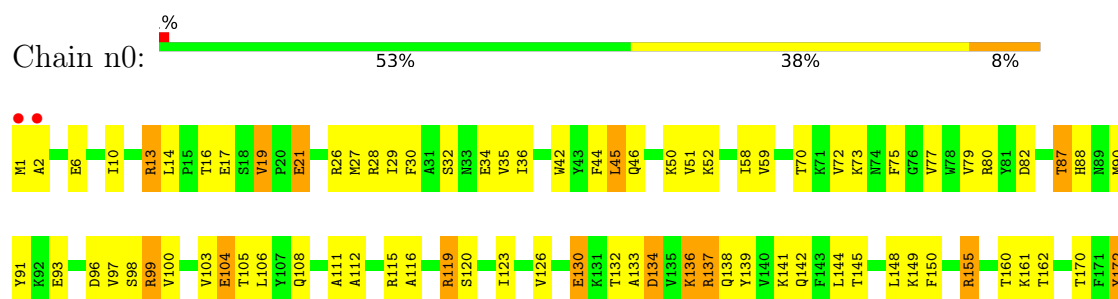
- Molecule 55: 60S ribosomal protein L19-A



- Molecule 56: 60S ribosomal protein L20-A



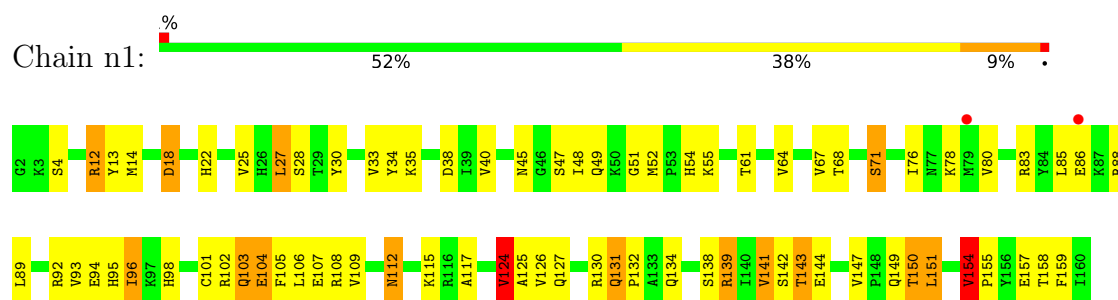
- Molecule 56: 60S ribosomal protein L20-A



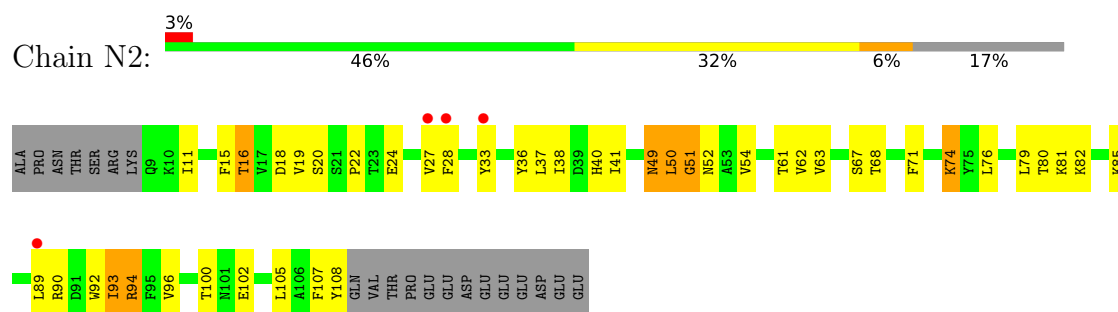
- Molecule 57: 60S ribosomal protein L21-A



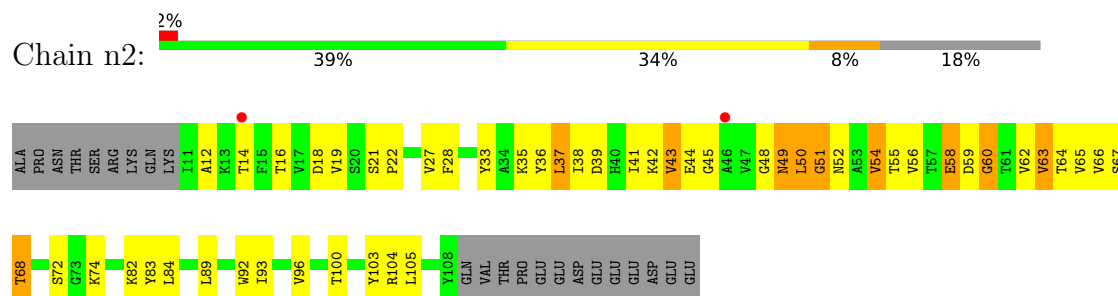
- Molecule 57: 60S ribosomal protein L21-A



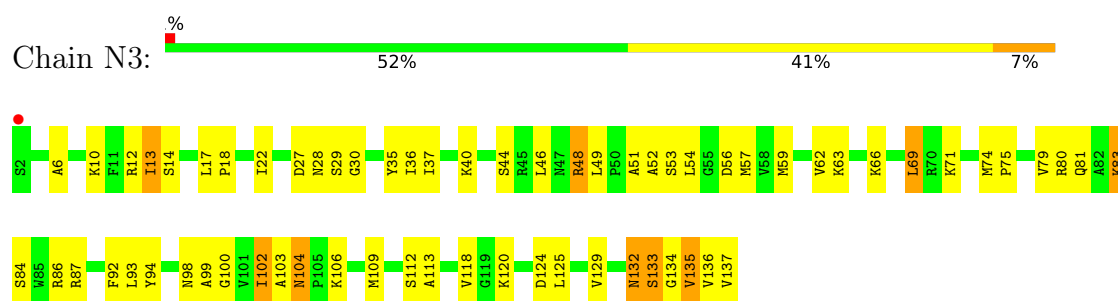
• Molecule 58: 60S ribosomal protein L22-A



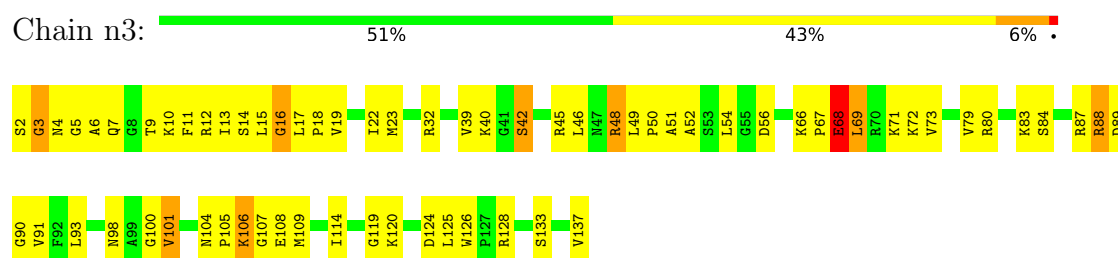
• Molecule 58: 60S ribosomal protein L22-A



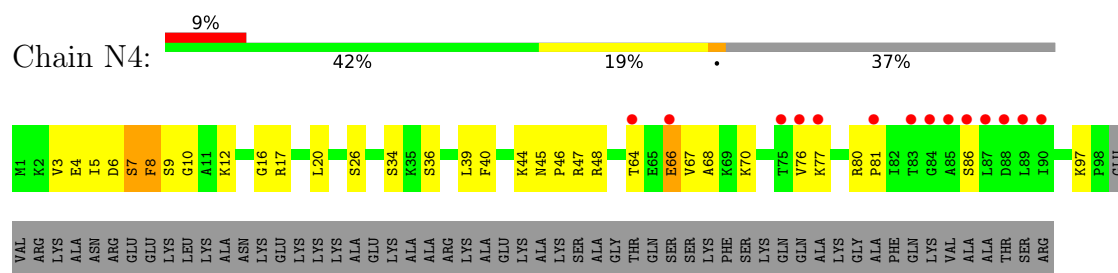
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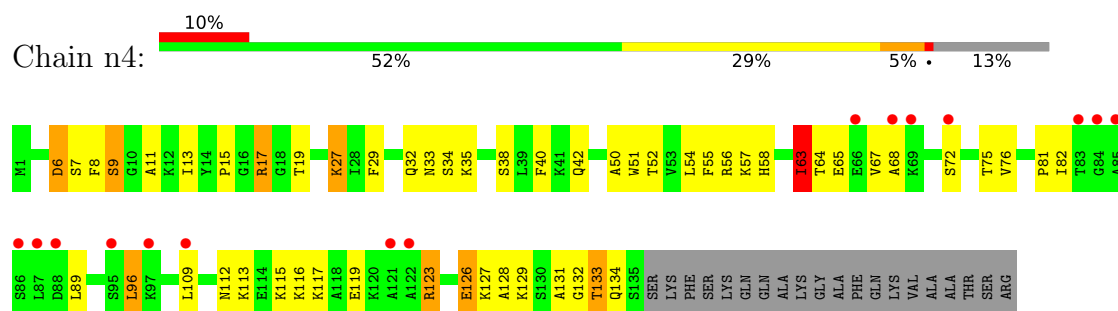
• Molecule 59: 60S ribosomal protein L23-A



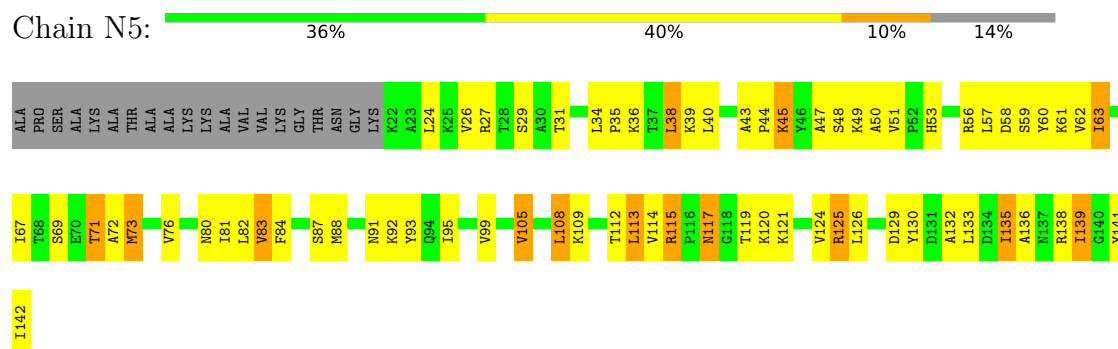
- Molecule 60: 60S ribosomal protein L24-A



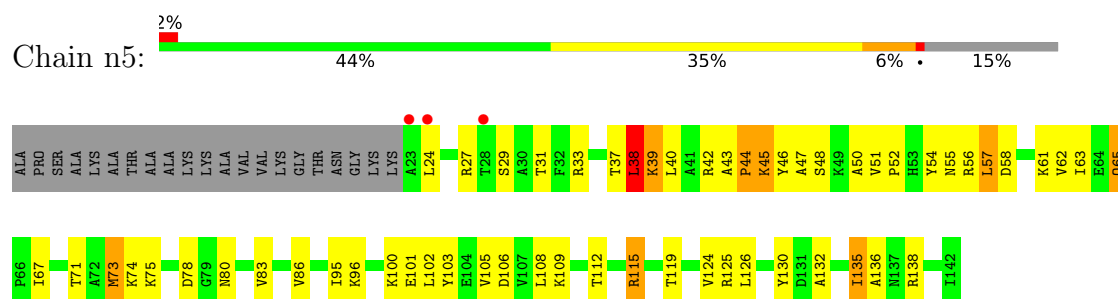
- Molecule 60: 60S ribosomal protein L24-A



- Molecule 61: 60S ribosomal protein L25

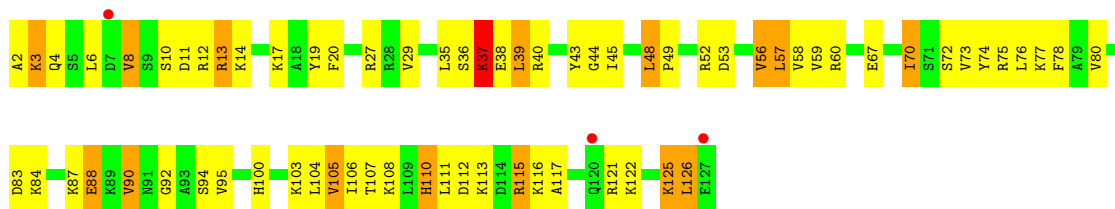


- Molecule 61: 60S ribosomal protein L25

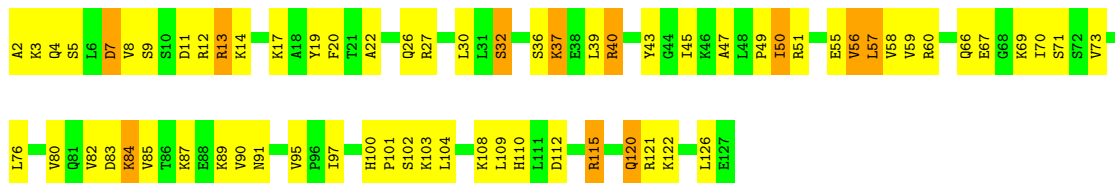


- Molecule 62: 60S ribosomal protein L26-A

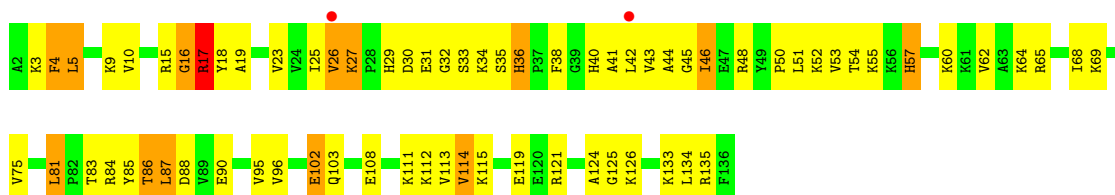




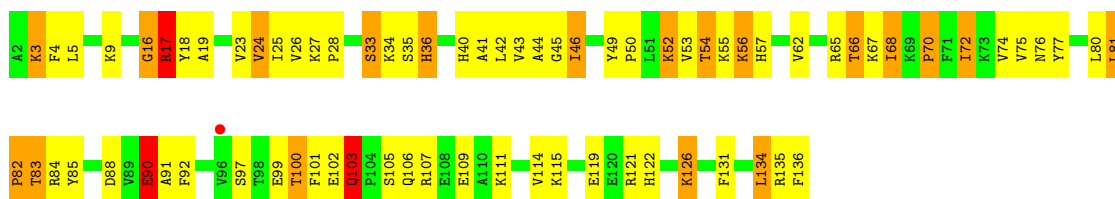
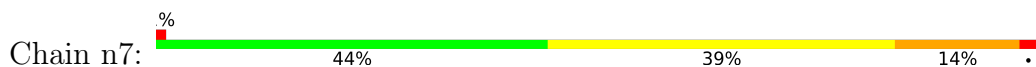
• Molecule 62: 60S ribosomal protein L26-A



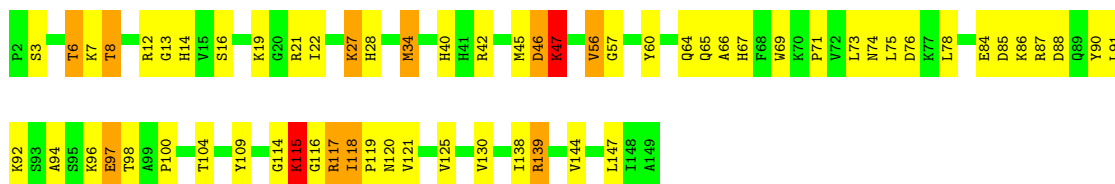
• Molecule 63: 60S ribosomal protein L27-A



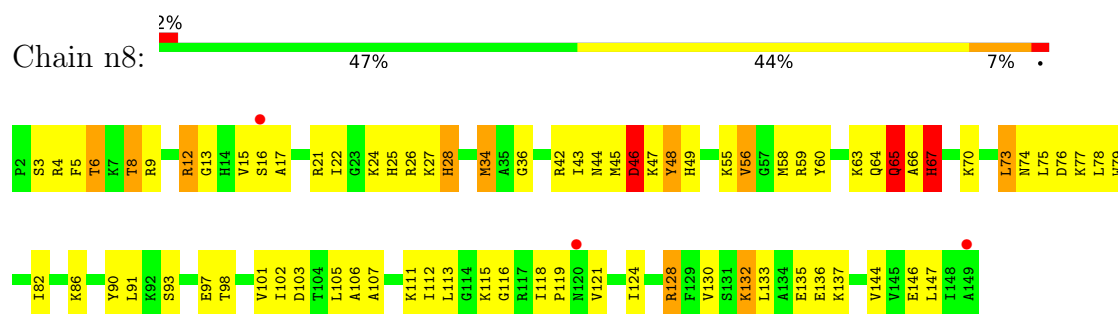
• Molecule 63: 60S ribosomal protein L27-A



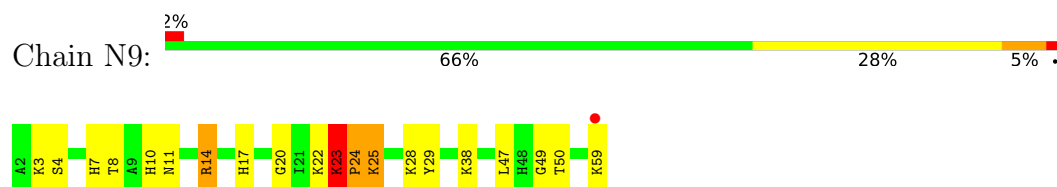
• Molecule 64: 60S ribosomal protein L28



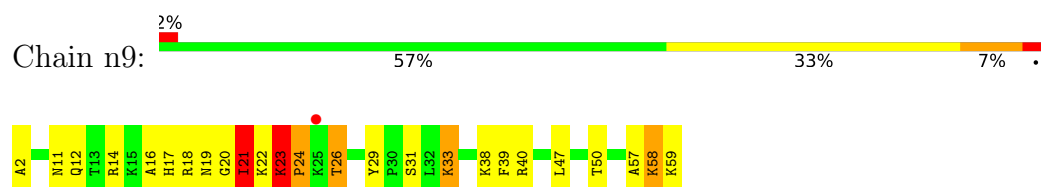
• Molecule 64: 60S ribosomal protein L28



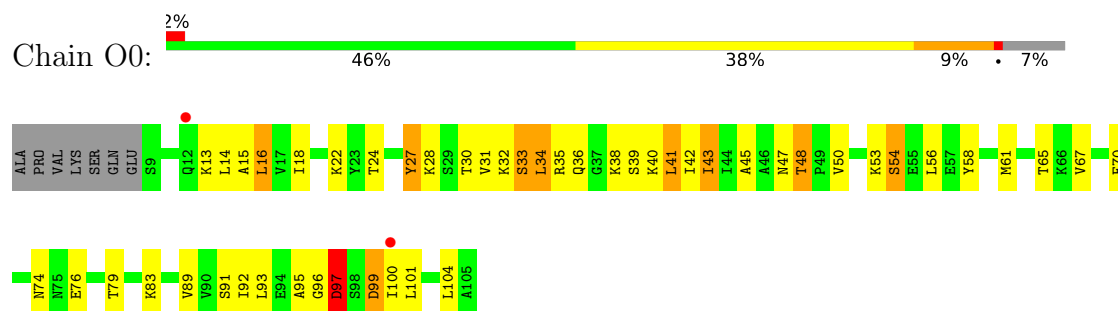
- Molecule 65: 60S ribosomal protein L29



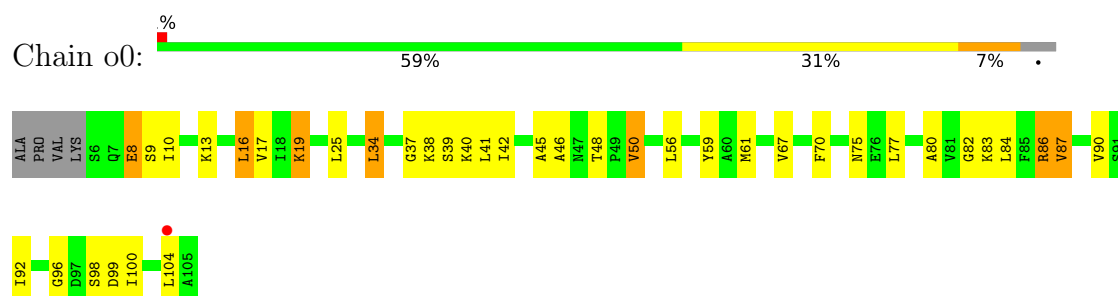
- Molecule 65: 60S ribosomal protein L29



- Molecule 66: 60S ribosomal protein L30

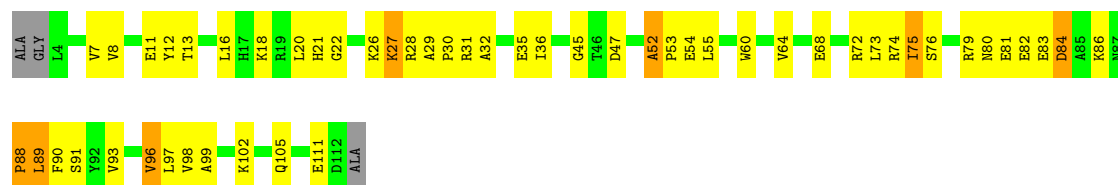


- Molecule 66: 60S ribosomal protein L30



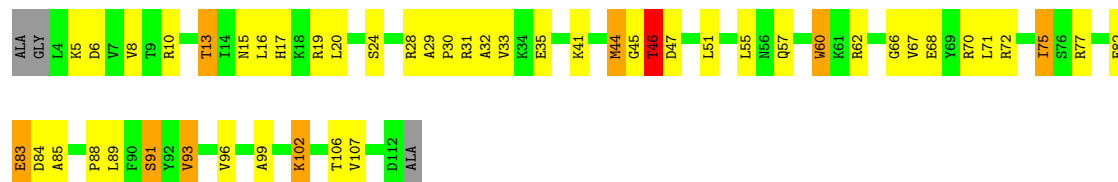
- Molecule 67: 60S ribosomal protein L31-A





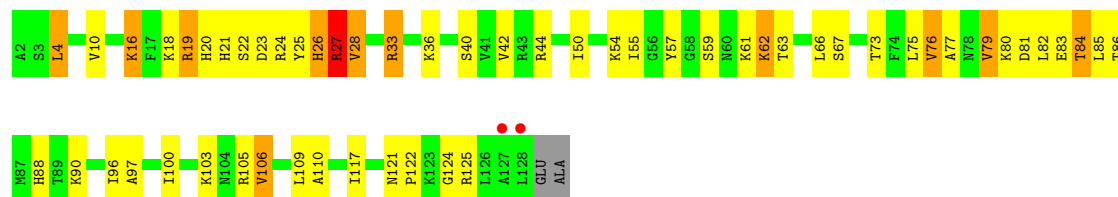
• Molecule 67: 60S ribosomal protein L31-A

Chain o1: 54% 36% 7% ..



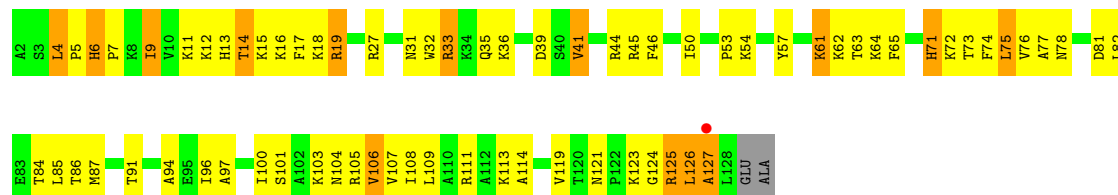
• Molecule 68: 60S ribosomal protein L32

Chain O2: 2% 55% 34% 9% ..



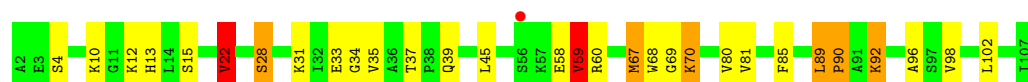
• Molecule 68: 60S ribosomal protein L32

Chain o2: 1% 43% 44% 11% .



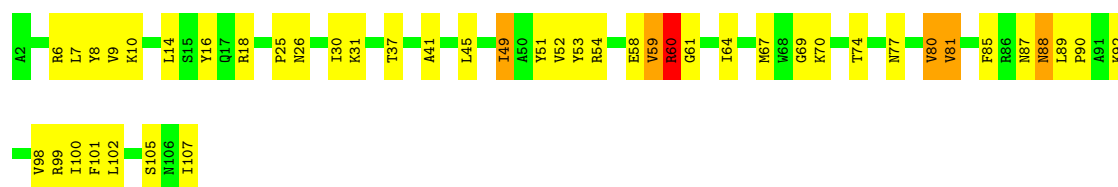
• Molecule 69: 60S ribosomal protein L33-A

Chain O3: 1% 72% 21% 6% .

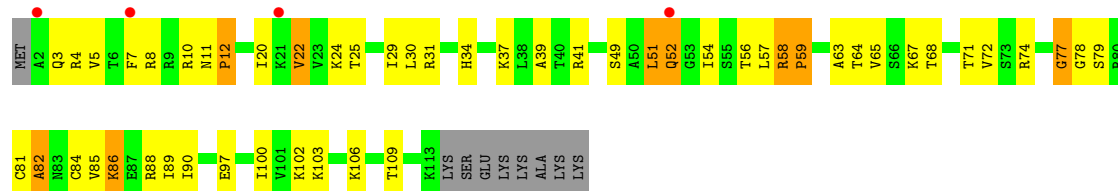


• Molecule 69: 60S ribosomal protein L33-A

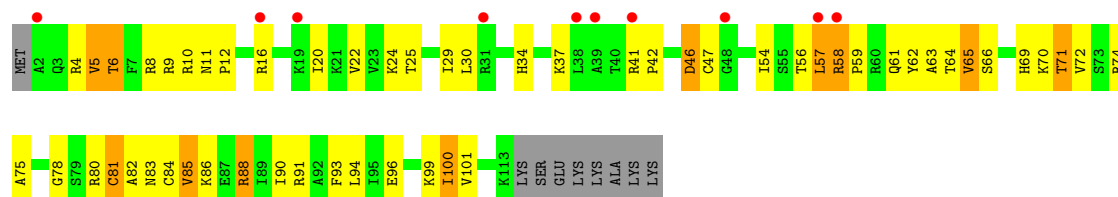
Chain o3: 58% 37% 5% .



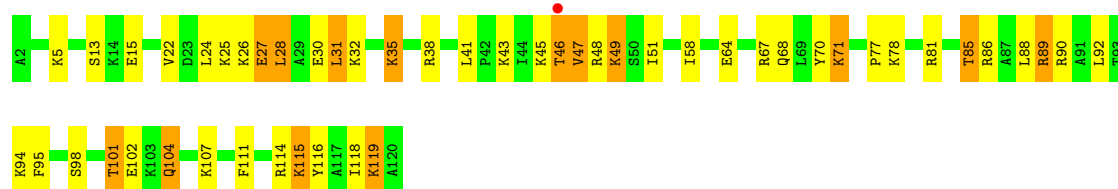
- Molecule 70: 60S ribosomal protein L34-A



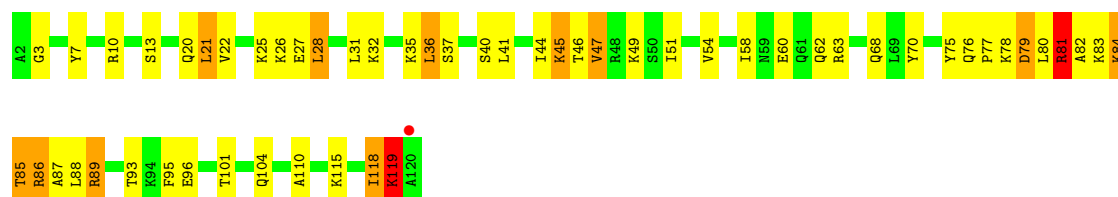
- Molecule 70: 60S ribosomal protein L34-A



- Molecule 71: 60S ribosomal protein L35-A

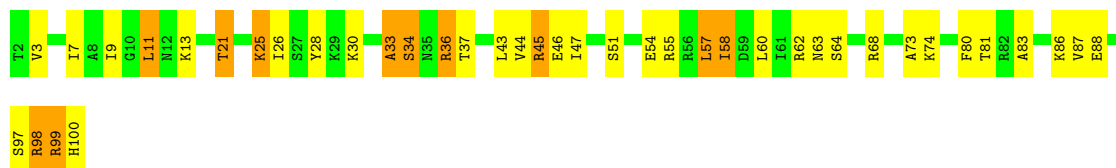


- Molecule 71: 60S ribosomal protein L35-A



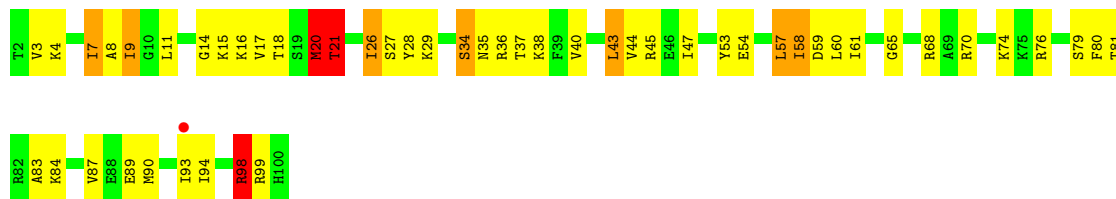
- Molecule 72: 60S ribosomal protein L36-A

Chain O6:  59% 30% 11%



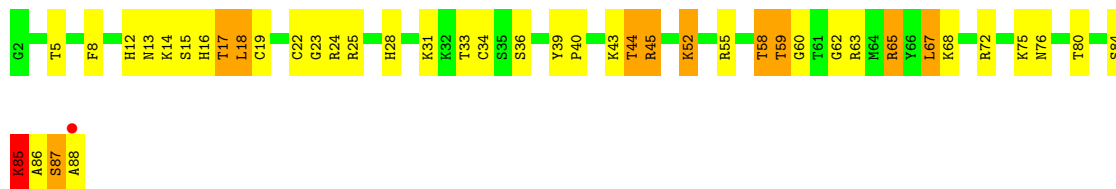
• Molecule 72: 60S ribosomal protein L36-A

Chain o6:  48% 41% 7% .



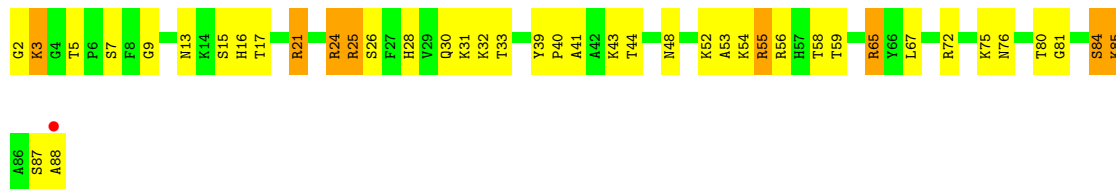
• Molecule 73: 60S ribosomal protein L37-A

Chain O7:  51% 37% 11% .



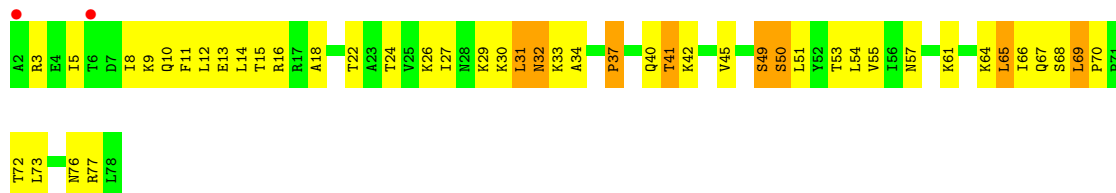
• Molecule 73: 60S ribosomal protein L37-A

Chain o7:  52% 39% 9%

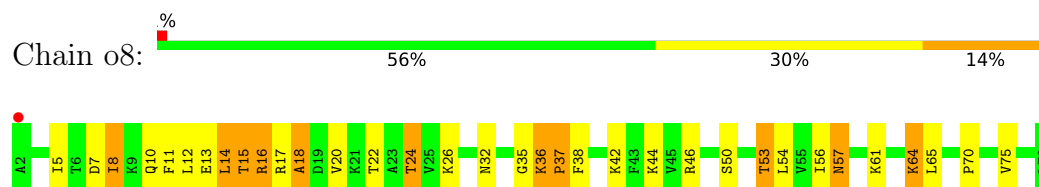


• Molecule 74: 60S ribosomal protein L38

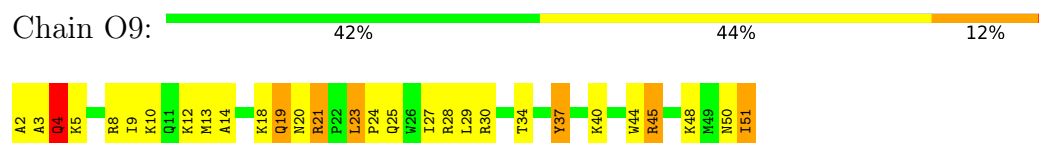
Chain O8:  40% 49% 10% 3%



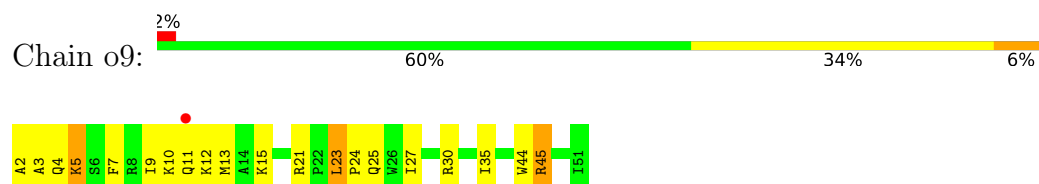
• Molecule 74: 60S ribosomal protein L38



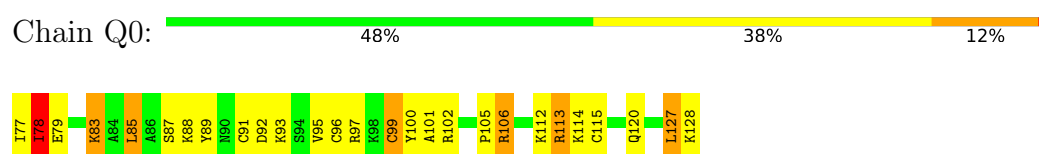
• Molecule 75: 60S ribosomal protein L39



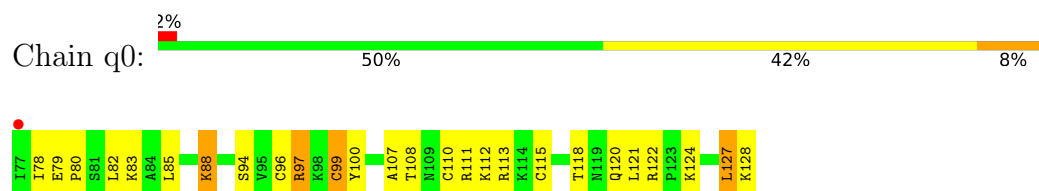
• Molecule 75: 60S ribosomal protein L39



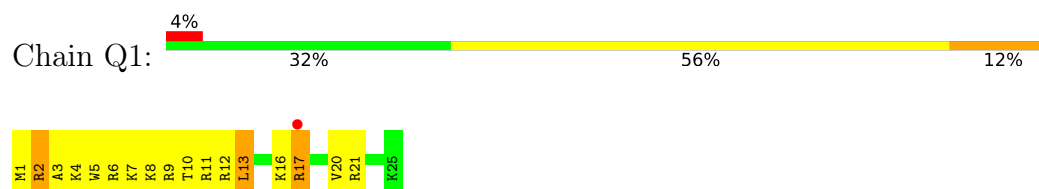
• Molecule 76: Ubiquitin-60S ribosomal protein L40



• Molecule 76: Ubiquitin-60S ribosomal protein L40

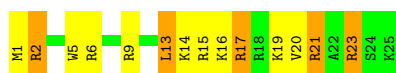


• Molecule 77: 60S ribosomal protein L41-A



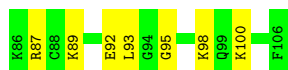
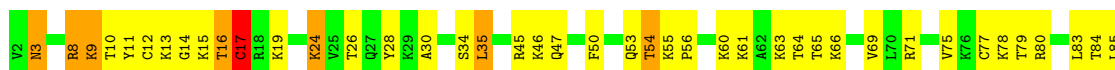
• Molecule 77: 60S ribosomal protein L41-A





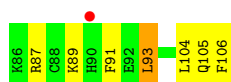
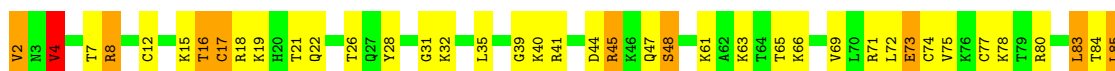
- Molecule 78: 60S ribosomal protein L42-A

Chain Q2: 53% 39% 7% .



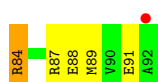
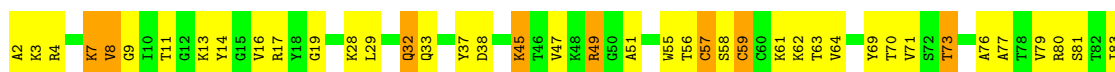
- Molecule 78: 60S ribosomal protein L42-A

Chain q2: % 55% 34% 10% .



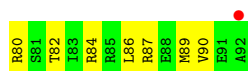
- Molecule 79: 60S ribosomal protein L43-A

Chain Q3: % 49% 41% 10%



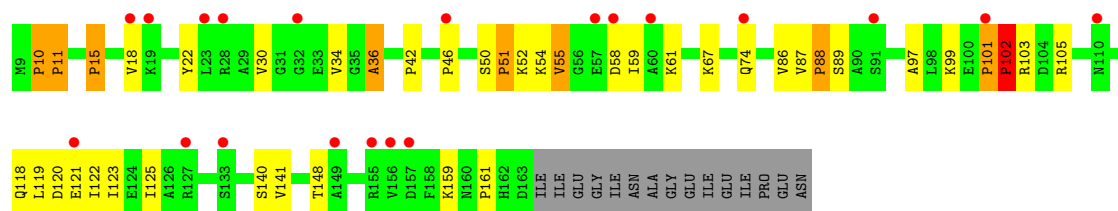
- Molecule 79: 60S ribosomal protein L43-A

Chain q3: % 49% 38% 12%

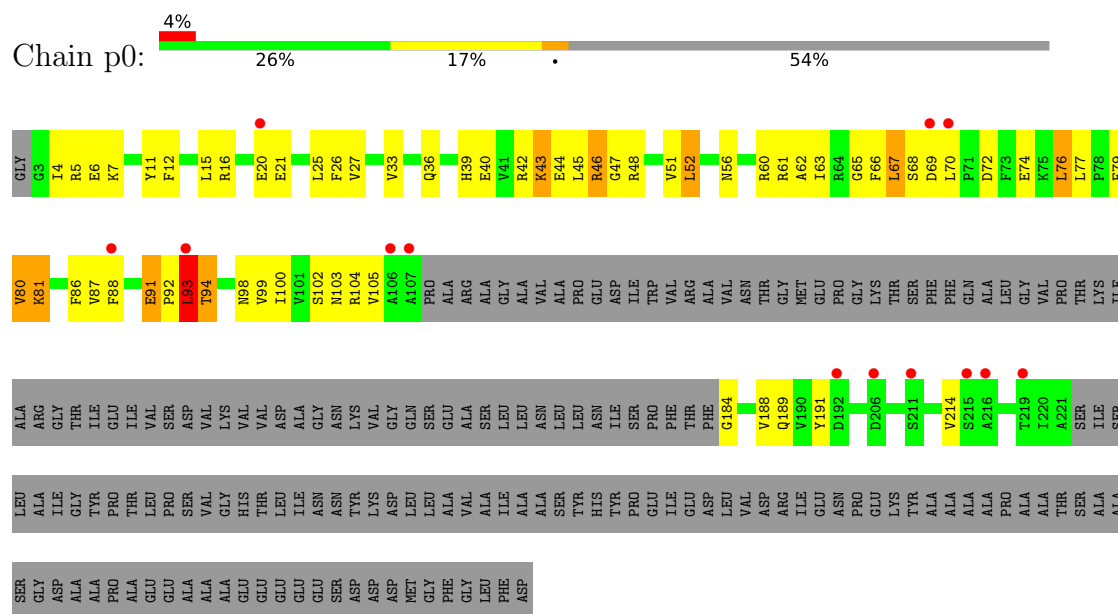


- Molecule 80: 60S ribosomal protein L12-A

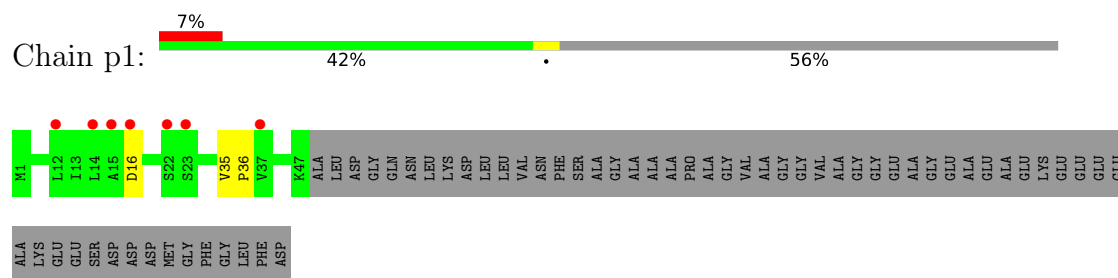
Chain m2: 12% 65% 20% 5% . 9%



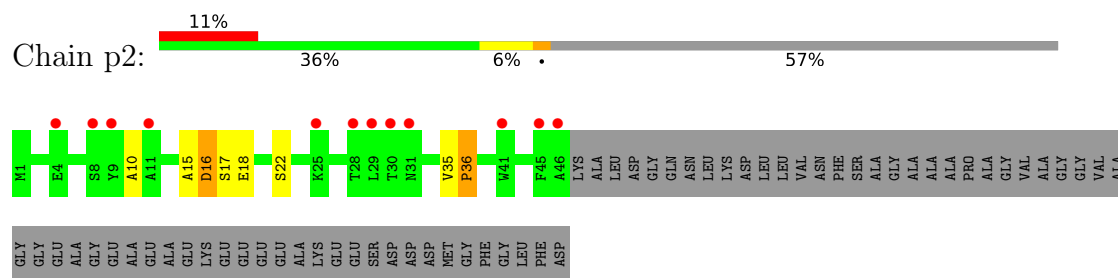
• Molecule 81: 60S acidic ribosomal protein P0



• Molecule 82: 60S acidic ribosomal protein P1-alpha

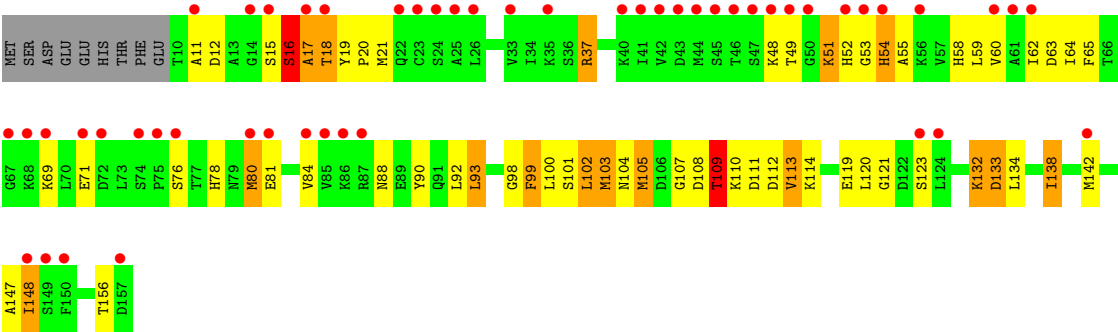


• Molecule 82: 60S acidic ribosomal protein P1-alpha

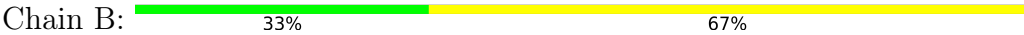


• Molecule 83: Eukaryotic translation initiation factor 5A-1





● Molecule 84: DNA (5'-R(*CP*CP*(NA))-3')



● Molecule 84: DNA (5'-R(*CP*CP*(NA))-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	438.00Å 289.05Å 305.26Å 90.00° 98.95° 90.00°	Depositor
Resolution (Å)	122.88 – 3.45 122.88 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (122.88-3.45) 99.9 (122.88-3.45)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.49Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.207 , 0.263 0.209 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	90.1	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 97.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	413121	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 5CT, 8AN, MG, OHX, SPS

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	0.25	0/42467	0.44	0/66169
1	6	0.30	0/42790	0.48	0/66673
2	S0	0.46	0/1617	0.95	5/2215 (0.2%)
2	s0	0.48	0/1623	0.96	4/2222 (0.2%)
3	S1	0.41	0/1735	0.85	3/2335 (0.1%)
3	s1	0.43	0/1748	0.93	7/2352 (0.3%)
4	S2	0.47	0/1665	0.93	4/2263 (0.2%)
4	s2	0.56	0/1665	1.02	10/2263 (0.4%)
5	S3	0.43	0/1759	0.88	2/2368 (0.1%)
5	s3	0.42	0/1759	0.87	6/2368 (0.3%)
6	S4	0.43	0/2109	0.89	7/2839 (0.2%)
6	s4	0.48	0/2109	0.94	4/2839 (0.1%)
7	S5	0.40	0/1629	0.87	3/2202 (0.1%)
7	s5	0.41	0/1629	0.91	6/2202 (0.3%)
8	S6	0.41	0/1823	0.82	0/2439
8	s6	0.47	0/1779	0.95	6/2379 (0.3%)
9	S7	0.41	0/1506	0.87	5/2028 (0.2%)
9	s7	0.45	0/1516	0.91	3/2043 (0.1%)
10	S8	0.45	0/1514	0.87	0/2021
10	s8	0.54	0/1514	0.96	2/2021 (0.1%)
11	S9	0.40	0/1519	0.85	2/2035 (0.1%)
11	s9	0.47	0/1519	0.95	5/2035 (0.2%)
12	C0	0.42	0/790	0.89	3/1069 (0.3%)
12	c0	0.40	0/777	0.95	4/1049 (0.4%)
13	C1	0.47	0/1240	0.93	2/1675 (0.1%)
13	c1	0.55	0/1194	0.89	1/1610 (0.1%)
14	C2	0.43	0/900	0.82	1/1224 (0.1%)
14	c2	0.35	0/900	0.77	0/1224
15	C3	0.44	0/1215	0.89	3/1638 (0.2%)
15	c3	0.50	0/1215	0.95	2/1638 (0.1%)
16	C4	0.42	0/901	0.88	1/1217 (0.1%)
16	c4	0.47	0/960	0.98	6/1290 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.45	0/998	1.05	10/1341 (0.7%)
17	c5	0.49	0/1060	0.97	4/1426 (0.3%)
18	C6	0.43	0/1125	0.89	3/1510 (0.2%)
18	c6	0.45	0/1131	0.88	3/1518 (0.2%)
19	C7	0.48	0/935	0.98	4/1254 (0.3%)
19	c7	0.42	0/914	0.91	1/1224 (0.1%)
20	C8	0.44	0/1211	0.86	3/1628 (0.2%)
20	c8	0.43	0/1211	0.87	2/1628 (0.1%)
21	C9	0.41	0/1130	0.86	0/1517
21	c9	0.44	0/1130	0.93	2/1517 (0.1%)
22	D0	0.43	0/865	0.90	5/1169 (0.4%)
22	d0	0.44	0/892	0.90	4/1205 (0.3%)
23	D1	0.44	0/693	0.84	0/935
23	d1	0.47	0/693	0.98	4/935 (0.4%)
24	D2	0.45	0/1038	0.92	3/1395 (0.2%)
24	d2	0.52	0/1038	0.96	3/1395 (0.2%)
25	D3	0.50	0/1139	0.90	0/1518
25	d3	0.59	0/1139	0.98	2/1518 (0.1%)
26	D4	0.43	0/1087	0.82	0/1449
26	d4	0.47	0/1087	0.94	0/1449
27	D5	0.46	0/571	0.92	0/768
27	d5	0.43	0/566	0.92	2/761 (0.3%)
28	D6	0.46	0/782	0.87	3/1047 (0.3%)
28	d6	0.51	0/782	0.93	0/1047
29	D7	0.45	0/620	0.96	3/838 (0.4%)
29	d7	0.46	0/620	0.98	4/838 (0.5%)
30	D8	0.37	0/499	0.81	0/670
30	d8	0.44	0/499	0.93	1/670 (0.1%)
31	D9	0.48	0/452	0.91	2/600 (0.3%)
31	d9	0.42	0/452	0.87	0/600
32	E0	0.40	0/483	0.82	0/643
32	e0	0.49	0/499	0.98	3/665 (0.5%)
33	E1	0.49	0/577	0.92	2/770 (0.3%)
33	e1	0.50	0/619	0.94	2/822 (0.2%)
34	SR	0.38	0/2489	0.81	0/3389
34	sR	0.37	0/2494	0.77	0/3395
35	SM	0.54	0/1113	1.03	7/1502 (0.5%)
35	sM	0.49	0/683	0.95	3/923 (0.3%)
36	1	0.36	0/75394	0.54	4/117545 (0.0%)
36	5	0.38	0/75414	0.55	2/117575 (0.0%)
37	3	0.32	0/2883	0.48	0/4491
37	7	0.39	0/2883	0.54	0/4491
38	4	0.34	0/3746	0.49	0/5832

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	8	0.34	0/3746	0.49	0/5832
39	L2	0.57	0/1948	1.02	5/2617 (0.2%)
39	l2	0.60	0/1946	1.01	4/2614 (0.2%)
40	L3	0.56	0/3146	0.97	8/4228 (0.2%)
40	l3	0.65	0/3146	0.98	7/4228 (0.2%)
41	L4	0.60	0/2800	1.07	18/3790 (0.5%)
41	l4	0.60	0/2800	1.05	12/3790 (0.3%)
42	L5	0.47	0/2425	0.89	5/3271 (0.2%)
42	l5	0.59	0/2408	0.99	10/3248 (0.3%)
43	L6	0.57	0/1260	0.95	4/1694 (0.2%)
43	l6	0.56	0/1269	0.90	1/1705 (0.1%)
44	L7	0.61	0/1821	0.99	5/2451 (0.2%)
44	l7	0.62	0/1828	1.03	8/2461 (0.3%)
45	L8	0.47	0/1836	0.94	6/2481 (0.2%)
45	l8	0.49	0/1796	0.93	8/2431 (0.3%)
46	L9	0.53	0/1539	0.94	1/2073 (0.0%)
46	l9	0.63	0/1539	0.95	0/2073
47	M0	0.55	0/1741	0.93	4/2335 (0.2%)
47	m0	0.63	0/1758	0.97	2/2358 (0.1%)
48	M1	0.47	0/1374	0.90	2/1842 (0.1%)
48	m1	0.55	0/1374	0.95	1/1842 (0.1%)
49	M3	0.56	0/1568	1.04	11/2106 (0.5%)
49	m3	0.57	0/1573	1.02	4/2113 (0.2%)
50	M4	0.57	0/1068	0.96	3/1438 (0.2%)
50	m4	0.62	0/1074	0.97	2/1446 (0.1%)
51	M5	0.56	0/1757	0.91	6/2354 (0.3%)
51	m5	0.54	0/1757	0.94	4/2354 (0.2%)
52	M6	0.70	0/1585	0.94	4/2128 (0.2%)
52	m6	0.80	0/1585	0.97	8/2128 (0.4%)
53	M7	0.62	0/1443	0.98	4/1944 (0.2%)
53	m7	0.67	0/1250	1.02	5/1683 (0.3%)
54	M8	0.62	0/1465	1.03	5/1965 (0.3%)
54	m8	0.60	0/1465	1.04	6/1965 (0.3%)
55	M9	0.47	0/1538	0.86	1/2050 (0.0%)
55	m9	0.54	0/1538	0.90	3/2050 (0.1%)
56	N0	0.57	0/1481	0.91	4/1990 (0.2%)
56	n0	0.64	0/1481	1.03	4/1990 (0.2%)
57	N1	0.55	0/1300	0.93	0/1743
57	n1	0.62	0/1300	0.98	7/1743 (0.4%)
58	N2	0.41	0/812	0.87	0/1099
58	n2	0.43	0/794	0.90	2/1076 (0.2%)
59	N3	0.59	0/1018	0.93	1/1369 (0.1%)
59	n3	0.68	0/1018	1.02	1/1369 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	N4	0.48	0/712	0.99	3/958 (0.3%)
60	n4	0.57	0/1052	0.96	0/1398
61	N5	0.51	0/979	0.90	2/1321 (0.2%)
61	n5	0.52	0/974	0.92	2/1314 (0.2%)
62	N6	0.53	0/1004	1.00	2/1341 (0.1%)
62	n6	0.52	0/1004	0.91	1/1341 (0.1%)
63	N7	0.43	0/1118	0.91	1/1497 (0.1%)
63	n7	0.46	0/1118	0.89	5/1497 (0.3%)
64	N8	0.60	0/1204	0.98	1/1612 (0.1%)
64	n8	0.61	0/1204	0.99	4/1612 (0.2%)
65	N9	0.54	0/473	1.05	2/629 (0.3%)
65	n9	0.66	0/473	1.24	2/629 (0.3%)
66	O0	0.41	0/750	0.82	0/1008
66	o0	0.48	0/774	0.95	2/1040 (0.2%)
67	O1	0.53	0/890	0.93	4/1196 (0.3%)
67	o1	0.59	0/897	0.99	2/1205 (0.2%)
68	O2	0.63	0/1041	0.94	0/1394
68	o2	0.65	0/1041	0.97	1/1394 (0.1%)
69	O3	0.64	0/868	1.01	5/1168 (0.4%)
69	o3	0.64	0/868	1.00	3/1168 (0.3%)
70	O4	0.51	0/890	0.95	2/1189 (0.2%)
70	o4	0.55	0/890	0.96	1/1189 (0.1%)
71	O5	0.51	0/978	0.95	0/1301
71	o5	0.48	0/974	0.91	0/1297
72	O6	0.53	0/778	0.89	0/1034
72	o6	0.54	0/777	0.97	2/1033 (0.2%)
73	O7	0.65	0/696	1.02	3/923 (0.3%)
73	o7	0.58	0/696	0.92	2/923 (0.2%)
74	O8	0.42	0/618	0.85	2/826 (0.2%)
74	o8	0.49	0/614	0.92	2/822 (0.2%)
75	O9	0.59	0/443	0.99	0/588
75	o9	0.54	0/443	0.86	0/588
76	Q0	0.55	0/423	0.98	2/562 (0.4%)
76	q0	0.67	0/423	1.01	4/562 (0.7%)
77	Q1	0.50	0/234	0.80	0/300
77	q1	0.64	0/234	0.95	0/300
78	Q2	0.62	1/860 (0.1%)	0.97	0/1136
78	q2	0.64	0/860	0.95	2/1136 (0.2%)
79	Q3	0.58	0/701	0.94	0/934
79	q3	0.59	0/701	0.96	1/934 (0.1%)
80	m2	0.52	0/736	1.16	10/1019 (1.0%)
81	p0	0.39	0/1092	0.88	1/1474 (0.1%)
82	p1	0.45	0/234	0.98	1/326 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
82	p2	0.49	0/229	0.93	1/319 (0.3%)
83	f	0.56	0/1121	0.92	3/1508 (0.2%)
84	B	0.46	0/40	0.67	0/60
84	C	0.36	0/43	0.55	0/64
All	All	0.43	1/433264 (0.0%)	0.71	475/635894 (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
9	s7	0	1
16	C4	0	1
17	c5	0	1
18	c6	0	1
19	C7	0	1
39	L2	0	2
40	l3	0	1
52	M6	0	1
53	m7	0	1
56	n0	0	1
65	N9	0	1
83	f	1	0
All	All	1	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	5.44	1.99	1.81

The worst 5 of 475 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	n9	23	LYS	CA-C-N	-11.42	105.57	119.84
65	n9	23	LYS	C-N-CA	-11.42	105.57	119.84
60	N4	80	ARG	CA-C-N	10.19	132.57	119.84
60	N4	80	ARG	C-N-CA	10.19	132.57	119.84
35	SM	38	PRO	CA-C-N	9.94	130.62	120.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
83	f	51	5CT	C2

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
19	C7	85	VAL	Peptide
39	L2	142	ASP	Peptide
39	L2	19	HIS	Peptide
52	M6	110	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	873	0
1	6	38260	0	19250	852	0
2	S0	1577	0	1567	84	0
2	s0	1583	0	1578	92	0
3	S1	1709	0	1784	84	0
3	s1	1722	0	1793	76	0
4	S2	1635	0	1723	69	0
4	s2	1635	0	1723	85	0
5	S3	1734	0	1817	73	0
5	s3	1734	0	1817	68	0
6	S4	2068	0	2154	97	0
6	s4	2068	0	2154	90	0
7	S5	1609	0	1675	65	0
7	s5	1609	0	1675	75	0
8	S6	1799	0	1879	57	0
8	s6	1755	0	1846	67	0
9	S7	1481	0	1572	61	0
9	s7	1491	0	1578	55	0
10	S8	1489	0	1525	58	0
10	s8	1489	0	1525	55	0
11	S9	1494	0	1573	58	0
11	s9	1494	0	1573	96	0
12	C0	773	0	729	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	c0	762	0	699	39	0
13	C1	1214	0	1259	43	0
13	c1	1168	0	1231	31	0
14	C2	892	0	891	38	0
14	c2	892	0	891	24	0
15	C3	1192	0	1255	55	0
15	c3	1192	0	1255	48	0
16	C4	891	0	883	51	0
16	c4	949	0	985	46	0
17	C5	977	0	1002	33	0
17	c5	1039	0	1050	49	0
18	C6	1105	0	1166	54	0
18	c6	1111	0	1171	59	0
19	C7	926	0	930	43	0
19	c7	906	0	909	36	0
20	C8	1192	0	1222	46	0
20	c8	1192	0	1222	56	0
21	C9	1112	0	1124	45	0
21	c9	1112	0	1124	41	0
22	D0	855	0	917	46	0
22	d0	882	0	939	30	0
23	D1	684	0	672	49	0
23	d1	684	0	672	39	0
24	D2	1021	0	1060	45	0
24	d2	1021	0	1060	46	0
25	D3	1121	0	1196	51	0
25	d3	1121	0	1196	46	0
26	D4	1073	0	1132	41	0
26	d4	1073	0	1132	40	0
27	D5	563	0	603	25	0
27	d5	558	0	598	23	0
28	D6	769	0	814	53	0
28	d6	769	0	814	32	0
29	D7	610	0	630	19	0
29	d7	610	0	631	23	0
30	D8	497	0	535	27	0
30	d8	497	0	535	25	0
31	D9	442	0	428	13	0
31	d9	442	0	428	13	0
32	E0	475	0	525	18	0
32	e0	491	0	542	24	0
33	E1	566	0	601	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	e1	608	0	656	28	0
34	SR	2436	0	2386	83	0
34	sR	2441	0	2392	73	0
35	SM	1104	0	996	32	0
35	sM	680	0	607	22	0
36	1	67355	0	33846	1394	0
36	5	67376	0	33856	1332	0
37	3	2579	0	1304	56	0
37	7	2579	0	1304	52	0
38	4	3353	0	1695	82	0
38	8	3353	0	1695	79	0
39	L2	1914	0	1981	80	0
39	l2	1912	0	1976	95	0
40	L3	3075	0	3142	161	0
40	l3	3075	0	3142	133	0
41	L4	2748	0	2859	129	0
41	l4	2748	0	2859	118	0
42	L5	2375	0	2325	105	0
42	l5	2359	0	2311	114	0
43	L6	1239	0	1326	56	0
43	l6	1248	0	1339	51	0
44	L7	1784	0	1862	84	0
44	l7	1791	0	1869	69	0
45	L8	1804	0	1875	56	0
45	l8	1764	0	1821	62	0
46	L9	1518	0	1587	74	0
46	l9	1518	0	1587	49	0
47	M0	1705	0	1736	87	0
47	m0	1722	0	1755	102	0
48	M1	1353	0	1383	55	0
48	m1	1353	0	1383	39	0
49	M3	1543	0	1608	66	0
49	m3	1548	0	1613	56	0
50	M4	1053	0	1149	60	0
50	m4	1059	0	1154	55	0
51	M5	1720	0	1779	78	0
51	m5	1720	0	1779	70	0
52	M6	1555	0	1659	54	0
52	m6	1555	0	1659	45	0
53	M7	1420	0	1437	68	0
53	m7	1227	0	1236	55	0
54	M8	1441	0	1543	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	m8	1441	0	1543	51	0
55	M9	1521	0	1616	69	0
55	m9	1521	0	1617	54	0
56	N0	1445	0	1487	64	0
56	n0	1445	0	1487	52	0
57	N1	1276	0	1323	49	0
57	n1	1276	0	1323	51	0
58	N2	796	0	812	26	0
58	n2	778	0	791	28	0
59	N3	1003	0	1048	44	0
59	n3	1003	0	1047	45	0
60	N4	699	0	640	16	0
60	n4	1038	0	1071	30	0
61	N5	964	0	1025	39	0
61	n5	959	0	1023	42	0
62	N6	993	0	1081	53	0
62	n6	993	0	1081	44	0
63	N7	1092	0	1155	56	0
63	n7	1092	0	1155	57	0
64	N8	1173	0	1215	43	0
64	n8	1173	0	1215	66	0
65	N9	462	0	491	9	0
65	n9	462	0	491	21	0
66	O0	742	0	797	31	0
66	o0	766	0	816	22	0
67	O1	876	0	912	22	0
67	o1	883	0	918	30	0
68	O2	1020	0	1090	36	0
68	o2	1020	0	1090	39	0
69	O3	850	0	880	24	0
69	o3	850	0	880	29	0
70	O4	880	0	945	38	0
70	o4	880	0	945	43	0
71	O5	969	0	1078	39	0
71	o5	965	0	1067	42	0
72	O6	771	0	849	28	0
72	o6	770	0	846	28	0
73	O7	681	0	683	32	0
73	o7	681	0	683	31	0
74	O8	612	0	682	20	0
74	o8	608	0	671	24	0
75	O9	436	0	475	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	o9	436	0	475	24	0
76	Q0	417	0	455	18	0
76	q0	417	0	456	16	0
77	Q1	233	0	284	17	0
77	q1	233	0	284	11	0
78	Q2	847	0	914	28	0
78	q2	847	0	914	34	0
79	Q3	694	0	734	34	0
79	q3	694	0	734	38	0
80	m2	739	0	343	7	0
81	p0	1077	0	1041	32	0
82	p1	235	0	119	0	0
82	p2	230	0	117	2	0
83	f	1122	0	1116	45	0
84	B	59	0	34	0	0
84	C	62	0	33	3	0
85	1	361	0	0	0	0
85	2	90	0	0	0	0
85	3	8	0	0	0	0
85	4	15	0	0	0	0
85	5	415	0	0	0	0
85	6	111	0	0	0	0
85	7	13	0	0	0	0
85	8	10	0	0	0	0
85	B	1	0	0	0	0
85	C	1	0	0	0	0
85	D3	1	0	0	0	0
85	L2	2	0	0	0	0
85	L3	1	0	0	0	0
85	L6	1	0	0	0	0
85	L7	3	0	0	0	0
85	M0	2	0	0	0	0
85	M5	2	0	0	0	0
85	M6	3	0	0	0	0
85	M7	4	0	0	0	0
85	M9	1	0	0	0	0
85	N3	1	0	0	0	0
85	N6	1	0	0	0	0
85	N8	3	0	0	0	0
85	O4	1	0	0	0	0
85	O7	2	0	0	0	0
85	Q2	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	S2	1	0	0	0	0
85	SM	1	0	0	0	0
85	c8	2	0	0	0	0
85	c9	1	0	0	0	0
85	d2	1	0	0	0	0
85	d3	1	0	0	0	0
85	d6	1	0	0	0	0
85	f	1	0	0	0	0
85	l2	2	0	0	0	0
85	l3	2	0	0	0	0
85	l4	1	0	0	0	0
85	l5	1	0	0	0	0
85	l7	2	0	0	0	0
85	m0	1	0	0	0	0
85	m3	1	0	0	0	0
85	m5	3	0	0	0	0
85	m7	3	0	0	0	0
85	n0	1	0	0	0	0
85	n3	1	0	0	0	0
85	n6	1	0	0	0	0
85	n8	2	0	0	0	0
85	o2	1	0	0	0	0
85	o3	1	0	0	0	0
85	o4	1	0	0	0	0
85	q1	1	0	0	0	0
85	q2	1	0	0	0	0
85	q3	1	0	0	0	0
85	s4	1	0	0	0	0
85	s8	2	0	0	0	0
86	1	2457	0	0	236	0
86	2	1134	0	0	124	0
86	3	77	0	0	3	0
86	4	126	0	0	14	0
86	5	2492	0	0	243	0
86	6	1204	0	0	118	0
86	7	77	0	0	4	0
86	8	147	0	0	11	0
86	C3	7	0	0	1	0
86	C5	7	0	0	4	0
86	C8	7	0	0	0	0
86	D9	7	0	0	0	0
86	L3	21	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	L4	7	0	0	3	0
86	L5	7	0	0	1	0
86	M0	14	0	0	5	0
86	M5	14	0	0	2	0
86	M6	7	0	0	0	0
86	M7	7	0	0	1	0
86	M8	7	0	0	0	0
86	M9	7	0	0	1	0
86	N8	7	0	0	0	0
86	N9	7	0	0	1	0
86	O1	7	0	0	2	0
86	O3	7	0	0	0	0
86	O4	7	0	0	2	0
86	O7	7	0	0	6	0
86	O9	7	0	0	1	0
86	Q2	7	0	0	2	0
86	S1	7	0	0	1	0
86	S6	7	0	0	3	0
86	S8	7	0	0	1	0
86	S9	7	0	0	2	0
86	SR	7	0	0	2	0
86	c3	7	0	0	2	0
86	c5	14	0	0	5	0
86	c8	7	0	0	1	0
86	d4	7	0	0	0	0
86	d9	7	0	0	0	0
86	l3	14	0	0	1	0
86	l4	14	0	0	5	0
86	l5	14	0	0	3	0
86	l9	7	0	0	0	0
86	m0	14	0	0	4	0
86	m1	7	0	0	0	0
86	m4	7	0	0	0	0
86	m5	21	0	0	1	0
86	m6	7	0	0	0	0
86	m7	7	0	0	1	0
86	m8	7	0	0	0	0
86	m9	7	0	0	0	0
86	n3	7	0	0	1	0
86	n9	7	0	0	1	0
86	o3	7	0	0	1	0
86	o6	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	o7	14	0	0	5	0
86	q2	7	0	0	1	0
86	s1	14	0	0	2	0
86	s4	7	0	0	0	0
86	s8	7	0	0	0	0
86	s9	7	0	0	2	0
86	sR	7	0	0	3	0
87	D6	1	0	0	0	0
87	D7	1	0	0	0	0
87	D9	1	0	0	0	0
87	E1	1	0	0	0	0
87	O7	1	0	0	0	0
87	Q0	1	0	0	1	0
87	Q2	1	0	0	0	0
87	Q3	1	0	0	0	0
87	d6	1	0	0	0	0
87	d7	1	0	0	0	0
87	d9	1	0	0	0	0
87	e1	1	0	0	0	0
87	o7	1	0	0	0	0
87	q0	1	0	0	1	0
87	q2	1	0	0	0	0
87	q3	1	0	0	0	0
88	1	23	0	18	1	0
88	5	23	0	18	5	0
89	1	7	0	7	0	0
89	5	7	0	7	0	0
89	B	7	0	7	0	0
89	C	7	0	7	0	0
90	5	6	0	0	0	0
90	f	6	0	0	0	0
All	All	413121	0	299177	10534	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 15.

The worst 5 of 10534 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)
76:Q0:96:CYS:SG	76:Q0:99:CYS:SG	2.31	1.29
78:q2:17:CYS:SG	78:q2:77:CYS:SG	2.32	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1:2208:A:N1	86:1:3940:OHX:N6	2.03	1.05
36:1:2403:G:OP2	86:1:4071:OHX:N5	1.95	0.99
73:O7:87:SER:O	86:O7:104:OHX:N3	1.96	0.98

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	157 (77%)	34 (17%)	13 (6%)	1	12
2	s0	204/251 (81%)	148 (72%)	31 (15%)	25 (12%)	0	4
3	S1	212/254 (84%)	154 (73%)	38 (18%)	20 (9%)	0	6
3	s1	214/254 (84%)	169 (79%)	30 (14%)	15 (7%)	1	10
4	S2	215/253 (85%)	169 (79%)	36 (17%)	10 (5%)	2	17
4	s2	215/253 (85%)	172 (80%)	25 (12%)	18 (8%)	0	7
5	S3	221/239 (92%)	186 (84%)	24 (11%)	11 (5%)	1	15
5	s3	221/239 (92%)	172 (78%)	36 (16%)	13 (6%)	1	13
6	S4	258/260 (99%)	197 (76%)	44 (17%)	17 (7%)	1	11
6	s4	258/260 (99%)	200 (78%)	42 (16%)	16 (6%)	1	12
7	S5	204/224 (91%)	153 (75%)	35 (17%)	16 (8%)	1	8
7	s5	204/224 (91%)	150 (74%)	41 (20%)	13 (6%)	1	12
8	S6	224/236 (95%)	189 (84%)	23 (10%)	12 (5%)	1	14
8	s6	216/236 (92%)	176 (82%)	32 (15%)	8 (4%)	2	21
9	S7	182/189 (96%)	127 (70%)	39 (21%)	16 (9%)	0	7
9	s7	184/189 (97%)	141 (77%)	29 (16%)	14 (8%)	1	8
10	S8	184/200 (92%)	150 (82%)	25 (14%)	9 (5%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	s8	184/200 (92%)	151 (82%)	27 (15%)	6 (3%)	3	23
11	S9	183/196 (93%)	148 (81%)	27 (15%)	8 (4%)	2	17
11	s9	183/196 (93%)	141 (77%)	33 (18%)	9 (5%)	1	16
12	C0	94/105 (90%)	69 (73%)	16 (17%)	9 (10%)	0	6
12	c0	92/105 (88%)	63 (68%)	14 (15%)	15 (16%)	0	2
13	C1	153/155 (99%)	122 (80%)	21 (14%)	10 (6%)	1	11
13	c1	144/155 (93%)	120 (83%)	19 (13%)	5 (4%)	3	23
14	C2	122/142 (86%)	71 (58%)	33 (27%)	18 (15%)	0	3
14	c2	122/142 (86%)	78 (64%)	30 (25%)	14 (12%)	0	5
15	C3	148/150 (99%)	120 (81%)	17 (12%)	11 (7%)	1	9
15	c3	148/150 (99%)	116 (78%)	20 (14%)	12 (8%)	1	8
16	C4	125/136 (92%)	89 (71%)	24 (19%)	12 (10%)	0	6
16	c4	126/136 (93%)	96 (76%)	16 (13%)	14 (11%)	0	5
17	C5	122/141 (86%)	99 (81%)	13 (11%)	10 (8%)	0	8
17	c5	133/141 (94%)	86 (65%)	38 (29%)	9 (7%)	1	10
18	C6	139/142 (98%)	118 (85%)	13 (9%)	8 (6%)	1	13
18	c6	140/142 (99%)	118 (84%)	13 (9%)	9 (6%)	1	12
19	C7	116/136 (85%)	90 (78%)	18 (16%)	8 (7%)	1	10
19	c7	113/136 (83%)	86 (76%)	18 (16%)	9 (8%)	1	8
20	C8	143/145 (99%)	111 (78%)	25 (18%)	7 (5%)	1	16
20	c8	143/145 (99%)	117 (82%)	19 (13%)	7 (5%)	1	16
21	C9	141/143 (99%)	116 (82%)	18 (13%)	7 (5%)	1	15
21	c9	141/143 (99%)	116 (82%)	21 (15%)	4 (3%)	4	26
22	D0	105/120 (88%)	89 (85%)	12 (11%)	4 (4%)	2	20
22	d0	108/120 (90%)	90 (83%)	13 (12%)	5 (5%)	2	17
23	D1	85/87 (98%)	64 (75%)	8 (9%)	13 (15%)	0	2
23	d1	85/87 (98%)	61 (72%)	17 (20%)	7 (8%)	0	8
24	D2	127/129 (98%)	106 (84%)	16 (13%)	5 (4%)	2	20
24	d2	127/129 (98%)	107 (84%)	17 (13%)	3 (2%)	4	29
25	D3	142/144 (99%)	104 (73%)	22 (16%)	16 (11%)	0	5
25	d3	142/144 (99%)	117 (82%)	24 (17%)	1 (1%)	18	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	D4	132/134 (98%)	106 (80%)	16 (12%)	10 (8%)	1	8
26	d4	132/134 (98%)	101 (76%)	20 (15%)	11 (8%)	0	8
27	D5	68/107 (64%)	50 (74%)	12 (18%)	6 (9%)	0	7
27	d5	67/107 (63%)	49 (73%)	16 (24%)	2 (3%)	3	25
28	D6	95/97 (98%)	57 (60%)	24 (25%)	14 (15%)	0	3
28	d6	95/97 (98%)	69 (73%)	14 (15%)	12 (13%)	0	4
29	D7	79/81 (98%)	69 (87%)	7 (9%)	3 (4%)	2	20
29	d7	79/81 (98%)	57 (72%)	16 (20%)	6 (8%)	1	8
30	D8	61/66 (92%)	47 (77%)	10 (16%)	4 (7%)	1	11
30	d8	61/66 (92%)	41 (67%)	11 (18%)	9 (15%)	0	3
31	D9	51/55 (93%)	37 (72%)	11 (22%)	3 (6%)	1	13
31	d9	51/55 (93%)	40 (78%)	8 (16%)	3 (6%)	1	13
32	E0	58/63 (92%)	41 (71%)	15 (26%)	2 (3%)	3	23
32	e0	60/63 (95%)	38 (63%)	15 (25%)	7 (12%)	0	5
33	E1	69/76 (91%)	38 (55%)	19 (28%)	12 (17%)	0	2
33	e1	74/76 (97%)	39 (53%)	12 (16%)	23 (31%)	0	0
34	SR	316/318 (99%)	260 (82%)	43 (14%)	13 (4%)	2	19
34	sR	316/318 (99%)	264 (84%)	38 (12%)	14 (4%)	2	17
35	SM	155/273 (57%)	107 (69%)	32 (21%)	16 (10%)	0	6
35	sM	98/273 (36%)	66 (67%)	23 (24%)	9 (9%)	0	7
39	L2	250/253 (99%)	217 (87%)	23 (9%)	10 (4%)	2	19
39	l2	250/253 (99%)	204 (82%)	33 (13%)	13 (5%)	1	14
40	L3	384/386 (100%)	315 (82%)	46 (12%)	23 (6%)	1	12
40	l3	384/386 (100%)	337 (88%)	35 (9%)	12 (3%)	3	25
41	L4	359/361 (99%)	285 (79%)	52 (14%)	22 (6%)	1	12
41	l4	359/361 (99%)	288 (80%)	53 (15%)	18 (5%)	1	15
42	L5	294/296 (99%)	229 (78%)	42 (14%)	23 (8%)	1	8
42	l5	292/296 (99%)	250 (86%)	35 (12%)	7 (2%)	4	29
43	L6	152/175 (87%)	132 (87%)	17 (11%)	3 (2%)	6	32
43	l6	153/175 (87%)	123 (80%)	25 (16%)	5 (3%)	3	23
44	L7	220/243 (90%)	173 (79%)	39 (18%)	8 (4%)	2	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	l7	221/243 (91%)	193 (87%)	23 (10%)	5 (2%)	5	30
45	L8	231/255 (91%)	184 (80%)	38 (16%)	9 (4%)	2	20
45	l8	229/255 (90%)	167 (73%)	48 (21%)	14 (6%)	1	12
46	L9	189/191 (99%)	159 (84%)	19 (10%)	11 (6%)	1	13
46	l9	189/191 (99%)	163 (86%)	21 (11%)	5 (3%)	4	27
47	M0	207/220 (94%)	167 (81%)	31 (15%)	9 (4%)	2	18
47	m0	209/220 (95%)	165 (79%)	33 (16%)	11 (5%)	1	14
48	M1	167/173 (96%)	134 (80%)	19 (11%)	14 (8%)	0	7
48	m1	167/173 (96%)	137 (82%)	19 (11%)	11 (7%)	1	11
49	M3	191/198 (96%)	153 (80%)	27 (14%)	11 (6%)	1	13
49	m3	192/198 (97%)	153 (80%)	24 (12%)	15 (8%)	1	8
50	M4	134/137 (98%)	114 (85%)	15 (11%)	5 (4%)	2	21
50	m4	135/137 (98%)	115 (85%)	16 (12%)	4 (3%)	3	25
51	M5	201/203 (99%)	176 (88%)	19 (10%)	6 (3%)	3	25
51	m5	201/203 (99%)	174 (87%)	23 (11%)	4 (2%)	6	32
52	M6	195/198 (98%)	173 (89%)	16 (8%)	6 (3%)	3	25
52	m6	195/198 (98%)	182 (93%)	9 (5%)	4 (2%)	5	31
53	M7	181/183 (99%)	150 (83%)	25 (14%)	6 (3%)	3	23
53	m7	153/183 (84%)	127 (83%)	25 (16%)	1 (1%)	18	51
54	M8	183/185 (99%)	151 (82%)	24 (13%)	8 (4%)	2	17
54	m8	183/185 (99%)	154 (84%)	20 (11%)	9 (5%)	1	16
55	M9	186/188 (99%)	160 (86%)	23 (12%)	3 (2%)	7	36
55	m9	186/188 (99%)	166 (89%)	13 (7%)	7 (4%)	2	20
56	N0	170/172 (99%)	155 (91%)	12 (7%)	3 (2%)	6	34
56	n0	170/172 (99%)	152 (89%)	15 (9%)	3 (2%)	6	34
57	N1	157/159 (99%)	137 (87%)	15 (10%)	5 (3%)	3	24
57	n1	157/159 (99%)	131 (83%)	24 (15%)	2 (1%)	9	39
58	N2	98/120 (82%)	72 (74%)	23 (24%)	3 (3%)	3	25
58	n2	96/120 (80%)	80 (83%)	11 (12%)	5 (5%)	1	14
59	N3	134/136 (98%)	117 (87%)	15 (11%)	2 (2%)	8	37
59	n3	134/136 (98%)	122 (91%)	7 (5%)	5 (4%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	N4	96/155 (62%)	68 (71%)	18 (19%)	10 (10%)	0	6
60	n4	133/155 (86%)	102 (77%)	22 (16%)	9 (7%)	1	10
61	N5	119/141 (84%)	99 (83%)	14 (12%)	6 (5%)	1	15
61	n5	118/141 (84%)	94 (80%)	19 (16%)	5 (4%)	2	19
62	N6	124/126 (98%)	107 (86%)	13 (10%)	4 (3%)	3	24
62	n6	124/126 (98%)	102 (82%)	21 (17%)	1 (1%)	16	49
63	N7	133/135 (98%)	114 (86%)	10 (8%)	9 (7%)	1	10
63	n7	133/135 (98%)	112 (84%)	12 (9%)	9 (7%)	1	10
64	N8	146/148 (99%)	118 (81%)	22 (15%)	6 (4%)	2	19
64	n8	146/148 (99%)	111 (76%)	24 (16%)	11 (8%)	1	9
65	N9	56/58 (97%)	41 (73%)	12 (21%)	3 (5%)	1	14
65	n9	56/58 (97%)	39 (70%)	12 (21%)	5 (9%)	0	7
66	O0	95/104 (91%)	80 (84%)	11 (12%)	4 (4%)	2	19
66	o0	98/104 (94%)	84 (86%)	11 (11%)	3 (3%)	3	25
67	O1	107/112 (96%)	89 (83%)	8 (8%)	10 (9%)	0	7
67	o1	107/112 (96%)	83 (78%)	18 (17%)	6 (6%)	1	13
68	O2	125/129 (97%)	104 (83%)	18 (14%)	3 (2%)	4	29
68	o2	125/129 (97%)	103 (82%)	16 (13%)	6 (5%)	2	16
69	O3	104/106 (98%)	96 (92%)	7 (7%)	1 (1%)	12	44
69	o3	104/106 (98%)	92 (88%)	9 (9%)	3 (3%)	3	26
70	O4	110/121 (91%)	88 (80%)	17 (16%)	5 (4%)	2	17
70	o4	110/121 (91%)	98 (89%)	11 (10%)	1 (1%)	14	46
71	O5	117/119 (98%)	93 (80%)	22 (19%)	2 (2%)	7	35
71	o5	117/119 (98%)	98 (84%)	14 (12%)	5 (4%)	2	18
72	O6	97/99 (98%)	78 (80%)	13 (13%)	6 (6%)	1	12
72	o6	97/99 (98%)	78 (80%)	14 (14%)	5 (5%)	1	14
73	O7	85/87 (98%)	64 (75%)	16 (19%)	5 (6%)	1	13
73	o7	85/87 (98%)	72 (85%)	11 (13%)	2 (2%)	4	29
74	O8	75/77 (97%)	62 (83%)	9 (12%)	4 (5%)	1	14
74	o8	75/77 (97%)	60 (80%)	12 (16%)	3 (4%)	2	19
75	O9	48/50 (96%)	40 (83%)	7 (15%)	1 (2%)	5	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
75	o9	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
76	Q0	50/52 (96%)	42 (84%)	7 (14%)	1 (2%)	6	32
76	q0	50/52 (96%)	46 (92%)	2 (4%)	2 (4%)	2	19
77	Q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
77	q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
78	Q2	103/105 (98%)	80 (78%)	17 (16%)	6 (6%)	1	13
78	q2	103/105 (98%)	95 (92%)	7 (7%)	1 (1%)	12	44
79	Q3	89/91 (98%)	71 (80%)	10 (11%)	8 (9%)	0	7
79	q3	89/91 (98%)	74 (83%)	12 (14%)	3 (3%)	3	23
80	m2	144/165 (87%)	67 (46%)	48 (33%)	29 (20%)	0	1
81	p0	139/311 (45%)	110 (79%)	20 (14%)	9 (6%)	1	11
82	p1	45/106 (42%)	26 (58%)	17 (38%)	2 (4%)	2	17
82	p2	44/106 (42%)	33 (75%)	6 (14%)	5 (11%)	0	5
83	f	145/157 (92%)	97 (67%)	34 (23%)	14 (10%)	0	6
All	All	22711/24683 (92%)	18197 (80%)	3231 (14%)	1283 (6%)	1	13

5 of 1283 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	158	VAL
2	S0	169	SER
2	S0	191	ARG
3	S1	82	ARG

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%)	140 (85%)	24 (15%)	3	17
2	s0	165/209 (79%)	140 (85%)	25 (15%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	S1	191/223 (86%)	162 (85%)	29 (15%)	3	16
3	s1	192/223 (86%)	158 (82%)	34 (18%)	2	11
4	S2	176/204 (86%)	143 (81%)	33 (19%)	1	9
4	s2	176/204 (86%)	133 (76%)	43 (24%)	1	4
5	S3	182/194 (94%)	145 (80%)	37 (20%)	1	7
5	s3	182/194 (94%)	156 (86%)	26 (14%)	3	18
6	S4	221/221 (100%)	190 (86%)	31 (14%)	3	19
6	s4	221/221 (100%)	180 (81%)	41 (19%)	1	9
7	S5	173/190 (91%)	147 (85%)	26 (15%)	3	17
7	s5	173/190 (91%)	145 (84%)	28 (16%)	2	14
8	S6	188/201 (94%)	159 (85%)	29 (15%)	2	16
8	s6	187/201 (93%)	159 (85%)	28 (15%)	3	17
9	S7	165/169 (98%)	142 (86%)	23 (14%)	3	19
9	s7	165/169 (98%)	136 (82%)	29 (18%)	2	11
10	S8	150/161 (93%)	125 (83%)	25 (17%)	2	13
10	s8	150/161 (93%)	126 (84%)	24 (16%)	2	14
11	S9	158/165 (96%)	131 (83%)	27 (17%)	2	12
11	s9	158/165 (96%)	132 (84%)	26 (16%)	2	14
12	C0	77/98 (79%)	68 (88%)	9 (12%)	5	25
12	c0	73/98 (74%)	62 (85%)	11 (15%)	3	17
13	C1	129/136 (95%)	110 (85%)	19 (15%)	3	17
13	c1	129/136 (95%)	105 (81%)	24 (19%)	1	9
14	C2	88/118 (75%)	70 (80%)	18 (20%)	1	7
14	c2	88/118 (75%)	75 (85%)	13 (15%)	3	17
15	C3	127/127 (100%)	97 (76%)	30 (24%)	1	4
15	c3	127/127 (100%)	109 (86%)	18 (14%)	3	18
16	C4	81/104 (78%)	63 (78%)	18 (22%)	1	5
16	c4	97/104 (93%)	77 (79%)	20 (21%)	1	7
17	C5	101/117 (86%)	86 (85%)	15 (15%)	3	17
17	c5	103/117 (88%)	84 (82%)	19 (18%)	1	9
18	C6	117/118 (99%)	96 (82%)	21 (18%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	c6	118/118 (100%)	101 (86%)	17 (14%)	3	18
19	C7	94/124 (76%)	78 (83%)	16 (17%)	2	12
19	c7	92/124 (74%)	77 (84%)	15 (16%)	2	14
20	C8	128/128 (100%)	103 (80%)	25 (20%)	1	8
20	c8	128/128 (100%)	102 (80%)	26 (20%)	1	7
21	C9	115/115 (100%)	95 (83%)	20 (17%)	2	12
21	c9	115/115 (100%)	99 (86%)	16 (14%)	3	19
22	D0	100/113 (88%)	74 (74%)	26 (26%)	0	3
22	d0	103/113 (91%)	78 (76%)	25 (24%)	1	4
23	D1	74/74 (100%)	59 (80%)	15 (20%)	1	7
23	d1	74/74 (100%)	55 (74%)	19 (26%)	0	3
24	D2	110/110 (100%)	83 (76%)	27 (24%)	1	4
24	d2	110/110 (100%)	91 (83%)	19 (17%)	2	12
25	D3	119/119 (100%)	95 (80%)	24 (20%)	1	7
25	d3	119/119 (100%)	97 (82%)	22 (18%)	1	9
26	D4	112/112 (100%)	95 (85%)	17 (15%)	3	16
26	d4	112/112 (100%)	92 (82%)	20 (18%)	2	10
27	D5	61/88 (69%)	49 (80%)	12 (20%)	1	8
27	d5	61/88 (69%)	50 (82%)	11 (18%)	2	10
28	D6	83/83 (100%)	63 (76%)	20 (24%)	1	4
28	d6	83/83 (100%)	75 (90%)	8 (10%)	8	31
29	D7	70/70 (100%)	65 (93%)	5 (7%)	13	40
29	d7	70/70 (100%)	56 (80%)	14 (20%)	1	7
30	D8	56/59 (95%)	45 (80%)	11 (20%)	1	8
30	d8	56/59 (95%)	41 (73%)	15 (27%)	0	3
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2	12
31	d9	47/48 (98%)	39 (83%)	8 (17%)	2	12
32	E0	51/54 (94%)	42 (82%)	9 (18%)	2	11
32	e0	53/54 (98%)	35 (66%)	18 (34%)	0	2
33	E1	62/66 (94%)	51 (82%)	11 (18%)	2	11
33	e1	66/66 (100%)	52 (79%)	14 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	SR	259/261 (99%)	235 (91%)	24 (9%)	8	32
34	sR	260/261 (100%)	236 (91%)	24 (9%)	8	32
35	SM	97/228 (42%)	76 (78%)	21 (22%)	1	6
35	sM	54/228 (24%)	46 (85%)	8 (15%)	3	17
39	L2	193/195 (99%)	153 (79%)	40 (21%)	1	6
39	l2	192/195 (98%)	150 (78%)	42 (22%)	1	6
40	L3	319/322 (99%)	252 (79%)	67 (21%)	1	6
40	l3	320/322 (99%)	254 (79%)	66 (21%)	1	7
41	L4	288/288 (100%)	232 (81%)	56 (19%)	1	8
41	l4	288/288 (100%)	235 (82%)	53 (18%)	1	9
42	L5	244/244 (100%)	201 (82%)	43 (18%)	2	11
42	l5	243/244 (100%)	195 (80%)	48 (20%)	1	7
43	L6	134/152 (88%)	111 (83%)	23 (17%)	2	12
43	l6	135/152 (89%)	109 (81%)	26 (19%)	1	8
44	L7	186/204 (91%)	157 (84%)	29 (16%)	2	15
44	l7	187/204 (92%)	157 (84%)	30 (16%)	2	14
45	L8	187/207 (90%)	157 (84%)	30 (16%)	2	14
45	l8	177/207 (86%)	151 (85%)	26 (15%)	3	17
46	L9	171/171 (100%)	131 (77%)	40 (23%)	1	4
46	l9	171/171 (100%)	141 (82%)	30 (18%)	2	11
47	M0	177/186 (95%)	144 (81%)	33 (19%)	1	9
47	m0	179/186 (96%)	144 (80%)	35 (20%)	1	8
48	M1	147/150 (98%)	116 (79%)	31 (21%)	1	6
48	m1	147/150 (98%)	117 (80%)	30 (20%)	1	7
49	M3	154/158 (98%)	131 (85%)	23 (15%)	3	17
49	m3	154/158 (98%)	136 (88%)	18 (12%)	5	25
50	M4	107/108 (99%)	87 (81%)	20 (19%)	1	9
50	m4	108/108 (100%)	85 (79%)	23 (21%)	1	6
51	M5	175/175 (100%)	145 (83%)	30 (17%)	2	12
51	m5	175/175 (100%)	149 (85%)	26 (15%)	3	17
52	M6	160/161 (99%)	138 (86%)	22 (14%)	3	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	m6	160/161 (99%)	140 (88%)	20 (12%)	4	22
53	M7	140/145 (97%)	105 (75%)	35 (25%)	0	4
53	m7	125/145 (86%)	101 (81%)	24 (19%)	1	8
54	M8	150/150 (100%)	127 (85%)	23 (15%)	3	16
54	m8	150/150 (100%)	129 (86%)	21 (14%)	3	19
55	M9	153/153 (100%)	129 (84%)	24 (16%)	2	15
55	m9	153/153 (100%)	133 (87%)	20 (13%)	4	21
56	N0	156/156 (100%)	128 (82%)	28 (18%)	2	10
56	n0	156/156 (100%)	121 (78%)	35 (22%)	1	5
57	N1	136/136 (100%)	106 (78%)	30 (22%)	1	5
57	n1	136/136 (100%)	107 (79%)	29 (21%)	1	6
58	N2	87/106 (82%)	75 (86%)	12 (14%)	3	19
58	n2	85/106 (80%)	69 (81%)	16 (19%)	1	9
59	N3	104/104 (100%)	89 (86%)	15 (14%)	3	18
59	n3	104/104 (100%)	87 (84%)	17 (16%)	2	14
60	N4	57/129 (44%)	55 (96%)	2 (4%)	32	58
60	n4	100/129 (78%)	86 (86%)	14 (14%)	3	19
61	N5	104/117 (89%)	76 (73%)	28 (27%)	0	3
61	n5	104/117 (89%)	88 (85%)	16 (15%)	2	16
62	N6	109/109 (100%)	84 (77%)	25 (23%)	1	5
62	n6	109/109 (100%)	88 (81%)	21 (19%)	1	8
63	N7	115/115 (100%)	100 (87%)	15 (13%)	4	21
63	n7	115/115 (100%)	93 (81%)	22 (19%)	1	8
64	N8	118/118 (100%)	97 (82%)	21 (18%)	2	10
64	n8	118/118 (100%)	96 (81%)	22 (19%)	1	9
65	N9	46/46 (100%)	38 (83%)	8 (17%)	2	12
65	n9	46/46 (100%)	39 (85%)	7 (15%)	3	16
66	O0	81/87 (93%)	65 (80%)	16 (20%)	1	7
66	o0	84/87 (97%)	70 (83%)	14 (17%)	2	13
67	O1	92/96 (96%)	76 (83%)	16 (17%)	2	12
67	o1	94/96 (98%)	78 (83%)	16 (17%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	O2	109/110 (99%)	85 (78%)	24 (22%)	1	5
68	o2	109/110 (99%)	83 (76%)	26 (24%)	1	4
69	O3	90/90 (100%)	78 (87%)	12 (13%)	4	21
69	o3	90/90 (100%)	79 (88%)	11 (12%)	5	23
70	O4	95/103 (92%)	81 (85%)	14 (15%)	3	17
70	o4	95/103 (92%)	76 (80%)	19 (20%)	1	7
71	O5	104/104 (100%)	82 (79%)	22 (21%)	1	6
71	o5	103/104 (99%)	84 (82%)	19 (18%)	1	9
72	O6	81/81 (100%)	63 (78%)	18 (22%)	1	5
72	o6	80/81 (99%)	57 (71%)	23 (29%)	0	2
73	O7	70/70 (100%)	56 (80%)	14 (20%)	1	7
73	o7	70/70 (100%)	53 (76%)	17 (24%)	1	4
74	O8	68/68 (100%)	49 (72%)	19 (28%)	0	3
74	o8	67/68 (98%)	56 (84%)	11 (16%)	2	14
75	O9	45/45 (100%)	35 (78%)	10 (22%)	1	5
75	o9	45/45 (100%)	39 (87%)	6 (13%)	4	21
76	Q0	47/47 (100%)	38 (81%)	9 (19%)	1	8
76	q0	47/47 (100%)	39 (83%)	8 (17%)	2	12
77	Q1	23/23 (100%)	18 (78%)	5 (22%)	1	6
77	q1	23/23 (100%)	17 (74%)	6 (26%)	0	3
78	Q2	90/90 (100%)	71 (79%)	19 (21%)	1	6
78	q2	90/90 (100%)	68 (76%)	22 (24%)	1	4
79	Q3	71/71 (100%)	61 (86%)	10 (14%)	3	19
79	q3	71/71 (100%)	58 (82%)	13 (18%)	2	10
81	p0	105/253 (42%)	86 (82%)	19 (18%)	2	10
83	f	123/132 (93%)	103 (84%)	20 (16%)	2	14
All	All	18849/20379 (92%)	15488 (82%)	3361 (18%)	2	10

5 of 3361 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	s5	119	ASP
30	d8	39	THR

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Mol	Chain	Res	Type
71	o5	21	LEU
9	s7	114	ARG
7	s5	102	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 194 such sidechains are listed below:

Mol	Chain	Res	Type
20	c8	137	HIS
43	l6	28	GLN
22	d0	98	GLN
34	sR	196	ASN
48	m1	20	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1777/1800 (98%)	463 (26%)	42 (2%)
1	6	1791/1800 (99%)	450 (25%)	35 (1%)
36	1	3145/3396 (92%)	688 (21%)	65 (2%)
36	5	3145/3396 (92%)	664 (21%)	65 (2%)
37	3	120/121 (99%)	20 (16%)	1 (0%)
37	7	120/121 (99%)	16 (13%)	1 (0%)
38	4	157/158 (99%)	33 (21%)	3 (1%)
38	8	157/158 (99%)	32 (20%)	1 (0%)
84	B	1/3 (33%)	1 (100%)	0
84	C	1/3 (33%)	0	0
All	All	10414/10956 (95%)	2367 (22%)	213 (2%)

5 of 2367 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	23	G
1	2	25	C
1	2	26	A

5 of 213 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	6	158	U
1	6	1657	U
36	5	3078	U
1	6	272	U
1	6	1031	U

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

3 non-standard protein/DNA/RNA residues are 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
84	8AN	C	76	84,85,89	21,24,25	1.52	4 (19%)	26,35,38	2.36	9 (34%)
84	8AN	B	76	84,85,89	21,24,25	1.50	4 (19%)	26,35,38	2.18	9 (34%)
83	5CT	f	51	83	13,14,15	2.48	3 (23%)	8,15,17	1.75	3 (37%)

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
84	8AN	C	76	84,85,89	-	3/7/25/26	0/3/3/3
84	8AN	B	76	84,85,89	-	2/7/25/26	0/3/3/3
83	5CT	f	51	83	1/1/2/4	6/13/14/16	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	f	51	5CT	O1-C2	-7.03	1.22	1.43
84	C	76	8AN	C5-C4	4.66	1.47	1.39
84	B	76	8AN	C5-C4	4.37	1.46	1.39
83	f	51	5CT	C1-NZ	-3.43	1.41	1.47
83	f	51	5CT	CB-CA	3.28	1.58	1.53

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	C	76	8AN	C5-C4-N3	-6.46	117.83	126.72
84	B	76	8AN	C5-C4-N3	-5.71	118.86	126.72
84	C	76	8AN	N3-C4-N9	5.42	136.39	127.17
84	B	76	8AN	N3-C4-N9	4.03	134.02	127.17
84	B	76	8AN	C4-C5-N7	-3.86	106.17	110.58

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
83	f	51	5CT	C2

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	f	51	5CT	CD-CE-NZ-C1
83	f	51	5CT	O1-C2-C3-C4
83	f	51	5CT	C2-C3-C4-N1
83	f	51	5CT	CG-CD-CE-NZ
83	f	51	5CT	NZ-C1-C2-O1

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	C	76	8AN	1	0
83	f	51	5CT	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2284 ligands modelled in this entry, 1109 are monoatomic - leaving 1175 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	6	2114	-	0,6,6	-	-	-		
86	OHX	5	3892	-	0,6,6	-	-	-		
86	OHX	6	2136	-	0,6,6	-	-	-		
86	OHX	1	4027	-	0,6,6	-	-	-		
86	OHX	6	2120	-	0,6,6	-	-	-		
86	OHX	5	3818	-	0,6,6	-	-	-		
86	OHX	5	4123	-	0,6,6	-	-	-		
86	OHX	1	4065	-	0,6,6	-	-	-		
86	OHX	4	229	-	0,6,6	-	-	-		
86	OHX	6	2035	-	0,6,6	-	-	-		
86	OHX	2	2065	-	0,6,6	-	-	-		
86	OHX	1	3776	-	0,6,6	-	-	-		
86	OHX	5	4114	-	0,6,6	-	-	-		
86	OHX	5	3838	-	0,6,6	-	-	-		
86	OHX	5	4133	-	0,6,6	-	-	-		
86	OHX	5	4015	-	0,6,6	-	-	-		
86	OHX	5	3904	-	0,6,6	-	-	-		
86	OHX	5	3820	-	0,6,6	-	-	-		
86	OHX	5	3998	-	0,6,6	-	-	-		
89	PRO	1	4114	89	6,7,8	0.60	0	7,8,10	1.08	0
86	OHX	1	3888	-	0,6,6	-	-	-		
86	OHX	5	3985	-	0,6,6	-	-	-		
86	OHX	5	3857	-	0,6,6	-	-	-		
86	OHX	6	2150	-	0,6,6	-	-	-		
86	OHX	4	224	-	0,6,6	-	-	-		
86	OHX	1	4066	-	0,6,6	-	-	-		
86	OHX	5	4046	-	0,6,6	-	-	-		
86	OHX	2	2144	-	0,6,6	-	-	-		
86	OHX	1	3860	-	0,6,6	-	-	-		
86	OHX	1	3957	-	0,6,6	-	-	-		
86	OHX	6	2028	-	0,6,6	-	-	-		
86	OHX	1	3793	-	0,6,6	-	-	-		
86	OHX	5	4158	-	0,6,6	-	-	-		
86	OHX	1	3963	-	0,6,6	-	-	-		
86	OHX	n3	202	-	0,6,6	-	-	-		
86	OHX	1	3953	-	0,6,6	-	-	-		
86	OHX	1	3931	-	0,6,6	-	-	-		
86	OHX	5	4016	-	0,6,6	-	-	-		
86	OHX	7	221	-	0,6,6	-	-	-		
86	OHX	1	3923	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	M7	205	-	0,6,6	-	-	-		
86	OHX	2	2134	-	0,6,6	-	-	-		
86	OHX	1	3875	-	0,6,6	-	-	-		
86	OHX	1	4047	-	0,6,6	-	-	-		
86	OHX	5	4076	-	0,6,6	-	-	-		
86	OHX	5	3880	-	0,6,6	-	-	-		
86	OHX	1	3782	-	0,6,6	-	-	-		
86	OHX	5	4122	-	0,6,6	-	-	-		
86	OHX	2	2152	-	0,6,6	-	-	-		
88	SPS	1	4113	85	20,23,23	3.70	13 (65%)	23,30,30	2.69	12 (52%)
86	OHX	1	4081	-	0,6,6	-	-	-		
86	OHX	1	4056	-	0,6,6	-	-	-		
86	OHX	6	2116	-	0,6,6	-	-	-		
86	OHX	2	2063	-	0,6,6	-	-	-		
86	OHX	5	4098	-	0,6,6	-	-	-		
86	OHX	2	2108	-	0,6,6	-	-	-		
86	OHX	2	2030	-	0,6,6	-	-	-		
86	OHX	1	3928	-	0,6,6	-	-	-		
86	OHX	1	4021	-	0,6,6	-	-	-		
86	OHX	1	3802	-	0,6,6	-	-	-		
86	OHX	2	2106	-	0,6,6	-	-	-		
86	OHX	5	3994	-	0,6,6	-	-	-		
86	OHX	5	3884	-	0,6,6	-	-	-		
86	OHX	1	3894	-	0,6,6	-	-	-		
86	OHX	6	2059	-	0,6,6	-	-	-		
86	OHX	2	2105	-	0,6,6	-	-	-		
86	OHX	2	2056	-	0,6,6	-	-	-		
86	OHX	1	3775	-	0,6,6	-	-	-		
86	OHX	1	3817	-	0,6,6	-	-	-		
86	OHX	5	4033	-	0,6,6	-	-	-		
86	OHX	5	4021	-	0,6,6	-	-	-		
86	OHX	5	4072	-	0,6,6	-	-	-		
86	OHX	2	2138	-	0,6,6	-	-	-		
86	OHX	5	3933	-	0,6,6	-	-	-		
86	OHX	8	216	-	0,6,6	-	-	-		
86	OHX	1	3827	-	0,6,6	-	-	-		
86	OHX	2	2120	-	0,6,6	-	-	-		
86	OHX	1	4072	-	0,6,6	-	-	-		
86	OHX	1	3766	-	0,6,6	-	-	-		
86	OHX	5	3910	-	0,6,6	-	-	-		
86	OHX	5	4020	-	0,6,6	-	-	-		
86	OHX	1	3770	-	0,6,6	-	-	-		
86	OHX	5	4099	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	l3	404	-	0,6,6	-	-	-		
86	OHX	1	3877	-	0,6,6	-	-	-		
86	OHX	1	3898	-	0,6,6	-	-	-		
86	OHX	O3	201	-	0,6,6	-	-	-		
86	OHX	1	3926	-	0,6,6	-	-	-		
86	OHX	1	4035	-	0,6,6	-	-	-		
86	OHX	6	2071	-	0,6,6	-	-	-		
86	OHX	5	4078	-	0,6,6	-	-	-		
86	OHX	1	3867	-	0,6,6	-	-	-		
86	OHX	1	3783	-	0,6,6	-	-	-		
86	OHX	1	3913	-	0,6,6	-	-	-		
86	OHX	4	218	-	0,6,6	-	-	-		
86	OHX	m5	304	-	0,6,6	-	-	-		
86	OHX	1	3807	-	0,6,6	-	-	-		
86	OHX	5	4097	-	0,6,6	-	-	-		
86	OHX	5	3932	-	0,6,6	-	-	-		
86	OHX	6	2109	-	0,6,6	-	-	-		
86	OHX	5	3859	-	0,6,6	-	-	-		
86	OHX	1	3795	-	0,6,6	-	-	-		
86	OHX	5	4001	-	0,6,6	-	-	-		
86	OHX	1	3905	-	0,6,6	-	-	-		
86	OHX	1	4109	-	0,6,6	-	-	-		
86	OHX	5	3972	-	0,6,6	-	-	-		
86	OHX	5	4058	-	0,6,6	-	-	-		
86	OHX	5	4146	-	0,6,6	-	-	-		
86	OHX	5	3991	-	0,6,6	-	-	-		
86	OHX	7	218	-	0,6,6	-	-	-		
86	OHX	1	4012	-	0,6,6	-	-	-		
86	OHX	1	3819	-	0,6,6	-	-	-		
86	OHX	6	2137	-	0,6,6	-	-	-		
86	OHX	5	3992	-	0,6,6	-	-	-		
86	OHX	5	4144	-	0,6,6	-	-	-		
86	OHX	8	213	-	0,6,6	-	-	-		
86	OHX	2	2099	-	0,6,6	-	-	-		
86	OHX	2	2036	-	0,6,6	-	-	-		
86	OHX	2	2094	-	0,6,6	-	-	-		
86	OHX	6	2042	-	0,6,6	-	-	-		
86	OHX	2	2139	-	0,6,6	-	-	-		
86	OHX	5	4084	36	0,6,6	-	-	-		
86	OHX	5	4080	-	0,6,6	-	-	-		
86	OHX	5	3896	-	0,6,6	-	-	-		
86	OHX	2	2034	-	0,6,6	-	-	-		
86	OHX	8	218	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4130	-	0,6,6	-	-	-		
86	OHX	1	4097	-	0,6,6	-	-	-		
86	OHX	1	3932	-	0,6,6	-	-	-		
86	OHX	5	3950	-	0,6,6	-	-	-		
86	OHX	2	2072	-	0,6,6	-	-	-		
86	OHX	5	3823	-	0,6,6	-	-	-		
86	OHX	6	2034	-	0,6,6	-	-	-		
86	OHX	2	2016	-	0,6,6	-	-	-		
86	OHX	1	3864	-	0,6,6	-	-	-		
86	OHX	2	2097	-	0,6,6	-	-	-		
86	OHX	2	2058	-	0,6,6	-	-	-		
86	OHX	1	3958	-	0,6,6	-	-	-		
86	OHX	1	4009	-	0,6,6	-	-	-		
86	OHX	1	4033	-	0,6,6	-	-	-		
86	OHX	1	3811	-	0,6,6	-	-	-		
86	OHX	3	216	-	0,6,6	-	-	-		
86	OHX	5	4003	-	0,6,6	-	-	-		
86	OHX	2	2075	-	0,6,6	-	-	-		
86	OHX	6	2039	-	0,6,6	-	-	-		
86	OHX	6	2031	-	0,6,6	-	-	-		
86	OHX	5	3897	-	0,6,6	-	-	-		
86	OHX	1	3803	-	0,6,6	-	-	-		
86	OHX	L3	402	-	0,6,6	-	-	-		
86	OHX	1	4074	-	0,6,6	-	-	-		
86	OHX	1	3950	-	0,6,6	-	-	-		
86	OHX	1	4073	-	0,6,6	-	-	-		
86	OHX	6	2118	-	0,6,6	-	-	-		
86	OHX	1	4005	-	0,6,6	-	-	-		
86	OHX	O4	202	-	0,6,6	-	-	-		
86	OHX	6	2064	-	0,6,6	-	-	-		
86	OHX	6	2021	-	0,6,6	-	-	-		
86	OHX	4	231	-	0,6,6	-	-	-		
86	OHX	5	3825	-	0,6,6	-	-	-		
86	OHX	5	3966	-	0,6,6	-	-	-		
86	OHX	5	4034	-	0,6,6	-	-	-		
86	OHX	6	2038	-	0,6,6	-	-	-		
86	OHX	5	3921	-	0,6,6	-	-	-		
86	OHX	c8	203	-	0,6,6	-	-	-		
86	OHX	5	3996	-	0,6,6	-	-	-		
86	OHX	5	4138	-	0,6,6	-	-	-		
86	OHX	5	4162	-	0,6,6	-	-	-		
86	OHX	1	4034	-	0,6,6	-	-	-		
86	OHX	2	2070	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4005	-	0,6,6	-	-	-		
86	OHX	5	3885	-	0,6,6	-	-	-		
86	OHX	1	3836	-	0,6,6	-	-	-		
86	OHX	2	2010	-	0,6,6	-	-	-		
86	OHX	1	3977	-	0,6,6	-	-	-		
86	OHX	6	2080	-	0,6,6	-	-	-		
86	OHX	6	2104	-	0,6,6	-	-	-		
86	OHX	5	4010	-	0,6,6	-	-	-		
86	OHX	4	221	-	0,6,6	-	-	-		
86	OHX	1	3911	-	0,6,6	-	-	-		
86	OHX	5	3827	-	0,6,6	-	-	-		
86	OHX	6	2167	-	0,6,6	-	-	-		
86	OHX	2	2039	-	0,6,6	-	-	-		
86	OHX	5	3829	-	0,6,6	-	-	-		
86	OHX	1	3970	-	0,6,6	-	-	-		
86	OHX	5	4028	-	0,6,6	-	-	-		
86	OHX	1	3855	-	0,6,6	-	-	-		
86	OHX	1	3872	-	0,6,6	-	-	-		
86	OHX	Q2	503	-	0,6,6	-	-	-		
86	OHX	6	2182	-	0,6,6	-	-	-		
86	OHX	5	3943	-	0,6,6	-	-	-		
86	OHX	1	4077	-	0,6,6	-	-	-		
86	OHX	2	2085	-	0,6,6	-	-	-		
86	OHX	sR	401	-	0,6,6	-	-	-		
86	OHX	5	3986	-	0,6,6	-	-	-		
86	OHX	5	3915	-	0,6,6	-	-	-		
86	OHX	1	3882	-	0,6,6	-	-	-		
86	OHX	6	2139	-	0,6,6	-	-	-		
86	OHX	5	3987	-	0,6,6	-	-	-		
86	OHX	1	3927	-	0,6,6	-	-	-		
86	OHX	6	2102	-	0,6,6	-	-	-		
86	OHX	5	4126	-	0,6,6	-	-	-		
86	OHX	L5	301	-	0,6,6	-	-	-		
86	OHX	O1	201	-	0,6,6	-	-	-		
86	OHX	5	3912	-	0,6,6	-	-	-		
86	OHX	2	1997	-	0,6,6	-	-	-		
86	OHX	2	2067	-	0,6,6	-	-	-		
86	OHX	1	3966	-	0,6,6	-	-	-		
86	OHX	1	3785	-	0,6,6	-	-	-		
86	OHX	1	3801	-	0,6,6	-	-	-		
86	OHX	1	3764	-	0,6,6	-	-	-		
86	OHX	1	3919	-	0,6,6	-	-	-		
86	OHX	1	3936	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2176	-	0,6,6	-	-	-		
86	OHX	5	3929	-	0,6,6	-	-	-		
86	OHX	5	4013	-	0,6,6	-	-	-		
86	OHX	5	4041	-	0,6,6	-	-	-		
86	OHX	2	2007	-	0,6,6	-	-	-		
86	OHX	6	2106	-	0,6,6	-	-	-		
86	OHX	5	3889	-	0,6,6	-	-	-		
86	OHX	d4	201	-	0,6,6	-	-	-		
86	OHX	5	3934	-	0,6,6	-	-	-		
86	OHX	8	220	-	0,6,6	-	-	-		
86	OHX	2	2031	-	0,6,6	-	-	-		
86	OHX	5	4105	-	0,6,6	-	-	-		
86	OHX	2	2025	-	0,6,6	-	-	-		
86	OHX	2	2088	-	0,6,6	-	-	-		
86	OHX	1	3993	-	0,6,6	-	-	-		
86	OHX	5	3965	-	0,6,6	-	-	-		
86	OHX	5	4156	-	0,6,6	-	-	-		
86	OHX	1	3850	-	0,6,6	-	-	-		
86	OHX	1	3907	-	0,6,6	-	-	-		
86	OHX	6	2151	-	0,6,6	-	-	-		
86	OHX	2	2116	-	0,6,6	-	-	-		
86	OHX	1	3797	-	0,6,6	-	-	-		
86	OHX	O9	101	-	0,6,6	-	-	-		
86	OHX	1	3863	-	0,6,6	-	-	-		
86	OHX	2	2000	-	0,6,6	-	-	-		
86	OHX	2	2017	-	0,6,6	-	-	-		
86	OHX	1	3973	-	0,6,6	-	-	-		
86	OHX	6	2158	-	0,6,6	-	-	-		
86	OHX	1	4087	-	0,6,6	-	-	-		
86	OHX	6	2094	-	0,6,6	-	-	-		
86	OHX	1	4020	-	0,6,6	-	-	-		
86	OHX	1	4006	-	0,6,6	-	-	-		
86	OHX	1	3772	-	0,6,6	-	-	-		
86	OHX	m7	204	-	0,6,6	-	-	-		
86	OHX	5	3995	-	0,6,6	-	-	-		
86	OHX	1	4053	-	0,6,6	-	-	-		
86	OHX	5	4094	-	0,6,6	-	-	-		
86	OHX	5	4029	-	0,6,6	-	-	-		
86	OHX	5	3883	-	0,6,6	-	-	-		
86	OHX	5	4011	-	0,6,6	-	-	-		
86	OHX	5	4145	-	0,6,6	-	-	-		
86	OHX	1	3828	-	0,6,6	-	-	-		
86	OHX	2	2032	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2055	-	0,6,6	-	-	-		
86	OHX	6	2036	-	0,6,6	-	-	-		
86	OHX	1	3954	-	0,6,6	-	-	-		
86	OHX	6	2097	-	0,6,6	-	-	-		
86	OHX	1	4068	-	0,6,6	-	-	-		
86	OHX	2	2041	-	0,6,6	-	-	-		
86	OHX	1	3831	-	0,6,6	-	-	-		
86	OHX	5	3988	-	0,6,6	-	-	-		
86	OHX	2	2143	-	0,6,6	-	-	-		
86	OHX	1	4018	-	0,6,6	-	-	-		
86	OHX	6	2065	-	0,6,6	-	-	-		
86	OHX	2	2102	-	0,6,6	-	-	-		
86	OHX	1	3870	-	0,6,6	-	-	-		
86	OHX	5	4061	-	0,6,6	-	-	-		
86	OHX	2	2068	-	0,6,6	-	-	-		
86	OHX	2	1998	-	0,6,6	-	-	-		
86	OHX	5	3881	-	0,6,6	-	-	-		
86	OHX	6	2053	-	0,6,6	-	-	-		
86	OHX	1	3995	-	0,6,6	-	-	-		
86	OHX	1	3787	-	0,6,6	-	-	-		
86	OHX	15	303	-	0,6,6	-	-	-		
86	OHX	7	220	-	0,6,6	-	-	-		
86	OHX	1	3971	-	0,6,6	-	-	-		
86	OHX	1	4016	-	0,6,6	-	-	-		
86	OHX	5	4153	-	0,6,6	-	-	-		
86	OHX	1	4024	-	0,6,6	-	-	-		
86	OHX	5	3862	-	0,6,6	-	-	-		
86	OHX	1	3769	-	0,6,6	-	-	-		
86	OHX	6	2165	-	0,6,6	-	-	-		
86	OHX	5	4040	-	0,6,6	-	-	-		
86	OHX	1	3839	-	0,6,6	-	-	-		
86	OHX	5	4070	-	0,6,6	-	-	-		
86	OHX	1	3837	-	0,6,6	-	-	-		
86	OHX	1	4091	-	0,6,6	-	-	-		
86	OHX	5	4067	-	0,6,6	-	-	-		
86	OHX	5	4120	-	0,6,6	-	-	-		
86	OHX	5	3952	-	0,6,6	-	-	-		
86	OHX	5	4085	-	0,6,6	-	-	-		
86	OHX	q2	203	-	0,6,6	-	-	-		
86	OHX	6	2146	-	0,6,6	-	-	-		
86	OHX	4	225	-	0,6,6	-	-	-		
86	OHX	1	3881	-	0,6,6	-	-	-		
86	OHX	1	3908	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4017	-	0,6,6	-	-	-		
86	OHX	5	4152	-	0,6,6	-	-	-		
86	OHX	5	4049	-	0,6,6	-	-	-		
86	OHX	1	3822	-	0,6,6	-	-	-		
86	OHX	m9	201	-	0,6,6	-	-	-		
86	OHX	1	3848	-	0,6,6	-	-	-		
86	OHX	4	227	-	0,6,6	-	-	-		
86	OHX	5	4172	-	0,6,6	-	-	-		
86	OHX	1	4070	-	0,6,6	-	-	-		
86	OHX	2	2011	-	0,6,6	-	-	-		
86	OHX	1	3873	-	0,6,6	-	-	-		
86	OHX	5	4057	-	0,6,6	-	-	-		
86	OHX	2	2135	-	0,6,6	-	-	-		
86	OHX	5	4139	-	0,6,6	-	-	-		
86	OHX	2	2110	-	0,6,6	-	-	-		
86	OHX	1	3996	-	0,6,6	-	-	-		
86	OHX	6	2101	-	0,6,6	-	-	-		
86	OHX	1	3940	-	0,6,6	-	-	-		
86	OHX	4	217	-	0,6,6	-	-	-		
86	OHX	2	2121	-	0,6,6	-	-	-		
86	OHX	1	3999	-	0,6,6	-	-	-		
86	OHX	6	2159	-	0,6,6	-	-	-		
86	OHX	1	3974	-	0,6,6	-	-	-		
86	OHX	2	1994	-	0,6,6	-	-	-		
86	OHX	5	3955	36	0,6,6	-	-	-		
86	OHX	5	3959	-	0,6,6	-	-	-		
86	OHX	1	4044	-	0,6,6	-	-	-		
86	OHX	5	3962	-	0,6,6	-	-	-		
86	OHX	5	4022	-	0,6,6	-	-	-		
89	PRO	5	4173	89	6,7,8	0.49	0	7,8,10	1.33	1 (14%)
86	OHX	1	3879	-	0,6,6	-	-	-		
86	OHX	1	3852	-	0,6,6	-	-	-		
86	OHX	4	222	-	0,6,6	-	-	-		
86	OHX	2	2046	-	0,6,6	-	-	-		
86	OHX	1	4076	-	0,6,6	-	-	-		
86	OHX	5	3931	-	0,6,6	-	-	-		
86	OHX	1	3878	-	0,6,6	-	-	-		
86	OHX	M0	303	-	0,6,6	-	-	-		
86	OHX	5	3834	-	0,6,6	-	-	-		
86	OHX	1	3891	-	0,6,6	-	-	-		
86	OHX	5	4116	-	0,6,6	-	-	-		
86	OHX	6	2164	-	0,6,6	-	-	-		
86	OHX	6	2180	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2029	-	0,6,6	-	-	-		
86	OHX	1	3845	-	0,6,6	-	-	-		
86	OHX	1	4057	-	0,6,6	-	-	-		
86	OHX	6	2032	-	0,6,6	-	-	-		
86	OHX	1	4095	-	0,6,6	-	-	-		
86	OHX	5	4064	-	0,6,6	-	-	-		
86	OHX	5	4121	-	0,6,6	-	-	-		
86	OHX	m4	201	-	0,6,6	-	-	-		
86	OHX	1	3858	-	0,6,6	-	-	-		
86	OHX	6	2041	-	0,6,6	-	-	-		
86	OHX	2	2042	-	0,6,6	-	-	-		
86	OHX	1	4111	-	0,6,6	-	-	-		
86	OHX	2	1991	-	0,6,6	-	-	-		
86	OHX	5	3891	-	0,6,6	-	-	-		
86	OHX	2	2014	-	0,6,6	-	-	-		
86	OHX	1	3955	-	0,6,6	-	-	-		
86	OHX	1	3990	-	0,6,6	-	-	-		
86	OHX	6	2067	1	0,6,6	-	-	-		
86	OHX	6	2012	-	0,6,6	-	-	-		
86	OHX	1	3821	-	0,6,6	-	-	-		
86	OHX	2	2061	-	0,6,6	-	-	-		
86	OHX	2	2089	-	0,6,6	-	-	-		
86	OHX	2	2095	-	0,6,6	-	-	-		
86	OHX	1	3997	-	0,6,6	-	-	-		
86	OHX	M9	202	-	0,6,6	-	-	-		
86	OHX	5	4052	-	0,6,6	-	-	-		
86	OHX	1	3820	-	0,6,6	-	-	-		
86	OHX	5	4163	-	0,6,6	-	-	-		
86	OHX	6	2014	-	0,6,6	-	-	-		
86	OHX	5	3830	-	0,6,6	-	-	-		
86	OHX	d9	102	-	0,6,6	-	-	-		
86	OHX	5	3821	-	0,6,6	-	-	-		
86	OHX	1	3929	-	0,6,6	-	-	-		
86	OHX	5	4063	-	0,6,6	-	-	-		
86	OHX	1	4045	-	0,6,6	-	-	-		
86	OHX	6	2060	-	0,6,6	-	-	-		
86	OHX	1	3982	-	0,6,6	-	-	-		
86	OHX	2	2123	-	0,6,6	-	-	-		
86	OHX	6	2078	-	0,6,6	-	-	-		
86	OHX	4	233	-	0,6,6	-	-	-		
86	OHX	5	4038	-	0,6,6	-	-	-		
86	OHX	1	4090	-	0,6,6	-	-	-		
86	OHX	1	3985	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2063	-	0,6,6	-	-	-		
86	OHX	6	2131	-	0,6,6	-	-	-		
86	OHX	1	4038	-	0,6,6	-	-	-		
86	OHX	5	3832	-	0,6,6	-	-	-		
86	OHX	1	4108	-	0,6,6	-	-	-		
86	OHX	2	2125	-	0,6,6	-	-	-		
86	OHX	1	3900	-	0,6,6	-	-	-		
86	OHX	c5	201	-	0,6,6	-	-	-		
86	OHX	5	4054	-	0,6,6	-	-	-		
86	OHX	5	3930	-	0,6,6	-	-	-		
86	OHX	2	2103	-	0,6,6	-	-	-		
86	OHX	5	3867	-	0,6,6	-	-	-		
86	OHX	5	3954	-	0,6,6	-	-	-		
86	OHX	2	2145	-	0,6,6	-	-	-		
86	OHX	5	4012	-	0,6,6	-	-	-		
86	OHX	1	3786	-	0,6,6	-	-	-		
86	OHX	6	2050	-	0,6,6	-	-	-		
86	OHX	1	4059	-	0,6,6	-	-	-		
86	OHX	2	2064	-	0,6,6	-	-	-		
86	OHX	2	2093	-	0,6,6	-	-	-		
86	OHX	1	4101	-	0,6,6	-	-	-		
86	OHX	O7	104	73	0,6,6	-	-	-		
86	OHX	5	3848	-	0,6,6	-	-	-		
86	OHX	1	3934	-	0,6,6	-	-	-		
86	OHX	1	3871	-	0,6,6	-	-	-		
86	OHX	5	4140	-	0,6,6	-	-	-		
86	OHX	1	3835	-	0,6,6	-	-	-		
86	OHX	6	2099	-	0,6,6	-	-	-		
86	OHX	1	3921	-	0,6,6	-	-	-		
86	OHX	5	3888	-	0,6,6	-	-	-		
86	OHX	5	4066	-	0,6,6	-	-	-		
86	OHX	3	215	-	0,6,6	-	-	-		
86	OHX	5	3873	-	0,6,6	-	-	-		
86	OHX	1	4096	-	0,6,6	-	-	-		
86	OHX	2	2027	-	0,6,6	-	-	-		
86	OHX	5	4161	-	0,6,6	-	-	-		
86	OHX	M5	304	-	0,6,6	-	-	-		
86	OHX	1	3869	-	0,6,6	-	-	-		
86	OHX	6	2153	-	0,6,6	-	-	-		
86	OHX	o3	202	-	0,6,6	-	-	-		
86	OHX	1	4069	-	0,6,6	-	-	-		
86	OHX	8	228	-	0,6,6	-	-	-		
86	OHX	5	4159	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2077	-	0,6,6	-	-	-		
86	OHX	1	3890	-	0,6,6	-	-	-		
86	OHX	5	3937	-	0,6,6	-	-	-		
86	OHX	2	2006	-	0,6,6	-	-	-		
86	OHX	6	2179	-	0,6,6	-	-	-		
86	OHX	M0	304	-	0,6,6	-	-	-		
86	OHX	2	2098	-	0,6,6	-	-	-		
86	OHX	5	3977	-	0,6,6	-	-	-		
86	OHX	2	2015	-	0,6,6	-	-	-		
86	OHX	2	2053	-	0,6,6	-	-	-		
86	OHX	1	3761	-	0,6,6	-	-	-		
86	OHX	5	4118	-	0,6,6	-	-	-		
86	OHX	1	3989	-	0,6,6	-	-	-		
86	OHX	5	4086	-	0,6,6	-	-	-		
86	OHX	1	3843	-	0,6,6	-	-	-		
86	OHX	1	4040	-	0,6,6	-	-	-		
86	OHX	1	4093	-	0,6,6	-	-	-		
86	OHX	6	2020	-	0,6,6	-	-	-		
86	OHX	2	2052	-	0,6,6	-	-	-		
86	OHX	1	3841	-	0,6,6	-	-	-		
86	OHX	5	3903	-	0,6,6	-	-	-		
86	OHX	1	4046	-	0,6,6	-	-	-		
86	OHX	1	3798	-	0,6,6	-	-	-		
86	OHX	6	2156	-	0,6,6	-	-	-		
86	OHX	5	3946	-	0,6,6	-	-	-		
86	OHX	6	2170	-	0,6,6	-	-	-		
86	OHX	3	217	-	0,6,6	-	-	-		
86	OHX	5	4073	-	0,6,6	-	-	-		
86	OHX	5	4027	-	0,6,6	-	-	-		
86	OHX	5	3886	-	0,6,6	-	-	-		
86	OHX	1	3889	-	0,6,6	-	-	-		
86	OHX	6	2044	-	0,6,6	-	-	-		
86	OHX	5	4169	-	0,6,6	-	-	-		
86	OHX	5	4000	-	0,6,6	-	-	-		
86	OHX	2	2009	-	0,6,6	-	-	-		
86	OHX	5	3911	-	0,6,6	-	-	-		
86	OHX	1	3886	-	0,6,6	-	-	-		
86	OHX	1	3847	-	0,6,6	-	-	-		
86	OHX	6	2075	-	0,6,6	-	-	-		
86	OHX	2	2033	-	0,6,6	-	-	-		
86	OHX	5	3928	-	0,6,6	-	-	-		
86	OHX	1	3938	-	0,6,6	-	-	-		
86	OHX	6	2115	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4095	-	0,6,6	-	-	-		
86	OHX	1	4031	-	0,6,6	-	-	-		
86	OHX	5	3860	-	0,6,6	-	-	-		
86	OHX	N9	101	-	0,6,6	-	-	-		
86	OHX	6	2140	-	0,6,6	-	-	-		
86	OHX	5	4081	-	0,6,6	-	-	-		
86	OHX	7	223	-	0,6,6	-	-	-		
86	OHX	5	4082	-	0,6,6	-	-	-		
86	OHX	2	2132	-	0,6,6	-	-	-		
86	OHX	1	4036	-	0,6,6	-	-	-		
86	OHX	1	4083	-	0,6,6	-	-	-		
86	OHX	5	3905	-	0,6,6	-	-	-		
86	OHX	5	4103	-	0,6,6	-	-	-		
86	OHX	5	4030	-	0,6,6	-	-	-		
86	OHX	1	3972	-	0,6,6	-	-	-		
86	OHX	1	4043	-	0,6,6	-	-	-		
86	OHX	6	2173	-	0,6,6	-	-	-		
86	OHX	5	4036	-	0,6,6	-	-	-		
86	OHX	1	3904	-	0,6,6	-	-	-		
86	OHX	5	4050	-	0,6,6	-	-	-		
86	OHX	1	3965	-	0,6,6	-	-	-		
86	OHX	6	2084	-	0,6,6	-	-	-		
86	OHX	5	4060	-	0,6,6	-	-	-		
86	OHX	5	3978	-	0,6,6	-	-	-		
86	OHX	6	2123	-	0,6,6	-	-	-		
86	OHX	5	4148	-	0,6,6	-	-	-		
86	OHX	1	3899	-	0,6,6	-	-	-		
86	OHX	5	4089	-	0,6,6	-	-	-		
86	OHX	8	212	-	0,6,6	-	-	-		
86	OHX	1	3969	-	0,6,6	-	-	-		
86	OHX	6	2166	-	0,6,6	-	-	-		
86	OHX	5	3890	-	0,6,6	-	-	-		
86	OHX	19	201	-	0,6,6	-	-	-		
86	OHX	1	4082	-	0,6,6	-	-	-		
86	OHX	2	2023	-	0,6,6	-	-	-		
86	OHX	2	2013	-	0,6,6	-	-	-		
86	OHX	5	3840	-	0,6,6	-	-	-		
86	OHX	5	3894	-	0,6,6	-	-	-		
86	OHX	5	4141	-	0,6,6	-	-	-		
86	OHX	6	2030	-	0,6,6	-	-	-		
86	OHX	1	3792	-	0,6,6	-	-	-		
86	OHX	7	224	-	0,6,6	-	-	-		
86	OHX	m5	305	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4050	-	0,6,6	-	-	-		
86	OHX	1	4002	-	0,6,6	-	-	-		
86	OHX	1	3916	-	0,6,6	-	-	-		
86	OHX	1	3906	-	0,6,6	-	-	-		
86	OHX	5	4026	-	0,6,6	-	-	-		
86	OHX	5	4037	-	0,6,6	-	-	-		
86	OHX	2	2084	-	0,6,6	-	-	-		
86	OHX	5	3865	-	0,6,6	-	-	-		
86	OHX	1	4049	-	0,6,6	-	-	-		
86	OHX	2	1995	-	0,6,6	-	-	-		
86	OHX	1	4037	-	0,6,6	-	-	-		
86	OHX	1	4064	-	0,6,6	-	-	-		
86	OHX	M8	201	-	0,6,6	-	-	-		
86	OHX	1	3917	-	0,6,6	-	-	-		
86	OHX	1	3856	-	0,6,6	-	-	-		
86	OHX	1	4098	-	0,6,6	-	-	-		
86	OHX	1	3865	-	0,6,6	-	-	-		
86	OHX	5	3842	-	0,6,6	-	-	-		
86	OHX	5	3973	-	0,6,6	-	-	-		
86	OHX	5	4074	-	0,6,6	-	-	-		
86	OHX	8	215	-	0,6,6	-	-	-		
86	OHX	2	2107	-	0,6,6	-	-	-		
86	OHX	5	4093	-	0,6,6	-	-	-		
86	OHX	5	3913	-	0,6,6	-	-	-		
86	OHX	2	2146	-	0,6,6	-	-	-		
86	OHX	1	3846	-	0,6,6	-	-	-		
86	OHX	6	2025	-	0,6,6	-	-	-		
86	OHX	1	3952	-	0,6,6	-	-	-		
86	OHX	5	3964	-	0,6,6	-	-	-		
86	OHX	1	3826	-	0,6,6	-	-	-		
86	OHX	1	3948	-	0,6,6	-	-	-		
86	OHX	5	4025	-	0,6,6	-	-	-		
86	OHX	1	3883	-	0,6,6	-	-	-		
86	OHX	6	2093	-	0,6,6	-	-	-		
86	OHX	6	2172	-	0,6,6	-	-	-		
86	OHX	5	4051	-	0,6,6	-	-	-		
86	OHX	1	4062	-	0,6,6	-	-	-		
86	OHX	8	231	-	0,6,6	-	-	-		
86	OHX	1	3816	-	0,6,6	-	-	-		
86	OHX	6	2073	-	0,6,6	-	-	-		
86	OHX	5	3909	-	0,6,6	-	-	-		
86	OHX	5	4019	-	0,6,6	-	-	-		
86	OHX	5	3927	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4041	-	0,6,6	-	-	-		
86	OHX	5	4047	-	0,6,6	-	-	-		
86	OHX	5	3831	-	0,6,6	-	-	-		
86	OHX	1	3790	-	0,6,6	-	-	-		
86	OHX	5	4167	-	0,6,6	-	-	-		
86	OHX	1	3861	-	0,6,6	-	-	-		
86	OHX	1	3789	-	0,6,6	-	-	-		
86	OHX	1	3829	-	0,6,6	-	-	-		
86	OHX	5	3869	-	0,6,6	-	-	-		
86	OHX	1	4028	-	0,6,6	-	-	-		
86	OHX	5	3939	-	0,6,6	-	-	-		
86	OHX	5	4129	-	0,6,6	-	-	-		
86	OHX	1	3991	-	0,6,6	-	-	-		
86	OHX	2	2148	-	0,6,6	-	-	-		
86	OHX	5	3864	-	0,6,6	-	-	-		
86	OHX	5	4100	-	0,6,6	-	-	-		
86	OHX	5	4032	-	0,6,6	-	-	-		
86	OHX	1	4078	-	0,6,6	-	-	-		
86	OHX	6	2098	-	0,6,6	-	-	-		
86	OHX	3	219	-	0,6,6	-	-	-		
86	OHX	2	2081	-	0,6,6	-	-	-		
86	OHX	6	2056	-	0,6,6	-	-	-		
86	OHX	5	3942	-	0,6,6	-	-	-		
86	OHX	5	4154	-	0,6,6	-	-	-		
86	OHX	2	2004	-	0,6,6	-	-	-		
86	OHX	1	3912	-	0,6,6	-	-	-		
86	OHX	1	3924	-	0,6,6	-	-	-		
86	OHX	5	4071	-	0,6,6	-	-	-		
86	OHX	15	302	-	0,6,6	-	-	-		
86	OHX	7	217	-	0,6,6	-	-	-		
86	OHX	2	2078	-	0,6,6	-	-	-		
86	OHX	6	2155	-	0,6,6	-	-	-		
89	PRO	B	101	84,89	6,7,8	0.68	0	7,8,10	1.31	1 (14%)
86	OHX	1	3851	-	0,6,6	-	-	-		
86	OHX	6	2013	-	0,6,6	-	-	-		
86	OHX	c3	201	-	0,6,6	-	-	-		
86	OHX	6	2152	-	0,6,6	-	-	-		
86	OHX	5	4137	-	0,6,6	-	-	-		
86	OHX	8	224	-	0,6,6	-	-	-		
86	OHX	5	3917	-	0,6,6	-	-	-		
86	OHX	5	3907	-	0,6,6	-	-	-		
86	OHX	1	4094	-	0,6,6	-	-	-		
86	OHX	6	2132	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4075	-	0,6,6	-	-	-		
86	OHX	s9	201	-	0,6,6	-	-	-		
86	OHX	SR	401	-	0,6,6	-	-	-		
86	OHX	1	3805	-	0,6,6	-	-	-		
86	OHX	5	3836	-	0,6,6	-	-	-		
86	OHX	5	3919	-	0,6,6	-	-	-		
86	OHX	1	3804	-	0,6,6	-	-	-		
86	OHX	5	3967	-	0,6,6	-	-	-		
86	OHX	5	4113	-	0,6,6	-	-	-		
86	OHX	1	3765	-	0,6,6	-	-	-		
86	OHX	6	2105	-	0,6,6	-	-	-		
86	OHX	5	4042	-	0,6,6	-	-	-		
86	OHX	2	1996	-	0,6,6	-	-	-		
86	OHX	1	3784	-	0,6,6	-	-	-		
86	OHX	5	4124	-	0,6,6	-	-	-		
86	OHX	2	2073	-	0,6,6	-	-	-		
86	OHX	5	4062	-	0,6,6	-	-	-		
86	OHX	5	4092	-	0,6,6	-	-	-		
86	OHX	5	3976	-	0,6,6	-	-	-		
86	OHX	5	3852	-	0,6,6	-	-	-		
86	OHX	14	403	-	0,6,6	-	-	-		
86	OHX	5	3870	-	0,6,6	-	-	-		
86	OHX	8	225	-	0,6,6	-	-	-		
86	OHX	2	2037	-	0,6,6	-	-	-		
86	OHX	2	2050	-	0,6,6	-	-	-		
86	OHX	1	3933	-	0,6,6	-	-	-		
86	OHX	6	2110	-	0,6,6	-	-	-		
86	OHX	5	3841	-	0,6,6	-	-	-		
86	OHX	5	3968	-	0,6,6	-	-	-		
86	OHX	2	1992	-	0,6,6	-	-	-		
86	OHX	5	4170	-	0,6,6	-	-	-		
86	OHX	5	3924	-	0,6,6	-	-	-		
86	OHX	1	3981	-	0,6,6	-	-	-		
86	OHX	5	4006	-	0,6,6	-	-	-		
86	OHX	2	2062	-	0,6,6	-	-	-		
86	OHX	5	3861	-	0,6,6	-	-	-		
86	OHX	5	4069	-	0,6,6	-	-	-		
86	OHX	5	4149	-	0,6,6	-	-	-		
86	OHX	1	4023	-	0,6,6	-	-	-		
86	OHX	5	4164	-	0,6,6	-	-	-		
86	OHX	2	2133	-	0,6,6	-	-	-		
86	OHX	1	3944	-	0,6,6	-	-	-		
86	OHX	6	2112	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	8	223	-	0,6,6	-	-	-		
86	OHX	1	4088	-	0,6,6	-	-	-		
86	OHX	1	3779	-	0,6,6	-	-	-		
86	OHX	6	2183	-	0,6,6	-	-	-		
86	OHX	2	2109	-	0,6,6	-	-	-		
86	OHX	2	2091	-	0,6,6	-	-	-		
86	OHX	2	2083	-	0,6,6	-	-	-		
86	OHX	1	4058	-	0,6,6	-	-	-		
86	OHX	1	4061	-	0,6,6	-	-	-		
86	OHX	1	4015	-	0,6,6	-	-	-		
86	OHX	5	3944	-	0,6,6	-	-	-		
86	OHX	4	216	-	0,6,6	-	-	-		
86	OHX	5	3953	-	0,6,6	-	-	-		
86	OHX	S6	301	-	0,6,6	-	-	-		
86	OHX	8	222	-	0,6,6	-	-	-		
86	OHX	1	3808	-	0,6,6	-	-	-		
86	OHX	2	2024	-	0,6,6	-	-	-		
86	OHX	1	3857	-	0,6,6	-	-	-		
86	OHX	5	3839	-	0,6,6	-	-	-		
86	OHX	5	4131	-	0,6,6	-	-	-		
86	OHX	5	3925	-	0,6,6	-	-	-		
86	OHX	6	2168	-	0,6,6	-	-	-		
86	OHX	5	4091	-	0,6,6	-	-	-		
86	OHX	5	3851	-	0,6,6	-	-	-		
86	OHX	2	2022	-	0,6,6	-	-	-		
86	OHX	1	3887	-	0,6,6	-	-	-		
86	OHX	5	3844	-	0,6,6	-	-	-		
86	OHX	5	4104	-	0,6,6	-	-	-		
86	OHX	1	4079	-	0,6,6	-	-	-		
86	OHX	1	4032	-	0,6,6	-	-	-		
86	OHX	s4	602	-	0,6,6	-	-	-		
86	OHX	5	4087	-	0,6,6	-	-	-		
86	OHX	1	3962	-	0,6,6	-	-	-		
86	OHX	m1	201	-	0,6,6	-	-	-		
86	OHX	m5	306	-	0,6,6	-	-	-		
86	OHX	2	2054	-	0,6,6	-	-	-		
86	OHX	1	4060	-	0,6,6	-	-	-		
86	OHX	6	2022	-	0,6,6	-	-	-		
86	OHX	2	2008	-	0,6,6	-	-	-		
86	OHX	5	4077	-	0,6,6	-	-	-		
86	OHX	2	2002	-	0,6,6	-	-	-		
86	OHX	2	2131	-	0,6,6	-	-	-		
86	OHX	1	3941	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	M5	303	-	0,6,6	-	-	-		
86	OHX	2	2113	-	0,6,6	-	-	-		
86	OHX	6	2054	-	0,6,6	-	-	-		
86	OHX	5	3898	-	0,6,6	-	-	-		
86	OHX	5	3926	-	0,6,6	-	-	-		
86	OHX	5	4024	-	0,6,6	-	-	-		
86	OHX	5	4035	-	0,6,6	-	-	-		
88	SPS	5	3403	-	20,23,23	3.60	14 (70%)	23,30,30	2.67	13 (56%)
86	OHX	1	4106	-	0,6,6	-	-	-		
86	OHX	5	4053	-	0,6,6	-	-	-		
86	OHX	6	2095	-	0,6,6	-	-	-		
86	OHX	2	2026	-	0,6,6	-	-	-		
86	OHX	5	4101	-	0,6,6	-	-	-		
86	OHX	2	2082	-	0,6,6	-	-	-		
86	OHX	1	3844	-	0,6,6	-	-	-		
86	OHX	2	2074	-	0,6,6	-	-	-		
86	OHX	1	3771	-	0,6,6	-	-	-		
86	OHX	1	3947	-	0,6,6	-	-	-		
86	OHX	1	3949	-	0,6,6	-	-	-		
86	OHX	1	4010	-	0,6,6	-	-	-		
86	OHX	6	2148	-	0,6,6	-	-	-		
86	OHX	6	2066	-	0,6,6	-	-	-		
86	OHX	6	2103	-	0,6,6	-	-	-		
86	OHX	2	2090	-	0,6,6	-	-	-		
86	OHX	5	3822	-	0,6,6	-	-	-		
86	OHX	5	3974	-	0,6,6	-	-	-		
86	OHX	5	3983	-	0,6,6	-	-	-		
86	OHX	6	2082	-	0,6,6	-	-	-		
86	OHX	5	4127	-	0,6,6	-	-	-		
86	OHX	1	3914	-	0,6,6	-	-	-		
86	OHX	7	216	-	0,6,6	-	-	-		
86	OHX	1	3920	-	0,6,6	-	-	-		
86	OHX	5	4090	-	0,6,6	-	-	-		
86	OHX	1	3892	-	0,6,6	-	-	-		
86	OHX	5	3866	-	0,6,6	-	-	-		
86	OHX	1	4055	-	0,6,6	-	-	-		
86	OHX	6	2072	-	0,6,6	-	-	-		
86	OHX	1	3806	-	0,6,6	-	-	-		
86	OHX	6	2149	-	0,6,6	-	-	-		
86	OHX	5	3923	-	0,6,6	-	-	-		
86	OHX	5	4044	-	0,6,6	-	-	-		
86	OHX	6	2177	-	0,6,6	-	-	-		
86	OHX	2	2137	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	3	212	-	0,6,6	-	-	-		
86	OHX	5	3922	-	0,6,6	-	-	-		
86	OHX	2	2071	-	0,6,6	-	-	-		
86	OHX	5	4048	-	0,6,6	-	-	-		
86	OHX	5	3854	-	0,6,6	-	-	-		
86	OHX	m8	201	-	0,6,6	-	-	-		
86	OHX	5	3938	-	0,6,6	-	-	-		
86	OHX	6	2081	-	0,6,6	-	-	-		
86	OHX	6	2058	-	0,6,6	-	-	-		
86	OHX	5	4160	-	0,6,6	-	-	-		
86	OHX	2	2040	-	0,6,6	-	-	-		
86	OHX	8	219	-	0,6,6	-	-	-		
86	OHX	6	2134	-	0,6,6	-	-	-		
86	OHX	1	4102	-	0,6,6	-	-	-		
86	OHX	1	3876	-	0,6,6	-	-	-		
86	OHX	5	4045	-	0,6,6	-	-	-		
86	OHX	1	4039	-	0,6,6	-	-	-		
86	OHX	5	3982	-	0,6,6	-	-	-		
86	OHX	6	2169	-	0,6,6	-	-	-		
86	OHX	8	230	-	0,6,6	-	-	-		
86	OHX	5	3961	-	0,6,6	-	-	-		
86	OHX	2	2092	-	0,6,6	-	-	-		
86	OHX	1	3951	-	0,6,6	-	-	-		
86	OHX	6	2089	-	0,6,6	-	-	-		
86	OHX	5	3941	-	0,6,6	-	-	-		
86	OHX	m6	201	-	0,6,6	-	-	-		
86	OHX	6	2171	-	0,6,6	-	-	-		
86	OHX	2	2118	-	0,6,6	-	-	-		
86	OHX	1	3780	-	0,6,6	-	-	-		
86	OHX	1	3895	-	0,6,6	-	-	-		
86	OHX	s1	301	-	0,6,6	-	-	-		
86	OHX	6	2162	-	0,6,6	-	-	-		
86	OHX	6	2016	-	0,6,6	-	-	-		
86	OHX	1	3818	-	0,6,6	-	-	-		
86	OHX	6	2107	-	0,6,6	-	-	-		
86	OHX	2	2119	-	0,6,6	-	-	-		
86	OHX	1	3853	-	0,6,6	-	-	-		
86	OHX	1	3833	-	0,6,6	-	-	-		
86	OHX	1	3814	-	0,6,6	-	-	-		
86	OHX	1	3880	-	0,6,6	-	-	-		
86	OHX	1	4026	-	0,6,6	-	-	-		
86	OHX	6	2100	-	0,6,6	-	-	-		
86	OHX	6	2154	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2175	-	0,6,6	-	-	-		
86	OHX	5	3879	-	0,6,6	-	-	-		
86	OHX	1	3945	-	0,6,6	-	-	-		
86	OHX	5	3895	-	0,6,6	-	-	-		
86	OHX	C3	201	-	0,6,6	-	-	-		
86	OHX	1	3838	-	0,6,6	-	-	-		
86	OHX	1	3930	-	0,6,6	-	-	-		
86	OHX	5	4068	-	0,6,6	-	-	-		
89	PRO	C	101	84,89	6,7,8	0.57	0	7,8,10	1.41	1 (14%)
86	OHX	2	2038	-	0,6,6	-	-	-		
86	OHX	1	3918	-	0,6,6	-	-	-		
86	OHX	5	3872	-	0,6,6	-	-	-		
86	OHX	5	4108	-	0,6,6	-	-	-		
86	OHX	1	4029	-	0,6,6	-	-	-		
86	OHX	2	2151	-	0,6,6	-	-	-		
86	OHX	5	3835	-	0,6,6	-	-	-		
86	OHX	5	4018	-	0,6,6	-	-	-		
86	OHX	2	1999	-	0,6,6	-	-	-		
86	OHX	5	4119	-	0,6,6	-	-	-		
86	OHX	5	3849	-	0,6,6	-	-	-		
86	OHX	2	2018	-	0,6,6	-	-	-		
86	OHX	2	2080	-	0,6,6	-	-	-		
86	OHX	5	4096	-	0,6,6	-	-	-		
86	OHX	1	3935	-	0,6,6	-	-	-		
86	OHX	6	2029	-	0,6,6	-	-	-		
86	OHX	m0	302	-	0,6,6	-	-	-		
86	OHX	1	4022	-	0,6,6	-	-	-		
86	OHX	6	2133	-	0,6,6	-	-	-		
86	OHX	2	2035	-	0,6,6	-	-	-		
86	OHX	5	4075	-	0,6,6	-	-	-		
86	OHX	6	2143	-	0,6,6	-	-	-		
86	OHX	s8	303	-	0,6,6	-	-	-		
86	OHX	5	3901	-	0,6,6	-	-	-		
86	OHX	6	2023	-	0,6,6	-	-	-		
86	OHX	6	2055	-	0,6,6	-	-	-		
86	OHX	2	2005	-	0,6,6	-	-	-		
86	OHX	5	3875	-	0,6,6	-	-	-		
86	OHX	1	3976	-	0,6,6	-	-	-		
86	OHX	5	3989	-	0,6,6	-	-	-		
86	OHX	1	3778	-	0,6,6	-	-	-		
86	OHX	6	2027	-	0,6,6	-	-	-		
86	OHX	2	2142	-	0,6,6	-	-	-		
86	OHX	6	2088	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3833	-	0,6,6	-	-	-		
86	OHX	2	2111	-	0,6,6	-	-	-		
86	OHX	1	3868	-	0,6,6	-	-	-		
86	OHX	5	3993	-	0,6,6	-	-	-		
86	OHX	6	2068	-	0,6,6	-	-	-		
86	OHX	1	3943	-	0,6,6	-	-	-		
86	OHX	5	4171	-	0,6,6	-	-	-		
86	OHX	6	2077	-	0,6,6	-	-	-		
86	OHX	5	4143	-	0,6,6	-	-	-		
86	OHX	2	2128	-	0,6,6	-	-	-		
86	OHX	1	3984	-	0,6,6	-	-	-		
86	OHX	1	4080	-	0,6,6	-	-	-		
86	OHX	4	223	-	0,6,6	-	-	-		
86	OHX	5	4059	-	0,6,6	-	-	-		
86	OHX	1	4104	-	0,6,6	-	-	-		
86	OHX	5	3949	-	0,6,6	-	-	-		
86	OHX	5	3957	-	0,6,6	-	-	-		
86	OHX	6	2121	-	0,6,6	-	-	-		
86	OHX	1	3987	-	0,6,6	-	-	-		
86	OHX	6	2138	-	0,6,6	-	-	-		
86	OHX	2	2127	-	0,6,6	-	-	-		
86	OHX	6	2052	-	0,6,6	-	-	-		
86	OHX	1	3884	-	0,6,6	-	-	-		
86	OHX	D9	102	-	0,6,6	-	-	-		
86	OHX	1	3824	-	0,6,6	-	-	-		
86	OHX	2	2003	-	0,6,6	-	-	-		
86	OHX	S1	301	-	0,6,6	-	-	-		
86	OHX	6	2074	-	0,6,6	-	-	-		
86	OHX	1	3859	-	0,6,6	-	-	-		
86	OHX	1	3975	-	0,6,6	-	-	-		
86	OHX	5	3863	-	0,6,6	-	-	-		
86	OHX	5	3877	-	0,6,6	-	-	-		
86	OHX	5	4128	-	0,6,6	-	-	-		
86	OHX	2	2086	-	0,6,6	-	-	-		
86	OHX	5	3828	-	0,6,6	-	-	-		
86	OHX	5	3971	-	0,6,6	-	-	-		
86	OHX	5	4150	-	0,6,6	-	-	-		
86	OHX	2	2019	-	0,6,6	-	-	-		
86	OHX	5	4166	-	0,6,6	-	-	-		
86	OHX	1	4099	-	0,6,6	-	-	-		
86	OHX	5	3918	-	0,6,6	-	-	-		
86	OHX	2	2021	-	0,6,6	-	-	-		
86	OHX	6	2108	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4056	-	0,6,6	-	-	-		
86	OHX	5	4043	-	0,6,6	-	-	-		
86	OHX	5	4004	-	0,6,6	-	-	-		
86	OHX	5	3847	-	0,6,6	-	-	-		
86	OHX	2	2066	-	0,6,6	-	-	-		
86	OHX	1	4042	-	0,6,6	-	-	-		
86	OHX	1	4092	-	0,6,6	-	-	-		
86	OHX	5	4134	-	0,6,6	-	-	-		
86	OHX	1	4004	-	0,6,6	-	-	-		
86	OHX	5	4109	-	0,6,6	-	-	-		
86	OHX	6	2061	-	0,6,6	-	-	-		
86	OHX	1	3777	-	0,6,6	-	-	-		
86	OHX	6	2163	-	0,6,6	-	-	-		
86	OHX	5	4009	-	0,6,6	-	-	-		
86	OHX	2	2012	-	0,6,6	-	-	-		
86	OHX	6	2046	-	0,6,6	-	-	-		
86	OHX	6	2040	-	0,6,6	-	-	-		
86	OHX	C8	201	-	0,6,6	-	-	-		
86	OHX	2	2150	-	0,6,6	-	-	-		
86	OHX	1	4089	-	0,6,6	-	-	-		
86	OHX	5	4110	-	0,6,6	-	-	-		
86	OHX	5	4079	-	0,6,6	-	-	-		
86	OHX	1	3788	-	0,6,6	-	-	-		
86	OHX	6	2181	-	0,6,6	-	-	-		
86	OHX	5	3824	-	0,6,6	-	-	-		
86	OHX	5	3956	-	0,6,6	-	-	-		
86	OHX	8	226	-	0,6,6	-	-	-		
86	OHX	2	2048	-	0,6,6	-	-	-		
86	OHX	1	3830	-	0,6,6	-	-	-		
86	OHX	6	2043	-	0,6,6	-	-	-		
86	OHX	6	2125	-	0,6,6	-	-	-		
86	OHX	6	2174	-	0,6,6	-	-	-		
86	OHX	5	4151	-	0,6,6	-	-	-		
86	OHX	o7	502	-	0,6,6	-	-	-		
86	OHX	1	3840	-	0,6,6	-	-	-		
86	OHX	1	4003	-	0,6,6	-	-	-		
86	OHX	6	2157	-	0,6,6	-	-	-		
86	OHX	L3	403	-	0,6,6	-	-	-		
86	OHX	5	3906	-	0,6,6	-	-	-		
86	OHX	6	2048	-	0,6,6	-	-	-		
86	OHX	1	3809	-	0,6,6	-	-	-		
86	OHX	1	3767	-	0,6,6	-	-	-		
86	OHX	5	3958	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3986	-	0,6,6	-	-	-		
86	OHX	5	3850	-	0,6,6	-	-	-		
86	OHX	5	3837	-	0,6,6	-	-	-		
86	OHX	5	4014	-	0,6,6	-	-	-		
86	OHX	6	2119	-	0,6,6	-	-	-		
86	OHX	1	3854	-	0,6,6	-	-	-		
86	OHX	6	2129	-	0,6,6	-	-	-		
86	OHX	6	2017	-	0,6,6	-	-	-		
86	OHX	5	3846	-	0,6,6	-	-	-		
86	OHX	1	3842	-	0,6,6	-	-	-		
86	OHX	5	3940	-	0,6,6	-	-	-		
86	OHX	5	3963	-	0,6,6	-	-	-		
86	OHX	6	2051	-	0,6,6	-	-	-		
86	OHX	1	3815	-	0,6,6	-	-	-		
86	OHX	5	3826	-	0,6,6	-	-	-		
86	OHX	M6	203	-	0,6,6	-	-	-		
86	OHX	5	3984	-	0,6,6	-	-	-		
86	OHX	5	4008	-	0,6,6	-	-	-		
86	OHX	1	3897	-	0,6,6	-	-	-		
86	OHX	1	4008	-	0,6,6	-	-	-		
86	OHX	5	4017	-	0,6,6	-	-	-		
86	OHX	2	2087	-	0,6,6	-	-	-		
86	OHX	2	2104	-	0,6,6	-	-	-		
86	OHX	2	2051	-	0,6,6	-	-	-		
86	OHX	2	2101	-	0,6,6	-	-	-		
86	OHX	6	2049	-	0,6,6	-	-	-		
86	OHX	5	3981	-	0,6,6	-	-	-		
86	OHX	1	4105	-	0,6,6	-	-	-		
86	OHX	2	2059	-	0,6,6	-	-	-		
86	OHX	5	4132	-	0,6,6	-	-	-		
86	OHX	5	3856	-	0,6,6	-	-	-		
86	OHX	5	4007	-	0,6,6	-	-	-		
86	OHX	1	3781	-	0,6,6	-	-	-		
86	OHX	1	4051	-	0,6,6	-	-	-		
86	OHX	1	3910	-	0,6,6	-	-	-		
86	OHX	6	2018	-	0,6,6	-	-	-		
86	OHX	5	3878	-	0,6,6	-	-	-		
86	OHX	3	213	-	0,6,6	-	-	-		
86	OHX	6	2076	-	0,6,6	-	-	-		
86	OHX	6	2086	-	0,6,6	-	-	-		
86	OHX	S9	201	-	0,6,6	-	-	-		
86	OHX	6	2113	-	0,6,6	-	-	-		
86	OHX	2	2047	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3885	-	0,6,6	-	-	-		
86	OHX	2	2117	-	0,6,6	-	-	-		
86	OHX	1	3909	-	0,6,6	-	-	-		
86	OHX	4	220	-	0,6,6	-	-	-		
86	OHX	6	2178	-	0,6,6	-	-	-		
86	OHX	6	2161	-	0,6,6	-	-	-		
86	OHX	5	3899	-	0,6,6	-	-	-		
86	OHX	5	3935	-	0,6,6	-	-	-		
86	OHX	2	2130	-	0,6,6	-	-	-		
86	OHX	4	226	-	0,6,6	-	-	-		
86	OHX	5	4111	-	0,6,6	-	-	-		
86	OHX	5	4135	-	0,6,6	-	-	-		
86	OHX	5	3855	-	0,6,6	-	-	-		
86	OHX	8	211	-	0,6,6	-	-	-		
86	OHX	5	3936	-	0,6,6	-	-	-		
86	OHX	1	3967	-	0,6,6	-	-	-		
86	OHX	1	3849	-	0,6,6	-	-	-		
86	OHX	1	4103	-	0,6,6	-	-	-		
86	OHX	6	2128	-	0,6,6	-	-	-		
86	OHX	S8	301	-	0,6,6	-	-	-		
86	OHX	5	3817	-	0,6,6	-	-	-		
86	OHX	1	3813	-	0,6,6	-	-	-		
86	OHX	1	3994	-	0,6,6	-	-	-		
86	OHX	1	4001	-	0,6,6	-	-	-		
86	OHX	5	3843	-	0,6,6	-	-	-		
86	OHX	6	2070	-	0,6,6	-	-	-		
86	OHX	5	3882	-	0,6,6	-	-	-		
86	OHX	8	221	-	0,6,6	-	-	-		
86	OHX	L3	404	-	0,6,6	-	-	-		
86	OHX	1	4100	-	0,6,6	-	-	-		
86	OHX	C5	201	17	0,6,6	-	-	-		
86	OHX	6	2111	-	0,6,6	-	-	-		
86	OHX	5	4155	-	0,6,6	-	-	-		
86	OHX	2	2149	-	0,6,6	-	-	-		
86	OHX	5	3960	-	0,6,6	-	-	-		
86	OHX	7	219	-	0,6,6	-	-	-		
86	OHX	4	230	-	0,6,6	-	-	-		
86	OHX	1	3896	-	0,6,6	-	-	-		
86	OHX	4	232	-	0,6,6	-	-	-		
86	OHX	2	2001	-	0,6,6	-	-	-		
86	OHX	2	2069	-	0,6,6	-	-	-		
86	OHX	1	3799	-	0,6,6	-	-	-		
86	OHX	1	3942	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2033	-	0,6,6	-	-	-		
86	OHX	6	2160	-	0,6,6	-	-	-		
86	OHX	5	3951	-	0,6,6	-	-	-		
86	OHX	1	3796	-	0,6,6	-	-	-		
86	OHX	5	3997	-	0,6,6	-	-	-		
86	OHX	1	3773	-	0,6,6	-	-	-		
86	OHX	o7	503	-	0,6,6	-	-	-		
86	OHX	2	2141	-	0,6,6	-	-	-		
86	OHX	2	2079	-	0,6,6	-	-	-		
86	OHX	5	3900	-	0,6,6	-	-	-		
86	OHX	6	2085	-	0,6,6	-	-	-		
86	OHX	2	2076	-	0,6,6	-	-	-		
86	OHX	1	3939	-	0,6,6	-	-	-		
86	OHX	5	3893	-	0,6,6	-	-	-		
86	OHX	c5	202	17	0,6,6	-	-	-		
86	OHX	7	215	-	0,6,6	-	-	-		
86	OHX	2	2147	-	0,6,6	-	-	-		
86	OHX	2	2126	-	0,6,6	-	-	-		
86	OHX	5	3980	-	0,6,6	-	-	-		
86	OHX	1	3983	-	0,6,6	-	-	-		
86	OHX	3	209	-	0,6,6	-	-	-		
86	OHX	5	3871	-	0,6,6	-	-	-		
86	OHX	5	4142	-	0,6,6	-	-	-		
86	OHX	1	4067	-	0,6,6	-	-	-		
86	OHX	5	3947	-	0,6,6	-	-	-		
86	OHX	7	214	-	0,6,6	-	-	-		
86	OHX	1	4013	-	0,6,6	-	-	-		
86	OHX	2	2122	-	0,6,6	-	-	-		
86	OHX	1	3946	-	0,6,6	-	-	-		
86	OHX	1	3925	-	0,6,6	-	-	-		
86	OHX	3	214	-	0,6,6	-	-	-		
86	OHX	8	217	-	0,6,6	-	-	-		
86	OHX	2	2100	-	0,6,6	-	-	-		
86	OHX	1	3810	-	0,6,6	-	-	-		
86	OHX	5	4065	-	0,6,6	-	-	-		
86	OHX	5	4125	-	0,6,6	-	-	-		
86	OHX	5	4165	-	0,6,6	-	-	-		
86	OHX	6	2087	-	0,6,6	-	-	-		
86	OHX	5	4136	-	0,6,6	-	-	-		
86	OHX	1	4000	-	0,6,6	-	-	-		
86	OHX	1	3968	-	0,6,6	-	-	-		
86	OHX	1	3800	-	0,6,6	-	-	-		
86	OHX	4	228	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	l3	403	-	0,6,6	-	-	-		
86	OHX	1	3791	-	0,6,6	-	-	-		
86	OHX	5	3887	-	0,6,6	-	-	-		
86	OHX	6	2037	-	0,6,6	-	-	-		
86	OHX	6	2135	-	0,6,6	-	-	-		
86	OHX	6	2057	-	0,6,6	-	-	-		
86	OHX	1	4025	-	0,6,6	-	-	-		
86	OHX	5	4002	-	0,6,6	-	-	-		
86	OHX	1	3960	-	0,6,6	-	-	-		
86	OHX	1	3959	-	0,6,6	-	-	-		
86	OHX	5	4147	-	0,6,6	-	-	-		
86	OHX	1	3794	-	0,6,6	-	-	-		
86	OHX	3	218	-	0,6,6	-	-	-		
86	OHX	1	3812	-	0,6,6	-	-	-		
86	OHX	2	2028	-	0,6,6	-	-	-		
86	OHX	2	2057	-	0,6,6	-	-	-		
86	OHX	1	3979	-	0,6,6	-	-	-		
86	OHX	1	4030	-	0,6,6	-	-	-		
86	OHX	6	2062	-	0,6,6	-	-	-		
86	OHX	5	3876	-	0,6,6	-	-	-		
86	OHX	5	4102	-	0,6,6	-	-	-		
86	OHX	1	4110	-	0,6,6	-	-	-		
86	OHX	1	4011	-	0,6,6	-	-	-		
86	OHX	8	227	-	0,6,6	-	-	-		
86	OHX	1	3956	-	0,6,6	-	-	-		
86	OHX	1	4071	36	0,6,6	-	-	-		
86	OHX	1	4084	-	0,6,6	-	-	-		
86	OHX	5	3979	-	0,6,6	-	-	-		
86	OHX	1	3978	-	0,6,6	-	-	-		
86	OHX	5	4088	-	0,6,6	-	-	-		
86	OHX	6	2083	-	0,6,6	-	-	-		
86	OHX	1	3998	-	0,6,6	-	-	-		
86	OHX	1	3862	-	0,6,6	-	-	-		
86	OHX	5	3970	-	0,6,6	-	-	-		
86	OHX	2	2044	-	0,6,6	-	-	-		
86	OHX	6	2024	-	0,6,6	-	-	-		
86	OHX	5	3853	-	0,6,6	-	-	-		
86	OHX	5	3908	-	0,6,6	-	-	-		
86	OHX	m0	303	-	0,6,6	-	-	-		
86	OHX	6	2047	-	0,6,6	-	-	-		
86	OHX	1	4107	-	0,6,6	-	-	-		
86	OHX	6	2079	-	0,6,6	-	-	-		
86	OHX	5	3914	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4014	-	0,6,6	-	-	-		
86	OHX	6	2092	-	0,6,6	-	-	-		
86	OHX	1	3964	-	0,6,6	-	-	-		
86	OHX	5	4106	-	0,6,6	-	-	-		
86	OHX	2	2114	-	0,6,6	-	-	-		
86	OHX	5	3874	-	0,6,6	-	-	-		
86	OHX	2	2129	-	0,6,6	-	-	-		
86	OHX	N8	204	-	0,6,6	-	-	-		
86	OHX	2	2136	-	0,6,6	-	-	-		
86	OHX	5	3819	-	0,6,6	-	-	-		
86	OHX	5	3845	-	0,6,6	-	-	-		
86	OHX	6	2096	-	0,6,6	-	-	-		
86	OHX	8	229	-	0,6,6	-	-	-		
86	OHX	1	3763	-	0,6,6	-	-	-		
86	OHX	2	2140	-	0,6,6	-	-	-		
86	OHX	1	3903	-	0,6,6	-	-	-		
86	OHX	5	4055	-	0,6,6	-	-	-		
86	OHX	2	2124	-	0,6,6	-	-	-		
86	OHX	5	4023	-	0,6,6	-	-	-		
86	OHX	2	2096	-	0,6,6	-	-	-		
86	OHX	2	2049	-	0,6,6	-	-	-		
86	OHX	1	3915	-	0,6,6	-	-	-		
86	OHX	5	4115	-	0,6,6	-	-	-		
86	OHX	5	3920	-	0,6,6	-	-	-		
86	OHX	2	2115	-	0,6,6	-	-	-		
86	OHX	1	4085	-	0,6,6	-	-	-		
86	OHX	1	3834	-	0,6,6	-	-	-		
86	OHX	L4	401	-	0,6,6	-	-	-		
86	OHX	6	2117	-	0,6,6	-	-	-		
86	OHX	6	2130	-	0,6,6	-	-	-		
86	OHX	4	219	-	0,6,6	-	-	-		
86	OHX	5	3969	-	0,6,6	-	-	-		
86	OHX	1	4007	-	0,6,6	-	-	-		
86	OHX	5	4083	-	0,6,6	-	-	-		
86	OHX	6	2090	-	0,6,6	-	-	-		
86	OHX	5	4157	-	0,6,6	-	-	-		
86	OHX	5	4039	-	0,6,6	-	-	-		
86	OHX	1	3774	-	0,6,6	-	-	-		
86	OHX	5	3902	-	0,6,6	-	-	-		
86	OHX	6	2141	-	0,6,6	-	-	-		
86	OHX	1	4052	-	0,6,6	-	-	-		
86	OHX	1	3992	-	0,6,6	-	-	-		
86	OHX	1	3866	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	3	211	-	0,6,6	-	-	-		
86	OHX	14	402	-	0,6,6	-	-	-		
86	OHX	1	3902	-	0,6,6	-	-	-		
86	OHX	5	3858	-	0,6,6	-	-	-		
86	OHX	1	4019	-	0,6,6	-	-	-		
86	OHX	n9	101	-	0,6,6	-	-	-		
86	OHX	6	2144	-	0,6,6	-	-	-		
86	OHX	1	3937	-	0,6,6	-	-	-		
86	OHX	2	2045	-	0,6,6	-	-	-		
86	OHX	2	2112	-	0,6,6	-	-	-		
86	OHX	1	3825	-	0,6,6	-	-	-		
86	OHX	1	3922	-	0,6,6	-	-	-		
86	OHX	6	2015	-	0,6,6	-	-	-		
86	OHX	5	3916	-	0,6,6	-	-	-		
86	OHX	5	3990	-	0,6,6	-	-	-		
86	OHX	6	2045	-	0,6,6	-	-	-		
86	OHX	1	3874	-	0,6,6	-	-	-		
86	OHX	6	2069	-	0,6,6	-	-	-		
86	OHX	2	2060	-	0,6,6	-	-	-		
86	OHX	5	3999	-	0,6,6	-	-	-		
86	OHX	7	222	-	0,6,6	-	-	-		
86	OHX	6	2124	-	0,6,6	-	-	-		
86	OHX	3	210	-	0,6,6	-	-	-		
86	OHX	2	1993	-	0,6,6	-	-	-		
86	OHX	1	3988	-	0,6,6	-	-	-		
86	OHX	1	3832	-	0,6,6	-	-	-		
86	OHX	2	2043	-	0,6,6	-	-	-		
86	OHX	1	3768	-	0,6,6	-	-	-		
86	OHX	1	3823	-	0,6,6	-	-	-		
86	OHX	5	4117	-	0,6,6	-	-	-		
86	OHX	1	3901	-	0,6,6	-	-	-		
86	OHX	1	4054	-	0,6,6	-	-	-		
86	OHX	5	3948	-	0,6,6	-	-	-		
86	OHX	6	2147	-	0,6,6	-	-	-		
86	OHX	1	3961	-	0,6,6	-	-	-		
86	OHX	1	4048	-	0,6,6	-	-	-		
86	OHX	1	4063	-	0,6,6	-	-	-		
86	OHX	6	2091	-	0,6,6	-	-	-		
86	OHX	6	2126	-	0,6,6	-	-	-		
86	OHX	5	4107	-	0,6,6	-	-	-		
86	OHX	6	2026	-	0,6,6	-	-	-		
86	OHX	5	4112	-	0,6,6	-	-	-		
86	OHX	2	2020	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	o6	201	-	0,6,6	-	-	-		
86	OHX	5	3975	-	0,6,6	-	-	-		
86	OHX	1	3762	-	0,6,6	-	-	-		
86	OHX	s1	302	-	0,6,6	-	-	-		
86	OHX	1	4086	-	0,6,6	-	-	-		
86	OHX	6	2122	-	0,6,6	-	-	-		
86	OHX	1	3893	-	0,6,6	-	-	-		
86	OHX	6	2019	-	0,6,6	-	-	-		
86	OHX	6	2142	-	0,6,6	-	-	-		
86	OHX	1	3980	-	0,6,6	-	-	-		
86	OHX	5	3945	-	0,6,6	-	-	-		
86	OHX	6	2145	-	0,6,6	-	-	-		
86	OHX	5	4168	-	0,6,6	-	-	-		
86	OHX	5	3868	-	0,6,6	-	-	-		
86	OHX	8	214	-	0,6,6	-	-	-		
86	OHX	6	2127	-	0,6,6	-	-	-		
86	OHX	5	4031	-	0,6,6	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	PRO	1	4114	89	-	0/0/9/11	0/1/1/1
89	PRO	C	101	84,89	-	0/0/9/11	0/1/1/1
89	PRO	B	101	84,89	-	0/0/9/11	0/1/1/1
88	SPS	5	3403	-	-	1/15/18/18	0/1/1/1
88	SPS	1	4113	85	-	3/15/18/18	0/1/1/1
89	PRO	5	4173	89	-	0/0/9/11	0/1/1/1

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4113	SPS	C9-C10	-8.17	1.31	1.48
88	5	3403	SPS	C9-C10	-8.01	1.31	1.48
88	5	3403	SPS	C9-C8	6.45	1.52	1.33
88	1	4113	SPS	C9-C8	6.30	1.51	1.33
88	5	3403	SPS	O13-C13	-5.44	1.19	1.42

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4113	SPS	C7-C5-C6	-5.55	119.27	126.47
88	5	3403	SPS	C7-C5-N4	5.47	119.78	113.42
88	1	4113	SPS	C7-C5-N4	4.99	119.22	113.42
88	5	3403	SPS	C7-C5-C6	-4.98	120.02	126.47
88	1	4113	SPS	C5-N4-C3	-4.47	120.24	123.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	1	4113	SPS	N11-C12-C13-O13
88	1	4113	SPS	C14-C12-C13-O13
88	1	4113	SPS	N11-C12-C14-S15
88	5	3403	SPS	N11-C12-C14-S15

There are no ring outliers.

578 monomers are involved in 838 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	4027	OHX	2	0
86	1	4065	OHX	1	0
86	4	229	OHX	1	0
86	1	3776	OHX	1	0
86	5	4114	OHX	3	0
86	5	4133	OHX	1	0
86	5	4015	OHX	2	0
86	5	3904	OHX	2	0
86	5	3998	OHX	1	0
86	6	2150	OHX	1	0
86	4	224	OHX	1	0
86	1	4066	OHX	2	0
86	5	4046	OHX	1	0
86	1	3860	OHX	1	0
86	1	3957	OHX	1	0
86	6	2028	OHX	2	0
86	1	3963	OHX	1	0
86	n3	202	OHX	1	0
86	7	221	OHX	1	0
86	M7	205	OHX	1	0
86	1	3875	OHX	1	0
86	5	4076	OHX	1	0
86	5	3880	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3782	OHX	1	0
88	1	4113	SPS	1	0
86	1	4081	OHX	1	0
86	2	2108	OHX	2	0
86	2	2106	OHX	1	0
86	1	3894	OHX	1	0
86	2	2105	OHX	1	0
86	1	3775	OHX	1	0
86	5	4072	OHX	1	0
86	2	2138	OHX	1	0
86	5	3933	OHX	2	0
86	8	216	OHX	1	0
86	2	2120	OHX	1	0
86	1	4072	OHX	1	0
86	1	3766	OHX	2	0
86	5	3910	OHX	1	0
86	1	3770	OHX	2	0
86	1	3877	OHX	2	0
86	1	3898	OHX	1	0
86	1	3783	OHX	1	0
86	1	3913	OHX	1	0
86	4	218	OHX	1	0
86	5	4097	OHX	1	0
86	6	2109	OHX	2	0
86	5	3859	OHX	1	0
86	5	4001	OHX	5	0
86	5	4058	OHX	2	0
86	7	218	OHX	1	0
86	1	3819	OHX	1	0
86	5	3992	OHX	1	0
86	5	4144	OHX	2	0
86	2	2099	OHX	4	0
86	2	2036	OHX	1	0
86	5	4084	OHX	5	0
86	5	3896	OHX	1	0
86	2	2034	OHX	2	0
86	8	218	OHX	1	0
86	5	4130	OHX	2	0
86	1	4097	OHX	2	0
86	1	3932	OHX	1	0
86	2	2072	OHX	1	0
86	5	3823	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	6	2034	OHX	1	0
86	2	2016	OHX	1	0
86	2	2097	OHX	1	0
86	2	2058	OHX	5	0
86	1	3958	OHX	1	0
86	1	4033	OHX	2	0
86	1	3811	OHX	1	0
86	3	216	OHX	1	0
86	2	2075	OHX	1	0
86	6	2039	OHX	2	0
86	6	2031	OHX	1	0
86	1	3803	OHX	1	0
86	L3	402	OHX	1	0
86	1	3950	OHX	3	0
86	O4	202	OHX	2	0
86	6	2064	OHX	1	0
86	5	3825	OHX	1	0
86	5	3966	OHX	1	0
86	6	2038	OHX	2	0
86	5	3921	OHX	1	0
86	c8	203	OHX	1	0
86	5	3996	OHX	2	0
86	5	4138	OHX	1	0
86	1	4034	OHX	1	0
86	5	4005	OHX	1	0
86	5	3885	OHX	1	0
86	6	2104	OHX	2	0
86	5	4010	OHX	1	0
86	4	221	OHX	1	0
86	1	3911	OHX	1	0
86	2	2039	OHX	3	0
86	1	3855	OHX	1	0
86	1	3872	OHX	1	0
86	Q2	503	OHX	2	0
86	5	3943	OHX	1	0
86	1	4077	OHX	1	0
86	sR	401	OHX	3	0
86	5	3986	OHX	1	0
86	5	3915	OHX	4	0
86	L5	301	OHX	1	0
86	O1	201	OHX	2	0
86	5	3912	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	2	1997	OHX	1	0
86	1	3785	OHX	1	0
86	1	3919	OHX	1	0
86	1	3936	OHX	1	0
86	5	3929	OHX	2	0
86	5	4013	OHX	1	0
86	5	4041	OHX	1	0
86	5	4105	OHX	1	0
86	1	3993	OHX	1	0
86	5	3965	OHX	1	0
86	1	3850	OHX	1	0
86	6	2151	OHX	1	0
86	2	2116	OHX	2	0
86	O9	101	OHX	1	0
86	1	3863	OHX	1	0
86	2	2000	OHX	1	0
86	1	4087	OHX	1	0
86	6	2094	OHX	2	0
86	m7	204	OHX	1	0
86	5	4011	OHX	2	0
86	1	3828	OHX	1	0
86	2	2032	OHX	1	0
86	2	2055	OHX	1	0
86	6	2036	OHX	1	0
86	2	2041	OHX	3	0
86	1	3831	OHX	1	0
86	5	3988	OHX	1	0
86	2	2143	OHX	1	0
86	1	4018	OHX	1	0
86	2	2102	OHX	1	0
86	1	3870	OHX	2	0
86	5	4061	OHX	2	0
86	5	3881	OHX	1	0
86	6	2053	OHX	1	0
86	1	3787	OHX	1	0
86	l5	303	OHX	3	0
86	5	4153	OHX	1	0
86	5	3862	OHX	1	0
86	1	3769	OHX	2	0
86	1	3839	OHX	1	0
86	5	4070	OHX	1	0
86	1	3837	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	4120	OHX	3	0
86	q2	203	OHX	1	0
86	4	225	OHX	1	0
86	1	3881	OHX	2	0
86	5	4152	OHX	1	0
86	5	4049	OHX	1	0
86	4	227	OHX	1	0
86	5	4172	OHX	1	0
86	1	4070	OHX	1	0
86	1	3873	OHX	1	0
86	2	2110	OHX	1	0
86	1	3996	OHX	1	0
86	6	2101	OHX	1	0
86	1	3940	OHX	5	0
86	4	217	OHX	1	0
86	1	3999	OHX	2	0
86	6	2159	OHX	1	0
86	1	3974	OHX	1	0
86	2	1994	OHX	2	0
86	5	3955	OHX	4	0
86	5	3959	OHX	1	0
86	1	4044	OHX	2	0
86	5	3962	OHX	1	0
86	2	2046	OHX	1	0
86	1	4076	OHX	3	0
86	1	3878	OHX	1	0
86	5	3834	OHX	2	0
86	6	2180	OHX	1	0
86	6	2032	OHX	1	0
86	5	4121	OHX	1	0
86	1	3858	OHX	2	0
86	6	2041	OHX	2	0
86	2	2042	OHX	1	0
86	2	1991	OHX	1	0
86	5	3891	OHX	1	0
86	2	2014	OHX	1	0
86	6	2067	OHX	4	0
86	1	3821	OHX	1	0
86	2	2061	OHX	1	0
86	2	2089	OHX	3	0
86	2	2095	OHX	1	0
86	1	3997	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	M9	202	OHX	1	0
86	5	4052	OHX	3	0
86	6	2014	OHX	2	0
86	5	3830	OHX	2	0
86	5	3821	OHX	1	0
86	6	2060	OHX	1	0
86	2	2123	OHX	2	0
86	6	2078	OHX	1	0
86	5	4038	OHX	1	0
86	6	2063	OHX	3	0
86	6	2131	OHX	1	0
86	1	4038	OHX	2	0
86	1	3900	OHX	1	0
86	c5	201	OHX	1	0
86	5	4054	OHX	1	0
86	5	3930	OHX	1	0
86	2	2145	OHX	1	0
86	5	4012	OHX	1	0
86	6	2050	OHX	1	0
86	2	2064	OHX	1	0
86	O7	104	OHX	6	0
86	1	3934	OHX	1	0
86	5	4140	OHX	2	0
86	1	3921	OHX	1	0
86	5	3888	OHX	1	0
86	5	4066	OHX	1	0
86	5	3873	OHX	3	0
86	1	4096	OHX	1	0
86	2	2027	OHX	1	0
86	M5	304	OHX	1	0
86	6	2153	OHX	1	0
86	o3	202	OHX	1	0
86	5	4159	OHX	1	0
86	2	2006	OHX	1	0
86	M0	304	OHX	5	0
86	5	3977	OHX	2	0
86	2	2015	OHX	1	0
86	5	4118	OHX	3	0
86	1	4040	OHX	1	0
86	6	2020	OHX	1	0
86	2	2052	OHX	2	0
86	1	4046	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	6	2156	OHX	2	0
86	5	3946	OHX	1	0
86	6	2170	OHX	3	0
86	5	4027	OHX	1	0
86	5	3886	OHX	1	0
86	1	3889	OHX	4	0
86	6	2044	OHX	1	0
86	5	4000	OHX	1	0
86	5	3911	OHX	1	0
86	1	3847	OHX	1	0
86	2	2033	OHX	1	0
86	5	3928	OHX	1	0
86	1	3938	OHX	2	0
86	6	2115	OHX	2	0
86	N9	101	OHX	1	0
86	5	4082	OHX	1	0
86	2	2132	OHX	1	0
86	1	4036	OHX	1	0
86	1	4083	OHX	1	0
86	5	3905	OHX	1	0
86	5	4103	OHX	2	0
86	1	4043	OHX	1	0
86	6	2173	OHX	1	0
86	1	3904	OHX	1	0
86	5	4060	OHX	1	0
86	5	3978	OHX	3	0
86	6	2123	OHX	2	0
86	5	4148	OHX	1	0
86	1	3899	OHX	1	0
86	5	3890	OHX	1	0
86	1	4082	OHX	6	0
86	2	2013	OHX	1	0
86	5	3894	OHX	3	0
86	5	4141	OHX	1	0
86	1	4050	OHX	1	0
86	1	3906	OHX	1	0
86	5	4037	OHX	1	0
86	2	2084	OHX	2	0
86	1	4049	OHX	1	0
86	2	1995	OHX	1	0
86	1	4037	OHX	2	0
86	1	3856	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	4098	OHX	1	0
86	5	3842	OHX	1	0
86	8	215	OHX	1	0
86	5	4093	OHX	2	0
86	1	3952	OHX	1	0
86	5	3964	OHX	1	0
86	1	3826	OHX	1	0
86	6	2172	OHX	1	0
86	8	231	OHX	1	0
86	1	3816	OHX	1	0
86	5	4019	OHX	2	0
86	5	4047	OHX	2	0
86	1	3790	OHX	1	0
86	1	3789	OHX	1	0
86	5	3869	OHX	1	0
86	5	3939	OHX	2	0
86	5	4129	OHX	1	0
86	1	3991	OHX	1	0
86	6	2056	OHX	1	0
86	5	4154	OHX	2	0
86	2	2078	OHX	1	0
86	c3	201	OHX	2	0
86	5	3907	OHX	1	0
86	6	2132	OHX	1	0
86	s9	201	OHX	2	0
86	SR	401	OHX	2	0
86	5	3836	OHX	1	0
86	5	3919	OHX	1	0
86	5	3967	OHX	1	0
86	1	3765	OHX	1	0
86	6	2105	OHX	1	0
86	14	403	OHX	2	0
86	5	3870	OHX	2	0
86	2	2050	OHX	1	0
86	6	2110	OHX	3	0
86	5	3841	OHX	1	0
86	2	1992	OHX	1	0
86	5	4170	OHX	2	0
86	1	3981	OHX	1	0
86	5	3861	OHX	1	0
86	5	4069	OHX	1	0
86	5	4149	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	4164	OHX	1	0
86	2	2133	OHX	1	0
86	6	2112	OHX	1	0
86	8	223	OHX	1	0
86	1	3779	OHX	2	0
86	6	2183	OHX	1	0
86	2	2109	OHX	1	0
86	2	2083	OHX	1	0
86	1	4058	OHX	1	0
86	1	4061	OHX	3	0
86	5	3944	OHX	1	0
86	5	3953	OHX	1	0
86	S6	301	OHX	3	0
86	8	222	OHX	1	0
86	5	3839	OHX	2	0
86	5	4131	OHX	1	0
86	5	3925	OHX	1	0
86	6	2168	OHX	1	0
86	1	3887	OHX	1	0
86	5	4104	OHX	1	0
86	1	4032	OHX	1	0
86	5	4087	OHX	1	0
86	m5	306	OHX	1	0
86	1	4060	OHX	3	0
86	6	2022	OHX	2	0
86	2	2008	OHX	3	0
86	2	2002	OHX	2	0
86	2	2131	OHX	4	0
86	M5	303	OHX	1	0
86	6	2054	OHX	1	0
86	5	3926	OHX	1	0
86	5	4024	OHX	1	0
88	5	3403	SPS	5	0
86	1	4106	OHX	1	0
86	5	4053	OHX	3	0
86	6	2095	OHX	1	0
86	2	2026	OHX	1	0
86	5	4101	OHX	1	0
86	2	2082	OHX	1	0
86	1	3844	OHX	1	0
86	2	2074	OHX	2	0
86	1	3771	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3949	OHX	1	0
86	6	2103	OHX	1	0
86	1	3920	OHX	1	0
86	1	4055	OHX	1	0
86	1	3806	OHX	1	0
86	6	2149	OHX	1	0
86	5	3923	OHX	1	0
86	5	3922	OHX	3	0
86	5	4048	OHX	1	0
86	6	2081	OHX	1	0
86	6	2058	OHX	1	0
86	6	2134	OHX	1	0
86	1	4102	OHX	1	0
86	5	3982	OHX	1	0
86	5	3961	OHX	1	0
86	2	2092	OHX	2	0
86	1	3951	OHX	3	0
86	6	2089	OHX	2	0
86	5	3941	OHX	1	0
86	s1	301	OHX	2	0
86	6	2107	OHX	1	0
86	2	2119	OHX	1	0
86	1	3853	OHX	2	0
86	1	3833	OHX	1	0
86	6	2175	OHX	1	0
86	5	3879	OHX	2	0
86	1	3945	OHX	3	0
86	5	3895	OHX	1	0
86	C3	201	OHX	1	0
86	1	3838	OHX	1	0
86	1	3930	OHX	1	0
86	2	2038	OHX	2	0
86	1	4029	OHX	1	0
86	2	2151	OHX	1	0
86	5	3835	OHX	2	0
86	5	3849	OHX	1	0
86	2	2018	OHX	1	0
86	2	2080	OHX	3	0
86	5	4096	OHX	3	0
86	1	3935	OHX	1	0
86	m0	302	OHX	2	0
86	2	2035	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	3901	OHX	1	0
86	6	2023	OHX	1	0
86	6	2055	OHX	1	0
86	2	2005	OHX	1	0
86	5	3875	OHX	1	0
86	5	3989	OHX	2	0
86	6	2027	OHX	2	0
86	2	2142	OHX	1	0
86	5	3833	OHX	1	0
86	1	3868	OHX	1	0
86	1	3943	OHX	1	0
86	5	4171	OHX	2	0
86	2	2128	OHX	1	0
86	1	3984	OHX	1	0
86	4	223	OHX	2	0
86	5	3949	OHX	1	0
86	5	3957	OHX	1	0
86	6	2138	OHX	1	0
86	2	2127	OHX	3	0
86	1	3884	OHX	3	0
86	1	3824	OHX	1	0
86	2	2003	OHX	1	0
86	S1	301	OHX	1	0
86	6	2074	OHX	2	0
86	1	3859	OHX	1	0
86	5	3877	OHX	1	0
86	5	3828	OHX	1	0
86	2	2019	OHX	1	0
86	5	4166	OHX	1	0
86	5	3918	OHX	4	0
86	6	2108	OHX	1	0
86	5	4056	OHX	1	0
86	2	2066	OHX	2	0
86	1	3777	OHX	2	0
86	5	4009	OHX	1	0
86	2	2012	OHX	1	0
86	6	2040	OHX	2	0
86	2	2150	OHX	2	0
86	1	3788	OHX	1	0
86	6	2181	OHX	3	0
86	5	3956	OHX	1	0
86	1	3830	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	o7	502	OHX	5	0
86	1	3840	OHX	1	0
86	1	4003	OHX	1	0
86	6	2157	OHX	1	0
86	L3	403	OHX	1	0
86	5	3906	OHX	2	0
86	1	3809	OHX	3	0
86	1	3986	OHX	1	0
86	5	3850	OHX	1	0
86	5	3837	OHX	1	0
86	5	4014	OHX	3	0
86	1	3854	OHX	4	0
86	6	2129	OHX	1	0
86	5	3846	OHX	1	0
86	5	3963	OHX	1	0
86	1	3815	OHX	1	0
86	5	3826	OHX	2	0
86	5	3984	OHX	1	0
86	1	3897	OHX	3	0
86	5	4017	OHX	1	0
86	2	2051	OHX	1	0
86	2	2101	OHX	2	0
86	2	2059	OHX	1	0
86	5	3856	OHX	1	0
86	1	3781	OHX	1	0
86	6	2018	OHX	1	0
86	5	3878	OHX	3	0
86	6	2086	OHX	1	0
86	S9	201	OHX	2	0
86	2	2117	OHX	1	0
86	4	220	OHX	1	0
86	5	3899	OHX	1	0
86	5	3935	OHX	1	0
86	2	2130	OHX	1	0
86	5	3855	OHX	1	0
86	8	211	OHX	1	0
86	5	3936	OHX	2	0
86	1	3967	OHX	2	0
86	1	3849	OHX	1	0
86	S8	301	OHX	1	0
86	5	3817	OHX	1	0
86	1	3813	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	4001	OHX	1	0
86	6	2070	OHX	1	0
86	1	4100	OHX	2	0
86	C5	201	OHX	4	0
86	6	2111	OHX	2	0
86	5	3960	OHX	1	0
86	4	230	OHX	1	0
86	2	2001	OHX	2	0
86	1	3942	OHX	2	0
86	6	2033	OHX	1	0
86	1	3796	OHX	1	0
86	5	3997	OHX	1	0
86	2	2079	OHX	1	0
86	5	3900	OHX	1	0
86	6	2085	OHX	1	0
86	2	2076	OHX	1	0
86	1	3939	OHX	1	0
86	c5	202	OHX	4	0
86	3	209	OHX	1	0
86	1	4067	OHX	1	0
86	2	2122	OHX	1	0
86	3	214	OHX	1	0
86	8	217	OHX	2	0
86	1	3810	OHX	1	0
86	5	4125	OHX	1	0
86	6	2087	OHX	1	0
86	1	4000	OHX	1	0
86	1	3800	OHX	1	0
86	4	228	OHX	1	0
86	l3	403	OHX	1	0
86	6	2037	OHX	1	0
86	6	2057	OHX	1	0
86	5	4002	OHX	5	0
86	1	3960	OHX	1	0
86	1	3794	OHX	1	0
86	1	3812	OHX	2	0
86	2	2057	OHX	1	0
86	1	3979	OHX	1	0
86	1	4030	OHX	2	0
86	5	3876	OHX	1	0
86	5	4102	OHX	1	0
86	1	4110	OHX	1	0

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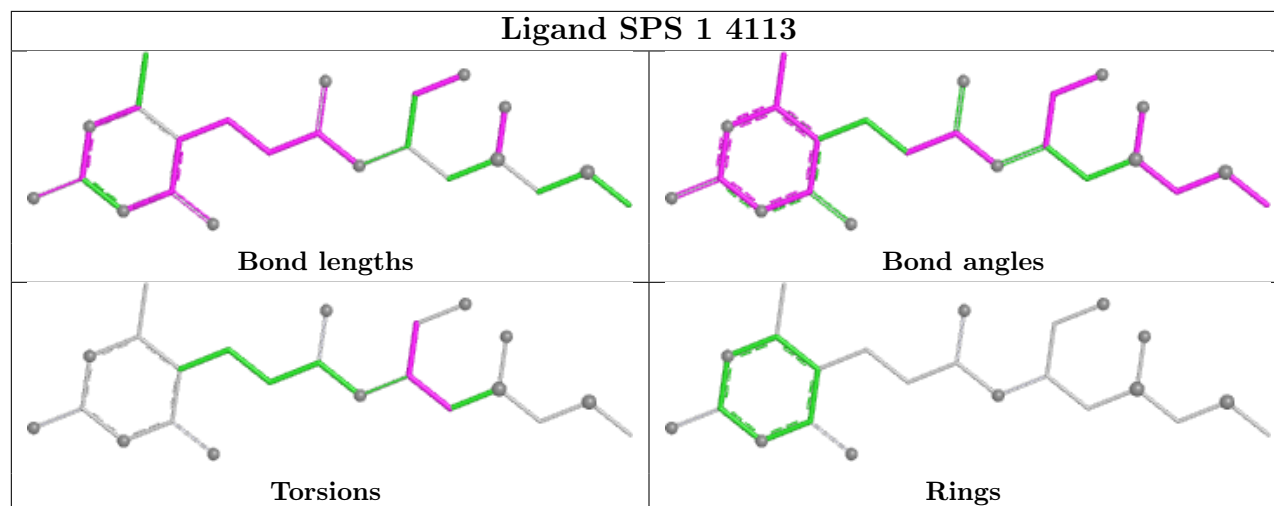
Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3956	OHX	1	0
86	1	4071	OHX	8	0
86	1	3978	OHX	1	0
86	5	4088	OHX	1	0
86	6	2083	OHX	2	0
86	5	3970	OHX	1	0
86	6	2024	OHX	1	0
86	m0	303	OHX	2	0
86	1	4107	OHX	1	0
86	1	4014	OHX	1	0
86	6	2092	OHX	2	0
86	1	3964	OHX	1	0
86	2	2136	OHX	1	0
86	5	3819	OHX	2	0
86	6	2096	OHX	3	0
86	8	229	OHX	2	0
86	1	3763	OHX	1	0
86	2	2124	OHX	1	0
86	2	2049	OHX	1	0
86	1	3915	OHX	1	0
86	1	4085	OHX	4	0
86	1	3834	OHX	1	0
86	L4	401	OHX	3	0
86	4	219	OHX	2	0
86	5	4157	OHX	1	0
86	1	3774	OHX	2	0
86	5	3902	OHX	2	0
86	6	2141	OHX	1	0
86	14	402	OHX	3	0
86	5	3858	OHX	1	0
86	1	4019	OHX	1	0
86	n9	101	OHX	1	0
86	1	3937	OHX	2	0
86	2	2112	OHX	1	0
86	1	3825	OHX	1	0
86	6	2015	OHX	1	0
86	6	2069	OHX	2	0
86	7	222	OHX	2	0
86	6	2124	OHX	5	0
86	2	1993	OHX	1	0
86	1	3768	OHX	1	0
86	1	3823	OHX	1	0

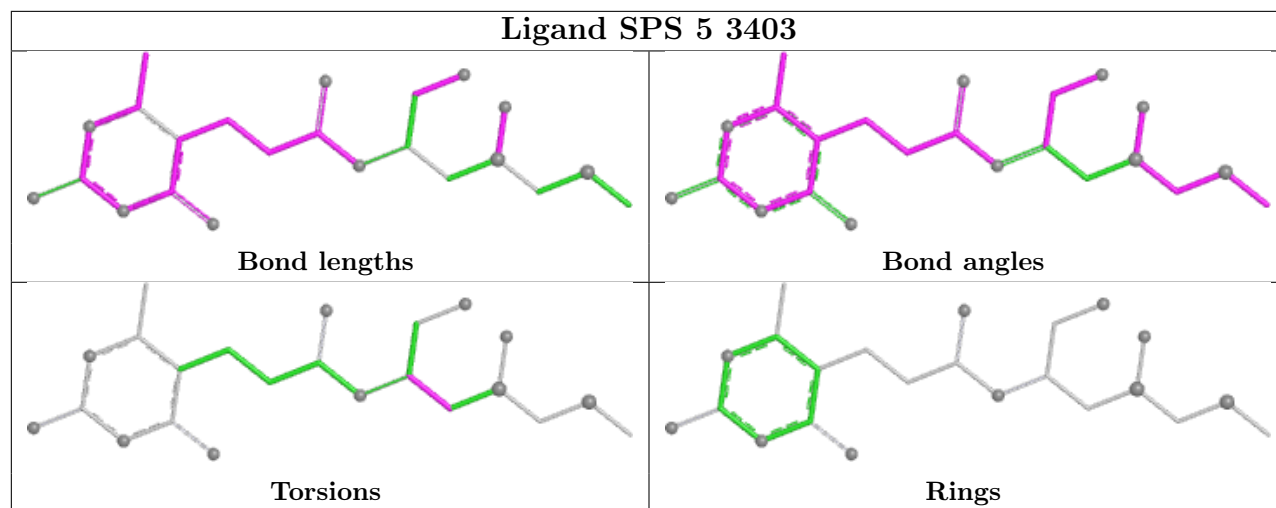
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	4117	OHX	2	0
86	5	3948	OHX	1	0
86	1	4048	OHX	1	0
86	5	4112	OHX	1	0
86	2	2020	OHX	1	0
86	1	3893	OHX	2	0
86	5	3945	OHX	1	0
86	6	2145	OHX	1	0
86	6	2127	OHX	2	0

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
1	2	2
80	m2	2

All 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	5.10
1	m2	23:LEU	C	28:ARG	N	3.71
1	m2	52:LYS	C	54:LYS	N	3.25
1	2	1685:G	O3'	1686:C	P	2.98

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	2	1781/1800 (98%)	0.08	29 (1%) 70 46	42, 100, 190, 245	1 (0%)
1	6	1795/1800 (99%)	-0.12	23 (1%) 75 51	33, 84, 172, 231	1 (0%)
2	S0	206/251 (82%)	0.73	9 (4%) 39 23	99, 112, 122, 125	0
2	s0	206/251 (82%)	0.50	7 (3%) 48 29	78, 93, 107, 115	0
3	S1	214/254 (84%)	0.92	22 (10%) 12 9	114, 152, 175, 179	0
3	s1	216/254 (85%)	0.26	4 (1%) 66 42	80, 93, 110, 126	0
4	S2	217/253 (85%)	0.55	9 (4%) 41 24	79, 95, 109, 118	0
4	s2	217/253 (85%)	0.38	10 (4%) 37 21	63, 79, 90, 99	0
5	S3	223/239 (93%)	0.45	7 (3%) 51 31	90, 103, 122, 135	0
5	s3	223/239 (93%)	0.36	6 (2%) 56 33	83, 108, 131, 139	0
6	S4	260/260 (100%)	0.51	8 (3%) 51 31	78, 101, 111, 133	0
6	s4	260/260 (100%)	0.23	3 (1%) 76 53	56, 79, 94, 113	0
7	S5	206/224 (91%)	0.61	13 (6%) 26 17	107, 122, 134, 144	0
7	s5	206/224 (91%)	0.51	6 (2%) 53 32	88, 106, 123, 134	0
8	S6	226/236 (95%)	0.79	22 (9%) 13 10	77, 113, 131, 142	0
8	s6	218/236 (92%)	0.35	10 (4%) 37 21	56, 85, 110, 123	0
9	S7	184/189 (97%)	0.68	6 (3%) 49 29	96, 127, 147, 152	0
9	s7	186/189 (98%)	0.30	3 (1%) 70 46	70, 103, 132, 139	0
10	S8	188/200 (94%)	0.49	2 (1%) 78 54	68, 88, 122, 139	0
10	s8	188/200 (94%)	0.35	8 (4%) 40 23	52, 69, 110, 129	0
11	S9	185/196 (94%)	0.61	7 (3%) 44 26	91, 107, 137, 157	0
11	s9	185/196 (94%)	0.65	11 (5%) 28 18	68, 87, 125, 146	0
12	C0	96/105 (91%)	0.64	5 (5%) 33 20	96, 121, 141, 151	0
12	c0	96/105 (91%)	0.91	14 (14%) 6 5	105, 136, 149, 150	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	C1	155/155 (100%)	0.58	9 (5%) 29 18	71, 84, 118, 130	0
13	c1	146/155 (94%)	0.50	8 (5%) 30 19	54, 66, 94, 115	0
14	C2	124/142 (87%)	0.95	14 (11%) 10 8	149, 161, 174, 180	0
14	c2	124/142 (87%)	0.97	16 (12%) 7 6	180, 196, 211, 215	0
15	C3	150/150 (100%)	0.38	4 (2%) 56 33	79, 94, 109, 115	0
15	c3	150/150 (100%)	0.14	2 (1%) 75 51	62, 76, 93, 96	0
16	C4	127/136 (93%)	1.15	15 (11%) 9 7	83, 146, 158, 162	0
16	c4	128/136 (94%)	0.34	0 100 100	64, 96, 104, 109	0
17	C5	124/141 (87%)	0.44	3 (2%) 59 37	87, 103, 120, 130	0
17	c5	135/141 (95%)	0.53	8 (5%) 28 18	72, 107, 122, 123	0
18	C6	141/142 (99%)	0.80	10 (7%) 22 15	92, 110, 116, 118	0
18	c6	142/142 (100%)	0.83	14 (9%) 13 9	82, 104, 118, 136	0
19	C7	120/136 (88%)	0.61	7 (5%) 29 18	95, 110, 129, 131	0
19	c7	117/136 (86%)	0.54	5 (4%) 40 23	85, 102, 114, 122	0
20	C8	145/145 (100%)	0.58	4 (2%) 55 33	85, 109, 135, 142	0
20	c8	145/145 (100%)	0.61	9 (6%) 26 17	83, 101, 117, 124	0
21	C9	143/143 (100%)	0.86	8 (5%) 30 19	95, 110, 125, 133	0
21	c9	143/143 (100%)	0.61	8 (5%) 30 19	82, 98, 115, 123	0
22	D0	107/120 (89%)	0.68	5 (4%) 36 21	86, 114, 136, 138	0
22	d0	110/120 (91%)	0.56	6 (5%) 30 19	85, 115, 144, 149	0
23	D1	87/87 (100%)	0.46	3 (3%) 48 29	96, 103, 117, 122	0
23	d1	87/87 (100%)	0.21	0 100 100	71, 82, 104, 111	0
24	D2	129/129 (100%)	0.65	2 (1%) 70 46	80, 92, 101, 111	0
24	d2	129/129 (100%)	0.05	0 100 100	59, 68, 75, 84	0
25	D3	144/144 (100%)	0.34	2 (1%) 73 49	70, 78, 90, 102	0
25	d3	144/144 (100%)	0.17	3 (2%) 63 39	52, 57, 70, 81	0
26	D4	134/134 (100%)	0.58	7 (5%) 33 20	89, 111, 123, 127	0
26	d4	134/134 (100%)	0.41	4 (2%) 52 31	65, 88, 100, 105	0
27	D5	70/107 (65%)	0.57	3 (4%) 40 23	118, 134, 141, 146	0
27	d5	69/107 (64%)	0.60	4 (5%) 29 18	98, 112, 124, 126	0
28	D6	97/97 (100%)	1.00	15 (15%) 5 5	86, 108, 160, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	d6	97/97 (100%)	0.60	3 (3%) 51 31	67, 84, 111, 116	0
29	D7	81/81 (100%)	0.74	4 (4%) 35 21	95, 113, 139, 143	0
29	d7	81/81 (100%)	0.49	4 (4%) 35 21	72, 90, 127, 128	0
30	D8	63/66 (95%)	0.62	4 (6%) 26 17	114, 131, 139, 144	0
30	d8	63/66 (95%)	0.51	3 (4%) 35 21	105, 118, 125, 128	0
31	D9	53/55 (96%)	0.76	4 (7%) 20 14	85, 90, 108, 114	0
31	d9	53/55 (96%)	0.67	3 (5%) 29 18	82, 92, 128, 145	0
32	E0	60/63 (95%)	0.37	1 (1%) 69 44	80, 110, 134, 137	0
32	e0	62/63 (98%)	0.62	7 (11%) 10 8	60, 88, 117, 120	0
33	E1	71/76 (93%)	0.89	8 (11%) 10 8	115, 142, 155, 157	0
33	e1	76/76 (100%)	1.07	14 (18%) 3 4	117, 168, 186, 187	0
34	SR	318/318 (100%)	0.69	27 (8%) 16 12	109, 122, 138, 156	0
34	sR	318/318 (100%)	0.59	12 (3%) 44 26	112, 127, 141, 153	0
35	SM	159/273 (58%)	0.57	11 (6%) 23 15	58, 100, 159, 163	0
35	sM	104/273 (38%)	0.61	5 (4%) 35 21	51, 115, 188, 197	0
36	1	3149/3396 (92%)	-0.32	28 (0%) 81 58	33, 58, 136, 238	0
36	5	3150/3396 (92%)	-0.43	22 (0%) 84 64	28, 52, 127, 213	0
37	3	121/121 (100%)	-0.31	0 100 100	42, 77, 90, 98	0
37	7	121/121 (100%)	-0.48	1 (0%) 82 61	33, 55, 66, 75	0
38	4	158/158 (100%)	-0.46	1 (0%) 85 66	42, 63, 102, 146	0
38	8	158/158 (100%)	-0.50	1 (0%) 85 66	42, 63, 101, 131	0
39	L2	252/253 (99%)	0.22	3 (1%) 76 53	40, 60, 78, 84	0
39	l2	252/253 (99%)	0.16	2 (0%) 82 61	36, 55, 73, 80	0
40	L3	386/386 (100%)	0.06	4 (1%) 79 56	37, 62, 77, 88	0
40	l3	386/386 (100%)	-0.16	7 (1%) 67 43	28, 45, 60, 81	0
41	L4	361/361 (100%)	0.06	8 (2%) 62 39	38, 54, 69, 74	0
41	l4	361/361 (100%)	0.02	5 (1%) 73 49	37, 56, 74, 82	0
42	L5	296/296 (100%)	0.32	3 (1%) 79 56	58, 80, 98, 119	0
42	l5	294/296 (99%)	0.04	6 (2%) 65 41	42, 56, 82, 97	0
43	L6	156/175 (89%)	0.04	2 (1%) 75 51	46, 56, 72, 87	0
43	l6	157/175 (89%)	-0.00	1 (0%) 85 66	48, 57, 78, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	L7	222/243 (91%)	-0.13	1 (0%) 87 70	38, 47, 77, 104	0
44	l7	223/243 (91%)	-0.22	1 (0%) 88 73	33, 45, 82, 112	0
45	L8	233/255 (91%)	0.43	8 (3%) 48 29	68, 84, 110, 120	0
45	l8	231/255 (90%)	0.41	6 (2%) 57 34	69, 82, 107, 117	0
46	L9	191/191 (100%)	0.15	2 (1%) 79 56	59, 71, 82, 94	0
46	l9	191/191 (100%)	-0.16	1 (0%) 87 70	41, 51, 68, 78	0
47	M0	211/220 (95%)	0.16	7 (3%) 49 29	44, 63, 94, 105	0
47	m0	213/220 (96%)	0.09	5 (2%) 61 38	39, 54, 78, 94	0
48	M1	169/173 (97%)	0.31	3 (1%) 67 43	68, 85, 97, 103	0
48	m1	169/173 (97%)	-0.04	1 (0%) 85 66	47, 66, 77, 81	0
49	M3	193/198 (97%)	-0.02	0 100 100	36, 63, 101, 122	0
49	m3	194/198 (97%)	0.08	4 (2%) 63 39	38, 67, 104, 119	0
50	M4	136/137 (99%)	-0.09	0 100 100	50, 59, 72, 83	0
50	m4	137/137 (100%)	-0.20	3 (2%) 62 39	43, 50, 66, 84	0
51	M5	203/203 (100%)	0.36	2 (0%) 79 56	39, 56, 67, 71	0
51	m5	203/203 (100%)	0.28	2 (0%) 79 56	40, 58, 68, 73	0
52	M6	197/198 (99%)	0.08	2 (1%) 79 56	25, 32, 46, 49	0
52	m6	197/198 (99%)	0.03	2 (1%) 79 56	18, 24, 45, 52	0
53	M7	183/183 (100%)	0.12	10 (5%) 30 19	44, 52, 105, 133	0
53	m7	155/183 (84%)	-0.17	0 100 100	36, 45, 55, 77	0
54	M8	185/185 (100%)	0.03	3 (1%) 70 46	42, 51, 68, 88	0
54	m8	185/185 (100%)	-0.04	0 100 100	39, 53, 64, 72	0
55	M9	188/188 (100%)	0.37	8 (4%) 40 23	64, 78, 147, 156	0
55	m9	188/188 (100%)	0.03	0 100 100	50, 62, 123, 138	0
56	N0	172/172 (100%)	-0.03	3 (1%) 69 44	37, 56, 70, 75	0
56	n0	172/172 (100%)	-0.29	2 (1%) 76 53	32, 45, 57, 67	0
57	N1	159/159 (100%)	0.03	1 (0%) 85 66	41, 56, 99, 105	0
57	n1	159/159 (100%)	-0.08	2 (1%) 75 51	37, 45, 82, 88	0
58	N2	100/120 (83%)	0.53	4 (4%) 42 25	94, 106, 112, 117	0
58	n2	98/120 (81%)	0.32	2 (2%) 65 41	74, 85, 93, 95	0
59	N3	136/136 (100%)	0.14	1 (0%) 84 64	49, 59, 73, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
59	n3	136/136 (100%)	-0.27	0 100 100	31, 41, 52, 57	0
60	N4	98/155 (63%)	0.72	14 (14%) 6 6	59, 74, 147, 155	0
60	n4	135/155 (87%)	0.50	15 (11%) 10 8	41, 93, 124, 142	0
61	N5	121/141 (85%)	0.15	0 100 100	59, 71, 86, 103	0
61	n5	120/141 (85%)	-0.01	3 (2%) 58 35	55, 68, 82, 97	0
62	N6	126/126 (100%)	0.22	3 (2%) 59 37	48, 64, 77, 85	0
62	n6	126/126 (100%)	0.13	0 100 100	50, 66, 82, 85	0
63	N7	135/135 (100%)	0.50	2 (1%) 72 48	83, 96, 107, 111	0
63	n7	135/135 (100%)	0.35	1 (0%) 84 64	78, 89, 101, 109	0
64	N8	148/148 (100%)	-0.15	0 100 100	32, 54, 76, 82	0
64	n8	148/148 (100%)	0.03	3 (2%) 65 41	34, 55, 72, 75	0
65	N9	58/58 (100%)	0.05	1 (1%) 69 44	36, 59, 97, 113	0
65	n9	58/58 (100%)	0.19	1 (1%) 69 44	36, 55, 76, 82	0
66	O0	97/104 (93%)	0.13	2 (2%) 63 39	83, 90, 106, 111	0
66	o0	100/104 (96%)	0.09	1 (1%) 79 56	69, 79, 98, 105	0
67	O1	109/112 (97%)	0.25	0 100 100	60, 73, 94, 101	0
67	o1	109/112 (97%)	-0.02	0 100 100	44, 56, 89, 97	0
68	O2	127/129 (98%)	-0.04	2 (1%) 70 46	34, 48, 63, 79	0
68	o2	127/129 (98%)	-0.04	1 (0%) 82 61	32, 52, 67, 78	0
69	O3	106/106 (100%)	0.05	1 (0%) 81 58	39, 46, 70, 82	0
69	o3	106/106 (100%)	-0.10	0 100 100	36, 44, 71, 82	0
70	O4	112/121 (92%)	0.62	4 (3%) 46 27	57, 74, 110, 117	0
70	o4	112/121 (92%)	0.60	10 (8%) 15 11	50, 66, 101, 108	0
71	O5	119/119 (100%)	0.22	1 (0%) 82 61	56, 73, 80, 83	0
71	o5	119/119 (100%)	0.14	1 (0%) 82 61	58, 71, 86, 96	0
72	O6	99/99 (100%)	0.18	0 100 100	59, 70, 100, 111	0
72	o6	99/99 (100%)	0.19	1 (1%) 79 56	62, 72, 91, 110	0
73	O7	87/87 (100%)	0.22	1 (1%) 78 54	41, 49, 70, 80	0
73	o7	87/87 (100%)	-0.03	1 (1%) 78 54	37, 48, 79, 85	0
74	O8	77/77 (100%)	0.35	2 (2%) 57 34	85, 97, 107, 108	0
74	o8	77/77 (100%)	0.11	1 (1%) 75 51	75, 85, 94, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	O9	50/50 (100%)	0.25	0 100 100	51, 57, 61, 62	0
75	o9	50/50 (100%)	0.02	1 (2%) 65 41	49, 54, 63, 64	0
76	Q0	52/52 (100%)	0.21	0 100 100	53, 59, 74, 82	0
76	q0	52/52 (100%)	-0.31	1 (1%) 66 42	38, 42, 52, 57	0
77	Q1	25/25 (100%)	0.53	1 (4%) 42 25	62, 66, 72, 74	0
77	q1	25/25 (100%)	0.01	0 100 100	49, 53, 54, 55	0
78	Q2	105/105 (100%)	-0.10	0 100 100	41, 55, 76, 97	0
78	q2	105/105 (100%)	-0.14	1 (0%) 79 56	40, 53, 69, 96	0
79	Q3	91/91 (100%)	0.16	1 (1%) 78 54	49, 65, 79, 85	0
79	q3	91/91 (100%)	0.03	2 (2%) 62 39	40, 55, 71, 81	0
80	m2	150/165 (90%)	1.13	20 (13%) 7 6	102, 138, 156, 161	0
81	p0	143/311 (45%)	0.81	13 (9%) 15 11	100, 125, 220, 229	0
82	p1	47/106 (44%)	1.32	7 (14%) 5 5	179, 224, 242, 245	0
82	p2	46/106 (43%)	1.55	12 (26%) 1 2	275, 283, 288, 289	0
83	f	147/157 (93%)	1.94	51 (34%) 1 1	23, 77, 157, 159	74 (50%)
84	B	2/3 (66%)	0.00	0 100 100	45, 45, 45, 48	0
84	C	2/3 (66%)	-0.11	0 100 100	40, 40, 40, 45	0
All	All	33488/35639 (93%)	0.14	914 (2%) 56 33	18, 74, 141, 289	76 (0%)

The worst 5 of 914 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
83	f	52	HIS	15.6
83	f	50	GLY	15.0
83	f	53	GLY	11.6
83	f	49	THR	10.0
13	c1	3	THR	8.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	5CT	f	51	15/16	0.80	0.54	44,44,44,44	15
84	8AN	C	76	22/23	0.96	0.09	40,42,43,43	0
84	8AN	B	76	22/23	0.97	0.08	44,44,45,45	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	2	1939	1/1	-0.07	0.35	130,130,130,130	0
85	MG	1	3405	1/1	-0.00	0.37	132,132,132,132	0
85	MG	2	1986	1/1	0.01	0.30	118,118,118,118	0
85	MG	2	1943	1/1	0.18	0.40	115,115,115,115	0
85	MG	5	3778	1/1	0.25	0.31	115,115,115,115	0
85	MG	2	1950	1/1	0.26	0.30	108,108,108,108	0
85	MG	6	1937	1/1	0.30	0.45	98,98,98,98	0
85	MG	5	3686	1/1	0.39	0.28	92,92,92,92	0
85	MG	1	3662	1/1	0.45	0.26	101,101,101,101	0
85	MG	1	3753	1/1	0.46	0.28	107,107,107,107	0
85	MG	2	1958	1/1	0.46	0.33	104,104,104,104	0
85	MG	6	1959	1/1	0.47	0.36	98,98,98,98	0
85	MG	5	3748	1/1	0.49	0.12	124,124,124,124	0
85	MG	2	1961	1/1	0.50	0.32	86,86,86,86	0
85	MG	5	3462	1/1	0.51	0.28	109,109,109,109	0
85	MG	2	1922	1/1	0.51	0.47	85,85,85,85	0
85	MG	2	1904	1/1	0.52	0.30	90,90,90,90	0
85	MG	2	1957	1/1	0.52	0.21	99,99,99,99	0
85	MG	O4	201	1/1	0.52	0.37	77,77,77,77	0
85	MG	6	1954	1/1	0.53	0.35	64,64,64,64	0
85	MG	2	1989	1/1	0.53	0.26	65,65,65,65	0
85	MG	6	1908	1/1	0.54	0.29	109,109,109,109	0
85	MG	2	1974	1/1	0.55	0.43	83,83,83,83	0
86	OHX	5	4123	7/7	0.56	0.28	76,76,76,76	5
85	MG	2	1912	1/1	0.57	0.43	88,88,88,88	0
86	OHX	6	2183	7/7	0.58	0.28	76,76,76,76	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3757	1/1	0.58	0.27	73,73,73,73	0
85	MG	2	1953	1/1	0.59	0.35	89,89,89,89	0
85	MG	1	3423	1/1	0.59	0.24	46,46,46,46	0
85	MG	2	1936	1/1	0.60	0.30	83,83,83,83	0
85	MG	5	3464	1/1	0.60	0.22	125,125,125,125	0
85	MG	6	1948	1/1	0.60	0.34	85,85,85,85	0
85	MG	6	1971	1/1	0.60	0.35	90,90,90,90	0
85	MG	6	1963	1/1	0.61	0.27	80,80,80,80	0
86	OHX	2	2145	7/7	0.61	0.19	103,103,103,103	4
85	MG	1	3635	1/1	0.62	0.45	88,88,88,88	0
85	MG	2	1955	1/1	0.62	0.36	62,62,62,62	0
85	MG	2	1924	1/1	0.62	0.30	100,100,100,100	0
85	MG	2	1945	1/1	0.62	0.24	107,107,107,107	0
85	MG	2	1969	1/1	0.63	0.36	108,108,108,108	0
85	MG	2	1941	1/1	0.63	0.32	100,100,100,100	0
85	MG	2	1967	1/1	0.63	0.15	93,93,93,93	0
85	MG	1	3560	1/1	0.63	0.48	46,46,46,46	0
85	MG	6	1984	1/1	0.64	0.28	109,109,109,109	0
85	MG	5	3667	1/1	0.64	0.33	86,86,86,86	0
85	MG	M7	201	1/1	0.64	0.43	71,71,71,71	0
85	MG	5	3503	1/1	0.65	0.34	57,57,57,57	0
86	OHX	2	2149	7/7	0.65	0.13	137,137,137,137	6
86	OHX	6	2178	7/7	0.65	0.15	145,145,145,145	6
85	MG	2	1909	1/1	0.65	0.39	83,83,83,83	0
86	OHX	2	2104	7/7	0.65	0.22	119,119,119,119	5
85	MG	6	1974	1/1	0.66	0.42	94,94,94,94	0
85	MG	5	3474	1/1	0.66	0.29	63,63,63,63	0
85	MG	17	2200	1/1	0.67	0.18	50,50,50,50	0
85	MG	2	1927	1/1	0.67	0.33	85,85,85,85	0
85	MG	2	1964	1/1	0.67	0.39	92,92,92,92	0
86	OHX	2	2147	7/7	0.67	0.14	116,116,116,116	6
85	MG	1	3729	1/1	0.67	0.15	69,69,69,69	0
86	OHX	3	219	7/7	0.67	0.18	82,82,82,82	5
85	MG	2	1978	1/1	0.67	0.33	74,74,74,74	0
85	MG	1	3537	1/1	0.67	0.27	57,57,57,57	0
85	MG	2	1952	1/1	0.67	0.33	64,64,64,64	0
85	MG	2	1933	1/1	0.68	0.41	70,70,70,70	0
85	MG	2	1968	1/1	0.68	0.30	101,101,101,101	0
85	MG	6	1938	1/1	0.68	0.25	60,60,60,60	0
85	MG	2	1925	1/1	0.68	0.35	67,67,67,67	0
86	OHX	M0	304	7/7	0.68	0.20	101,101,101,101	6
85	MG	5	3628	1/1	0.68	0.40	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3424	1/1	0.68	0.22	59,59,59,59	0
86	OHX	2	2123	7/7	0.68	0.16	121,121,121,121	5
85	MG	3	205	1/1	0.69	0.37	68,68,68,68	0
85	MG	2	1913	1/1	0.69	0.40	79,79,79,79	0
85	MG	2	1919	1/1	0.69	0.39	62,62,62,62	0
85	MG	6	1972	1/1	0.69	0.26	81,81,81,81	0
85	MG	5	3540	1/1	0.69	0.39	62,62,62,62	0
85	MG	1	3434	1/1	0.69	0.29	62,62,62,62	0
85	MG	6	1957	1/1	0.69	0.34	94,94,94,94	0
86	OHX	2	2141	7/7	0.69	0.19	90,90,90,90	6
85	MG	2	1905	1/1	0.70	0.39	63,63,63,63	0
86	OHX	1	3871	7/7	0.70	0.34	61,61,61,61	2
86	OHX	2	2121	7/7	0.70	0.26	94,94,94,94	4
85	MG	1	3672	1/1	0.70	0.29	76,76,76,76	0
85	MG	s4	601	1/1	0.70	0.29	66,66,66,66	0
85	MG	6	1910	1/1	0.70	0.30	91,91,91,91	0
85	MG	1	3660	1/1	0.70	0.23	82,82,82,82	0
85	MG	6	1931	1/1	0.71	0.25	92,92,92,92	0
85	MG	2	1954	1/1	0.71	0.20	105,105,105,105	0
85	MG	2	1951	1/1	0.71	0.43	71,71,71,71	0
85	MG	6	1980	1/1	0.71	0.11	76,76,76,76	0
86	OHX	1	4044	7/7	0.71	0.19	108,108,108,108	4
86	OHX	1	4106	7/7	0.71	0.13	72,72,72,72	4
85	MG	6	1960	1/1	0.71	0.23	65,65,65,65	0
86	OHX	2	2117	7/7	0.71	0.15	93,93,93,93	4
86	OHX	6	2175	7/7	0.71	0.23	100,100,100,100	6
85	MG	2	1988	1/1	0.71	0.28	88,88,88,88	0
85	MG	c9	201	1/1	0.71	0.17	83,83,83,83	0
85	MG	5	3446	1/1	0.71	0.22	64,64,64,64	0
86	OHX	5	4147	7/7	0.71	0.16	89,89,89,89	7
86	OHX	1	4013	7/7	0.72	0.35	54,54,54,54	3
85	MG	3	206	1/1	0.72	0.29	65,65,65,65	0
86	OHX	1	4093	7/7	0.72	0.17	64,64,64,64	4
85	MG	6	1986	1/1	0.72	0.40	93,93,93,93	0
85	MG	2	1973	1/1	0.72	0.33	80,80,80,80	0
85	MG	c8	202	1/1	0.72	0.39	84,84,84,84	0
86	OHX	6	2137	7/7	0.72	0.19	95,95,95,95	4
86	OHX	6	2149	7/7	0.72	0.19	95,95,95,95	6
85	MG	6	1967	1/1	0.72	0.27	76,76,76,76	0
85	MG	2	1911	1/1	0.72	0.55	77,77,77,77	0
85	MG	2	1962	1/1	0.72	0.25	88,88,88,88	0
85	MG	2	1929	1/1	0.72	0.33	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	2	1987	1/1	0.72	0.31	104,104,104,104	0
86	OHX	5	4150	7/7	0.72	0.24	62,62,62,62	5
86	OHX	5	4165	7/7	0.72	0.32	51,51,51,51	3
85	MG	6	1987	1/1	0.73	0.34	77,77,77,77	0
85	MG	2	1901	1/1	0.73	0.30	87,87,87,87	0
86	OHX	5	4062	7/7	0.73	0.24	56,56,56,56	3
85	MG	1	3566	1/1	0.73	0.40	47,47,47,47	0
85	MG	2	1970	1/1	0.73	0.32	65,65,65,65	0
85	MG	5	3422	1/1	0.73	0.34	44,44,44,44	0
86	OHX	1	4104	7/7	0.73	0.12	73,73,73,73	6
85	MG	6	1929	1/1	0.74	0.25	49,49,49,49	0
85	MG	5	3690	1/1	0.74	0.20	75,75,75,75	0
86	OHX	5	4034	7/7	0.74	0.19	66,66,66,66	4
85	MG	5	3424	1/1	0.74	0.28	56,56,56,56	0
86	OHX	5	4086	7/7	0.74	0.20	70,70,70,70	4
85	MG	1	3472	1/1	0.74	0.27	42,42,42,42	0
85	MG	6	1916	1/1	0.74	0.24	66,66,66,66	0
86	OHX	1	4067	7/7	0.74	0.16	107,107,107,107	7
85	MG	6	1962	1/1	0.74	0.15	93,93,93,93	0
86	OHX	8	228	7/7	0.74	0.19	73,73,73,73	5
85	MG	1	3700	1/1	0.75	0.23	51,51,51,51	0
85	MG	1	3607	1/1	0.75	0.33	85,85,85,85	0
86	OHX	L3	404	7/7	0.75	0.15	84,84,84,84	6
85	MG	1	3409	1/1	0.75	0.32	52,52,52,52	0
85	MG	6	1927	1/1	0.75	0.31	63,63,63,63	0
86	OHX	2	2151	7/7	0.75	0.16	112,112,112,112	7
86	OHX	2	2152	7/7	0.75	0.11	122,122,122,122	6
85	MG	3	201	1/1	0.75	0.20	80,80,80,80	0
86	OHX	1	3995	7/7	0.75	0.24	50,50,50,50	2
85	MG	2	1944	1/1	0.75	0.22	102,102,102,102	0
86	OHX	1	4021	7/7	0.75	0.22	58,58,58,58	3
86	OHX	1	4039	7/7	0.75	0.10	278,278,278,278	6
86	OHX	5	4119	7/7	0.75	0.29	52,52,52,52	3
85	MG	1	3661	1/1	0.75	0.27	51,51,51,51	0
85	MG	2	1946	1/1	0.75	0.20	108,108,108,108	0
86	OHX	1	4089	7/7	0.75	0.28	55,55,55,55	6
85	MG	2	1959	1/1	0.75	0.26	87,87,87,87	0
86	OHX	5	4172	7/7	0.75	0.26	45,45,45,45	3
85	MG	5	3680	1/1	0.75	0.24	70,70,70,70	0
86	OHX	8	229	7/7	0.75	0.14	101,101,101,101	6
86	OHX	m1	201	7/7	0.75	0.14	78,78,78,78	3
85	MG	1	3407	1/1	0.76	0.36	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	6	1903	1/1	0.76	0.22	88,88,88,88	0
85	MG	2	1938	1/1	0.76	0.35	72,72,72,72	0
86	OHX	5	3948	7/7	0.76	0.28	49,49,49,49	2
85	MG	5	3739	1/1	0.76	0.13	109,109,109,109	0
85	MG	6	1979	1/1	0.76	0.23	101,101,101,101	0
85	MG	2	1949	1/1	0.76	0.41	86,86,86,86	0
85	MG	5	3547	1/1	0.76	0.39	53,53,53,53	0
85	MG	14	401	1/1	0.76	0.10	42,42,42,42	0
85	MG	5	3567	1/1	0.76	0.23	37,37,37,37	0
86	OHX	1	3965	7/7	0.76	0.27	56,56,56,56	3
86	OHX	1	3983	7/7	0.76	0.14	77,77,77,77	2
86	OHX	6	2131	7/7	0.76	0.18	89,89,89,89	6
85	MG	1	3714	1/1	0.76	0.12	46,46,46,46	0
85	MG	1	3576	1/1	0.76	0.36	46,46,46,46	0
86	OHX	8	230	7/7	0.76	0.20	68,68,68,68	3
86	OHX	19	201	7/7	0.76	0.17	61,61,61,61	2
86	OHX	6	2169	7/7	0.76	0.22	89,89,89,89	4
85	MG	5	3674	1/1	0.77	0.11	65,65,65,65	0
85	MG	5	3507	1/1	0.77	0.34	38,38,38,38	0
85	MG	5	3685	1/1	0.77	0.28	48,48,48,48	0
85	MG	1	3487	1/1	0.77	0.27	49,49,49,49	0
86	OHX	5	4083	7/7	0.77	0.31	53,53,53,53	3
86	OHX	1	4108	7/7	0.77	0.19	59,59,59,59	5
86	OHX	2	2120	7/7	0.77	0.18	87,87,87,87	3
85	MG	1	3517	1/1	0.77	0.36	46,46,46,46	0
85	MG	5	3712	1/1	0.77	0.21	67,67,67,67	0
86	OHX	6	2114	7/7	0.77	0.20	66,66,66,66	3
85	MG	1	3447	1/1	0.77	0.27	51,51,51,51	0
86	OHX	6	2133	7/7	0.77	0.15	125,125,125,125	6
86	OHX	1	4036	7/7	0.77	0.15	83,83,83,83	6
85	MG	5	3571	1/1	0.77	0.34	34,34,34,34	0
85	MG	6	1947	1/1	0.77	0.30	50,50,50,50	0
85	MG	6	2011	1/1	0.77	0.27	48,48,48,48	0
86	OHX	1	4070	7/7	0.77	0.12	111,111,111,111	6
85	MG	2	1932	1/1	0.78	0.41	64,64,64,64	0
86	OHX	1	3928	7/7	0.78	0.23	49,49,49,49	3
85	MG	5	3684	1/1	0.78	0.11	62,62,62,62	0
85	MG	2	1981	1/1	0.78	0.22	79,79,79,79	0
86	OHX	3	217	7/7	0.78	0.22	78,78,78,78	4
85	MG	5	3518	1/1	0.78	0.39	38,38,38,38	0
85	MG	1	3464	1/1	0.78	0.31	38,38,38,38	0
85	MG	2	1985	1/1	0.78	0.37	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4139	7/7	0.78	0.12	108,108,108,108	5
86	OHX	N8	204	7/7	0.78	0.15	90,90,90,90	7
85	MG	5	3722	1/1	0.78	0.30	41,41,41,41	0
85	MG	2	1965	1/1	0.78	0.39	76,76,76,76	0
86	OHX	5	4169	7/7	0.78	0.16	81,81,81,81	7
85	MG	6	1961	1/1	0.78	0.32	95,95,95,95	0
85	MG	6	1909	1/1	0.78	0.26	53,53,53,53	0
85	MG	6	1943	1/1	0.78	0.41	70,70,70,70	0
86	OHX	1	4075	7/7	0.78	0.18	75,75,75,75	5
86	OHX	1	4079	7/7	0.78	0.13	108,108,108,108	6
85	MG	1	3586	1/1	0.78	0.39	45,45,45,45	0
86	OHX	2	2083	7/7	0.79	0.17	87,87,87,87	2
86	OHX	2	2103	7/7	0.79	0.19	118,118,118,118	4
85	MG	2	1937	1/1	0.79	0.22	80,80,80,80	0
85	MG	6	1913	1/1	0.79	0.30	79,79,79,79	0
85	MG	1	3417	1/1	0.79	0.40	78,78,78,78	0
85	MG	6	1919	1/1	0.79	0.35	64,64,64,64	0
86	OHX	1	4073	7/7	0.79	0.14	71,71,71,71	5
85	MG	1	3739	1/1	0.79	0.25	72,72,72,72	0
85	MG	6	1928	1/1	0.79	0.15	57,57,57,57	0
86	OHX	5	4078	7/7	0.79	0.23	68,68,68,68	3
86	OHX	2	2142	7/7	0.79	0.14	132,132,132,132	7
85	MG	2	1907	1/1	0.79	0.40	62,62,62,62	0
86	OHX	1	4096	7/7	0.79	0.18	80,80,80,80	4
85	MG	6	1906	1/1	0.79	0.26	76,76,76,76	0
85	MG	6	1988	1/1	0.79	0.29	80,80,80,80	0
86	OHX	5	4143	7/7	0.79	0.23	50,50,50,50	4
86	OHX	2	2150	7/7	0.79	0.11	151,151,151,151	7
86	OHX	1	4111	7/7	0.79	0.11	104,104,104,104	7
86	OHX	5	4153	7/7	0.79	0.27	35,35,35,35	4
85	MG	5	3531	1/1	0.79	0.27	55,55,55,55	0
86	OHX	5	4166	7/7	0.79	0.25	49,49,49,49	4
85	MG	6	1996	1/1	0.79	0.23	70,70,70,70	0
85	MG	6	1932	1/1	0.79	0.12	72,72,72,72	0
85	MG	1	3538	1/1	0.79	0.40	39,39,39,39	0
85	MG	8	205	1/1	0.79	0.14	43,43,43,43	0
85	MG	8	210	1/1	0.79	0.09	48,48,48,48	0
85	MG	6	1964	1/1	0.79	0.20	82,82,82,82	0
85	MG	2	1966	1/1	0.79	0.26	74,74,74,74	0
87	ZN	d7	101	1/1	0.79	0.17	147,147,147,147	0
86	OHX	s1	302	7/7	0.80	0.17	99,99,99,99	6
85	MG	1	3401	1/1	0.80	0.32	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	4	205	1/1	0.80	0.25	58,58,58,58	0
85	MG	1	3694	1/1	0.80	0.19	46,46,46,46	0
85	MG	1	3595	1/1	0.80	0.42	78,78,78,78	0
85	MG	5	3548	1/1	0.80	0.30	25,25,25,25	0
86	OHX	1	4107	7/7	0.80	0.14	91,91,91,91	6
85	MG	6	1901	1/1	0.80	0.41	52,52,52,52	0
85	MG	1	3701	1/1	0.80	0.17	52,52,52,52	0
85	MG	5	3591	1/1	0.80	0.31	42,42,42,42	0
85	MG	2	1928	1/1	0.80	0.41	71,71,71,71	0
85	MG	1	3551	1/1	0.80	0.22	38,38,38,38	0
85	MG	1	3507	1/1	0.80	0.38	30,30,30,30	0
85	MG	6	1946	1/1	0.80	0.31	53,53,53,53	0
86	OHX	5	4159	7/7	0.80	0.26	48,48,48,48	4
86	OHX	1	4032	7/7	0.80	0.20	52,52,52,52	3
85	MG	1	3415	1/1	0.80	0.28	43,43,43,43	0
85	MG	1	3533	1/1	0.80	0.25	49,49,49,49	0
85	MG	6	1981	1/1	0.80	0.35	54,54,54,54	0
86	OHX	2	2135	7/7	0.80	0.10	188,188,188,188	6
85	MG	5	3481	1/1	0.80	0.37	76,76,76,76	0
85	MG	6	1915	1/1	0.80	0.34	75,75,75,75	0
86	OHX	6	2177	7/7	0.80	0.11	141,141,141,141	7
86	OHX	2	2143	7/7	0.80	0.22	84,84,84,84	5
85	MG	1	3669	1/1	0.80	0.23	59,59,59,59	0
85	MG	5	3715	1/1	0.81	0.33	62,62,62,62	0
85	MG	6	1990	1/1	0.81	0.30	79,79,79,79	0
85	MG	6	1992	1/1	0.81	0.26	61,61,61,61	0
85	MG	2	1916	1/1	0.81	0.33	63,63,63,63	0
86	OHX	5	4054	7/7	0.81	0.16	50,50,50,50	2
85	MG	2	1914	1/1	0.81	0.33	83,83,83,83	0
86	OHX	1	4094	7/7	0.81	0.16	77,77,77,77	4
85	MG	1	3473	1/1	0.81	0.26	56,56,56,56	0
85	MG	1	3760	1/1	0.81	0.15	62,62,62,62	0
86	OHX	5	4091	7/7	0.81	0.14	45,45,45,45	2
86	OHX	5	4108	7/7	0.81	0.24	66,66,66,66	3
85	MG	6	1940	1/1	0.81	0.42	36,36,36,36	0
86	OHX	S6	301	7/7	0.81	0.15	117,117,117,117	7
86	OHX	1	3867	7/7	0.81	0.24	51,51,51,51	4
85	MG	2	1920	1/1	0.81	0.34	76,76,76,76	0
85	MG	5	3600	1/1	0.81	0.12	37,37,37,37	0
86	OHX	5	4149	7/7	0.81	0.09	145,145,145,145	7
85	MG	1	3544	1/1	0.81	0.20	55,55,55,55	0
85	MG	1	3674	1/1	0.81	0.26	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	2	1960	1/1	0.81	0.19	76,76,76,76	0
86	OHX	2	2112	7/7	0.81	0.16	121,121,121,121	6
85	MG	6	1918	1/1	0.81	0.35	41,41,41,41	0
85	MG	5	3469	1/1	0.81	0.14	38,38,38,38	1
85	MG	1	3609	1/1	0.81	0.22	44,44,44,44	0
85	MG	M9	201	1/1	0.81	0.20	75,75,75,75	0
85	MG	1	3557	1/1	0.81	0.39	55,55,55,55	0
86	OHX	1	4061	7/7	0.81	0.17	72,72,72,72	4
86	OHX	2	2137	7/7	0.81	0.10	219,219,219,219	7
86	OHX	1	4069	7/7	0.81	0.21	58,58,58,58	5
85	MG	1	3652	1/1	0.81	0.18	48,48,48,48	0
86	OHX	5	4061	7/7	0.82	0.21	55,55,55,55	4
85	MG	1	3570	1/1	0.82	0.26	46,46,46,46	0
85	MG	1	3597	1/1	0.82	0.28	47,47,47,47	0
85	MG	1	3602	1/1	0.82	0.32	58,58,58,58	0
85	MG	2	1940	1/1	0.82	0.47	80,80,80,80	0
85	MG	1	3460	1/1	0.82	0.36	49,49,49,49	0
86	OHX	6	2110	7/7	0.82	0.19	112,112,112,112	6
86	OHX	5	4111	7/7	0.82	0.15	74,74,74,74	7
85	MG	1	3612	1/1	0.82	0.28	55,55,55,55	0
86	OHX	2	2109	7/7	0.82	0.14	105,105,105,105	6
85	MG	1	3751	1/1	0.82	0.28	67,67,67,67	0
86	OHX	5	4140	7/7	0.82	0.18	88,88,88,88	7
86	OHX	6	2135	7/7	0.82	0.28	94,94,94,94	7
85	MG	5	3629	1/1	0.82	0.12	35,35,35,35	0
85	MG	5	3640	1/1	0.82	0.20	50,50,50,50	0
86	OHX	6	2162	7/7	0.82	0.19	114,114,114,114	5
85	MG	1	3587	1/1	0.82	0.33	35,35,35,35	0
86	OHX	6	2174	7/7	0.82	0.11	92,92,92,92	6
86	OHX	5	4161	7/7	0.82	0.13	123,123,123,123	7
86	OHX	2	2122	7/7	0.82	0.20	91,91,91,91	7
85	MG	1	3692	1/1	0.82	0.31	61,61,61,61	0
86	OHX	2	2128	7/7	0.82	0.17	115,115,115,115	7
86	OHX	5	4171	7/7	0.82	0.18	90,90,90,90	5
86	OHX	2	2133	7/7	0.82	0.10	214,214,214,214	6
86	OHX	7	224	7/7	0.82	0.16	54,54,54,54	5
85	MG	5	3790	1/1	0.82	0.25	69,69,69,69	0
85	MG	5	3809	1/1	0.82	0.27	42,42,42,42	0
86	OHX	5	4008	7/7	0.82	0.20	66,66,66,66	3
86	OHX	1	4029	7/7	0.82	0.15	82,82,82,82	3
86	OHX	5	4048	7/7	0.82	0.19	69,69,69,69	3
86	OHX	m4	201	7/7	0.82	0.15	108,108,108,108	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	6	1905	1/1	0.82	0.27	51,51,51,51	0
86	OHX	5	4082	7/7	0.83	0.13	92,92,92,92	3
85	MG	5	3514	1/1	0.83	0.28	35,35,35,35	0
86	OHX	6	2097	7/7	0.83	0.23	49,49,49,49	1
85	MG	6	1936	1/1	0.83	0.28	76,76,76,76	0
85	MG	5	3441	1/1	0.83	0.29	30,30,30,30	0
85	MG	2	1931	1/1	0.83	0.41	65,65,65,65	0
85	MG	5	3542	1/1	0.83	0.42	46,46,46,46	0
85	MG	5	3451	1/1	0.83	0.20	40,40,40,40	0
86	OHX	5	4125	7/7	0.83	0.27	48,48,48,48	5
86	OHX	5	4127	7/7	0.83	0.27	44,44,44,44	3
86	OHX	5	4128	7/7	0.83	0.18	47,47,47,47	4
86	OHX	5	4137	7/7	0.83	0.15	50,50,50,50	4
86	OHX	2	2105	7/7	0.83	0.15	87,87,87,87	3
85	MG	5	3695	1/1	0.83	0.23	54,54,54,54	0
86	OHX	6	2161	7/7	0.83	0.21	84,84,84,84	6
86	OHX	1	4078	7/7	0.83	0.10	167,167,167,167	7
86	OHX	6	2165	7/7	0.83	0.18	74,74,74,74	6
86	OHX	6	2167	7/7	0.83	0.20	73,73,73,73	7
85	MG	6	2002	1/1	0.83	0.10	66,66,66,66	0
85	MG	6	2003	1/1	0.83	0.20	96,96,96,96	0
85	MG	1	3690	1/1	0.83	0.29	63,63,63,63	0
86	OHX	5	4164	7/7	0.83	0.19	61,61,61,61	7
86	OHX	1	3915	7/7	0.83	0.18	66,66,66,66	4
85	MG	5	3724	1/1	0.83	0.29	35,35,35,35	0
86	OHX	6	2182	7/7	0.83	0.20	113,113,113,113	7
85	MG	2	1923	1/1	0.83	0.32	45,45,45,45	0
85	MG	1	3433	1/1	0.83	0.30	34,34,34,34	0
86	OHX	2	2124	7/7	0.83	0.12	128,128,128,128	6
85	MG	5	3485	1/1	0.83	0.18	38,38,38,38	0
86	OHX	1	4110	7/7	0.83	0.30	55,55,55,55	5
86	OHX	1	4016	7/7	0.83	0.23	56,56,56,56	3
85	MG	2	1908	1/1	0.83	0.16	90,90,90,90	0
85	MG	1	3532	1/1	0.83	0.35	42,42,42,42	0
85	MG	5	3508	1/1	0.83	0.37	31,31,31,31	0
85	MG	5	3673	1/1	0.83	0.33	78,78,78,78	0
85	MG	6	1933	1/1	0.84	0.33	56,56,56,56	0
85	MG	6	1934	1/1	0.84	0.29	43,43,43,43	0
85	MG	5	3638	1/1	0.84	0.17	50,50,50,50	0
86	OHX	1	4042	7/7	0.84	0.09	70,70,70,70	5
86	OHX	2	2114	7/7	0.84	0.17	103,103,103,103	4
85	MG	1	3523	1/1	0.84	0.33	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4065	7/7	0.84	0.19	59,59,59,59	5
85	MG	5	3663	1/1	0.84	0.24	48,48,48,48	0
85	MG	1	3426	1/1	0.84	0.28	52,52,52,52	0
85	MG	1	3465	1/1	0.84	0.29	28,28,28,28	0
85	MG	6	1982	1/1	0.84	0.28	53,53,53,53	0
85	MG	1	3741	1/1	0.84	0.29	46,46,46,46	0
85	MG	5	3479	1/1	0.84	0.28	70,70,70,70	0
85	MG	2	1935	1/1	0.84	0.24	70,70,70,70	0
86	OHX	1	4086	7/7	0.84	0.21	65,65,65,65	4
85	MG	5	3483	1/1	0.84	0.29	52,52,52,52	0
86	OHX	1	4092	7/7	0.84	0.22	47,47,47,47	3
85	MG	2	1942	1/1	0.84	0.22	69,69,69,69	0
85	MG	5	3502	1/1	0.84	0.40	31,31,31,31	0
86	OHX	5	4107	7/7	0.84	0.17	81,81,81,81	5
85	MG	5	3697	1/1	0.84	0.10	61,61,61,61	0
85	MG	1	3758	1/1	0.84	0.28	48,48,48,48	0
85	MG	1	3445	1/1	0.84	0.37	57,57,57,57	0
85	MG	1	4112	1/1	0.84	0.11	44,44,44,44	0
85	MG	5	3510	1/1	0.84	0.22	39,39,39,39	0
85	MG	1	3497	1/1	0.84	0.35	25,25,25,25	0
85	MG	1	3505	1/1	0.84	0.35	38,38,38,38	0
86	OHX	5	4132	7/7	0.84	0.21	45,45,45,45	4
85	MG	2	1948	1/1	0.84	0.30	72,72,72,72	0
85	MG	6	2004	1/1	0.84	0.28	74,74,74,74	0
85	MG	5	3782	1/1	0.84	0.18	48,48,48,48	0
85	MG	6	1921	1/1	0.84	0.33	66,66,66,66	0
85	MG	1	3414	1/1	0.84	0.40	43,43,43,43	0
86	OHX	6	2080	7/7	0.84	0.20	82,82,82,82	1
86	OHX	1	3924	7/7	0.84	0.20	71,71,71,71	4
85	MG	7	212	1/1	0.84	0.27	51,51,51,51	0
86	OHX	5	4158	7/7	0.84	0.18	35,35,35,35	3
86	OHX	1	3955	7/7	0.84	0.21	71,71,71,71	3
86	OHX	6	2118	7/7	0.84	0.22	89,89,89,89	5
86	OHX	1	3963	7/7	0.84	0.27	51,51,51,51	3
85	MG	M6	201	1/1	0.84	0.13	34,34,34,34	0
85	MG	5	3557	1/1	0.84	0.35	29,29,29,29	0
85	MG	1	3630	1/1	0.84	0.24	76,76,76,76	0
86	OHX	6	2148	7/7	0.84	0.21	54,54,54,54	3
85	MG	5	3420	1/1	0.84	0.33	26,26,26,26	0
86	OHX	6	2150	7/7	0.84	0.15	78,78,78,78	6
86	OHX	6	2152	7/7	0.84	0.17	107,107,107,107	5
85	MG	5	3590	1/1	0.84	0.28	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4018	7/7	0.84	0.13	69,69,69,69	3
86	OHX	l5	302	7/7	0.84	0.14	105,105,105,105	4
85	MG	1	3567	1/1	0.84	0.20	48,48,48,48	0
86	OHX	m0	302	7/7	0.84	0.24	49,49,49,49	3
86	OHX	1	4028	7/7	0.84	0.15	58,58,58,58	3
85	MG	1	3710	1/1	0.84	0.09	46,46,46,46	0
86	OHX	6	2173	7/7	0.84	0.15	64,64,64,64	5
85	MG	5	3598	1/1	0.85	0.25	48,48,48,48	0
86	OHX	sR	401	7/7	0.85	0.13	129,129,129,129	6
86	OHX	5	3936	7/7	0.85	0.21	49,49,49,49	3
85	MG	5	3800	1/1	0.85	0.11	70,70,70,70	0
85	MG	6	1953	1/1	0.85	0.36	63,63,63,63	0
86	OHX	C3	201	7/7	0.85	0.14	100,100,100,100	5
86	OHX	5	4046	7/7	0.85	0.09	53,53,53,53	5
86	OHX	1	4095	7/7	0.85	0.23	55,55,55,55	5
85	MG	5	3602	1/1	0.85	0.24	30,30,30,30	0
86	OHX	1	4098	7/7	0.85	0.13	61,61,61,61	5
86	OHX	1	4102	7/7	0.85	0.16	65,65,65,65	3
86	OHX	1	4103	7/7	0.85	0.21	53,53,53,53	5
85	MG	5	3619	1/1	0.85	0.25	47,47,47,47	0
85	MG	1	3712	1/1	0.85	0.34	44,44,44,44	0
85	MG	1	3571	1/1	0.85	0.35	53,53,53,53	0
86	OHX	5	4087	7/7	0.85	0.30	39,39,39,39	5
85	MG	5	3632	1/1	0.85	0.11	36,36,36,36	0
86	OHX	2	2065	7/7	0.85	0.19	106,106,106,106	5
85	MG	N3	201	1/1	0.85	0.31	36,36,36,36	0
86	OHX	2	2101	7/7	0.85	0.17	110,110,110,110	5
86	OHX	5	4117	7/7	0.85	0.23	40,40,40,40	5
85	MG	1	3488	1/1	0.85	0.35	37,37,37,37	0
85	MG	5	3659	1/1	0.85	0.28	39,39,39,39	0
86	OHX	1	4000	7/7	0.85	0.22	55,55,55,55	3
86	OHX	1	4009	7/7	0.85	0.09	131,131,131,131	7
85	MG	5	3501	1/1	0.85	0.25	42,42,42,42	0
85	MG	2	1906	1/1	0.85	0.27	68,68,68,68	0
86	OHX	5	4136	7/7	0.85	0.10	180,180,180,180	7
85	MG	1	3542	1/1	0.85	0.35	50,50,50,50	0
86	OHX	1	4019	7/7	0.85	0.20	47,47,47,47	2
85	MG	2	1917	1/1	0.85	0.35	54,54,54,54	0
86	OHX	5	4142	7/7	0.85	0.12	58,58,58,58	4
86	OHX	6	2120	7/7	0.85	0.11	70,70,70,70	3
86	OHX	1	4027	7/7	0.85	0.15	75,75,75,75	3
85	MG	2	1976	1/1	0.85	0.24	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3555	1/1	0.85	0.33	26,26,26,26	0
85	MG	1	3604	1/1	0.85	0.39	39,39,39,39	0
86	OHX	5	4154	7/7	0.85	0.10	111,111,111,111	6
85	MG	5	3401	1/1	0.85	0.20	53,53,53,53	0
85	MG	1	3512	1/1	0.85	0.31	31,31,31,31	0
85	MG	1	3693	1/1	0.85	0.28	49,49,49,49	0
85	MG	1	3430	1/1	0.85	0.27	57,57,57,57	0
86	OHX	6	2157	7/7	0.85	0.12	90,90,90,90	7
86	OHX	6	2158	7/7	0.85	0.10	131,131,131,131	7
85	MG	6	1945	1/1	0.85	0.33	51,51,51,51	0
86	OHX	1	4063	7/7	0.85	0.10	159,159,159,159	7
85	MG	2	1977	1/1	0.85	0.23	72,72,72,72	0
86	OHX	6	2166	7/7	0.85	0.14	66,66,66,66	4
85	MG	2	1956	1/1	0.85	0.42	70,70,70,70	0
85	MG	5	3564	1/1	0.85	0.40	27,27,27,27	0
85	MG	2	1934	1/1	0.85	0.28	80,80,80,80	0
85	MG	5	3747	1/1	0.85	0.25	51,51,51,51	0
85	MG	6	1949	1/1	0.85	0.28	77,77,77,77	0
85	MG	5	3589	1/1	0.85	0.36	28,28,28,28	0
85	MG	6	1950	1/1	0.85	0.43	66,66,66,66	0
86	OHX	1	4085	7/7	0.85	0.10	61,61,61,61	6
87	ZN	D7	101	1/1	0.85	0.16	161,161,161,161	0
85	MG	5	3472	1/1	0.85	0.24	39,39,39,39	0
85	MG	3	208	1/1	0.86	0.19	42,42,42,42	0
86	OHX	1	4077	7/7	0.86	0.12	62,62,62,62	4
86	OHX	6	2181	7/7	0.86	0.15	117,117,117,117	7
85	MG	4	203	1/1	0.86	0.32	57,57,57,57	0
85	MG	1	3534	1/1	0.86	0.29	69,69,69,69	0
85	MG	4	214	1/1	0.86	0.26	41,41,41,41	0
86	OHX	c5	202	7/7	0.86	0.16	109,109,109,109	6
85	MG	4	215	1/1	0.86	0.36	55,55,55,55	0
85	MG	5	3592	1/1	0.86	0.39	35,35,35,35	0
85	MG	5	3596	1/1	0.86	0.18	47,47,47,47	0
86	OHX	5	3970	7/7	0.86	0.21	80,80,80,80	3
85	MG	1	3715	1/1	0.86	0.31	46,46,46,46	0
85	MG	6	1926	1/1	0.86	0.20	65,65,65,65	0
85	MG	1	3561	1/1	0.86	0.24	22,22,22,22	0
85	MG	1	3483	1/1	0.86	0.25	54,54,54,54	0
85	MG	1	3421	1/1	0.86	0.26	58,58,58,58	0
86	OHX	1	4101	7/7	0.86	0.14	66,66,66,66	4
85	MG	SM	301	1/1	0.86	0.28	58,58,58,58	0
86	OHX	1	3927	7/7	0.86	0.21	51,51,51,51	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3491	1/1	0.86	0.35	51,51,51,51	0
86	OHX	2	2049	7/7	0.86	0.15	100,100,100,100	4
85	MG	6	1902	1/1	0.86	0.35	40,40,40,40	0
86	OHX	2	2074	7/7	0.86	0.14	85,85,85,85	3
86	OHX	1	4109	7/7	0.86	0.19	48,48,48,48	4
86	OHX	1	3974	7/7	0.86	0.24	63,63,63,63	5
86	OHX	1	3975	7/7	0.86	0.12	88,88,88,88	3
86	OHX	2	2076	7/7	0.86	0.15	87,87,87,87	5
86	OHX	5	4115	7/7	0.86	0.18	63,63,63,63	6
86	OHX	1	3986	7/7	0.86	0.16	76,76,76,76	3
86	OHX	4	228	7/7	0.86	0.23	51,51,51,51	4
86	OHX	4	232	7/7	0.86	0.15	73,73,73,73	5
86	OHX	1	3989	7/7	0.86	0.18	94,94,94,94	5
86	OHX	2	2081	7/7	0.86	0.17	120,120,120,120	6
86	OHX	M9	202	7/7	0.86	0.12	77,77,77,77	3
85	MG	6	2006	1/1	0.86	0.32	67,67,67,67	0
86	OHX	2	2092	7/7	0.86	0.18	73,73,73,73	5
86	OHX	6	2091	7/7	0.86	0.24	83,83,83,83	3
86	OHX	2	2093	7/7	0.86	0.21	110,110,110,110	5
85	MG	6	2009	1/1	0.86	0.22	64,64,64,64	0
85	MG	1	3546	1/1	0.86	0.34	36,36,36,36	0
85	MG	6	1935	1/1	0.86	0.36	44,44,44,44	0
85	MG	1	3529	1/1	0.86	0.30	34,34,34,34	0
85	MG	5	3513	1/1	0.86	0.23	37,37,37,37	0
85	MG	1	3432	1/1	0.86	0.16	49,49,49,49	0
86	OHX	5	4152	7/7	0.86	0.16	76,76,76,76	5
85	MG	5	3515	1/1	0.86	0.24	42,42,42,42	0
85	MG	d6	102	1/1	0.86	0.21	68,68,68,68	0
85	MG	5	3526	1/1	0.86	0.35	29,29,29,29	0
86	OHX	1	4038	7/7	0.86	0.28	56,56,56,56	4
85	MG	1	3659	1/1	0.86	0.12	78,78,78,78	0
86	OHX	5	4162	7/7	0.86	0.12	100,100,100,100	7
85	MG	5	3406	1/1	0.86	0.09	47,47,47,47	0
85	MG	5	3417	1/1	0.86	0.27	64,64,64,64	0
86	OHX	1	4045	7/7	0.86	0.17	54,54,54,54	1
86	OHX	5	4168	7/7	0.86	0.17	64,64,64,64	5
86	OHX	1	4046	7/7	0.86	0.12	50,50,50,50	2
86	OHX	1	4050	7/7	0.86	0.23	58,58,58,58	5
86	OHX	6	2163	7/7	0.86	0.18	61,61,61,61	4
86	OHX	6	2164	7/7	0.86	0.18	44,44,44,44	5
85	MG	1	3592	1/1	0.86	0.18	61,61,61,61	0
85	MG	5	3714	1/1	0.86	0.14	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	6	1978	1/1	0.86	0.22	77,77,77,77	0
86	OHX	8	231	7/7	0.86	0.23	62,62,62,62	5
86	OHX	6	2168	7/7	0.86	0.16	76,76,76,76	3
85	MG	5	3719	1/1	0.86	0.27	63,63,63,63	1
86	OHX	6	2171	7/7	0.86	0.22	53,53,53,53	7
85	MG	2	1926	1/1	0.86	0.22	76,76,76,76	0
85	MG	5	3431	1/1	0.86	0.20	41,41,41,41	0
85	MG	5	3733	1/1	0.86	0.19	50,50,50,50	0
86	OHX	6	2176	7/7	0.86	0.16	62,62,62,62	7
86	OHX	2	2079	7/7	0.87	0.23	82,82,82,82	3
86	OHX	5	4026	7/7	0.87	0.21	54,54,54,54	4
86	OHX	5	4033	7/7	0.87	0.16	98,98,98,98	7
85	MG	1	3504	1/1	0.87	0.36	42,42,42,42	0
85	MG	1	3439	1/1	0.87	0.25	60,60,60,60	0
86	OHX	1	3990	7/7	0.87	0.14	92,92,92,92	6
85	MG	6	1917	1/1	0.87	0.33	64,64,64,64	0
86	OHX	5	4055	7/7	0.87	0.19	56,56,56,56	4
86	OHX	5	4059	7/7	0.87	0.20	47,47,47,47	3
85	MG	1	3613	1/1	0.87	0.32	58,58,58,58	0
85	MG	6	2007	1/1	0.87	0.24	51,51,51,51	0
85	MG	1	3619	1/1	0.87	0.22	53,53,53,53	0
86	OHX	5	4081	7/7	0.87	0.19	35,35,35,35	3
85	MG	4	202	1/1	0.87	0.16	64,64,64,64	0
85	MG	6	1922	1/1	0.87	0.14	55,55,55,55	0
85	MG	2	1979	1/1	0.87	0.13	70,70,70,70	0
85	MG	1	3474	1/1	0.87	0.26	48,48,48,48	0
85	MG	5	3523	1/1	0.87	0.35	29,29,29,29	0
86	OHX	5	4105	7/7	0.87	0.12	84,84,84,84	4
86	OHX	6	2083	7/7	0.87	0.21	94,94,94,94	7
85	MG	4	211	1/1	0.87	0.10	54,54,54,54	0
85	MG	1	3641	1/1	0.87	0.24	49,49,49,49	0
85	MG	5	3703	1/1	0.87	0.29	58,58,58,58	0
85	MG	5	3705	1/1	0.87	0.21	66,66,66,66	0
85	MG	5	3535	1/1	0.87	0.31	36,36,36,36	0
85	MG	1	3642	1/1	0.87	0.31	32,32,32,32	0
86	OHX	5	4124	7/7	0.87	0.23	51,51,51,51	6
86	OHX	2	2126	7/7	0.87	0.11	64,64,64,64	4
85	MG	5	3407	1/1	0.87	0.31	35,35,35,35	0
85	MG	5	3413	1/1	0.87	0.31	36,36,36,36	0
85	MG	1	3419	1/1	0.87	0.12	36,36,36,36	0
85	MG	1	3519	1/1	0.87	0.33	49,49,49,49	0
86	OHX	1	4058	7/7	0.87	0.20	100,100,100,100	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	2	2140	7/7	0.87	0.17	85,85,85,85	5
86	OHX	1	4062	7/7	0.87	0.22	51,51,51,51	3
86	OHX	6	2154	7/7	0.87	0.22	49,49,49,49	3
86	OHX	6	2155	7/7	0.87	0.17	71,71,71,71	3
86	OHX	5	4144	7/7	0.87	0.20	65,65,65,65	5
85	MG	5	3421	1/1	0.87	0.28	38,38,38,38	0
85	MG	1	3717	1/1	0.87	0.34	59,59,59,59	0
86	OHX	1	4066	7/7	0.87	0.16	63,63,63,63	6
85	MG	1	3719	1/1	0.87	0.20	65,65,65,65	0
85	MG	5	3585	1/1	0.87	0.38	35,35,35,35	0
86	OHX	2	2146	7/7	0.87	0.17	87,87,87,87	7
86	OHX	5	4155	7/7	0.87	0.09	97,97,97,97	7
85	MG	1	3454	1/1	0.87	0.33	31,31,31,31	0
85	MG	5	3777	1/1	0.87	0.12	41,41,41,41	0
85	MG	1	3413	1/1	0.87	0.31	41,41,41,41	0
85	MG	D3	201	1/1	0.87	0.12	54,54,54,54	0
85	MG	1	3496	1/1	0.87	0.33	41,41,41,41	0
86	OHX	1	4080	7/7	0.87	0.21	57,57,57,57	4
85	MG	5	3594	1/1	0.87	0.34	35,35,35,35	0
85	MG	6	1985	1/1	0.87	0.15	55,55,55,55	0
85	MG	7	201	1/1	0.87	0.34	41,41,41,41	0
85	MG	1	3752	1/1	0.87	0.22	64,64,64,64	0
85	MG	1	3564	1/1	0.87	0.24	30,30,30,30	0
86	OHX	7	220	7/7	0.87	0.17	73,73,73,73	1
85	MG	1	3755	1/1	0.87	0.13	45,45,45,45	0
86	OHX	8	218	7/7	0.87	0.20	63,63,63,63	4
85	MG	5	3614	1/1	0.87	0.38	41,41,41,41	0
85	MG	2	1963	1/1	0.87	0.18	83,83,83,83	0
85	MG	1	3676	1/1	0.87	0.21	52,52,52,52	0
85	MG	6	1993	1/1	0.87	0.11	66,66,66,66	0
86	OHX	s8	303	7/7	0.87	0.14	105,105,105,105	3
86	OHX	2	2069	7/7	0.87	0.16	115,115,115,115	4
85	MG	1	3684	1/1	0.87	0.43	52,52,52,52	0
85	MG	6	1997	1/1	0.87	0.24	53,53,53,53	0
86	OHX	1	3978	7/7	0.87	0.19	77,77,77,77	3
86	OHX	1	3980	7/7	0.87	0.16	51,51,51,51	1
86	OHX	5	3975	7/7	0.87	0.22	85,85,85,85	3
85	MG	5	3709	1/1	0.88	0.19	51,51,51,51	0
85	MG	1	3577	1/1	0.88	0.21	39,39,39,39	0
86	OHX	5	4043	7/7	0.88	0.29	38,38,38,38	4
85	MG	5	3494	1/1	0.88	0.30	45,45,45,45	0
85	MG	5	3498	1/1	0.88	0.24	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3718	1/1	0.88	0.26	26,26,26,26	1
85	MG	6	1912	1/1	0.88	0.30	39,39,39,39	0
85	MG	1	3451	1/1	0.88	0.22	53,53,53,53	0
86	OHX	1	4023	7/7	0.88	0.15	73,73,73,73	3
86	OHX	1	4026	7/7	0.88	0.13	52,52,52,52	5
86	OHX	5	4069	7/7	0.88	0.18	58,58,58,58	5
86	OHX	5	4070	7/7	0.88	0.14	73,73,73,73	3
85	MG	1	3485	1/1	0.88	0.21	58,58,58,58	0
86	OHX	5	4079	7/7	0.88	0.21	54,54,54,54	5
85	MG	6	1944	1/1	0.88	0.30	63,63,63,63	0
86	OHX	6	2088	7/7	0.88	0.16	99,99,99,99	3
85	MG	5	3734	1/1	0.88	0.21	45,45,45,45	0
85	MG	5	3735	1/1	0.88	0.26	37,37,37,37	0
86	OHX	6	2102	7/7	0.88	0.20	97,97,97,97	4
85	MG	1	3721	1/1	0.88	0.28	43,43,43,43	0
86	OHX	5	4095	7/7	0.88	0.10	41,41,41,41	2
86	OHX	5	4104	7/7	0.88	0.18	68,68,68,68	6
86	OHX	2	2134	7/7	0.88	0.13	74,74,74,74	4
85	MG	1	3678	1/1	0.88	0.32	53,53,53,53	0
85	MG	5	3617	1/1	0.88	0.32	35,35,35,35	0
86	OHX	6	2121	7/7	0.88	0.20	86,86,86,86	5
86	OHX	6	2123	7/7	0.88	0.17	70,70,70,70	4
86	OHX	5	4116	7/7	0.88	0.16	52,52,52,52	4
86	OHX	6	2126	7/7	0.88	0.20	53,53,53,53	3
86	OHX	2	2139	7/7	0.88	0.11	114,114,114,114	6
85	MG	6	1983	1/1	0.88	0.38	57,57,57,57	0
85	MG	1	3631	1/1	0.88	0.18	42,42,42,42	0
86	OHX	1	4049	7/7	0.88	0.21	61,61,61,61	5
85	MG	1	3453	1/1	0.88	0.29	39,39,39,39	0
85	MG	5	3630	1/1	0.88	0.28	56,56,56,56	0
86	OHX	1	4059	7/7	0.88	0.17	72,72,72,72	4
86	OHX	5	4133	7/7	0.88	0.23	34,34,34,34	3
86	OHX	5	4134	7/7	0.88	0.09	157,157,157,157	7
85	MG	1	3748	1/1	0.88	0.32	67,67,67,67	0
85	MG	2	1910	1/1	0.88	0.39	69,69,69,69	0
85	MG	5	3802	1/1	0.88	0.19	44,44,44,44	0
86	OHX	6	2156	7/7	0.88	0.08	150,150,150,150	5
85	MG	6	1923	1/1	0.88	0.35	46,46,46,46	0
85	MG	5	3815	1/1	0.88	0.20	44,44,44,44	0
86	OHX	6	2159	7/7	0.88	0.13	93,93,93,93	5
85	MG	5	3643	1/1	0.88	0.20	64,64,64,64	0
86	OHX	5	4148	7/7	0.88	0.14	100,100,100,100	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3648	1/1	0.88	0.18	37,37,37,37	0
85	MG	5	3652	1/1	0.88	0.27	35,35,35,35	0
85	MG	1	3458	1/1	0.88	0.31	51,51,51,51	0
86	OHX	1	3856	7/7	0.88	0.19	76,76,76,76	3
85	MG	1	3539	1/1	0.88	0.38	44,44,44,44	0
85	MG	5	3664	1/1	0.88	0.21	62,62,62,62	0
86	OHX	1	3883	7/7	0.88	0.17	71,71,71,71	1
86	OHX	1	3899	7/7	0.88	0.27	52,52,52,52	4
86	OHX	1	4082	7/7	0.88	0.18	63,63,63,63	5
85	MG	o3	201	1/1	0.88	0.45	51,51,51,51	0
85	MG	C	102	1/1	0.88	0.31	39,39,39,39	0
86	OHX	1	4088	7/7	0.88	0.16	92,92,92,92	7
85	MG	1	3696	1/1	0.88	0.27	30,30,30,30	0
85	MG	5	3672	1/1	0.88	0.40	62,62,62,62	0
86	OHX	1	3949	7/7	0.88	0.14	111,111,111,111	7
85	MG	1	3603	1/1	0.88	0.18	63,63,63,63	0
85	MG	1	3492	1/1	0.88	0.28	32,32,32,32	0
85	MG	1	3709	1/1	0.88	0.15	48,48,48,48	0
86	OHX	1	3971	7/7	0.88	0.20	47,47,47,47	4
85	MG	1	3449	1/1	0.88	0.31	57,57,57,57	0
86	OHX	c3	201	7/7	0.88	0.12	84,84,84,84	4
85	MG	3	202	1/1	0.88	0.36	56,56,56,56	0
85	MG	5	3566	1/1	0.88	0.30	31,31,31,31	0
85	MG	1	3526	1/1	0.88	0.27	45,45,45,45	0
85	MG	5	3569	1/1	0.88	0.27	38,38,38,38	0
85	MG	6	1969	1/1	0.88	0.31	55,55,55,55	0
85	MG	5	3700	1/1	0.88	0.14	43,43,43,43	0
86	OHX	5	3986	7/7	0.88	0.31	58,58,58,58	5
86	OHX	5	4006	7/7	0.88	0.23	109,109,109,109	5
85	MG	6	1970	1/1	0.88	0.36	64,64,64,64	0
85	MG	1	3476	1/1	0.88	0.38	43,43,43,43	0
86	OHX	2	2107	7/7	0.89	0.15	66,66,66,66	4
86	OHX	5	4040	7/7	0.89	0.10	149,149,149,149	6
85	MG	5	3444	1/1	0.89	0.19	34,34,34,34	0
85	MG	1	3599	1/1	0.89	0.08	32,32,32,32	0
85	MG	5	3448	1/1	0.89	0.23	36,36,36,36	0
85	MG	1	3448	1/1	0.89	0.23	49,49,49,49	0
86	OHX	O9	101	7/7	0.89	0.18	51,51,51,51	6
86	OHX	6	2071	7/7	0.89	0.24	58,58,58,58	4
86	OHX	5	4060	7/7	0.89	0.18	45,45,45,45	5
86	OHX	2	2119	7/7	0.89	0.15	62,62,62,62	3
85	MG	5	3458	1/1	0.89	0.30	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3584	1/1	0.89	0.23	27,27,27,27	0
85	MG	5	3460	1/1	0.89	0.10	36,36,36,36	0
86	OHX	5	4072	7/7	0.89	0.22	40,40,40,40	4
85	MG	5	3586	1/1	0.89	0.30	29,29,29,29	0
85	MG	1	3531	1/1	0.89	0.28	40,40,40,40	0
86	OHX	2	2125	7/7	0.89	0.11	147,147,147,147	6
86	OHX	6	2111	7/7	0.89	0.12	73,73,73,73	5
85	MG	1	3502	1/1	0.89	0.29	30,30,30,30	0
85	MG	1	3680	1/1	0.89	0.29	45,45,45,45	0
86	OHX	2	2131	7/7	0.89	0.12	109,109,109,109	5
85	MG	1	3681	1/1	0.89	0.35	37,37,37,37	0
86	OHX	5	4092	7/7	0.89	0.19	33,33,33,33	2
85	MG	1	3466	1/1	0.89	0.22	37,37,37,37	0
85	MG	5	3476	1/1	0.89	0.22	42,42,42,42	0
85	MG	1	3689	1/1	0.89	0.08	44,44,44,44	0
85	MG	1	3608	1/1	0.89	0.30	46,46,46,46	0
85	MG	1	3486	1/1	0.89	0.22	39,39,39,39	0
86	OHX	6	2136	7/7	0.89	0.29	62,62,62,62	4
86	OHX	1	4055	7/7	0.89	0.15	81,81,81,81	5
86	OHX	6	2138	7/7	0.89	0.11	120,120,120,120	7
86	OHX	6	2146	7/7	0.89	0.21	48,48,48,48	4
85	MG	5	3612	1/1	0.89	0.18	40,40,40,40	0
85	MG	1	3535	1/1	0.89	0.27	39,39,39,39	0
85	MG	5	3759	1/1	0.89	0.26	46,46,46,46	0
85	MG	1	3506	1/1	0.89	0.29	32,32,32,32	0
86	OHX	6	2153	7/7	0.89	0.14	67,67,67,67	3
85	MG	1	3618	1/1	0.89	0.20	39,39,39,39	0
86	OHX	5	4130	7/7	0.89	0.09	171,171,171,171	7
85	MG	1	3455	1/1	0.89	0.28	29,29,29,29	0
85	MG	5	3784	1/1	0.89	0.12	35,35,35,35	0
85	MG	5	3789	1/1	0.89	0.16	49,49,49,49	0
85	MG	1	3621	1/1	0.89	0.35	52,52,52,52	0
85	MG	4	208	1/1	0.89	0.29	37,37,37,37	0
85	MG	2	1915	1/1	0.89	0.28	57,57,57,57	0
85	MG	1	3572	1/1	0.89	0.36	57,57,57,57	0
85	MG	1	3575	1/1	0.89	0.31	32,32,32,32	0
85	MG	5	3405	1/1	0.89	0.26	49,49,49,49	0
85	MG	1	3540	1/1	0.89	0.30	41,41,41,41	0
85	MG	5	3649	1/1	0.89	0.22	47,47,47,47	0
85	MG	2	1980	1/1	0.89	0.20	104,104,104,104	0
86	OHX	1	3905	7/7	0.89	0.18	57,57,57,57	1
85	MG	5	3408	1/1	0.89	0.14	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	l5	301	1/1	0.89	0.20	63,63,63,63	0
85	MG	1	3647	1/1	0.89	0.29	64,64,64,64	0
85	MG	1	3580	1/1	0.89	0.32	35,35,35,35	0
85	MG	5	3666	1/1	0.89	0.27	54,54,54,54	0
86	OHX	5	4157	7/7	0.89	0.17	44,44,44,44	5
85	MG	1	3475	1/1	0.89	0.33	44,44,44,44	0
85	MG	1	3545	1/1	0.89	0.27	31,31,31,31	0
85	MG	1	3493	1/1	0.89	0.31	42,42,42,42	0
86	OHX	6	2179	7/7	0.89	0.17	61,61,61,61	7
86	OHX	1	3968	7/7	0.89	0.17	72,72,72,72	3
86	OHX	1	4099	7/7	0.89	0.10	53,53,53,53	3
85	MG	5	3423	1/1	0.89	0.17	43,43,43,43	0
85	MG	5	3543	1/1	0.89	0.31	41,41,41,41	0
85	MG	5	3681	1/1	0.89	0.09	43,43,43,43	0
85	MG	5	3682	1/1	0.89	0.14	45,45,45,45	0
86	OHX	1	4105	7/7	0.89	0.32	46,46,46,46	5
85	MG	5	3683	1/1	0.89	0.15	38,38,38,38	0
85	MG	5	3545	1/1	0.89	0.27	57,57,57,57	0
86	OHX	5	3941	7/7	0.89	0.22	34,34,34,34	4
85	MG	1	3549	1/1	0.89	0.23	59,59,59,59	0
86	OHX	1	3988	7/7	0.89	0.16	87,87,87,87	5
85	MG	1	3742	1/1	0.89	0.18	44,44,44,44	0
85	MG	5	3687	1/1	0.89	0.27	37,37,37,37	0
86	OHX	5	3995	7/7	0.89	0.15	88,88,88,88	5
85	MG	5	3555	1/1	0.89	0.22	54,54,54,54	0
85	MG	2	1930	1/1	0.89	0.39	72,72,72,72	0
86	OHX	5	4019	7/7	0.89	0.18	76,76,76,76	6
86	OHX	1	4002	7/7	0.89	0.17	65,65,65,65	7
86	OHX	m9	201	7/7	0.89	0.10	61,61,61,61	6
86	OHX	o6	201	7/7	0.89	0.22	68,68,68,68	4
86	OHX	5	4032	7/7	0.89	0.15	71,71,71,71	4
86	OHX	4	231	7/7	0.89	0.11	75,75,75,75	5
85	MG	5	3625	1/1	0.90	0.22	51,51,51,51	0
85	MG	5	3781	1/1	0.90	0.25	43,43,43,43	0
85	MG	1	3437	1/1	0.90	0.28	44,44,44,44	0
85	MG	2	1921	1/1	0.90	0.22	63,63,63,63	0
85	MG	1	3410	1/1	0.90	0.22	39,39,39,39	0
86	OHX	5	3988	7/7	0.90	0.16	64,64,64,64	5
85	MG	5	3631	1/1	0.90	0.25	52,52,52,52	0
86	OHX	S8	301	7/7	0.90	0.10	115,115,115,115	7
85	MG	5	3791	1/1	0.90	0.17	46,46,46,46	0
86	OHX	5	4011	7/7	0.90	0.13	120,120,120,120	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3792	1/1	0.90	0.27	55,55,55,55	0
85	MG	5	3509	1/1	0.90	0.34	25,25,25,25	0
85	MG	5	3633	1/1	0.90	0.22	34,34,34,34	0
85	MG	5	3803	1/1	0.90	0.17	35,35,35,35	0
86	OHX	1	3884	7/7	0.90	0.17	74,74,74,74	4
85	MG	1	3508	1/1	0.90	0.17	38,38,38,38	0
85	MG	1	3671	1/1	0.90	0.26	47,47,47,47	0
86	OHX	1	3908	7/7	0.90	0.16	91,91,91,91	3
85	MG	1	3723	1/1	0.90	0.18	67,67,67,67	0
86	OHX	5	4050	7/7	0.90	0.18	45,45,45,45	3
85	MG	7	210	1/1	0.90	0.26	43,43,43,43	0
86	OHX	3	214	7/7	0.90	0.19	83,83,83,83	4
85	MG	5	3646	1/1	0.90	0.28	56,56,56,56	0
85	MG	8	202	1/1	0.90	0.19	42,42,42,42	0
86	OHX	4	226	7/7	0.90	0.12	106,106,106,106	5
85	MG	1	3726	1/1	0.90	0.23	64,64,64,64	0
85	MG	M6	202	1/1	0.90	0.11	40,40,40,40	0
85	MG	1	3581	1/1	0.90	0.38	29,29,29,29	0
86	OHX	1	3964	7/7	0.90	0.16	71,71,71,71	4
86	OHX	5	4075	7/7	0.90	0.14	47,47,47,47	3
86	OHX	L5	301	7/7	0.90	0.17	88,88,88,88	6
85	MG	1	3735	1/1	0.90	0.10	49,49,49,49	0
86	OHX	5	4080	7/7	0.90	0.18	55,55,55,55	3
85	MG	5	3530	1/1	0.90	0.27	31,31,31,31	0
85	MG	17	2201	1/1	0.90	0.16	46,46,46,46	0
86	OHX	O4	202	7/7	0.90	0.14	82,82,82,82	5
86	OHX	1	3973	7/7	0.90	0.15	63,63,63,63	5
85	MG	m5	302	1/1	0.90	0.15	46,46,46,46	0
85	MG	1	3614	1/1	0.90	0.25	54,54,54,54	0
85	MG	5	3426	1/1	0.90	0.23	45,45,45,45	0
86	OHX	6	2086	7/7	0.90	0.19	70,70,70,70	5
86	OHX	5	4098	7/7	0.90	0.11	106,106,106,106	5
86	OHX	5	4100	7/7	0.90	0.16	46,46,46,46	5
86	OHX	2	2011	7/7	0.90	0.15	83,83,83,83	3
85	MG	5	3539	1/1	0.90	0.30	33,33,33,33	0
86	OHX	6	2095	7/7	0.90	0.16	99,99,99,99	3
86	OHX	2	2064	7/7	0.90	0.15	135,135,135,135	5
85	MG	5	3670	1/1	0.90	0.17	35,35,35,35	0
85	MG	5	3429	1/1	0.90	0.21	31,31,31,31	0
85	MG	N6	201	1/1	0.90	0.29	70,70,70,70	0
85	MG	5	3432	1/1	0.90	0.12	32,32,32,32	0
85	MG	1	3616	1/1	0.90	0.18	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4122	7/7	0.90	0.14	52,52,52,52	3
85	MG	5	3546	1/1	0.90	0.37	46,46,46,46	0
85	MG	6	1939	1/1	0.90	0.25	34,34,34,34	0
86	OHX	6	2122	7/7	0.90	0.14	77,77,77,77	4
86	OHX	2	2086	7/7	0.90	0.13	112,112,112,112	5
86	OHX	6	2125	7/7	0.90	0.13	52,52,52,52	5
86	OHX	2	2088	7/7	0.90	0.17	91,91,91,91	6
85	MG	Q2	502	1/1	0.90	0.28	63,63,63,63	0
85	MG	1	3583	1/1	0.90	0.31	31,31,31,31	0
86	OHX	2	2095	7/7	0.90	0.13	75,75,75,75	5
86	OHX	2	2098	7/7	0.90	0.15	111,111,111,111	6
85	MG	1	3743	1/1	0.90	0.15	50,50,50,50	0
85	MG	5	3454	1/1	0.90	0.12	59,59,59,59	0
85	MG	1	3744	1/1	0.90	0.19	44,44,44,44	0
86	OHX	5	4141	7/7	0.90	0.16	49,49,49,49	4
85	MG	6	1904	1/1	0.90	0.29	59,59,59,59	0
86	OHX	1	4030	7/7	0.90	0.10	130,130,130,130	6
85	MG	1	3481	1/1	0.90	0.21	40,40,40,40	0
86	OHX	1	4033	7/7	0.90	0.17	66,66,66,66	5
85	MG	1	3516	1/1	0.90	0.35	33,33,33,33	0
86	OHX	2	2111	7/7	0.90	0.13	112,112,112,112	5
85	MG	5	3577	1/1	0.90	0.30	31,31,31,31	0
85	MG	5	3466	1/1	0.90	0.20	37,37,37,37	0
86	OHX	2	2115	7/7	0.90	0.18	91,91,91,91	6
86	OHX	2	2116	7/7	0.90	0.10	127,127,127,127	7
85	MG	5	3467	1/1	0.90	0.20	47,47,47,47	0
86	OHX	1	4047	7/7	0.90	0.15	101,101,101,101	5
85	MG	1	3622	1/1	0.90	0.28	44,44,44,44	0
85	MG	5	3588	1/1	0.90	0.26	29,29,29,29	0
86	OHX	5	4160	7/7	0.90	0.21	37,37,37,37	5
86	OHX	1	4052	7/7	0.90	0.16	58,58,58,58	4
85	MG	5	3470	1/1	0.90	0.29	56,56,56,56	0
85	MG	1	3624	1/1	0.90	0.14	33,33,33,33	0
85	MG	1	3446	1/1	0.90	0.20	41,41,41,41	0
85	MG	1	3469	1/1	0.90	0.28	41,41,41,41	0
85	MG	1	3520	1/1	0.90	0.27	35,35,35,35	0
85	MG	1	3501	1/1	0.90	0.28	26,26,26,26	0
85	MG	1	3600	1/1	0.90	0.15	60,60,60,60	0
86	OHX	2	2129	7/7	0.90	0.18	87,87,87,87	5
86	OHX	2	2130	7/7	0.90	0.11	84,84,84,84	4
85	MG	1	3644	1/1	0.90	0.29	52,52,52,52	0
85	MG	1	3543	1/1	0.90	0.10	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	8	223	7/7	0.90	0.15	75,75,75,75	5
85	MG	5	3605	1/1	0.90	0.25	33,33,33,33	0
85	MG	5	3495	1/1	0.90	0.17	33,33,33,33	0
85	MG	1	3411	1/1	0.90	0.20	43,43,43,43	0
86	OHX	2	2138	7/7	0.90	0.18	67,67,67,67	5
85	MG	5	3750	1/1	0.90	0.22	37,37,37,37	0
85	MG	5	3753	1/1	0.90	0.23	30,30,30,30	0
85	MG	1	3657	1/1	0.90	0.26	49,49,49,49	0
85	MG	5	3618	1/1	0.90	0.25	34,34,34,34	0
85	MG	5	3769	1/1	0.90	0.16	50,50,50,50	0
86	OHX	m8	201	7/7	0.90	0.19	47,47,47,47	3
86	OHX	d4	201	7/7	0.90	0.11	90,90,90,90	6
85	MG	5	3770	1/1	0.90	0.23	47,47,47,47	0
86	OHX	5	3926	7/7	0.90	0.15	60,60,60,60	4
85	MG	1	3428	1/1	0.90	0.18	52,52,52,52	0
86	OHX	5	3971	7/7	0.91	0.15	41,41,41,41	7
85	MG	1	3598	1/1	0.91	0.25	39,39,39,39	0
85	MG	5	3639	1/1	0.91	0.18	36,36,36,36	0
85	MG	5	3807	1/1	0.91	0.18	54,54,54,54	0
85	MG	5	3808	1/1	0.91	0.13	36,36,36,36	0
86	OHX	5	4005	7/7	0.91	0.19	82,82,82,82	3
85	MG	5	3409	1/1	0.91	0.22	45,45,45,45	0
85	MG	1	3450	1/1	0.91	0.16	31,31,31,31	0
86	OHX	1	3891	7/7	0.91	0.10	103,103,103,103	5
86	OHX	5	4016	7/7	0.91	0.16	62,62,62,62	7
86	OHX	5	4017	7/7	0.91	0.18	36,36,36,36	2
85	MG	5	3644	1/1	0.91	0.19	34,34,34,34	0
86	OHX	5	4024	7/7	0.91	0.14	66,66,66,66	5
85	MG	2	1972	1/1	0.91	0.06	57,57,57,57	0
86	OHX	5	4030	7/7	0.91	0.15	70,70,70,70	5
85	MG	1	3452	1/1	0.91	0.30	55,55,55,55	0
86	OHX	1	3914	7/7	0.91	0.14	79,79,79,79	3
85	MG	5	3516	1/1	0.91	0.33	21,21,21,21	0
85	MG	4	204	1/1	0.91	0.32	64,64,64,64	0
85	MG	5	3657	1/1	0.91	0.21	33,33,33,33	0
86	OHX	5	4045	7/7	0.91	0.17	48,48,48,48	2
85	MG	1	3422	1/1	0.91	0.22	32,32,32,32	0
86	OHX	1	3930	7/7	0.91	0.14	118,118,118,118	2
86	OHX	3	215	7/7	0.91	0.13	90,90,90,90	3
86	OHX	1	3947	7/7	0.91	0.14	80,80,80,80	3
85	MG	6	1975	1/1	0.91	0.16	90,90,90,90	0
86	OHX	5	4057	7/7	0.91	0.17	50,50,50,50	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	3952	7/7	0.91	0.11	140,140,140,140	5
85	MG	1	3403	1/1	0.91	0.20	42,42,42,42	0
86	OHX	4	230	7/7	0.91	0.11	45,45,45,45	3
85	MG	1	3478	1/1	0.91	0.19	60,60,60,60	0
85	MG	2	1947	1/1	0.91	0.14	76,76,76,76	0
86	OHX	4	233	7/7	0.91	0.15	65,65,65,65	5
85	MG	n6	201	1/1	0.91	0.16	56,56,56,56	0
86	OHX	1	3966	7/7	0.91	0.22	35,35,35,35	3
85	MG	1	3444	1/1	0.91	0.25	35,35,35,35	0
85	MG	L6	201	1/1	0.91	0.18	57,57,57,57	0
85	MG	5	3541	1/1	0.91	0.25	41,41,41,41	0
86	OHX	2	2036	7/7	0.91	0.11	145,145,145,145	5
85	MG	5	3433	1/1	0.91	0.26	37,37,37,37	0
86	OHX	2	2058	7/7	0.91	0.18	67,67,67,67	4
86	OHX	5	4085	7/7	0.91	0.10	143,143,143,143	7
85	MG	5	3676	1/1	0.91	0.18	51,51,51,51	0
86	OHX	1	3981	7/7	0.91	0.21	53,53,53,53	3
86	OHX	5	4090	7/7	0.91	0.16	51,51,51,51	4
85	MG	5	3434	1/1	0.91	0.25	33,33,33,33	0
86	OHX	6	2087	7/7	0.91	0.11	109,109,109,109	6
85	MG	5	3436	1/1	0.91	0.15	44,44,44,44	0
86	OHX	1	3987	7/7	0.91	0.14	73,73,73,73	5
86	OHX	5	4099	7/7	0.91	0.12	73,73,73,73	5
85	MG	M0	301	1/1	0.91	0.23	41,41,41,41	0
85	MG	5	3442	1/1	0.91	0.18	32,32,32,32	0
85	MG	2	1983	1/1	0.91	0.11	84,84,84,84	0
85	MG	5	3549	1/1	0.91	0.11	43,43,43,43	0
85	MG	5	3551	1/1	0.91	0.27	32,32,32,32	0
86	OHX	6	2112	7/7	0.91	0.21	66,66,66,66	4
85	MG	1	3728	1/1	0.91	0.18	47,47,47,47	0
86	OHX	2	2087	7/7	0.91	0.14	89,89,89,89	5
86	OHX	1	4010	7/7	0.91	0.21	44,44,44,44	5
85	MG	1	3462	1/1	0.91	0.22	44,44,44,44	0
85	MG	5	3693	1/1	0.91	0.25	38,38,38,38	0
85	MG	1	3673	1/1	0.91	0.20	39,39,39,39	0
85	MG	5	3565	1/1	0.91	0.25	32,32,32,32	0
86	OHX	1	4020	7/7	0.91	0.14	47,47,47,47	3
86	OHX	6	2127	7/7	0.91	0.17	58,58,58,58	5
85	MG	1	3736	1/1	0.91	0.09	50,50,50,50	0
86	OHX	6	2132	7/7	0.91	0.13	94,94,94,94	6
86	OHX	5	4131	7/7	0.91	0.10	64,64,64,64	5
85	MG	5	3455	1/1	0.91	0.23	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	6	1989	1/1	0.91	0.20	57,57,57,57	0
85	MG	1	3513	1/1	0.91	0.28	34,34,34,34	0
85	MG	5	3710	1/1	0.91	0.18	55,55,55,55	0
85	MG	1	3578	1/1	0.91	0.31	60,60,60,60	0
86	OHX	6	2143	7/7	0.91	0.19	51,51,51,51	3
85	MG	5	3463	1/1	0.91	0.12	39,39,39,39	0
86	OHX	2	2110	7/7	0.91	0.15	112,112,112,112	5
85	MG	O7	103	1/1	0.91	0.22	49,49,49,49	0
86	OHX	1	4035	7/7	0.91	0.12	65,65,65,65	4
85	MG	5	3716	1/1	0.91	0.20	34,34,34,34	0
85	MG	1	3515	1/1	0.91	0.24	28,28,28,28	0
85	MG	2	1971	1/1	0.91	0.19	81,81,81,81	0
85	MG	5	3468	1/1	0.91	0.22	47,47,47,47	0
85	MG	1	3429	1/1	0.91	0.21	36,36,36,36	0
85	MG	5	3726	1/1	0.91	0.08	46,46,46,46	0
85	MG	1	3683	1/1	0.91	0.35	39,39,39,39	1
85	MG	1	3585	1/1	0.91	0.41	20,20,20,20	0
85	MG	1	3490	1/1	0.91	0.30	34,34,34,34	0
85	MG	1	3627	1/1	0.91	0.26	41,41,41,41	0
85	MG	5	3743	1/1	0.91	0.12	32,32,32,32	0
85	MG	5	3746	1/1	0.91	0.33	76,76,76,76	0
85	MG	6	2008	1/1	0.91	0.39	61,61,61,61	0
85	MG	2	1975	1/1	0.91	0.33	60,60,60,60	0
85	MG	5	3749	1/1	0.91	0.23	30,30,30,30	0
85	MG	1	3588	1/1	0.91	0.22	39,39,39,39	0
85	MG	6	1955	1/1	0.91	0.28	60,60,60,60	0
85	MG	5	3756	1/1	0.91	0.16	42,42,42,42	0
85	MG	5	3608	1/1	0.91	0.34	50,50,50,50	0
85	MG	5	3493	1/1	0.91	0.33	42,42,42,42	0
85	MG	c8	201	1/1	0.91	0.11	91,91,91,91	0
85	MG	1	3467	1/1	0.91	0.14	42,42,42,42	0
85	MG	5	3773	1/1	0.91	0.12	52,52,52,52	0
86	OHX	7	222	7/7	0.91	0.18	38,38,38,38	4
86	OHX	7	223	7/7	0.91	0.16	54,54,54,54	4
86	OHX	1	4074	7/7	0.91	0.20	38,38,38,38	3
85	MG	5	3496	1/1	0.91	0.18	35,35,35,35	0
85	MG	5	3497	1/1	0.91	0.21	36,36,36,36	0
86	OHX	8	226	7/7	0.91	0.13	47,47,47,47	3
85	MG	5	3623	1/1	0.91	0.06	42,42,42,42	0
85	MG	1	3639	1/1	0.91	0.25	56,56,56,56	0
85	MG	1	3524	1/1	0.91	0.28	44,44,44,44	0
85	MG	5	3788	1/1	0.91	0.24	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	l3	404	7/7	0.91	0.09	72,72,72,72	4
86	OHX	1	4083	7/7	0.91	0.09	45,45,45,45	4
86	OHX	1	4084	7/7	0.91	0.24	42,42,42,42	5
85	MG	6	1914	1/1	0.91	0.27	62,62,62,62	0
85	MG	1	3420	1/1	0.91	0.29	45,45,45,45	0
86	OHX	5	3917	7/7	0.91	0.23	49,49,49,49	3
85	MG	5	3506	1/1	0.91	0.36	27,27,27,27	0
85	MG	3	204	1/1	0.91	0.35	33,33,33,33	0
85	MG	5	3793	1/1	0.91	0.20	37,37,37,37	0
85	MG	5	3797	1/1	0.91	0.13	39,39,39,39	0
85	MG	1	3707	1/1	0.91	0.27	48,48,48,48	0
85	MG	1	3479	1/1	0.92	0.16	45,45,45,45	0
86	OHX	5	3991	7/7	0.92	0.11	37,37,37,37	3
86	OHX	5	3993	7/7	0.92	0.16	38,38,38,38	4
85	MG	6	1925	1/1	0.92	0.24	49,49,49,49	0
86	OHX	2	2053	7/7	0.92	0.15	107,107,107,107	4
86	OHX	1	3939	7/7	0.92	0.13	54,54,54,54	3
85	MG	5	3613	1/1	0.92	0.24	42,42,42,42	0
86	OHX	2	2061	7/7	0.92	0.24	88,88,88,88	5
86	OHX	1	3951	7/7	0.92	0.12	159,159,159,159	7
85	MG	5	3517	1/1	0.92	0.18	28,28,28,28	0
85	MG	1	3711	1/1	0.92	0.20	54,54,54,54	0
85	MG	5	3519	1/1	0.92	0.32	35,35,35,35	0
86	OHX	3	213	7/7	0.92	0.16	82,82,82,82	5
85	MG	M7	202	1/1	0.92	0.34	40,40,40,40	0
86	OHX	5	4031	7/7	0.92	0.12	85,85,85,85	4
85	MG	5	3620	1/1	0.92	0.33	39,39,39,39	0
86	OHX	2	2077	7/7	0.92	0.14	108,108,108,108	7
85	MG	5	3621	1/1	0.92	0.13	36,36,36,36	0
86	OHX	1	3970	7/7	0.92	0.11	68,68,68,68	1
85	MG	6	1966	1/1	0.92	0.22	56,56,56,56	0
85	MG	5	3725	1/1	0.92	0.15	51,51,51,51	0
85	MG	5	3624	1/1	0.92	0.11	31,31,31,31	0
85	MG	5	3527	1/1	0.92	0.21	32,32,32,32	0
85	MG	M7	203	1/1	0.92	0.17	46,46,46,46	0
85	MG	5	3461	1/1	0.92	0.33	57,57,57,57	0
85	MG	1	3675	1/1	0.92	0.20	49,49,49,49	0
86	OHX	M0	303	7/7	0.92	0.19	55,55,55,55	4
85	MG	1	3558	1/1	0.92	0.23	35,35,35,35	0
86	OHX	2	2097	7/7	0.92	0.12	73,73,73,73	5
85	MG	1	3480	1/1	0.92	0.39	46,46,46,46	0
86	OHX	O3	201	7/7	0.92	0.22	52,52,52,52	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3679	1/1	0.92	0.20	59,59,59,59	0
85	MG	5	3634	1/1	0.92	0.10	36,36,36,36	0
85	MG	1	3418	1/1	0.92	0.16	47,47,47,47	0
86	OHX	1	3993	7/7	0.92	0.15	94,94,94,94	7
85	MG	1	3720	1/1	0.92	0.20	48,48,48,48	0
86	OHX	1	3998	7/7	0.92	0.15	107,107,107,107	4
85	MG	1	3470	1/1	0.92	0.21	46,46,46,46	0
85	MG	5	3642	1/1	0.92	0.11	39,39,39,39	0
86	OHX	1	4004	7/7	0.92	0.17	75,75,75,75	5
85	MG	1	3655	1/1	0.92	0.22	44,44,44,44	0
85	MG	1	3724	1/1	0.92	0.19	55,55,55,55	0
86	OHX	1	4012	7/7	0.92	0.15	64,64,64,64	1
86	OHX	6	2103	7/7	0.92	0.15	67,67,67,67	4
86	OHX	5	4089	7/7	0.92	0.24	47,47,47,47	3
86	OHX	6	2107	7/7	0.92	0.12	81,81,81,81	5
85	MG	5	3763	1/1	0.92	0.12	38,38,38,38	0
85	MG	5	3473	1/1	0.92	0.22	30,30,30,30	0
85	MG	5	3412	1/1	0.92	0.20	47,47,47,47	0
86	OHX	5	4097	7/7	0.92	0.13	75,75,75,75	6
85	MG	5	3475	1/1	0.92	0.16	51,51,51,51	0
85	MG	5	3651	1/1	0.92	0.08	42,42,42,42	0
85	MG	5	3552	1/1	0.92	0.26	52,52,52,52	0
85	MG	5	3653	1/1	0.92	0.14	47,47,47,47	0
86	OHX	1	4025	7/7	0.92	0.13	56,56,56,56	3
85	MG	3	207	1/1	0.92	0.34	66,66,66,66	0
85	MG	1	3548	1/1	0.92	0.25	30,30,30,30	0
85	MG	5	3661	1/1	0.92	0.15	64,64,64,64	0
86	OHX	5	4112	7/7	0.92	0.19	51,51,51,51	6
85	MG	6	1941	1/1	0.92	0.29	57,57,57,57	0
86	OHX	6	2130	7/7	0.92	0.09	153,153,153,153	7
85	MG	1	3463	1/1	0.92	0.25	39,39,39,39	0
86	OHX	1	4031	7/7	0.92	0.12	65,65,65,65	6
85	MG	1	3584	1/1	0.92	0.30	33,33,33,33	0
85	MG	1	3477	1/1	0.92	0.28	41,41,41,41	0
85	MG	5	3669	1/1	0.92	0.22	36,36,36,36	1
85	MG	5	3794	1/1	0.92	0.10	45,45,45,45	0
86	OHX	5	4126	7/7	0.92	0.12	98,98,98,98	3
85	MG	1	3629	1/1	0.92	0.13	33,33,33,33	0
85	MG	4	206	1/1	0.92	0.23	44,44,44,44	0
86	OHX	6	2145	7/7	0.92	0.11	92,92,92,92	4
85	MG	5	3801	1/1	0.92	0.25	44,44,44,44	0
85	MG	5	3427	1/1	0.92	0.27	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3580	1/1	0.92	0.38	38,38,38,38	0
85	MG	5	3675	1/1	0.92	0.28	34,34,34,34	1
86	OHX	5	4135	7/7	0.92	0.16	54,54,54,54	4
85	MG	4	207	1/1	0.92	0.30	41,41,41,41	0
85	MG	1	3663	1/1	0.92	0.29	44,44,44,44	0
85	MG	5	3499	1/1	0.92	0.14	42,42,42,42	0
85	MG	4	210	1/1	0.92	0.24	63,63,63,63	0
85	MG	7	209	1/1	0.92	0.20	54,54,54,54	0
86	OHX	1	4056	7/7	0.92	0.15	85,85,85,85	5
86	OHX	1	4057	7/7	0.92	0.09	109,109,109,109	5
86	OHX	2	2144	7/7	0.92	0.16	103,103,103,103	6
86	OHX	6	2160	7/7	0.92	0.18	69,69,69,69	5
85	MG	1	3695	1/1	0.92	0.31	58,58,58,58	0
85	MG	1	3665	1/1	0.92	0.24	48,48,48,48	0
85	MG	7	213	1/1	0.92	0.13	49,49,49,49	0
86	OHX	2	2148	7/7	0.92	0.29	69,69,69,69	6
86	OHX	1	4064	7/7	0.92	0.23	39,39,39,39	3
85	MG	S2	301	1/1	0.92	0.31	62,62,62,62	0
85	MG	5	3439	1/1	0.92	0.26	30,30,30,30	0
85	MG	8	206	1/1	0.92	0.15	47,47,47,47	0
85	MG	8	209	1/1	0.92	0.24	55,55,55,55	0
85	MG	6	1956	1/1	0.92	0.30	44,44,44,44	0
85	MG	5	3688	1/1	0.92	0.19	47,47,47,47	0
85	MG	5	3595	1/1	0.92	0.38	28,28,28,28	0
86	OHX	D9	102	7/7	0.92	0.14	97,97,97,97	6
86	OHX	1	3849	7/7	0.92	0.19	48,48,48,48	5
85	MG	1	3556	1/1	0.92	0.22	29,29,29,29	0
85	MG	5	3597	1/1	0.92	0.16	44,44,44,44	0
85	MG	m0	301	1/1	0.92	0.20	33,33,33,33	0
86	OHX	1	4081	7/7	0.92	0.34	43,43,43,43	5
86	OHX	1	3875	7/7	0.92	0.23	53,53,53,53	3
86	OHX	1	3877	7/7	0.92	0.13	95,95,95,95	2
85	MG	m5	301	1/1	0.92	0.11	56,56,56,56	0
85	MG	5	3443	1/1	0.92	0.23	44,44,44,44	0
85	MG	m7	201	1/1	0.92	0.10	36,36,36,36	0
85	MG	n3	201	1/1	0.92	0.25	25,25,25,25	0
86	OHX	1	3900	7/7	0.92	0.14	57,57,57,57	3
86	OHX	8	222	7/7	0.92	0.13	100,100,100,100	5
86	OHX	1	4091	7/7	0.92	0.11	42,42,42,42	4
86	OHX	5	3916	7/7	0.92	0.15	77,77,77,77	3
86	OHX	1	3904	7/7	0.92	0.20	59,59,59,59	3
85	MG	5	3512	1/1	0.92	0.35	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3573	1/1	0.92	0.35	40,40,40,40	0
86	OHX	5	3938	7/7	0.92	0.15	50,50,50,50	3
86	OHX	1	3912	7/7	0.92	0.13	126,126,126,126	4
85	MG	q1	101	1/1	0.92	0.29	50,50,50,50	0
86	OHX	5	3949	7/7	0.92	0.20	56,56,56,56	4
86	OHX	5	3950	7/7	0.92	0.17	95,95,95,95	4
86	OHX	5	3963	7/7	0.92	0.13	62,62,62,62	5
86	OHX	5	3967	7/7	0.92	0.21	49,49,49,49	5
85	MG	1	3590	1/1	0.92	0.20	43,43,43,43	0
86	OHX	1	3916	7/7	0.92	0.19	54,54,54,54	4
86	OHX	1	4100	7/7	0.92	0.17	38,38,38,38	3
86	OHX	5	3977	7/7	0.92	0.24	58,58,58,58	4
85	MG	5	3708	1/1	0.92	0.09	50,50,50,50	0
85	MG	5	3410	1/1	0.93	0.15	29,29,29,29	0
85	MG	5	3570	1/1	0.93	0.25	29,29,29,29	0
86	OHX	1	4087	7/7	0.93	0.18	44,44,44,44	6
85	MG	8	203	1/1	0.93	0.16	57,57,57,57	0
85	MG	5	3411	1/1	0.93	0.31	44,44,44,44	0
86	OHX	5	3957	7/7	0.93	0.20	46,46,46,46	3
85	MG	5	3575	1/1	0.93	0.32	36,36,36,36	0
85	MG	8	207	1/1	0.93	0.18	43,43,43,43	0
85	MG	5	3484	1/1	0.93	0.35	28,28,28,28	0
85	MG	5	3578	1/1	0.93	0.29	35,35,35,35	0
86	OHX	1	3886	7/7	0.93	0.19	56,56,56,56	4
85	MG	1	3482	1/1	0.93	0.30	33,33,33,33	0
86	OHX	5	3978	7/7	0.93	0.13	69,69,69,69	4
86	OHX	5	3979	7/7	0.93	0.18	67,67,67,67	3
86	OHX	5	3982	7/7	0.93	0.14	58,58,58,58	3
86	OHX	1	4097	7/7	0.93	0.13	42,42,42,42	6
85	MG	5	3488	1/1	0.93	0.29	44,44,44,44	0
85	MG	5	3490	1/1	0.93	0.17	40,40,40,40	0
85	MG	5	3491	1/1	0.93	0.13	41,41,41,41	0
85	MG	5	3587	1/1	0.93	0.26	30,30,30,30	0
86	OHX	1	3907	7/7	0.93	0.16	71,71,71,71	3
85	MG	5	3492	1/1	0.93	0.22	30,30,30,30	0
85	MG	L7	303	1/1	0.93	0.13	50,50,50,50	0
85	MG	5	3691	1/1	0.93	0.23	38,38,38,38	0
86	OHX	5	4013	7/7	0.93	0.11	119,119,119,119	4
85	MG	m7	202	1/1	0.93	0.34	33,33,33,33	0
85	MG	1	3740	1/1	0.93	0.15	62,62,62,62	0
85	MG	5	3694	1/1	0.93	0.17	55,55,55,55	0
86	OHX	1	3925	7/7	0.93	0.11	96,96,96,96	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	6	1976	1/1	0.93	0.07	32,32,32,32	0
85	MG	o4	201	1/1	0.93	0.39	53,53,53,53	0
85	MG	6	1977	1/1	0.93	0.11	57,57,57,57	0
85	MG	1	3691	1/1	0.93	0.18	64,64,64,64	0
85	MG	1	3651	1/1	0.93	0.19	49,49,49,49	0
86	OHX	2	2022	7/7	0.93	0.18	78,78,78,78	4
86	OHX	3	218	7/7	0.93	0.16	54,54,54,54	5
86	OHX	5	4042	7/7	0.93	0.15	43,43,43,43	3
86	OHX	2	2035	7/7	0.93	0.11	116,116,116,116	5
85	MG	1	3442	1/1	0.93	0.25	52,52,52,52	0
86	OHX	1	3953	7/7	0.93	0.12	58,58,58,58	2
86	OHX	2	2043	7/7	0.93	0.14	100,100,100,100	4
86	OHX	1	3958	7/7	0.93	0.14	45,45,45,45	4
86	OHX	2	2047	7/7	0.93	0.15	80,80,80,80	4
85	MG	5	3706	1/1	0.93	0.24	32,32,32,32	0
85	MG	5	3425	1/1	0.93	0.15	41,41,41,41	0
86	OHX	2	2054	7/7	0.93	0.17	103,103,103,103	5
86	OHX	1	3967	7/7	0.93	0.09	82,82,82,82	3
86	OHX	2	2057	7/7	0.93	0.10	79,79,79,79	1
86	OHX	M8	201	7/7	0.93	0.14	47,47,47,47	3
86	OHX	5	4063	7/7	0.93	0.15	39,39,39,39	3
85	MG	1	3654	1/1	0.93	0.21	39,39,39,39	0
85	MG	1	3745	1/1	0.93	0.13	53,53,53,53	0
85	MG	5	3711	1/1	0.93	0.20	32,32,32,32	0
86	OHX	5	4074	7/7	0.93	0.14	77,77,77,77	6
85	MG	1	3747	1/1	0.93	0.11	48,48,48,48	0
86	OHX	2	2068	7/7	0.93	0.16	103,103,103,103	7
86	OHX	6	2043	7/7	0.93	0.17	90,90,90,90	5
86	OHX	6	2051	7/7	0.93	0.12	131,131,131,131	5
85	MG	5	3604	1/1	0.93	0.21	33,33,33,33	0
86	OHX	6	2073	7/7	0.93	0.18	69,69,69,69	5
86	OHX	6	2077	7/7	0.93	0.17	98,98,98,98	5
86	OHX	6	2078	7/7	0.93	0.15	60,60,60,60	5
86	OHX	2	2072	7/7	0.93	0.08	187,187,187,187	7
85	MG	2	1903	1/1	0.93	0.22	43,43,43,43	0
85	MG	5	3607	1/1	0.93	0.15	36,36,36,36	0
85	MG	1	3591	1/1	0.93	0.39	53,53,53,53	0
85	MG	5	3610	1/1	0.93	0.16	49,49,49,49	0
85	MG	5	3720	1/1	0.93	0.23	34,34,34,34	0
86	OHX	6	2092	7/7	0.93	0.23	69,69,69,69	4
85	MG	5	3721	1/1	0.93	0.25	36,36,36,36	0
85	MG	1	3699	1/1	0.93	0.16	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3554	1/1	0.93	0.28	37,37,37,37	0
85	MG	1	3416	1/1	0.93	0.29	43,43,43,43	0
86	OHX	2	2089	7/7	0.93	0.11	116,116,116,116	7
86	OHX	1	3999	7/7	0.93	0.08	215,215,215,215	2
86	OHX	5	4106	7/7	0.93	0.14	32,32,32,32	4
86	OHX	2	2090	7/7	0.93	0.11	94,94,94,94	6
85	MG	1	3757	1/1	0.93	0.19	55,55,55,55	0
86	OHX	5	4110	7/7	0.93	0.11	133,133,133,133	5
86	OHX	1	4003	7/7	0.93	0.13	63,63,63,63	3
86	OHX	6	2117	7/7	0.93	0.10	65,65,65,65	3
86	OHX	5	4114	7/7	0.93	0.11	55,55,55,55	4
85	MG	5	3731	1/1	0.93	0.31	55,55,55,55	0
86	OHX	1	4005	7/7	0.93	0.18	40,40,40,40	4
85	MG	1	3596	1/1	0.93	0.28	46,46,46,46	0
85	MG	6	1991	1/1	0.93	0.11	77,77,77,77	0
86	OHX	1	4011	7/7	0.93	0.09	62,62,62,62	3
85	MG	1	3759	1/1	0.93	0.10	48,48,48,48	0
85	MG	5	3738	1/1	0.93	0.08	42,42,42,42	0
86	OHX	1	4014	7/7	0.93	0.09	60,60,60,60	3
85	MG	1	3431	1/1	0.93	0.09	47,47,47,47	0
86	OHX	1	4017	7/7	0.93	0.09	46,46,46,46	2
85	MG	1	3509	1/1	0.93	0.28	33,33,33,33	0
86	OHX	5	4129	7/7	0.93	0.19	37,37,37,37	3
85	MG	5	3744	1/1	0.93	0.25	57,57,57,57	0
85	MG	1	3626	1/1	0.93	0.22	46,46,46,46	0
85	MG	5	3520	1/1	0.93	0.26	30,30,30,30	0
85	MG	5	3627	1/1	0.93	0.24	47,47,47,47	0
85	MG	5	3449	1/1	0.93	0.11	32,32,32,32	0
86	OHX	6	2140	7/7	0.93	0.10	74,74,74,74	6
85	MG	5	3524	1/1	0.93	0.25	48,48,48,48	0
86	OHX	6	2144	7/7	0.93	0.13	85,85,85,85	7
86	OHX	5	4138	7/7	0.93	0.20	44,44,44,44	5
85	MG	1	3541	1/1	0.93	0.32	28,28,28,28	0
85	MG	5	3452	1/1	0.93	0.24	29,29,29,29	0
85	MG	5	3453	1/1	0.93	0.19	33,33,33,33	0
85	MG	6	1952	1/1	0.93	0.51	53,53,53,53	0
86	OHX	2	2118	7/7	0.93	0.09	143,143,143,143	7
85	MG	5	3760	1/1	0.93	0.07	53,53,53,53	0
85	MG	1	3628	1/1	0.93	0.21	41,41,41,41	0
85	MG	5	3635	1/1	0.93	0.07	50,50,50,50	0
85	MG	5	3537	1/1	0.93	0.25	26,26,26,26	0
85	MG	1	3579	1/1	0.93	0.10	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3459	1/1	0.93	0.20	34,34,34,34	0
85	MG	1	3716	1/1	0.93	0.07	65,65,65,65	0
85	MG	5	3780	1/1	0.93	0.16	30,30,30,30	0
86	OHX	2	2127	7/7	0.93	0.10	128,128,128,128	7
85	MG	1	3601	1/1	0.93	0.15	72,72,72,72	0
85	MG	1	3559	1/1	0.93	0.28	22,22,22,22	0
85	MG	6	2010	1/1	0.93	0.19	53,53,53,53	0
85	MG	5	3647	1/1	0.93	0.17	55,55,55,55	0
86	OHX	2	2132	7/7	0.93	0.13	87,87,87,87	3
85	MG	1	3634	1/1	0.93	0.28	41,41,41,41	0
85	MG	1	3498	1/1	0.93	0.32	45,45,45,45	0
85	MG	5	3650	1/1	0.93	0.34	29,29,29,29	0
85	MG	1	3636	1/1	0.93	0.35	53,53,53,53	0
85	MG	1	3637	1/1	0.93	0.36	46,46,46,46	0
86	OHX	6	2172	7/7	0.93	0.14	69,69,69,69	3
85	MG	1	3725	1/1	0.93	0.12	38,38,38,38	0
85	MG	5	3796	1/1	0.93	0.21	42,42,42,42	0
85	MG	1	3530	1/1	0.93	0.27	41,41,41,41	0
85	MG	5	3554	1/1	0.93	0.28	32,32,32,32	0
85	MG	6	1965	1/1	0.93	0.10	48,48,48,48	0
85	MG	5	3662	1/1	0.93	0.25	42,42,42,42	0
85	MG	5	3556	1/1	0.93	0.22	33,33,33,33	0
85	MG	5	3804	1/1	0.93	0.28	49,49,49,49	0
85	MG	1	3459	1/1	0.93	0.24	60,60,60,60	0
85	MG	5	3558	1/1	0.93	0.31	31,31,31,31	0
85	MG	5	3561	1/1	0.93	0.33	26,26,26,26	0
85	MG	1	3412	1/1	0.93	0.10	68,68,68,68	0
86	OHX	s9	201	7/7	0.93	0.15	71,71,71,71	5
85	MG	5	3816	1/1	0.93	0.20	39,39,39,39	0
86	OHX	c5	201	7/7	0.93	0.07	129,129,129,129	6
85	MG	1	3503	1/1	0.93	0.30	37,37,37,37	0
85	MG	7	205	1/1	0.93	0.34	26,26,26,26	0
86	OHX	d9	102	7/7	0.93	0.17	106,106,106,106	6
85	MG	5	3671	1/1	0.93	0.09	84,84,84,84	0
86	OHX	5	3876	7/7	0.93	0.20	43,43,43,43	3
86	OHX	5	3889	7/7	0.93	0.27	42,42,42,42	3
85	MG	1	3646	1/1	0.93	0.10	39,39,39,39	0
86	OHX	C5	201	7/7	0.93	0.08	122,122,122,122	7
85	MG	1	3737	1/1	0.93	0.26	63,63,63,63	0
86	OHX	SR	401	7/7	0.93	0.09	144,144,144,144	6
86	OHX	6	2113	7/7	0.94	0.11	67,67,67,67	3
85	MG	1	3562	1/1	0.94	0.34	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	2	2094	7/7	0.94	0.17	87,87,87,87	5
86	OHX	5	4036	7/7	0.94	0.17	38,38,38,38	5
86	OHX	5	4038	7/7	0.94	0.12	106,106,106,106	4
86	OHX	5	4039	7/7	0.94	0.17	72,72,72,72	4
85	MG	5	3660	1/1	0.94	0.17	46,46,46,46	0
85	MG	5	3456	1/1	0.94	0.18	31,31,31,31	0
85	MG	7	203	1/1	0.94	0.29	54,54,54,54	0
85	MG	5	3418	1/1	0.94	0.19	36,36,36,36	0
86	OHX	2	2102	7/7	0.94	0.10	118,118,118,118	5
85	MG	1	3563	1/1	0.94	0.14	41,41,41,41	0
86	OHX	1	3932	7/7	0.94	0.17	57,57,57,57	5
86	OHX	5	4053	7/7	0.94	0.08	65,65,65,65	5
86	OHX	1	3933	7/7	0.94	0.09	91,91,91,91	4
86	OHX	1	3938	7/7	0.94	0.16	53,53,53,53	3
86	OHX	1	4072	7/7	0.94	0.28	47,47,47,47	3
85	MG	L2	301	1/1	0.94	0.16	37,37,37,37	0
86	OHX	1	3945	7/7	0.94	0.18	57,57,57,57	5
85	MG	7	211	1/1	0.94	0.07	57,57,57,57	0
85	MG	5	3606	1/1	0.94	0.07	39,39,39,39	1
86	OHX	2	2108	7/7	0.94	0.12	79,79,79,79	5
86	OHX	5	4067	7/7	0.94	0.16	34,34,34,34	4
85	MG	5	3550	1/1	0.94	0.37	44,44,44,44	0
86	OHX	6	2139	7/7	0.94	0.10	86,86,86,86	3
85	MG	5	3737	1/1	0.94	0.17	40,40,40,40	0
86	OHX	5	4073	7/7	0.94	0.15	44,44,44,44	4
86	OHX	6	2142	7/7	0.94	0.14	95,95,95,95	7
85	MG	5	3668	1/1	0.94	0.07	33,33,33,33	0
86	OHX	5	4077	7/7	0.94	0.18	32,32,32,32	3
86	OHX	1	3956	7/7	0.94	0.12	57,57,57,57	5
85	MG	8	204	1/1	0.94	0.31	44,44,44,44	0
86	OHX	2	2113	7/7	0.94	0.08	152,152,152,152	7
85	MG	1	3643	1/1	0.94	0.22	38,38,38,38	0
85	MG	5	3741	1/1	0.94	0.14	66,66,66,66	0
85	MG	5	3742	1/1	0.94	0.11	31,31,31,31	1
86	OHX	6	2151	7/7	0.94	0.12	65,65,65,65	4
85	MG	1	3499	1/1	0.94	0.21	37,37,37,37	0
85	MG	5	3611	1/1	0.94	0.12	38,38,38,38	0
85	MG	5	3505	1/1	0.94	0.41	25,25,25,25	0
85	MG	1	3605	1/1	0.94	0.18	44,44,44,44	0
85	MG	M5	301	1/1	0.94	0.17	42,42,42,42	0
85	MG	6	1973	1/1	0.94	0.42	51,51,51,51	0
86	OHX	5	4093	7/7	0.94	0.14	55,55,55,55	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3730	1/1	0.94	0.12	36,36,36,36	0
85	MG	5	3751	1/1	0.94	0.30	53,53,53,53	0
85	MG	5	3678	1/1	0.94	0.27	37,37,37,37	0
85	MG	m5	303	1/1	0.94	0.21	67,67,67,67	0
85	MG	5	3755	1/1	0.94	0.23	55,55,55,55	0
86	OHX	1	3984	7/7	0.94	0.08	127,127,127,127	7
86	OHX	1	3985	7/7	0.94	0.17	38,38,38,38	2
85	MG	1	3731	1/1	0.94	0.14	57,57,57,57	0
85	MG	5	3563	1/1	0.94	0.32	44,44,44,44	0
85	MG	1	3606	1/1	0.94	0.17	43,43,43,43	0
85	MG	n8	201	1/1	0.94	0.18	37,37,37,37	0
85	MG	n8	202	1/1	0.94	0.23	50,50,50,50	0
85	MG	5	3622	1/1	0.94	0.18	62,62,62,62	0
85	MG	1	3461	1/1	0.94	0.15	57,57,57,57	0
85	MG	5	3765	1/1	0.94	0.13	39,39,39,39	0
85	MG	5	3766	1/1	0.94	0.08	27,27,27,27	0
86	OHX	2	2010	7/7	0.94	0.15	101,101,101,101	4
86	OHX	3	211	7/7	0.94	0.15	64,64,64,64	3
85	MG	5	3767	1/1	0.94	0.13	43,43,43,43	0
85	MG	5	3471	1/1	0.94	0.16	51,51,51,51	0
86	OHX	2	2034	7/7	0.94	0.13	119,119,119,119	4
86	OHX	6	2180	7/7	0.94	0.12	97,97,97,97	6
85	MG	6	1920	1/1	0.94	0.31	46,46,46,46	0
85	MG	5	3568	1/1	0.94	0.26	22,22,22,22	0
85	MG	1	3708	1/1	0.94	0.11	42,42,42,42	0
86	OHX	2	2044	7/7	0.94	0.13	98,98,98,98	6
86	OHX	s4	602	7/7	0.94	0.11	76,76,76,76	3
85	MG	1	3404	1/1	0.94	0.23	57,57,57,57	0
85	MG	5	3438	1/1	0.94	0.29	39,39,39,39	0
86	OHX	2	2050	7/7	0.94	0.11	129,129,129,129	6
86	OHX	2	2051	7/7	0.94	0.15	101,101,101,101	5
86	OHX	2	2052	7/7	0.94	0.16	90,90,90,90	5
86	OHX	c8	203	7/7	0.94	0.14	99,99,99,99	5
85	MG	5	3572	1/1	0.94	0.22	21,21,21,21	0
86	OHX	L4	401	7/7	0.94	0.08	67,67,67,67	7
85	MG	1	3569	1/1	0.94	0.27	39,39,39,39	0
86	OHX	5	3871	7/7	0.94	0.17	72,72,72,72	2
86	OHX	2	2055	7/7	0.94	0.10	63,63,63,63	5
85	MG	5	3576	1/1	0.94	0.16	28,28,28,28	0
86	OHX	5	3909	7/7	0.94	0.12	77,77,77,77	4
86	OHX	5	3910	7/7	0.94	0.17	57,57,57,57	3
86	OHX	M7	205	7/7	0.94	0.13	57,57,57,57	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	6	1924	1/1	0.94	0.34	48,48,48,48	0
86	OHX	5	3919	7/7	0.94	0.18	73,73,73,73	3
85	MG	5	3521	1/1	0.94	0.32	44,44,44,44	0
86	OHX	5	4151	7/7	0.94	0.12	53,53,53,53	4
85	MG	5	3579	1/1	0.94	0.15	17,17,17,17	0
85	MG	1	3611	1/1	0.94	0.10	41,41,41,41	0
86	OHX	1	3825	7/7	0.94	0.18	91,91,91,91	5
86	OHX	5	3942	7/7	0.94	0.16	50,50,50,50	5
86	OHX	5	4156	7/7	0.94	0.14	49,49,49,49	6
86	OHX	2	2067	7/7	0.94	0.08	132,132,132,132	4
86	OHX	6	2029	7/7	0.94	0.15	68,68,68,68	2
85	MG	1	3547	1/1	0.94	0.32	32,32,32,32	0
86	OHX	6	2050	7/7	0.94	0.12	87,87,87,87	5
85	MG	1	3440	1/1	0.94	0.40	49,49,49,49	0
86	OHX	6	2066	7/7	0.94	0.10	162,162,162,162	3
86	OHX	5	3969	7/7	0.94	0.14	105,105,105,105	5
85	MG	2	1982	1/1	0.94	0.24	46,46,46,46	0
86	OHX	6	2072	7/7	0.94	0.19	76,76,76,76	3
86	OHX	5	4167	7/7	0.94	0.16	38,38,38,38	3
86	OHX	5	3972	7/7	0.94	0.13	89,89,89,89	1
85	MG	5	3795	1/1	0.94	0.10	41,41,41,41	0
86	OHX	5	3976	7/7	0.94	0.10	115,115,115,115	3
85	MG	5	3486	1/1	0.94	0.18	51,51,51,51	0
85	MG	5	3447	1/1	0.94	0.17	31,31,31,31	0
85	MG	5	3489	1/1	0.94	0.23	39,39,39,39	0
86	OHX	5	3981	7/7	0.94	0.11	69,69,69,69	3
85	MG	1	3686	1/1	0.94	0.16	35,35,35,35	0
86	OHX	1	4041	7/7	0.94	0.16	46,46,46,46	4
86	OHX	8	219	7/7	0.94	0.13	80,80,80,80	2
85	MG	1	3615	1/1	0.94	0.27	68,68,68,68	0
86	OHX	5	3989	7/7	0.94	0.12	158,158,158,158	5
86	OHX	8	224	7/7	0.94	0.14	95,95,95,95	7
86	OHX	1	3897	7/7	0.94	0.16	49,49,49,49	5
86	OHX	6	2090	7/7	0.94	0.12	91,91,91,91	7
86	OHX	5	3994	7/7	0.94	0.11	42,42,42,42	4
86	OHX	1	3898	7/7	0.94	0.17	89,89,89,89	5
86	OHX	2	2084	7/7	0.94	0.16	95,95,95,95	5
85	MG	1	3511	1/1	0.94	0.33	36,36,36,36	0
86	OHX	14	403	7/7	0.94	0.11	51,51,51,51	7
86	OHX	1	4048	7/7	0.94	0.11	116,116,116,116	5
86	OHX	15	303	7/7	0.94	0.12	90,90,90,90	6
86	OHX	6	2098	7/7	0.94	0.17	87,87,87,87	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	3903	7/7	0.94	0.16	53,53,53,53	3
86	OHX	m0	303	7/7	0.94	0.15	96,96,96,96	5
85	MG	1	3638	1/1	0.94	0.27	48,48,48,48	0
86	OHX	6	2104	7/7	0.94	0.12	91,91,91,91	5
86	OHX	m7	204	7/7	0.94	0.12	47,47,47,47	5
86	OHX	6	2106	7/7	0.94	0.12	85,85,85,85	4
85	MG	1	3553	1/1	0.94	0.23	24,24,24,24	0
86	OHX	o3	202	7/7	0.94	0.16	52,52,52,52	3
85	MG	1	3666	1/1	0.94	0.29	65,65,65,65	0
85	MG	5	3544	1/1	0.94	0.33	48,48,48,48	0
85	MG	5	3810	1/1	0.94	0.12	50,50,50,50	0
86	OHX	5	3985	7/7	0.95	0.11	55,55,55,55	2
85	MG	o2	201	1/1	0.95	0.15	35,35,35,35	1
86	OHX	6	2039	7/7	0.95	0.13	126,126,126,126	5
85	MG	1	3702	1/1	0.95	0.14	45,45,45,45	0
85	MG	1	3704	1/1	0.95	0.15	59,59,59,59	0
85	MG	5	3761	1/1	0.95	0.18	38,38,38,38	0
86	OHX	6	2057	7/7	0.95	0.14	58,58,58,58	2
86	OHX	6	2060	7/7	0.95	0.09	96,96,96,96	1
86	OHX	5	3997	7/7	0.95	0.11	62,62,62,62	5
86	OHX	5	3999	7/7	0.95	0.21	38,38,38,38	5
86	OHX	5	4001	7/7	0.95	0.18	41,41,41,41	4
85	MG	q2	201	1/1	0.95	0.06	43,43,43,43	1
86	OHX	2	2136	7/7	0.95	0.17	74,74,74,74	6
85	MG	B	102	1/1	0.95	0.23	38,38,38,38	0
86	OHX	5	4009	7/7	0.95	0.23	41,41,41,41	3
85	MG	1	3738	1/1	0.95	0.13	41,41,41,41	0
86	OHX	6	2074	7/7	0.95	0.11	70,70,70,70	2
85	MG	5	3764	1/1	0.95	0.17	43,43,43,43	0
85	MG	5	3562	1/1	0.95	0.22	27,27,27,27	0
86	OHX	2	2019	7/7	0.95	0.13	81,81,81,81	3
86	OHX	5	4020	7/7	0.95	0.18	47,47,47,47	1
86	OHX	5	4022	7/7	0.95	0.16	37,37,37,37	1
86	OHX	6	2081	7/7	0.95	0.11	74,74,74,74	6
86	OHX	6	2082	7/7	0.95	0.12	99,99,99,99	5
86	OHX	5	4027	7/7	0.95	0.14	49,49,49,49	3
86	OHX	5	4028	7/7	0.95	0.15	72,72,72,72	4
85	MG	5	3404	1/1	0.95	0.24	33,33,33,33	0
86	OHX	2	2027	7/7	0.95	0.14	75,75,75,75	4
86	OHX	2	2030	7/7	0.95	0.10	98,98,98,98	5
86	OHX	2	2032	7/7	0.95	0.14	102,102,102,102	6
85	MG	4	201	1/1	0.95	0.17	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3768	1/1	0.95	0.18	34,34,34,34	0
86	OHX	5	4037	7/7	0.95	0.10	93,93,93,93	5
85	MG	1	3677	1/1	0.95	0.12	46,46,46,46	0
86	OHX	6	2094	7/7	0.95	0.15	109,109,109,109	6
86	OHX	1	4022	7/7	0.95	0.12	71,71,71,71	6
86	OHX	2	2037	7/7	0.95	0.17	73,73,73,73	4
86	OHX	1	4024	7/7	0.95	0.14	42,42,42,42	3
86	OHX	2	2040	7/7	0.95	0.15	89,89,89,89	3
85	MG	1	3550	1/1	0.95	0.24	33,33,33,33	0
86	OHX	5	4047	7/7	0.95	0.10	28,28,28,28	1
85	MG	5	3689	1/1	0.95	0.28	40,40,40,40	0
86	OHX	6	2105	7/7	0.95	0.10	81,81,81,81	4
86	OHX	5	4051	7/7	0.95	0.13	64,64,64,64	6
85	MG	5	3774	1/1	0.95	0.30	55,55,55,55	0
86	OHX	2	2048	7/7	0.95	0.08	141,141,141,141	5
86	OHX	S9	201	7/7	0.95	0.13	94,94,94,94	6
85	MG	1	3468	1/1	0.95	0.27	39,39,39,39	0
85	MG	1	3489	1/1	0.95	0.22	67,67,67,67	0
85	MG	1	3500	1/1	0.95	0.33	30,30,30,30	0
85	MG	1	3527	1/1	0.95	0.25	31,31,31,31	0
86	OHX	6	2115	7/7	0.95	0.11	58,58,58,58	2
86	OHX	6	2116	7/7	0.95	0.14	61,61,61,61	2
86	OHX	5	4064	7/7	0.95	0.11	52,52,52,52	3
86	OHX	1	3807	7/7	0.95	0.21	73,73,73,73	2
86	OHX	1	4037	7/7	0.95	0.15	84,84,84,84	7
86	OHX	6	2119	7/7	0.95	0.16	60,60,60,60	3
86	OHX	5	4071	7/7	0.95	0.10	45,45,45,45	3
85	MG	2	1990	1/1	0.95	0.17	49,49,49,49	0
86	OHX	1	3843	7/7	0.95	0.15	55,55,55,55	2
85	MG	4	209	1/1	0.95	0.22	51,51,51,51	0
85	MG	5	3786	1/1	0.95	0.12	35,35,35,35	0
86	OHX	5	4076	7/7	0.95	0.08	43,43,43,43	3
86	OHX	1	3859	7/7	0.95	0.17	53,53,53,53	2
86	OHX	1	3862	7/7	0.95	0.10	83,83,83,83	3
86	OHX	1	3866	7/7	0.95	0.14	69,69,69,69	3
86	OHX	6	2128	7/7	0.95	0.14	53,53,53,53	4
86	OHX	6	2129	7/7	0.95	0.11	58,58,58,58	5
86	OHX	2	2056	7/7	0.95	0.17	99,99,99,99	4
86	OHX	1	3870	7/7	0.95	0.17	67,67,67,67	3
86	OHX	5	4084	7/7	0.95	0.20	35,35,35,35	6
85	MG	5	3698	1/1	0.95	0.24	42,42,42,42	0
85	MG	5	3573	1/1	0.95	0.35	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	6	2134	7/7	0.95	0.07	163,163,163,163	7
86	OHX	1	4051	7/7	0.95	0.13	58,58,58,58	3
86	OHX	2	2060	7/7	0.95	0.14	89,89,89,89	6
86	OHX	1	4054	7/7	0.95	0.20	77,77,77,77	6
85	MG	5	3702	1/1	0.95	0.12	54,54,54,54	0
85	MG	5	3574	1/1	0.95	0.25	37,37,37,37	0
86	OHX	5	4094	7/7	0.95	0.16	36,36,36,36	3
85	MG	5	3704	1/1	0.95	0.25	2,2,2,2	0
86	OHX	5	4096	7/7	0.95	0.07	119,119,119,119	7
86	OHX	1	3887	7/7	0.95	0.10	131,131,131,131	5
86	OHX	1	3888	7/7	0.95	0.15	71,71,71,71	3
86	OHX	1	3890	7/7	0.95	0.12	48,48,48,48	3
85	MG	5	3415	1/1	0.95	0.28	44,44,44,44	0
86	OHX	5	4101	7/7	0.95	0.11	69,69,69,69	3
86	OHX	5	4103	7/7	0.95	0.15	40,40,40,40	5
86	OHX	1	3893	7/7	0.95	0.10	155,155,155,155	6
86	OHX	6	2147	7/7	0.95	0.13	64,64,64,64	4
85	MG	5	3416	1/1	0.95	0.26	31,31,31,31	0
85	MG	5	3637	1/1	0.95	0.09	36,36,36,36	0
86	OHX	2	2070	7/7	0.95	0.09	108,108,108,108	5
86	OHX	5	4109	7/7	0.95	0.15	53,53,53,53	5
86	OHX	2	2071	7/7	0.95	0.10	72,72,72,72	6
86	OHX	1	4068	7/7	0.95	0.11	39,39,39,39	3
86	OHX	1	3902	7/7	0.95	0.22	53,53,53,53	3
86	OHX	5	4113	7/7	0.95	0.15	52,52,52,52	6
85	MG	1	3617	1/1	0.95	0.18	41,41,41,41	0
86	OHX	1	4071	7/7	0.95	0.19	42,42,42,42	3
85	MG	1	3687	1/1	0.95	0.35	46,46,46,46	0
86	OHX	2	2075	7/7	0.95	0.11	80,80,80,80	6
86	OHX	5	4118	7/7	0.95	0.20	49,49,49,49	4
86	OHX	1	3906	7/7	0.95	0.15	65,65,65,65	4
85	MG	5	3419	1/1	0.95	0.12	36,36,36,36	0
86	OHX	1	4076	7/7	0.95	0.24	45,45,45,45	5
85	MG	4	213	1/1	0.95	0.23	64,64,64,64	0
85	MG	5	3581	1/1	0.95	0.29	24,24,24,24	0
85	MG	6	1951	1/1	0.95	0.43	43,43,43,43	0
85	MG	5	3645	1/1	0.95	0.24	31,31,31,31	0
85	MG	5	3717	1/1	0.95	0.31	16,16,16,16	0
86	OHX	1	3919	7/7	0.95	0.10	106,106,106,106	3
86	OHX	1	3920	7/7	0.95	0.14	43,43,43,43	3
85	MG	1	3749	1/1	0.95	0.20	17,17,17,17	0
85	MG	1	3750	1/1	0.95	0.27	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	6	2170	7/7	0.95	0.09	83,83,83,83	7
85	MG	1	3688	1/1	0.95	0.23	39,39,39,39	0
85	MG	5	3814	1/1	0.95	0.23	42,42,42,42	0
85	MG	L3	401	1/1	0.95	0.20	41,41,41,41	0
85	MG	1	3406	1/1	0.95	0.15	44,44,44,44	0
86	OHX	1	4090	7/7	0.95	0.15	47,47,47,47	4
85	MG	5	3723	1/1	0.95	0.28	52,52,52,52	0
86	OHX	1	3935	7/7	0.95	0.11	71,71,71,71	2
86	OHX	1	3937	7/7	0.95	0.12	110,110,110,110	6
85	MG	5	3532	1/1	0.95	0.22	35,35,35,35	0
85	MG	7	204	1/1	0.95	0.23	44,44,44,44	0
85	MG	1	3514	1/1	0.95	0.18	35,35,35,35	0
86	OHX	5	4145	7/7	0.95	0.14	70,70,70,70	7
85	MG	7	208	1/1	0.95	0.30	45,45,45,45	0
86	OHX	2	2099	7/7	0.95	0.08	185,185,185,185	7
86	OHX	2	2100	7/7	0.95	0.11	83,83,83,83	4
85	MG	6	1958	1/1	0.95	0.21	44,44,44,44	0
85	MG	5	3728	1/1	0.95	0.12	44,44,44,44	0
86	OHX	1	3954	7/7	0.95	0.10	122,122,122,122	3
85	MG	5	3730	1/1	0.95	0.07	41,41,41,41	0
85	MG	5	3654	1/1	0.95	0.30	31,31,31,31	0
85	MG	5	3430	1/1	0.95	0.21	36,36,36,36	0
86	OHX	1	3959	7/7	0.95	0.09	112,112,112,112	3
86	OHX	1	3961	7/7	0.95	0.17	45,45,45,45	5
86	OHX	2	2106	7/7	0.95	0.11	78,78,78,78	3
85	MG	1	3640	1/1	0.95	0.21	62,62,62,62	0
85	MG	1	3484	1/1	0.95	0.17	52,52,52,52	0
85	MG	M5	302	1/1	0.95	0.22	47,47,47,47	0
85	MG	5	3487	1/1	0.95	0.17	37,37,37,37	0
86	OHX	5	4163	7/7	0.95	0.14	36,36,36,36	4
86	OHX	3	212	7/7	0.95	0.14	86,86,86,86	3
85	MG	5	3599	1/1	0.95	0.23	39,39,39,39	0
86	OHX	5	3914	7/7	0.95	0.15	74,74,74,74	4
86	OHX	1	3969	7/7	0.95	0.13	65,65,65,65	4
85	MG	1	3438	1/1	0.95	0.09	33,33,33,33	0
86	OHX	3	216	7/7	0.95	0.14	49,49,49,49	5
86	OHX	5	4170	7/7	0.95	0.17	71,71,71,71	3
86	OHX	5	3922	7/7	0.95	0.09	119,119,119,119	6
85	MG	1	3494	1/1	0.95	0.17	42,42,42,42	0
86	OHX	5	3928	7/7	0.95	0.09	146,146,146,146	3
86	OHX	5	3932	7/7	0.95	0.10	139,139,139,139	5
85	MG	5	3603	1/1	0.95	0.21	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	l3	402	1/1	0.95	0.16	39,39,39,39	1
86	OHX	8	215	7/7	0.95	0.14	60,60,60,60	3
86	OHX	5	3939	7/7	0.95	0.13	92,92,92,92	2
86	OHX	5	3940	7/7	0.95	0.13	62,62,62,62	2
86	OHX	8	221	7/7	0.95	0.13	62,62,62,62	3
85	MG	1	3625	1/1	0.95	0.12	41,41,41,41	0
86	OHX	4	227	7/7	0.95	0.12	103,103,103,103	6
86	OHX	5	3945	7/7	0.95	0.14	46,46,46,46	3
86	OHX	1	3977	7/7	0.95	0.09	72,72,72,72	7
85	MG	5	3745	1/1	0.95	0.27	34,34,34,34	0
85	MG	1	3456	1/1	0.95	0.18	32,32,32,32	0
86	OHX	5	3951	7/7	0.95	0.17	67,67,67,67	5
86	OHX	5	3952	7/7	0.95	0.10	100,100,100,100	2
85	MG	1	3697	1/1	0.95	0.10	42,42,42,42	0
85	MG	1	3457	1/1	0.95	0.17	32,32,32,32	0
85	MG	m3	201	1/1	0.95	0.17	40,40,40,40	0
85	MG	6	1968	1/1	0.95	0.18	48,48,48,48	0
85	MG	3	203	1/1	0.95	0.26	42,42,42,42	0
85	MG	5	3445	1/1	0.95	0.19	38,38,38,38	0
85	MG	5	3752	1/1	0.95	0.25	40,40,40,40	0
86	OHX	5	3974	7/7	0.95	0.13	53,53,53,53	4
85	MG	s8	302	1/1	0.95	0.32	49,49,49,49	0
85	MG	1	3649	1/1	0.95	0.17	37,37,37,37	0
86	OHX	1	3992	7/7	0.95	0.10	52,52,52,52	3
85	MG	1	3610	1/1	0.95	0.09	45,45,45,45	0
85	MG	5	3615	1/1	0.95	0.29	35,35,35,35	0
86	OHX	1	3996	7/7	0.95	0.12	64,64,64,64	5
85	MG	5	3758	1/1	0.95	0.06	36,36,36,36	0
86	OHX	5	3983	7/7	0.95	0.16	46,46,46,46	3
89	PRO	1	4114	7/8	0.95	0.17	41,41,51,51	0
85	MG	6	1995	1/1	0.96	0.22	47,47,47,47	0
85	MG	1	3705	1/1	0.96	0.16	33,33,33,33	0
86	OHX	1	3829	7/7	0.96	0.16	59,59,59,59	2
86	OHX	1	3834	7/7	0.96	0.13	62,62,62,62	3
86	OHX	5	4056	7/7	0.96	0.14	40,40,40,40	6
86	OHX	1	3997	7/7	0.96	0.12	55,55,55,55	5
86	OHX	5	4058	7/7	0.96	0.32	36,36,36,36	6
86	OHX	3	210	7/7	0.96	0.16	51,51,51,51	5
86	OHX	1	3841	7/7	0.96	0.17	70,70,70,70	3
85	MG	l2	301	1/1	0.96	0.24	37,37,37,37	0
86	OHX	1	3848	7/7	0.96	0.13	76,76,76,76	3
86	OHX	1	4001	7/7	0.96	0.11	61,61,61,61	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	12	302	1/1	0.96	0.25	45,45,45,45	0
86	OHX	1	3853	7/7	0.96	0.13	54,54,54,54	3
85	MG	4	212	1/1	0.96	0.07	60,60,60,60	0
86	OHX	1	3858	7/7	0.96	0.10	98,98,98,98	4
85	MG	5	3553	1/1	0.96	0.18	26,26,26,26	0
86	OHX	4	222	7/7	0.96	0.09	61,61,61,61	3
86	OHX	2	2080	7/7	0.96	0.15	91,91,91,91	4
85	MG	6	1998	1/1	0.96	0.21	42,42,42,42	0
86	OHX	2	2082	7/7	0.96	0.10	90,90,90,90	5
86	OHX	4	229	7/7	0.96	0.10	60,60,60,60	3
85	MG	6	1999	1/1	0.96	0.29	36,36,36,36	0
85	MG	5	3655	1/1	0.96	0.23	42,42,42,42	0
86	OHX	1	4015	7/7	0.96	0.14	47,47,47,47	2
85	MG	5	3656	1/1	0.96	0.42	41,41,41,41	0
85	MG	1	3633	1/1	0.96	0.11	59,59,59,59	0
85	MG	5	3658	1/1	0.96	0.20	27,27,27,27	0
85	MG	1	3732	1/1	0.96	0.21	35,35,35,35	0
85	MG	5	3465	1/1	0.96	0.30	44,44,44,44	0
86	OHX	2	2091	7/7	0.96	0.15	89,89,89,89	5
86	OHX	M5	304	7/7	0.96	0.17	72,72,72,72	4
85	MG	1	3667	1/1	0.96	0.16	58,58,58,58	0
85	MG	5	3511	1/1	0.96	0.22	43,43,43,43	0
85	MG	m7	203	1/1	0.96	0.23	34,34,34,34	0
85	MG	6	1907	1/1	0.96	0.32	51,51,51,51	0
86	OHX	2	2096	7/7	0.96	0.10	108,108,108,108	6
85	MG	1	3648	1/1	0.96	0.11	42,42,42,42	0
85	MG	1	3565	1/1	0.96	0.38	40,40,40,40	0
86	OHX	6	2025	7/7	0.96	0.15	62,62,62,62	2
85	MG	1	3650	1/1	0.96	0.17	47,47,47,47	0
86	OHX	1	3901	7/7	0.96	0.14	62,62,62,62	4
85	MG	6	1911	1/1	0.96	0.35	49,49,49,49	0
86	OHX	5	3869	7/7	0.96	0.14	35,35,35,35	4
86	OHX	6	2044	7/7	0.96	0.10	46,46,46,46	2
86	OHX	5	3874	7/7	0.96	0.14	62,62,62,62	3
86	OHX	5	4102	7/7	0.96	0.09	45,45,45,45	5
86	OHX	6	2045	7/7	0.96	0.15	91,91,91,91	5
85	MG	1	3443	1/1	0.96	0.14	46,46,46,46	0
86	OHX	5	3895	7/7	0.96	0.15	63,63,63,63	3
86	OHX	5	3902	7/7	0.96	0.13	72,72,72,72	3
85	MG	1	3552	1/1	0.96	0.38	37,37,37,37	0
86	OHX	1	4034	7/7	0.96	0.15	75,75,75,75	3
85	MG	5	3727	1/1	0.96	0.19	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	6	2064	7/7	0.96	0.12	98,98,98,98	5
86	OHX	6	2065	7/7	0.96	0.10	138,138,138,138	5
85	MG	s8	301	1/1	0.96	0.12	52,52,52,52	0
86	OHX	6	2067	7/7	0.96	0.10	154,154,154,154	3
85	MG	q3	502	1/1	0.96	0.27	48,48,48,48	0
85	MG	5	3729	1/1	0.96	0.07	47,47,47,47	0
86	OHX	5	3929	7/7	0.96	0.20	41,41,41,41	4
85	MG	1	3623	1/1	0.96	0.17	57,57,57,57	0
86	OHX	1	3913	7/7	0.96	0.06	54,54,54,54	3
86	OHX	6	2076	7/7	0.96	0.10	52,52,52,52	5
86	OHX	5	4120	7/7	0.96	0.15	64,64,64,64	5
86	OHX	2	1999	7/7	0.96	0.11	113,113,113,113	2
86	OHX	1	4043	7/7	0.96	0.10	39,39,39,39	2
86	OHX	2	2004	7/7	0.96	0.11	135,135,135,135	5
86	OHX	2	2007	7/7	0.96	0.13	94,94,94,94	5
86	OHX	1	3918	7/7	0.96	0.10	91,91,91,91	5
85	MG	1	3568	1/1	0.96	0.24	36,36,36,36	0
85	MG	5	3522	1/1	0.96	0.31	36,36,36,36	0
86	OHX	1	3922	7/7	0.96	0.10	82,82,82,82	3
86	OHX	2	2016	7/7	0.96	0.12	96,96,96,96	4
86	OHX	2	2017	7/7	0.96	0.14	74,74,74,74	4
86	OHX	5	3955	7/7	0.96	0.09	149,149,149,149	4
85	MG	5	3437	1/1	0.96	0.34	34,34,34,34	0
86	OHX	5	3960	7/7	0.96	0.20	44,44,44,44	3
86	OHX	1	4053	7/7	0.96	0.09	43,43,43,43	3
86	OHX	5	3964	7/7	0.96	0.10	107,107,107,107	2
86	OHX	5	3966	7/7	0.96	0.14	50,50,50,50	4
86	OHX	6	2093	7/7	0.96	0.09	45,45,45,45	2
86	OHX	2	2020	7/7	0.96	0.10	117,117,117,117	3
86	OHX	2	2021	7/7	0.96	0.11	99,99,99,99	5
85	MG	5	3480	1/1	0.96	0.07	47,47,47,47	0
86	OHX	2	2023	7/7	0.96	0.09	106,106,106,106	4
86	OHX	6	2099	7/7	0.96	0.11	81,81,81,81	5
86	OHX	1	3934	7/7	0.96	0.12	54,54,54,54	3
85	MG	5	3736	1/1	0.96	0.17	35,35,35,35	1
86	OHX	1	3936	7/7	0.96	0.16	54,54,54,54	3
86	OHX	2	2029	7/7	0.96	0.14	98,98,98,98	5
85	MG	2	1902	1/1	0.96	0.27	49,49,49,49	0
85	MG	5	3806	1/1	0.96	0.18	37,37,37,37	0
86	OHX	6	2108	7/7	0.96	0.08	109,109,109,109	6
86	OHX	1	3941	7/7	0.96	0.10	51,51,51,51	3
86	OHX	1	3942	7/7	0.96	0.12	94,94,94,94	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3718	1/1	0.96	0.20	52,52,52,52	0
85	MG	5	3528	1/1	0.96	0.36	21,21,21,21	0
86	OHX	1	3948	7/7	0.96	0.10	37,37,37,37	2
85	MG	5	3440	1/1	0.96	0.15	36,36,36,36	0
85	MG	d3	201	1/1	0.96	0.17	50,50,50,50	0
86	OHX	2	2039	7/7	0.96	0.14	103,103,103,103	7
85	MG	5	3811	1/1	0.96	0.12	30,30,30,30	0
86	OHX	5	3996	7/7	0.96	0.14	52,52,52,52	3
86	OHX	2	2041	7/7	0.96	0.08	141,141,141,141	6
86	OHX	5	3998	7/7	0.96	0.17	43,43,43,43	5
86	OHX	2	2042	7/7	0.96	0.11	68,68,68,68	5
85	MG	5	3812	1/1	0.96	0.13	32,32,32,32	0
86	OHX	5	4003	7/7	0.96	0.13	54,54,54,54	3
85	MG	5	3813	1/1	0.96	0.19	31,31,31,31	0
86	OHX	2	2045	7/7	0.96	0.12	95,95,95,95	4
86	OHX	6	2124	7/7	0.96	0.09	103,103,103,103	6
86	OHX	2	2046	7/7	0.96	0.14	83,83,83,83	7
86	OHX	1	3962	7/7	0.96	0.12	59,59,59,59	2
86	OHX	5	4012	7/7	0.96	0.15	41,41,41,41	4
86	OHX	7	216	7/7	0.96	0.14	62,62,62,62	3
85	MG	M6	204	1/1	0.96	0.10	37,37,37,37	0
86	OHX	5	4015	7/7	0.96	0.10	36,36,36,36	4
85	MG	5	3533	1/1	0.96	0.33	28,28,28,28	0
85	MG	1	3402	1/1	0.96	0.27	36,36,36,36	0
85	MG	2	1918	1/1	0.96	0.27	68,68,68,68	0
86	OHX	8	217	7/7	0.96	0.09	78,78,78,78	5
85	MG	5	3636	1/1	0.96	0.27	43,43,43,43	0
85	MG	1	3698	1/1	0.96	0.13	42,42,42,42	0
85	MG	M7	204	1/1	0.96	0.10	46,46,46,46	0
86	OHX	5	4025	7/7	0.96	0.14	50,50,50,50	2
85	MG	7	207	1/1	0.96	0.20	55,55,55,55	0
85	MG	1	3593	1/1	0.96	0.25	50,50,50,50	0
86	OHX	1	3972	7/7	0.96	0.10	55,55,55,55	4
86	OHX	5	4029	7/7	0.96	0.09	76,76,76,76	4
85	MG	5	3692	1/1	0.96	0.11	38,38,38,38	0
85	MG	1	3594	1/1	0.96	0.24	48,48,48,48	0
85	MG	1	3682	1/1	0.96	0.14	36,36,36,36	0
86	OHX	2	2059	7/7	0.96	0.13	101,101,101,101	4
86	OHX	6	2141	7/7	0.96	0.07	151,151,151,151	7
86	OHX	5	4035	7/7	0.96	0.13	40,40,40,40	3
85	MG	N8	201	1/1	0.96	0.11	33,33,33,33	0
86	OHX	1	3979	7/7	0.96	0.08	197,197,197,197	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3696	1/1	0.96	0.15	45,45,45,45	0
86	OHX	2	2062	7/7	0.96	0.14	109,109,109,109	6
86	OHX	2	2063	7/7	0.96	0.07	153,153,153,153	7
86	OHX	5	4041	7/7	0.96	0.10	73,73,73,73	4
85	MG	N8	202	1/1	0.96	0.32	47,47,47,47	0
85	MG	1	3522	1/1	0.96	0.24	31,31,31,31	0
85	MG	1	3703	1/1	0.96	0.08	40,40,40,40	0
85	MG	5	3701	1/1	0.96	0.15	38,38,38,38	0
85	MG	1	3754	1/1	0.96	0.34	71,71,71,71	0
86	OHX	o7	502	7/7	0.96	0.15	83,83,83,83	4
85	MG	1	3427	1/1	0.96	0.30	42,42,42,42	0
86	OHX	5	4049	7/7	0.96	0.19	37,37,37,37	3
85	MG	8	208	1/1	0.96	0.26	51,51,51,51	0
89	PRO	B	101	7/8	0.96	0.13	32,32,56,56	0
86	OHX	1	3864	7/7	0.97	0.12	104,104,104,104	3
86	OHX	2	2033	7/7	0.97	0.16	78,78,78,78	3
85	MG	5	3762	1/1	0.97	0.29	38,38,38,38	0
86	OHX	1	3869	7/7	0.97	0.10	92,92,92,92	3
85	MG	1	3510	1/1	0.97	0.15	39,39,39,39	0
85	MG	L7	301	1/1	0.97	0.18	38,38,38,38	0
86	OHX	1	3872	7/7	0.97	0.12	44,44,44,44	4
86	OHX	1	3873	7/7	0.97	0.15	53,53,53,53	5
86	OHX	1	3874	7/7	0.97	0.10	50,50,50,50	3
86	OHX	1	3994	7/7	0.97	0.10	54,54,54,54	5
85	MG	L7	302	1/1	0.97	0.11	50,50,50,50	0
86	OHX	1	3876	7/7	0.97	0.14	41,41,41,41	2
85	MG	1	3408	1/1	0.97	0.19	25,25,25,25	0
86	OHX	5	4044	7/7	0.97	0.11	51,51,51,51	3
86	OHX	1	3879	7/7	0.97	0.15	44,44,44,44	2
86	OHX	1	3881	7/7	0.97	0.12	86,86,86,86	4
86	OHX	1	3882	7/7	0.97	0.12	64,64,64,64	3
85	MG	8	201	1/1	0.97	0.11	43,43,43,43	0
85	MG	1	3685	1/1	0.97	0.17	43,43,43,43	0
86	OHX	1	3885	7/7	0.97	0.13	53,53,53,53	3
85	MG	5	3665	1/1	0.97	0.18	43,43,43,43	0
86	OHX	5	4052	7/7	0.97	0.12	67,67,67,67	5
85	MG	M0	302	1/1	0.97	0.17	50,50,50,50	0
86	OHX	1	4006	7/7	0.97	0.14	48,48,48,48	5
86	OHX	1	4007	7/7	0.97	0.08	43,43,43,43	4
86	OHX	4	217	7/7	0.97	0.12	61,61,61,61	3
86	OHX	4	220	7/7	0.97	0.09	81,81,81,81	2
86	OHX	4	221	7/7	0.97	0.12	84,84,84,84	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4008	7/7	0.97	0.13	47,47,47,47	5
86	OHX	4	223	7/7	0.97	0.09	61,61,61,61	3
86	OHX	4	224	7/7	0.97	0.09	86,86,86,86	3
86	OHX	4	225	7/7	0.97	0.12	44,44,44,44	3
85	MG	1	3722	1/1	0.97	0.05	43,43,43,43	0
86	OHX	1	3889	7/7	0.97	0.12	48,48,48,48	2
86	OHX	5	4066	7/7	0.97	0.12	38,38,38,38	4
85	MG	5	3529	1/1	0.97	0.23	45,45,45,45	0
86	OHX	5	4068	7/7	0.97	0.10	49,49,49,49	3
85	MG	5	3414	1/1	0.97	0.16	33,33,33,33	0
86	OHX	1	3892	7/7	0.97	0.11	65,65,65,65	3
85	MG	5	3775	1/1	0.97	0.09	40,40,40,40	0
86	OHX	1	3895	7/7	0.97	0.12	57,57,57,57	4
86	OHX	1	3896	7/7	0.97	0.18	49,49,49,49	2
86	OHX	L3	403	7/7	0.97	0.10	72,72,72,72	5
85	MG	5	3450	1/1	0.97	0.31	45,45,45,45	0
85	MG	2	1984	1/1	0.97	0.08	67,67,67,67	0
85	MG	5	3779	1/1	0.97	0.23	35,35,35,35	0
85	MG	5	3626	1/1	0.97	0.24	42,42,42,42	0
85	MG	l3	401	1/1	0.97	0.31	27,27,27,27	0
85	MG	6	2001	1/1	0.97	0.10	48,48,48,48	0
86	OHX	M6	203	7/7	0.97	0.15	43,43,43,43	2
85	MG	1	3746	1/1	0.97	0.23	43,43,43,43	0
85	MG	5	3536	1/1	0.97	0.38	29,29,29,29	0
85	MG	5	3785	1/1	0.97	0.16	57,57,57,57	0
85	MG	6	1942	1/1	0.97	0.41	43,43,43,43	0
86	OHX	O1	201	7/7	0.97	0.14	93,93,93,93	3
85	MG	5	3787	1/1	0.97	0.06	33,33,33,33	0
86	OHX	5	4088	7/7	0.97	0.10	39,39,39,39	4
85	MG	5	3583	1/1	0.97	0.43	23,23,23,23	0
86	OHX	O7	104	7/7	0.97	0.12	78,78,78,78	4
86	OHX	1	3909	7/7	0.97	0.12	73,73,73,73	4
86	OHX	1	3910	7/7	0.97	0.10	81,81,81,81	4
86	OHX	1	3911	7/7	0.97	0.12	61,61,61,61	3
86	OHX	6	2037	7/7	0.97	0.10	101,101,101,101	3
85	MG	5	3538	1/1	0.97	0.29	32,32,32,32	0
86	OHX	6	2041	7/7	0.97	0.16	56,56,56,56	4
85	MG	1	3670	1/1	0.97	0.32	38,38,38,38	0
86	OHX	5	3845	7/7	0.97	0.13	48,48,48,48	2
86	OHX	5	3846	7/7	0.97	0.14	37,37,37,37	3
86	OHX	5	3856	7/7	0.97	0.15	65,65,65,65	3
86	OHX	5	3858	7/7	0.97	0.14	72,72,72,72	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	3866	7/7	0.97	0.14	60,60,60,60	3
85	MG	1	3653	1/1	0.97	0.11	55,55,55,55	0
85	MG	1	3521	1/1	0.97	0.35	43,43,43,43	0
86	OHX	5	3872	7/7	0.97	0.16	82,82,82,82	3
86	OHX	6	2046	7/7	0.97	0.11	60,60,60,60	2
86	OHX	5	3875	7/7	0.97	0.12	49,49,49,49	2
86	OHX	6	2049	7/7	0.97	0.10	97,97,97,97	3
85	MG	1	3727	1/1	0.97	0.18	48,48,48,48	0
86	OHX	1	3917	7/7	0.97	0.08	54,54,54,54	4
86	OHX	5	3900	7/7	0.97	0.15	52,52,52,52	3
86	OHX	6	2052	7/7	0.97	0.11	67,67,67,67	3
86	OHX	5	3905	7/7	0.97	0.11	51,51,51,51	4
86	OHX	6	2053	7/7	0.97	0.13	92,92,92,92	5
86	OHX	6	2054	7/7	0.97	0.09	87,87,87,87	3
86	OHX	6	2055	7/7	0.97	0.09	113,113,113,113	4
86	OHX	5	3915	7/7	0.97	0.16	39,39,39,39	4
86	OHX	6	2056	7/7	0.97	0.10	73,73,73,73	3
85	MG	1	3435	1/1	0.97	0.32	25,25,25,25	0
86	OHX	5	3918	7/7	0.97	0.10	36,36,36,36	2
86	OHX	5	4121	7/7	0.97	0.13	68,68,68,68	7
86	OHX	6	2059	7/7	0.97	0.10	61,61,61,61	3
86	OHX	2	2066	7/7	0.97	0.08	160,160,160,160	7
86	OHX	5	3924	7/7	0.97	0.15	43,43,43,43	5
86	OHX	6	2061	7/7	0.97	0.10	86,86,86,86	4
86	OHX	6	2062	7/7	0.97	0.09	117,117,117,117	4
86	OHX	6	2063	7/7	0.97	0.07	147,147,147,147	6
86	OHX	5	3930	7/7	0.97	0.10	55,55,55,55	2
86	OHX	1	4040	7/7	0.97	0.13	52,52,52,52	4
85	MG	n0	201	1/1	0.97	0.15	41,41,41,41	0
85	MG	5	3500	1/1	0.97	0.05	40,40,40,40	0
85	MG	1	3656	1/1	0.97	0.18	46,46,46,46	0
86	OHX	6	2068	7/7	0.97	0.11	103,103,103,103	4
86	OHX	6	2069	7/7	0.97	0.11	73,73,73,73	4
86	OHX	6	2070	7/7	0.97	0.12	87,87,87,87	3
86	OHX	5	3943	7/7	0.97	0.12	44,44,44,44	2
85	MG	1	3620	1/1	0.97	0.13	32,32,32,32	0
86	OHX	5	3946	7/7	0.97	0.10	109,109,109,109	4
86	OHX	1	3926	7/7	0.97	0.18	57,57,57,57	4
85	MG	5	3798	1/1	0.97	0.16	42,42,42,42	0
85	MG	5	3799	1/1	0.97	0.21	42,42,42,42	0
86	OHX	6	2075	7/7	0.97	0.09	76,76,76,76	3
85	MG	5	3641	1/1	0.97	0.31	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3740	1/1	0.97	0.18	45,45,45,45	0
86	OHX	5	3956	7/7	0.97	0.08	40,40,40,40	2
86	OHX	5	4146	7/7	0.97	0.09	71,71,71,71	5
85	MG	1	3658	1/1	0.97	0.11	42,42,42,42	0
85	MG	5	3504	1/1	0.97	0.25	28,28,28,28	0
86	OHX	5	3961	7/7	0.97	0.10	74,74,74,74	1
86	OHX	5	3962	7/7	0.97	0.09	47,47,47,47	4
86	OHX	2	2078	7/7	0.97	0.07	115,115,115,115	7
85	MG	1	3436	1/1	0.97	0.22	39,39,39,39	0
86	OHX	5	3965	7/7	0.97	0.11	49,49,49,49	4
85	MG	f	1001	1/1	0.97	0.13	53,53,53,53	0
86	OHX	6	2084	7/7	0.97	0.12	104,104,104,104	5
86	OHX	5	3968	7/7	0.97	0.11	47,47,47,47	4
85	MG	5	3428	1/1	0.97	0.35	45,45,45,45	0
85	MG	1	3756	1/1	0.97	0.22	53,53,53,53	0
86	OHX	1	3940	7/7	0.97	0.12	77,77,77,77	5
86	OHX	6	2089	7/7	0.97	0.10	56,56,56,56	4
85	MG	1	3733	1/1	0.97	0.12	40,40,40,40	0
86	OHX	2	2002	7/7	0.97	0.12	101,101,101,101	3
86	OHX	1	3944	7/7	0.97	0.11	48,48,48,48	4
86	OHX	2	2085	7/7	0.97	0.09	103,103,103,103	4
86	OHX	1	3946	7/7	0.97	0.07	69,69,69,69	3
85	MG	N8	203	1/1	0.97	0.15	30,30,30,30	0
86	OHX	5	3980	7/7	0.97	0.13	55,55,55,55	3
86	OHX	6	2096	7/7	0.97	0.13	94,94,94,94	5
85	MG	1	3713	1/1	0.97	0.22	40,40,40,40	0
85	MG	d2	201	1/1	0.97	0.20	59,59,59,59	0
86	OHX	5	3984	7/7	0.97	0.12	56,56,56,56	4
86	OHX	C8	201	7/7	0.97	0.10	111,111,111,111	4
86	OHX	6	2101	7/7	0.97	0.10	62,62,62,62	2
85	MG	5	3699	1/1	0.97	0.26	39,39,39,39	0
86	OHX	7	221	7/7	0.97	0.12	50,50,50,50	4
85	MG	O7	101	1/1	0.97	0.08	62,62,62,62	0
85	MG	5	3435	1/1	0.97	0.15	33,33,33,33	0
86	OHX	1	3808	7/7	0.97	0.12	74,74,74,74	3
86	OHX	1	3811	7/7	0.97	0.14	79,79,79,79	2
86	OHX	8	216	7/7	0.97	0.10	85,85,85,85	3
86	OHX	1	3957	7/7	0.97	0.09	49,49,49,49	5
86	OHX	1	3817	7/7	0.97	0.12	109,109,109,109	5
86	OHX	6	2109	7/7	0.97	0.10	99,99,99,99	6
86	OHX	1	3820	7/7	0.97	0.18	47,47,47,47	4
86	OHX	1	3960	7/7	0.97	0.11	42,42,42,42	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	3821	7/7	0.97	0.14	66,66,66,66	5
86	OHX	5	4002	7/7	0.97	0.12	70,70,70,70	4
86	OHX	2	2018	7/7	0.97	0.09	74,74,74,74	5
86	OHX	8	227	7/7	0.97	0.11	59,59,59,59	3
85	MG	1	3645	1/1	0.97	0.32	51,51,51,51	0
86	OHX	1	3831	7/7	0.97	0.15	48,48,48,48	3
86	OHX	1	3832	7/7	0.97	0.13	80,80,80,80	3
86	OHX	1	3833	7/7	0.97	0.11	71,71,71,71	4
86	OHX	5	4010	7/7	0.97	0.07	72,72,72,72	5
86	OHX	14	402	7/7	0.97	0.08	69,69,69,69	5
85	MG	1	3471	1/1	0.97	0.31	45,45,45,45	0
85	MG	5	3402	1/1	0.97	0.10	54,54,54,54	0
86	OHX	1	3842	7/7	0.97	0.10	80,80,80,80	3
86	OHX	5	4014	7/7	0.97	0.10	48,48,48,48	3
85	MG	7	202	1/1	0.97	0.36	19,19,19,19	0
86	OHX	1	3845	7/7	0.97	0.09	123,123,123,123	3
85	MG	1	3441	1/1	0.97	0.08	52,52,52,52	0
86	OHX	2	2024	7/7	0.97	0.10	100,100,100,100	6
86	OHX	m5	306	7/7	0.97	0.10	76,76,76,76	3
86	OHX	1	3852	7/7	0.97	0.12	70,70,70,70	3
86	OHX	2	2026	7/7	0.97	0.11	103,103,103,103	4
86	OHX	5	4023	7/7	0.97	0.11	39,39,39,39	2
86	OHX	1	3976	7/7	0.97	0.11	41,41,41,41	4
86	OHX	1	3855	7/7	0.97	0.11	87,87,87,87	3
85	MG	5	3477	1/1	0.97	0.25	27,27,27,27	0
86	OHX	q2	203	7/7	0.97	0.15	47,47,47,47	2
86	OHX	1	3857	7/7	0.97	0.14	54,54,54,54	4
87	ZN	E1	501	1/1	0.97	0.04	145,145,145,145	0
85	MG	5	3707	1/1	0.97	0.32	64,64,64,64	0
88	SPS	5	3403	23/23	0.97	0.10	35,38,52,54	23
85	MG	1	3582	1/1	0.97	0.42	27,27,27,27	0
89	PRO	5	4173	7/8	0.97	0.11	35,35,45,45	0
85	MG	1	3536	1/1	0.97	0.21	29,29,29,29	0
86	OHX	1	3931	7/7	0.98	0.12	43,43,43,43	4
86	OHX	5	3903	7/7	0.98	0.12	91,91,91,91	2
86	OHX	5	4065	7/7	0.98	0.13	39,39,39,39	3
86	OHX	5	3904	7/7	0.98	0.16	49,49,49,49	2
86	OHX	1	3836	7/7	0.98	0.12	98,98,98,98	3
86	OHX	5	3906	7/7	0.98	0.11	60,60,60,60	4
86	OHX	6	2100	7/7	0.98	0.10	71,71,71,71	3
86	OHX	1	3839	7/7	0.98	0.12	64,64,64,64	3
86	OHX	5	3912	7/7	0.98	0.10	107,107,107,107	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	3913	7/7	0.98	0.08	77,77,77,77	3
86	OHX	1	3840	7/7	0.98	0.11	85,85,85,85	3
86	OHX	2	2025	7/7	0.98	0.11	79,79,79,79	5
85	MG	5	3713	1/1	0.98	0.23	38,38,38,38	0
85	MG	1	3495	1/1	0.98	0.34	34,34,34,34	0
86	OHX	4	218	7/7	0.98	0.09	55,55,55,55	2
86	OHX	4	219	7/7	0.98	0.13	60,60,60,60	4
86	OHX	5	3920	7/7	0.98	0.08	36,36,36,36	2
86	OHX	5	3921	7/7	0.98	0.11	57,57,57,57	2
86	OHX	1	3844	7/7	0.98	0.10	98,98,98,98	5
85	MG	6	1930	1/1	0.98	0.36	45,45,45,45	0
86	OHX	5	3925	7/7	0.98	0.08	56,56,56,56	3
86	OHX	1	3846	7/7	0.98	0.08	119,119,119,119	3
86	OHX	5	3927	7/7	0.98	0.10	64,64,64,64	5
85	MG	6	2005	1/1	0.98	0.06	88,88,88,88	0
86	OHX	2	2031	7/7	0.98	0.10	81,81,81,81	4
86	OHX	1	3943	7/7	0.98	0.09	97,97,97,97	6
86	OHX	5	3931	7/7	0.98	0.10	54,54,54,54	4
85	MG	5	3534	1/1	0.98	0.24	25,25,25,25	0
86	OHX	5	3933	7/7	0.98	0.09	94,94,94,94	4
86	OHX	5	3934	7/7	0.98	0.11	38,38,38,38	2
86	OHX	5	3935	7/7	0.98	0.11	45,45,45,45	1
85	MG	1	3664	1/1	0.98	0.22	39,39,39,39	0
86	OHX	5	3937	7/7	0.98	0.09	53,53,53,53	2
85	MG	5	3609	1/1	0.98	0.09	35,35,35,35	0
85	MG	5	3478	1/1	0.98	0.26	21,21,21,21	0
85	MG	5	3771	1/1	0.98	0.22	36,36,36,36	0
85	MG	5	3772	1/1	0.98	0.27	37,37,37,37	0
86	OHX	1	3950	7/7	0.98	0.09	41,41,41,41	4
86	OHX	2	2038	7/7	0.98	0.08	119,119,119,119	6
86	OHX	5	3944	7/7	0.98	0.13	42,42,42,42	3
86	OHX	L3	402	7/7	0.98	0.10	59,59,59,59	4
86	OHX	1	3861	7/7	0.98	0.10	60,60,60,60	3
86	OHX	5	3947	7/7	0.98	0.13	45,45,45,45	3
85	MG	1	3589	1/1	0.98	0.12	40,40,40,40	0
86	OHX	1	3863	7/7	0.98	0.11	42,42,42,42	3
85	MG	1	3528	1/1	0.98	0.28	47,47,47,47	0
85	MG	1	3425	1/1	0.98	0.41	27,27,27,27	0
85	MG	5	3805	1/1	0.98	0.10	37,37,37,37	0
86	OHX	5	3953	7/7	0.98	0.10	45,45,45,45	3
86	OHX	5	3954	7/7	0.98	0.09	49,49,49,49	2
86	OHX	1	3868	7/7	0.98	0.11	53,53,53,53	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3776	1/1	0.98	0.05	75,75,75,75	0
85	MG	5	3677	1/1	0.98	0.06	29,29,29,29	0
86	OHX	5	3958	7/7	0.98	0.12	42,42,42,42	2
86	OHX	5	3959	7/7	0.98	0.10	61,61,61,61	4
86	OHX	2	1991	7/7	0.98	0.11	88,88,88,88	0
86	OHX	2	1992	7/7	0.98	0.08	98,98,98,98	1
86	OHX	2	1993	7/7	0.98	0.12	96,96,96,96	2
86	OHX	2	1994	7/7	0.98	0.10	97,97,97,97	2
86	OHX	2	1996	7/7	0.98	0.13	101,101,101,101	5
86	OHX	2	1997	7/7	0.98	0.11	107,107,107,107	5
86	OHX	2	1998	7/7	0.98	0.12	116,116,116,116	2
86	OHX	1	4060	7/7	0.98	0.10	65,65,65,65	4
86	OHX	Q2	503	7/7	0.98	0.12	46,46,46,46	2
86	OHX	6	2016	7/7	0.98	0.11	83,83,83,83	4
86	OHX	6	2020	7/7	0.98	0.11	100,100,100,100	4
86	OHX	1	3878	7/7	0.98	0.10	58,58,58,58	3
85	MG	5	3482	1/1	0.98	0.32	37,37,37,37	0
86	OHX	5	3973	7/7	0.98	0.13	39,39,39,39	4
86	OHX	6	2031	7/7	0.98	0.11	80,80,80,80	4
86	OHX	6	2032	7/7	0.98	0.11	117,117,117,117	2
86	OHX	6	2033	7/7	0.98	0.14	56,56,56,56	5
86	OHX	6	2035	7/7	0.98	0.11	82,82,82,82	3
86	OHX	6	2036	7/7	0.98	0.09	58,58,58,58	3
86	OHX	1	3880	7/7	0.98	0.11	47,47,47,47	5
85	MG	5	3679	1/1	0.98	0.17	31,31,31,31	1
86	OHX	6	2040	7/7	0.98	0.09	123,123,123,123	5
85	MG	5	3525	1/1	0.98	0.32	31,31,31,31	0
86	OHX	S1	301	7/7	0.98	0.10	121,121,121,121	2
86	OHX	2	2005	7/7	0.98	0.10	99,99,99,99	3
86	OHX	2	2006	7/7	0.98	0.10	93,93,93,93	3
85	MG	5	3616	1/1	0.98	0.05	42,42,42,42	0
86	OHX	5	3987	7/7	0.98	0.12	41,41,41,41	3
86	OHX	6	2047	7/7	0.98	0.10	67,67,67,67	5
86	OHX	6	2048	7/7	0.98	0.10	65,65,65,65	4
86	OHX	5	3990	7/7	0.98	0.10	44,44,44,44	4
86	OHX	2	2008	7/7	0.98	0.09	89,89,89,89	5
86	OHX	5	3992	7/7	0.98	0.13	80,80,80,80	5
85	MG	5	3754	1/1	0.98	0.23	51,51,51,51	0
85	MG	5	3783	1/1	0.98	0.03	38,38,38,38	0
86	OHX	2	2012	7/7	0.98	0.09	87,87,87,87	3
86	OHX	2	2013	7/7	0.98	0.11	94,94,94,94	4
86	OHX	1	3982	7/7	0.98	0.12	47,47,47,47	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	3776	7/7	0.98	0.12	55,55,55,55	1
86	OHX	1	3782	7/7	0.98	0.13	71,71,71,71	4
86	OHX	1	3894	7/7	0.98	0.06	132,132,132,132	7
86	OHX	6	2058	7/7	0.98	0.07	72,72,72,72	2
86	OHX	1	3787	7/7	0.98	0.14	72,72,72,72	3
86	OHX	5	4004	7/7	0.98	0.07	55,55,55,55	2
86	OHX	1	3792	7/7	0.98	0.11	74,74,74,74	3
86	OHX	1	3793	7/7	0.98	0.14	68,68,68,68	4
86	OHX	5	4007	7/7	0.98	0.09	40,40,40,40	3
86	OHX	1	3794	7/7	0.98	0.11	69,69,69,69	2
86	OHX	1	3795	7/7	0.98	0.12	85,85,85,85	2
86	OHX	1	3991	7/7	0.98	0.09	57,57,57,57	3
86	OHX	1	3796	7/7	0.98	0.11	57,57,57,57	4
86	OHX	1	3798	7/7	0.98	0.10	69,69,69,69	1
86	OHX	1	3799	7/7	0.98	0.12	78,78,78,78	3
86	OHX	1	3800	7/7	0.98	0.14	44,44,44,44	3
86	OHX	1	3801	7/7	0.98	0.12	71,71,71,71	3
86	OHX	7	214	7/7	0.98	0.10	70,70,70,70	1
86	OHX	7	215	7/7	0.98	0.11	60,60,60,60	5
86	OHX	1	3805	7/7	0.98	0.09	93,93,93,93	4
86	OHX	7	218	7/7	0.98	0.13	67,67,67,67	3
86	OHX	7	219	7/7	0.98	0.08	67,67,67,67	2
86	OHX	2	2014	7/7	0.98	0.06	130,130,130,130	7
86	OHX	2	2015	7/7	0.98	0.06	90,90,90,90	4
86	OHX	1	3810	7/7	0.98	0.12	62,62,62,62	3
86	OHX	5	4021	7/7	0.98	0.11	36,36,36,36	2
85	MG	5	3457	1/1	0.98	0.17	38,38,38,38	0
86	OHX	8	214	7/7	0.98	0.11	62,62,62,62	4
86	OHX	1	3812	7/7	0.98	0.11	88,88,88,88	3
86	OHX	1	3813	7/7	0.98	0.10	52,52,52,52	2
86	OHX	1	3814	7/7	0.98	0.14	76,76,76,76	3
86	OHX	1	3815	7/7	0.98	0.10	85,85,85,85	3
86	OHX	6	2079	7/7	0.98	0.09	51,51,51,51	3
86	OHX	8	220	7/7	0.98	0.09	44,44,44,44	3
86	OHX	1	3816	7/7	0.98	0.15	62,62,62,62	5
85	MG	5	3559	1/1	0.98	0.31	22,22,22,22	0
86	OHX	1	3819	7/7	0.98	0.09	81,81,81,81	3
85	MG	5	3560	1/1	0.98	0.38	27,27,27,27	0
86	OHX	8	225	7/7	0.98	0.08	40,40,40,40	3
86	OHX	5	3843	7/7	0.98	0.11	64,64,64,64	1
85	MG	1	3632	1/1	0.98	0.25	47,47,47,47	0
86	OHX	6	2085	7/7	0.98	0.12	76,76,76,76	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	3855	7/7	0.98	0.13	71,71,71,71	3
85	MG	6	2000	1/1	0.98	0.28	48,48,48,48	0
86	OHX	1	3826	7/7	0.98	0.11	84,84,84,84	4
86	OHX	13	403	7/7	0.98	0.10	50,50,50,50	3
86	OHX	5	3860	7/7	0.98	0.10	88,88,88,88	3
86	OHX	5	3862	7/7	0.98	0.10	47,47,47,47	2
86	OHX	5	3865	7/7	0.98	0.10	86,86,86,86	1
86	OHX	1	3921	7/7	0.98	0.08	82,82,82,82	3
86	OHX	5	3867	7/7	0.98	0.08	126,126,126,126	2
86	OHX	5	3868	7/7	0.98	0.13	74,74,74,74	2
85	MG	5	3601	1/1	0.98	0.23	26,26,26,26	0
86	OHX	1	3923	7/7	0.98	0.09	40,40,40,40	3
86	OHX	1	3830	7/7	0.98	0.12	99,99,99,99	3
85	MG	1	3734	1/1	0.98	0.34	35,35,35,35	1
86	OHX	m5	305	7/7	0.98	0.14	54,54,54,54	3
85	MG	1	3706	1/1	0.98	0.12	38,38,38,38	0
86	OHX	m6	201	7/7	0.98	0.13	36,36,36,36	3
86	OHX	2	2073	7/7	0.98	0.09	63,63,63,63	6
86	OHX	5	3879	7/7	0.98	0.10	59,59,59,59	3
86	OHX	5	3881	7/7	0.98	0.08	96,96,96,96	2
86	OHX	n3	202	7/7	0.98	0.08	60,60,60,60	3
86	OHX	5	3882	7/7	0.98	0.10	89,89,89,89	3
86	OHX	5	3884	7/7	0.98	0.10	63,63,63,63	3
85	MG	7	206	1/1	0.98	0.14	34,34,34,34	0
86	OHX	o7	503	7/7	0.98	0.14	62,62,62,62	1
86	OHX	5	3890	7/7	0.98	0.11	69,69,69,69	3
86	OHX	5	3891	7/7	0.98	0.11	66,66,66,66	4
86	OHX	5	3892	7/7	0.98	0.14	63,63,63,63	3
87	ZN	Q0	500	1/1	0.98	0.03	54,54,54,54	0
86	OHX	5	3894	7/7	0.98	0.15	50,50,50,50	2
87	ZN	e1	501	1/1	0.98	0.05	173,173,173,173	0
87	ZN	q2	202	1/1	0.98	0.08	71,71,71,71	0
88	SPS	1	4113	23/23	0.98	0.07	39,42,55,58	0
86	OHX	1	3929	7/7	0.98	0.10	53,53,53,53	4
86	OHX	5	3896	7/7	0.98	0.10	42,42,42,42	4
86	OHX	5	3899	7/7	0.98	0.12	49,49,49,49	3
86	OHX	1	3835	7/7	0.98	0.14	62,62,62,62	1
89	PRO	C	101	7/8	0.98	0.09	29,29,51,51	0
86	OHX	1	3788	7/7	0.99	0.08	58,58,58,58	4
86	OHX	5	3861	7/7	0.99	0.09	46,46,46,46	3
86	OHX	1	3789	7/7	0.99	0.07	74,74,74,74	2
86	OHX	5	3863	7/7	0.99	0.10	85,85,85,85	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	3864	7/7	0.99	0.07	88,88,88,88	3
86	OHX	4	216	7/7	0.99	0.10	59,59,59,59	3
86	OHX	1	3790	7/7	0.99	0.09	48,48,48,48	3
86	OHX	1	3791	7/7	0.99	0.10	41,41,41,41	2
86	OHX	2	2001	7/7	0.99	0.07	120,120,120,120	2
85	MG	5	3582	1/1	0.99	0.35	31,31,31,31	0
86	OHX	5	3870	7/7	0.99	0.12	76,76,76,76	5
86	OHX	2	2003	7/7	0.99	0.11	76,76,76,76	5
85	MG	1	3574	1/1	0.99	0.33	30,30,30,30	0
86	OHX	5	3873	7/7	0.99	0.08	58,58,58,58	4
86	OHX	1	3847	7/7	0.99	0.10	56,56,56,56	3
85	MG	1	3668	1/1	0.99	0.04	38,38,38,38	1
86	OHX	5	4000	7/7	0.99	0.07	45,45,45,45	2
86	OHX	1	3797	7/7	0.99	0.07	54,54,54,54	2
86	OHX	5	3877	7/7	0.99	0.07	62,62,62,62	3
86	OHX	5	3878	7/7	0.99	0.11	73,73,73,73	3
86	OHX	1	3850	7/7	0.99	0.12	47,47,47,47	3
86	OHX	5	3880	7/7	0.99	0.08	47,47,47,47	3
86	OHX	1	3851	7/7	0.99	0.08	46,46,46,46	3
85	MG	1	3518	1/1	0.99	0.33	31,31,31,31	0
86	OHX	5	3883	7/7	0.99	0.08	53,53,53,53	1
85	MG	5	3593	1/1	0.99	0.30	22,22,22,22	0
86	OHX	5	3885	7/7	0.99	0.07	78,78,78,78	3
86	OHX	5	3886	7/7	0.99	0.12	79,79,79,79	3
86	OHX	5	3887	7/7	0.99	0.08	44,44,44,44	2
86	OHX	5	3888	7/7	0.99	0.10	43,43,43,43	3
86	OHX	1	3854	7/7	0.99	0.09	43,43,43,43	4
86	OHX	2	1995	7/7	0.99	0.13	76,76,76,76	2
86	OHX	2	2009	7/7	0.99	0.10	89,89,89,89	4
86	OHX	1	3802	7/7	0.99	0.08	60,60,60,60	2
86	OHX	5	4018	7/7	0.99	0.09	48,48,48,48	4
86	OHX	5	3893	7/7	0.99	0.10	59,59,59,59	2
86	OHX	1	3803	7/7	0.99	0.09	73,73,73,73	3
86	OHX	1	3804	7/7	0.99	0.11	62,62,62,62	1
85	MG	6	1994	1/1	0.99	0.35	49,49,49,49	0
86	OHX	5	3897	7/7	0.99	0.09	46,46,46,46	5
86	OHX	5	3898	7/7	0.99	0.09	58,58,58,58	4
86	OHX	1	3806	7/7	0.99	0.12	52,52,52,52	2
85	MG	L2	302	1/1	0.99	0.19	41,41,41,41	0
86	OHX	5	3901	7/7	0.99	0.11	43,43,43,43	3
85	MG	5	3732	1/1	0.99	0.14	30,30,30,30	0
86	OHX	1	3865	7/7	0.99	0.08	75,75,75,75	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	3809	7/7	0.99	0.11	80,80,80,80	2
86	OHX	1	3763	7/7	0.99	0.10	58,58,58,58	2
86	OHX	1	3765	7/7	0.99	0.11	65,65,65,65	2
86	OHX	5	3907	7/7	0.99	0.09	63,63,63,63	3
86	OHX	5	3908	7/7	0.99	0.09	45,45,45,45	4
86	OHX	1	3766	7/7	0.99	0.09	61,61,61,61	2
86	OHX	1	3767	7/7	0.99	0.11	77,77,77,77	2
86	OHX	5	3911	7/7	0.99	0.10	44,44,44,44	4
86	OHX	1	3769	7/7	0.99	0.07	64,64,64,64	2
86	OHX	N9	101	7/7	0.99	0.08	64,64,64,64	1
86	OHX	1	3771	7/7	0.99	0.07	59,59,59,59	2
86	OHX	1	3772	7/7	0.99	0.08	67,67,67,67	2
86	OHX	1	3773	7/7	0.99	0.10	49,49,49,49	2
86	OHX	1	3818	7/7	0.99	0.09	62,62,62,62	2
86	OHX	1	3774	7/7	0.99	0.09	71,71,71,71	3
86	OHX	1	3775	7/7	0.99	0.12	66,66,66,66	2
86	OHX	6	2012	7/7	0.99	0.12	70,70,70,70	3
86	OHX	6	2013	7/7	0.99	0.08	87,87,87,87	2
86	OHX	6	2014	7/7	0.99	0.09	76,76,76,76	3
86	OHX	5	3923	7/7	0.99	0.13	41,41,41,41	1
86	OHX	7	217	7/7	0.99	0.08	40,40,40,40	1
86	OHX	6	2015	7/7	0.99	0.07	78,78,78,78	3
85	MG	1	3525	1/1	0.99	0.41	35,35,35,35	0
86	OHX	6	2018	7/7	0.99	0.09	90,90,90,90	2
86	OHX	6	2019	7/7	0.99	0.12	79,79,79,79	2
86	OHX	1	3822	7/7	0.99	0.09	50,50,50,50	4
86	OHX	6	2021	7/7	0.99	0.08	69,69,69,69	3
86	OHX	6	2022	7/7	0.99	0.07	67,67,67,67	2
86	OHX	8	212	7/7	0.99	0.10	57,57,57,57	3
86	OHX	8	213	7/7	0.99	0.07	57,57,57,57	2
86	OHX	6	2023	7/7	0.99	0.10	80,80,80,80	3
86	OHX	6	2024	7/7	0.99	0.07	99,99,99,99	3
86	OHX	1	3823	7/7	0.99	0.09	111,111,111,111	4
86	OHX	6	2026	7/7	0.99	0.10	66,66,66,66	1
86	OHX	6	2027	7/7	0.99	0.10	76,76,76,76	2
86	OHX	6	2028	7/7	0.99	0.08	63,63,63,63	2
86	OHX	1	3824	7/7	0.99	0.09	68,68,68,68	3
86	OHX	6	2030	7/7	0.99	0.09	57,57,57,57	2
86	OHX	1	3777	7/7	0.99	0.10	61,61,61,61	3
86	OHX	s1	301	7/7	0.99	0.10	95,95,95,95	2
86	OHX	1	3778	7/7	0.99	0.09	64,64,64,64	1
86	OHX	1	3827	7/7	0.99	0.08	45,45,45,45	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	6	2034	7/7	0.99	0.09	66,66,66,66	5
86	OHX	1	3828	7/7	0.99	0.09	63,63,63,63	2
86	OHX	1	3780	7/7	0.99	0.08	75,75,75,75	1
86	OHX	1	3781	7/7	0.99	0.09	76,76,76,76	2
86	OHX	6	2038	7/7	0.99	0.09	61,61,61,61	5
86	OHX	3	209	7/7	0.99	0.08	76,76,76,76	4
86	OHX	2	2028	7/7	0.99	0.07	108,108,108,108	5
86	OHX	1	3783	7/7	0.99	0.08	83,83,83,83	2
86	OHX	6	2042	7/7	0.99	0.11	62,62,62,62	3
86	OHX	5	3819	7/7	0.99	0.14	51,51,51,51	3
86	OHX	5	3821	7/7	0.99	0.11	64,64,64,64	2
86	OHX	5	3823	7/7	0.99	0.14	53,53,53,53	2
86	OHX	5	3825	7/7	0.99	0.09	58,58,58,58	1
86	OHX	5	3827	7/7	0.99	0.09	80,80,80,80	1
86	OHX	5	3828	7/7	0.99	0.09	50,50,50,50	3
86	OHX	5	3830	7/7	0.99	0.09	67,67,67,67	0
86	OHX	5	3831	7/7	0.99	0.09	61,61,61,61	1
86	OHX	5	3832	7/7	0.99	0.09	56,56,56,56	2
86	OHX	5	3833	7/7	0.99	0.08	59,59,59,59	2
86	OHX	5	3834	7/7	0.99	0.11	51,51,51,51	1
86	OHX	5	3835	7/7	0.99	0.07	54,54,54,54	1
86	OHX	5	3836	7/7	0.99	0.11	65,65,65,65	3
86	OHX	5	3839	7/7	0.99	0.08	64,64,64,64	2
86	OHX	5	3840	7/7	0.99	0.09	65,65,65,65	2
86	OHX	n9	101	7/7	0.99	0.08	62,62,62,62	2
86	OHX	1	3784	7/7	0.99	0.11	73,73,73,73	2
86	OHX	5	3844	7/7	0.99	0.10	62,62,62,62	2
86	OHX	1	3785	7/7	0.99	0.11	59,59,59,59	2
86	OHX	1	3786	7/7	0.99	0.10	94,94,94,94	3
86	OHX	5	3847	7/7	0.99	0.10	48,48,48,48	1
87	ZN	D6	500	1/1	0.99	0.04	103,103,103,103	0
86	OHX	5	3848	7/7	0.99	0.09	54,54,54,54	1
87	ZN	D9	101	1/1	0.99	0.03	89,89,89,89	0
86	OHX	5	3849	7/7	0.99	0.08	100,100,100,100	3
86	OHX	5	3850	7/7	0.99	0.10	51,51,51,51	2
87	ZN	Q2	501	1/1	0.99	0.08	77,77,77,77	0
87	ZN	d6	101	1/1	0.99	0.07	84,84,84,84	0
86	OHX	5	3851	7/7	0.99	0.11	55,55,55,55	4
87	ZN	d9	101	1/1	0.99	0.03	91,91,91,91	0
86	OHX	5	3852	7/7	0.99	0.12	55,55,55,55	2
86	OHX	5	3853	7/7	0.99	0.08	56,56,56,56	3
86	OHX	5	3854	7/7	0.99	0.07	78,78,78,78	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	2	2000	7/7	0.99	0.10	105,105,105,105	3
86	OHX	1	3837	7/7	0.99	0.09	60,60,60,60	2
86	OHX	5	3857	7/7	0.99	0.10	54,54,54,54	1
86	OHX	1	3838	7/7	0.99	0.10	52,52,52,52	3
86	OHX	5	3859	7/7	0.99	0.10	55,55,55,55	1
86	OHX	5	3842	7/7	1.00	0.07	38,38,38,38	3
86	OHX	1	3768	7/7	1.00	0.08	52,52,52,52	2
86	OHX	8	211	7/7	1.00	0.07	64,64,64,64	1
86	OHX	5	3824	7/7	1.00	0.08	62,62,62,62	2
86	OHX	1	3779	7/7	1.00	0.07	49,49,49,49	4
86	OHX	5	3826	7/7	1.00	0.08	46,46,46,46	1
86	OHX	1	3762	7/7	1.00	0.08	55,55,55,55	3
86	OHX	1	3770	7/7	1.00	0.09	61,61,61,61	2
86	OHX	5	3829	7/7	1.00	0.08	44,44,44,44	5
87	ZN	O7	102	1/1	1.00	0.01	47,47,47,47	0
86	OHX	1	3860	7/7	1.00	0.09	38,38,38,38	2
86	OHX	M5	303	7/7	1.00	0.09	61,61,61,61	2
87	ZN	Q3	501	1/1	1.00	0.02	78,78,78,78	0
86	OHX	1	3761	7/7	1.00	0.08	57,57,57,57	1
86	OHX	5	3817	7/7	1.00	0.10	53,53,53,53	4
86	OHX	m5	304	7/7	1.00	0.08	61,61,61,61	2
86	OHX	5	3818	7/7	1.00	0.06	57,57,57,57	0
87	ZN	o7	501	1/1	1.00	0.02	45,45,45,45	0
87	ZN	q0	500	1/1	1.00	0.02	42,42,42,42	0
86	OHX	1	3764	7/7	1.00	0.10	65,65,65,65	2
87	ZN	q3	501	1/1	1.00	0.02	62,62,62,62	0
86	OHX	5	3820	7/7	1.00	0.10	52,52,52,52	3
86	OHX	5	3837	7/7	1.00	0.07	71,71,71,71	0
86	OHX	5	3838	7/7	1.00	0.07	58,58,58,58	2
86	OHX	6	2017	7/7	1.00	0.09	59,59,59,59	2
86	OHX	5	3822	7/7	1.00	0.09	61,61,61,61	2
86	OHX	5	3841	7/7	1.00	0.06	51,51,51,51	1

6.5 Other polymers [i](#)

There are no such residues in this entry.