



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2026 – 03:39 AM UTC

PDB ID : 4U52 / pdb_00004u52
Title : Crystal structure of Nagilactone C bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 3.00 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

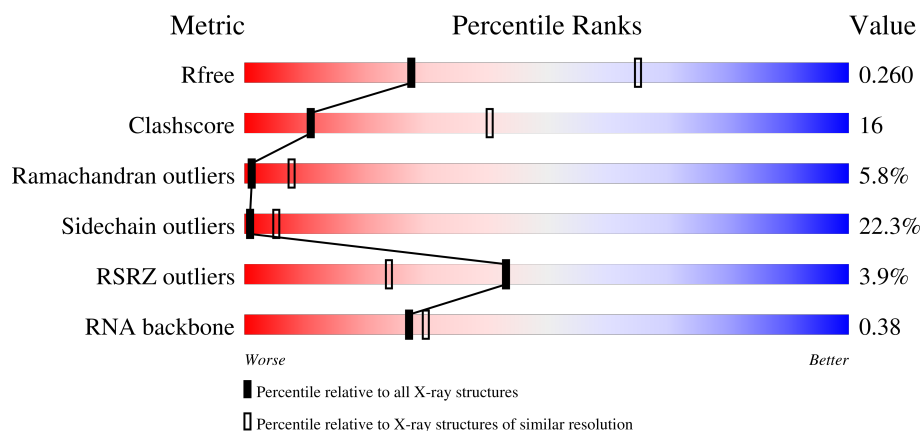
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	5% 37% 44% 17% .
1	6	1800	5% 41% 42% 16%
2	S0	251	6% 31% 37% 12% . 18%
2	s0	251	4% 33% 33% 12% . 18%

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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	

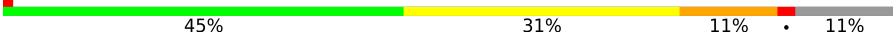
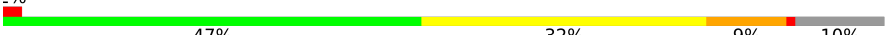
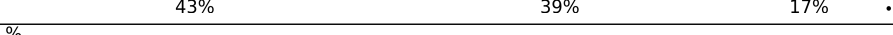
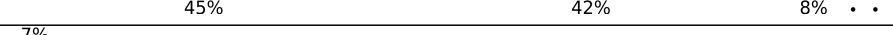
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Mol	Chain	Length	Quality of chain
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	

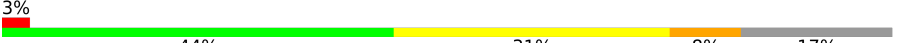
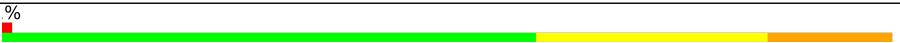
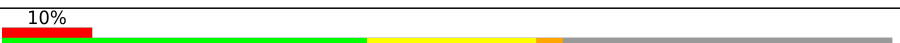
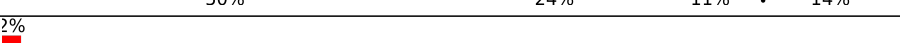
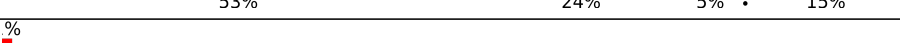
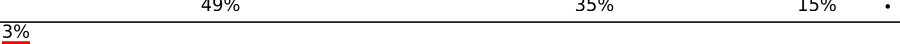
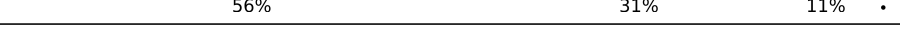
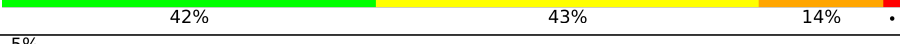
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Mol	Chain	Length	Quality of chain
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	

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Mol	Chain	Length	Quality of chain
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	
65	n9	58	

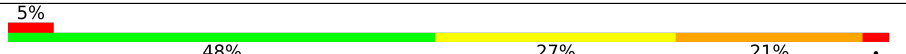
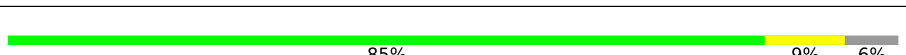
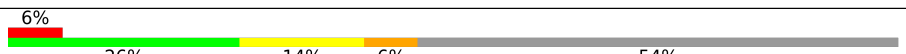
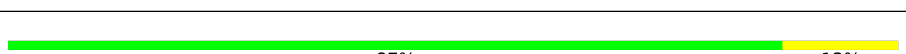
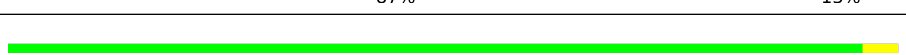
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Mol	Chain	Length	Quality of chain
66	O0	104	 47% 36% 10% 7%
66	o0	104	 47% 37% 12% 4%
67	O1	112	 56% 30% 11% 3%
67	o1	112	 54% 32% 10% 2%
68	O2	129	 50% 36% 12% 2%
68	o2	129	 47% 38% 13% 2%
69	O3	106	 51% 40% 8% 1%
69	o3	106	 51% 37% 12% 2%
70	O4	119	 51% 31% 11% 4%
70	o4	119	 49% 37% 8% 4%
71	O5	119	 50% 38% 12% 3%
71	o5	119	 47% 36% 16% 3%
72	O6	99	 51% 29% 18% 3%
72	o6	99	 54% 35% 11% 2%
73	O7	87	 47% 44% 8% 5%
73	o7	87	 53% 40% 7% 5%
74	O8	77	 52% 32% 16% 3%
74	o8	77	 44% 39% 17% 3%
75	O9	50	 48% 36% 14% 4%
75	o9	50	 36% 42% 20% 2%
76	Q0	52	 60% 25% 12% 3%
76	q0	52	 63% 25% 12% 0%
77	Q1	25	 20% 52% 28% 0%
77	q1	25	 28% 48% 24% 0%
78	Q2	105	 55% 36% 7% 3%

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Mol	Chain	Length	Quality of chain
78	q2	105	
79	Q3	91	
79	q3	91	
80	e0	62	
81	m2	160	
82	p0	311	
83	p1	47	
84	p2	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	1	3405	-	-	-	X
85	MG	1	3624	-	-	-	X
85	MG	1	3649	-	-	-	X
85	MG	1	3803	-	-	-	X
85	MG	1	3813	-	-	-	X
85	MG	2	1913	-	-	-	X
85	MG	2	1915	-	-	-	X
85	MG	2	1924	-	-	-	X
85	MG	2	1926	-	-	-	X
85	MG	2	1928	-	-	-	X
85	MG	2	1945	-	-	-	X
85	MG	2	1951	-	-	-	X
85	MG	2	1953	-	-	-	X
85	MG	2	1959	-	-	-	X
85	MG	2	1968	-	-	-	X
85	MG	2	1969	-	-	-	X
85	MG	2	1975	-	-	-	X
85	MG	2	1978	-	-	-	X
85	MG	2	1980	-	-	-	X
85	MG	2	1987	-	-	-	X
85	MG	2	1995	-	-	-	X
85	MG	2	2003	-	-	-	X
85	MG	2	2007	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	2	2017	-	-	-	X
85	MG	2	2020	-	-	-	X
85	MG	4	204	-	-	-	X
85	MG	4	222	-	-	-	X
85	MG	5	3466	-	-	-	X
85	MG	5	3662	-	-	-	X
85	MG	5	3708	-	-	-	X
85	MG	5	3779	-	-	-	X
85	MG	5	3780	-	-	-	X
85	MG	5	3806	-	-	-	X
85	MG	5	3881	-	-	-	X
85	MG	6	1920	-	-	-	X
85	MG	6	1924	-	-	-	X
85	MG	6	1933	-	-	-	X
85	MG	6	2015	-	-	-	X
85	MG	6	2041	-	-	-	X
85	MG	6	2042	-	-	-	X
85	MG	6	2047	-	-	-	X
85	MG	M0	302	-	-	-	X
85	MG	M3	202	-	-	-	X
86	OHX	1	3938	-	-	X	-
86	OHX	1	3957	-	-	X	-
86	OHX	1	3959	-	-	X	-
86	OHX	1	3970	-	-	X	-
86	OHX	1	3974	-	-	X	-
86	OHX	1	4000	-	-	X	-
86	OHX	1	4016	-	-	X	-
86	OHX	1	4025	-	-	X	-
86	OHX	1	4028	-	-	X	-
86	OHX	1	4039	-	-	X	-
86	OHX	1	4040	-	-	X	-
86	OHX	1	4047	-	-	X	-
86	OHX	1	4050	-	-	X	-
86	OHX	1	4052	-	-	X	-
86	OHX	1	4053	-	-	X	-
86	OHX	1	4057	-	-	X	-
86	OHX	1	4063	-	-	X	-
86	OHX	1	4076	-	-	X	-
86	OHX	1	4080	-	-	X	-
86	OHX	1	4110	-	-	X	-
86	OHX	1	4123	-	-	X	-
86	OHX	1	4136	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	1	4142	-	-	X	-
86	OHX	1	4146	-	-	X	-
86	OHX	1	4150	-	-	X	-
86	OHX	1	4151	-	-	X	-
86	OHX	1	4152	-	-	X	-
86	OHX	1	4156	-	-	X	-
86	OHX	1	4158	-	-	X	-
86	OHX	1	4159	-	-	X	-
86	OHX	1	4163	-	-	X	-
86	OHX	1	4168	-	-	X	-
86	OHX	1	4177	-	-	X	-
86	OHX	1	4193	-	-	X	-
86	OHX	2	2032	-	-	X	-
86	OHX	2	2045	-	-	X	-
86	OHX	2	2076	-	-	X	-
86	OHX	2	2084	-	-	X	-
86	OHX	2	2086	-	-	X	-
86	OHX	2	2091	-	-	X	-
86	OHX	2	2096	-	-	X	-
86	OHX	2	2099	-	-	X	-
86	OHX	2	2109	-	-	X	-
86	OHX	2	2116	-	-	X	-
86	OHX	2	2132	-	-	X	-
86	OHX	2	2147	-	-	X	-
86	OHX	2	2155	-	-	X	-
86	OHX	2	2158	-	-	X	-
86	OHX	2	2162	-	-	X	-
86	OHX	3	218	-	-	X	-
86	OHX	5	3944	-	-	X	-
86	OHX	5	3963	-	-	X	-
86	OHX	5	3974	-	-	X	-
86	OHX	5	3979	-	-	X	-
86	OHX	5	4000	-	-	X	-
86	OHX	5	4009	-	-	X	-
86	OHX	5	4019	-	-	X	-
86	OHX	5	4031	-	-	X	-
86	OHX	5	4032	-	-	X	-
86	OHX	5	4053	-	-	X	-
86	OHX	5	4063	-	-	X	-
86	OHX	5	4064	-	-	X	-
86	OHX	5	4072	-	-	X	-
86	OHX	5	4074	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	5	4079	-	-	X	-
86	OHX	5	4089	-	-	X	-
86	OHX	5	4092	-	-	X	-
86	OHX	5	4093	-	-	X	-
86	OHX	5	4117	-	-	X	-
86	OHX	5	4127	-	-	X	-
86	OHX	5	4136	-	-	X	-
86	OHX	5	4142	-	-	X	-
86	OHX	5	4145	-	-	X	-
86	OHX	5	4189	-	-	X	-
86	OHX	5	4191	-	-	X	-
86	OHX	5	4192	-	-	X	-
86	OHX	5	4198	-	-	X	-
86	OHX	5	4199	-	-	X	-
86	OHX	5	4200	-	-	X	-
86	OHX	5	4201	-	-	X	-
86	OHX	5	4203	-	-	X	-
86	OHX	5	4217	-	-	X	-
86	OHX	5	4237	-	-	X	-
86	OHX	5	4244	-	-	X	-
86	OHX	6	2062	-	-	X	-
86	OHX	6	2123	-	-	X	-
86	OHX	6	2128	-	-	X	-
86	OHX	6	2150	-	-	X	-
86	OHX	6	2153	-	-	X	-
86	OHX	6	2174	-	-	X	-
86	OHX	7	221	-	-	X	-
86	OHX	7	226	-	-	X	-
86	OHX	8	217	-	-	X	-
86	OHX	8	218	-	-	X	-
86	OHX	8	226	-	-	X	-
86	OHX	8	227	-	-	X	-
86	OHX	C1	201	-	-	X	-
86	OHX	C5	201	-	-	X	-
86	OHX	O7	104	-	-	X	-
86	OHX	q1	101	-	-	X	-

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411206 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O4	110	GLU	-	expression tag	UNP P87262
O4	111	ALA	-	expression tag	UNP P87262
O4	112	ALA	-	expression tag	UNP P87262
O4	113	LYS	-	expression tag	UNP P87262
O4	114	SER	-	expression tag	UNP P87262
O4	115	GLU	-	expression tag	UNP P87262
O4	116	LYS	-	expression tag	UNP P87262
O4	117	LYS	-	expression tag	UNP P87262
O4	118	ALA	-	expression tag	UNP P87262
O4	119	LYS	-	expression tag	UNP P87262
O4	120	LYS	-	expression tag	UNP P87262

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Chain	Residue	Modelled	Actual	Comment	Reference
o4	110	GLU	-	expression tag	UNP P87262
o4	111	ALA	-	expression tag	UNP P87262
o4	112	ALA	-	expression tag	UNP P87262
o4	113	LYS	-	expression tag	UNP P87262
o4	114	SER	-	expression tag	UNP P87262
o4	115	GLU	-	expression tag	UNP P87262
o4	116	LYS	-	expression tag	UNP P87262
o4	117	LYS	-	expression tag	UNP P87262
o4	118	ALA	-	expression tag	UNP P87262
o4	119	LYS	-	expression tag	UNP P87262
o4	120	LYS	-	expression tag	UNP P87262

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e0	62	VAL	-	expression tag	UNP P0CX33
e0	63	GLN	-	expression tag	UNP P0CX33

- Molecule 81 is a protein called Unknown Protein m2.

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

- Molecule 82 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 83 is a protein called Unknown Protein p1.

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

- Molecule 84 is a protein called Unknown Protein p2.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	2	125	Total	Mg	0	0
			125	125		
85	S8	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	D0	1	Total 1	Mg 1	0	0
85	D3	1	Total 1	Mg 1	0	0
85	SM	1	Total 1	Mg 1	0	0
85	1	469	Total 469	Mg 469	0	0
85	3	14	Total 14	Mg 14	0	0
85	4	22	Total 22	Mg 22	0	0
85	L2	3	Total 3	Mg 3	0	0
85	L3	2	Total 2	Mg 2	0	0
85	L4	2	Total 2	Mg 2	0	0
85	L5	1	Total 1	Mg 1	0	0
85	L7	3	Total 3	Mg 3	0	0
85	L8	1	Total 1	Mg 1	0	0
85	M0	2	Total 2	Mg 2	0	0
85	M1	1	Total 1	Mg 1	0	0
85	M3	3	Total 3	Mg 3	0	0
85	M4	1	Total 1	Mg 1	0	0
85	M5	3	Total 3	Mg 3	0	0
85	M6	1	Total 1	Mg 1	0	0
85	M7	3	Total 3	Mg 3	0	0
85	M8	1	Total 1	Mg 1	0	0
85	M9	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	N0	1	Total 1	Mg 1	0	0
85	N3	3	Total 3	Mg 3	0	0
85	N5	1	Total 1	Mg 1	0	0
85	N6	1	Total 1	Mg 1	0	0
85	N8	5	Total 5	Mg 5	0	0
85	N9	1	Total 1	Mg 1	0	0
85	O1	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	O7	2	Total 2	Mg 2	0	0
85	6	150	Total 150	Mg 150	0	0
85	s1	1	Total 1	Mg 1	0	0
85	s8	2	Total 2	Mg 2	0	0
85	c7	2	Total 2	Mg 2	0	0
85	c8	2	Total 2	Mg 2	0	0
85	d3	2	Total 2	Mg 2	0	0
85	d6	1	Total 1	Mg 1	0	0
85	sM	2	Total 2	Mg 2	0	0
85	5	502	Total 502	Mg 502	0	0
85	7	17	Total 17	Mg 17	0	0
85	8	15	Total 15	Mg 15	0	0

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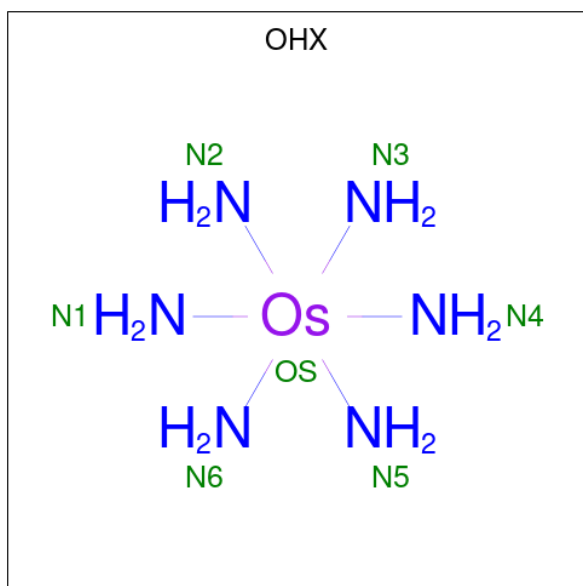
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	l2	3	Total 3	Mg 3	0	0
85	l3	2	Total 2	Mg 2	0	0
85	l4	1	Total 1	Mg 1	0	0
85	l5	1	Total 1	Mg 1	0	0
85	l7	1	Total 1	Mg 1	0	0
85	l8	1	Total 1	Mg 1	0	0
85	l9	1	Total 1	Mg 1	0	0
85	m0	1	Total 1	Mg 1	0	0
85	m1	2	Total 2	Mg 2	0	0
85	m5	4	Total 4	Mg 4	0	0
85	m6	1	Total 1	Mg 1	0	0
85	m7	5	Total 5	Mg 5	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	5	Total 5	Mg 5	0	0
85	n9	1	Total 1	Mg 1	0	0
85	o1	1	Total 1	Mg 1	0	0
85	o3	1	Total 1	Mg 1	0	0
85	o4	2	Total 2	Mg 2	0	0
85	q0	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		

- 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	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
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	S8	1	Total 7	N 6	Os 1	0	0
86	S9	1	Total 7	N 6	Os 1	0	0
86	C1	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
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
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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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
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
			7	6	1		
86	1	1	Total	N	Os	0	0
			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
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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
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	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	L3	1	Total 7	N 6	Os 1	0	0
86	L4	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	M6	1	Total 7	N 6	Os 1	0	0
86	M7	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	N9	1	Total 7	N 6	Os 1	0	0
86	O2	1	Total 7	N 6	Os 1	0	0
86	O3	1	Total 7	N 6	Os 1	0	0
86	O7	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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	m9	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n6	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	q1	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).

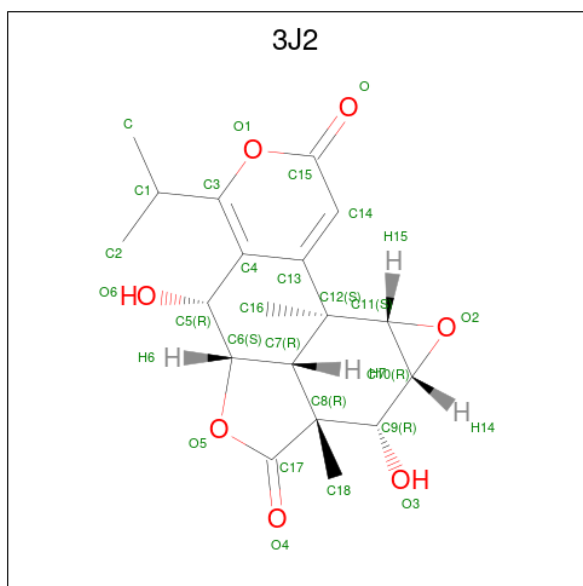
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	D6	1	Total	Zn	0	0
			1	1		
87	D7	1	Total	Zn	0	0
			1	1		
87	D9	1	Total	Zn	0	0
			1	1		
87	E1	1	Total	Zn	0	0
			1	1		
87	O7	1	Total	Zn	0	0
			1	1		
87	Q0	1	Total	Zn	0	0
			1	1		
87	Q2	1	Total	Zn	0	0
			1	1		
87	Q3	1	Total	Zn	0	0
			1	1		
87	d6	1	Total	Zn	0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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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		

- Molecule 88 is Nagilactone C (CCD ID: 3J2) (formula: C₁₉H₂₂O₇).

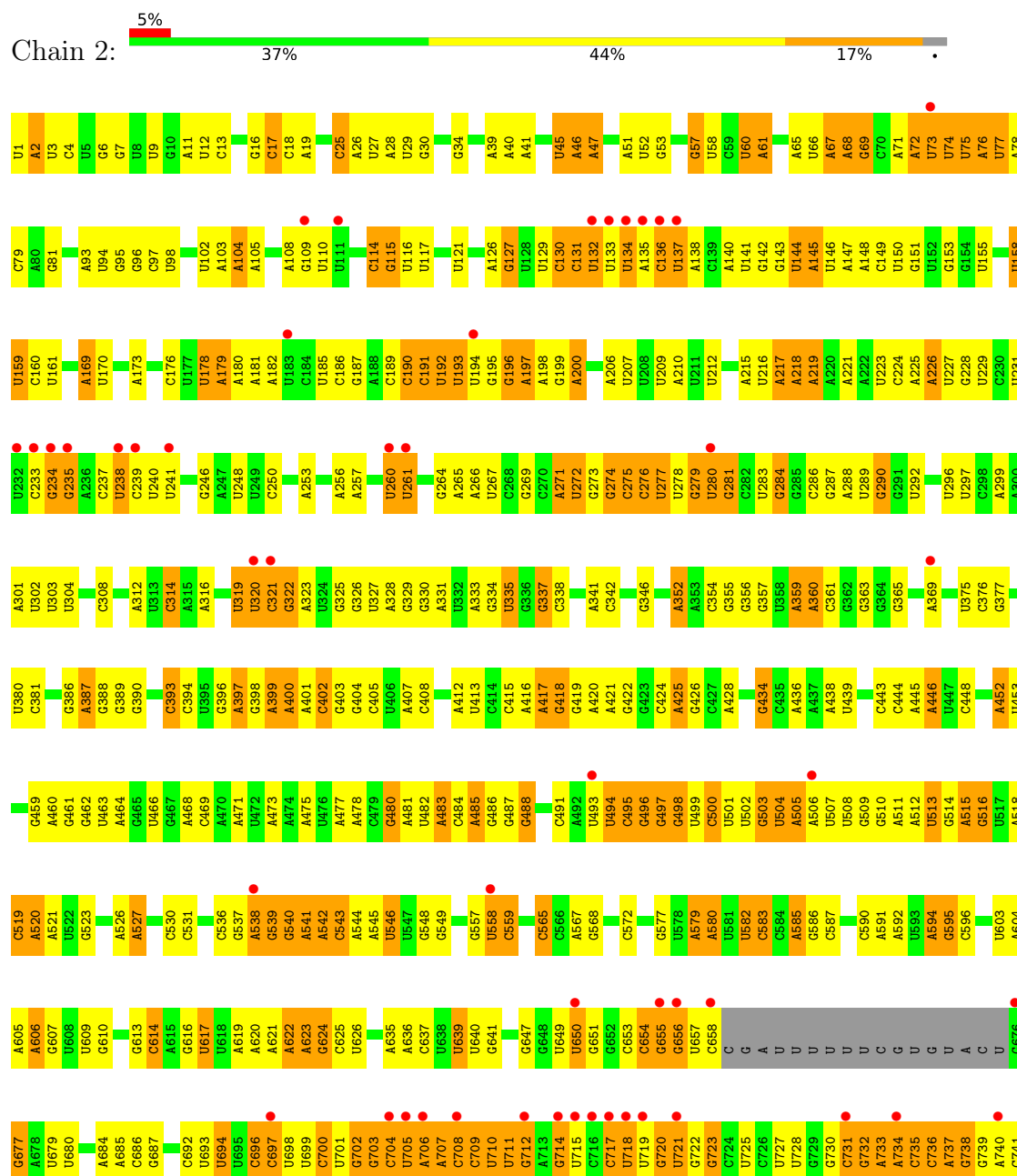


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	1	1	Total	C O	0	0
			26 19 7			
88	5	1	Total	C O	0	0
			26 19 7			

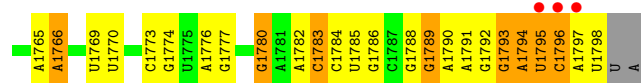
3 Residue-property plots

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.

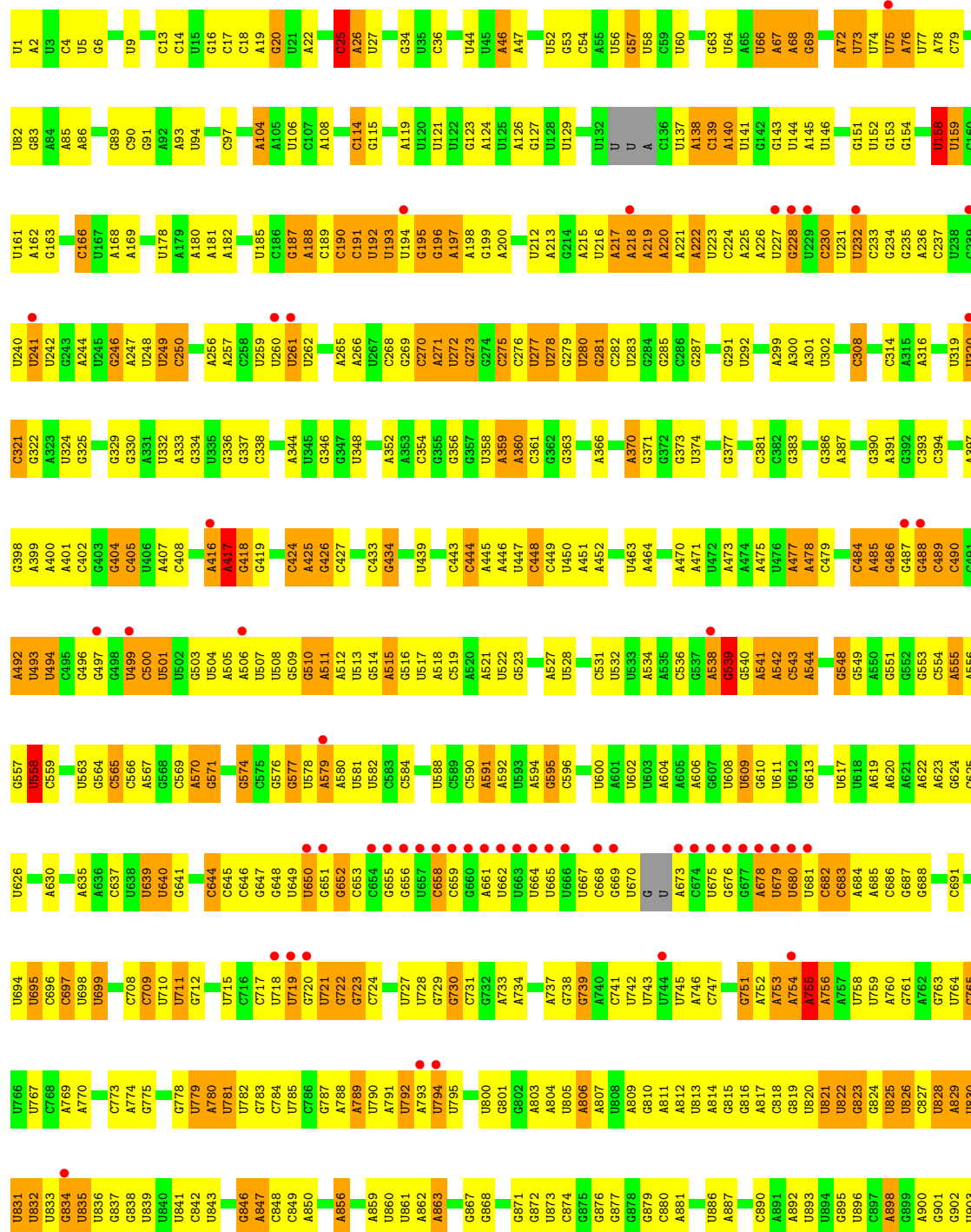
• Molecule 1: 18S ribosomal RNA

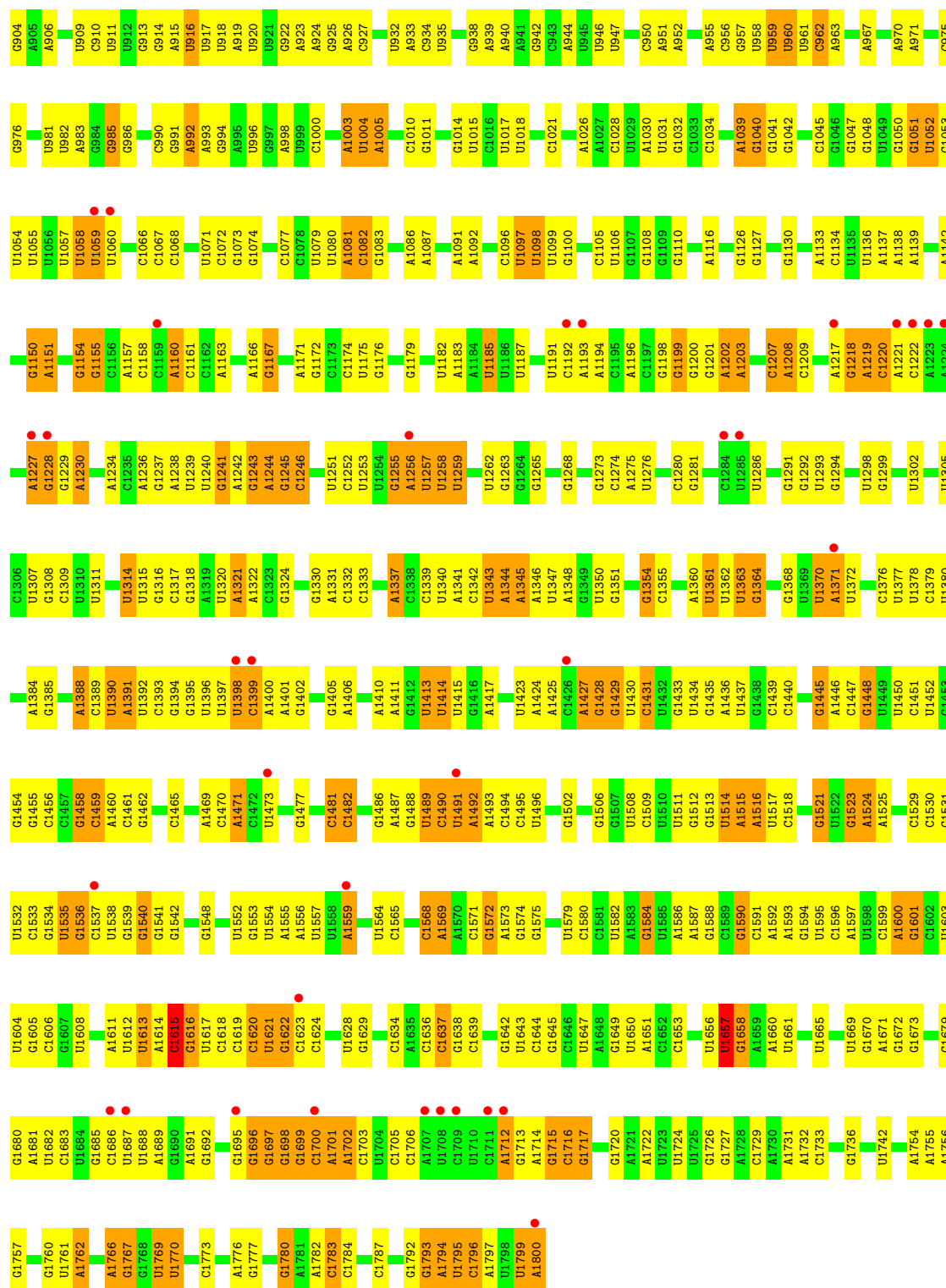






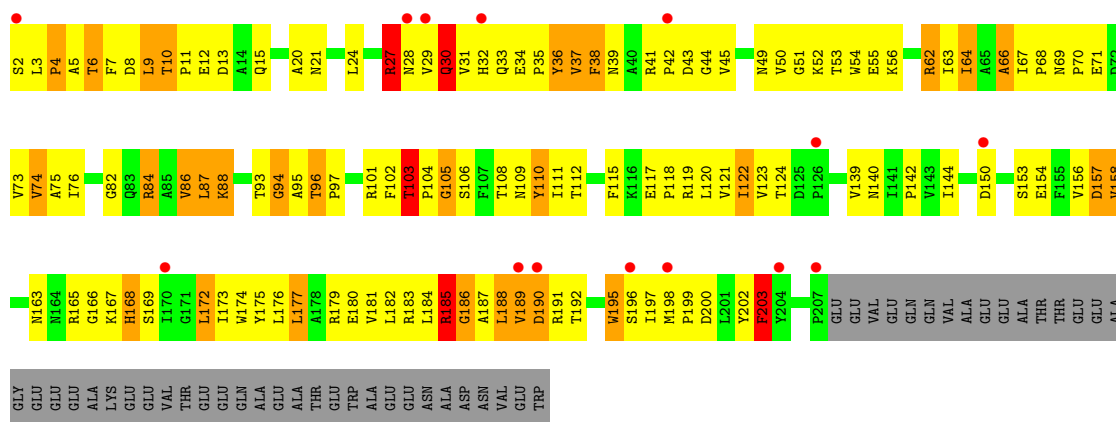
● Molecule 1: 18S ribosomal RNA



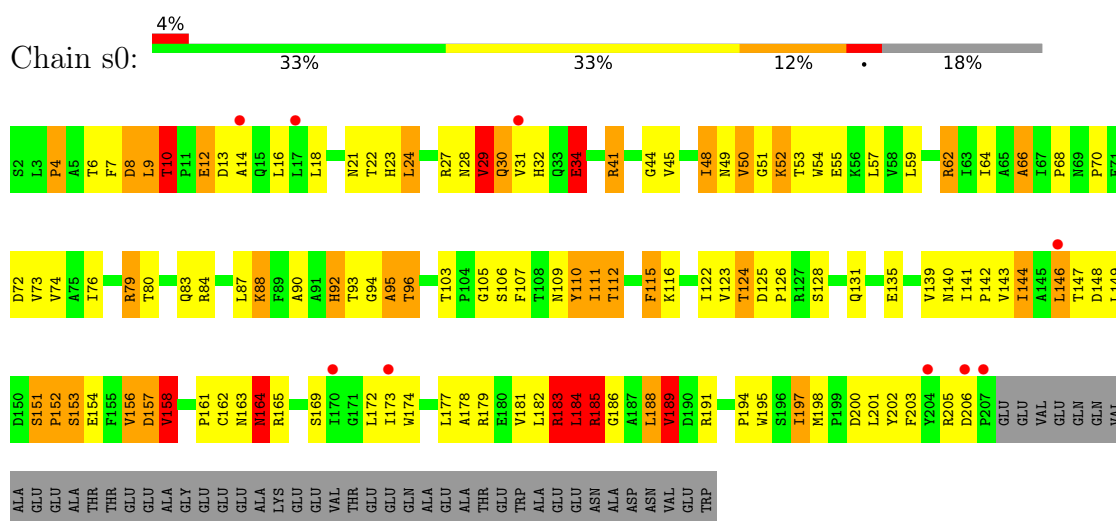


• Molecule 2: 40S ribosomal protein S0-A

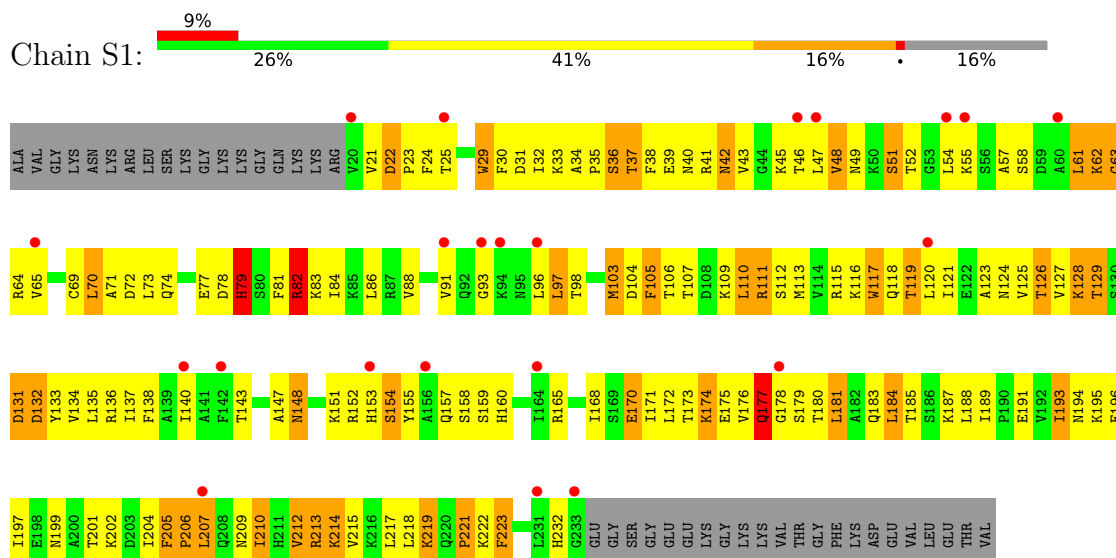




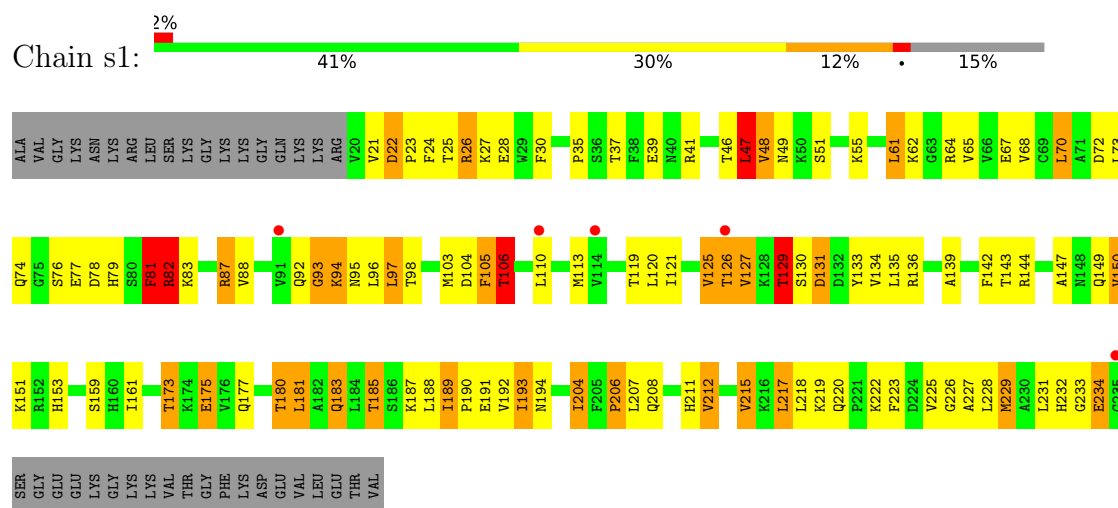
• Molecule 2: 40S ribosomal protein S0-A



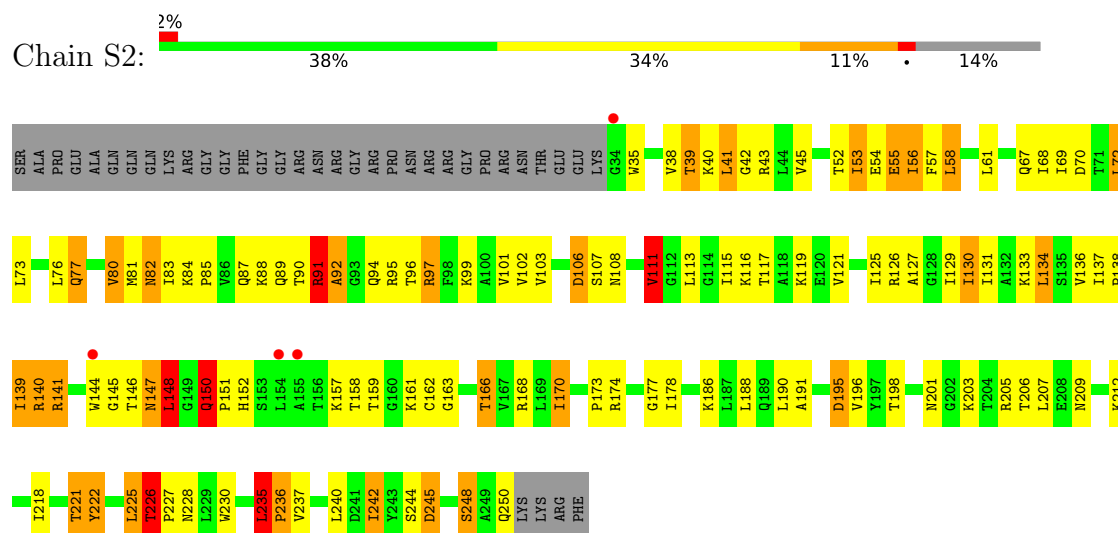
• Molecule 3: 40S ribosomal protein S1-A



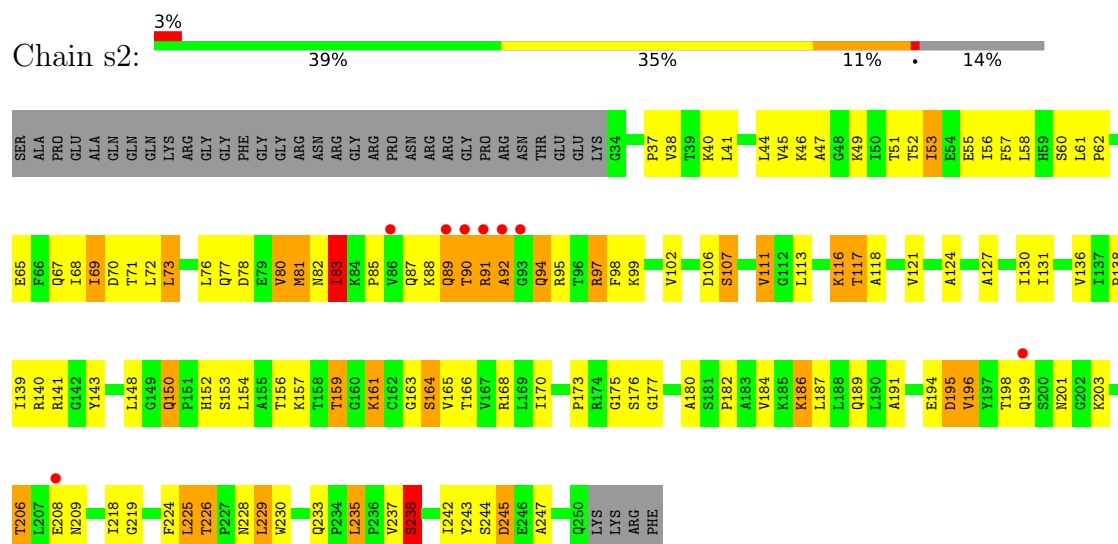
• Molecule 3: 40S ribosomal protein S1-A



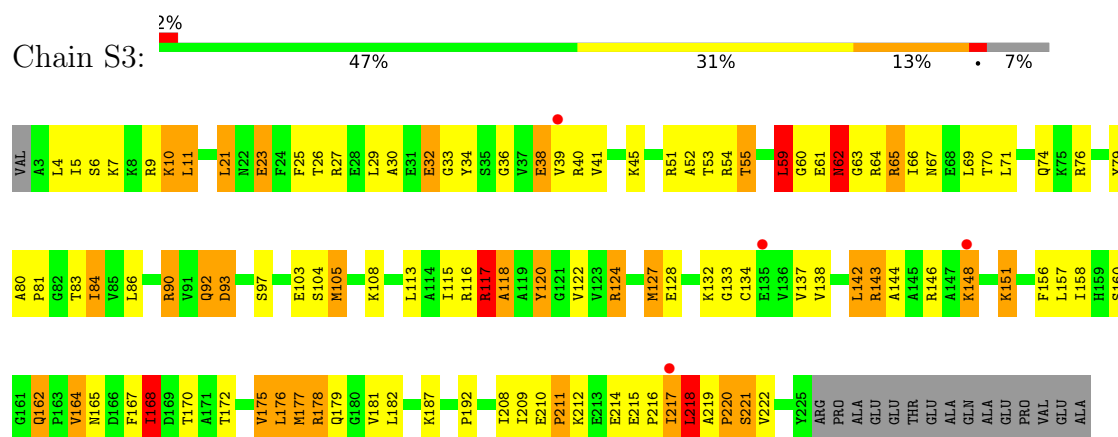
- Molecule 4: 40S ribosomal protein S2



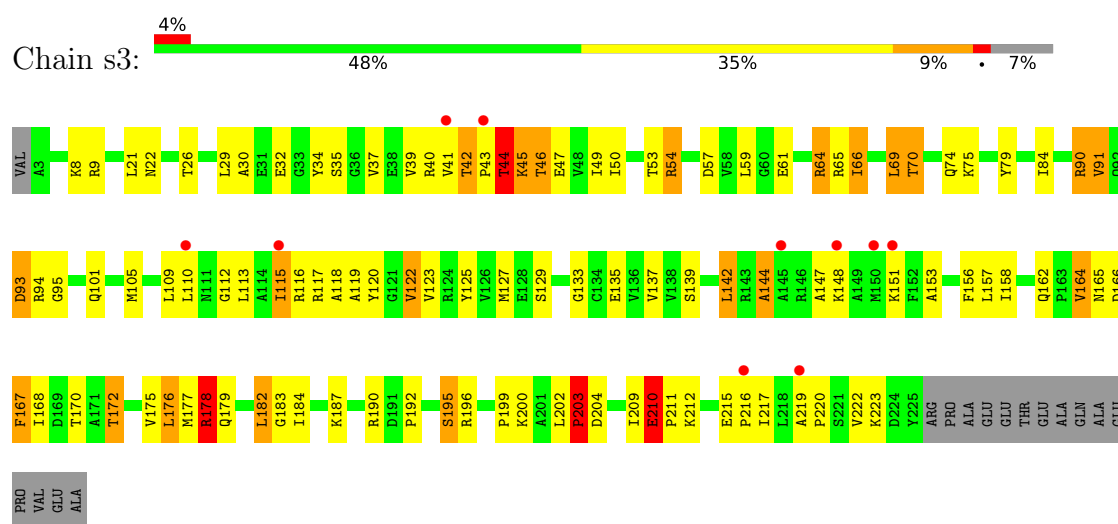
- Molecule 4: 40S ribosomal protein S2



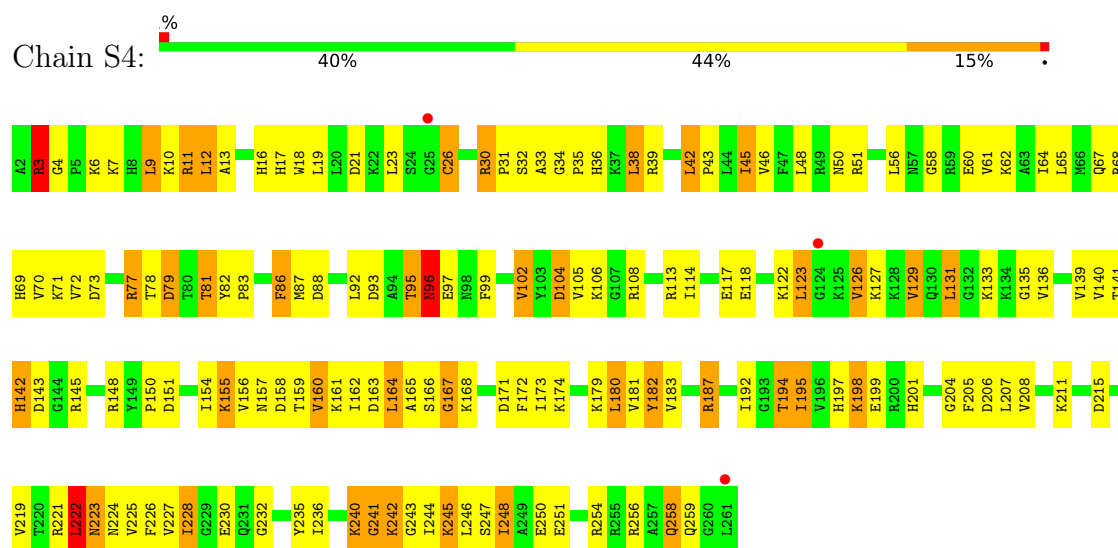
- Molecule 5: 40S ribosomal protein S3



• Molecule 5: 40S ribosomal protein S3

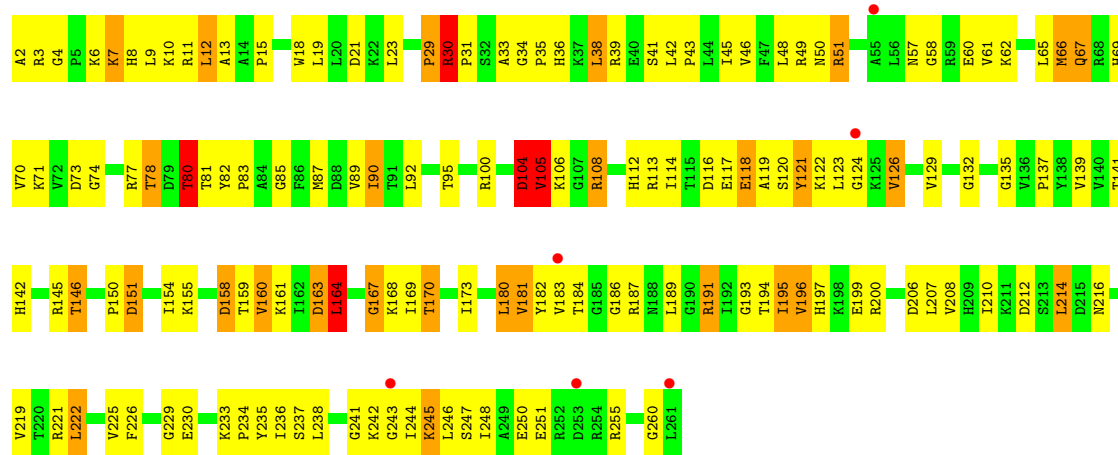


• Molecule 6: 40S ribosomal protein S4-A

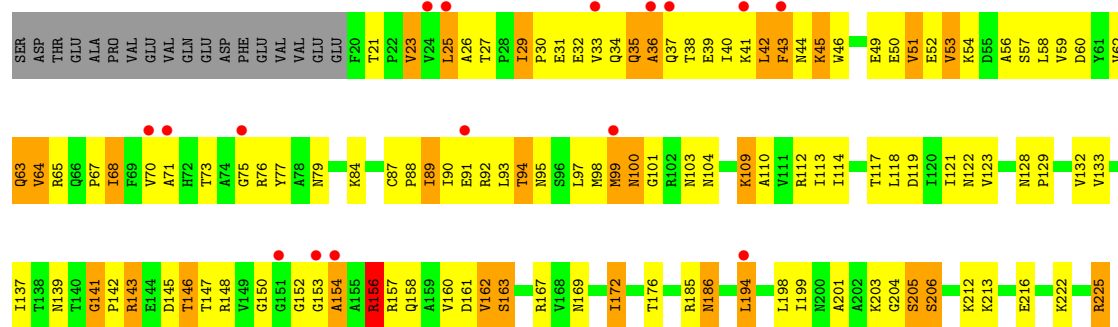


• Molecule 6: 40S ribosomal protein S4-A

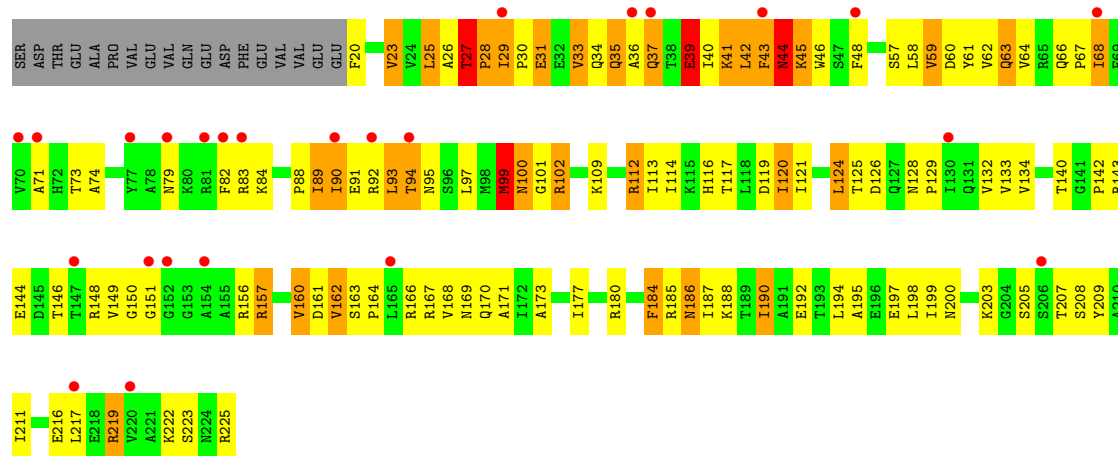




• Molecule 7: 40S ribosomal protein S5

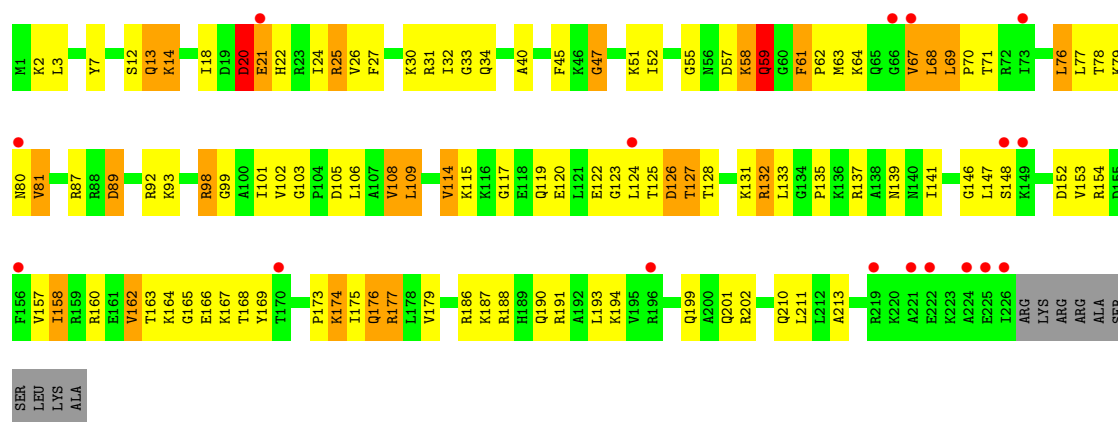


• Molecule 7: 40S ribosomal protein S5

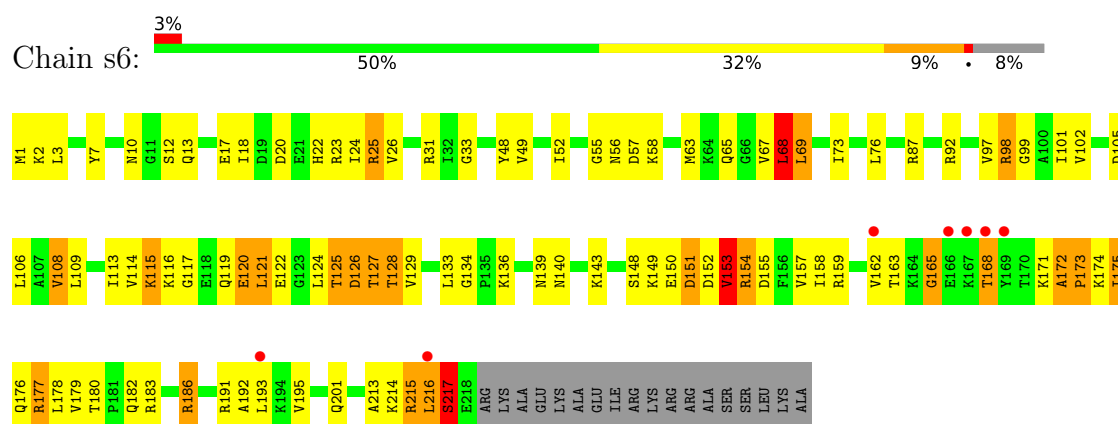


• Molecule 8: 40S ribosomal protein S6-A

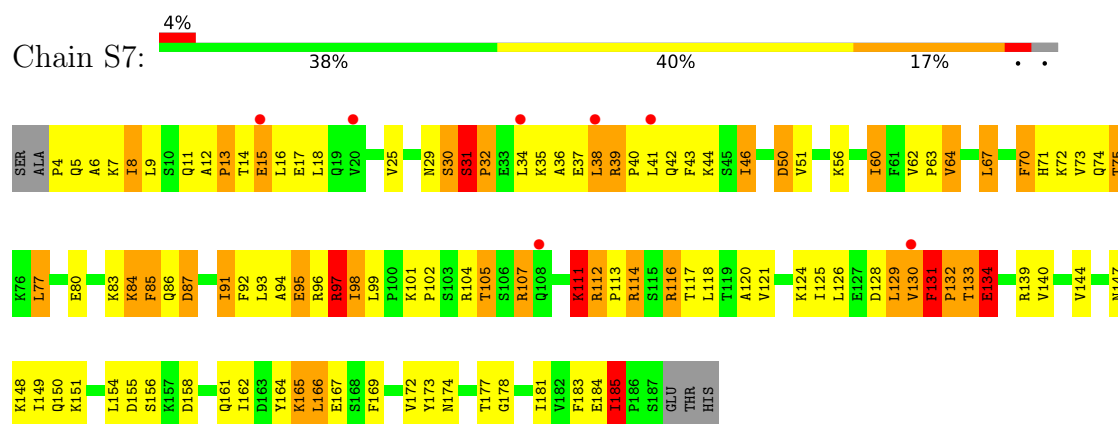




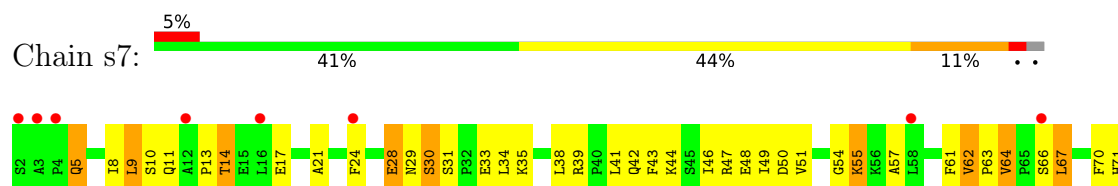
• Molecule 8: 40S ribosomal protein S6-A

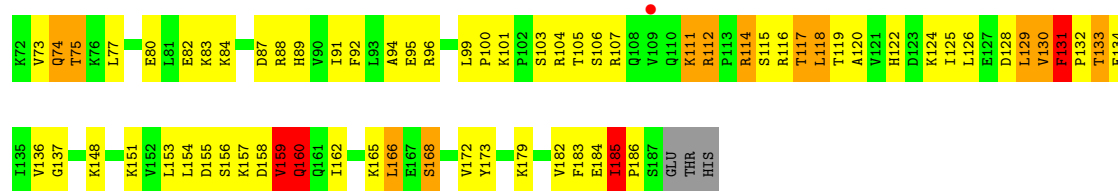


• Molecule 9: 40S ribosomal protein S7-A

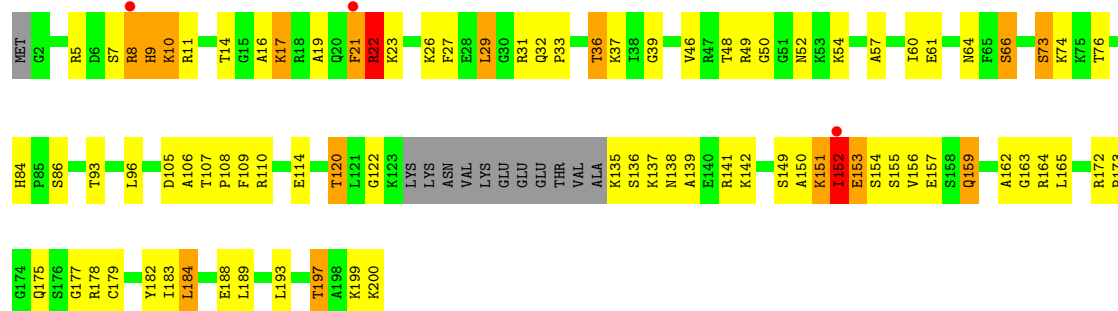


• Molecule 9: 40S ribosomal protein S7-A

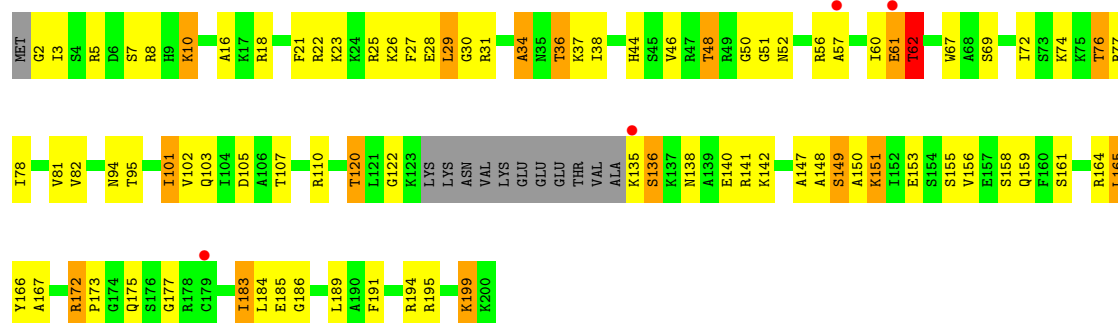




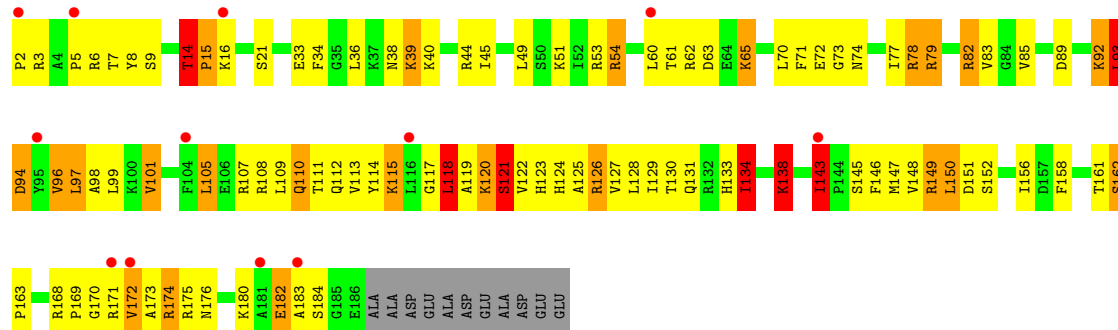
• Molecule 10: 40S ribosomal protein S8-A



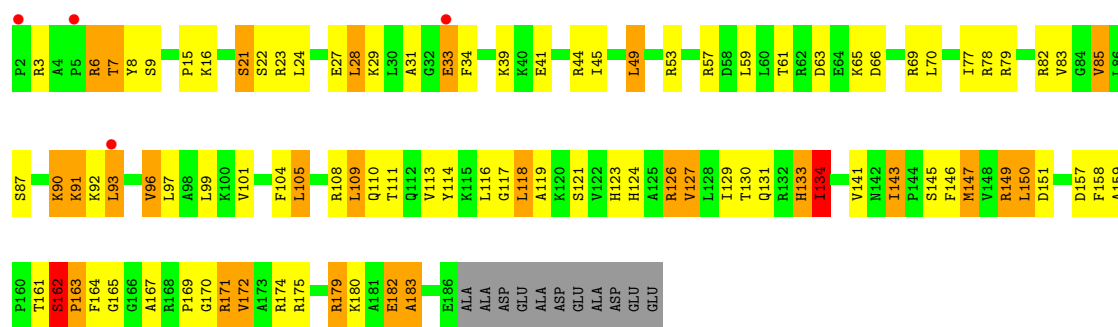
• Molecule 10: 40S ribosomal protein S8-A



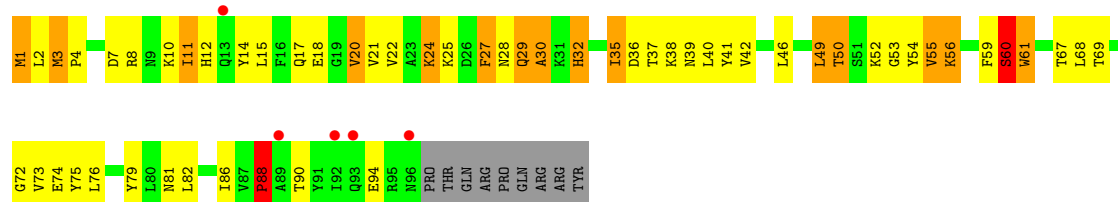
• Molecule 11: 40S ribosomal protein S9-A



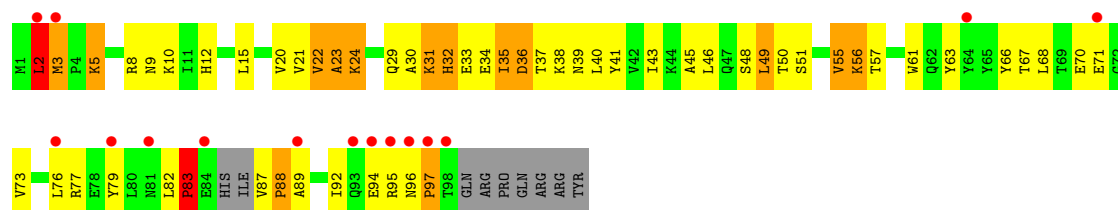
• Molecule 11: 40S ribosomal protein S9-A



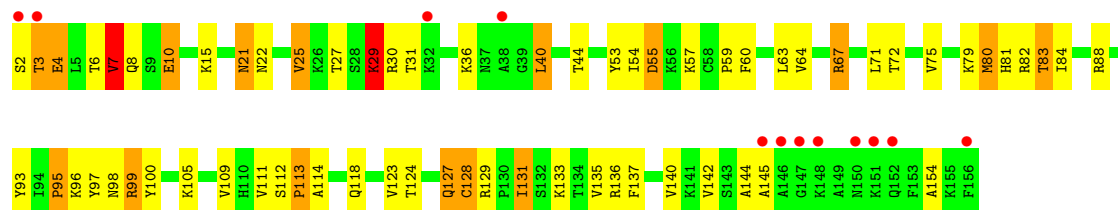
• Molecule 12: 40S ribosomal protein S10-A



• Molecule 12: 40S ribosomal protein S10-A

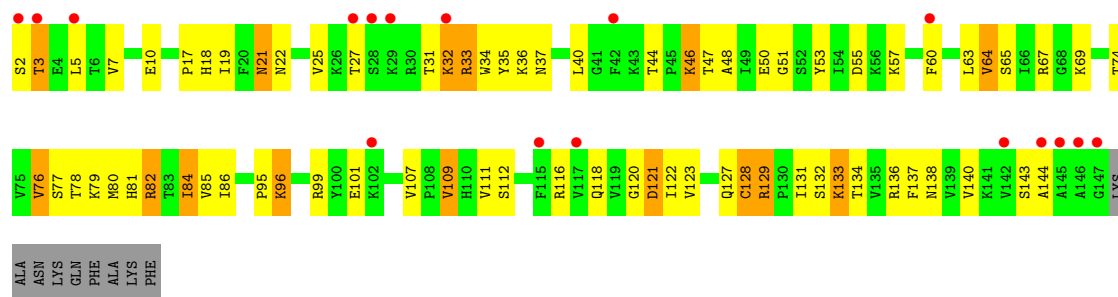


• Molecule 13: 40S ribosomal protein S11-A

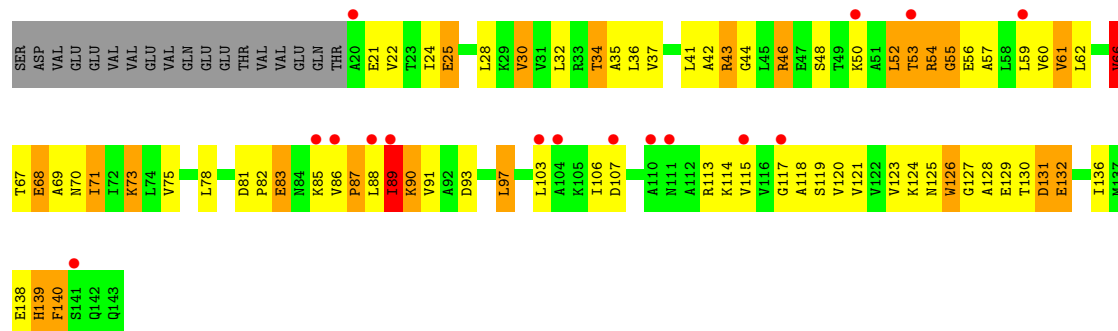


• Molecule 13: 40S ribosomal protein S11-A

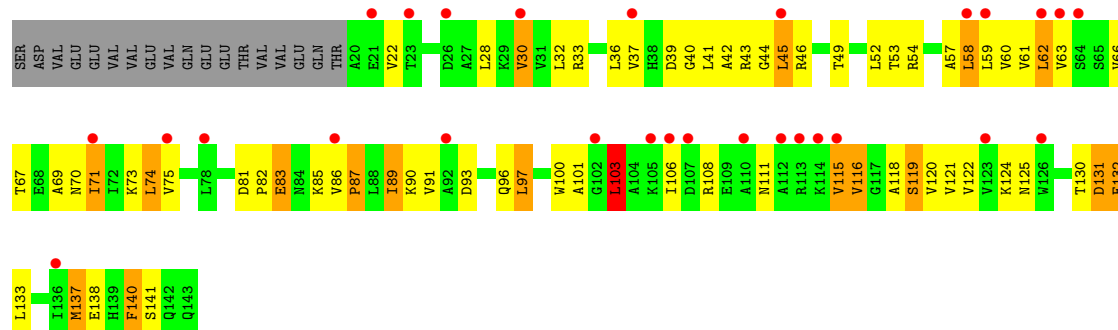




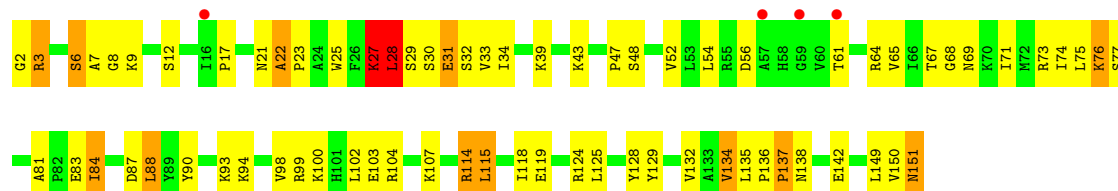
• Molecule 14: 40S ribosomal protein S12



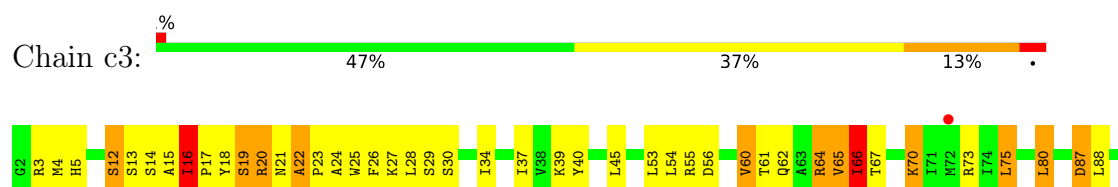
• Molecule 14: 40S ribosomal protein S12



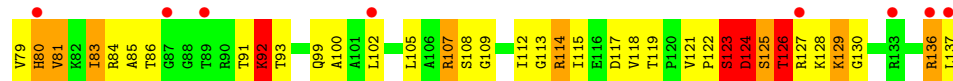
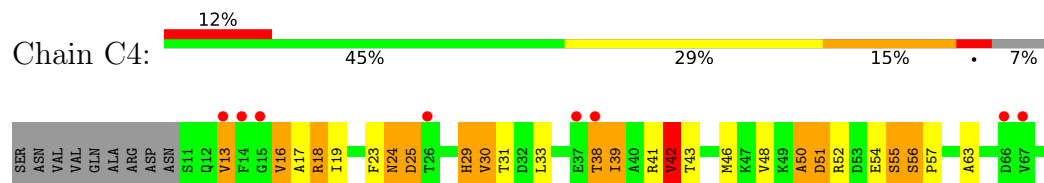
• Molecule 15: 40S ribosomal protein S13



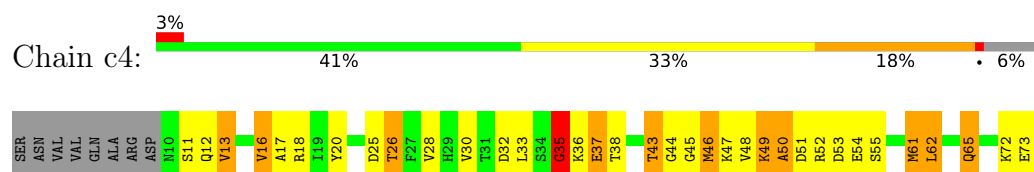
• Molecule 15: 40S ribosomal protein S13



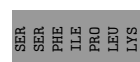
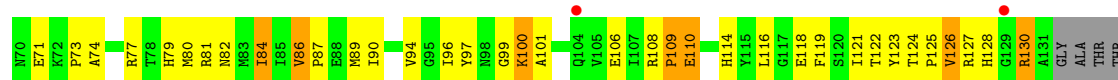
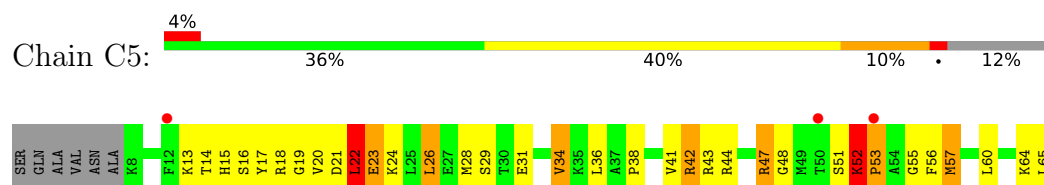
• Molecule 16: 40S ribosomal protein S14-A



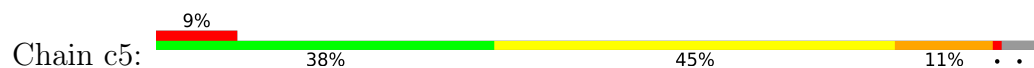
• Molecule 16: 40S ribosomal protein S14-A

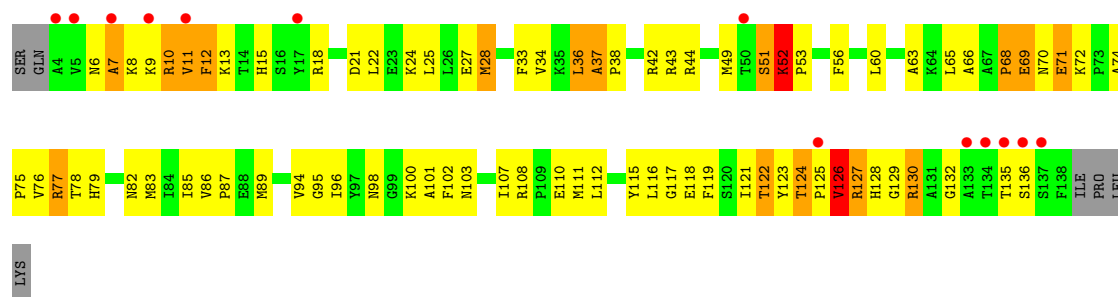


• Molecule 17: 40S ribosomal protein S15



• Molecule 17: 40S ribosomal protein S15





- Molecule 18: 40S ribosomal protein S16-A



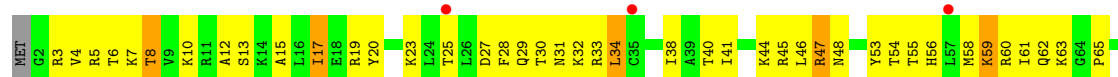
- Molecule 18: 40S ribosomal protein S16-A

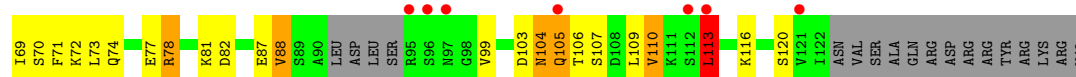


- Molecule 19: 40S ribosomal protein S17-A

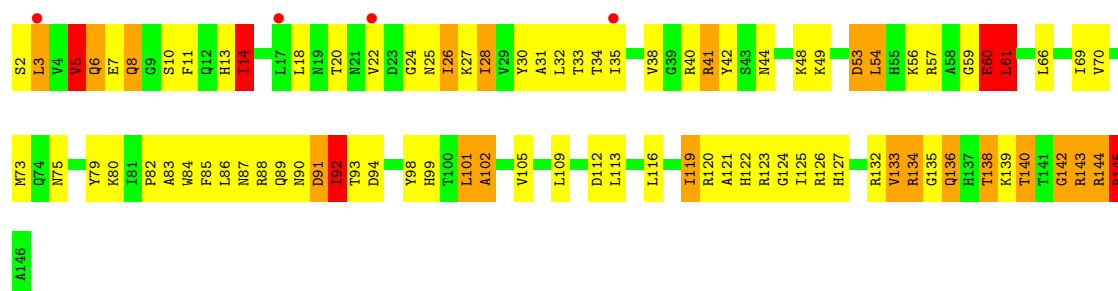


- Molecule 19: 40S ribosomal protein S17-A

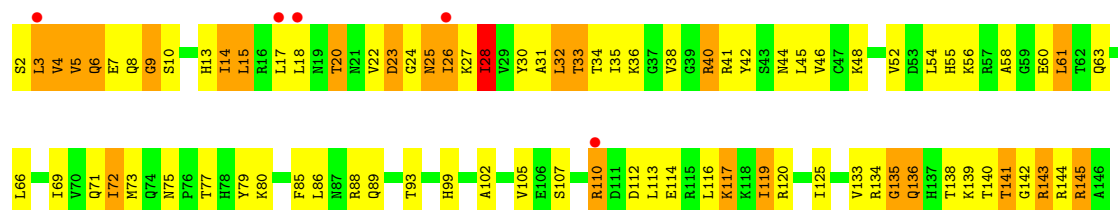




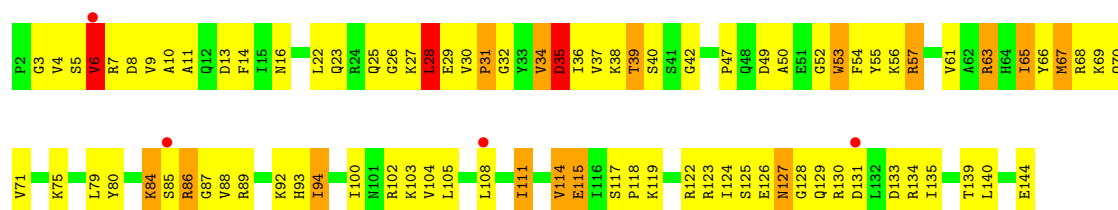
• Molecule 20: 40S ribosomal protein S18-A



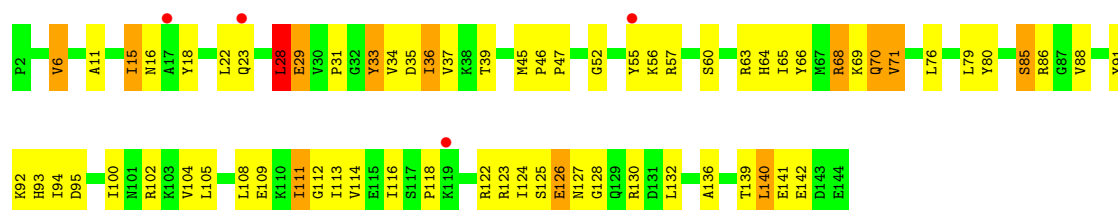
• Molecule 20: 40S ribosomal protein S18-A



• Molecule 21: 40S ribosomal protein S19-A



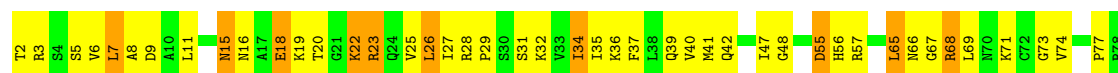
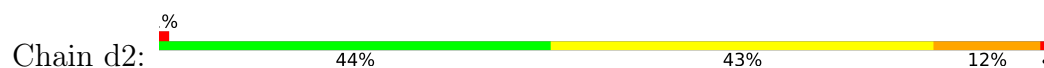
• Molecule 21: 40S ribosomal protein S19-A



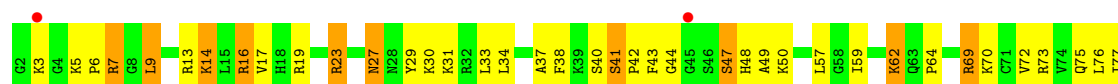
• Molecule 22: 40S ribosomal protein S20



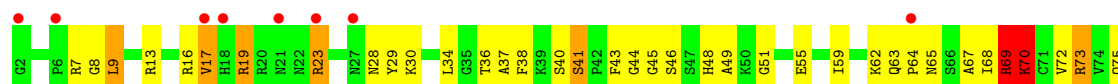
- Molecule 24: 40S ribosomal protein S22-A



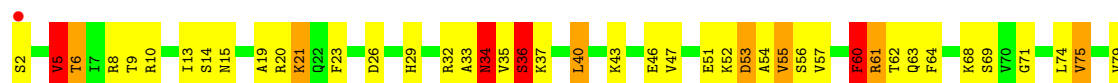
- Molecule 25: 40S ribosomal protein S23-A



- Molecule 26: 40S ribosomal protein S24-A

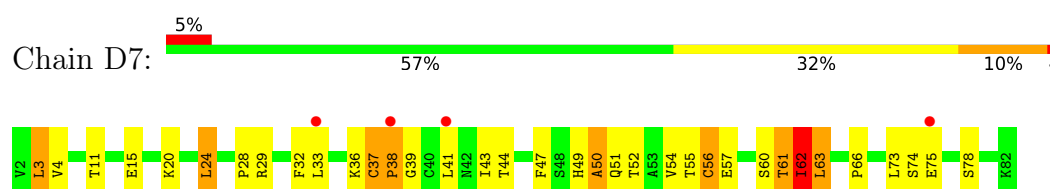


- Molecule 27: 40S ribosomal protein S25-A

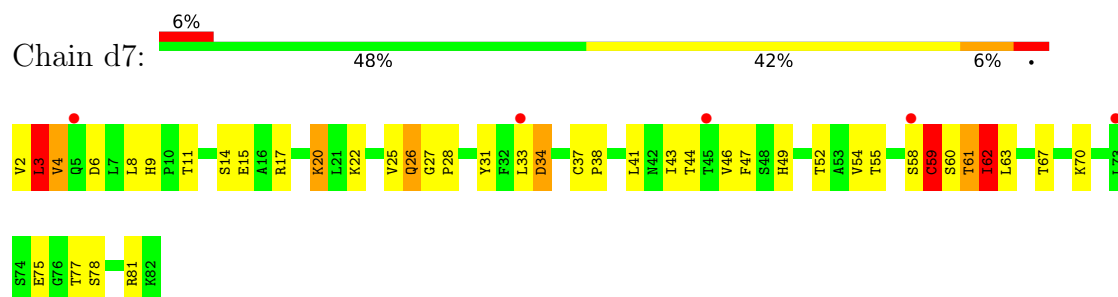


- Molecule 28: 40S ribosomal protein S26-A

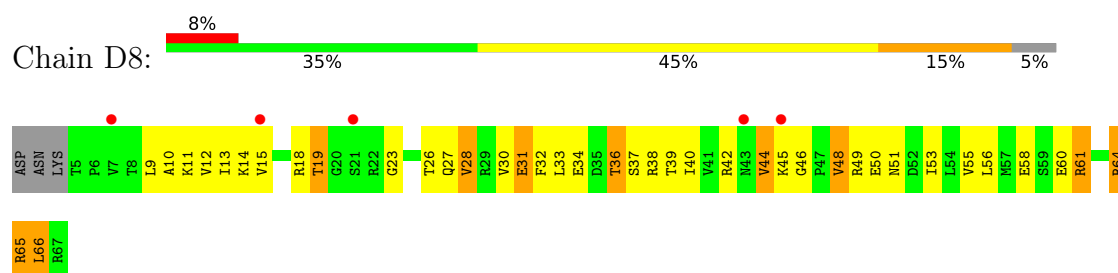




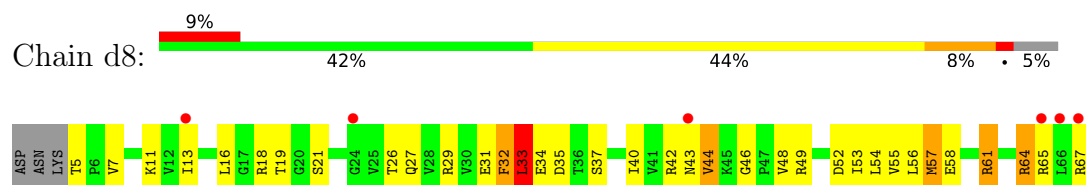
- Molecule 29: 40S ribosomal protein S27-A



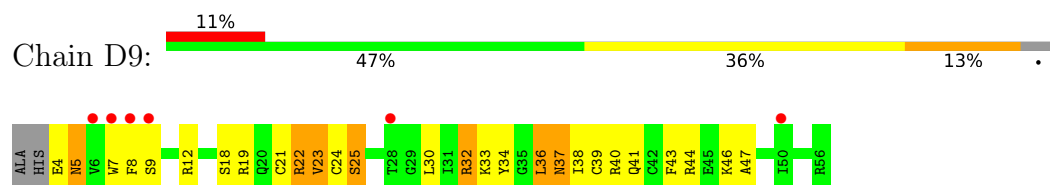
- Molecule 30: 40S ribosomal protein S28-A



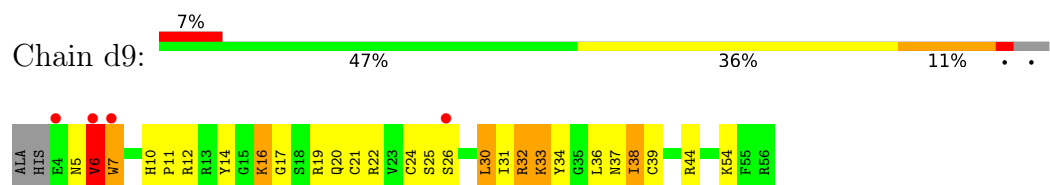
- Molecule 30: 40S ribosomal protein S28-A



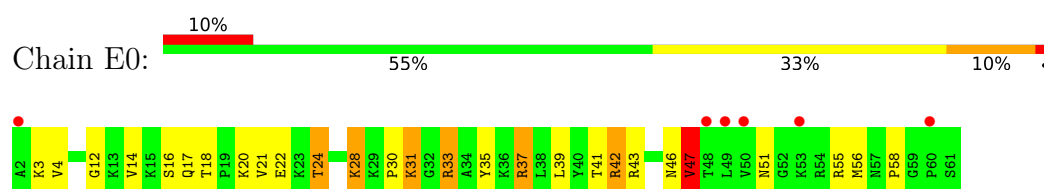
- Molecule 31: 40S ribosomal protein S29-A



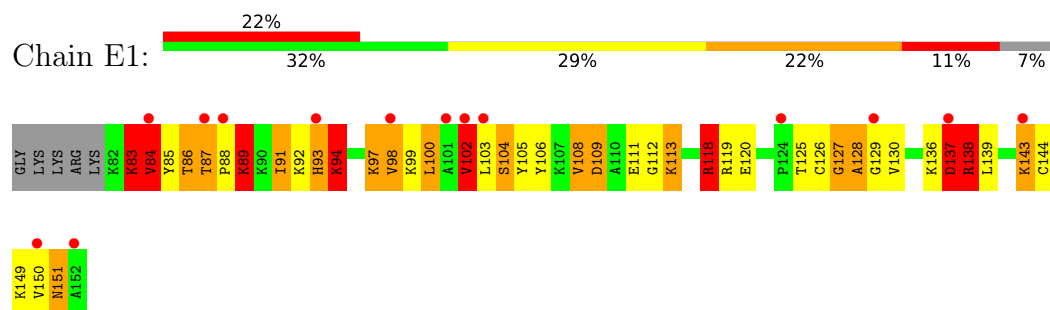
- Molecule 31: 40S ribosomal protein S29-A



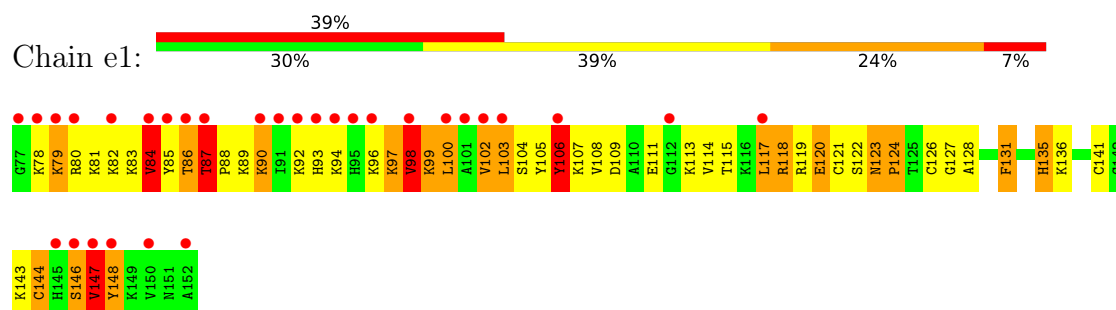
- Molecule 32: 40S ribosomal protein S30-A



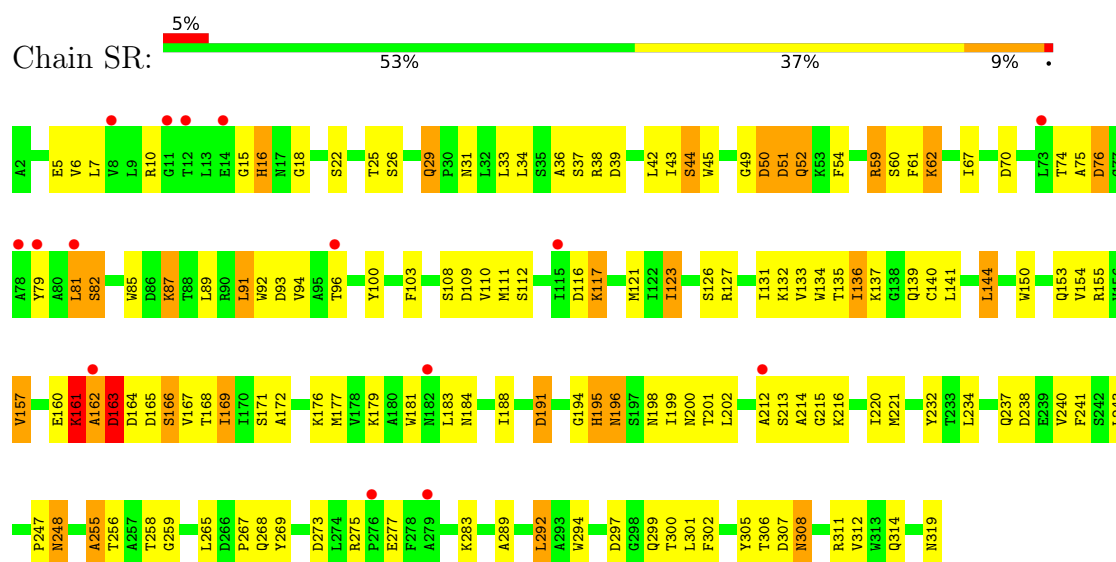
• Molecule 33: Ubiquitin-40S ribosomal protein S31



• Molecule 33: Ubiquitin-40S ribosomal protein S31

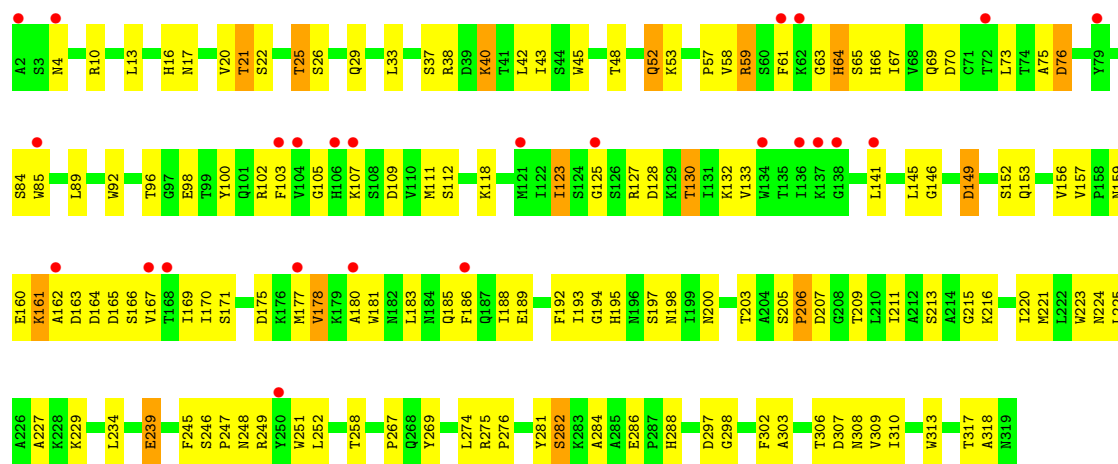


• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

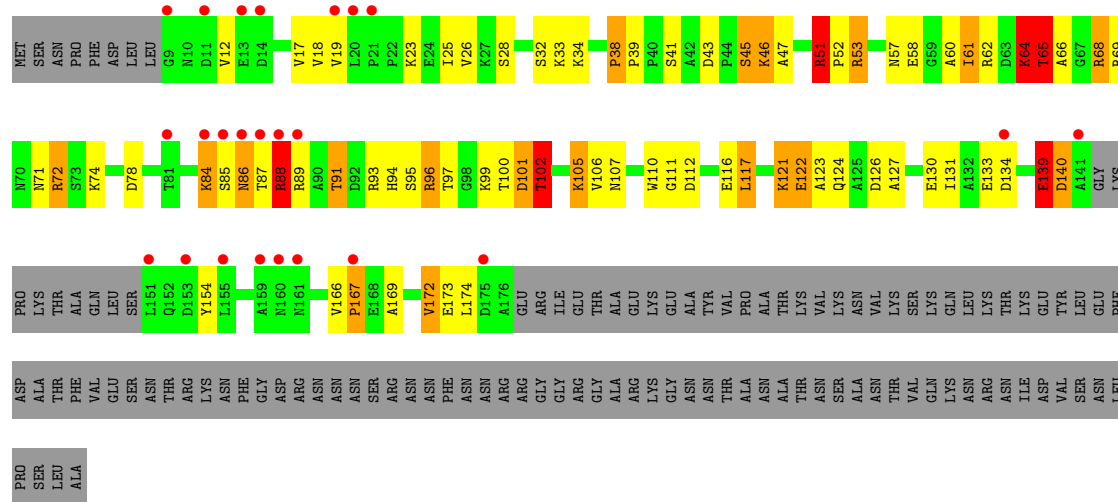
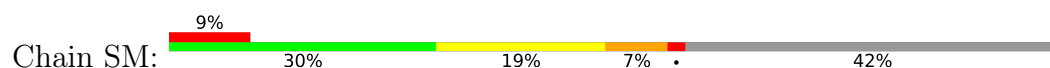


• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

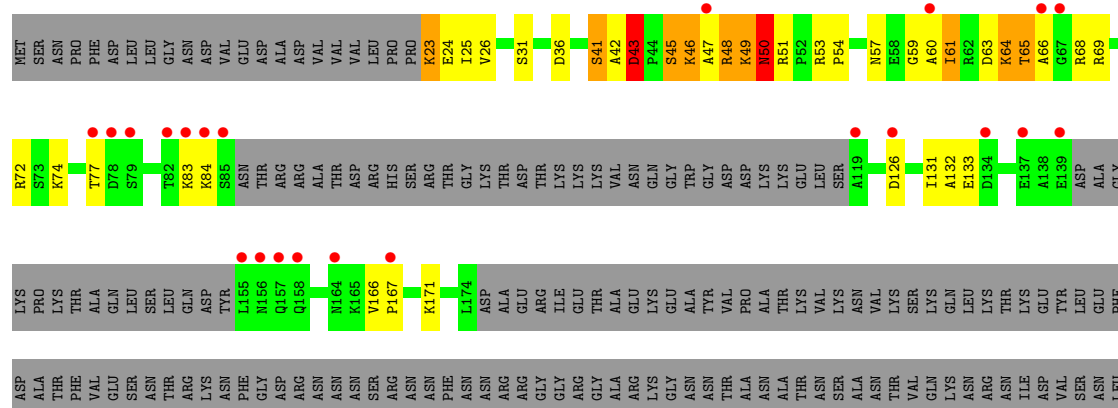




• Molecule 35: Suppressor protein STM1

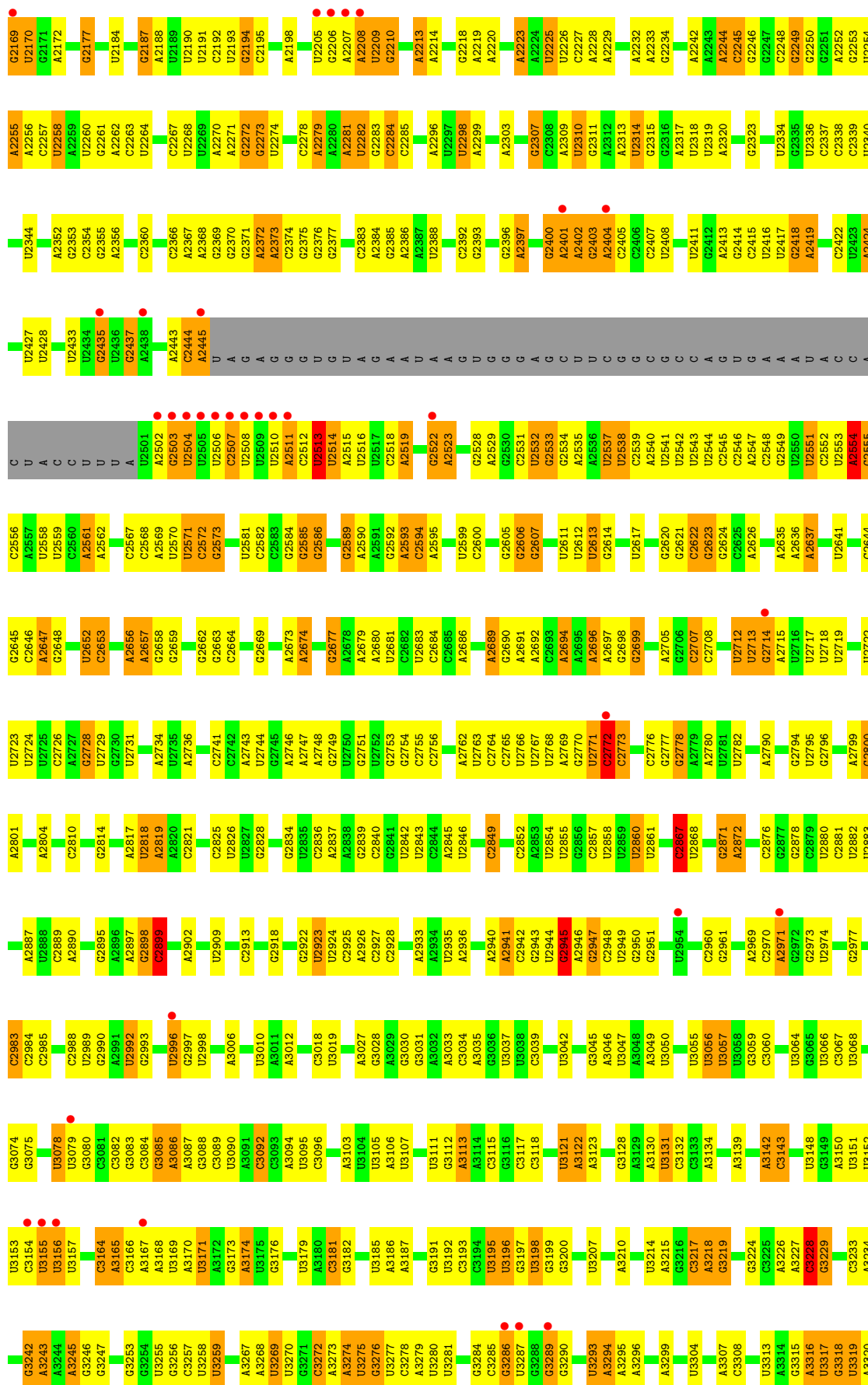


• Molecule 35: Suppressor protein STM1







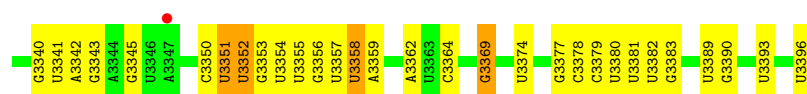


Chain 5:

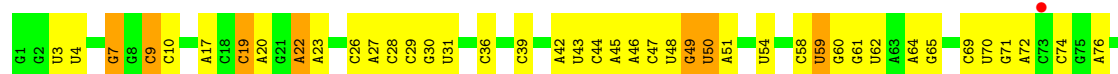
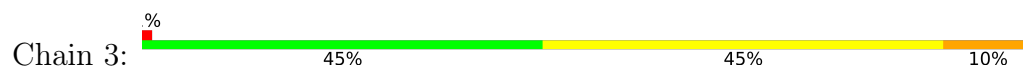




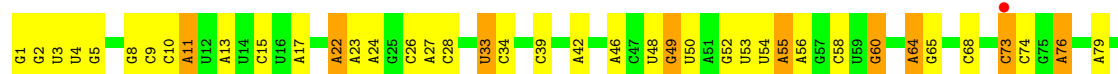
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G3263	G3112	G3112	G3028	C2942	A2947	G2754	G2663	C2572	A	G2442	U2205	G2272	U2206
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G3188	G3188	C3115	A3033	G2950	U2854	A2762	A2675	A2580	U2506	A	C2374	U2208	C2208
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C3194	C3194	U3121	U3038	U2953	U2859	U2767	U2681	G2586	U2509	G	C2385	A2280	C2212
U3195	U3195	A3122	C3039	U2954	U2860	U2768	U2682	U2587	A2510	A	G	U2282	A2213
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C3237	C3072	G2990	A3072	G2990	G2912	G2815	A2727	U2642	U2543	C	A2418	U2336	G2248
G3238	G3073	A2991	A3073	A2991	G2912	G2816	U2728	U2643	U2543	G	G2419	G2249	G2249
C3239	G3074	U2996	G3074	U2996	U2915	A2817	U2729	U2643	U2543	U	U2421	G2250	G2250
G3240	U3075	G2997	U3075	G2997	U2916	U2818	G2732	A2646	A2547	G	C2422	G2251	G2251
G3241	U3076	U2998	U3076	U2998	U2916	U2819	A2733	C2648	C2546	A	U2423	A2341	A2252
G3242	C3084	C3001	C3084	C3001	U2923	C2821	A2734	C2644	C2549	A	A2424	C2350	U2254
A3243	G3085	A3006	A3086	A3006	U2924	U2822	A2736	C2644	C2552	U	G2425	U2351	A2255
A3244	A3086	A3006	A3086	A3006	C2925	U2823	A2736	C2644	U2553	A	U2426	A2352	A2256
A3245	C3089	A3012	C3089	A3012	C2926	U2824	A2739	U2648	A2554	C	U2428	G2353	C2257
G3246	U3090	U3013	U3090	U3013	C2927	U2825	U2740	U2648	C2555	C	G2429	G2354	U2258
G3247	C3091	U3014	C3091	U3014	C2928	U2826	C2741	U2652	C2556	A	A2429	C2355	U2259
U3252	G3092	A3174	A3092	A3174	U2932	A2837	G2745	C2653	C2557	C	C2430	G2356	G2261
G3253	C3093	U3175	C3093	U3175	U2933	A2838	A2746	C2654	A2562	U	C2431	A2357	A2262
A3254	A3094	G3177	A3094	G3177	U2934	U2839	A2747	U2655	U2563	C	A2432	A2358	G2263
G3255	U3095	C3018	U3095	C3018	U2935	C2840	A2748	A2657	A2564	A	U2433	C2359	U2264
G3256	C3097	G3022	C3097	G3022	A2936	U2843	A2749	G2658	C2566	C	G2434	U2360	U2265
U3259	C3097	A3180	C3097	A3180	G2937	U2844	G2751	G2660	C2567	U	U2436	A2363	G2267
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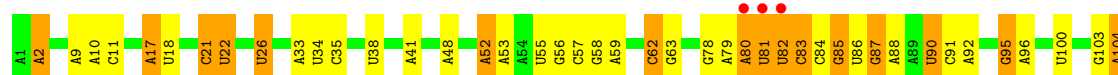
- Molecule 37: 5S ribosomal RNA



- Molecule 37: 5S ribosomal RNA



- Molecule 38: 5.8S ribosomal RNA

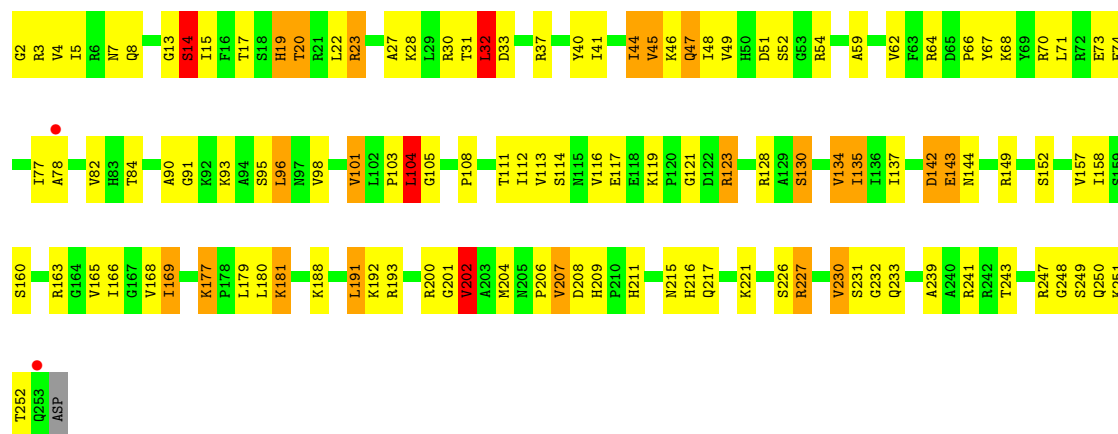


- Molecule 38: 5.8S ribosomal RNA

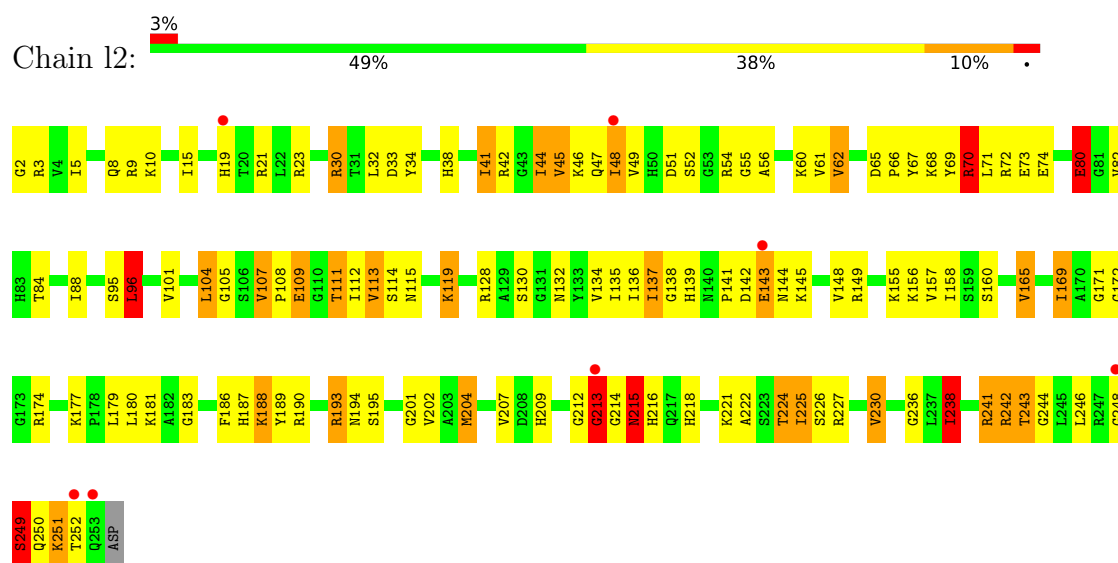


- Molecule 39: 60S ribosomal protein L2-A

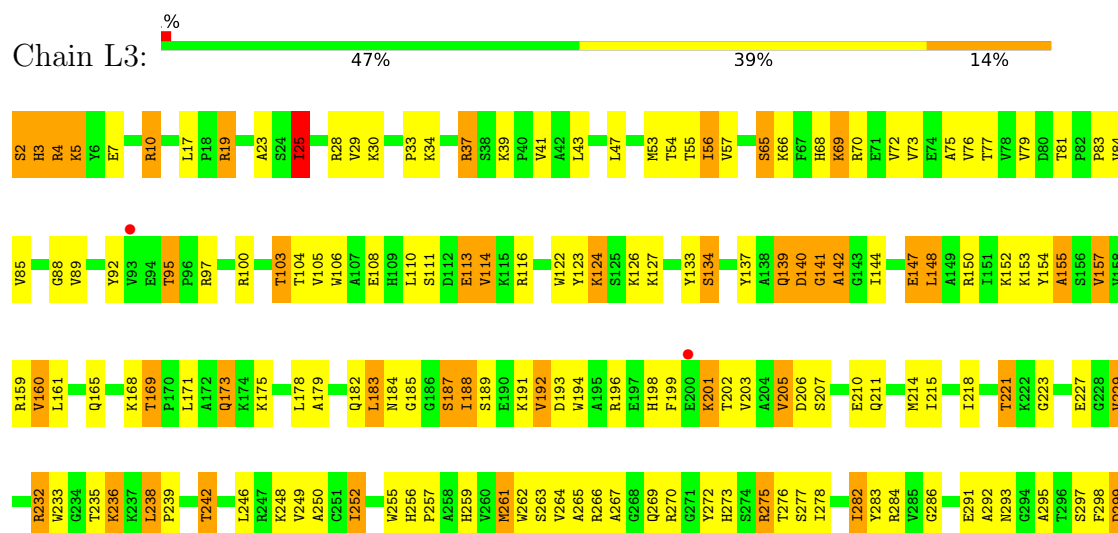


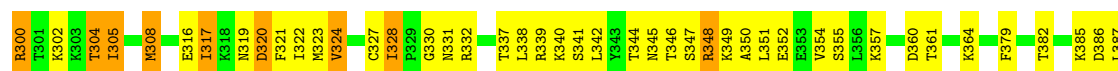


• Molecule 39: 60S ribosomal protein L2-A



• Molecule 40: 60S ribosomal protein L3

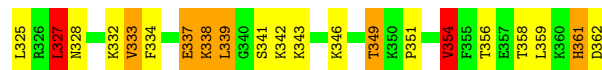
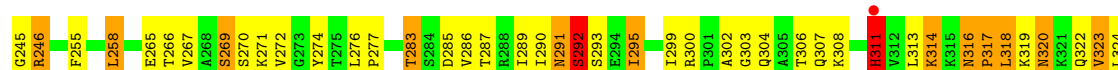
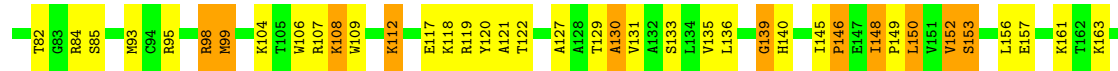
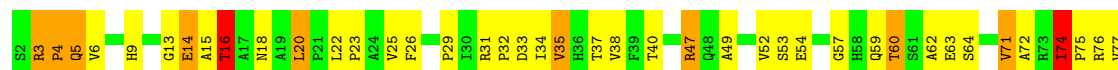




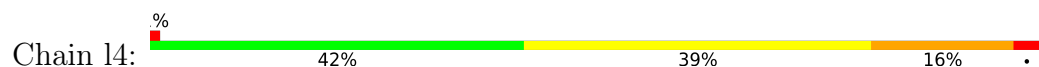
• Molecule 40: 60S ribosomal protein L3

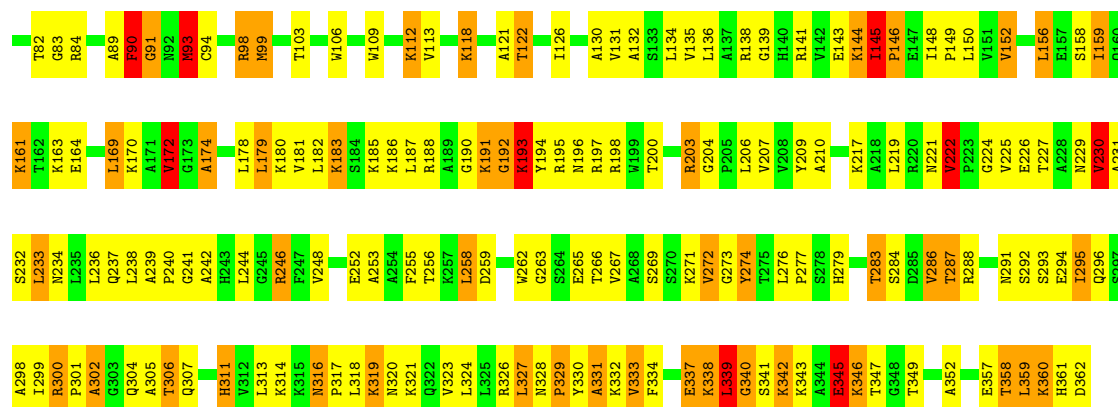


• Molecule 41: 60S ribosomal protein L4-A

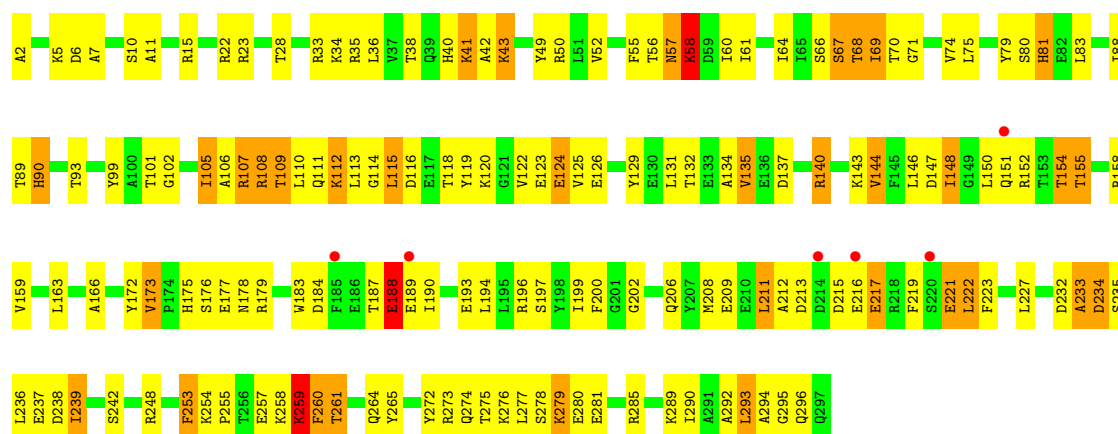


• Molecule 41: 60S ribosomal protein L4-A

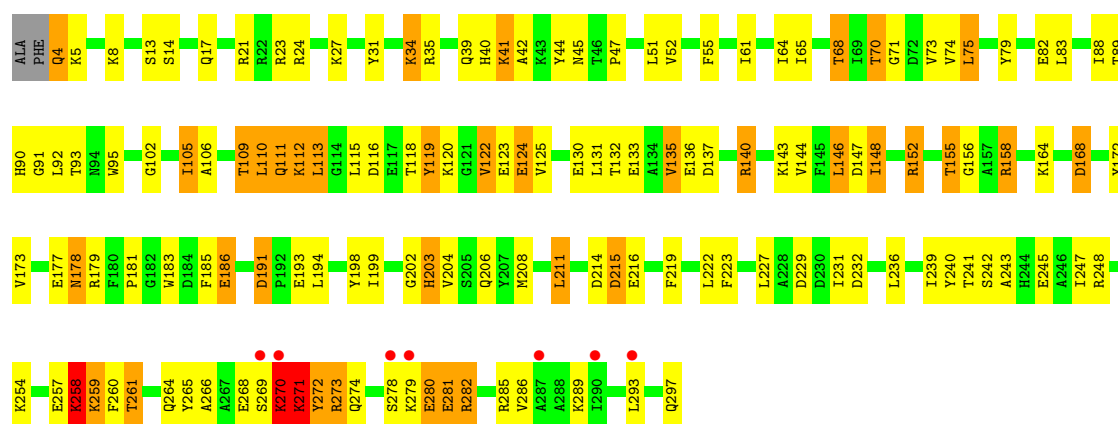




• Molecule 42: 60S ribosomal protein L5

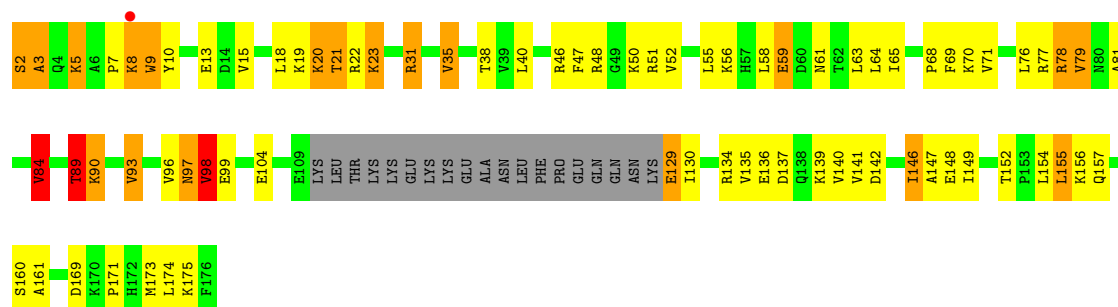


• Molecule 42: 60S ribosomal protein L5

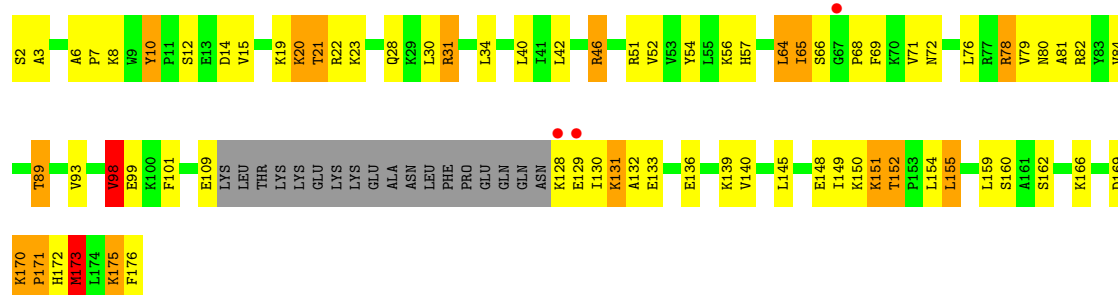


• Molecule 43: 60S ribosomal protein L6-A

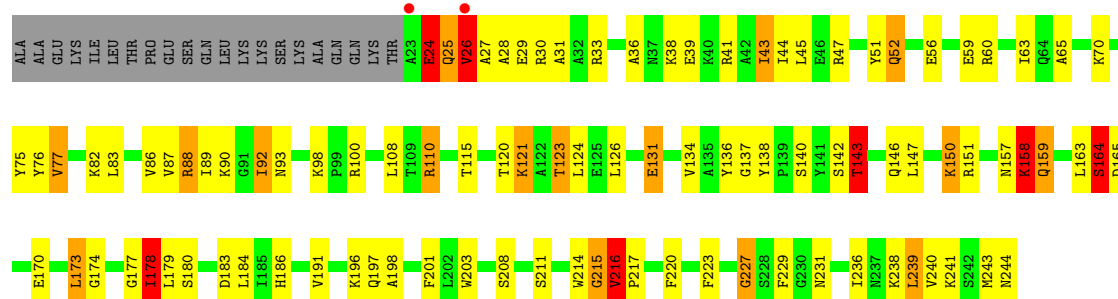




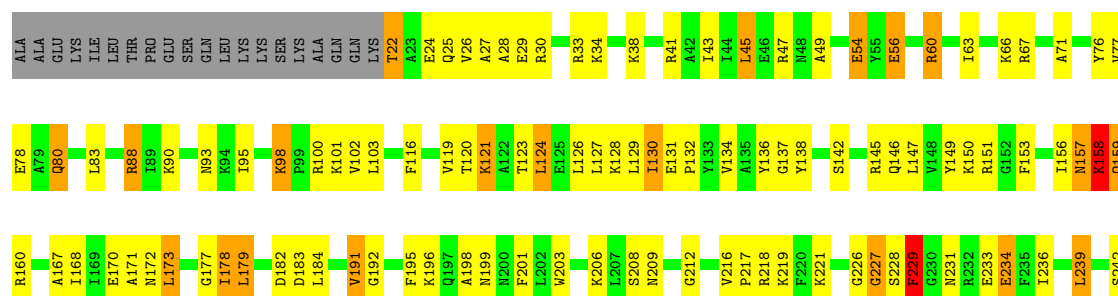
• Molecule 43: 60S ribosomal protein L6-A



• Molecule 44: 60S ribosomal protein L7-A



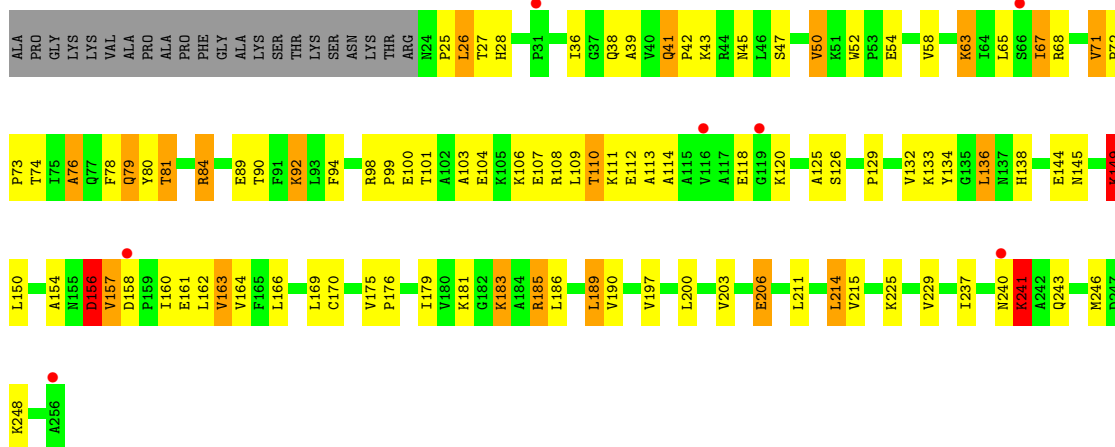
• Molecule 44: 60S ribosomal protein L7-A





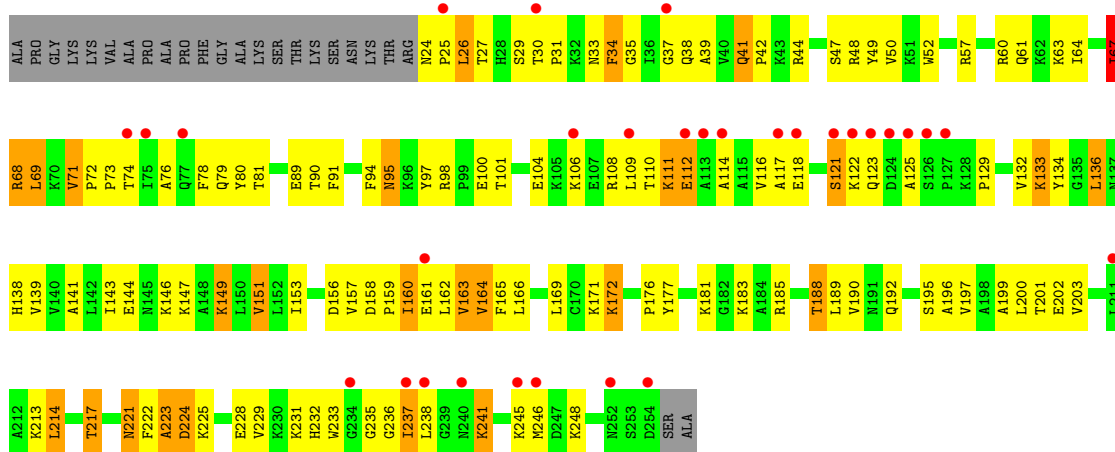
• Molecule 45: 60S ribosomal protein L8-A

Chain L8: 3% 53% 30% 8% 9%



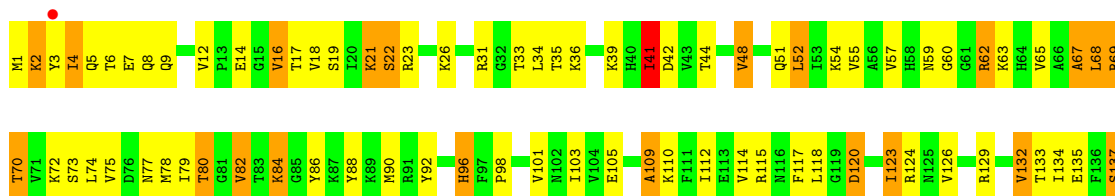
• Molecule 45: 60S ribosomal protein L8-A

Chain l8: 12% 40% 40% 10% 9%



• Molecule 46: 60S ribosomal protein L9-A

Chain L9: 43% 39% 17%

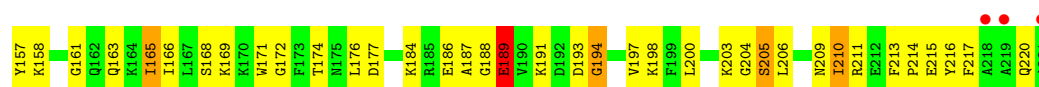
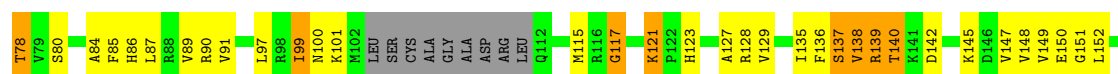




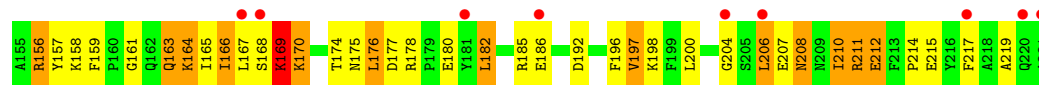
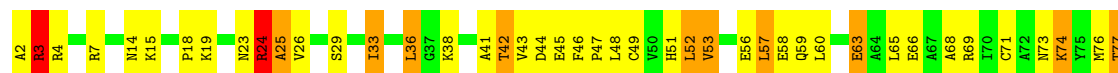
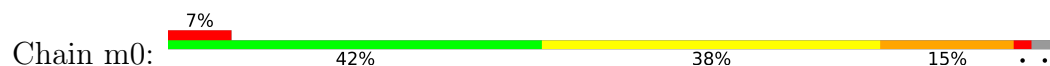
• Molecule 46: 60S ribosomal protein L9-A



• Molecule 47: 60S ribosomal protein L10

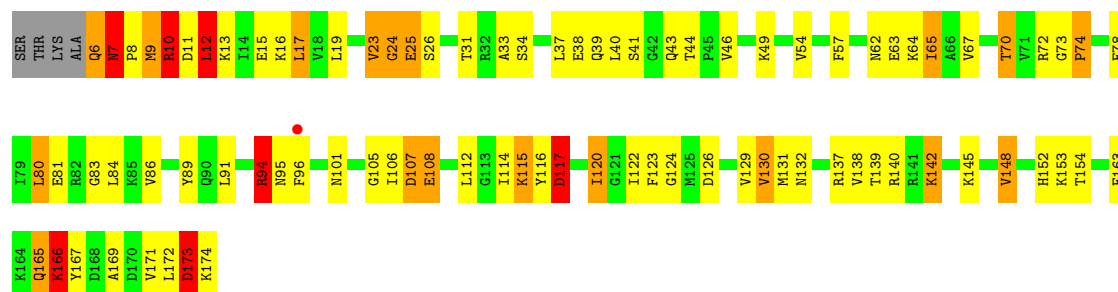


• Molecule 47: 60S ribosomal protein L10

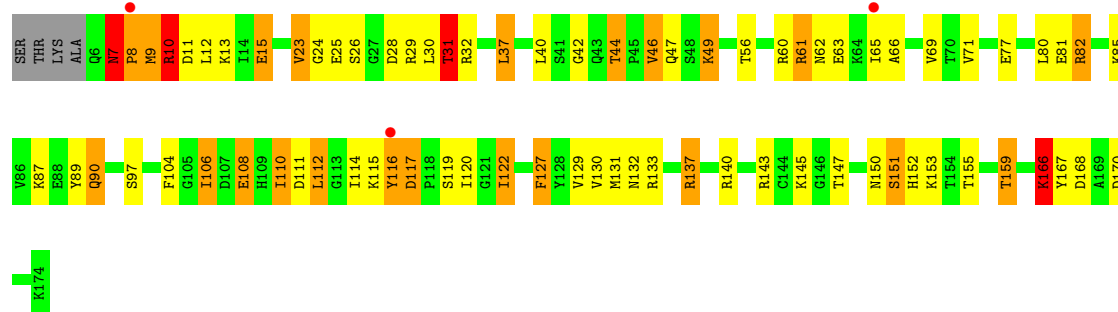


• Molecule 48: 60S ribosomal protein L11-B

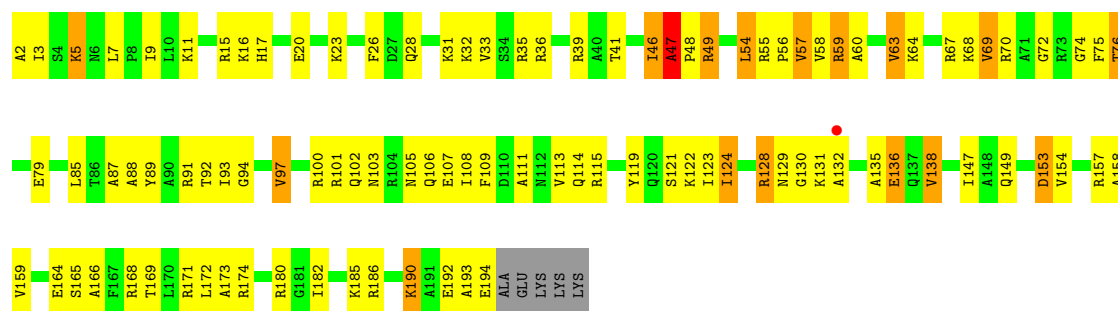




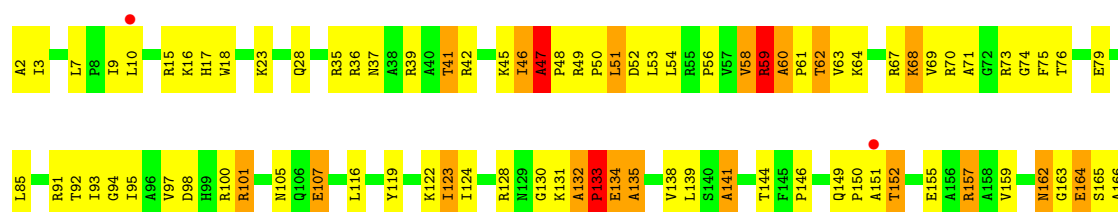
• Molecule 48: 60S ribosomal protein L11-B



• Molecule 49: 60S ribosomal protein L13-A



• Molecule 49: 60S ribosomal protein L13-A





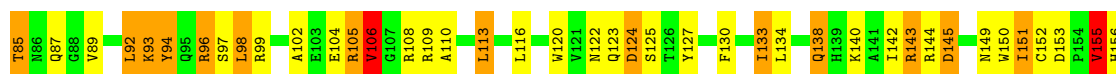
- Molecule 50: 60S ribosomal protein L14-A



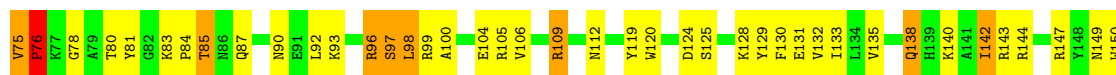
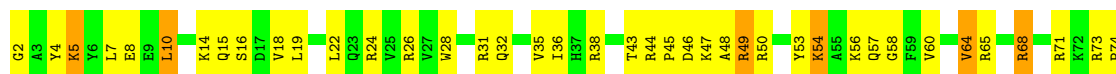
- Molecule 50: 60S ribosomal protein L14-A



- Molecule 51: 60S ribosomal protein L15-A



- Molecule 51: 60S ribosomal protein L15-A

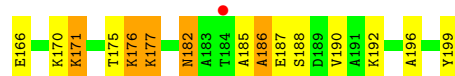




- Molecule 52: 60S ribosomal protein L16-A



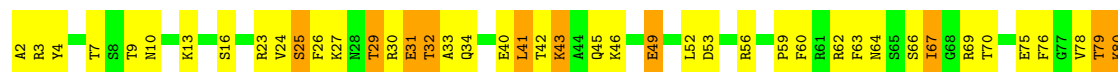
- Molecule 52: 60S ribosomal protein L16-A

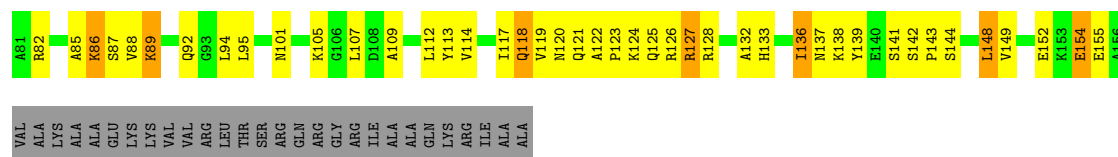


- Molecule 53: 60S ribosomal protein L17-A

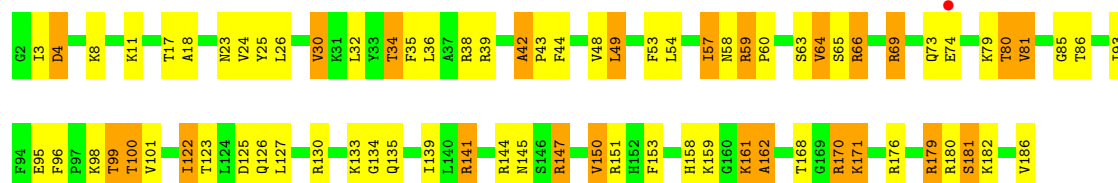


- Molecule 53: 60S ribosomal protein L17-A

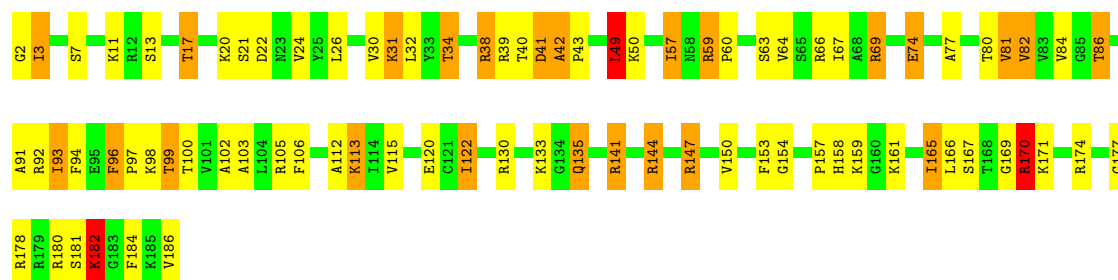




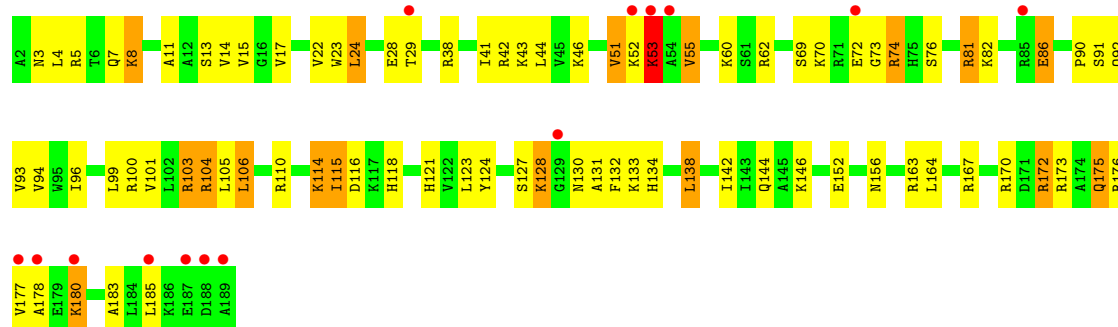
- Molecule 54: 60S ribosomal protein L18-A



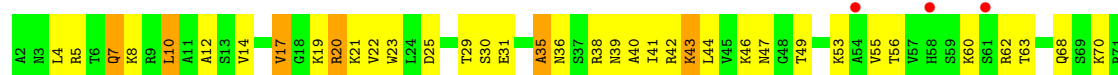
- Molecule 54: 60S ribosomal protein L18-A

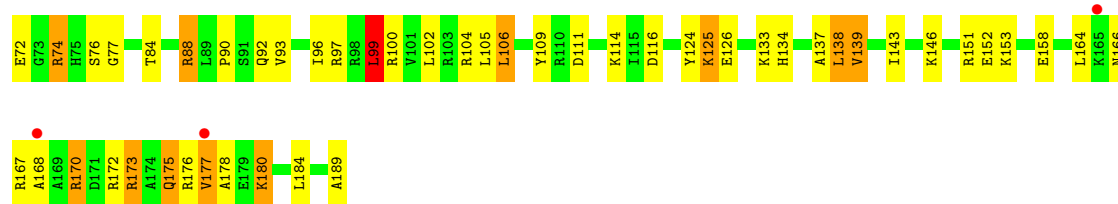


- Molecule 55: 60S ribosomal protein L19-A

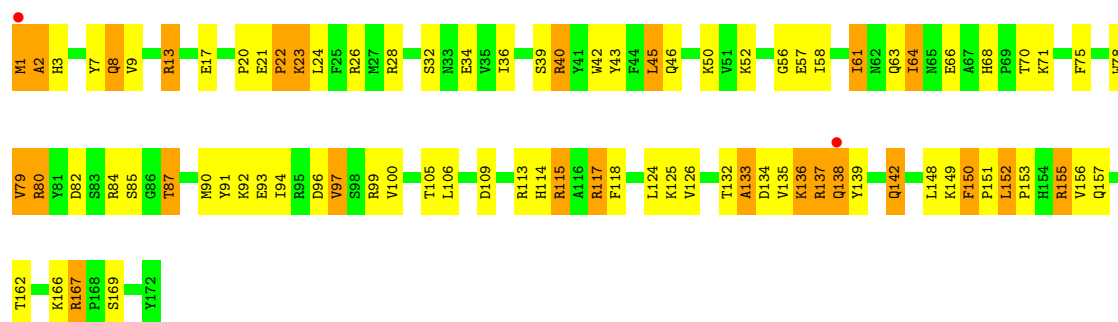


- Molecule 55: 60S ribosomal protein L19-A

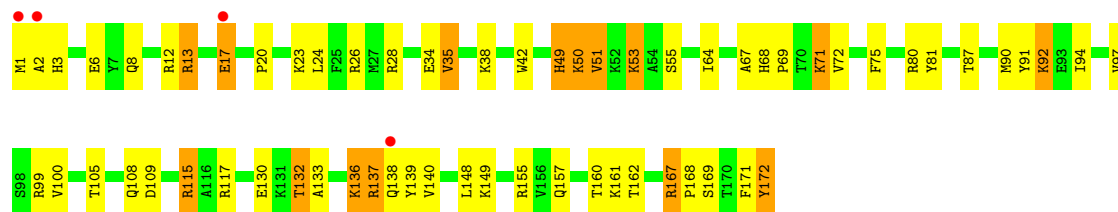




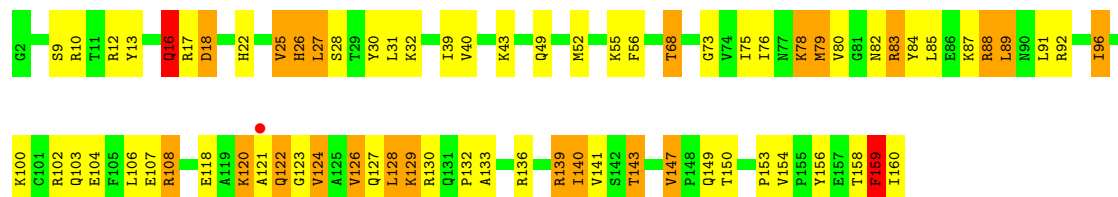
• Molecule 56: 60S ribosomal protein L20-A



• Molecule 56: 60S ribosomal protein L20-A



• Molecule 57: 60S ribosomal protein L21-A

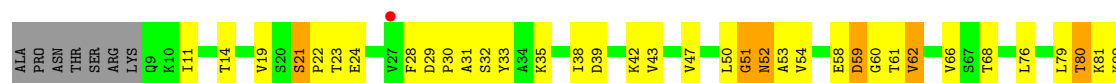


• Molecule 57: 60S ribosomal protein L21-A

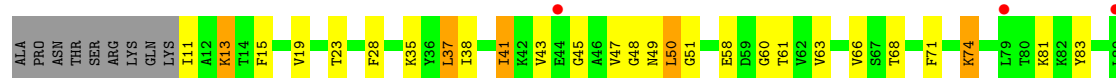




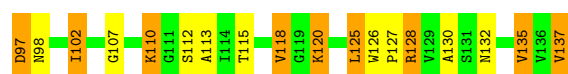
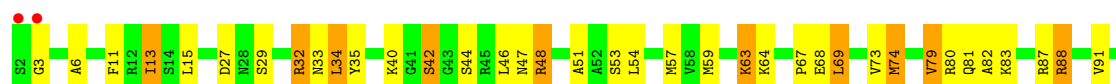
• Molecule 58: 60S ribosomal protein L22-A



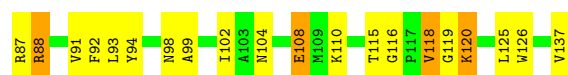
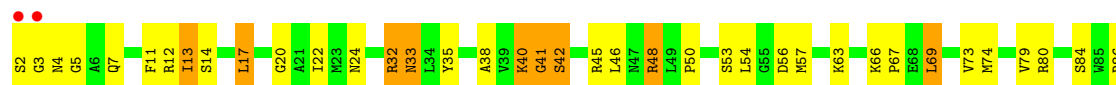
• Molecule 58: 60S ribosomal protein L22-A



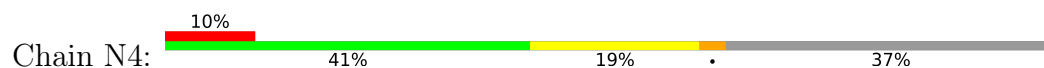
• Molecule 59: 60S ribosomal protein L23-A

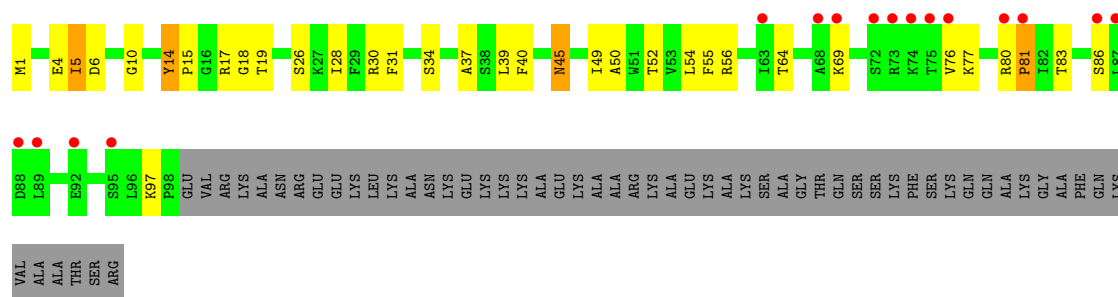


• Molecule 59: 60S ribosomal protein L23-A

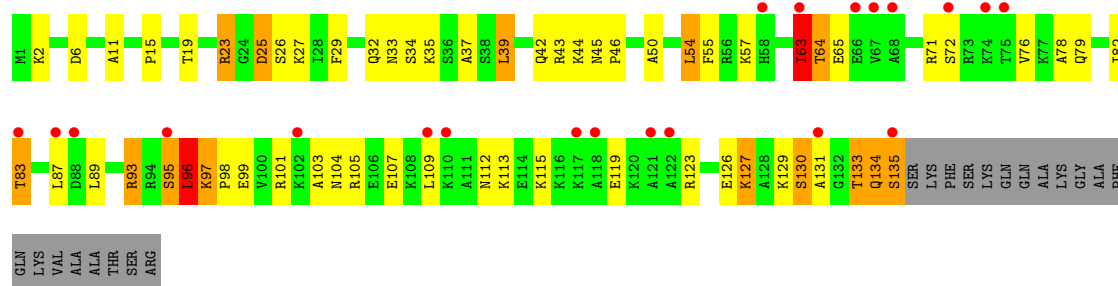


• Molecule 60: 60S ribosomal protein L24-A

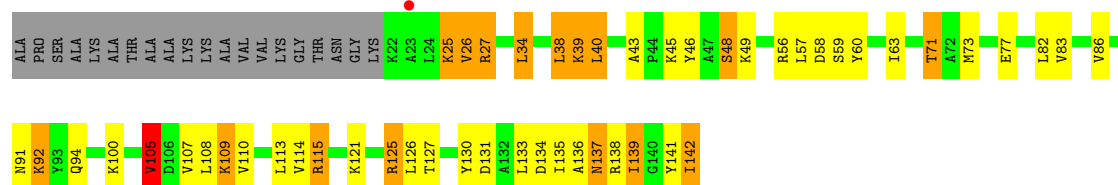




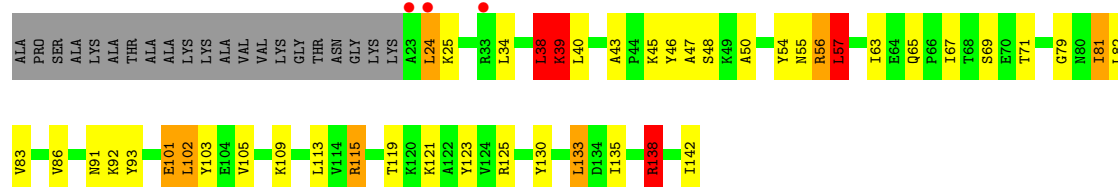
• Molecule 60: 60S ribosomal protein L24-A



• Molecule 61: 60S ribosomal protein L25



• Molecule 61: 60S ribosomal protein L25

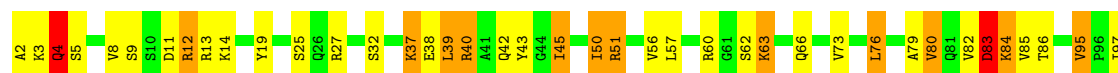


• Molecule 62: 60S ribosomal protein L26-A

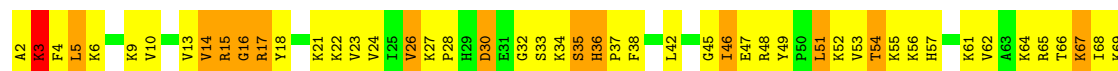
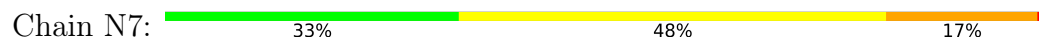




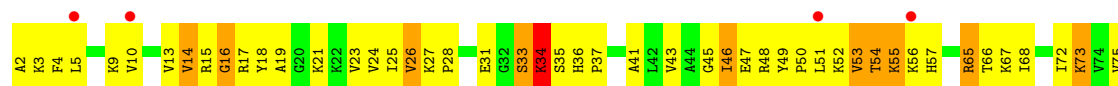
• Molecule 62: 60S ribosomal protein L26-A



• Molecule 63: 60S ribosomal protein L27-A



• Molecule 63: 60S ribosomal protein L27-A

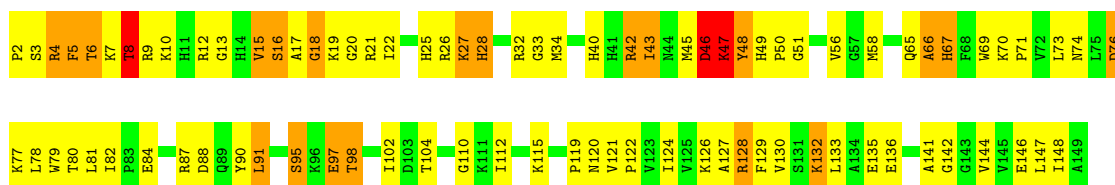


• Molecule 64: 60S ribosomal protein L28

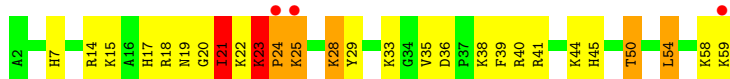


• Molecule 64: 60S ribosomal protein L28

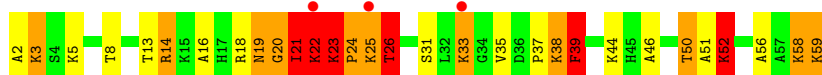




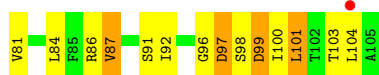
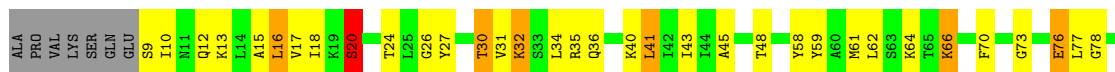
• Molecule 65: 60S ribosomal protein L29



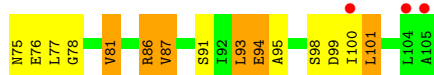
• Molecule 65: 60S ribosomal protein L29



• Molecule 66: 60S ribosomal protein L30



• Molecule 66: 60S ribosomal protein L30

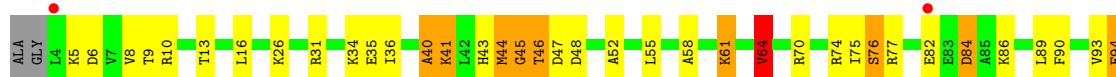


• Molecule 67: 60S ribosomal protein L31-A

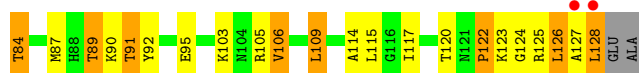




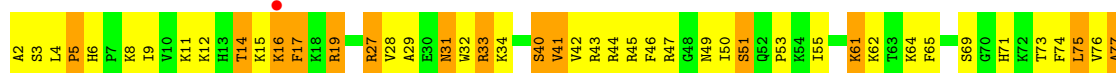
- Molecule 67: 60S ribosomal protein L31-A



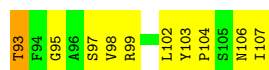
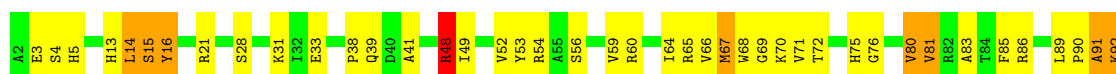
- Molecule 68: 60S ribosomal protein L32



- Molecule 68: 60S ribosomal protein L32

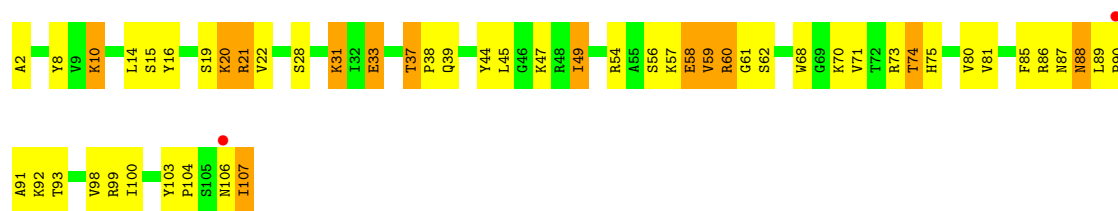


- Molecule 69: 60S ribosomal protein L33-A

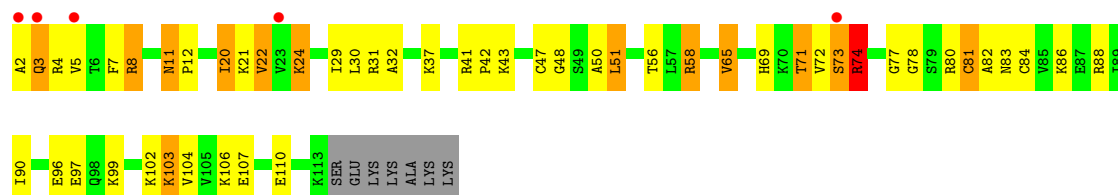


- Molecule 69: 60S ribosomal protein L33-A

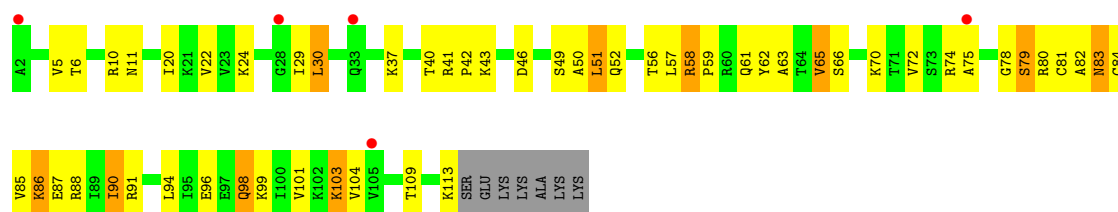




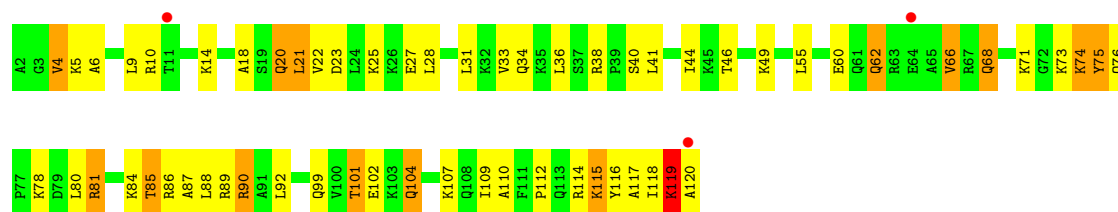
• Molecule 70: 60S ribosomal protein L34-A



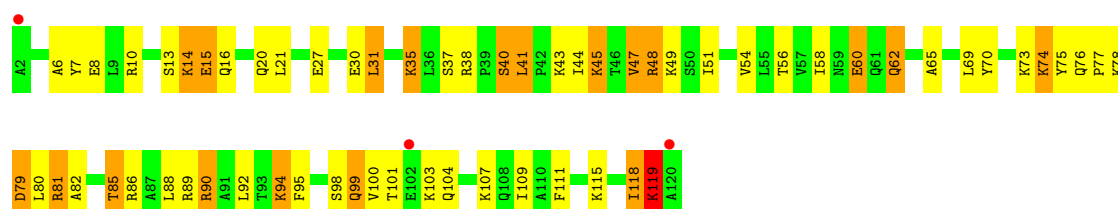
• Molecule 70: 60S ribosomal protein L34-A



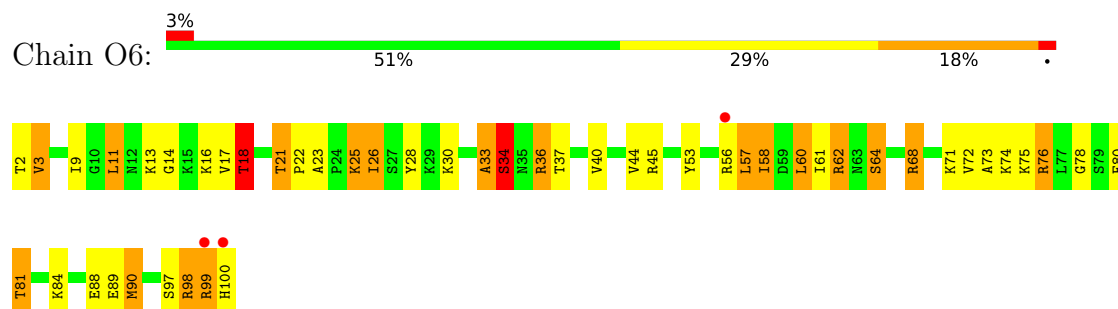
• Molecule 71: 60S ribosomal protein L35-A



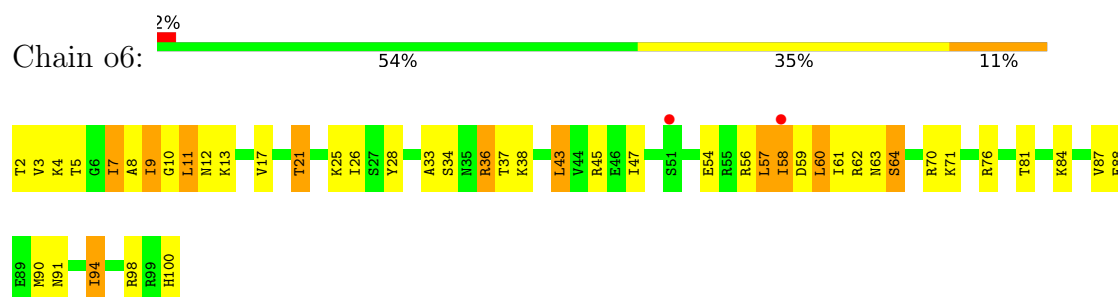
• Molecule 71: 60S ribosomal protein L35-A



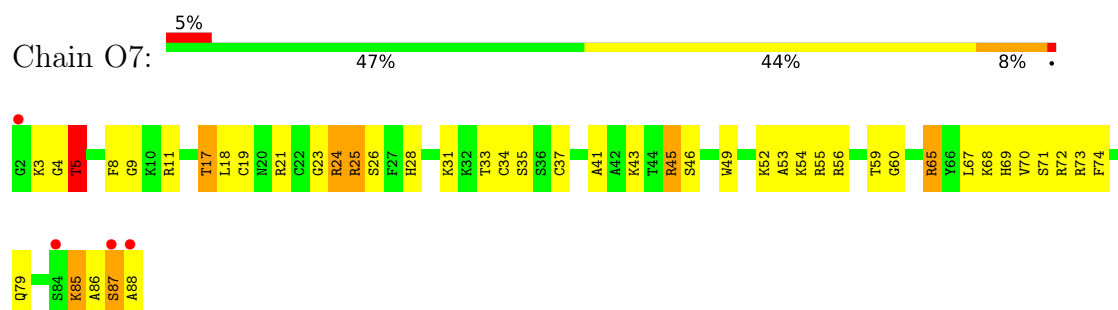
- Molecule 72: 60S ribosomal protein L36-A



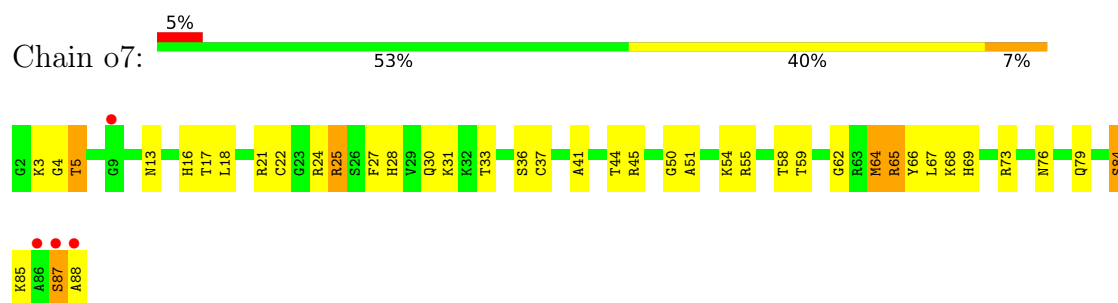
- Molecule 72: 60S ribosomal protein L36-A



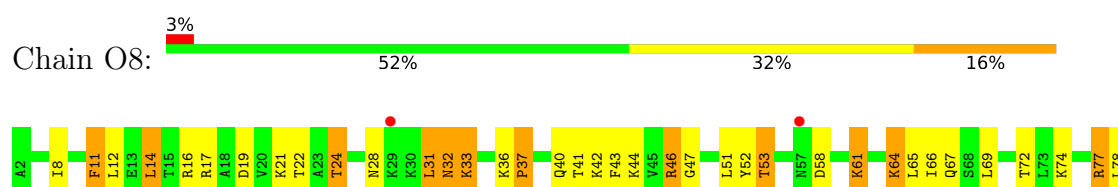
- Molecule 73: 60S ribosomal protein L37-A



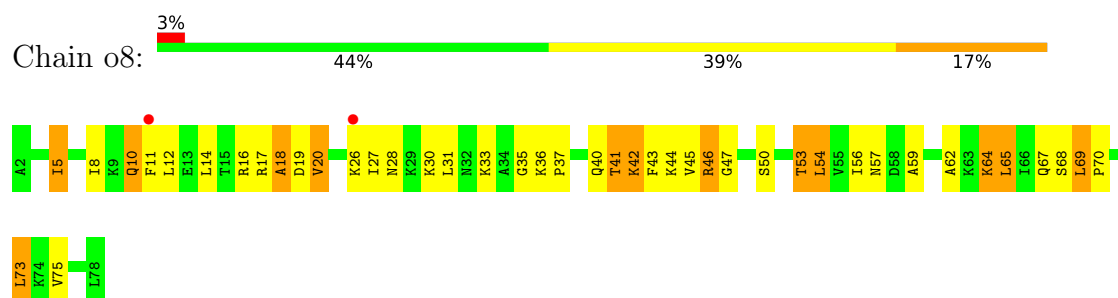
- Molecule 73: 60S ribosomal protein L37-A



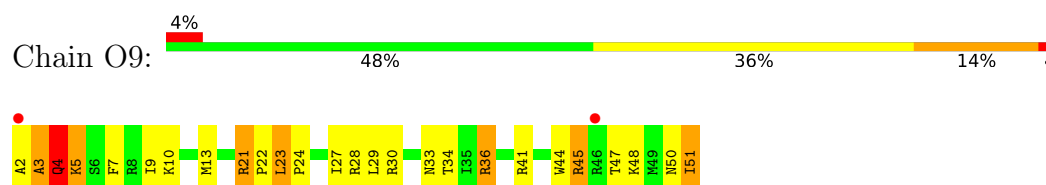
- Molecule 74: 60S ribosomal protein L38



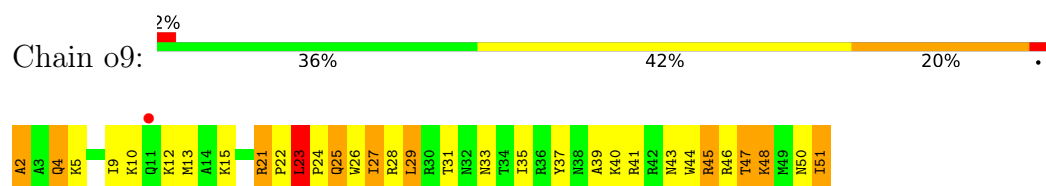
• Molecule 74: 60S ribosomal protein L38



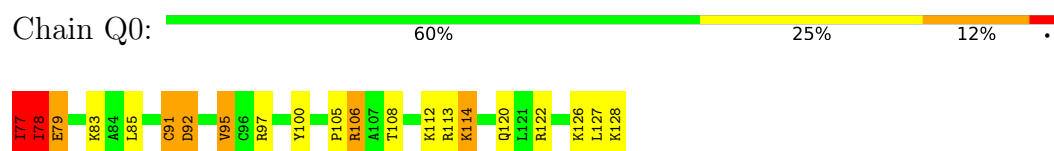
• Molecule 75: 60S ribosomal protein L39



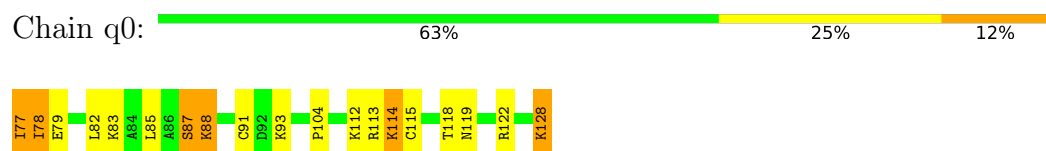
• Molecule 75: 60S ribosomal protein L39



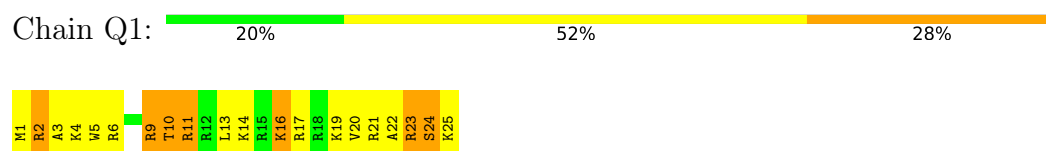
• Molecule 76: Ubiquitin-60S ribosomal protein L40



• Molecule 76: Ubiquitin-60S ribosomal protein L40



• Molecule 77: 60S ribosomal protein L41-A

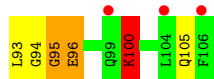


• Molecule 77: 60S ribosomal protein L41-A

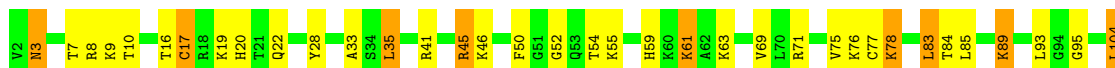




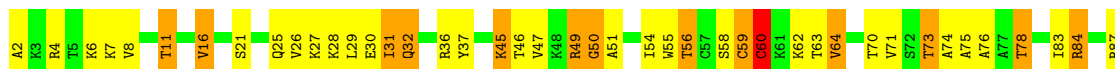
- Molecule 78: 60S ribosomal protein L42-A



- Molecule 78: 60S ribosomal protein L42-A



- Molecule 79: 60S ribosomal protein L43-A



- Molecule 79: 60S ribosomal protein L43-A



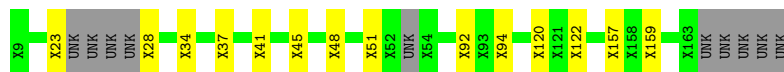
- Molecule 80: 40S ribosomal protein S30-A





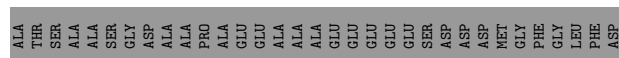
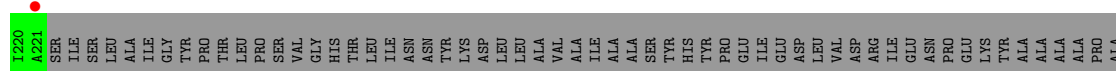
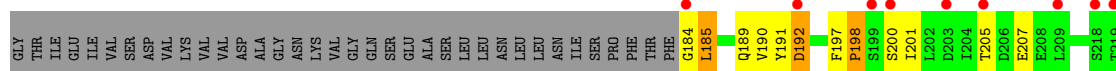
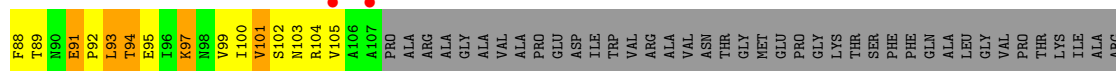
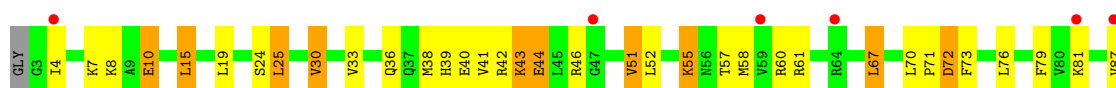
• Molecule 81: Unknown Protein m2

Chain m2: 85% 9% 6%



• Molecule 82: 60S acidic ribosomal protein P0

Chain p0: 6% 26% 14% 6% 54%



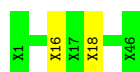
• Molecule 83: Unknown Protein p1

Chain p1: 87% 13%



• Molecule 84: Unknown Protein p2

Chain p2: 96%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	435.39Å 286.22Å 303.33Å 90.00° 98.97° 90.00°	Depositor
Resolution (Å)	299.62 – 3.00 299.62 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (299.62-3.00) 99.9 (299.62-3.00)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.207 , 0.258 0.211 , 0.260	Depositor DCC
R_{free} test set	29190 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 110.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	411206	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, OHX, 3J2

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	0.48	0/41698	0.67	6/64972 (0.0%)
1	6	0.52	0/42765	0.69	10/66634 (0.0%)
2	S0	0.66	0/1617	1.09	12/2215 (0.5%)
2	s0	0.67	0/1623	1.13	9/2222 (0.4%)
3	S1	0.56	0/1735	0.99	6/2335 (0.3%)
3	s1	0.69	1/1748 (0.1%)	1.08	6/2352 (0.3%)
4	S2	0.70	0/1665	1.12	9/2263 (0.4%)
4	s2	0.83	0/1665	1.11	3/2263 (0.1%)
5	S3	0.68	0/1759	1.10	10/2368 (0.4%)
5	s3	0.59	0/1759	1.02	8/2368 (0.3%)
6	S4	0.72	0/2109	1.06	10/2839 (0.4%)
6	s4	0.72	0/2109	1.15	13/2839 (0.5%)
7	S5	0.58	0/1629	1.01	7/2202 (0.3%)
7	s5	0.63	0/1629	1.05	6/2202 (0.3%)
8	S6	0.67	0/1823	1.06	5/2439 (0.2%)
8	s6	0.75	0/1779	1.07	6/2379 (0.3%)
9	S7	0.62	0/1506	1.07	9/2028 (0.4%)
9	s7	0.66	1/1516 (0.1%)	1.11	8/2043 (0.4%)
10	S8	0.83	0/1514	1.10	4/2021 (0.2%)
10	s8	0.85	0/1514	1.11	7/2021 (0.3%)
11	S9	0.67	0/1519	1.11	8/2035 (0.4%)
11	s9	0.73	0/1519	1.11	8/2035 (0.4%)
12	C0	0.56	0/790	1.01	3/1069 (0.3%)
12	c0	0.52	0/777	1.03	3/1049 (0.3%)
13	C1	0.82	0/1239	1.08	1/1673 (0.1%)
13	c1	0.83	0/1194	1.18	1/1610 (0.1%)
14	C2	0.58	0/900	0.96	1/1224 (0.1%)
14	c2	0.46	0/900	0.86	0/1224
15	C3	0.75	0/1215	1.10	7/1638 (0.4%)
15	c3	0.77	0/1215	1.17	12/1638 (0.7%)
16	C4	0.58	0/901	1.03	5/1217 (0.4%)
16	c4	0.75	0/960	1.16	8/1290 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.70	0/998	1.10	4/1341 (0.3%)
17	c5	0.68	1/1060 (0.1%)	1.17	6/1426 (0.4%)
18	C6	0.63	0/1125	1.07	3/1510 (0.2%)
18	c6	0.67	0/1131	1.08	6/1518 (0.4%)
19	C7	0.67	0/935	1.08	5/1254 (0.4%)
19	c7	0.64	0/914	1.09	0/1224
20	C8	0.62	0/1211	1.02	2/1628 (0.1%)
20	c8	0.64	0/1211	1.04	4/1628 (0.2%)
21	C9	0.62	0/1130	1.01	2/1517 (0.1%)
21	c9	0.64	0/1130	1.01	1/1517 (0.1%)
22	D0	0.68	0/865	1.03	3/1169 (0.3%)
22	d0	0.68	0/892	1.04	4/1205 (0.3%)
23	D1	0.67	0/693	1.01	0/935
23	d1	0.71	0/693	1.13	1/935 (0.1%)
24	D2	0.75	0/1038	1.14	6/1395 (0.4%)
24	d2	0.85	0/1038	1.12	5/1395 (0.4%)
25	D3	0.91	0/1139	1.24	11/1518 (0.7%)
25	d3	0.97	0/1139	1.15	5/1518 (0.3%)
26	D4	0.65	0/1087	1.02	4/1449 (0.3%)
26	d4	0.71	0/1087	1.11	2/1449 (0.1%)
27	D5	0.56	0/571	1.13	6/768 (0.8%)
27	d5	0.59	0/566	1.09	1/761 (0.1%)
28	D6	0.63	0/782	1.10	5/1047 (0.5%)
28	d6	0.79	0/782	1.13	2/1047 (0.2%)
29	D7	0.63	0/620	1.09	5/838 (0.6%)
29	d7	0.67	0/620	1.04	2/838 (0.2%)
30	D8	0.52	0/499	1.00	2/670 (0.3%)
30	d8	0.56	0/499	1.03	1/670 (0.1%)
31	D9	0.77	0/452	1.12	1/600 (0.2%)
31	d9	0.67	0/452	0.99	0/600
32	E0	0.64	0/483	1.05	0/643
33	E1	0.70	0/577	1.24	5/770 (0.6%)
33	e1	0.60	0/619	1.10	4/822 (0.5%)
34	SR	0.56	1/2494 (0.0%)	0.91	4/3393 (0.1%)
34	sR	0.55	0/2495	0.89	2/3395 (0.1%)
35	SM	0.79	0/1113	1.20	6/1502 (0.4%)
35	sM	0.71	0/683	1.14	1/923 (0.1%)
36	1	0.74	0/75394	0.84	34/117545 (0.0%)
36	5	0.75	0/75414	0.85	29/117575 (0.0%)
37	3	0.59	0/2883	0.73	0/4491
37	7	0.74	0/2883	0.83	1/4491 (0.0%)
38	4	0.73	0/3746	0.83	0/5832
38	8	0.66	0/3746	0.79	0/5832

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	1.10	0/1948	1.27	10/2617 (0.4%)
39	l2	1.08	3/1946 (0.2%)	1.33	12/2614 (0.5%)
40	L3	1.05	0/3146	1.27	12/4228 (0.3%)
40	l3	1.20	5/3146 (0.2%)	1.33	31/4228 (0.7%)
41	L4	1.16	3/2800 (0.1%)	1.40	23/3790 (0.6%)
41	l4	1.11	0/2800	1.40	37/3790 (1.0%)
42	L5	0.77	0/2425	1.07	5/3271 (0.2%)
42	l5	1.00	1/2408 (0.0%)	1.24	12/3248 (0.4%)
43	L6	1.12	1/1260 (0.1%)	1.21	6/1694 (0.4%)
43	l6	1.10	0/1269	1.23	3/1705 (0.2%)
44	L7	1.16	2/1821 (0.1%)	1.36	19/2451 (0.8%)
44	l7	1.17	4/1828 (0.2%)	1.38	23/2461 (0.9%)
45	L8	0.82	0/1836	1.13	12/2481 (0.5%)
45	l8	0.73	0/1795	1.07	5/2429 (0.2%)
46	L9	0.95	0/1539	1.21	7/2073 (0.3%)
46	l9	1.08	0/1539	1.24	12/2073 (0.6%)
47	M0	0.99	2/1741 (0.1%)	1.22	8/2335 (0.3%)
47	m0	1.10	1/1758 (0.1%)	1.26	7/2358 (0.3%)
48	M1	0.71	0/1374	1.16	8/1842 (0.4%)
48	m1	0.94	0/1374	1.20	10/1842 (0.5%)
49	M3	1.12	4/1568 (0.3%)	1.37	20/2106 (0.9%)
49	m3	1.03	1/1573 (0.1%)	1.29	14/2113 (0.7%)
50	M4	1.09	0/1068	1.27	7/1438 (0.5%)
50	m4	1.20	0/1074	1.32	11/1446 (0.8%)
51	M5	1.15	5/1757 (0.3%)	1.31	14/2354 (0.6%)
51	m5	0.97	1/1757 (0.1%)	1.26	14/2354 (0.6%)
52	M6	1.24	1/1585 (0.1%)	1.32	7/2128 (0.3%)
52	m6	1.37	4/1585 (0.3%)	1.45	14/2128 (0.7%)
53	M7	1.13	1/1443 (0.1%)	1.35	8/1944 (0.4%)
53	m7	1.25	1/1250 (0.1%)	1.37	6/1683 (0.4%)
54	M8	1.12	0/1465	1.38	11/1965 (0.6%)
54	m8	1.11	1/1465 (0.1%)	1.39	12/1965 (0.6%)
55	M9	0.86	0/1538	1.07	0/2050
55	m9	0.87	0/1538	1.10	2/2050 (0.1%)
56	N0	1.06	1/1481 (0.1%)	1.25	11/1990 (0.6%)
56	n0	1.20	1/1481 (0.1%)	1.28	5/1990 (0.3%)
57	N1	1.02	0/1300	1.22	7/1743 (0.4%)
57	n1	1.12	1/1300 (0.1%)	1.30	7/1743 (0.4%)
58	N2	0.58	0/812	1.00	4/1099 (0.4%)
58	n2	0.63	0/794	1.02	0/1076
59	N3	1.08	0/1018	1.24	2/1369 (0.1%)
59	n3	1.23	1/1018 (0.1%)	1.42	7/1369 (0.5%)
60	N4	0.91	0/712	1.52	6/958 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.92	0/1052	1.19	0/1398
61	N5	0.96	0/979	1.25	4/1321 (0.3%)
61	n5	0.92	0/974	1.26	5/1314 (0.4%)
62	N6	1.05	0/1004	1.30	6/1341 (0.4%)
62	n6	1.04	1/1004 (0.1%)	1.26	1/1341 (0.1%)
63	N7	0.75	0/1118	1.12	3/1497 (0.2%)
63	n7	0.64	0/1118	1.10	4/1497 (0.3%)
64	N8	1.16	0/1204	1.36	9/1612 (0.6%)
64	n8	1.14	1/1204 (0.1%)	1.34	8/1612 (0.5%)
65	N9	0.98	0/473	1.29	6/629 (1.0%)
65	n9	1.25	2/473 (0.4%)	1.51	9/629 (1.4%)
66	O0	0.70	0/751	1.06	1/1008 (0.1%)
66	o0	0.68	0/775	1.02	2/1040 (0.2%)
67	O1	0.93	0/890	1.18	3/1196 (0.3%)
67	o1	1.04	0/897	1.23	4/1205 (0.3%)
68	O2	1.25	2/1041 (0.2%)	1.36	6/1394 (0.4%)
68	o2	1.29	5/1041 (0.5%)	1.34	6/1394 (0.4%)
69	O3	1.28	1/868 (0.1%)	1.36	7/1168 (0.6%)
69	o3	1.26	3/868 (0.3%)	1.35	5/1168 (0.4%)
70	O4	0.94	1/890 (0.1%)	1.18	7/1189 (0.6%)
70	o4	0.86	0/890	1.19	2/1189 (0.2%)
71	O5	1.04	1/978 (0.1%)	1.30	2/1301 (0.2%)
71	o5	0.86	0/974	1.15	9/1297 (0.7%)
72	O6	0.97	2/778 (0.3%)	1.26	4/1034 (0.4%)
72	o6	0.82	0/777	1.14	2/1033 (0.2%)
73	O7	1.23	1/696 (0.1%)	1.37	5/923 (0.5%)
73	o7	1.05	1/696 (0.1%)	1.25	1/923 (0.1%)
74	O8	0.74	0/618	1.04	0/826
74	o8	0.68	0/614	1.05	0/822
75	O9	1.12	0/443	1.13	0/588
75	o9	1.00	0/443	1.34	3/588 (0.5%)
76	Q0	1.05	0/423	1.23	1/562 (0.2%)
76	q0	1.23	0/423	1.35	4/562 (0.7%)
77	Q1	0.90	0/234	1.10	0/300
77	q1	1.07	0/234	1.17	0/300
78	Q2	1.05	1/860 (0.1%)	1.21	1/1136 (0.1%)
78	q2	0.99	0/860	1.25	6/1136 (0.5%)
79	Q3	1.02	0/701	1.31	1/934 (0.1%)
79	q3	0.99	0/701	1.25	1/934 (0.1%)
80	e0	0.76	0/499	1.21	2/665 (0.3%)
82	p0	0.58	0/1092	0.99	2/1474 (0.1%)
All	All	0.78	71/430073 (0.0%)	0.96	989/631362 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	S1	0	1
3	s1	0	1
5	s3	0	1
6	S4	0	1
7	S5	0	1
7	s5	0	2
9	S7	0	2
9	s7	0	1
16	C4	0	1
16	c4	0	1
18	c6	0	2
19	c7	0	1
22	d0	0	1
26	d4	0	1
27	D5	0	2
28	D6	0	2
33	E1	0	1
33	e1	0	1
39	L2	0	1
39	l2	0	3
41	L4	0	1
41	l4	0	1
42	L5	0	2
42	l5	0	1
43	L6	0	1
44	L7	0	1
44	l7	0	1
45	l8	0	1
48	M1	0	1
49	M3	0	1
51	M5	0	1
52	M6	0	1
52	m6	0	1
53	M7	0	1
56	N0	0	1
56	n0	0	1
57	N1	0	1
59	n3	0	1
60	n4	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
63	N7	0	1
64	N8	0	1
64	n8	0	2
65	N9	0	1
65	n9	0	2
67	O1	0	2
67	o1	0	1
71	o5	0	1
72	O6	0	2
75	O9	0	1
75	o9	0	1
76	Q0	0	1
78	Q2	0	2
All	All	0	65

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	8.78	2.10	1.81
51	M5	183	THR	CA-C	-8.37	1.45	1.53
64	n8	15	VAL	CA-CB	-8.23	1.46	1.54
47	M0	127	ALA	CA-CB	-7.99	1.42	1.53
34	SR	161	LYS	CA-C	7.85	1.63	1.52

The worst 5 of 989 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	N4	80	ARG	CA-C-N	19.07	143.68	119.84
60	N4	80	ARG	C-N-CA	19.07	143.68	119.84
54	M8	18	ALA	CA-C-N	-14.31	106.28	120.31
54	M8	18	ALA	C-N-CA	-14.31	106.28	120.31
52	m6	108	ILE	CA-C-N	14.09	134.89	120.38

There are no chirality outliers.

5 of 65 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	S1	177	GLN	Peptide
6	S4	167	GLY	Peptide
7	S5	49	GLU	Peptide
9	S7	131	PHE	Peptide

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Mol	Chain	Res	Type	Group
9	S7	31	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37283	0	18757	961	1
1	6	38238	0	19240	924	0
2	S0	1577	0	1567	90	0
2	s0	1583	0	1578	89	0
3	S1	1709	0	1784	113	0
3	s1	1722	0	1793	69	0
4	S2	1635	0	1723	100	0
4	s2	1635	0	1723	69	0
5	S3	1734	0	1817	76	0
5	s3	1734	0	1817	65	0
6	S4	2068	0	2154	100	0
6	s4	2068	0	2154	112	0
7	S5	1609	0	1675	90	0
7	s5	1609	0	1675	110	0
8	S6	1799	0	1879	88	0
8	s6	1755	0	1845	74	0
9	S7	1481	0	1572	87	0
9	s7	1491	0	1578	67	0
10	S8	1489	0	1525	65	0
10	s8	1489	0	1525	60	0
11	S9	1494	0	1573	74	0
11	s9	1494	0	1573	70	0
12	C0	773	0	729	43	0
12	c0	762	0	699	33	0
13	C1	1213	0	1257	46	0
13	c1	1168	0	1233	36	0
14	C2	892	0	891	46	0
14	c2	892	0	891	30	0
15	C3	1192	0	1255	42	0
15	c3	1192	0	1255	64	0
16	C4	891	0	883	62	0
16	c4	949	0	985	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	C5	977	0	1002	55	0
17	c5	1039	0	1050	62	0
18	C6	1105	0	1166	62	0
18	c6	1111	0	1171	68	0
19	C7	926	0	930	43	0
19	c7	906	0	909	47	0
20	C8	1192	0	1222	61	0
20	c8	1192	0	1222	65	0
21	C9	1112	0	1124	73	0
21	c9	1112	0	1124	47	0
22	D0	855	0	917	51	0
22	d0	882	0	939	48	0
23	D1	684	0	672	41	0
23	d1	684	0	672	44	0
24	D2	1021	0	1060	67	0
24	d2	1021	0	1060	59	0
25	D3	1121	0	1196	62	0
25	d3	1121	0	1196	44	0
26	D4	1073	0	1132	53	0
26	d4	1073	0	1132	47	0
27	D5	563	0	603	29	0
27	d5	558	0	598	28	0
28	D6	769	0	814	62	0
28	d6	769	0	814	46	0
29	D7	610	0	631	21	0
29	d7	610	0	632	28	0
30	D8	497	0	535	25	0
30	d8	497	0	535	32	0
31	D9	442	0	428	25	0
31	d9	442	0	428	22	0
32	E0	475	0	525	14	0
33	E1	566	0	602	39	0
33	e1	608	0	656	34	0
34	SR	2441	0	2397	97	0
34	sR	2442	0	2392	82	0
35	SM	1104	0	996	59	0
35	sM	680	0	607	34	0
36	1	67355	0	33835	1325	0
36	5	67376	0	33849	1306	1
37	3	2579	0	1304	55	0
37	7	2579	0	1304	52	0
38	4	3353	0	1695	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	8	3353	0	1695	84	0
39	L2	1914	0	1981	88	0
39	l2	1912	0	1976	86	0
40	L3	3075	0	3142	148	0
40	l3	3075	0	3142	148	0
41	L4	2748	0	2859	117	0
41	l4	2748	0	2859	141	0
42	L5	2375	0	2325	113	0
42	l5	2359	0	2311	97	0
43	L6	1239	0	1326	48	0
43	l6	1248	0	1339	54	0
44	L7	1784	0	1862	74	0
44	l7	1791	0	1869	66	0
45	L8	1804	0	1877	68	0
45	l8	1763	0	1819	92	0
46	L9	1518	0	1587	76	0
46	l9	1518	0	1587	76	0
47	M0	1705	0	1736	66	0
47	m0	1722	0	1755	90	0
48	M1	1353	0	1383	55	0
48	m1	1353	0	1383	44	0
49	M3	1543	0	1608	69	0
49	m3	1548	0	1613	72	0
50	M4	1053	0	1149	54	0
50	m4	1059	0	1154	36	0
51	M5	1720	0	1779	77	0
51	m5	1720	0	1779	94	0
52	M6	1555	0	1659	42	0
52	m6	1555	0	1659	73	0
53	M7	1420	0	1437	73	0
53	m7	1227	0	1236	55	0
54	M8	1441	0	1543	56	0
54	m8	1441	0	1543	57	0
55	M9	1521	0	1617	65	0
55	m9	1521	0	1617	51	0
56	N0	1445	0	1487	59	0
56	n0	1445	0	1487	39	0
57	N1	1276	0	1323	49	0
57	n1	1276	0	1323	55	0
58	N2	796	0	812	26	0
58	n2	778	0	791	21	0
59	N3	1003	0	1048	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	n3	1003	0	1048	42	0
60	N4	699	0	640	19	0
60	n4	1038	0	1071	37	0
61	N5	964	0	1025	39	0
61	n5	959	0	1023	29	0
62	N6	993	0	1081	36	0
62	n6	993	0	1081	36	0
63	N7	1092	0	1155	66	0
63	n7	1092	0	1155	60	0
64	N8	1173	0	1215	58	0
64	n8	1173	0	1215	79	0
65	N9	462	0	491	14	0
65	n9	462	0	491	22	0
66	O0	743	0	797	31	0
66	o0	767	0	816	30	0
67	O1	876	0	912	24	0
67	o1	883	0	918	23	0
68	O2	1020	0	1090	38	0
68	o2	1020	0	1090	36	0
69	O3	850	0	880	41	0
69	o3	850	0	880	34	0
70	O4	880	0	945	38	0
70	o4	880	0	945	39	0
71	O5	969	0	1078	40	0
71	o5	965	0	1067	47	0
72	O6	771	0	849	33	0
72	o6	770	0	846	22	0
73	O7	681	0	683	35	0
73	o7	681	0	683	30	0
74	O8	612	0	682	21	0
74	o8	608	0	671	27	0
75	O9	436	0	475	31	0
75	o9	436	0	475	30	0
76	Q0	417	0	455	13	0
76	q0	417	0	455	10	0
77	Q1	233	0	284	24	0
77	q1	233	0	284	19	0
78	Q2	847	0	916	27	0
78	q2	847	0	914	27	0
79	Q3	694	0	734	33	0
79	q3	694	0	734	26	0
80	e0	491	0	542	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	m2	750	0	171	7	0
82	p0	1077	0	1041	37	0
83	p1	235	0	51	4	0
84	p2	230	0	51	1	0
85	1	469	0	0	0	0
85	2	125	0	0	0	0
85	3	14	0	0	0	0
85	4	22	0	0	0	0
85	5	502	0	0	0	0
85	6	150	0	0	0	0
85	7	17	0	0	0	0
85	8	15	0	0	0	0
85	D0	1	0	0	0	0
85	D3	1	0	0	0	0
85	L2	3	0	0	0	0
85	L3	2	0	0	0	0
85	L4	2	0	0	0	0
85	L5	1	0	0	0	0
85	L7	3	0	0	0	0
85	L8	1	0	0	0	0
85	M0	2	0	0	0	0
85	M1	1	0	0	0	0
85	M3	3	0	0	0	0
85	M4	1	0	0	0	0
85	M5	3	0	0	0	0
85	M6	1	0	0	0	0
85	M7	3	0	0	0	0
85	M8	1	0	0	0	0
85	M9	1	0	0	0	0
85	N0	1	0	0	0	0
85	N3	3	0	0	0	0
85	N5	1	0	0	0	0
85	N6	1	0	0	0	0
85	N8	5	0	0	0	0
85	N9	1	0	0	0	0
85	O1	1	0	0	0	0
85	O3	1	0	0	0	0
85	O4	1	0	0	0	0
85	O7	2	0	0	0	0
85	S8	1	0	0	0	0
85	SM	1	0	0	0	0
85	c7	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	c8	2	0	0	0	0
85	d3	2	0	0	0	0
85	d6	1	0	0	0	0
85	l2	3	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	1	0	0	0	0
85	l8	1	0	0	0	0
85	l9	1	0	0	0	0
85	m0	1	0	0	0	0
85	m1	2	0	0	0	0
85	m5	4	0	0	0	0
85	m6	1	0	0	0	0
85	m7	5	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	5	0	0	0	0
85	n9	1	0	0	0	0
85	o1	1	0	0	0	0
85	o3	1	0	0	0	0
85	o4	2	0	0	0	0
85	q0	1	0	0	0	0
85	q3	1	0	0	0	0
85	s1	1	0	0	0	0
85	s8	2	0	0	0	0
85	sM	2	0	0	0	0
86	1	2422	0	0	309	0
86	2	1099	0	0	150	0
86	3	77	0	0	9	0
86	4	112	0	0	7	0
86	5	2478	0	0	252	0
86	6	1120	0	0	119	0
86	7	84	0	0	9	0
86	8	112	0	0	22	0
86	C1	7	0	0	6	0
86	C3	7	0	0	0	0
86	C5	7	0	0	4	0
86	C8	7	0	0	0	0
86	D9	7	0	0	1	0
86	L3	21	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	L4	7	0	0	1	0
86	M0	7	0	0	0	0
86	M5	7	0	0	1	0
86	M6	7	0	0	0	0
86	M7	14	0	0	2	0
86	M8	7	0	0	0	0
86	M9	7	0	0	1	0
86	N9	7	0	0	0	0
86	O2	7	0	0	0	0
86	O3	7	0	0	2	0
86	O7	14	0	0	6	0
86	O9	7	0	0	3	0
86	Q2	7	0	0	3	0
86	S8	7	0	0	1	0
86	S9	7	0	0	2	0
86	SR	7	0	0	0	0
86	c3	7	0	0	1	0
86	c5	7	0	0	1	0
86	c8	7	0	0	0	0
86	d4	7	0	0	1	0
86	d9	7	0	0	0	0
86	l3	14	0	0	1	0
86	l4	14	0	0	3	0
86	l5	21	0	0	0	0
86	l9	7	0	0	0	0
86	m0	14	0	0	2	0
86	m1	7	0	0	2	0
86	m5	7	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	1	0
86	n3	7	0	0	0	0
86	n6	7	0	0	0	0
86	n9	7	0	0	0	0
86	o3	7	0	0	1	0
86	o7	7	0	0	1	0
86	q1	7	0	0	6	0
86	q2	7	0	0	2	0
86	s1	14	0	0	1	0
86	s4	7	0	0	0	0
86	s8	7	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	sR	7	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	0	0
87	Q2	1	0	0	1	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	0	0
87	q2	1	0	0	0	0
87	q3	1	0	0	0	0
88	1	26	0	21	3	0
88	5	26	0	22	2	0
All	All	411206	0	297306	11436	1

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 16.

The worst 5 of 11436 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)
52:m6:66:LYS:NZ	52:m6:66:LYS:CE	1.68	1.52
78:Q2:17:CYS:SG	78:Q2:17:CYS:CB	2.10	1.39
40:l3:41:VAL:HA	40:l3:185:GLY:HA3	1.24	1.18
42:l5:152:ARG:HH11	42:l5:152:ARG:HG3	1.12	1.11
36:1:3182:G:OP1	52:M6:160:ARG:NH2	1.87	1.06

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1353:U:O2'	36:5:3165:A:OP1[2_546]	2.14	0.06

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	145 (71%)	36 (18%)	23 (11%)	0	1
2	s0	204/251 (81%)	151 (74%)	28 (14%)	25 (12%)	0	1
3	S1	212/254 (84%)	144 (68%)	40 (19%)	28 (13%)	0	1
3	s1	214/254 (84%)	169 (79%)	31 (14%)	14 (6%)	1	5
4	S2	215/253 (85%)	180 (84%)	23 (11%)	12 (6%)	1	8
4	s2	215/253 (85%)	183 (85%)	20 (9%)	12 (6%)	1	8
5	S3	221/239 (92%)	175 (79%)	32 (14%)	14 (6%)	1	6
5	s3	221/239 (92%)	182 (82%)	22 (10%)	17 (8%)	1	4
6	S4	258/260 (99%)	202 (78%)	36 (14%)	20 (8%)	1	4
6	s4	258/260 (99%)	211 (82%)	31 (12%)	16 (6%)	1	6
7	S5	204/224 (91%)	158 (78%)	25 (12%)	21 (10%)	0	2
7	s5	204/224 (91%)	152 (74%)	37 (18%)	15 (7%)	1	4
8	S6	224/236 (95%)	187 (84%)	28 (12%)	9 (4%)	2	14
8	s6	216/236 (92%)	180 (83%)	26 (12%)	10 (5%)	2	11
9	S7	182/189 (96%)	136 (75%)	28 (15%)	18 (10%)	0	2
9	s7	184/189 (97%)	133 (72%)	37 (20%)	14 (8%)	1	4
10	S8	184/200 (92%)	160 (87%)	16 (9%)	8 (4%)	2	12
10	s8	184/200 (92%)	157 (85%)	18 (10%)	9 (5%)	1	10
11	S9	183/196 (93%)	150 (82%)	25 (14%)	8 (4%)	2	12
11	s9	183/196 (93%)	143 (78%)	28 (15%)	12 (7%)	1	5
12	C0	94/105 (90%)	69 (73%)	16 (17%)	9 (10%)	0	2
12	c0	92/105 (88%)	67 (73%)	9 (10%)	16 (17%)	0	0
13	C1	153/155 (99%)	123 (80%)	19 (12%)	11 (7%)	1	4
13	c1	144/155 (93%)	121 (84%)	13 (9%)	10 (7%)	1	5
14	C2	122/142 (86%)	70 (57%)	28 (23%)	24 (20%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	c2	122/142 (86%)	73 (60%)	32 (26%)	17 (14%)	0	1
15	C3	148/150 (99%)	120 (81%)	22 (15%)	6 (4%)	2	13
15	c3	148/150 (99%)	117 (79%)	20 (14%)	11 (7%)	1	4
16	C4	125/136 (92%)	81 (65%)	28 (22%)	16 (13%)	0	1
16	c4	126/136 (93%)	99 (79%)	14 (11%)	13 (10%)	0	2
17	C5	122/141 (86%)	91 (75%)	18 (15%)	13 (11%)	0	2
17	c5	133/141 (94%)	95 (71%)	20 (15%)	18 (14%)	0	1
18	C6	139/142 (98%)	111 (80%)	14 (10%)	14 (10%)	0	2
18	c6	140/142 (99%)	115 (82%)	17 (12%)	8 (6%)	1	8
19	C7	116/136 (85%)	86 (74%)	18 (16%)	12 (10%)	0	2
19	c7	113/136 (83%)	86 (76%)	20 (18%)	7 (6%)	1	6
20	C8	143/145 (99%)	110 (77%)	20 (14%)	13 (9%)	0	2
20	c8	143/145 (99%)	112 (78%)	22 (15%)	9 (6%)	1	6
21	C9	141/143 (99%)	116 (82%)	17 (12%)	8 (6%)	1	8
21	c9	141/143 (99%)	120 (85%)	18 (13%)	3 (2%)	5	27
22	D0	105/120 (88%)	81 (77%)	16 (15%)	8 (8%)	1	4
22	d0	108/120 (90%)	80 (74%)	19 (18%)	9 (8%)	0	3
23	D1	85/87 (98%)	62 (73%)	15 (18%)	8 (9%)	0	2
23	d1	85/87 (98%)	68 (80%)	9 (11%)	8 (9%)	0	2
24	D2	127/129 (98%)	100 (79%)	23 (18%)	4 (3%)	3	19
24	d2	127/129 (98%)	112 (88%)	13 (10%)	2 (2%)	7	34
25	D3	142/144 (99%)	112 (79%)	17 (12%)	13 (9%)	0	2
25	d3	142/144 (99%)	121 (85%)	16 (11%)	5 (4%)	3	16
26	D4	132/134 (98%)	108 (82%)	17 (13%)	7 (5%)	1	9
26	d4	132/134 (98%)	104 (79%)	16 (12%)	12 (9%)	0	2
27	D5	68/107 (64%)	46 (68%)	13 (19%)	9 (13%)	0	1
27	d5	67/107 (63%)	52 (78%)	12 (18%)	3 (4%)	2	12
28	D6	95/97 (98%)	55 (58%)	24 (25%)	16 (17%)	0	0
28	d6	95/97 (98%)	73 (77%)	12 (13%)	10 (10%)	0	2
29	D7	79/81 (98%)	60 (76%)	14 (18%)	5 (6%)	1	6
29	d7	79/81 (98%)	63 (80%)	9 (11%)	7 (9%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	D8	61/66 (92%)	47 (77%)	12 (20%)	2 (3%)	3	17
30	d8	61/66 (92%)	44 (72%)	13 (21%)	4 (7%)	1	5
31	D9	51/55 (93%)	43 (84%)	5 (10%)	3 (6%)	1	7
31	d9	51/55 (93%)	37 (72%)	9 (18%)	5 (10%)	0	2
32	E0	58/60 (97%)	44 (76%)	11 (19%)	3 (5%)	1	9
33	E1	69/76 (91%)	30 (44%)	19 (28%)	20 (29%)	0	0
33	e1	74/76 (97%)	37 (50%)	16 (22%)	21 (28%)	0	0
34	SR	316/318 (99%)	263 (83%)	45 (14%)	8 (2%)	4	23
34	sR	316/318 (99%)	256 (81%)	48 (15%)	12 (4%)	2	15
35	SM	155/273 (57%)	103 (66%)	29 (19%)	23 (15%)	0	0
35	sM	98/273 (36%)	57 (58%)	28 (29%)	13 (13%)	0	1
39	L2	250/253 (99%)	222 (89%)	19 (8%)	9 (4%)	2	16
39	l2	250/253 (99%)	211 (84%)	29 (12%)	10 (4%)	2	14
40	L3	384/386 (100%)	339 (88%)	29 (8%)	16 (4%)	2	13
40	l3	384/386 (100%)	342 (89%)	29 (8%)	13 (3%)	3	17
41	L4	359/361 (99%)	301 (84%)	39 (11%)	19 (5%)	1	9
41	l4	359/361 (99%)	303 (84%)	36 (10%)	20 (6%)	1	8
42	L5	294/296 (99%)	235 (80%)	37 (13%)	22 (8%)	1	4
42	l5	292/296 (99%)	247 (85%)	34 (12%)	11 (4%)	2	15
43	L6	152/175 (87%)	137 (90%)	12 (8%)	3 (2%)	6	28
43	l6	153/175 (87%)	129 (84%)	20 (13%)	4 (3%)	4	23
44	L7	220/243 (90%)	192 (87%)	20 (9%)	8 (4%)	2	16
44	l7	221/243 (91%)	201 (91%)	14 (6%)	6 (3%)	4	22
45	L8	231/255 (91%)	188 (81%)	36 (16%)	7 (3%)	3	19
45	l8	229/255 (90%)	180 (79%)	33 (14%)	16 (7%)	1	4
46	L9	189/191 (99%)	164 (87%)	21 (11%)	4 (2%)	5	27
46	l9	189/191 (99%)	169 (89%)	16 (8%)	4 (2%)	5	27
47	M0	207/220 (94%)	174 (84%)	25 (12%)	8 (4%)	2	14
47	m0	209/220 (95%)	167 (80%)	26 (12%)	16 (8%)	1	4
48	M1	167/173 (96%)	130 (78%)	21 (13%)	16 (10%)	0	2
48	m1	167/173 (96%)	139 (83%)	17 (10%)	11 (7%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	M3	191/198 (96%)	165 (86%)	17 (9%)	9 (5%)	2	11
49	m3	192/198 (97%)	152 (79%)	26 (14%)	14 (7%)	1	4
50	M4	134/137 (98%)	114 (85%)	10 (8%)	10 (8%)	1	4
50	m4	135/137 (98%)	122 (90%)	11 (8%)	2 (2%)	8	35
51	M5	201/203 (99%)	179 (89%)	17 (8%)	5 (2%)	4	23
51	m5	201/203 (99%)	180 (90%)	16 (8%)	5 (2%)	4	23
52	M6	195/198 (98%)	182 (93%)	10 (5%)	3 (2%)	8	35
52	m6	195/198 (98%)	172 (88%)	15 (8%)	8 (4%)	2	13
53	M7	181/183 (99%)	149 (82%)	21 (12%)	11 (6%)	1	7
53	m7	153/183 (84%)	133 (87%)	17 (11%)	3 (2%)	6	28
54	M8	183/185 (99%)	161 (88%)	16 (9%)	6 (3%)	3	17
54	m8	183/185 (99%)	148 (81%)	24 (13%)	11 (6%)	1	7
55	M9	186/188 (99%)	162 (87%)	21 (11%)	3 (2%)	7	34
55	m9	186/188 (99%)	156 (84%)	25 (13%)	5 (3%)	4	22
56	N0	170/172 (99%)	154 (91%)	14 (8%)	2 (1%)	10	40
56	n0	170/172 (99%)	153 (90%)	15 (9%)	2 (1%)	10	40
57	N1	157/159 (99%)	135 (86%)	13 (8%)	9 (6%)	1	8
57	n1	157/159 (99%)	140 (89%)	11 (7%)	6 (4%)	2	15
58	N2	98/120 (82%)	75 (76%)	18 (18%)	5 (5%)	1	10
58	n2	96/120 (80%)	77 (80%)	16 (17%)	3 (3%)	3	19
59	N3	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	8	35
59	n3	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
60	N4	96/155 (62%)	72 (75%)	16 (17%)	8 (8%)	0	3
60	n4	133/155 (86%)	101 (76%)	21 (16%)	11 (8%)	0	3
61	N5	119/141 (84%)	100 (84%)	17 (14%)	2 (2%)	7	32
61	n5	118/141 (84%)	103 (87%)	7 (6%)	8 (7%)	1	5
62	N6	124/126 (98%)	114 (92%)	8 (6%)	2 (2%)	7	34
62	n6	124/126 (98%)	109 (88%)	12 (10%)	3 (2%)	4	24
63	N7	133/135 (98%)	102 (77%)	21 (16%)	10 (8%)	1	4
63	n7	133/135 (98%)	101 (76%)	20 (15%)	12 (9%)	0	3
64	N8	146/148 (99%)	121 (83%)	18 (12%)	7 (5%)	2	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	n8	146/148 (99%)	128 (88%)	14 (10%)	4 (3%)	4	22
65	N9	56/58 (97%)	43 (77%)	12 (21%)	1 (2%)	6	31
65	n9	56/58 (97%)	40 (71%)	9 (16%)	7 (12%)	0	1
66	O0	95/104 (91%)	88 (93%)	5 (5%)	2 (2%)	5	27
66	o0	98/104 (94%)	88 (90%)	8 (8%)	2 (2%)	6	28
67	O1	107/112 (96%)	95 (89%)	8 (8%)	4 (4%)	2	15
67	o1	107/112 (96%)	86 (80%)	14 (13%)	7 (6%)	1	5
68	O2	125/129 (97%)	113 (90%)	11 (9%)	1 (1%)	16	50
68	o2	125/129 (97%)	108 (86%)	12 (10%)	5 (4%)	2	14
69	O3	104/106 (98%)	95 (91%)	8 (8%)	1 (1%)	12	45
69	o3	104/106 (98%)	98 (94%)	4 (4%)	2 (2%)	6	30
70	O4	110/119 (92%)	100 (91%)	6 (6%)	4 (4%)	2	16
70	o4	110/119 (92%)	99 (90%)	7 (6%)	4 (4%)	2	16
71	O5	117/119 (98%)	108 (92%)	7 (6%)	2 (2%)	7	32
71	o5	117/119 (98%)	104 (89%)	7 (6%)	6 (5%)	1	10
72	O6	97/99 (98%)	79 (81%)	13 (13%)	5 (5%)	1	9
72	o6	97/99 (98%)	85 (88%)	10 (10%)	2 (2%)	5	27
73	O7	85/87 (98%)	71 (84%)	11 (13%)	3 (4%)	3	16
73	o7	85/87 (98%)	73 (86%)	10 (12%)	2 (2%)	4	24
74	O8	75/77 (97%)	62 (83%)	9 (12%)	4 (5%)	1	9
74	o8	75/77 (97%)	57 (76%)	15 (20%)	3 (4%)	2	14
75	O9	48/50 (96%)	42 (88%)	4 (8%)	2 (4%)	2	13
75	o9	48/50 (96%)	45 (94%)	2 (4%)	1 (2%)	5	27
76	Q0	50/52 (96%)	47 (94%)	1 (2%)	2 (4%)	2	14
76	q0	50/52 (96%)	46 (92%)	3 (6%)	1 (2%)	6	28
77	Q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	2	12
77	q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
78	Q2	103/105 (98%)	84 (82%)	12 (12%)	7 (7%)	1	5
78	q2	103/105 (98%)	91 (88%)	12 (12%)	0	100	100
79	Q3	89/91 (98%)	74 (83%)	11 (12%)	4 (4%)	2	12
79	q3	89/91 (98%)	80 (90%)	7 (8%)	2 (2%)	5	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	e0	60/62 (97%)	46 (77%)	8 (13%)	6 (10%)	0	2
82	p0	139/311 (45%)	113 (81%)	22 (16%)	4 (3%)	3	20
All	All	22333/24141 (92%)	18316 (82%)	2723 (12%)	1294 (6%)	1	8

5 of 1294 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	5	ALA
2	S0	30	GLN
2	S0	39	ASN
2	S0	66	ALA

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%)	130 (79%)	34 (21%)	1	7
2	s0	165/209 (79%)	118 (72%)	47 (28%)	0	2
3	S1	191/223 (86%)	148 (78%)	43 (22%)	1	5
3	s1	192/223 (86%)	151 (79%)	41 (21%)	1	6
4	S2	176/204 (86%)	131 (74%)	45 (26%)	0	3
4	s2	176/204 (86%)	126 (72%)	50 (28%)	0	2
5	S3	182/194 (94%)	131 (72%)	51 (28%)	0	2
5	s3	182/194 (94%)	149 (82%)	33 (18%)	2	9
6	S4	221/221 (100%)	172 (78%)	49 (22%)	1	5
6	s4	221/221 (100%)	180 (81%)	41 (19%)	1	9
7	S5	173/190 (91%)	137 (79%)	36 (21%)	1	7
7	s5	173/190 (91%)	132 (76%)	41 (24%)	1	4
8	S6	188/201 (94%)	145 (77%)	43 (23%)	1	5
8	s6	187/201 (93%)	148 (79%)	39 (21%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	S7	165/169 (98%)	128 (78%)	37 (22%)	1	5
9	s7	165/169 (98%)	131 (79%)	34 (21%)	1	7
10	S8	150/161 (93%)	130 (87%)	20 (13%)	4	18
10	s8	150/161 (93%)	126 (84%)	24 (16%)	2	12
11	S9	158/165 (96%)	116 (73%)	42 (27%)	0	3
11	s9	158/165 (96%)	125 (79%)	33 (21%)	1	7
12	C0	77/98 (79%)	58 (75%)	19 (25%)	1	4
12	c0	73/98 (74%)	60 (82%)	13 (18%)	2	10
13	C1	129/136 (95%)	106 (82%)	23 (18%)	2	10
13	c1	129/136 (95%)	99 (77%)	30 (23%)	1	4
14	C2	88/118 (75%)	62 (70%)	26 (30%)	0	2
14	c2	88/118 (75%)	63 (72%)	25 (28%)	0	2
15	C3	127/127 (100%)	102 (80%)	25 (20%)	1	8
15	c3	127/127 (100%)	103 (81%)	24 (19%)	1	9
16	C4	81/104 (78%)	54 (67%)	27 (33%)	0	1
16	c4	97/104 (93%)	72 (74%)	25 (26%)	0	3
17	C5	101/117 (86%)	78 (77%)	23 (23%)	1	5
17	c5	103/117 (88%)	85 (82%)	18 (18%)	2	10
18	C6	117/118 (99%)	86 (74%)	31 (26%)	0	3
18	c6	118/118 (100%)	90 (76%)	28 (24%)	1	4
19	C7	94/124 (76%)	76 (81%)	18 (19%)	1	8
19	c7	92/124 (74%)	71 (77%)	21 (23%)	1	5
20	C8	128/128 (100%)	97 (76%)	31 (24%)	1	4
20	c8	128/128 (100%)	94 (73%)	34 (27%)	0	3
21	C9	115/115 (100%)	88 (76%)	27 (24%)	1	4
21	c9	115/115 (100%)	95 (83%)	20 (17%)	2	10
22	D0	100/113 (88%)	69 (69%)	31 (31%)	0	1
22	d0	103/113 (91%)	76 (74%)	27 (26%)	0	3
23	D1	74/74 (100%)	59 (80%)	15 (20%)	1	7
23	d1	74/74 (100%)	60 (81%)	14 (19%)	1	9
24	D2	110/110 (100%)	83 (76%)	27 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	d2	110/110 (100%)	93 (84%)	17 (16%)	2	13
25	D3	119/119 (100%)	97 (82%)	22 (18%)	1	9
25	d3	119/119 (100%)	94 (79%)	25 (21%)	1	6
26	D4	112/112 (100%)	86 (77%)	26 (23%)	1	4
26	d4	112/112 (100%)	88 (79%)	24 (21%)	1	6
27	D5	61/88 (69%)	42 (69%)	19 (31%)	0	1
27	d5	61/88 (69%)	52 (85%)	9 (15%)	3	15
28	D6	83/83 (100%)	63 (76%)	20 (24%)	1	4
28	d6	83/83 (100%)	68 (82%)	15 (18%)	2	9
29	D7	70/70 (100%)	59 (84%)	11 (16%)	2	13
29	d7	70/70 (100%)	53 (76%)	17 (24%)	1	4
30	D8	56/59 (95%)	39 (70%)	17 (30%)	0	1
30	d8	56/59 (95%)	48 (86%)	8 (14%)	3	16
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2	11
31	d9	47/48 (98%)	36 (77%)	11 (23%)	1	4
32	E0	51/51 (100%)	36 (71%)	15 (29%)	0	2
33	E1	62/66 (94%)	39 (63%)	23 (37%)	0	1
33	e1	66/66 (100%)	45 (68%)	21 (32%)	0	1
34	SR	260/261 (100%)	218 (84%)	42 (16%)	2	12
34	sR	260/261 (100%)	226 (87%)	34 (13%)	4	19
35	SM	97/228 (42%)	67 (69%)	30 (31%)	0	1
35	sM	54/228 (24%)	44 (82%)	10 (18%)	1	9
39	L2	193/195 (99%)	151 (78%)	42 (22%)	1	6
39	l2	192/195 (98%)	141 (73%)	51 (27%)	0	3
40	L3	320/322 (99%)	246 (77%)	74 (23%)	1	5
40	l3	320/322 (99%)	246 (77%)	74 (23%)	1	5
41	L4	288/288 (100%)	214 (74%)	74 (26%)	0	3
41	l4	288/288 (100%)	217 (75%)	71 (25%)	1	4
42	L5	244/244 (100%)	189 (78%)	55 (22%)	1	5
42	l5	243/244 (100%)	187 (77%)	56 (23%)	1	5
43	L6	134/152 (88%)	104 (78%)	30 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	l6	135/152 (89%)	105 (78%)	30 (22%)	1	5
44	L7	186/204 (91%)	157 (84%)	29 (16%)	2	13
44	l7	187/204 (92%)	157 (84%)	30 (16%)	2	12
45	L8	187/207 (90%)	155 (83%)	32 (17%)	2	11
45	l8	177/207 (86%)	143 (81%)	34 (19%)	1	8
46	L9	171/171 (100%)	124 (72%)	47 (28%)	0	2
46	l9	171/171 (100%)	130 (76%)	41 (24%)	1	4
47	M0	177/186 (95%)	135 (76%)	42 (24%)	1	4
47	m0	179/186 (96%)	135 (75%)	44 (25%)	1	4
48	M1	147/150 (98%)	113 (77%)	34 (23%)	1	5
48	m1	147/150 (98%)	111 (76%)	36 (24%)	1	4
49	M3	154/158 (98%)	127 (82%)	27 (18%)	2	10
49	m3	154/158 (98%)	124 (80%)	30 (20%)	1	8
50	M4	107/108 (99%)	86 (80%)	21 (20%)	1	8
50	m4	108/108 (100%)	85 (79%)	23 (21%)	1	6
51	M5	175/175 (100%)	145 (83%)	30 (17%)	2	11
51	m5	175/175 (100%)	146 (83%)	29 (17%)	2	12
52	M6	160/161 (99%)	131 (82%)	29 (18%)	2	9
52	m6	160/161 (99%)	120 (75%)	40 (25%)	0	3
53	M7	140/145 (97%)	106 (76%)	34 (24%)	1	4
53	m7	125/145 (86%)	91 (73%)	34 (27%)	0	2
54	M8	150/150 (100%)	118 (79%)	32 (21%)	1	6
54	m8	150/150 (100%)	114 (76%)	36 (24%)	1	4
55	M9	153/153 (100%)	123 (80%)	30 (20%)	1	8
55	m9	153/153 (100%)	114 (74%)	39 (26%)	0	3
56	N0	156/156 (100%)	125 (80%)	31 (20%)	1	7
56	n0	156/156 (100%)	128 (82%)	28 (18%)	2	10
57	N1	136/136 (100%)	100 (74%)	36 (26%)	0	3
57	n1	136/136 (100%)	106 (78%)	30 (22%)	1	5
58	N2	87/106 (82%)	73 (84%)	14 (16%)	2	12
58	n2	85/106 (80%)	72 (85%)	13 (15%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	N3	104/104 (100%)	79 (76%)	25 (24%)	1	4
59	n3	104/104 (100%)	85 (82%)	19 (18%)	2	9
60	N4	57/129 (44%)	51 (90%)	6 (10%)	6	27
60	n4	100/129 (78%)	82 (82%)	18 (18%)	2	10
61	N5	104/117 (89%)	79 (76%)	25 (24%)	1	4
61	n5	104/117 (89%)	83 (80%)	21 (20%)	1	7
62	N6	109/109 (100%)	75 (69%)	34 (31%)	0	1
62	n6	109/109 (100%)	83 (76%)	26 (24%)	1	4
63	N7	115/115 (100%)	81 (70%)	34 (30%)	0	2
63	n7	115/115 (100%)	79 (69%)	36 (31%)	0	1
64	N8	118/118 (100%)	94 (80%)	24 (20%)	1	7
64	n8	118/118 (100%)	95 (80%)	23 (20%)	1	8
65	N9	46/46 (100%)	32 (70%)	14 (30%)	0	1
65	n9	46/46 (100%)	30 (65%)	16 (35%)	0	1
66	O0	81/87 (93%)	67 (83%)	14 (17%)	2	10
66	o0	84/87 (97%)	62 (74%)	22 (26%)	0	3
67	O1	92/96 (96%)	71 (77%)	21 (23%)	1	5
67	o1	94/96 (98%)	71 (76%)	23 (24%)	1	4
68	O2	109/110 (99%)	83 (76%)	26 (24%)	1	4
68	o2	109/110 (99%)	84 (77%)	25 (23%)	1	5
69	O3	90/90 (100%)	76 (84%)	14 (16%)	2	13
69	o3	90/90 (100%)	73 (81%)	17 (19%)	1	9
70	O4	95/101 (94%)	78 (82%)	17 (18%)	2	10
70	o4	95/101 (94%)	79 (83%)	16 (17%)	2	11
71	O5	104/104 (100%)	74 (71%)	30 (29%)	0	2
71	o5	103/104 (99%)	81 (79%)	22 (21%)	1	6
72	O6	81/81 (100%)	55 (68%)	26 (32%)	0	1
72	o6	80/81 (99%)	54 (68%)	26 (32%)	0	1
73	O7	70/70 (100%)	59 (84%)	11 (16%)	2	13
73	o7	70/70 (100%)	58 (83%)	12 (17%)	2	11
74	O8	68/68 (100%)	51 (75%)	17 (25%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	o8	67/68 (98%)	47 (70%)	20 (30%)	0	2
75	O9	45/45 (100%)	35 (78%)	10 (22%)	1	5
75	o9	45/45 (100%)	32 (71%)	13 (29%)	0	2
76	Q0	47/47 (100%)	35 (74%)	12 (26%)	0	3
76	q0	47/47 (100%)	36 (77%)	11 (23%)	1	4
77	Q1	23/23 (100%)	15 (65%)	8 (35%)	0	1
77	q1	23/23 (100%)	14 (61%)	9 (39%)	0	1
78	Q2	90/90 (100%)	69 (77%)	21 (23%)	1	4
78	q2	90/90 (100%)	73 (81%)	17 (19%)	1	9
79	Q3	71/71 (100%)	53 (75%)	18 (25%)	0	3
79	q3	71/71 (100%)	55 (78%)	16 (22%)	1	5
80	e0	53/53 (100%)	40 (76%)	13 (24%)	1	4
82	p0	105/253 (42%)	81 (77%)	24 (23%)	1	5
All	All	18728/20239 (92%)	14555 (78%)	4173 (22%)	1	5

5 of 4173 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
57	n1	71	SER
62	n6	66	GLN
57	n1	35	LYS
82	p0	57	THR
53	M7	181	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 182 such sidechains are listed below:

Mol	Chain	Res	Type
18	c6	74	HIS
41	l4	48	GLN
20	c8	89	GLN
28	d6	80	HIS
44	l7	194	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	517 (29%)	56 (3%)
1	6	1792/1800 (99%)	466 (26%)	53 (2%)
36	1	3145/3396 (92%)	711 (22%)	92 (2%)
36	5	3145/3396 (92%)	723 (22%)	94 (2%)
37	3	120/121 (99%)	24 (20%)	2 (1%)
37	7	120/121 (99%)	23 (19%)	1 (0%)
38	4	157/158 (99%)	41 (26%)	4 (2%)
38	8	157/158 (99%)	41 (26%)	4 (2%)
All	All	10383/10950 (94%)	2546 (24%)	306 (2%)

5 of 2546 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A

5 of 306 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	5	1027	A
36	5	3078	U
36	5	1238	C
36	5	2112	U
36	5	3357	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2562 ligands modelled in this entry, 1429 are monoatomic - leaving 1133 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	1	3991	-	0,6,6	-	-	-		
86	OHX	1	3957	-	0,6,6	-	-	-		
86	OHX	1	3863	-	0,6,6	-	-	-		
86	OHX	5	3904	-	0,6,6	-	-	-		
86	OHX	2	2155	-	0,6,6	-	-	-		
86	OHX	1	3964	-	0,6,6	-	-	-		
86	OHX	1	3905	-	0,6,6	-	-	-		
86	OHX	6	2139	-	0,6,6	-	-	-		
86	OHX	L4	403	-	0,6,6	-	-	-		
86	OHX	5	4161	-	0,6,6	-	-	-		
86	OHX	1	4092	-	0,6,6	-	-	-		
86	OHX	5	4175	-	0,6,6	-	-	-		
86	OHX	15	303	-	0,6,6	-	-	-		
86	OHX	1	3966	-	0,6,6	-	-	-		
86	OHX	5	3949	-	0,6,6	-	-	-		
86	OHX	6	2172	-	0,6,6	-	-	-		
86	OHX	1	4161	-	0,6,6	-	-	-		
86	OHX	5	4240	-	0,6,6	-	-	-		
86	OHX	5	4208	-	0,6,6	-	-	-		
86	OHX	5	4163	-	0,6,6	-	-	-		
86	OHX	1	4070	-	0,6,6	-	-	-		
86	OHX	1	4139	-	0,6,6	-	-	-		
86	OHX	4	223	-	0,6,6	-	-	-		
86	OHX	1	3938	-	0,6,6	-	-	-		
86	OHX	5	3964	-	0,6,6	-	-	-		
86	OHX	3	221	-	0,6,6	-	-	-		
86	OHX	5	4245	-	0,6,6	-	-	-		
86	OHX	5	4035	-	0,6,6	-	-	-		
86	OHX	2	2025	-	0,6,6	-	-	-		
86	OHX	1	3970	-	0,6,6	-	-	-		
86	OHX	5	4072	-	0,6,6	-	-	-		
86	OHX	1	4194	-	0,6,6	-	-	-		
86	OHX	5	4126	-	0,6,6	-	-	-		
86	OHX	1	3962	-	0,6,6	-	-	-		
86	OHX	5	4187	-	0,6,6	-	-	-		
86	OHX	8	228	-	0,6,6	-	-	-		
86	OHX	2	2050	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3925	-	0,6,6	-	-	-		
86	OHX	2	2033	-	0,6,6	-	-	-		
86	OHX	1	3986	-	0,6,6	-	-	-		
86	OHX	6	2167	-	0,6,6	-	-	-		
86	OHX	5	3921	-	0,6,6	-	-	-		
86	OHX	1	3922	-	0,6,6	-	-	-		
86	OHX	5	4145	-	0,6,6	-	-	-		
86	OHX	3	219	-	0,6,6	-	-	-		
86	OHX	s1	302	-	0,6,6	-	-	-		
86	OHX	5	3902	-	0,6,6	-	-	-		
86	OHX	5	4141	-	0,6,6	-	-	-		
86	OHX	1	3864	-	0,6,6	-	-	-		
86	OHX	5	4140	-	0,6,6	-	-	-		
86	OHX	6	2126	-	0,6,6	-	-	-		
86	OHX	1	3980	-	0,6,6	-	-	-		
86	OHX	1	4145	-	0,6,6	-	-	-		
86	OHX	5	4151	-	0,6,6	-	-	-		
86	OHX	5	4124	-	0,6,6	-	-	-		
86	OHX	1	4208	-	0,6,6	-	-	-		
88	3J2	5	4254	-	29,30,30	0.90	1 (3%)	35,52,52	1.60	6 (17%)
86	OHX	5	4242	-	0,6,6	-	-	-		
86	OHX	5	4121	-	0,6,6	-	-	-		
86	OHX	1	3891	-	0,6,6	-	-	-		
86	OHX	1	4068	-	0,6,6	-	-	-		
86	OHX	1	4047	-	0,6,6	-	-	-		
86	OHX	5	4056	-	0,6,6	-	-	-		
86	OHX	5	4080	-	0,6,6	-	-	-		
86	OHX	1	4063	-	0,6,6	-	-	-		
86	OHX	1	3912	-	0,6,6	-	-	-		
86	OHX	5	3919	-	0,6,6	-	-	-		
86	OHX	6	2103	-	0,6,6	-	-	-		
86	OHX	c5	201	-	0,6,6	-	-	-		
86	OHX	5	4246	-	0,6,6	-	-	-		
86	OHX	2	2079	-	0,6,6	-	-	-		
86	OHX	1	4167	-	0,6,6	-	-	-		
86	OHX	6	2159	-	0,6,6	-	-	-		
86	OHX	5	4172	-	0,6,6	-	-	-		
86	OHX	5	4201	-	0,6,6	-	-	-		
86	OHX	1	3921	-	0,6,6	-	-	-		
86	OHX	1	4170	-	0,6,6	-	-	-		
86	OHX	1	4086	-	0,6,6	-	-	-		
86	OHX	6	2069	-	0,6,6	-	-	-		
86	OHX	6	2156	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3958	-	0,6,6	-	-	-		
86	OHX	2	2168	-	0,6,6	-	-	-		
86	OHX	1	3990	-	0,6,6	-	-	-		
86	OHX	M6	202	-	0,6,6	-	-	-		
86	OHX	6	2090	-	0,6,6	-	-	-		
86	OHX	5	4058	-	0,6,6	-	-	-		
86	OHX	5	4243	-	0,6,6	-	-	-		
86	OHX	2	2109	-	0,6,6	-	-	-		
86	OHX	2	2040	-	0,6,6	-	-	-		
86	OHX	1	4166	-	0,6,6	-	-	-		
86	OHX	O2	201	-	0,6,6	-	-	-		
86	OHX	5	4052	-	0,6,6	-	-	-		
88	3J2	1	4209	-	29,30,30	1.34	3 (10%)	35,52,52	1.62	4 (11%)
86	OHX	4	235	-	0,6,6	-	-	-		
86	OHX	5	3973	-	0,6,6	-	-	-		
86	OHX	1	3954	-	0,6,6	-	-	-		
86	OHX	6	2194	-	0,6,6	-	-	-		
86	OHX	5	4235	-	0,6,6	-	-	-		
86	OHX	1	4157	-	0,6,6	-	-	-		
86	OHX	1	4014	-	0,6,6	-	-	-		
86	OHX	5	4182	-	0,6,6	-	-	-		
86	OHX	1	4101	-	0,6,6	-	-	-		
86	OHX	5	3936	-	0,6,6	-	-	-		
86	OHX	1	4080	-	0,6,6	-	-	-		
86	OHX	5	4032	-	0,6,6	-	-	-		
86	OHX	5	4045	-	0,6,6	-	-	-		
86	OHX	2	2084	-	0,6,6	-	-	-		
86	OHX	5	4122	-	0,6,6	-	-	-		
86	OHX	2	2094	-	0,6,6	-	-	-		
86	OHX	1	3989	-	0,6,6	-	-	-		
86	OHX	5	4222	-	0,6,6	-	-	-		
86	OHX	2	2114	-	0,6,6	-	-	-		
86	OHX	6	2165	-	0,6,6	-	-	-		
86	OHX	5	4139	-	0,6,6	-	-	-		
86	OHX	7	225	-	0,6,6	-	-	-		
86	OHX	6	2119	-	0,6,6	-	-	-		
86	OHX	5	4239	-	0,6,6	-	-	-		
86	OHX	8	216	-	0,6,6	-	-	-		
86	OHX	8	224	-	0,6,6	-	-	-		
86	OHX	1	4013	-	0,6,6	-	-	-		
86	OHX	m8	201	-	0,6,6	-	-	-		
86	OHX	6	2155	-	0,6,6	-	-	-		
86	OHX	5	4205	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4169	-	0,6,6	-	-	-		
86	OHX	1	3871	-	0,6,6	-	-	-		
86	OHX	1	3898	-	0,6,6	-	-	-		
86	OHX	6	2140	-	0,6,6	-	-	-		
86	OHX	15	304	-	0,6,6	-	-	-		
86	OHX	5	4188	-	0,6,6	-	-	-		
86	OHX	2	2103	-	0,6,6	-	-	-		
86	OHX	5	4044	-	0,6,6	-	-	-		
86	OHX	1	4009	-	0,6,6	-	-	-		
86	OHX	5	4042	-	0,6,6	-	-	-		
86	OHX	5	4022	-	0,6,6	-	-	-		
86	OHX	1	4188	-	0,6,6	-	-	-		
86	OHX	1	3952	-	0,6,6	-	-	-		
86	OHX	1	3971	-	0,6,6	-	-	-		
86	OHX	1	4040	-	0,6,6	-	-	-		
86	OHX	6	2182	-	0,6,6	-	-	-		
86	OHX	5	3986	-	0,6,6	-	-	-		
86	OHX	5	3928	-	0,6,6	-	-	-		
86	OHX	6	2197	-	0,6,6	-	-	-		
86	OHX	8	218	-	0,6,6	-	-	-		
86	OHX	1	3936	-	0,6,6	-	-	-		
86	OHX	2	2102	-	0,6,6	-	-	-		
86	OHX	2	2152	-	0,6,6	-	-	-		
86	OHX	2	2058	-	0,6,6	-	-	-		
86	OHX	1	4103	-	0,6,6	-	-	-		
86	OHX	2	2063	-	0,6,6	-	-	-		
86	OHX	2	2051	-	0,6,6	-	-	-		
86	OHX	1	3896	-	0,6,6	-	-	-		
86	OHX	6	2096	-	0,6,6	-	-	-		
86	OHX	5	3934	-	0,6,6	-	-	-		
86	OHX	5	4103	-	0,6,6	-	-	-		
86	OHX	1	4034	-	0,6,6	-	-	-		
86	OHX	1	4124	-	0,6,6	-	-	-		
86	OHX	1	4137	-	0,6,6	-	-	-		
86	OHX	2	2121	-	0,6,6	-	-	-		
86	OHX	1	4169	-	0,6,6	-	-	-		
86	OHX	1	4191	-	0,6,6	-	-	-		
86	OHX	6	2056	-	0,6,6	-	-	-		
86	OHX	6	2163	-	0,6,6	-	-	-		
86	OHX	5	4041	-	0,6,6	-	-	-		
86	OHX	5	4066	-	0,6,6	-	-	-		
86	OHX	5	4186	-	0,6,6	-	-	-		
86	OHX	6	2207	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4093	-	0,6,6	-	-	-		
86	OHX	5	4247	-	0,6,6	-	-	-		
86	OHX	1	4115	-	0,6,6	-	-	-		
86	OHX	2	2147	86	0,6,6	-	-	-		
86	OHX	5	4030	-	0,6,6	-	-	-		
86	OHX	5	3941	-	0,6,6	-	-	-		
86	OHX	6	2127	-	0,6,6	-	-	-		
86	OHX	1	4042	-	0,6,6	-	-	-		
86	OHX	1	4134	-	0,6,6	-	-	-		
86	OHX	1	3895	-	0,6,6	-	-	-		
86	OHX	2	2085	-	0,6,6	-	-	-		
86	OHX	8	226	-	0,6,6	-	-	-		
86	OHX	6	2100	-	0,6,6	-	-	-		
86	OHX	6	2105	-	0,6,6	-	-	-		
86	OHX	c8	203	-	0,6,6	-	-	-		
86	OHX	1	3928	-	0,6,6	-	-	-		
86	OHX	5	4074	-	0,6,6	-	-	-		
86	OHX	O7	105	-	0,6,6	-	-	-		
86	OHX	5	3982	-	0,6,6	-	-	-		
86	OHX	5	4127	-	0,6,6	-	-	-		
86	OHX	5	4147	-	0,6,6	-	-	-		
86	OHX	5	3988	-	0,6,6	-	-	-		
86	OHX	5	3999	-	0,6,6	-	-	-		
86	OHX	5	4097	-	0,6,6	-	-	-		
86	OHX	1	4076	-	0,6,6	-	-	-		
86	OHX	1	3982	-	0,6,6	-	-	-		
86	OHX	2	2060	-	0,6,6	-	-	-		
86	OHX	1	3919	-	0,6,6	-	-	-		
86	OHX	6	2128	-	0,6,6	-	-	-		
86	OHX	5	4006	-	0,6,6	-	-	-		
86	OHX	1	3920	-	0,6,6	-	-	-		
86	OHX	2	2032	86	0,6,6	-	-	-		
86	OHX	5	4190	-	0,6,6	-	-	-		
86	OHX	5	4142	-	0,6,6	-	-	-		
86	OHX	1	4066	-	0,6,6	-	-	-		
86	OHX	1	3973	-	0,6,6	-	-	-		
86	OHX	1	4041	-	0,6,6	-	-	-		
86	OHX	2	2024	-	0,6,6	-	-	-		
86	OHX	6	2196	-	0,6,6	-	-	-		
86	OHX	5	4108	-	0,6,6	-	-	-		
86	OHX	6	2092	-	0,6,6	-	-	-		
86	OHX	1	4030	-	0,6,6	-	-	-		
86	OHX	5	4039	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4206	-	0,6,6	-	-	-		
86	OHX	6	2070	-	0,6,6	-	-	-		
86	OHX	2	2172	-	0,6,6	-	-	-		
86	OHX	1	4000	86	0,6,6	-	-	-		
86	OHX	1	4165	-	0,6,6	-	-	-		
86	OHX	2	2175	-	0,6,6	-	-	-		
86	OHX	3	220	-	0,6,6	-	-	-		
86	OHX	1	3934	-	0,6,6	-	-	-		
86	OHX	4	233	-	0,6,6	-	-	-		
86	OHX	5	3913	-	0,6,6	-	-	-		
86	OHX	6	2166	-	0,6,6	-	-	-		
86	OHX	5	4057	-	0,6,6	-	-	-		
86	OHX	5	4250	-	0,6,6	-	-	-		
86	OHX	6	2160	-	0,6,6	-	-	-		
86	OHX	2	2036	-	0,6,6	-	-	-		
86	OHX	1	4074	-	0,6,6	-	-	-		
86	OHX	1	3868	-	0,6,6	-	-	-		
86	OHX	1	3903	-	0,6,6	-	-	-		
86	OHX	1	4147	-	0,6,6	-	-	-		
86	OHX	5	4179	-	0,6,6	-	-	-		
86	OHX	5	4218	-	0,6,6	-	-	-		
86	OHX	1	3999	-	0,6,6	-	-	-		
86	OHX	2	2090	-	0,6,6	-	-	-		
86	OHX	1	4097	-	0,6,6	-	-	-		
86	OHX	1	4177	-	0,6,6	-	-	-		
86	OHX	2	2165	-	0,6,6	-	-	-		
86	OHX	1	3881	-	0,6,6	-	-	-		
86	OHX	5	4078	-	0,6,6	-	-	-		
86	OHX	5	4116	-	0,6,6	-	-	-		
86	OHX	5	3992	-	0,6,6	-	-	-		
86	OHX	5	4049	-	0,6,6	-	-	-		
86	OHX	5	4081	-	0,6,6	-	-	-		
86	OHX	1	4116	-	0,6,6	-	-	-		
86	OHX	2	2067	-	0,6,6	-	-	-		
86	OHX	6	2071	-	0,6,6	-	-	-		
86	OHX	d4	201	-	0,6,6	-	-	-		
86	OHX	1	4190	-	0,6,6	-	-	-		
86	OHX	6	2073	-	0,6,6	-	-	-		
86	OHX	M8	202	-	0,6,6	-	-	-		
86	OHX	5	4173	-	0,6,6	-	-	-		
86	OHX	1	4158	-	0,6,6	-	-	-		
86	OHX	1	3901	-	0,6,6	-	-	-		
86	OHX	6	2149	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3952	-	0,6,6	-	-	-		
86	OHX	1	3927	-	0,6,6	-	-	-		
86	OHX	2	2028	-	0,6,6	-	-	-		
86	OHX	1	4201	-	0,6,6	-	-	-		
86	OHX	5	4204	-	0,6,6	-	-	-		
86	OHX	2	2116	-	0,6,6	-	-	-		
86	OHX	1	3960	-	0,6,6	-	-	-		
86	OHX	2	2031	-	0,6,6	-	-	-		
86	OHX	1	4039	-	0,6,6	-	-	-		
86	OHX	1	4022	-	0,6,6	-	-	-		
86	OHX	L3	405	-	0,6,6	-	-	-		
86	OHX	5	4252	-	0,6,6	-	-	-		
86	OHX	6	2184	-	0,6,6	-	-	-		
86	OHX	6	2076	-	0,6,6	-	-	-		
86	OHX	5	3998	-	0,6,6	-	-	-		
86	OHX	1	3977	-	0,6,6	-	-	-		
86	OHX	5	4028	-	0,6,6	-	-	-		
86	OHX	6	2138	-	0,6,6	-	-	-		
86	OHX	6	2131	-	0,6,6	-	-	-		
86	OHX	5	4203	-	0,6,6	-	-	-		
86	OHX	5	4249	-	0,6,6	-	-	-		
86	OHX	1	3918	-	0,6,6	-	-	-		
86	OHX	5	4135	-	0,6,6	-	-	-		
86	OHX	2	2146	-	0,6,6	-	-	-		
86	OHX	5	4047	-	0,6,6	-	-	-		
86	OHX	m0	302	-	0,6,6	-	-	-		
86	OHX	4	228	-	0,6,6	-	-	-		
86	OHX	5	4202	-	0,6,6	-	-	-		
86	OHX	2	2055	-	0,6,6	-	-	-		
86	OHX	2	2042	-	0,6,6	-	-	-		
86	OHX	6	2083	-	0,6,6	-	-	-		
86	OHX	2	2163	-	0,6,6	-	-	-		
86	OHX	2	2056	-	0,6,6	-	-	-		
86	OHX	1	4096	-	0,6,6	-	-	-		
86	OHX	5	4237	-	0,6,6	-	-	-		
86	OHX	5	4034	-	0,6,6	-	-	-		
86	OHX	1	4105	-	0,6,6	-	-	-		
86	OHX	2	2174	-	0,6,6	-	-	-		
86	OHX	1	4035	-	0,6,6	-	-	-		
86	OHX	5	4194	-	0,6,6	-	-	-		
86	OHX	8	220	-	0,6,6	-	-	-		
86	OHX	C3	201	-	0,6,6	-	-	-		
86	OHX	2	2069	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	7	222	-	0,6,6	-	-	-		
86	OHX	5	3915	-	0,6,6	-	-	-		
86	OHX	19	202	-	0,6,6	-	-	-		
86	OHX	4	232	-	0,6,6	-	-	-		
86	OHX	6	2145	-	0,6,6	-	-	-		
86	OHX	1	4057	-	0,6,6	-	-	-		
86	OHX	m7	206	-	0,6,6	-	-	-		
86	OHX	1	4045	-	0,6,6	-	-	-		
86	OHX	5	4215	-	0,6,6	-	-	-		
86	OHX	1	4122	-	0,6,6	-	-	-		
86	OHX	4	224	-	0,6,6	-	-	-		
86	OHX	1	3876	-	0,6,6	-	-	-		
86	OHX	5	4033	-	0,6,6	-	-	-		
86	OHX	2	2030	-	0,6,6	-	-	-		
86	OHX	6	2106	-	0,6,6	-	-	-		
86	OHX	6	2130	-	0,6,6	-	-	-		
86	OHX	2	2123	-	0,6,6	-	-	-		
86	OHX	5	3944	86	0,6,6	-	-	-		
86	OHX	6	2060	-	0,6,6	-	-	-		
86	OHX	1	3968	-	0,6,6	-	-	-		
86	OHX	7	221	-	0,6,6	-	-	-		
86	OHX	1	4136	-	0,6,6	-	-	-		
86	OHX	2	2127	-	0,6,6	-	-	-		
86	OHX	2	2128	-	0,6,6	-	-	-		
86	OHX	1	3923	-	0,6,6	-	-	-		
86	OHX	1	3907	-	0,6,6	-	-	-		
86	OHX	1	3993	-	0,6,6	-	-	-		
86	OHX	1	4202	-	0,6,6	-	-	-		
86	OHX	1	4206	-	0,6,6	-	-	-		
86	OHX	N9	102	-	0,6,6	-	-	-		
86	OHX	5	4000	-	0,6,6	-	-	-		
86	OHX	5	4054	-	0,6,6	-	-	-		
86	OHX	1	4123	-	0,6,6	-	-	-		
86	OHX	5	4031	-	0,6,6	-	-	-		
86	OHX	5	4138	-	0,6,6	-	-	-		
86	OHX	5	4143	-	0,6,6	-	-	-		
86	OHX	5	4196	-	0,6,6	-	-	-		
86	OHX	5	4019	-	0,6,6	-	-	-		
86	OHX	5	4114	-	0,6,6	-	-	-		
86	OHX	5	4207	-	0,6,6	-	-	-		
86	OHX	2	2092	-	0,6,6	-	-	-		
86	OHX	2	2082	-	0,6,6	-	-	-		
86	OHX	6	2205	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4025	-	0,6,6	-	-	-		
86	OHX	6	2168	-	0,6,6	-	-	-		
86	OHX	2	2113	-	0,6,6	-	-	-		
86	OHX	1	4087	-	0,6,6	-	-	-		
86	OHX	5	4227	-	0,6,6	-	-	-		
86	OHX	5	3984	-	0,6,6	-	-	-		
86	OHX	2	2166	-	0,6,6	-	-	-		
86	OHX	1	3873	-	0,6,6	-	-	-		
86	OHX	2	2160	-	0,6,6	-	-	-		
86	OHX	5	4002	-	0,6,6	-	-	-		
86	OHX	5	4216	-	0,6,6	-	-	-		
86	OHX	1	3897	-	0,6,6	-	-	-		
86	OHX	1	3996	-	0,6,6	-	-	-		
86	OHX	5	3965	-	0,6,6	-	-	-		
86	OHX	2	2122	-	0,6,6	-	-	-		
86	OHX	5	4155	-	0,6,6	-	-	-		
86	OHX	5	3972	-	0,6,6	-	-	-		
86	OHX	5	4225	-	0,6,6	-	-	-		
86	OHX	M5	304	-	0,6,6	-	-	-		
86	OHX	2	2070	-	0,6,6	-	-	-		
86	OHX	1	3914	-	0,6,6	-	-	-		
86	OHX	5	3940	-	0,6,6	-	-	-		
86	OHX	2	2071	-	0,6,6	-	-	-		
86	OHX	4	226	-	0,6,6	-	-	-		
86	OHX	1	4113	-	0,6,6	-	-	-		
86	OHX	2	2135	-	0,6,6	-	-	-		
86	OHX	5	3937	-	0,6,6	-	-	-		
86	OHX	1	4088	-	0,6,6	-	-	-		
86	OHX	5	4076	-	0,6,6	-	-	-		
86	OHX	7	229	-	0,6,6	-	-	-		
86	OHX	1	4025	-	0,6,6	-	-	-		
86	OHX	1	4084	-	0,6,6	-	-	-		
86	OHX	6	2164	-	0,6,6	-	-	-		
86	OHX	1	4183	-	0,6,6	-	-	-		
86	OHX	1	3865	-	0,6,6	-	-	-		
86	OHX	M9	202	-	0,6,6	-	-	-		
86	OHX	1	3916	-	0,6,6	-	-	-		
86	OHX	1	4032	-	0,6,6	-	-	-		
86	OHX	6	2052	-	0,6,6	-	-	-		
86	OHX	5	4164	-	0,6,6	-	-	-		
86	OHX	1	3983	-	0,6,6	-	-	-		
86	OHX	5	4125	-	0,6,6	-	-	-		
86	OHX	5	4234	86	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3959	-	0,6,6	-	-	-		
86	OHX	5	4105	-	0,6,6	-	-	-		
86	OHX	2	2029	-	0,6,6	-	-	-		
86	OHX	6	2055	-	0,6,6	-	-	-		
86	OHX	6	2107	-	0,6,6	-	-	-		
86	OHX	6	2102	-	0,6,6	-	-	-		
86	OHX	6	2195	-	0,6,6	-	-	-		
86	OHX	2	2086	-	0,6,6	-	-	-		
86	OHX	1	4198	-	0,6,6	-	-	-		
86	OHX	5	4217	-	0,6,6	-	-	-		
86	OHX	1	4008	-	0,6,6	-	-	-		
86	OHX	6	2132	-	0,6,6	-	-	-		
86	OHX	1	4130	-	0,6,6	-	-	-		
86	OHX	6	2051	-	0,6,6	-	-	-		
86	OHX	5	3935	-	0,6,6	-	-	-		
86	OHX	2	2039	-	0,6,6	-	-	-		
86	OHX	6	2154	-	0,6,6	-	-	-		
86	OHX	1	4053	-	0,6,6	-	-	-		
86	OHX	5	3948	-	0,6,6	-	-	-		
86	OHX	S8	302	-	0,6,6	-	-	-		
86	OHX	7	228	-	0,6,6	-	-	-		
86	OHX	1	4140	-	0,6,6	-	-	-		
86	OHX	1	4002	-	0,6,6	-	-	-		
86	OHX	1	4192	-	0,6,6	-	-	-		
86	OHX	2	2068	-	0,6,6	-	-	-		
86	OHX	1	3948	-	0,6,6	-	-	-		
86	OHX	2	2101	-	0,6,6	-	-	-		
86	OHX	2	2145	-	0,6,6	-	-	-		
86	OHX	1	4180	-	0,6,6	-	-	-		
86	OHX	M7	204	-	0,6,6	-	-	-		
86	OHX	2	2037	-	0,6,6	-	-	-		
86	OHX	6	2116	-	0,6,6	-	-	-		
86	OHX	5	3943	-	0,6,6	-	-	-		
86	OHX	5	4159	-	0,6,6	-	-	-		
86	OHX	5	4168	-	0,6,6	-	-	-		
86	OHX	6	2078	-	0,6,6	-	-	-		
86	OHX	5	4001	-	0,6,6	-	-	-		
86	OHX	1	4021	-	0,6,6	-	-	-		
86	OHX	5	4195	-	0,6,6	-	-	-		
86	OHX	2	2130	-	0,6,6	-	-	-		
86	OHX	1	3963	-	0,6,6	-	-	-		
86	OHX	6	2181	-	0,6,6	-	-	-		
86	OHX	3	216	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2085	-	0,6,6	-	-	-		
86	OHX	1	3972	-	0,6,6	-	-	-		
86	OHX	2	2131	-	0,6,6	-	-	-		
86	OHX	5	3930	-	0,6,6	-	-	-		
86	OHX	1	4054	-	0,6,6	-	-	-		
86	OHX	5	3985	-	0,6,6	-	-	-		
86	OHX	6	2112	-	0,6,6	-	-	-		
86	OHX	5	4150	-	0,6,6	-	-	-		
86	OHX	1	4083	-	0,6,6	-	-	-		
86	OHX	5	4131	-	0,6,6	-	-	-		
86	OHX	2	2104	-	0,6,6	-	-	-		
86	OHX	1	3877	-	0,6,6	-	-	-		
86	OHX	5	3995	-	0,6,6	-	-	-		
86	OHX	5	4149	-	0,6,6	-	-	-		
86	OHX	1	3882	-	0,6,6	-	-	-		
86	OHX	6	2086	-	0,6,6	-	-	-		
86	OHX	2	2073	-	0,6,6	-	-	-		
86	OHX	1	3995	-	0,6,6	-	-	-		
86	OHX	6	2200	-	0,6,6	-	-	-		
86	OHX	2	2157	-	0,6,6	-	-	-		
86	OHX	1	3951	-	0,6,6	-	-	-		
86	OHX	5	4018	-	0,6,6	-	-	-		
86	OHX	5	4086	-	0,6,6	-	-	-		
86	OHX	6	2099	-	0,6,6	-	-	-		
86	OHX	5	4170	-	0,6,6	-	-	-		
86	OHX	1	4018	-	0,6,6	-	-	-		
86	OHX	5	4091	-	0,6,6	-	-	-		
86	OHX	5	4077	-	0,6,6	-	-	-		
86	OHX	1	4168	86	0,6,6	-	-	-		
86	OHX	5	4223	-	0,6,6	-	-	-		
86	OHX	1	4159	-	0,6,6	-	-	-		
86	OHX	1	3888	-	0,6,6	-	-	-		
86	OHX	6	2142	-	0,6,6	-	-	-		
86	OHX	5	4117	-	0,6,6	-	-	-		
86	OHX	5	4059	-	0,6,6	-	-	-		
86	OHX	1	4001	-	0,6,6	-	-	-		
86	OHX	1	4055	-	0,6,6	-	-	-		
86	OHX	1	4195	-	0,6,6	-	-	-		
86	OHX	2	2076	-	0,6,6	-	-	-		
86	OHX	5	4226	-	0,6,6	-	-	-		
86	OHX	6	2175	-	0,6,6	-	-	-		
86	OHX	4	227	-	0,6,6	-	-	-		
86	OHX	1	4016	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4187	-	0,6,6	-	-	-		
86	OHX	1	3985	-	0,6,6	-	-	-		
86	OHX	5	4144	-	0,6,6	-	-	-		
86	OHX	1	4028	-	0,6,6	-	-	-		
86	OHX	1	4102	-	0,6,6	-	-	-		
86	OHX	1	4110	-	0,6,6	-	-	-		
86	OHX	5	4211	-	0,6,6	-	-	-		
86	OHX	5	4065	-	0,6,6	-	-	-		
86	OHX	7	224	-	0,6,6	-	-	-		
86	OHX	2	2054	-	0,6,6	-	-	-		
86	OHX	6	2104	-	0,6,6	-	-	-		
86	OHX	1	3892	-	0,6,6	-	-	-		
86	OHX	5	3955	-	0,6,6	-	-	-		
86	OHX	5	4113	-	0,6,6	-	-	-		
86	OHX	5	3969	-	0,6,6	-	-	-		
86	OHX	1	4091	-	0,6,6	-	-	-		
86	OHX	5	4236	-	0,6,6	-	-	-		
86	OHX	5	4198	-	0,6,6	-	-	-		
86	OHX	5	3956	-	0,6,6	-	-	-		
86	OHX	13	404	-	0,6,6	-	-	-		
86	OHX	2	2180	-	0,6,6	-	-	-		
86	OHX	1	4117	-	0,6,6	-	-	-		
86	OHX	2	2089	-	0,6,6	-	-	-		
86	OHX	6	2113	-	0,6,6	-	-	-		
86	OHX	5	4214	-	0,6,6	-	-	-		
86	OHX	2	2052	-	0,6,6	-	-	-		
86	OHX	5	4104	-	0,6,6	-	-	-		
86	OHX	2	2062	-	0,6,6	-	-	-		
86	OHX	n9	102	-	0,6,6	-	-	-		
86	OHX	2	2027	-	0,6,6	-	-	-		
86	OHX	2	2096	-	0,6,6	-	-	-		
86	OHX	2	2107	-	0,6,6	-	-	-		
86	OHX	5	4073	-	0,6,6	-	-	-		
86	OHX	5	3942	-	0,6,6	-	-	-		
86	OHX	5	4036	-	0,6,6	-	-	-		
86	OHX	2	2142	-	0,6,6	-	-	-		
86	OHX	5	4189	-	0,6,6	-	-	-		
86	OHX	6	2122	-	0,6,6	-	-	-		
86	OHX	1	4073	-	0,6,6	-	-	-		
86	OHX	1	3885	-	0,6,6	-	-	-		
86	OHX	6	2146	-	0,6,6	-	-	-		
86	OHX	5	4241	-	0,6,6	-	-	-		
86	OHX	1	4175	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4191	-	0,6,6	-	-	-		
86	OHX	6	2192	-	0,6,6	-	-	-		
86	OHX	5	3927	-	0,6,6	-	-	-		
86	OHX	1	3941	-	0,6,6	-	-	-		
86	OHX	1	4037	-	0,6,6	-	-	-		
86	OHX	1	4205	-	0,6,6	-	-	-		
86	OHX	5	4093	-	0,6,6	-	-	-		
86	OHX	5	4071	-	0,6,6	-	-	-		
86	OHX	2	2066	-	0,6,6	-	-	-		
86	OHX	5	4003	-	0,6,6	-	-	-		
86	OHX	5	4248	-	0,6,6	-	-	-		
86	OHX	5	3967	-	0,6,6	-	-	-		
86	OHX	6	2203	-	0,6,6	-	-	-		
86	OHX	5	4075	-	0,6,6	-	-	-		
86	OHX	2	2154	-	0,6,6	-	-	-		
86	OHX	1	3880	-	0,6,6	-	-	-		
86	OHX	8	229	-	0,6,6	-	-	-		
86	OHX	5	3963	-	0,6,6	-	-	-		
86	OHX	6	2067	-	0,6,6	-	-	-		
86	OHX	8	227	-	0,6,6	-	-	-		
86	OHX	6	2188	-	0,6,6	-	-	-		
86	OHX	5	4079	-	0,6,6	-	-	-		
86	OHX	6	2179	-	0,6,6	-	-	-		
86	OHX	5	4050	-	0,6,6	-	-	-		
86	OHX	1	4036	-	0,6,6	-	-	-		
86	OHX	5	3947	-	0,6,6	-	-	-		
86	OHX	2	2112	-	0,6,6	-	-	-		
86	OHX	1	3869	-	0,6,6	-	-	-		
86	OHX	1	3956	-	0,6,6	-	-	-		
86	OHX	1	4131	-	0,6,6	-	-	-		
86	OHX	1	3947	-	0,6,6	-	-	-		
86	OHX	6	2120	-	0,6,6	-	-	-		
86	OHX	5	4088	-	0,6,6	-	-	-		
86	OHX	5	4146	-	0,6,6	-	-	-		
86	OHX	1	3909	-	0,6,6	-	-	-		
86	OHX	2	2099	-	0,6,6	-	-	-		
86	OHX	1	3987	-	0,6,6	-	-	-		
86	OHX	6	2077	-	0,6,6	-	-	-		
86	OHX	5	4090	-	0,6,6	-	-	-		
86	OHX	5	4185	-	0,6,6	-	-	-		
86	OHX	6	2110	-	0,6,6	-	-	-		
86	OHX	2	2126	-	0,6,6	-	-	-		
86	OHX	s8	303	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3944	-	0,6,6	-	-	-		
86	OHX	1	4144	-	0,6,6	-	-	-		
86	OHX	6	2151	-	0,6,6	-	-	-		
86	OHX	5	4010	-	0,6,6	-	-	-		
86	OHX	6	2137	-	0,6,6	-	-	-		
86	OHX	1	4079	-	0,6,6	-	-	-		
86	OHX	2	2164	-	0,6,6	-	-	-		
86	OHX	6	2066	-	0,6,6	-	-	-		
86	OHX	5	4165	-	0,6,6	-	-	-		
86	OHX	5	4210	-	0,6,6	-	-	-		
86	OHX	5	3903	-	0,6,6	-	-	-		
86	OHX	5	3946	-	0,6,6	-	-	-		
86	OHX	1	3904	-	0,6,6	-	-	-		
86	OHX	2	2075	-	0,6,6	-	-	-		
86	OHX	1	4162	-	0,6,6	-	-	-		
86	OHX	1	4050	-	0,6,6	-	-	-		
86	OHX	2	2129	-	0,6,6	-	-	-		
86	OHX	1	4143	-	0,6,6	-	-	-		
86	OHX	1	3949	-	0,6,6	-	-	-		
86	OHX	1	4186	-	0,6,6	-	-	-		
86	OHX	1	4111	-	0,6,6	-	-	-		
86	OHX	6	2124	-	0,6,6	-	-	-		
86	OHX	5	4158	-	0,6,6	-	-	-		
86	OHX	5	3901	-	0,6,6	-	-	-		
86	OHX	1	4012	-	0,6,6	-	-	-		
86	OHX	5	4137	-	0,6,6	-	-	-		
86	OHX	2	2091	-	0,6,6	-	-	-		
86	OHX	1	3870	-	0,6,6	-	-	-		
86	OHX	1	4004	-	0,6,6	-	-	-		
86	OHX	1	4104	-	0,6,6	-	-	-		
86	OHX	6	2198	-	0,6,6	-	-	-		
86	OHX	5	3960	-	0,6,6	-	-	-		
86	OHX	1	4128	-	0,6,6	-	-	-		
86	OHX	5	3939	-	0,6,6	-	-	-		
86	OHX	5	4115	-	0,6,6	-	-	-		
86	OHX	5	4199	-	0,6,6	-	-	-		
86	OHX	1	4185	-	0,6,6	-	-	-		
86	OHX	6	2065	-	0,6,6	-	-	-		
86	OHX	5	4023	-	0,6,6	-	-	-		
86	OHX	5	4101	-	0,6,6	-	-	-		
86	OHX	q1	101	-	0,6,6	-	-	-		
86	OHX	l5	302	-	0,6,6	-	-	-		
86	OHX	5	4092	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	m5	305	-	0,6,6	-	-	-		
86	OHX	1	4193	-	0,6,6	-	-	-		
86	OHX	2	2074	-	0,6,6	-	-	-		
86	OHX	1	4149	-	0,6,6	-	-	-		
86	OHX	1	4155	-	0,6,6	-	-	-		
86	OHX	6	2150	-	0,6,6	-	-	-		
86	OHX	5	4060	-	0,6,6	-	-	-		
86	OHX	5	4221	-	0,6,6	-	-	-		
86	OHX	1	3889	-	0,6,6	-	-	-		
86	OHX	5	4040	-	0,6,6	-	-	-		
86	OHX	sR	401	-	0,6,6	-	-	-		
86	OHX	2	2151	-	0,6,6	-	-	-		
86	OHX	6	2098	-	0,6,6	-	-	-		
86	OHX	5	4007	-	0,6,6	-	-	-		
86	OHX	5	4043	-	0,6,6	-	-	-		
86	OHX	5	4119	-	0,6,6	-	-	-		
86	OHX	5	4181	-	0,6,6	-	-	-		
86	OHX	3	215	-	0,6,6	-	-	-		
86	OHX	5	4160	-	0,6,6	-	-	-		
86	OHX	5	4109	-	0,6,6	-	-	-		
86	OHX	C1	201	-	0,6,6	-	-	-		
86	OHX	1	4075	-	0,6,6	-	-	-		
86	OHX	8	231	-	0,6,6	-	-	-		
86	OHX	5	3961	-	0,6,6	-	-	-		
86	OHX	2	2097	-	0,6,6	-	-	-		
86	OHX	5	4046	-	0,6,6	-	-	-		
86	OHX	1	3913	-	0,6,6	-	-	-		
86	OHX	5	4171	-	0,6,6	-	-	-		
86	OHX	2	2133	-	0,6,6	-	-	-		
86	OHX	1	3939	-	0,6,6	-	-	-		
86	OHX	O7	104	-	0,6,6	-	-	-		
86	OHX	1	4179	-	0,6,6	-	-	-		
86	OHX	6	2101	-	0,6,6	-	-	-		
86	OHX	o7	502	-	0,6,6	-	-	-		
86	OHX	5	4094	-	0,6,6	-	-	-		
86	OHX	2	2169	-	0,6,6	-	-	-		
86	OHX	6	2185	-	0,6,6	-	-	-		
86	OHX	5	4089	-	0,6,6	-	-	-		
86	OHX	6	2089	-	0,6,6	-	-	-		
86	OHX	2	2047	-	0,6,6	-	-	-		
86	OHX	1	3992	-	0,6,6	-	-	-		
86	OHX	1	4065	-	0,6,6	-	-	-		
86	OHX	5	4197	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3998	-	0,6,6	-	-	-		
86	OHX	1	4106	-	0,6,6	-	-	-		
86	OHX	n6	202	-	0,6,6	-	-	-		
86	OHX	5	4136	-	0,6,6	-	-	-		
86	OHX	M7	205	-	0,6,6	-	-	-		
86	OHX	6	2081	-	0,6,6	-	-	-		
86	OHX	5	4067	-	0,6,6	-	-	-		
86	OHX	6	2074	-	0,6,6	-	-	-		
86	OHX	5	3923	-	0,6,6	-	-	-		
86	OHX	5	4153	-	0,6,6	-	-	-		
86	OHX	5	3907	-	0,6,6	-	-	-		
86	OHX	6	2135	-	0,6,6	-	-	-		
86	OHX	5	3931	-	0,6,6	-	-	-		
86	OHX	3	223	-	0,6,6	-	-	-		
86	OHX	2	2120	-	0,6,6	-	-	-		
86	OHX	5	4238	-	0,6,6	-	-	-		
86	OHX	6	2202	-	0,6,6	-	-	-		
86	OHX	SR	401	-	0,6,6	-	-	-		
86	OHX	1	3961	-	0,6,6	-	-	-		
86	OHX	2	2150	-	0,6,6	-	-	-		
86	OHX	4	225	-	0,6,6	-	-	-		
86	OHX	6	2144	-	0,6,6	-	-	-		
86	OHX	5	4253	-	0,6,6	-	-	-		
86	OHX	2	2077	-	0,6,6	-	-	-		
86	OHX	1	4156	-	0,6,6	-	-	-		
86	OHX	6	2157	-	0,6,6	-	-	-		
86	OHX	2	2179	-	0,6,6	-	-	-		
86	OHX	1	3930	-	0,6,6	-	-	-		
86	OHX	2	2098	-	0,6,6	-	-	-		
86	OHX	5	4024	-	0,6,6	-	-	-		
86	OHX	5	4015	-	0,6,6	-	-	-		
86	OHX	5	4213	-	0,6,6	-	-	-		
86	OHX	1	3969	-	0,6,6	-	-	-		
86	OHX	6	2178	-	0,6,6	-	-	-		
86	OHX	1	4178	-	0,6,6	-	-	-		
86	OHX	5	4011	-	0,6,6	-	-	-		
86	OHX	1	4094	-	0,6,6	-	-	-		
86	OHX	14	403	-	0,6,6	-	-	-		
86	OHX	6	2075	-	0,6,6	-	-	-		
86	OHX	6	2191	-	0,6,6	-	-	-		
86	OHX	2	2059	-	0,6,6	-	-	-		
86	OHX	1	4089	-	0,6,6	-	-	-		
86	OHX	1	4033	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3886	-	0,6,6	-	-	-		
86	OHX	5	4129	-	0,6,6	-	-	-		
86	OHX	l3	403	-	0,6,6	-	-	-		
86	OHX	6	2057	-	0,6,6	-	-	-		
86	OHX	1	4197	-	0,6,6	-	-	-		
86	OHX	6	2169	-	0,6,6	-	-	-		
86	OHX	5	3996	-	0,6,6	-	-	-		
86	OHX	5	4004	-	0,6,6	-	-	-		
86	OHX	5	4064	-	0,6,6	-	-	-		
86	OHX	1	4199	-	0,6,6	-	-	-		
86	OHX	6	2186	-	0,6,6	-	-	-		
86	OHX	S9	201	-	0,6,6	-	-	-		
86	OHX	1	4082	-	0,6,6	-	-	-		
86	OHX	5	3914	-	0,6,6	-	-	-		
86	OHX	1	4023	-	0,6,6	-	-	-		
86	OHX	Q2	502	-	0,6,6	-	-	-		
86	OHX	6	2121	-	0,6,6	-	-	-		
86	OHX	1	4189	-	0,6,6	-	-	-		
86	OHX	5	4193	-	0,6,6	-	-	-		
86	OHX	o3	202	-	0,6,6	-	-	-		
86	OHX	1	3967	-	0,6,6	-	-	-		
86	OHX	2	2093	-	0,6,6	-	-	-		
86	OHX	6	2147	-	0,6,6	-	-	-		
86	OHX	4	229	-	0,6,6	-	-	-		
86	OHX	1	3878	-	0,6,6	-	-	-		
86	OHX	5	4148	-	0,6,6	-	-	-		
86	OHX	5	4085	-	0,6,6	-	-	-		
86	OHX	2	2140	-	0,6,6	-	-	-		
86	OHX	1	4121	-	0,6,6	-	-	-		
86	OHX	1	4024	-	0,6,6	-	-	-		
86	OHX	6	2125	-	0,6,6	-	-	-		
86	OHX	5	3929	-	0,6,6	-	-	-		
86	OHX	1	4015	-	0,6,6	-	-	-		
86	OHX	1	3917	-	0,6,6	-	-	-		
86	OHX	1	4007	-	0,6,6	-	-	-		
86	OHX	1	3979	-	0,6,6	-	-	-		
86	OHX	2	2141	-	0,6,6	-	-	-		
86	OHX	1	4011	-	0,6,6	-	-	-		
86	OHX	6	2187	-	0,6,6	-	-	-		
86	OHX	5	3951	-	0,6,6	-	-	-		
86	OHX	1	4160	-	0,6,6	-	-	-		
86	OHX	1	4146	-	0,6,6	-	-	-		
86	OHX	C8	201	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3984	-	0,6,6	-	-	-		
86	OHX	1	4069	-	0,6,6	-	-	-		
86	OHX	1	4081	-	0,6,6	-	-	-		
86	OHX	1	4129	-	0,6,6	-	-	-		
86	OHX	6	2062	-	0,6,6	-	-	-		
86	OHX	1	4173	-	0,6,6	-	-	-		
86	OHX	5	3975	-	0,6,6	-	-	-		
86	OHX	5	4232	-	0,6,6	-	-	-		
86	OHX	5	4095	-	0,6,6	-	-	-		
86	OHX	2	2043	-	0,6,6	-	-	-		
86	OHX	5	4008	-	0,6,6	-	-	-		
86	OHX	5	4130	-	0,6,6	-	-	-		
86	OHX	1	4019	-	0,6,6	-	-	-		
86	OHX	5	3912	-	0,6,6	-	-	-		
86	OHX	5	4132	-	0,6,6	-	-	-		
86	OHX	5	3905	-	0,6,6	-	-	-		
86	OHX	6	2111	-	0,6,6	-	-	-		
86	OHX	6	2133	-	0,6,6	-	-	-		
86	OHX	6	2053	-	0,6,6	-	-	-		
86	OHX	7	218	-	0,6,6	-	-	-		
86	OHX	1	3902	-	0,6,6	-	-	-		
86	OHX	5	4048	-	0,6,6	-	-	-		
86	OHX	6	2158	-	0,6,6	-	-	-		
86	OHX	2	2115	-	0,6,6	-	-	-		
86	OHX	5	4133	-	0,6,6	-	-	-		
86	OHX	5	4192	-	0,6,6	-	-	-		
86	OHX	5	3926	-	0,6,6	-	-	-		
86	OHX	2	2171	-	0,6,6	-	-	-		
86	OHX	6	2049	-	0,6,6	-	-	-		
86	OHX	5	4180	-	0,6,6	-	-	-		
86	OHX	1	4046	-	0,6,6	-	-	-		
86	OHX	5	3933	-	0,6,6	-	-	-		
86	OHX	1	3929	-	0,6,6	-	-	-		
86	OHX	1	3997	-	0,6,6	-	-	-		
86	OHX	2	2110	-	0,6,6	-	-	-		
86	OHX	1	4067	-	0,6,6	-	-	-		
86	OHX	5	4162	-	0,6,6	-	-	-		
86	OHX	6	2118	-	0,6,6	-	-	-		
86	OHX	5	3970	-	0,6,6	-	-	-		
86	OHX	2	2137	-	0,6,6	-	-	-		
86	OHX	5	4026	-	0,6,6	-	-	-		
86	OHX	5	4228	-	0,6,6	-	-	-		
86	OHX	4	238	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3883	-	0,6,6	-	-	-		
86	OHX	1	3975	-	0,6,6	-	-	-		
86	OHX	5	3925	-	0,6,6	-	-	-		
86	OHX	m6	202	-	0,6,6	-	-	-		
86	OHX	2	2106	-	0,6,6	-	-	-		
86	OHX	2	2125	-	0,6,6	-	-	-		
86	OHX	5	4112	-	0,6,6	-	-	-		
86	OHX	1	4095	-	0,6,6	-	-	-		
86	OHX	5	3922	-	0,6,6	-	-	-		
86	OHX	1	3908	-	0,6,6	-	-	-		
86	OHX	5	3980	-	0,6,6	-	-	-		
86	OHX	1	4132	-	0,6,6	-	-	-		
86	OHX	1	3915	-	0,6,6	-	-	-		
86	OHX	2	2124	-	0,6,6	-	-	-		
86	OHX	3	222	-	0,6,6	-	-	-		
86	OHX	6	2177	-	0,6,6	-	-	-		
86	OHX	1	3887	-	0,6,6	-	-	-		
86	OHX	1	4133	-	0,6,6	-	-	-		
86	OHX	1	3926	-	0,6,6	-	-	-		
86	OHX	6	2097	-	0,6,6	-	-	-		
86	OHX	1	4164	-	0,6,6	-	-	-		
86	OHX	5	3983	-	0,6,6	-	-	-		
86	OHX	1	4060	-	0,6,6	-	-	-		
86	OHX	1	4031	-	0,6,6	-	-	-		
86	OHX	1	4064	-	0,6,6	-	-	-		
86	OHX	1	4118	-	0,6,6	-	-	-		
86	OHX	3	225	-	0,6,6	-	-	-		
86	OHX	2	2065	-	0,6,6	-	-	-		
86	OHX	6	2058	-	0,6,6	-	-	-		
86	OHX	5	3910	-	0,6,6	-	-	-		
86	OHX	1	4163	-	0,6,6	-	-	-		
86	OHX	5	4096	-	0,6,6	-	-	-		
86	OHX	2	2111	-	0,6,6	-	-	-		
86	OHX	5	4200	-	0,6,6	-	-	-		
86	OHX	5	3976	-	0,6,6	-	-	-		
86	OHX	2	2053	-	0,6,6	-	-	-		
86	OHX	5	4021	-	0,6,6	-	-	-		
86	OHX	2	2064	-	0,6,6	-	-	-		
86	OHX	4	231	-	0,6,6	-	-	-		
86	OHX	5	4176	-	0,6,6	-	-	-		
86	OHX	2	2144	-	0,6,6	-	-	-		
86	OHX	8	219	-	0,6,6	-	-	-		
86	OHX	1	4072	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2057	-	0,6,6	-	-	-		
86	OHX	5	4016	-	0,6,6	-	-	-		
86	OHX	1	4126	-	0,6,6	-	-	-		
86	OHX	6	2117	-	0,6,6	-	-	-		
86	OHX	5	4167	-	0,6,6	-	-	-		
86	OHX	6	2143	-	0,6,6	-	-	-		
86	OHX	8	222	-	0,6,6	-	-	-		
86	OHX	L3	404	-	0,6,6	-	-	-		
86	OHX	2	2153	-	0,6,6	-	-	-		
86	OHX	1	4029	-	0,6,6	-	-	-		
86	OHX	6	2183	-	0,6,6	-	-	-		
86	OHX	5	3932	-	0,6,6	-	-	-		
86	OHX	5	4110	-	0,6,6	-	-	-		
86	OHX	1	4114	-	0,6,6	-	-	-		
86	OHX	6	2129	-	0,6,6	-	-	-		
86	OHX	1	4127	-	0,6,6	-	-	-		
86	OHX	6	2174	-	0,6,6	-	-	-		
86	OHX	5	3906	-	0,6,6	-	-	-		
86	OHX	1	4049	-	0,6,6	-	-	-		
86	OHX	5	3911	-	0,6,6	-	-	-		
86	OHX	5	4166	-	0,6,6	-	-	-		
86	OHX	1	4135	-	0,6,6	-	-	-		
86	OHX	6	2148	-	0,6,6	-	-	-		
86	OHX	5	4174	-	0,6,6	-	-	-		
86	OHX	5	4157	-	0,6,6	-	-	-		
86	OHX	1	3910	-	0,6,6	-	-	-		
86	OHX	6	2123	-	0,6,6	-	-	-		
86	OHX	2	2035	-	0,6,6	-	-	-		
86	OHX	1	4200	-	0,6,6	-	-	-		
86	OHX	6	2176	-	0,6,6	-	-	-		
86	OHX	6	2204	-	0,6,6	-	-	-		
86	OHX	1	3879	-	0,6,6	-	-	-		
86	OHX	1	4176	-	0,6,6	-	-	-		
86	OHX	8	217	-	0,6,6	-	-	-		
86	OHX	5	4183	-	0,6,6	-	-	-		
86	OHX	m0	303	-	0,6,6	-	-	-		
86	OHX	8	221	-	0,6,6	-	-	-		
86	OHX	5	4107	-	0,6,6	-	-	-		
86	OHX	2	2138	-	0,6,6	-	-	-		
86	OHX	2	2095	-	0,6,6	-	-	-		
86	OHX	1	4150	-	0,6,6	-	-	-		
86	OHX	6	2193	-	0,6,6	-	-	-		
86	OHX	2	2081	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3933	-	0,6,6	-	-	-		
86	OHX	1	4107	-	0,6,6	-	-	-		
86	OHX	6	2072	-	0,6,6	-	-	-		
86	OHX	6	2087	-	0,6,6	-	-	-		
86	OHX	1	4062	-	0,6,6	-	-	-		
86	OHX	5	4224	-	0,6,6	-	-	-		
86	OHX	5	3924	-	0,6,6	-	-	-		
86	OHX	5	3945	-	0,6,6	-	-	-		
86	OHX	5	3997	-	0,6,6	-	-	-		
86	OHX	5	4098	-	0,6,6	-	-	-		
86	OHX	5	4009	-	0,6,6	-	-	-		
86	OHX	1	4125	-	0,6,6	-	-	-		
86	OHX	2	2083	-	0,6,6	-	-	-		
86	OHX	L3	403	-	0,6,6	-	-	-		
86	OHX	6	2082	-	0,6,6	-	-	-		
86	OHX	1	4026	-	0,6,6	-	-	-		
86	OHX	2	2158	-	0,6,6	-	-	-		
86	OHX	6	2108	-	0,6,6	-	-	-		
86	OHX	5	3971	-	0,6,6	-	-	-		
86	OHX	5	4037	-	0,6,6	-	-	-		
86	OHX	5	4070	-	0,6,6	-	-	-		
86	OHX	1	3935	-	0,6,6	-	-	-		
86	OHX	1	4151	-	0,6,6	-	-	-		
86	OHX	1	4058	-	0,6,6	-	-	-		
86	OHX	6	2161	-	0,6,6	-	-	-		
86	OHX	1	3955	-	0,6,6	-	-	-		
86	OHX	1	4052	-	0,6,6	-	-	-		
86	OHX	1	4112	-	0,6,6	-	-	-		
86	OHX	7	220	-	0,6,6	-	-	-		
86	OHX	5	3900	-	0,6,6	-	-	-		
86	OHX	1	4078	-	0,6,6	-	-	-		
86	OHX	2	2178	-	0,6,6	-	-	-		
86	OHX	C5	201	-	0,6,6	-	-	-		
86	OHX	1	4182	-	0,6,6	-	-	-		
86	OHX	1	4056	-	0,6,6	-	-	-		
86	OHX	6	2141	-	0,6,6	-	-	-		
86	OHX	O3	202	-	0,6,6	-	-	-		
86	OHX	1	4141	-	0,6,6	-	-	-		
86	OHX	5	3938	-	0,6,6	-	-	-		
86	OHX	1	3866	-	0,6,6	-	-	-		
86	OHX	3	217	-	0,6,6	-	-	-		
86	OHX	6	2170	-	0,6,6	-	-	-		
86	OHX	6	2091	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2132	-	0,6,6	-	-	-		
86	OHX	6	2173	-	0,6,6	-	-	-		
86	OHX	8	230	-	0,6,6	-	-	-		
86	OHX	6	2095	-	0,6,6	-	-	-		
86	OHX	1	3943	-	0,6,6	-	-	-		
86	OHX	1	4148	-	0,6,6	-	-	-		
86	OHX	5	4152	-	0,6,6	-	-	-		
86	OHX	5	3974	-	0,6,6	-	-	-		
86	OHX	5	3978	-	0,6,6	-	-	-		
86	OHX	1	4044	-	0,6,6	-	-	-		
86	OHX	5	4027	-	0,6,6	-	-	-		
86	OHX	6	2171	-	0,6,6	-	-	-		
86	OHX	5	4069	-	0,6,6	-	-	-		
86	OHX	2	2078	-	0,6,6	-	-	-		
86	OHX	1	4003	-	0,6,6	-	-	-		
86	OHX	2	2080	-	0,6,6	-	-	-		
86	OHX	M0	303	-	0,6,6	-	-	-		
86	OHX	1	3942	-	0,6,6	-	-	-		
86	OHX	14	402	-	0,6,6	-	-	-		
86	OHX	6	2059	-	0,6,6	-	-	-		
86	OHX	2	2117	-	0,6,6	-	-	-		
86	OHX	2	2143	-	0,6,6	-	-	-		
86	OHX	2	2167	-	0,6,6	-	-	-		
86	OHX	2	2162	-	0,6,6	-	-	-		
86	OHX	1	4184	-	0,6,6	-	-	-		
86	OHX	2	2048	-	0,6,6	-	-	-		
86	OHX	5	3968	-	0,6,6	-	-	-		
86	OHX	3	224	-	0,6,6	-	-	-		
86	OHX	1	4174	-	0,6,6	-	-	-		
86	OHX	5	4111	-	0,6,6	-	-	-		
86	OHX	5	4017	-	0,6,6	-	-	-		
86	OHX	5	4177	-	0,6,6	-	-	-		
86	OHX	5	4012	-	0,6,6	-	-	-		
86	OHX	d9	102	-	0,6,6	-	-	-		
86	OHX	2	2119	-	0,6,6	-	-	-		
86	OHX	5	4219	-	0,6,6	-	-	-		
86	OHX	7	223	-	0,6,6	-	-	-		
86	OHX	1	4152	-	0,6,6	-	-	-		
86	OHX	n3	202	-	0,6,6	-	-	-		
86	OHX	1	4017	-	0,6,6	-	-	-		
86	OHX	5	3950	-	0,6,6	-	-	-		
86	OHX	5	3994	-	0,6,6	-	-	-		
86	OHX	6	2093	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	4	237	-	0,6,6	-	-	-		
86	OHX	2	2049	-	0,6,6	-	-	-		
86	OHX	2	2045	-	0,6,6	-	-	-		
86	OHX	1	3874	-	0,6,6	-	-	-		
86	OHX	1	3906	-	0,6,6	-	-	-		
86	OHX	5	4038	-	0,6,6	-	-	-		
86	OHX	2	2118	-	0,6,6	-	-	-		
86	OHX	O9	101	-	0,6,6	-	-	-		
86	OHX	2	2088	-	0,6,6	-	-	-		
86	OHX	3	218	-	0,6,6	-	-	-		
86	OHX	5	4229	-	0,6,6	-	-	-		
86	OHX	1	4098	-	0,6,6	-	-	-		
86	OHX	7	219	-	0,6,6	-	-	-		
86	OHX	5	4100	-	0,6,6	-	-	-		
86	OHX	2	2134	-	0,6,6	-	-	-		
86	OHX	2	2148	-	0,6,6	-	-	-		
86	OHX	1	3988	-	0,6,6	-	-	-		
86	OHX	5	4156	-	0,6,6	-	-	-		
86	OHX	2	2159	-	0,6,6	-	-	-		
86	OHX	2	2041	-	0,6,6	-	-	-		
86	OHX	5	4029	-	0,6,6	-	-	-		
86	OHX	1	4006	-	0,6,6	-	-	-		
86	OHX	5	4230	-	0,6,6	-	-	-		
86	OHX	1	3937	-	0,6,6	-	-	-		
86	OHX	8	223	-	0,6,6	-	-	-		
86	OHX	2	2176	-	0,6,6	-	-	-		
86	OHX	1	3893	-	0,6,6	-	-	-		
86	OHX	2	2156	-	0,6,6	-	-	-		
86	OHX	1	4142	-	0,6,6	-	-	-		
86	OHX	6	2088	-	0,6,6	-	-	-		
86	OHX	1	3900	-	0,6,6	-	-	-		
86	OHX	6	2162	-	0,6,6	-	-	-		
86	OHX	5	4013	-	0,6,6	-	-	-		
86	OHX	2	2044	-	0,6,6	-	-	-		
86	OHX	2	2177	-	0,6,6	-	-	-		
86	OHX	1	4108	-	0,6,6	-	-	-		
86	OHX	1	3950	-	0,6,6	-	-	-		
86	OHX	1	3994	-	0,6,6	-	-	-		
86	OHX	5	3989	-	0,6,6	-	-	-		
86	OHX	6	2136	-	0,6,6	-	-	-		
86	OHX	6	2115	-	0,6,6	-	-	-		
86	OHX	6	2208	-	0,6,6	-	-	-		
86	OHX	s4	301	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4061	-	0,6,6	-	-	-		
86	OHX	5	3977	-	0,6,6	-	-	-		
86	OHX	5	4178	-	0,6,6	-	-	-		
86	OHX	1	3981	-	0,6,6	-	-	-		
86	OHX	5	4084	-	0,6,6	-	-	-		
86	OHX	5	3918	-	0,6,6	-	-	-		
86	OHX	1	3940	-	0,6,6	-	-	-		
86	OHX	5	4106	-	0,6,6	-	-	-		
86	OHX	1	4100	-	0,6,6	-	-	-		
86	OHX	1	3974	-	0,6,6	-	-	-		
86	OHX	2	2105	-	0,6,6	-	-	-		
86	OHX	5	4055	-	0,6,6	-	-	-		
86	OHX	2	2072	-	0,6,6	-	-	-		
86	OHX	2	2161	-	0,6,6	-	-	-		
86	OHX	2	2170	-	0,6,6	-	-	-		
86	OHX	1	4027	-	0,6,6	-	-	-		
86	OHX	s1	303	-	0,6,6	-	-	-		
86	OHX	6	2134	-	0,6,6	-	-	-		
86	OHX	5	3917	-	0,6,6	-	-	-		
86	OHX	5	4020	-	0,6,6	-	-	-		
86	OHX	1	4077	-	0,6,6	-	-	-		
86	OHX	5	4231	-	0,6,6	-	-	-		
86	OHX	1	4196	-	0,6,6	-	-	-		
86	OHX	6	2054	-	0,6,6	-	-	-		
86	OHX	1	3875	-	0,6,6	-	-	-		
86	OHX	1	3976	-	0,6,6	-	-	-		
86	OHX	D9	102	-	0,6,6	-	-	-		
86	OHX	6	2199	-	0,6,6	-	-	-		
86	OHX	1	4071	-	0,6,6	-	-	-		
86	OHX	1	4043	-	0,6,6	-	-	-		
86	OHX	4	236	-	0,6,6	-	-	-		
86	OHX	1	4059	-	0,6,6	-	-	-		
86	OHX	1	4119	-	0,6,6	-	-	-		
86	OHX	1	4204	-	0,6,6	-	-	-		
86	OHX	5	3953	-	0,6,6	-	-	-		
86	OHX	5	4120	-	0,6,6	-	-	-		
86	OHX	1	4109	-	0,6,6	-	-	-		
86	OHX	6	2109	-	0,6,6	-	-	-		
86	OHX	5	4053	-	0,6,6	-	-	-		
86	OHX	6	2080	-	0,6,6	-	-	-		
86	OHX	7	227	-	0,6,6	-	-	-		
86	OHX	c3	201	-	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	5	4123	-	0,6,6	-	-	-		
86	OHX	5	4128	-	0,6,6	-	-	-		
86	OHX	1	3911	-	0,6,6	-	-	-		
86	OHX	1	4061	-	0,6,6	-	-	-		
86	OHX	5	3957	-	0,6,6	-	-	-		
86	OHX	1	4172	-	0,6,6	-	-	-		
86	OHX	1	3867	-	0,6,6	-	-	-		
86	OHX	1	4048	-	0,6,6	-	-	-		
86	OHX	1	3890	-	0,6,6	-	-	-		
86	OHX	2	2173	-	0,6,6	-	-	-		
86	OHX	5	4051	-	0,6,6	-	-	-		
86	OHX	1	3978	-	0,6,6	-	-	-		
86	OHX	5	3958	-	0,6,6	-	-	-		
86	OHX	5	4220	-	0,6,6	-	-	-		
86	OHX	5	4251	-	0,6,6	-	-	-		
86	OHX	6	2061	-	0,6,6	-	-	-		
86	OHX	5	4102	-	0,6,6	-	-	-		
86	OHX	1	4051	-	0,6,6	-	-	-		
86	OHX	1	4181	-	0,6,6	-	-	-		
86	OHX	6	2084	-	0,6,6	-	-	-		
86	OHX	6	2094	-	0,6,6	-	-	-		
86	OHX	5	4154	-	0,6,6	-	-	-		
86	OHX	1	3894	-	0,6,6	-	-	-		
86	OHX	2	2136	-	0,6,6	-	-	-		
86	OHX	1	4203	-	0,6,6	-	-	-		
86	OHX	5	3993	-	0,6,6	-	-	-		
86	OHX	5	3909	-	0,6,6	-	-	-		
86	OHX	5	4082	-	0,6,6	-	-	-		
86	OHX	6	2050	-	0,6,6	-	-	-		
86	OHX	6	2189	-	0,6,6	-	-	-		
86	OHX	6	2068	-	0,6,6	-	-	-		
86	OHX	6	2153	-	0,6,6	-	-	-		
86	OHX	q2	502	-	0,6,6	-	-	-		
86	OHX	2	2087	-	0,6,6	-	-	-		
86	OHX	1	3965	-	0,6,6	-	-	-		
86	OHX	1	4038	-	0,6,6	-	-	-		
86	OHX	1	4085	-	0,6,6	-	-	-		
86	OHX	1	4090	-	0,6,6	-	-	-		
86	OHX	4	234	-	0,6,6	-	-	-		
86	OHX	5	3920	-	0,6,6	-	-	-		
86	OHX	5	4083	-	0,6,6	-	-	-		
86	OHX	5	4099	-	0,6,6	-	-	-		
86	OHX	2	2108	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4120	-	0,6,6	-	-	-		
86	OHX	5	4087	-	0,6,6	-	-	-		
86	OHX	1	4010	-	0,6,6	-	-	-		
86	OHX	5	4005	-	0,6,6	-	-	-		
86	OHX	1	3924	-	0,6,6	-	-	-		
86	OHX	1	3945	-	0,6,6	-	-	-		
86	OHX	2	2100	-	0,6,6	-	-	-		
86	OHX	5	4118	-	0,6,6	-	-	-		
86	OHX	2	2026	-	0,6,6	-	-	-		
86	OHX	1	4005	-	0,6,6	-	-	-		
86	OHX	5	4244	-	0,6,6	-	-	-		
86	OHX	1	3946	-	0,6,6	-	-	-		
86	OHX	7	226	-	0,6,6	-	-	-		
86	OHX	5	3979	-	0,6,6	-	-	-		
86	OHX	4	230	-	0,6,6	-	-	-		
86	OHX	6	2152	-	0,6,6	-	-	-		
86	OHX	5	3916	-	0,6,6	-	-	-		
86	OHX	1	3932	-	0,6,6	-	-	-		
86	OHX	1	3931	-	0,6,6	-	-	-		
86	OHX	6	2063	-	0,6,6	-	-	-		
86	OHX	2	2034	-	0,6,6	-	-	-		
86	OHX	6	2206	-	0,6,6	-	-	-		
86	OHX	6	2079	-	0,6,6	-	-	-		
86	OHX	2	2038	-	0,6,6	-	-	-		
86	OHX	2	2139	-	0,6,6	-	-	-		
86	OHX	1	3884	-	0,6,6	-	-	-		
86	OHX	1	4171	-	0,6,6	-	-	-		
86	OHX	2	2061	-	0,6,6	-	-	-		
86	OHX	5	4068	-	0,6,6	-	-	-		
86	OHX	5	4233	-	0,6,6	-	-	-		
86	OHX	1	4099	-	0,6,6	-	-	-		
86	OHX	1	4138	-	0,6,6	-	-	-		
86	OHX	5	4063	-	0,6,6	-	-	-		
86	OHX	5	3987	-	0,6,6	-	-	-		
86	OHX	1	4207	-	0,6,6	-	-	-		
86	OHX	6	2114	-	0,6,6	-	-	-		
86	OHX	6	2064	-	0,6,6	-	-	-		
86	OHX	5	3966	-	0,6,6	-	-	-		
86	OHX	5	4212	-	0,6,6	-	-	-		
86	OHX	8	225	-	0,6,6	-	-	-		
86	OHX	m9	201	-	0,6,6	-	-	-		
86	OHX	5	3959	-	0,6,6	-	-	-		
86	OHX	5	4062	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3899	-	0,6,6	-	-	-		
86	OHX	1	4020	-	0,6,6	-	-	-		
86	OHX	6	2190	-	0,6,6	-	-	-		
86	OHX	1	3872	-	0,6,6	-	-	-		
86	OHX	1	4154	-	0,6,6	-	-	-		
86	OHX	1	4153	-	0,6,6	-	-	-		
86	OHX	5	4184	-	0,6,6	-	-	-		
86	OHX	5	3990	-	0,6,6	-	-	-		
86	OHX	m1	203	-	0,6,6	-	-	-		
86	OHX	5	4134	-	0,6,6	-	-	-		
86	OHX	5	3962	-	0,6,6	-	-	-		
86	OHX	5	4209	-	0,6,6	-	-	-		
86	OHX	1	3953	-	0,6,6	-	-	-		
86	OHX	2	2046	-	0,6,6	-	-	-		
86	OHX	6	2201	-	0,6,6	-	-	-		
86	OHX	5	3981	-	0,6,6	-	-	-		
86	OHX	5	3991	-	0,6,6	-	-	-		
86	OHX	5	3954	-	0,6,6	-	-	-		
86	OHX	5	3908	-	0,6,6	-	-	-		
86	OHX	2	2149	-	0,6,6	-	-	-		
86	OHX	5	4014	-	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
88	3J2	1	4209	-	-	0/4/65/65	0/5/5/5
88	3J2	5	4254	-	-	0/4/65/65	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4209	3J2	C1-C3	4.76	1.57	1.50
88	1	4209	3J2	C4-C3	4.01	1.41	1.34
88	1	4209	3J2	C10-C9	2.15	1.56	1.53
88	5	4254	3J2	C-C1	2.13	1.59	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	5	4254	3J2	C18-C8-C9	-4.85	99.90	108.96
88	1	4209	3J2	O2-C11-C12	4.80	123.51	117.68
88	1	4209	3J2	O6-C5-C6	-4.38	97.42	109.24
88	5	4254	3J2	C15-C14-C13	3.83	124.48	121.71
88	1	4209	3J2	C18-C8-C9	-3.24	102.89	108.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

541 monomers are involved in 923 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3957	OHX	5	0
86	2	2155	OHX	4	0
86	1	3964	OHX	1	0
86	6	2139	OHX	1	0
86	L4	403	OHX	1	0
86	5	4161	OHX	1	0
86	1	3966	OHX	1	0
86	1	4070	OHX	1	0
86	1	4139	OHX	1	0
86	1	3938	OHX	7	0
86	3	221	OHX	1	0
86	5	4245	OHX	1	0
86	1	3970	OHX	7	0
86	5	4072	OHX	5	0
86	1	4194	OHX	1	0
86	5	4187	OHX	1	0
86	8	228	OHX	1	0
86	5	3921	OHX	1	0
86	5	4145	OHX	5	0
86	s1	302	OHX	1	0
86	5	3902	OHX	1	0
86	5	4141	OHX	2	0
86	6	2126	OHX	1	0
86	1	3980	OHX	2	0
88	5	4254	3J2	2	0
86	1	4068	OHX	1	0
86	1	4047	OHX	5	0
86	1	4063	OHX	6	0
86	5	3919	OHX	2	0
86	6	2103	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	c5	201	OHX	1	0
86	5	4246	OHX	1	0
86	2	2079	OHX	1	0
86	6	2159	OHX	1	0
86	5	4172	OHX	2	0
86	5	4201	OHX	5	0
86	1	4170	OHX	3	0
86	1	4086	OHX	1	0
86	6	2156	OHX	1	0
86	2	2168	OHX	1	0
86	2	2109	OHX	5	0
86	2	2040	OHX	2	0
86	5	4052	OHX	2	0
88	1	4209	3J2	3	0
86	5	3973	OHX	2	0
86	6	2194	OHX	2	0
86	1	4014	OHX	1	0
86	5	4182	OHX	1	0
86	1	4080	OHX	8	0
86	5	4032	OHX	4	0
86	2	2084	OHX	6	0
86	1	3989	OHX	3	0
86	5	4139	OHX	1	0
86	5	4205	OHX	1	0
86	5	4169	OHX	1	0
86	1	3871	OHX	1	0
86	1	3898	OHX	1	0
86	5	4042	OHX	2	0
86	5	4022	OHX	2	0
86	1	4188	OHX	1	0
86	1	3971	OHX	1	0
86	1	4040	OHX	6	0
86	5	3928	OHX	1	0
86	6	2197	OHX	1	0
86	8	218	OHX	8	0
86	2	2063	OHX	2	0
86	5	3934	OHX	1	0
86	1	4034	OHX	1	0
86	1	4124	OHX	1	0
86	1	4137	OHX	3	0
86	2	2121	OHX	3	0
86	6	2056	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	2	2147	OHX	6	0
86	5	3941	OHX	1	0
86	6	2127	OHX	1	0
86	1	4042	OHX	2	0
86	1	4134	OHX	1	0
86	2	2085	OHX	2	0
86	8	226	OHX	6	0
86	6	2105	OHX	2	0
86	5	4074	OHX	5	0
86	O7	105	OHX	1	0
86	5	4127	OHX	6	0
86	5	3988	OHX	2	0
86	5	3999	OHX	1	0
86	1	4076	OHX	7	0
86	1	3982	OHX	1	0
86	2	2060	OHX	1	0
86	1	3919	OHX	1	0
86	6	2128	OHX	8	0
86	2	2032	OHX	8	0
86	5	4190	OHX	1	0
86	5	4142	OHX	6	0
86	1	4066	OHX	1	0
86	2	2024	OHX	1	0
86	6	2196	OHX	1	0
86	5	4108	OHX	2	0
86	1	4030	OHX	1	0
86	5	4039	OHX	1	0
86	2	2172	OHX	2	0
86	1	4000	OHX	8	0
86	1	4165	OHX	2	0
86	3	220	OHX	1	0
86	6	2166	OHX	1	0
86	5	4250	OHX	1	0
86	2	2036	OHX	1	0
86	1	4074	OHX	1	0
86	1	3868	OHX	2	0
86	5	4179	OHX	3	0
86	1	3999	OHX	2	0
86	2	2090	OHX	1	0
86	1	4177	OHX	5	0
86	1	3881	OHX	1	0
86	5	4078	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	4049	OHX	1	0
86	1	4116	OHX	1	0
86	6	2071	OHX	2	0
86	d4	201	OHX	1	0
86	1	4190	OHX	1	0
86	6	2073	OHX	1	0
86	5	4173	OHX	1	0
86	1	4158	OHX	4	0
86	6	2149	OHX	1	0
86	5	3952	OHX	1	0
86	2	2028	OHX	1	0
86	1	4201	OHX	1	0
86	2	2116	OHX	6	0
86	1	3960	OHX	1	0
86	1	4039	OHX	5	0
86	L3	405	OHX	1	0
86	6	2076	OHX	2	0
86	5	3998	OHX	1	0
86	5	4028	OHX	1	0
86	6	2131	OHX	1	0
86	5	4203	OHX	5	0
86	2	2146	OHX	1	0
86	5	4047	OHX	1	0
86	2	2055	OHX	1	0
86	5	4237	OHX	6	0
86	1	4105	OHX	2	0
86	1	4035	OHX	2	0
86	5	4194	OHX	1	0
86	7	222	OHX	1	0
86	1	4057	OHX	4	0
86	m7	206	OHX	1	0
86	5	4033	OHX	1	0
86	6	2106	OHX	1	0
86	2	2123	OHX	1	0
86	5	3944	OHX	5	0
86	7	221	OHX	5	0
86	1	4136	OHX	6	0
86	2	2127	OHX	1	0
86	1	4202	OHX	2	0
86	1	4206	OHX	1	0
86	5	4000	OHX	6	0
86	1	4123	OHX	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	4031	OHX	5	0
86	5	4143	OHX	1	0
86	5	4019	OHX	7	0
86	5	4207	OHX	1	0
86	5	4025	OHX	2	0
86	6	2168	OHX	1	0
86	1	4087	OHX	1	0
86	1	3873	OHX	1	0
86	5	4002	OHX	1	0
86	M5	304	OHX	1	0
86	2	2070	OHX	1	0
86	1	3914	OHX	1	0
86	2	2071	OHX	2	0
86	1	4025	OHX	6	0
86	1	4084	OHX	1	0
86	1	4183	OHX	1	0
86	M9	202	OHX	1	0
86	5	4234	OHX	2	0
86	1	3959	OHX	7	0
86	2	2086	OHX	6	0
86	5	4217	OHX	8	0
86	2	2039	OHX	2	0
86	6	2154	OHX	2	0
86	1	4053	OHX	4	0
86	S8	302	OHX	1	0
86	1	4140	OHX	1	0
86	1	4002	OHX	1	0
86	2	2145	OHX	2	0
86	1	4180	OHX	3	0
86	M7	204	OHX	1	0
86	2	2037	OHX	2	0
86	5	3943	OHX	1	0
86	5	4159	OHX	1	0
86	6	2078	OHX	1	0
86	5	4001	OHX	3	0
86	1	4021	OHX	1	0
86	5	4195	OHX	1	0
86	2	2130	OHX	1	0
86	6	2181	OHX	2	0
86	3	216	OHX	1	0
86	6	2085	OHX	1	0
86	1	3972	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	4054	OHX	1	0
86	5	3985	OHX	1	0
86	6	2112	OHX	1	0
86	2	2104	OHX	2	0
86	1	3877	OHX	1	0
86	1	3882	OHX	1	0
86	6	2086	OHX	1	0
86	2	2073	OHX	1	0
86	1	3995	OHX	1	0
86	5	4086	OHX	1	0
86	5	4091	OHX	1	0
86	1	4168	OHX	10	0
86	1	4159	OHX	6	0
86	1	3888	OHX	1	0
86	5	4117	OHX	5	0
86	1	4195	OHX	1	0
86	2	2076	OHX	7	0
86	1	4016	OHX	7	0
86	1	4187	OHX	1	0
86	1	4028	OHX	7	0
86	1	4102	OHX	1	0
86	1	4110	OHX	6	0
86	5	4211	OHX	1	0
86	5	4065	OHX	1	0
86	7	224	OHX	1	0
86	6	2104	OHX	2	0
86	1	3892	OHX	1	0
86	1	4091	OHX	1	0
86	5	4198	OHX	8	0
86	5	3956	OHX	1	0
86	13	404	OHX	1	0
86	2	2180	OHX	1	0
86	6	2113	OHX	1	0
86	5	4214	OHX	2	0
86	2	2052	OHX	1	0
86	2	2027	OHX	1	0
86	2	2096	OHX	4	0
86	2	2142	OHX	1	0
86	5	4189	OHX	6	0
86	6	2122	OHX	1	0
86	1	3885	OHX	1	0
86	6	2146	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	4241	OHX	3	0
86	1	4175	OHX	1	0
86	5	4191	OHX	6	0
86	6	2192	OHX	2	0
86	1	4205	OHX	1	0
86	5	4093	OHX	6	0
86	1	3880	OHX	2	0
86	8	229	OHX	1	0
86	5	3963	OHX	4	0
86	8	227	OHX	6	0
86	6	2188	OHX	3	0
86	5	4079	OHX	5	0
86	1	4036	OHX	3	0
86	1	3956	OHX	2	0
86	1	4131	OHX	1	0
86	1	3947	OHX	1	0
86	6	2120	OHX	1	0
86	5	4088	OHX	1	0
86	5	4146	OHX	1	0
86	2	2099	OHX	8	0
86	6	2077	OHX	1	0
86	5	4090	OHX	1	0
86	5	4185	OHX	1	0
86	6	2110	OHX	1	0
86	2	2126	OHX	1	0
86	s8	303	OHX	1	0
86	6	2151	OHX	1	0
86	5	4165	OHX	1	0
86	5	3903	OHX	1	0
86	2	2075	OHX	2	0
86	1	4050	OHX	6	0
86	1	4186	OHX	1	0
86	1	4111	OHX	1	0
86	6	2124	OHX	1	0
86	5	4158	OHX	2	0
86	5	4137	OHX	1	0
86	2	2091	OHX	8	0
86	1	3870	OHX	1	0
86	1	4004	OHX	3	0
86	6	2198	OHX	1	0
86	5	3960	OHX	1	0
86	1	4128	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	4199	OHX	7	0
86	5	4101	OHX	2	0
86	q1	101	OHX	6	0
86	5	4092	OHX	6	0
86	m5	305	OHX	1	0
86	1	4193	OHX	7	0
86	2	2074	OHX	1	0
86	1	4155	OHX	1	0
86	6	2150	OHX	7	0
86	5	4007	OHX	1	0
86	5	4043	OHX	1	0
86	5	4181	OHX	1	0
86	5	4109	OHX	1	0
86	C1	201	OHX	6	0
86	5	3961	OHX	1	0
86	2	2097	OHX	1	0
86	1	3913	OHX	1	0
86	2	2133	OHX	1	0
86	O7	104	OHX	5	0
86	1	4179	OHX	1	0
86	o7	502	OHX	1	0
86	2	2169	OHX	1	0
86	5	4089	OHX	5	0
86	6	2089	OHX	2	0
86	2	2047	OHX	1	0
86	1	4065	OHX	2	0
86	1	3998	OHX	2	0
86	5	4136	OHX	5	0
86	M7	205	OHX	1	0
86	5	4153	OHX	1	0
86	5	4238	OHX	1	0
86	6	2202	OHX	1	0
86	1	3961	OHX	1	0
86	2	2150	OHX	1	0
86	2	2077	OHX	1	0
86	1	4156	OHX	4	0
86	6	2157	OHX	2	0
86	1	3930	OHX	2	0
86	5	4024	OHX	1	0
86	1	3969	OHX	1	0
86	6	2178	OHX	1	0
86	5	4011	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	4094	OHX	1	0
86	14	403	OHX	1	0
86	6	2191	OHX	1	0
86	2	2059	OHX	2	0
86	1	4033	OHX	3	0
86	5	4129	OHX	1	0
86	5	4064	OHX	7	0
86	1	4199	OHX	3	0
86	6	2186	OHX	1	0
86	S9	201	OHX	2	0
86	1	4082	OHX	1	0
86	5	3914	OHX	2	0
86	1	4023	OHX	1	0
86	Q2	502	OHX	3	0
86	1	4189	OHX	1	0
86	5	4193	OHX	1	0
86	o3	202	OHX	1	0
86	2	2093	OHX	3	0
86	6	2147	OHX	1	0
86	4	229	OHX	2	0
86	1	4121	OHX	1	0
86	1	4024	OHX	2	0
86	1	3979	OHX	1	0
86	6	2187	OHX	1	0
86	1	4160	OHX	1	0
86	1	4146	OHX	6	0
86	1	3984	OHX	2	0
86	1	4069	OHX	1	0
86	1	4081	OHX	3	0
86	1	4129	OHX	1	0
86	6	2062	OHX	6	0
86	5	3975	OHX	1	0
86	5	4095	OHX	2	0
86	2	2043	OHX	1	0
86	5	4130	OHX	1	0
86	5	3912	OHX	1	0
86	6	2111	OHX	2	0
86	6	2133	OHX	1	0
86	6	2053	OHX	1	0
86	2	2115	OHX	2	0
86	5	4192	OHX	6	0
86	5	3926	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	2	2171	OHX	2	0
86	5	4180	OHX	1	0
86	5	3933	OHX	1	0
86	1	3929	OHX	1	0
86	2	2110	OHX	1	0
86	5	4162	OHX	1	0
86	5	3970	OHX	1	0
86	2	2137	OHX	1	0
86	5	4026	OHX	1	0
86	5	4228	OHX	1	0
86	4	238	OHX	1	0
86	1	3883	OHX	1	0
86	5	4112	OHX	1	0
86	6	2177	OHX	1	0
86	1	3926	OHX	3	0
86	1	4164	OHX	2	0
86	1	4031	OHX	1	0
86	1	4118	OHX	2	0
86	3	225	OHX	1	0
86	2	2065	OHX	1	0
86	5	3910	OHX	1	0
86	1	4163	OHX	4	0
86	2	2111	OHX	3	0
86	5	4200	OHX	7	0
86	2	2053	OHX	1	0
86	5	4021	OHX	3	0
86	4	231	OHX	2	0
86	2	2144	OHX	1	0
86	1	4072	OHX	1	0
86	6	2117	OHX	1	0
86	5	4167	OHX	1	0
86	8	222	OHX	1	0
86	L3	404	OHX	1	0
86	2	2153	OHX	2	0
86	1	4029	OHX	2	0
86	5	4110	OHX	2	0
86	1	4114	OHX	1	0
86	6	2129	OHX	1	0
86	1	4127	OHX	2	0
86	6	2174	OHX	10	0
86	5	3906	OHX	1	0
86	1	4135	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	6	2123	OHX	8	0
86	2	2035	OHX	1	0
86	1	4200	OHX	1	0
86	1	4176	OHX	1	0
86	8	217	OHX	4	0
86	5	4183	OHX	2	0
86	m0	303	OHX	2	0
86	1	4150	OHX	6	0
86	6	2193	OHX	3	0
86	1	3933	OHX	1	0
86	1	4062	OHX	1	0
86	5	4224	OHX	3	0
86	5	4098	OHX	1	0
86	5	4009	OHX	6	0
86	2	2083	OHX	2	0
86	L3	403	OHX	1	0
86	6	2082	OHX	1	0
86	1	4026	OHX	3	0
86	2	2158	OHX	4	0
86	6	2108	OHX	1	0
86	5	3971	OHX	1	0
86	5	4037	OHX	2	0
86	1	3935	OHX	1	0
86	1	4151	OHX	6	0
86	1	4058	OHX	1	0
86	1	4052	OHX	5	0
86	7	220	OHX	1	0
86	5	3900	OHX	1	0
86	C5	201	OHX	4	0
86	6	2141	OHX	2	0
86	O3	202	OHX	2	0
86	6	2091	OHX	1	0
86	2	2132	OHX	8	0
86	6	2095	OHX	1	0
86	1	3943	OHX	1	0
86	1	4148	OHX	1	0
86	5	4152	OHX	1	0
86	5	3974	OHX	4	0
86	5	4027	OHX	1	0
86	1	4003	OHX	2	0
86	14	402	OHX	2	0
86	2	2117	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	2	2167	OHX	1	0
86	2	2162	OHX	6	0
86	1	4184	OHX	1	0
86	2	2048	OHX	2	0
86	3	224	OHX	1	0
86	2	2119	OHX	1	0
86	7	223	OHX	1	0
86	1	4152	OHX	7	0
86	1	4017	OHX	1	0
86	6	2093	OHX	1	0
86	2	2049	OHX	1	0
86	2	2045	OHX	7	0
86	1	3906	OHX	1	0
86	O9	101	OHX	3	0
86	2	2088	OHX	1	0
86	3	218	OHX	5	0
86	5	4156	OHX	1	0
86	8	223	OHX	1	0
86	1	3893	OHX	1	0
86	2	2156	OHX	1	0
86	1	4142	OHX	6	0
86	6	2162	OHX	3	0
86	5	4013	OHX	1	0
86	1	3950	OHX	2	0
86	1	3994	OHX	2	0
86	6	2115	OHX	1	0
86	6	2208	OHX	1	0
86	1	3981	OHX	2	0
86	1	3940	OHX	1	0
86	1	3974	OHX	6	0
86	2	2072	OHX	2	0
86	1	4196	OHX	1	0
86	1	3976	OHX	1	0
86	D9	102	OHX	1	0
86	6	2199	OHX	1	0
86	1	4071	OHX	1	0
86	1	4043	OHX	1	0
86	1	4204	OHX	1	0
86	5	4053	OHX	6	0
86	c3	201	OHX	1	0
86	1	3911	OHX	2	0
86	1	4061	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	3957	OHX	2	0
86	1	3890	OHX	1	0
86	2	2173	OHX	2	0
86	5	3958	OHX	1	0
86	1	4051	OHX	3	0
86	6	2084	OHX	1	0
86	6	2094	OHX	1	0
86	2	2136	OHX	1	0
86	6	2068	OHX	1	0
86	6	2153	OHX	6	0
86	q2	502	OHX	2	0
86	2	2087	OHX	1	0
86	1	3965	OHX	1	0
86	1	4038	OHX	2	0
86	1	4090	OHX	1	0
86	4	234	OHX	2	0
86	5	4087	OHX	1	0
86	1	4010	OHX	2	0
86	5	4005	OHX	1	0
86	5	4118	OHX	1	0
86	1	4005	OHX	1	0
86	5	4244	OHX	5	0
86	1	3946	OHX	3	0
86	7	226	OHX	4	0
86	5	3979	OHX	8	0
86	6	2152	OHX	1	0
86	1	3932	OHX	3	0
86	6	2079	OHX	1	0
86	2	2038	OHX	1	0
86	2	2139	OHX	1	0
86	1	4171	OHX	1	0
86	2	2061	OHX	1	0
86	1	4099	OHX	1	0
86	1	4138	OHX	1	0
86	5	4063	OHX	5	0
86	5	3987	OHX	1	0
86	6	2114	OHX	2	0
86	6	2064	OHX	1	0
86	m9	201	OHX	1	0
86	5	4062	OHX	1	0
86	1	3899	OHX	1	0
86	6	2190	OHX	1	0

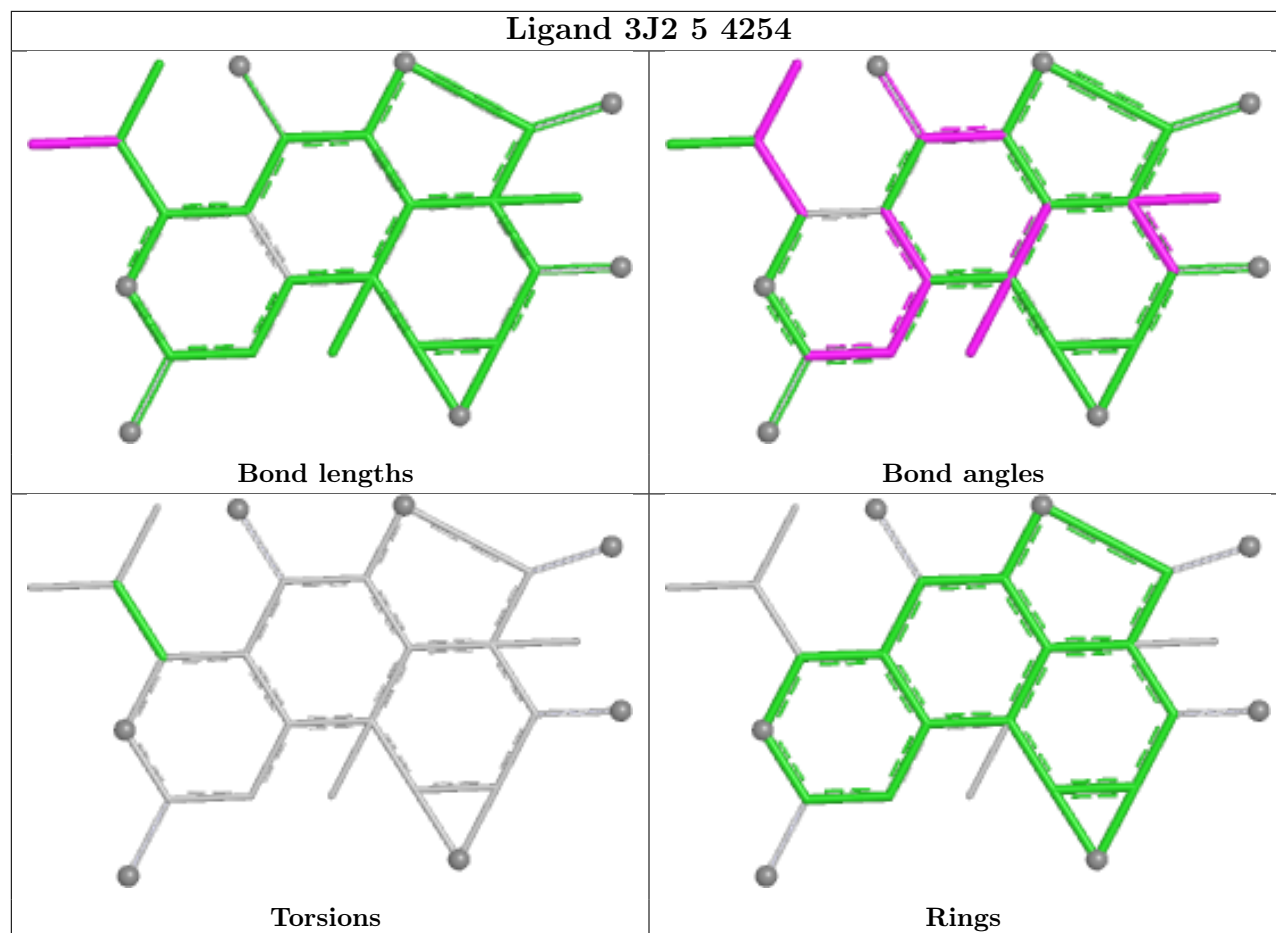
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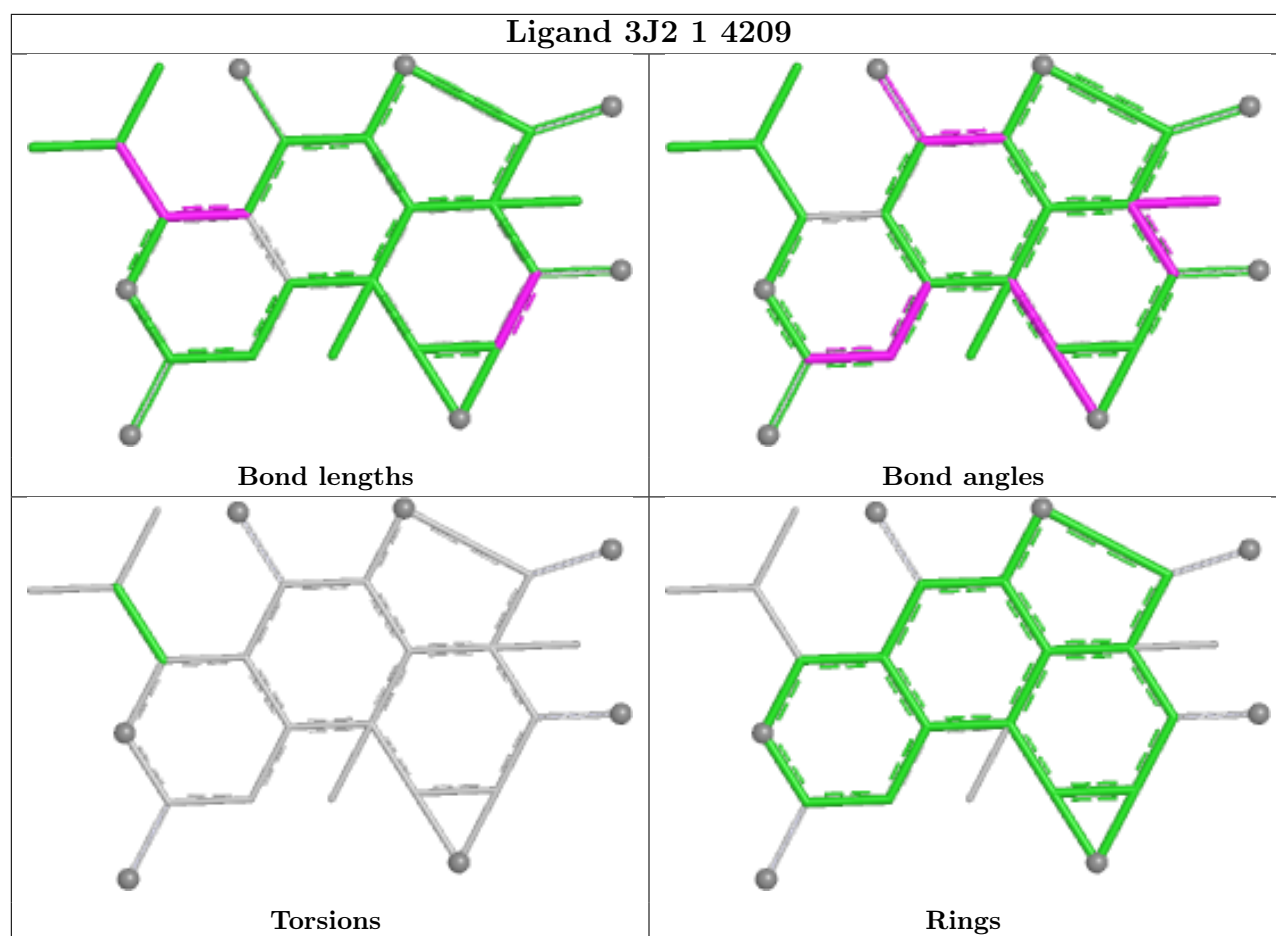
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	4154	OHX	1	0
86	m1	203	OHX	2	0
86	5	4209	OHX	1	0
86	1	3953	OHX	1	0
86	2	2046	OHX	1	0
86	5	3908	OHX	1	0
86	2	2149	OHX	3	0

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.

Ligand 3J2 5 4254





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	1750/1800 (97%)	0.38	87 (4%) 34 18	40, 71, 144, 248	0
1	6	1795/1800 (99%)	0.29	88 (4%) 35 18	32, 64, 158, 254	0
2	S0	206/251 (82%)	0.73	14 (6%) 23 12	77, 91, 106, 127	0
2	s0	206/251 (82%)	0.47	9 (4%) 39 21	63, 82, 97, 107	0
3	S1	214/254 (84%)	1.00	22 (10%) 12 6	79, 111, 138, 142	0
3	s1	216/254 (85%)	0.33	5 (2%) 61 38	56, 69, 93, 103	0
4	S2	217/253 (85%)	0.38	4 (1%) 67 44	55, 70, 87, 99	0
4	s2	217/253 (85%)	0.39	8 (3%) 45 25	47, 63, 77, 92	0
5	S3	223/239 (93%)	0.38	4 (1%) 67 44	60, 75, 101, 122	0
5	s3	223/239 (93%)	0.55	10 (4%) 38 20	61, 88, 116, 129	0
6	S4	260/260 (100%)	0.36	3 (1%) 76 55	46, 71, 84, 121	0
6	s4	260/260 (100%)	0.32	6 (2%) 61 38	40, 65, 85, 121	0
7	S5	206/224 (91%)	0.89	16 (7%) 19 10	77, 99, 117, 137	0
7	s5	206/224 (91%)	0.86	25 (12%) 8 5	59, 84, 107, 126	0
8	S6	226/236 (95%)	0.59	17 (7%) 20 10	48, 80, 103, 143	0
8	s6	218/236 (92%)	0.43	7 (3%) 50 29	40, 70, 94, 117	0
9	S7	184/189 (97%)	0.67	7 (3%) 44 24	67, 96, 128, 138	0
9	s7	186/189 (98%)	0.67	9 (4%) 35 19	59, 91, 123, 135	0
10	S8	188/200 (94%)	0.24	3 (1%) 70 47	41, 54, 90, 108	0
10	s8	188/200 (94%)	0.36	4 (2%) 63 40	36, 56, 99, 112	0
11	S9	185/196 (94%)	0.75	12 (6%) 25 13	64, 80, 118, 154	0
11	s9	185/196 (94%)	0.46	4 (2%) 62 39	54, 70, 105, 140	0
12	C0	96/105 (91%)	0.59	5 (5%) 33 17	66, 86, 115, 126	0
12	c0	96/105 (91%)	1.02	15 (15%) 5 3	78, 108, 128, 145	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	C1	155/155 (100%)	0.42	12 (7%)	19 10	44, 54, 128, 138	0
13	c1	146/155 (94%)	0.66	17 (11%)	9 5	40, 55, 86, 111	0
14	C2	124/142 (87%)	1.12	16 (12%)	7 5	108, 125, 144, 162	0
14	c2	124/142 (87%)	1.45	28 (22%)	2 1	151, 168, 191, 198	0
15	C3	150/150 (100%)	0.41	4 (2%)	56 33	51, 69, 83, 94	0
15	c3	150/150 (100%)	0.30	2 (1%)	75 53	48, 63, 81, 94	0
16	C4	127/136 (93%)	1.26	17 (13%)	7 4	54, 111, 128, 131	0
16	c4	128/136 (94%)	0.62	4 (3%)	51 30	39, 71, 79, 83	0
17	C5	124/141 (87%)	0.53	5 (4%)	42 23	59, 74, 114, 131	0
17	c5	135/141 (95%)	0.72	13 (9%)	13 7	63, 81, 106, 124	0
18	C6	141/142 (99%)	0.73	5 (3%)	47 27	66, 89, 95, 99	0
18	c6	142/142 (100%)	0.73	13 (9%)	14 8	53, 74, 92, 115	0
19	C7	120/136 (88%)	0.76	8 (6%)	24 12	75, 94, 121, 127	0
19	c7	117/136 (86%)	0.85	10 (8%)	16 8	66, 82, 112, 122	0
20	C8	145/145 (100%)	0.55	4 (2%)	55 32	59, 85, 112, 123	0
20	c8	145/145 (100%)	0.47	5 (3%)	48 27	57, 73, 105, 122	0
21	C9	143/143 (100%)	0.59	4 (2%)	55 32	69, 84, 102, 112	0
21	c9	143/143 (100%)	0.25	4 (2%)	55 32	54, 68, 91, 110	0
22	D0	107/120 (89%)	0.96	10 (9%)	14 7	57, 91, 131, 136	0
22	d0	110/120 (91%)	0.90	7 (6%)	25 13	54, 92, 136, 147	0
23	D1	87/87 (100%)	0.39	2 (2%)	61 38	73, 80, 99, 113	0
23	d1	87/87 (100%)	0.15	1 (1%)	78 57	60, 68, 89, 97	0
24	D2	129/129 (100%)	0.24	2 (1%)	70 47	52, 64, 73, 84	0
24	d2	129/129 (100%)	0.06	1 (0%)	82 64	45, 55, 63, 75	0
25	D3	144/144 (100%)	0.19	2 (1%)	73 51	42, 48, 58, 75	0
25	d3	144/144 (100%)	0.06	8 (5%)	30 15	36, 40, 52, 68	0
26	D4	134/134 (100%)	0.59	5 (3%)	45 25	56, 83, 100, 110	0
26	d4	134/134 (100%)	0.49	5 (3%)	45 25	48, 72, 89, 114	0
27	D5	70/107 (65%)	1.01	8 (11%)	10 6	94, 111, 127, 132	0
27	d5	69/107 (64%)	0.70	5 (7%)	21 11	80, 101, 116, 120	0
28	D6	97/97 (100%)	1.19	17 (17%)	4 3	59, 75, 133, 138	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	d6	97/97 (100%)	0.45	3 (3%)	51	30	44, 57, 85, 93	0
29	D7	81/81 (100%)	0.63	4 (4%)	35	18	67, 81, 121, 128	0
29	d7	81/81 (100%)	0.64	5 (6%)	26	14	57, 75, 124, 127	0
30	D8	63/66 (95%)	1.05	5 (7%)	18	10	93, 113, 129, 134	0
30	d8	63/66 (95%)	0.87	6 (9%)	14	7	79, 98, 116, 134	0
31	D9	53/55 (96%)	0.58	6 (11%)	10	6	59, 63, 82, 88	0
31	d9	53/55 (96%)	0.71	4 (7%)	20	10	58, 65, 104, 120	0
32	E0	60/60 (100%)	0.65	6 (10%)	12	7	48, 78, 135, 141	0
33	E1	71/76 (93%)	1.36	17 (23%)	2	1	86, 106, 121, 124	0
33	e1	76/76 (100%)	1.93	30 (39%)	1	1	128, 140, 151, 152	0
34	SR	318/318 (100%)	0.60	15 (4%)	36	19	58, 95, 118, 141	0
34	sR	318/318 (100%)	0.87	25 (7%)	18	10	82, 105, 122, 139	0
35	SM	159/273 (58%)	0.94	24 (15%)	5	3	51, 75, 129, 138	0
35	sM	104/273 (38%)	1.16	22 (21%)	2	1	44, 84, 157, 169	0
36	1	3149/3396 (92%)	-0.22	102 (3%)	50	29	14, 36, 116, 249	0
36	5	3150/3396 (92%)	-0.24	83 (2%)	57	34	14, 36, 105, 236	0
37	3	121/121 (100%)	-0.32	1 (0%)	82	64	29, 54, 69, 72	0
37	7	121/121 (100%)	-0.11	1 (0%)	82	64	22, 38, 51, 58	0
38	4	158/158 (100%)	-0.41	4 (2%)	58	35	19, 36, 72, 114	0
38	8	158/158 (100%)	0.24	6 (3%)	44	24	25, 45, 79, 105	0
39	L2	252/253 (99%)	-0.12	2 (0%)	82	64	20, 33, 48, 57	0
39	l2	252/253 (99%)	0.20	7 (2%)	55	32	23, 40, 56, 67	0
40	L3	386/386 (100%)	-0.15	2 (0%)	87	72	19, 38, 50, 83	0
40	l3	386/386 (100%)	-0.13	4 (1%)	79	59	15, 28, 40, 73	0
41	L4	361/361 (100%)	-0.24	1 (0%)	90	79	17, 30, 48, 59	0
41	l4	361/361 (100%)	-0.03	2 (0%)	85	69	19, 35, 52, 70	0
42	L5	296/296 (100%)	0.14	6 (2%)	65	41	37, 59, 77, 106	0
42	l5	294/296 (99%)	0.27	7 (2%)	59	36	28, 42, 69, 113	0
43	L6	156/175 (89%)	-0.16	1 (0%)	85	69	26, 33, 52, 72	0
43	l6	157/175 (89%)	-0.01	3 (1%)	66	43	27, 34, 52, 65	0
44	L7	222/243 (91%)	-0.33	2 (0%)	81	61	21, 28, 56, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	l7	223/243 (91%)	-0.22	0 100 100	18, 25, 64, 115	0
45	L8	233/255 (91%)	0.28	7 (3%) 52 30	41, 54, 91, 109	0
45	l8	231/255 (90%)	0.94	30 (12%) 7 4	53, 67, 100, 112	0
46	L9	191/191 (100%)	-0.12	2 (1%) 79 59	34, 44, 55, 75	0
46	l9	191/191 (100%)	0.04	2 (1%) 79 59	25, 34, 55, 79	0
47	M0	211/220 (95%)	-0.02	3 (1%) 73 51	26, 42, 77, 99	0
47	m0	213/220 (96%)	0.72	15 (7%) 22 12	27, 43, 67, 86	0
48	M1	169/173 (97%)	0.12	1 (0%) 85 69	46, 64, 75, 85	0
48	m1	169/173 (97%)	0.24	3 (1%) 67 44	31, 47, 59, 72	0
49	M3	193/198 (97%)	-0.13	1 (0%) 87 72	19, 39, 81, 106	0
49	m3	194/198 (97%)	0.33	3 (1%) 72 49	26, 48, 86, 110	0
50	M4	136/137 (99%)	-0.23	2 (1%) 72 49	27, 35, 47, 55	0
50	m4	137/137 (100%)	-0.17	4 (2%) 53 31	26, 29, 49, 59	0
51	M5	203/203 (100%)	-0.17	0 100 100	20, 32, 43, 47	0
51	m5	203/203 (100%)	0.27	0 100 100	25, 42, 53, 58	0
52	M6	197/198 (99%)	-0.26	1 (0%) 87 72	21, 27, 44, 46	0
52	m6	197/198 (99%)	-0.30	1 (0%) 87 72	16, 20, 44, 50	0
53	M7	183/183 (100%)	0.14	11 (6%) 27 14	22, 30, 93, 142	0
53	m7	155/183 (84%)	-0.22	0 100 100	19, 26, 36, 69	0
54	M8	185/185 (100%)	-0.17	1 (0%) 87 72	22, 32, 48, 68	0
54	m8	185/185 (100%)	-0.01	0 100 100	23, 34, 43, 49	0
55	M9	188/188 (100%)	0.35	14 (7%) 20 10	35, 50, 143, 153	0
55	m9	188/188 (100%)	0.51	6 (3%) 50 29	34, 47, 122, 132	0
56	N0	172/172 (100%)	-0.21	2 (1%) 76 55	26, 34, 46, 56	0
56	n0	172/172 (100%)	-0.20	4 (2%) 61 38	22, 28, 37, 44	0
57	N1	159/159 (100%)	-0.10	1 (0%) 85 69	25, 35, 81, 91	0
57	n1	159/159 (100%)	-0.06	1 (0%) 85 69	22, 28, 67, 74	0
58	N2	100/120 (83%)	0.58	4 (4%) 42 23	65, 83, 97, 132	0
58	n2	98/120 (81%)	0.81	5 (5%) 33 17	59, 73, 82, 85	0
59	N3	136/136 (100%)	-0.22	2 (1%) 72 49	24, 33, 44, 51	0
59	n3	136/136 (100%)	-0.20	2 (1%) 72 49	17, 27, 40, 44	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	N4	98/155 (63%)	0.70	16 (16%) 4 3	34, 47, 138, 143	0
60	n4	135/155 (87%)	0.83	21 (15%) 5 3	27, 79, 124, 144	0
61	N5	121/141 (85%)	-0.04	1 (0%) 82 64	32, 42, 61, 87	0
61	n5	120/141 (85%)	0.41	3 (2%) 58 35	36, 49, 71, 80	0
62	N6	126/126 (100%)	-0.26	1 (0%) 82 64	22, 38, 49, 53	0
62	n6	126/126 (100%)	0.34	4 (3%) 50 29	28, 43, 58, 65	0
63	N7	135/135 (100%)	0.15	0 100 100	51, 65, 79, 90	0
63	n7	135/135 (100%)	1.03	10 (7%) 20 10	62, 75, 95, 105	0
64	N8	148/148 (100%)	-0.28	1 (0%) 84 66	15, 33, 56, 66	0
64	n8	148/148 (100%)	-0.02	0 100 100	17, 38, 52, 55	0
65	N9	58/58 (100%)	0.21	3 (5%) 33 17	23, 40, 89, 103	0
65	n9	58/58 (100%)	0.40	3 (5%) 33 17	21, 38, 63, 69	0
66	O0	97/104 (93%)	0.02	1 (1%) 79 59	49, 59, 86, 97	0
66	o0	100/104 (96%)	0.64	4 (4%) 42 23	57, 67, 94, 98	0
67	O1	109/112 (97%)	0.07	3 (2%) 55 32	32, 44, 83, 94	0
67	o1	109/112 (97%)	0.07	2 (1%) 67 44	27, 38, 72, 93	0
68	O2	127/129 (98%)	-0.23	2 (1%) 70 47	15, 29, 38, 56	0
68	o2	127/129 (98%)	-0.06	3 (2%) 59 36	17, 32, 43, 67	0
69	O3	106/106 (100%)	-0.28	0 100 100	21, 25, 47, 57	0
69	o3	106/106 (100%)	-0.23	2 (1%) 66 43	18, 25, 48, 54	0
70	O4	112/119 (94%)	0.25	5 (4%) 38 20	31, 47, 92, 111	0
70	o4	112/119 (94%)	0.68	5 (4%) 38 20	36, 54, 95, 108	0
71	O5	119/119 (100%)	0.02	3 (2%) 58 35	31, 45, 52, 57	0
71	o5	119/119 (100%)	0.48	3 (2%) 58 35	38, 52, 63, 71	0
72	O6	99/99 (100%)	0.13	3 (3%) 52 30	36, 46, 82, 98	0
72	o6	99/99 (100%)	0.43	2 (2%) 65 41	43, 57, 81, 95	0
73	O7	87/87 (100%)	-0.01	4 (4%) 37 20	21, 25, 49, 71	0
73	o7	87/87 (100%)	0.42	4 (4%) 37 20	23, 31, 57, 93	0
74	O8	77/77 (100%)	0.20	2 (2%) 57 34	55, 67, 95, 106	0
74	o8	77/77 (100%)	0.89	2 (2%) 57 34	59, 72, 97, 101	0
75	O9	50/50 (100%)	-0.01	2 (4%) 42 23	29, 32, 40, 41	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	o9	50/50 (100%)	0.20	1 (2%) 65 41	34, 38, 45, 51	0
76	Q0	52/52 (100%)	-0.23	0 100 100	30, 35, 47, 56	0
76	q0	52/52 (100%)	-0.25	0 100 100	21, 25, 34, 41	0
77	Q1	25/25 (100%)	0.12	0 100 100	40, 42, 45, 47	0
77	q1	25/25 (100%)	0.05	0 100 100	32, 36, 44, 50	0
78	Q2	105/105 (100%)	-0.05	3 (2%) 53 31	24, 39, 60, 83	0
78	q2	105/105 (100%)	-0.02	1 (0%) 79 59	27, 38, 50, 78	0
79	Q3	91/91 (100%)	-0.20	1 (1%) 78 57	27, 36, 50, 63	0
79	q3	91/91 (100%)	0.12	1 (1%) 78 57	29, 41, 54, 63	0
80	e0	62/62 (100%)	0.40	3 (4%) 35 19	44, 69, 112, 130	0
81	m2	0/160	-	-	-	-
82	p0	143/311 (45%)	1.23	18 (12%) 8 5	78, 94, 173, 179	0
83	p1	0/47	-	-	-	-
84	p2	0/46	-	-	-	-
All	All	33063/35344 (93%)	0.21	1305 (3%) 43 24	14, 53, 117, 254	0

The worst 5 of 1305 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
47	m0	111	LEU	8.0
7	S5	37	GLN	7.7
73	o7	88	ALA	7.3
1	6	662	U	7.2
82	p0	192	ASP	7.1

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
85	MG	1	3803	1/1	-0.73	0.44	193,193,193,193	0
85	MG	6	1924	1/1	-0.06	0.50	92,92,92,92	0
85	MG	2	2003	1/1	-0.00	0.52	114,114,114,114	0
85	MG	2	1953	1/1	0.22	0.46	94,94,94,94	0
85	MG	5	3804	1/1	0.23	0.25	139,139,139,139	0
85	MG	6	2015	1/1	0.24	0.47	125,125,125,125	0
85	MG	6	2042	1/1	0.28	0.60	100,100,100,100	0
85	MG	5	3772	1/1	0.42	0.38	87,87,87,87	0
85	MG	1	3858	1/1	0.42	0.23	125,125,125,125	0
85	MG	2	1968	1/1	0.43	0.52	104,104,104,104	0
85	MG	1	3649	1/1	0.44	0.48	95,95,95,95	0
85	MG	6	2041	1/1	0.45	0.55	88,88,88,88	0
85	MG	1	3813	1/1	0.47	0.51	101,101,101,101	0
85	MG	2	1963	1/1	0.48	0.21	127,127,127,127	0
85	MG	1	3405	1/1	0.48	0.43	89,89,89,89	0
85	MG	6	2047	1/1	0.49	0.50	79,79,79,79	0
85	MG	5	3466	1/1	0.49	0.46	86,86,86,86	0
85	MG	2	1954	1/1	0.50	0.34	85,85,85,85	0
85	MG	5	3708	1/1	0.50	0.44	83,83,83,83	0
85	MG	2	1989	1/1	0.51	0.28	77,77,77,77	0
85	MG	4	222	1/1	0.52	0.48	76,76,76,76	0
85	MG	2	2018	1/1	0.53	0.30	62,62,62,62	0
85	MG	2	1969	1/1	0.54	0.43	78,78,78,78	0
85	MG	5	3881	1/1	0.54	0.49	77,77,77,77	0
85	MG	6	1909	1/1	0.56	0.37	88,88,88,88	0
85	MG	1	3624	1/1	0.56	0.44	87,87,87,87	0
85	MG	2	1987	1/1	0.56	0.42	88,88,88,88	0
85	MG	6	2022	1/1	0.56	0.33	104,104,104,104	0
85	MG	M3	202	1/1	0.57	0.43	83,83,83,83	0
85	MG	5	3686	1/1	0.59	0.22	67,67,67,67	0
85	MG	5	3780	1/1	0.59	0.41	60,60,60,60	0
85	MG	5	3792	1/1	0.63	0.31	80,80,80,80	0
85	MG	2	1951	1/1	0.63	0.43	79,79,79,79	0
85	MG	6	1934	1/1	0.63	0.33	65,65,65,65	0
85	MG	5	3795	1/1	0.64	0.33	59,59,59,59	0
85	MG	6	2037	1/1	0.64	0.36	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3732	1/1	0.64	0.27	69,69,69,69	0
85	MG	6	1966	1/1	0.65	0.38	75,75,75,75	0
85	MG	2	1975	1/1	0.65	0.53	73,73,73,73	0
85	MG	5	3896	1/1	0.65	0.23	100,100,100,100	0
85	MG	1	3419	1/1	0.66	0.36	70,70,70,70	0
85	MG	1	3530	1/1	0.66	0.36	48,48,48,48	0
85	MG	6	1985	1/1	0.66	0.28	72,72,72,72	0
85	MG	6	2000	1/1	0.66	0.36	91,91,91,91	0
85	MG	2	1933	1/1	0.67	0.36	58,58,58,58	0
85	MG	5	3806	1/1	0.67	0.41	75,75,75,75	0
85	MG	6	1904	1/1	0.67	0.39	57,57,57,57	0
85	MG	2	2023	1/1	0.67	0.25	93,93,93,93	0
87	ZN	d7	101	1/1	0.67	0.19	155,155,155,155	0
85	MG	6	1907	1/1	0.68	0.32	59,59,59,59	0
85	MG	1	3591	1/1	0.68	0.31	57,57,57,57	0
85	MG	5	3677	1/1	0.68	0.26	82,82,82,82	0
85	MG	2	1945	1/1	0.68	0.40	69,69,69,69	0
85	MG	2	1990	1/1	0.68	0.37	44,44,44,44	0
85	MG	2	1914	1/1	0.68	0.39	51,51,51,51	0
86	OHX	5	4239	7/7	0.68	0.23	137,137,137,137	0
85	MG	2	1943	1/1	0.68	0.13	53,53,53,53	0
85	MG	6	1920	1/1	0.69	0.43	57,57,57,57	0
85	MG	2	1991	1/1	0.69	0.36	98,98,98,98	0
85	MG	2	1972	1/1	0.69	0.36	70,70,70,70	0
85	MG	1	3674	1/1	0.69	0.39	59,59,59,59	0
85	MG	5	3662	1/1	0.69	0.50	58,58,58,58	0
85	MG	6	1977	1/1	0.69	0.25	60,60,60,60	0
85	MG	5	3421	1/1	0.70	0.36	82,82,82,82	0
85	MG	5	3769	1/1	0.70	0.19	90,90,90,90	0
85	MG	1	3479	1/1	0.70	0.38	67,67,67,67	0
85	MG	2	1980	1/1	0.70	0.42	57,57,57,57	0
86	OHX	2	2163	7/7	0.70	0.21	141,141,141,141	0
85	MG	M0	302	1/1	0.70	0.43	43,43,43,43	0
86	OHX	5	4243	7/7	0.70	0.16	213,213,213,213	0
85	MG	2	1966	1/1	0.70	0.25	69,69,69,69	0
85	MG	5	3649	1/1	0.71	0.31	75,75,75,75	0
85	MG	6	2046	1/1	0.71	0.32	53,53,53,53	0
85	MG	o4	202	1/1	0.71	0.24	61,61,61,61	0
85	MG	2	2017	1/1	0.71	0.44	67,67,67,67	0
85	MG	2	1928	1/1	0.71	0.44	66,66,66,66	0
85	MG	2	1960	1/1	0.71	0.31	52,52,52,52	0
85	MG	5	3475	1/1	0.71	0.34	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3754	1/1	0.72	0.34	80,80,80,80	0
85	MG	1	3546	1/1	0.72	0.21	51,51,51,51	0
86	OHX	5	4229	7/7	0.72	0.32	100,100,100,100	0
85	MG	6	1930	1/1	0.72	0.34	50,50,50,50	0
85	MG	6	2038	1/1	0.72	0.23	71,71,71,71	0
85	MG	4	201	1/1	0.72	0.29	42,42,42,42	0
85	MG	6	1989	1/1	0.73	0.20	42,42,42,42	0
85	MG	2	2010	1/1	0.73	0.34	59,59,59,59	0
85	MG	6	2008	1/1	0.73	0.12	50,50,50,50	0
85	MG	7	214	1/1	0.73	0.22	80,80,80,80	0
85	MG	1	3847	1/1	0.73	0.29	49,49,49,49	0
85	MG	1	3493	1/1	0.73	0.23	68,68,68,68	0
85	MG	1	3528	1/1	0.73	0.33	35,35,35,35	0
85	MG	5	3613	1/1	0.73	0.21	38,38,38,38	0
85	MG	4	204	1/1	0.73	0.46	49,49,49,49	0
86	OHX	14	402	7/7	0.73	0.22	117,117,117,117	0
85	MG	2	1995	1/1	0.73	0.47	78,78,78,78	0
85	MG	2	1964	1/1	0.74	0.32	80,80,80,80	0
85	MG	2	1948	1/1	0.74	0.28	72,72,72,72	0
85	MG	5	3886	1/1	0.74	0.29	46,46,46,46	0
85	MG	2	1940	1/1	0.74	0.27	50,50,50,50	0
85	MG	6	1963	1/1	0.75	0.36	71,71,71,71	0
85	MG	6	2005	1/1	0.75	0.26	80,80,80,80	0
85	MG	1	3660	1/1	0.75	0.10	46,46,46,46	0
86	OHX	1	4167	7/7	0.75	0.30	107,107,107,107	0
86	OHX	1	4182	7/7	0.75	0.19	161,161,161,161	0
85	MG	6	1973	1/1	0.75	0.32	58,58,58,58	0
86	OHX	5	4235	7/7	0.75	0.22	126,126,126,126	0
85	MG	5	3420	1/1	0.75	0.30	56,56,56,56	0
85	MG	2	2002	1/1	0.75	0.27	87,87,87,87	0
85	MG	6	1936	1/1	0.75	0.34	76,76,76,76	0
85	MG	6	1950	1/1	0.75	0.30	38,38,38,38	0
85	MG	3	209	1/1	0.76	0.33	51,51,51,51	0
85	MG	6	1967	1/1	0.76	0.30	64,64,64,64	0
85	MG	6	1968	1/1	0.76	0.33	64,64,64,64	0
85	MG	2	2019	1/1	0.76	0.38	60,60,60,60	0
85	MG	1	3442	1/1	0.76	0.26	75,75,75,75	0
85	MG	2	2020	1/1	0.76	0.42	61,61,61,61	0
85	MG	5	3685	1/1	0.76	0.32	54,54,54,54	0
85	MG	2	1978	1/1	0.76	0.47	77,77,77,77	0
85	MG	1	3648	1/1	0.76	0.26	49,49,49,49	0
86	OHX	6	2194	7/7	0.76	0.22	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	5	4164	7/7	0.76	0.18	169,169,169,169	0
86	OHX	5	4196	7/7	0.76	0.20	129,129,129,129	0
85	MG	6	2048	1/1	0.76	0.39	68,68,68,68	0
85	MG	c7	201	1/1	0.76	0.30	64,64,64,64	0
85	MG	5	3404	1/1	0.76	0.22	37,37,37,37	0
85	MG	1	3499	1/1	0.76	0.29	56,56,56,56	0
85	MG	2	1908	1/1	0.76	0.38	55,55,55,55	0
85	MG	5	3449	1/1	0.76	0.22	56,56,56,56	0
85	MG	2	1913	1/1	0.77	0.41	70,70,70,70	0
85	MG	5	3779	1/1	0.77	0.43	61,61,61,61	0
86	OHX	S9	201	7/7	0.77	0.25	110,110,110,110	0
85	MG	2	1992	1/1	0.77	0.28	82,82,82,82	0
85	MG	1	3511	1/1	0.77	0.37	33,33,33,33	0
86	OHX	1	4185	7/7	0.77	0.28	109,109,109,109	0
86	OHX	6	2188	7/7	0.77	0.25	110,110,110,110	0
85	MG	6	1933	1/1	0.77	0.46	61,61,61,61	0
85	MG	6	2032	1/1	0.77	0.27	92,92,92,92	0
86	OHX	5	4188	7/7	0.77	0.19	137,137,137,137	0
85	MG	2	1926	1/1	0.77	0.46	71,71,71,71	0
85	MG	5	3875	1/1	0.77	0.31	31,31,31,31	0
86	OHX	5	4232	7/7	0.77	0.29	96,96,96,96	0
85	MG	3	208	1/1	0.77	0.21	68,68,68,68	0
85	MG	1	3634	1/1	0.77	0.39	61,61,61,61	0
85	MG	5	3888	1/1	0.77	0.21	27,27,27,27	0
85	MG	5	3732	1/1	0.77	0.21	57,57,57,57	0
85	MG	1	3635	1/1	0.77	0.11	34,34,34,34	0
85	MG	5	3734	1/1	0.78	0.32	64,64,64,64	0
85	MG	1	3507	1/1	0.78	0.30	20,20,20,20	0
86	OHX	2	2100	7/7	0.78	0.21	124,124,124,124	0
85	MG	5	3842	1/1	0.78	0.10	40,40,40,40	0
86	OHX	2	2164	7/7	0.78	0.25	117,117,117,117	0
86	OHX	5	4231	7/7	0.78	0.21	138,138,138,138	0
85	MG	1	3830	1/1	0.78	0.36	43,43,43,43	0
86	OHX	1	4130	7/7	0.78	0.24	98,98,98,98	0
85	MG	5	3497	1/1	0.78	0.22	38,38,38,38	0
85	MG	5	3605	1/1	0.78	0.17	39,39,39,39	0
85	MG	2	1959	1/1	0.78	0.47	80,80,80,80	0
87	ZN	D7	101	1/1	0.78	0.19	156,156,156,156	0
85	MG	6	1981	1/1	0.78	0.34	60,60,60,60	0
85	MG	2	1924	1/1	0.79	0.41	67,67,67,67	0
85	MG	2	1998	1/1	0.79	0.19	63,63,63,63	0
85	MG	5	3822	1/1	0.79	0.27	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
85	MG	5	3705	1/1	0.79	0.21	39,39,39,39	0
86	OHX	1	4190	7/7	0.79	0.22	108,108,108,108	0
86	OHX	6	2151	7/7	0.79	0.22	109,109,109,109	0
85	MG	5	3847	1/1	0.79	0.10	42,42,42,42	0
86	OHX	6	2192	7/7	0.79	0.22	125,125,125,125	0
85	MG	5	3872	1/1	0.79	0.26	43,43,43,43	0
86	OHX	s1	303	7/7	0.79	0.19	141,141,141,141	0
85	MG	6	1923	1/1	0.79	0.34	61,61,61,61	0
85	MG	5	3728	1/1	0.79	0.21	81,81,81,81	0
85	MG	2	1915	1/1	0.79	0.44	56,56,56,56	0
86	OHX	5	4207	7/7	0.79	0.25	114,114,114,114	0
86	OHX	5	4224	7/7	0.79	0.28	95,95,95,95	0
85	MG	2	1983	1/1	0.79	0.34	66,66,66,66	0
85	MG	4	216	1/1	0.79	0.15	39,39,39,39	0
85	MG	2	2007	1/1	0.79	0.45	60,60,60,60	0
85	MG	7	216	1/1	0.79	0.35	55,55,55,55	0
86	OHX	5	4237	7/7	0.79	0.23	115,115,115,115	0
85	MG	1	3836	1/1	0.79	0.33	44,44,44,44	0
85	MG	1	3839	1/1	0.79	0.24	36,36,36,36	0
85	MG	5	3790	1/1	0.79	0.14	35,35,35,35	0
85	MG	2	1927	1/1	0.79	0.36	53,53,53,53	0
85	MG	1	3696	1/1	0.79	0.37	60,60,60,60	0
85	MG	2	1930	1/1	0.80	0.25	55,55,55,55	0
85	MG	2	1909	1/1	0.80	0.37	58,58,58,58	0
86	OHX	6	2195	7/7	0.80	0.20	139,139,139,139	0
85	MG	3	203	1/1	0.80	0.27	76,76,76,76	0
85	MG	5	3464	1/1	0.80	0.11	28,28,28,28	0
85	MG	2	1976	1/1	0.80	0.28	44,44,44,44	0
85	MG	5	3469	1/1	0.80	0.20	101,101,101,101	0
85	MG	5	3809	1/1	0.80	0.17	44,44,44,44	0
85	MG	5	3722	1/1	0.80	0.23	43,43,43,43	0
85	MG	2	1952	1/1	0.80	0.27	85,85,85,85	0
85	MG	2	1938	1/1	0.80	0.27	55,55,55,55	0
86	OHX	1	4181	7/7	0.80	0.22	121,121,121,121	0
85	MG	5	3582	1/1	0.80	0.31	32,32,32,32	0
85	MG	6	2210	1/1	0.80	0.30	58,58,58,58	0
85	MG	1	3474	1/1	0.80	0.36	63,63,63,63	0
86	OHX	L4	403	7/7	0.80	0.21	106,106,106,106	0
86	OHX	5	4249	7/7	0.80	0.21	128,128,128,128	0
86	OHX	7	227	7/7	0.80	0.21	127,127,127,127	0
85	MG	5	3775	1/1	0.80	0.18	46,46,46,46	0
86	OHX	14	403	7/7	0.80	0.21	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	6	1914	1/1	0.80	0.27	61,61,61,61	0
86	OHX	6	2189	7/7	0.80	0.16	146,146,146,146	0
85	MG	1	3662	1/1	0.81	0.11	35,35,35,35	0
85	MG	5	3812	1/1	0.81	0.15	69,69,69,69	0
86	OHX	6	2197	7/7	0.81	0.16	152,152,152,152	0
86	OHX	6	2200	7/7	0.81	0.16	148,148,148,148	0
86	OHX	6	2204	7/7	0.81	0.21	126,126,126,126	0
85	MG	5	3747	1/1	0.81	0.32	30,30,30,30	0
85	MG	2	1931	1/1	0.81	0.40	44,44,44,44	0
85	MG	6	1986	1/1	0.81	0.30	64,64,64,64	0
85	MG	6	1922	1/1	0.81	0.32	50,50,50,50	0
86	OHX	1	4165	7/7	0.81	0.20	125,125,125,125	0
85	MG	5	3479	1/1	0.81	0.35	50,50,50,50	0
86	OHX	1	4171	7/7	0.81	0.19	122,122,122,122	0
85	MG	5	3696	1/1	0.81	0.09	28,28,28,28	0
85	MG	6	1991	1/1	0.81	0.26	67,67,67,67	0
85	MG	5	3502	1/1	0.81	0.20	33,33,33,33	0
86	OHX	5	4236	7/7	0.81	0.12	197,197,197,197	0
86	OHX	1	4187	7/7	0.81	0.18	120,120,120,120	0
85	MG	5	3423	1/1	0.81	0.14	31,31,31,31	0
86	OHX	1	4195	7/7	0.81	0.22	115,115,115,115	0
85	MG	2	1939	1/1	0.81	0.22	54,54,54,54	0
85	MG	5	3455	1/1	0.81	0.28	89,89,89,89	0
86	OHX	6	2187	7/7	0.81	0.21	121,121,121,121	0
85	MG	8	208	1/1	0.81	0.23	44,44,44,44	0
85	MG	8	213	1/1	0.81	0.24	42,42,42,42	0
85	MG	o4	201	1/1	0.81	0.25	55,55,55,55	0
85	MG	5	3893	1/1	0.82	0.29	42,42,42,42	0
85	MG	1	3838	1/1	0.82	0.32	49,49,49,49	0
85	MG	1	3697	1/1	0.82	0.30	31,31,31,31	0
85	MG	2	1986	1/1	0.82	0.22	49,49,49,49	0
85	MG	7	217	1/1	0.82	0.22	39,39,39,39	0
85	MG	5	3660	1/1	0.82	0.32	20,20,20,20	0
85	MG	6	2031	1/1	0.82	0.48	74,74,74,74	0
85	MG	m1	201	1/1	0.82	0.27	50,50,50,50	0
85	MG	5	3431	1/1	0.82	0.32	65,65,65,65	0
85	MG	1	3440	1/1	0.82	0.08	29,29,29,29	0
86	OHX	6	2203	7/7	0.82	0.21	123,123,123,123	0
85	MG	3	201	1/1	0.82	0.35	54,54,54,54	0
86	OHX	2	2146	7/7	0.82	0.21	114,114,114,114	0
86	OHX	2	2159	7/7	0.82	0.12	255,255,255,255	0
85	MG	5	3458	1/1	0.82	0.22	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	N5	201	1/1	0.82	0.28	50,50,50,50	0
85	MG	5	3814	1/1	0.82	0.19	50,50,50,50	0
85	MG	1	3615	1/1	0.82	0.15	45,45,45,45	0
86	OHX	5	4226	7/7	0.82	0.20	116,116,116,116	0
86	OHX	1	4145	7/7	0.82	0.19	126,126,126,126	0
85	MG	1	3521	1/1	0.82	0.26	65,65,65,65	0
85	MG	6	1940	1/1	0.82	0.47	72,72,72,72	0
85	MG	5	3854	1/1	0.82	0.17	71,71,71,71	0
85	MG	2	1971	1/1	0.82	0.34	58,58,58,58	0
85	MG	6	1958	1/1	0.82	0.35	43,43,43,43	0
85	MG	1	3469	1/1	0.82	0.27	35,35,35,35	0
85	MG	5	3569	1/1	0.82	0.32	21,21,21,21	0
86	OHX	5	4246	7/7	0.82	0.24	104,104,104,104	0
85	MG	6	2006	1/1	0.82	0.28	66,66,66,66	0
86	OHX	1	4192	7/7	0.82	0.25	108,108,108,108	0
85	MG	5	3892	1/1	0.82	0.16	99,99,99,99	0
86	OHX	1	4199	7/7	0.82	0.23	101,101,101,101	0
86	OHX	4	235	7/7	0.82	0.20	122,122,122,122	0
86	OHX	4	238	7/7	0.82	0.26	106,106,106,106	0
85	MG	6	1939	1/1	0.83	0.37	52,52,52,52	0
85	MG	6	1912	1/1	0.83	0.31	51,51,51,51	0
85	MG	1	3734	1/1	0.83	0.25	50,50,50,50	0
86	OHX	1	4160	7/7	0.83	0.24	98,98,98,98	0
85	MG	6	1952	1/1	0.83	0.30	56,56,56,56	0
85	MG	2	1937	1/1	0.83	0.36	47,47,47,47	0
85	MG	6	1961	1/1	0.83	0.39	57,57,57,57	0
85	MG	5	3473	1/1	0.83	0.27	48,48,48,48	0
85	MG	1	3417	1/1	0.83	0.25	36,36,36,36	0
86	OHX	1	4183	7/7	0.83	0.19	117,117,117,117	0
85	MG	2	1977	1/1	0.83	0.35	73,73,73,73	0
86	OHX	5	4213	7/7	0.83	0.19	123,123,123,123	0
85	MG	c8	202	1/1	0.83	0.25	59,59,59,59	0
86	OHX	5	4225	7/7	0.83	0.24	110,110,110,110	0
86	OHX	1	4189	7/7	0.83	0.21	114,114,114,114	0
85	MG	1	3684	1/1	0.83	0.33	70,70,70,70	0
85	MG	5	3551	1/1	0.83	0.14	34,34,34,34	0
85	MG	2	2021	1/1	0.83	0.46	64,64,64,64	0
85	MG	1	3441	1/1	0.83	0.24	15,15,15,15	0
86	OHX	1	4204	7/7	0.83	0.27	97,97,97,97	0
85	MG	2	1981	1/1	0.83	0.36	46,46,46,46	0
85	MG	5	3858	1/1	0.83	0.31	74,74,74,74	0
86	OHX	5	4241	7/7	0.83	0.21	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4242	7/7	0.83	0.15	164,164,164,164	0
85	MG	5	3864	1/1	0.83	0.33	58,58,58,58	0
86	OHX	6	2139	7/7	0.83	0.21	108,108,108,108	0
86	OHX	5	4247	7/7	0.83	0.21	136,136,136,136	0
86	OHX	2	2160	7/7	0.83	0.19	134,134,134,134	0
86	OHX	6	2183	7/7	0.83	0.18	130,130,130,130	0
86	OHX	8	228	7/7	0.83	0.22	103,103,103,103	0
85	MG	5	3770	1/1	0.83	0.25	55,55,55,55	0
85	MG	6	1911	1/1	0.83	0.29	69,69,69,69	0
86	OHX	2	2178	7/7	0.83	0.17	152,152,152,152	0
86	OHX	2	2180	7/7	0.83	0.21	132,132,132,132	0
86	OHX	1	4191	7/7	0.84	0.16	149,149,149,149	0
85	MG	5	3695	1/1	0.84	0.24	56,56,56,56	0
85	MG	2	1907	1/1	0.84	0.43	42,42,42,42	0
85	MG	2	1901	1/1	0.84	0.41	62,62,62,62	0
85	MG	1	3657	1/1	0.84	0.10	19,19,19,19	0
85	MG	1	3850	1/1	0.84	0.12	64,64,64,64	0
85	MG	6	1988	1/1	0.84	0.15	57,57,57,57	0
85	MG	1	3522	1/1	0.84	0.34	24,24,24,24	0
86	OHX	M9	202	7/7	0.84	0.15	142,142,142,142	0
85	MG	2	1950	1/1	0.84	0.43	54,54,54,54	0
85	MG	6	1929	1/1	0.84	0.31	51,51,51,51	0
86	OHX	6	2167	7/7	0.84	0.13	181,181,181,181	0
85	MG	5	3758	1/1	0.84	0.26	55,55,55,55	0
85	MG	8	210	1/1	0.84	0.13	34,34,34,34	0
85	MG	6	2002	1/1	0.84	0.15	87,87,87,87	0
85	MG	1	3664	1/1	0.84	0.45	66,66,66,66	0
86	OHX	6	2190	7/7	0.84	0.20	120,120,120,120	0
85	MG	1	3667	1/1	0.84	0.24	64,64,64,64	0
85	MG	1	3477	1/1	0.84	0.19	27,27,27,27	0
85	MG	6	1935	1/1	0.84	0.23	54,54,54,54	0
86	OHX	2	2135	7/7	0.84	0.21	109,109,109,109	0
85	MG	3	213	1/1	0.84	0.36	49,49,49,49	0
86	OHX	2	2151	7/7	0.84	0.19	133,133,133,133	0
86	OHX	2	2152	7/7	0.84	0.15	162,162,162,162	0
86	OHX	6	2207	7/7	0.84	0.23	123,123,123,123	0
86	OHX	6	2208	7/7	0.84	0.21	118,118,118,118	0
85	MG	6	1938	1/1	0.84	0.22	36,36,36,36	0
86	OHX	d4	201	7/7	0.84	0.16	133,133,133,133	0
85	MG	5	3791	1/1	0.84	0.11	45,45,45,45	0
85	MG	2	1955	1/1	0.84	0.27	52,52,52,52	0
85	MG	6	2036	1/1	0.84	0.21	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	2	2177	7/7	0.84	0.16	151,151,151,151	0
85	MG	1	3583	1/1	0.84	0.33	40,40,40,40	0
86	OHX	5	4221	7/7	0.84	0.21	112,112,112,112	0
86	OHX	2	2179	7/7	0.84	0.21	115,115,115,115	0
85	MG	1	3484	1/1	0.84	0.30	38,38,38,38	0
85	MG	1	3607	1/1	0.84	0.34	47,47,47,47	0
86	OHX	1	4123	7/7	0.84	0.18	122,122,122,122	0
85	MG	1	3613	1/1	0.84	0.16	32,32,32,32	0
86	OHX	1	4137	7/7	0.84	0.24	102,102,102,102	0
85	MG	5	3813	1/1	0.84	0.12	45,45,45,45	0
85	MG	5	3644	1/1	0.84	0.13	47,47,47,47	0
86	OHX	1	4161	7/7	0.84	0.12	188,188,188,188	0
85	MG	1	3748	1/1	0.84	0.16	32,32,32,32	0
86	OHX	1	4166	7/7	0.84	0.18	139,139,139,139	0
85	MG	2	1957	1/1	0.84	0.37	60,60,60,60	0
85	MG	2	2000	1/1	0.84	0.25	59,59,59,59	0
86	OHX	1	4178	7/7	0.84	0.22	108,108,108,108	0
85	MG	5	3848	1/1	0.84	0.26	37,37,37,37	0
85	MG	1	3502	1/1	0.84	0.38	34,34,34,34	0
85	MG	5	3681	1/1	0.84	0.39	71,71,71,71	0
86	OHX	1	4184	7/7	0.84	0.24	97,97,97,97	0
85	MG	5	3861	1/1	0.84	0.11	29,29,29,29	0
85	MG	5	3682	1/1	0.84	0.08	18,18,18,18	0
85	MG	2	1905	1/1	0.84	0.42	52,52,52,52	0
85	MG	1	3638	1/1	0.84	0.15	48,48,48,48	0
85	MG	2	1994	1/1	0.85	0.15	59,59,59,59	0
85	MG	15	301	1/1	0.85	0.19	50,50,50,50	0
85	MG	1	3694	1/1	0.85	0.17	38,38,38,38	0
85	MG	2	1929	1/1	0.85	0.43	54,54,54,54	0
85	MG	2	1996	1/1	0.85	0.33	48,48,48,48	0
85	MG	1	3707	1/1	0.85	0.18	40,40,40,40	0
86	OHX	6	2159	7/7	0.85	0.17	134,134,134,134	0
85	MG	1	3710	1/1	0.85	0.26	51,51,51,51	0
86	OHX	6	2177	7/7	0.85	0.25	100,100,100,100	0
86	OHX	6	2181	7/7	0.85	0.24	103,103,103,103	0
86	OHX	2	2141	7/7	0.85	0.18	132,132,132,132	0
85	MG	5	3784	1/1	0.85	0.22	20,20,20,20	0
85	MG	1	3471	1/1	0.85	0.10	28,28,28,28	0
85	MG	2	1903	1/1	0.85	0.32	39,39,39,39	0
86	OHX	2	2154	7/7	0.85	0.16	141,141,141,141	0
86	OHX	2	2156	7/7	0.85	0.18	118,118,118,118	0
86	OHX	2	2157	7/7	0.85	0.12	212,212,212,212	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	4	219	1/1	0.85	0.27	44,44,44,44	0
85	MG	1	3742	1/1	0.85	0.14	35,35,35,35	0
85	MG	2	1919	1/1	0.85	0.48	63,63,63,63	0
85	MG	6	1960	1/1	0.85	0.37	38,38,38,38	0
86	OHX	2	2165	7/7	0.85	0.14	153,153,153,153	0
85	MG	1	3540	1/1	0.85	0.35	52,52,52,52	0
85	MG	1	3766	1/1	0.85	0.20	80,80,80,80	0
85	MG	6	1902	1/1	0.85	0.31	46,46,46,46	0
86	OHX	s8	303	7/7	0.85	0.15	136,136,136,136	0
85	MG	1	3770	1/1	0.85	0.17	40,40,40,40	0
85	MG	5	3673	1/1	0.85	0.29	53,53,53,53	0
86	OHX	5	4183	7/7	0.85	0.20	105,105,105,105	0
86	OHX	1	4091	7/7	0.85	0.17	118,118,118,118	0
85	MG	5	3829	1/1	0.85	0.26	36,36,36,36	0
86	OHX	5	4197	7/7	0.85	0.23	103,103,103,103	0
85	MG	2	1912	1/1	0.85	0.27	54,54,54,54	0
85	MG	6	1969	1/1	0.85	0.28	36,36,36,36	0
86	OHX	5	4219	7/7	0.85	0.21	114,114,114,114	0
86	OHX	5	4220	7/7	0.85	0.14	151,151,151,151	0
85	MG	c7	202	1/1	0.85	0.36	65,65,65,65	0
86	OHX	5	4222	7/7	0.85	0.18	132,132,132,132	0
86	OHX	1	4153	7/7	0.85	0.19	116,116,116,116	0
85	MG	2	1979	1/1	0.85	0.31	46,46,46,46	0
85	MG	5	3857	1/1	0.85	0.32	66,66,66,66	0
85	MG	sM	302	1/1	0.85	0.14	30,30,30,30	0
85	MG	5	3689	1/1	0.85	0.14	37,37,37,37	0
85	MG	2	1936	1/1	0.85	0.37	47,47,47,47	0
85	MG	1	3604	1/1	0.85	0.14	44,44,44,44	0
85	MG	5	3702	1/1	0.85	0.12	42,42,42,42	0
85	MG	6	1982	1/1	0.85	0.41	58,58,58,58	0
85	MG	1	3665	1/1	0.85	0.12	45,45,45,45	0
85	MG	5	3424	1/1	0.85	0.24	47,47,47,47	0
85	MG	2	1944	1/1	0.85	0.20	53,53,53,53	0
85	MG	5	3731	1/1	0.85	0.09	27,27,27,27	0
85	MG	1	3842	1/1	0.85	0.32	36,36,36,36	0
85	MG	7	208	1/1	0.85	0.09	54,54,54,54	0
85	MG	1	3668	1/1	0.85	0.26	41,41,41,41	0
85	MG	2	2011	1/1	0.85	0.34	59,59,59,59	0
86	OHX	8	227	7/7	0.85	0.20	115,115,115,115	0
85	MG	5	3757	1/1	0.85	0.25	53,53,53,53	0
85	MG	8	202	1/1	0.85	0.16	22,22,22,22	0
85	MG	1	3678	1/1	0.85	0.12	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	m1	203	7/7	0.85	0.18	119,119,119,119	0
85	MG	5	3761	1/1	0.85	0.29	59,59,59,59	0
86	OHX	1	4207	7/7	0.85	0.25	103,103,103,103	0
85	MG	5	3816	1/1	0.86	0.13	30,30,30,30	0
86	OHX	6	2170	7/7	0.86	0.13	156,156,156,156	0
86	OHX	6	2173	7/7	0.86	0.16	124,124,124,124	0
85	MG	5	3448	1/1	0.86	0.28	49,49,49,49	0
85	MG	1	3704	1/1	0.86	0.31	55,55,55,55	0
85	MG	6	2033	1/1	0.86	0.21	65,65,65,65	0
86	OHX	6	2185	7/7	0.86	0.23	115,115,115,115	0
85	MG	1	3408	1/1	0.86	0.30	24,24,24,24	0
85	MG	5	3459	1/1	0.86	0.19	21,21,21,21	0
85	MG	2	1997	1/1	0.86	0.25	83,83,83,83	0
85	MG	5	3704	1/1	0.86	0.07	39,39,39,39	0
86	OHX	6	2191	7/7	0.86	0.16	136,136,136,136	0
85	MG	3	211	1/1	0.86	0.10	57,57,57,57	0
85	MG	1	3832	1/1	0.86	0.14	29,29,29,29	0
85	MG	6	1941	1/1	0.86	0.24	42,42,42,42	0
85	MG	6	2045	1/1	0.86	0.29	43,43,43,43	0
86	OHX	6	2198	7/7	0.86	0.16	152,152,152,152	0
86	OHX	1	4126	7/7	0.86	0.19	124,124,124,124	0
85	MG	2	1970	1/1	0.86	0.31	61,61,61,61	0
85	MG	5	3491	1/1	0.86	0.44	51,51,51,51	0
86	OHX	1	4140	7/7	0.86	0.17	127,127,127,127	0
85	MG	D0	201	1/1	0.86	0.41	61,61,61,61	0
85	MG	5	3737	1/1	0.86	0.21	36,36,36,36	0
86	OHX	1	4155	7/7	0.86	0.17	126,126,126,126	0
86	OHX	c3	201	7/7	0.86	0.15	128,128,128,128	0
85	MG	5	3745	1/1	0.86	0.25	43,43,43,43	0
86	OHX	5	4137	7/7	0.86	0.18	105,105,105,105	0
86	OHX	5	4157	7/7	0.86	0.21	113,113,113,113	0
86	OHX	5	4159	7/7	0.86	0.24	99,99,99,99	0
85	MG	4	212	1/1	0.86	0.24	43,43,43,43	0
86	OHX	5	4171	7/7	0.86	0.18	133,133,133,133	0
86	OHX	5	4179	7/7	0.86	0.19	110,110,110,110	0
85	MG	5	3519	1/1	0.86	0.30	26,26,26,26	0
85	MG	6	1995	1/1	0.86	0.27	49,49,49,49	0
86	OHX	5	4195	7/7	0.86	0.26	100,100,100,100	0
85	MG	5	3553	1/1	0.86	0.24	23,23,23,23	0
86	OHX	1	4169	7/7	0.86	0.14	146,146,146,146	0
86	OHX	5	4202	7/7	0.86	0.18	110,110,110,110	0
85	MG	5	3762	1/1	0.86	0.17	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4173	7/7	0.86	0.20	122,122,122,122	0
85	MG	5	3560	1/1	0.86	0.29	19,19,19,19	0
85	MG	2	1946	1/1	0.86	0.18	48,48,48,48	0
85	MG	8	206	1/1	0.86	0.24	42,42,42,42	0
85	MG	5	3570	1/1	0.86	0.26	17,17,17,17	0
85	MG	1	3549	1/1	0.86	0.15	26,26,26,26	0
85	MG	5	3593	1/1	0.86	0.28	27,27,27,27	0
85	MG	1	3563	1/1	0.86	0.28	33,33,33,33	0
86	OHX	5	4228	7/7	0.86	0.16	133,133,133,133	0
85	MG	5	3782	1/1	0.86	0.28	68,68,68,68	0
86	OHX	5	4230	7/7	0.86	0.12	158,158,158,158	0
85	MG	1	3764	1/1	0.86	0.17	48,48,48,48	0
85	MG	1	3407	1/1	0.86	0.25	30,30,30,30	0
86	OHX	2	2094	7/7	0.86	0.18	121,121,121,121	0
85	MG	M7	201	1/1	0.86	0.45	55,55,55,55	0
86	OHX	2	2134	7/7	0.86	0.15	132,132,132,132	0
86	OHX	5	4238	7/7	0.86	0.24	103,103,103,103	0
85	MG	5	3654	1/1	0.86	0.21	47,47,47,47	0
85	MG	5	3655	1/1	0.86	0.13	32,32,32,32	0
86	OHX	3	223	7/7	0.86	0.15	146,146,146,146	0
85	MG	6	2020	1/1	0.86	0.33	42,42,42,42	0
86	OHX	4	236	7/7	0.86	0.19	112,112,112,112	0
86	OHX	4	237	7/7	0.86	0.21	102,102,102,102	0
86	OHX	2	2148	7/7	0.86	0.14	158,158,158,158	0
86	OHX	5	4250	7/7	0.86	0.20	101,101,101,101	0
85	MG	1	3702	1/1	0.86	0.29	50,50,50,50	0
86	OHX	M7	205	7/7	0.86	0.21	106,106,106,106	0
85	MG	6	2027	1/1	0.86	0.14	60,60,60,60	0
86	OHX	6	2109	7/7	0.86	0.21	100,100,100,100	0
86	OHX	6	2119	7/7	0.86	0.20	115,115,115,115	0
86	OHX	l5	304	7/7	0.86	0.20	115,115,115,115	0
85	MG	6	1972	1/1	0.86	0.23	60,60,60,60	0
85	MG	5	3434	1/1	0.86	0.36	72,72,72,72	0
85	MG	5	3441	1/1	0.86	0.25	21,21,21,21	0
85	MG	6	1915	1/1	0.87	0.39	55,55,55,55	0
85	MG	6	1916	1/1	0.87	0.45	59,59,59,59	0
85	MG	1	3554	1/1	0.87	0.23	21,21,21,21	0
85	MG	5	3504	1/1	0.87	0.31	43,43,43,43	0
85	MG	1	3614	1/1	0.87	0.14	26,26,26,26	0
86	OHX	1	4107	7/7	0.87	0.19	109,109,109,109	0
85	MG	5	3885	1/1	0.87	0.44	53,53,53,53	0
86	OHX	1	4125	7/7	0.87	0.15	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3535	1/1	0.87	0.32	25,25,25,25	0
85	MG	5	3540	1/1	0.87	0.30	26,26,26,26	0
86	OHX	1	4134	7/7	0.87	0.21	101,101,101,101	0
85	MG	1	3787	1/1	0.87	0.24	54,54,54,54	0
86	OHX	6	2201	7/7	0.87	0.20	119,119,119,119	0
85	MG	1	3802	1/1	0.87	0.11	21,21,21,21	0
86	OHX	1	4142	7/7	0.87	0.19	111,111,111,111	0
85	MG	6	1926	1/1	0.87	0.28	42,42,42,42	0
85	MG	c8	201	1/1	0.87	0.33	64,64,64,64	0
85	MG	4	202	1/1	0.87	0.35	44,44,44,44	0
86	OHX	1	4156	7/7	0.87	0.17	122,122,122,122	0
85	MG	5	3571	1/1	0.87	0.28	29,29,29,29	0
85	MG	d6	102	1/1	0.87	0.19	47,47,47,47	0
86	OHX	5	4052	7/7	0.87	0.36	92,92,92,92	0
86	OHX	5	4110	7/7	0.87	0.20	102,102,102,102	0
85	MG	1	3699	1/1	0.87	0.11	31,31,31,31	0
86	OHX	5	4147	7/7	0.87	0.21	107,107,107,107	0
85	MG	5	3601	1/1	0.87	0.12	56,56,56,56	0
85	MG	1	3560	1/1	0.87	0.25	32,32,32,32	0
85	MG	8	209	1/1	0.87	0.15	51,51,51,51	0
86	OHX	5	4168	7/7	0.87	0.19	105,105,105,105	0
85	MG	4	213	1/1	0.87	0.27	46,46,46,46	0
85	MG	5	3614	1/1	0.87	0.12	31,31,31,31	0
86	OHX	5	4181	7/7	0.87	0.19	112,112,112,112	0
86	OHX	5	4182	7/7	0.87	0.18	119,119,119,119	0
86	OHX	1	4176	7/7	0.87	0.22	106,106,106,106	0
85	MG	5	3637	1/1	0.87	0.13	41,41,41,41	0
86	OHX	1	4180	7/7	0.87	0.23	99,99,99,99	0
85	MG	2	1917	1/1	0.87	0.37	45,45,45,45	0
85	MG	m5	301	1/1	0.87	0.27	38,38,38,38	0
85	MG	n6	201	1/1	0.87	0.20	47,47,47,47	0
86	OHX	5	4204	7/7	0.87	0.19	115,115,115,115	0
85	MG	n8	204	1/1	0.87	0.16	30,30,30,30	0
86	OHX	5	4212	7/7	0.87	0.20	106,106,106,106	0
85	MG	1	3627	1/1	0.87	0.14	46,46,46,46	0
86	OHX	5	4218	7/7	0.87	0.18	114,114,114,114	0
85	MG	1	3404	1/1	0.87	0.35	53,53,53,53	0
85	MG	L3	402	1/1	0.87	0.16	38,38,38,38	0
85	MG	1	3712	1/1	0.87	0.41	70,70,70,70	0
86	OHX	2	2120	7/7	0.87	0.20	110,110,110,110	0
85	MG	5	3802	1/1	0.87	0.20	54,54,54,54	0
85	MG	1	3446	1/1	0.87	0.20	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4196	7/7	0.87	0.22	108,108,108,108	0
86	OHX	1	4197	7/7	0.87	0.22	109,109,109,109	0
86	OHX	2	2138	7/7	0.87	0.15	139,139,139,139	0
85	MG	5	3664	1/1	0.87	0.12	31,31,31,31	0
86	OHX	2	2145	7/7	0.87	0.15	139,139,139,139	0
85	MG	1	3637	1/1	0.87	0.17	44,44,44,44	0
86	OHX	5	4233	7/7	0.87	0.15	144,144,144,144	0
85	MG	N0	201	1/1	0.87	0.25	36,36,36,36	0
86	OHX	2	2150	7/7	0.87	0.15	134,134,134,134	0
85	MG	6	1957	1/1	0.87	0.43	52,52,52,52	0
85	MG	1	3845	1/1	0.87	0.27	38,38,38,38	0
85	MG	1	3735	1/1	0.87	0.25	23,23,23,23	0
85	MG	1	3848	1/1	0.87	0.09	29,29,29,29	0
85	MG	1	3677	1/1	0.87	0.10	34,34,34,34	0
85	MG	1	3497	1/1	0.87	0.26	30,30,30,30	0
86	OHX	5	4245	7/7	0.87	0.17	130,130,130,130	0
85	MG	1	3456	1/1	0.87	0.26	18,18,18,18	0
85	MG	5	3699	1/1	0.87	0.10	25,25,25,25	0
86	OHX	5	4248	7/7	0.87	0.20	120,120,120,120	0
85	MG	1	3609	1/1	0.87	0.11	31,31,31,31	0
85	MG	1	3765	1/1	0.87	0.22	38,38,38,38	0
86	OHX	2	2166	7/7	0.87	0.15	144,144,144,144	0
86	OHX	2	2169	7/7	0.87	0.18	129,129,129,129	0
86	OHX	2	2172	7/7	0.87	0.20	120,120,120,120	0
86	OHX	6	2176	7/7	0.87	0.19	122,122,122,122	0
86	OHX	2	2175	7/7	0.87	0.17	144,144,144,144	0
86	OHX	2	2176	7/7	0.87	0.21	111,111,111,111	0
86	OHX	6	2182	7/7	0.87	0.18	116,116,116,116	0
86	OHX	m8	201	7/7	0.87	0.22	104,104,104,104	0
85	MG	5	3486	1/1	0.87	0.23	38,38,38,38	0
86	OHX	6	2184	7/7	0.87	0.21	109,109,109,109	0
86	OHX	2	2174	7/7	0.88	0.17	132,132,132,132	0
86	OHX	6	2178	7/7	0.88	0.16	131,131,131,131	0
85	MG	6	1925	1/1	0.88	0.43	40,40,40,40	0
85	MG	2	1932	1/1	0.88	0.28	48,48,48,48	0
85	MG	6	2001	1/1	0.88	0.12	44,44,44,44	0
85	MG	1	3620	1/1	0.88	0.06	27,27,27,27	0
85	MG	1	3547	1/1	0.88	0.14	30,30,30,30	0
86	OHX	6	2186	7/7	0.88	0.20	111,111,111,111	0
85	MG	1	3780	1/1	0.88	0.19	34,34,34,34	0
85	MG	5	3690	1/1	0.88	0.22	35,35,35,35	0
86	OHX	1	4077	7/7	0.88	0.18	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4090	7/7	0.88	0.20	98,98,98,98	0
85	MG	1	3625	1/1	0.88	0.20	25,25,25,25	0
86	OHX	1	4105	7/7	0.88	0.19	104,104,104,104	0
85	MG	6	2011	1/1	0.88	0.15	43,43,43,43	0
86	OHX	1	4111	7/7	0.88	0.20	102,102,102,102	0
86	OHX	1	4116	7/7	0.88	0.19	105,105,105,105	0
85	MG	1	3626	1/1	0.88	0.14	26,26,26,26	0
86	OHX	6	2199	7/7	0.88	0.16	131,131,131,131	0
85	MG	4	215	1/1	0.88	0.21	43,43,43,43	0
85	MG	1	3686	1/1	0.88	0.13	27,27,27,27	0
86	OHX	1	4127	7/7	0.88	0.17	130,130,130,130	0
86	OHX	1	4129	7/7	0.88	0.20	108,108,108,108	0
85	MG	5	3890	1/1	0.88	0.13	79,79,79,79	0
85	MG	4	218	1/1	0.88	0.20	51,51,51,51	0
85	MG	1	3808	1/1	0.88	0.13	24,24,24,24	0
86	OHX	1	4138	7/7	0.88	0.16	110,110,110,110	0
85	MG	5	3894	1/1	0.88	0.22	40,40,40,40	0
86	OHX	1	4141	7/7	0.88	0.19	115,115,115,115	0
85	MG	5	3716	1/1	0.88	0.21	51,51,51,51	0
86	OHX	5	4095	7/7	0.88	0.17	119,119,119,119	0
85	MG	5	3898	1/1	0.88	0.16	23,23,23,23	0
86	OHX	1	4148	7/7	0.88	0.20	107,107,107,107	0
86	OHX	5	4141	7/7	0.88	0.20	96,96,96,96	0
86	OHX	1	4149	7/7	0.88	0.21	112,112,112,112	0
86	OHX	5	4153	7/7	0.88	0.35	86,86,86,86	0
85	MG	7	207	1/1	0.88	0.13	48,48,48,48	0
85	MG	5	3718	1/1	0.88	0.40	53,53,53,53	0
86	OHX	5	4160	7/7	0.88	0.21	95,95,95,95	0
86	OHX	5	4163	7/7	0.88	0.19	117,117,117,117	0
85	MG	1	3500	1/1	0.88	0.38	63,63,63,63	0
85	MG	6	1942	1/1	0.88	0.25	28,28,28,28	0
85	MG	6	1946	1/1	0.88	0.40	56,56,56,56	0
86	OHX	5	4176	7/7	0.88	0.20	112,112,112,112	0
86	OHX	1	4162	7/7	0.88	0.37	85,85,85,85	0
85	MG	1	3818	1/1	0.88	0.19	48,48,48,48	0
85	MG	8	203	1/1	0.88	0.34	31,31,31,31	0
85	MG	8	204	1/1	0.88	0.27	48,48,48,48	0
86	OHX	5	4186	7/7	0.88	0.22	102,102,102,102	0
85	MG	5	3733	1/1	0.88	0.18	35,35,35,35	0
86	OHX	5	4190	7/7	0.88	0.18	108,108,108,108	0
85	MG	1	3418	1/1	0.88	0.35	40,40,40,40	0
85	MG	5	3525	1/1	0.88	0.18	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	1	4175	7/7	0.88	0.21	103,103,103,103	0
85	MG	5	3744	1/1	0.88	0.16	34,34,34,34	0
85	MG	6	2039	1/1	0.88	0.31	59,59,59,59	0
86	OHX	5	4205	7/7	0.88	0.20	110,110,110,110	0
86	OHX	5	4206	7/7	0.88	0.21	112,112,112,112	0
85	MG	6	2040	1/1	0.88	0.37	47,47,47,47	0
86	OHX	5	4211	7/7	0.88	0.32	85,85,85,85	0
85	MG	5	3549	1/1	0.88	0.31	43,43,43,43	0
85	MG	2	1920	1/1	0.88	0.18	51,51,51,51	0
85	MG	1	3636	1/1	0.88	0.27	41,41,41,41	0
85	MG	5	3557	1/1	0.88	0.24	39,39,39,39	0
85	MG	1	3422	1/1	0.88	0.19	21,21,21,21	0
85	MG	1	3570	1/1	0.88	0.39	34,34,34,34	0
85	MG	q3	502	1/1	0.88	0.36	66,66,66,66	0
86	OHX	5	4223	7/7	0.88	0.17	112,112,112,112	0
85	MG	N8	201	1/1	0.88	0.10	18,18,18,18	0
85	MG	O1	201	1/1	0.88	0.31	49,49,49,49	0
86	OHX	2	2116	7/7	0.88	0.17	115,115,115,115	0
86	OHX	1	4194	7/7	0.88	0.21	99,99,99,99	0
85	MG	1	3647	1/1	0.88	0.14	35,35,35,35	0
85	MG	1	3581	1/1	0.88	0.24	26,26,26,26	0
85	MG	1	3426	1/1	0.88	0.17	29,29,29,29	0
85	MG	6	1970	1/1	0.88	0.27	51,51,51,51	0
86	OHX	1	4203	7/7	0.88	0.25	99,99,99,99	0
85	MG	1	3719	1/1	0.88	0.24	39,39,39,39	0
85	MG	1	3650	1/1	0.88	0.22	57,57,57,57	0
86	OHX	1	4208	7/7	0.88	0.21	116,116,116,116	0
85	MG	5	3616	1/1	0.88	0.20	33,33,33,33	0
86	OHX	3	224	7/7	0.88	0.22	103,103,103,103	0
86	OHX	5	4240	7/7	0.88	0.15	116,116,116,116	0
85	MG	5	3629	1/1	0.88	0.07	29,29,29,29	0
85	MG	1	3856	1/1	0.88	0.24	50,50,50,50	0
85	MG	5	3642	1/1	0.88	0.27	41,41,41,41	0
85	MG	1	3857	1/1	0.88	0.14	38,38,38,38	0
86	OHX	L3	405	7/7	0.88	0.15	130,130,130,130	0
85	MG	5	3418	1/1	0.88	0.32	14,14,14,14	0
85	MG	5	3811	1/1	0.88	0.09	33,33,33,33	0
85	MG	2	1935	1/1	0.88	0.36	39,39,39,39	0
85	MG	1	3524	1/1	0.88	0.18	27,27,27,27	0
85	MG	2	2014	1/1	0.88	0.47	64,64,64,64	0
86	OHX	7	229	7/7	0.88	0.16	109,109,109,109	0
86	OHX	2	2161	7/7	0.88	0.17	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	2	1904	1/1	0.88	0.35	55,55,55,55	0
86	OHX	8	230	7/7	0.88	0.21	95,95,95,95	0
85	MG	1	3535	1/1	0.88	0.28	34,34,34,34	0
85	MG	5	3669	1/1	0.88	0.17	24,24,24,24	0
86	OHX	15	303	7/7	0.88	0.18	117,117,117,117	0
85	MG	5	3833	1/1	0.88	0.14	60,60,60,60	0
86	OHX	m0	303	7/7	0.88	0.27	92,92,92,92	0
86	OHX	6	2171	7/7	0.88	0.25	96,96,96,96	0
85	MG	1	3410	1/1	0.88	0.25	35,35,35,35	0
86	OHX	6	2175	7/7	0.88	0.17	122,122,122,122	0
85	MG	5	3676	1/1	0.88	0.11	25,25,25,25	0
86	OHX	6	2168	7/7	0.89	0.17	120,120,120,120	0
86	OHX	2	2158	7/7	0.89	0.23	91,91,91,91	0
85	MG	5	3552	1/1	0.89	0.38	33,33,33,33	0
85	MG	1	3544	1/1	0.89	0.23	28,28,28,28	0
85	MG	6	2025	1/1	0.89	0.23	46,46,46,46	0
85	MG	6	1928	1/1	0.89	0.35	61,61,61,61	0
85	MG	5	3563	1/1	0.89	0.33	21,21,21,21	0
85	MG	5	3796	1/1	0.89	0.10	44,44,44,44	0
85	MG	1	3859	1/1	0.89	0.30	55,55,55,55	0
85	MG	2	2182	1/1	0.89	0.26	70,70,70,70	0
86	OHX	2	2171	7/7	0.89	0.17	122,122,122,122	0
85	MG	6	1932	1/1	0.89	0.23	37,37,37,37	0
86	OHX	2	2173	7/7	0.89	0.18	117,117,117,117	0
85	MG	5	3808	1/1	0.89	0.27	24,24,24,24	0
85	MG	5	3573	1/1	0.89	0.43	31,31,31,31	0
85	MG	5	3577	1/1	0.89	0.39	31,31,31,31	0
85	MG	2	2016	1/1	0.89	0.43	57,57,57,57	0
85	MG	1	3420	1/1	0.89	0.45	66,66,66,66	0
85	MG	D3	201	1/1	0.89	0.18	41,41,41,41	0
85	MG	1	3424	1/1	0.89	0.26	33,33,33,33	0
85	MG	5	3818	1/1	0.89	0.08	49,49,49,49	0
86	OHX	C3	201	7/7	0.89	0.14	131,131,131,131	0
86	OHX	6	2196	7/7	0.89	0.16	131,131,131,131	0
86	OHX	D9	102	7/7	0.89	0.20	118,118,118,118	0
86	OHX	1	4058	7/7	0.89	0.20	96,96,96,96	0
85	MG	5	3821	1/1	0.89	0.09	34,34,34,34	0
85	MG	6	1937	1/1	0.89	0.28	38,38,38,38	0
85	MG	3	212	1/1	0.89	0.15	54,54,54,54	0
86	OHX	1	4096	7/7	0.89	0.16	129,129,129,129	0
85	MG	1	3490	1/1	0.89	0.24	45,45,45,45	0
85	MG	1	3750	1/1	0.89	0.18	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4109	7/7	0.89	0.12	148,148,148,148	0
85	MG	5	3845	1/1	0.89	0.11	22,22,22,22	0
85	MG	5	3636	1/1	0.89	0.25	39,39,39,39	0
86	OHX	1	4119	7/7	0.89	0.18	107,107,107,107	0
85	MG	2	1988	1/1	0.89	0.28	63,63,63,63	0
86	OHX	d9	102	7/7	0.89	0.17	135,135,135,135	0
85	MG	1	3580	1/1	0.89	0.18	27,27,27,27	0
85	MG	2	1961	1/1	0.89	0.28	46,46,46,46	0
86	OHX	5	4099	7/7	0.89	0.19	101,101,101,101	0
86	OHX	5	4100	7/7	0.89	0.16	125,125,125,125	0
85	MG	5	3646	1/1	0.89	0.26	40,40,40,40	0
85	MG	2	1962	1/1	0.89	0.45	67,67,67,67	0
86	OHX	5	4139	7/7	0.89	0.16	112,112,112,112	0
86	OHX	5	4140	7/7	0.89	0.20	104,104,104,104	0
85	MG	5	3650	1/1	0.89	0.36	58,58,58,58	0
85	MG	s8	301	1/1	0.89	0.18	42,42,42,42	0
86	OHX	5	4149	7/7	0.89	0.17	122,122,122,122	0
86	OHX	5	4151	7/7	0.89	0.17	112,112,112,112	0
86	OHX	1	4136	7/7	0.89	0.20	103,103,103,103	0
85	MG	5	3873	1/1	0.89	0.31	36,36,36,36	0
85	MG	6	1951	1/1	0.89	0.37	59,59,59,59	0
85	MG	4	214	1/1	0.89	0.12	27,27,27,27	0
85	MG	5	3661	1/1	0.89	0.24	36,36,36,36	0
85	MG	1	3769	1/1	0.89	0.12	39,39,39,39	0
86	OHX	5	4167	7/7	0.89	0.15	124,124,124,124	0
86	OHX	1	4143	7/7	0.89	0.16	127,127,127,127	0
86	OHX	1	4144	7/7	0.89	0.17	112,112,112,112	0
85	MG	1	3663	1/1	0.89	0.15	26,26,26,26	0
85	MG	1	3779	1/1	0.89	0.19	41,41,41,41	0
85	MG	2	1921	1/1	0.89	0.37	37,37,37,37	0
85	MG	1	3602	1/1	0.89	0.24	26,26,26,26	0
86	OHX	1	4154	7/7	0.89	0.20	99,99,99,99	0
85	MG	5	3405	1/1	0.89	0.17	19,19,19,19	0
85	MG	1	3443	1/1	0.89	0.34	42,42,42,42	0
85	MG	5	3897	1/1	0.89	0.25	34,34,34,34	0
86	OHX	5	4191	7/7	0.89	0.20	94,94,94,94	0
85	MG	2	1958	1/1	0.89	0.36	58,58,58,58	0
85	MG	1	3448	1/1	0.89	0.10	27,27,27,27	0
85	MG	1	3516	1/1	0.89	0.29	27,27,27,27	0
85	MG	7	209	1/1	0.89	0.21	43,43,43,43	0
86	OHX	5	4203	7/7	0.89	0.21	101,101,101,101	0
85	MG	1	3449	1/1	0.89	0.24	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3454	1/1	0.89	0.26	42,42,42,42	0
86	OHX	1	4170	7/7	0.89	0.18	108,108,108,108	0
85	MG	1	3685	1/1	0.89	0.25	37,37,37,37	0
85	MG	1	3835	1/1	0.89	0.34	37,37,37,37	0
86	OHX	1	4174	7/7	0.89	0.09	213,213,213,213	0
85	MG	6	1979	1/1	0.89	0.30	38,38,38,38	0
86	OHX	5	4216	7/7	0.89	0.21	113,113,113,113	0
85	MG	O3	201	1/1	0.89	0.27	56,56,56,56	0
85	MG	8	205	1/1	0.89	0.35	40,40,40,40	0
86	OHX	1	4179	7/7	0.89	0.16	117,117,117,117	0
85	MG	5	3454	1/1	0.89	0.13	35,35,35,35	0
85	MG	O7	103	1/1	0.89	0.16	27,27,27,27	0
85	MG	5	3706	1/1	0.89	0.14	29,29,29,29	0
85	MG	1	3413	1/1	0.89	0.47	47,47,47,47	0
85	MG	5	3709	1/1	0.89	0.15	31,31,31,31	0
85	MG	1	3623	1/1	0.89	0.27	42,42,42,42	0
85	MG	l8	301	1/1	0.89	0.30	59,59,59,59	0
85	MG	6	1987	1/1	0.89	0.22	40,40,40,40	0
85	MG	m1	202	1/1	0.89	0.25	46,46,46,46	0
85	MG	6	1906	1/1	0.89	0.30	40,40,40,40	0
85	MG	m7	202	1/1	0.89	0.14	24,24,24,24	0
85	MG	5	3727	1/1	0.89	0.11	25,25,25,25	0
85	MG	1	3457	1/1	0.89	0.17	30,30,30,30	0
85	MG	5	3471	1/1	0.89	0.15	33,33,33,33	0
85	MG	6	1990	1/1	0.89	0.19	69,69,69,69	0
85	MG	1	3840	1/1	0.89	0.23	40,40,40,40	0
86	OHX	1	4202	7/7	0.89	0.21	100,100,100,100	0
85	MG	1	3458	1/1	0.89	0.26	45,45,45,45	0
85	MG	5	3481	1/1	0.89	0.23	32,32,32,32	0
85	MG	1	3531	1/1	0.89	0.24	17,17,17,17	0
85	MG	1	3846	1/1	0.89	0.29	35,35,35,35	0
85	MG	1	3701	1/1	0.89	0.24	48,48,48,48	0
85	MG	5	3499	1/1	0.89	0.28	28,28,28,28	0
86	OHX	2	2136	7/7	0.89	0.19	103,103,103,103	0
85	MG	1	3467	1/1	0.89	0.26	33,33,33,33	0
85	MG	1	3631	1/1	0.89	0.07	18,18,18,18	0
86	OHX	2	2143	7/7	0.89	0.17	113,113,113,113	0
86	OHX	5	4251	7/7	0.89	0.17	129,129,129,129	0
86	OHX	5	4252	7/7	0.89	0.16	123,123,123,123	0
86	OHX	5	4253	7/7	0.89	0.14	139,139,139,139	0
85	MG	1	3853	1/1	0.89	0.27	28,28,28,28	0
86	OHX	7	228	7/7	0.89	0.25	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3854	1/1	0.89	0.18	83,83,83,83	0
85	MG	1	3632	1/1	0.89	0.20	49,49,49,49	0
85	MG	5	3537	1/1	0.89	0.31	25,25,25,25	0
85	MG	6	2018	1/1	0.89	0.23	42,42,42,42	0
86	OHX	8	231	7/7	0.89	0.20	106,106,106,106	0
85	MG	5	3776	1/1	0.89	0.21	44,44,44,44	0
86	OHX	6	2138	7/7	0.89	0.16	113,113,113,113	0
86	OHX	2	2153	7/7	0.89	0.18	117,117,117,117	0
86	OHX	6	2143	7/7	0.89	0.19	109,109,109,109	0
86	OHX	6	2147	7/7	0.89	0.19	107,107,107,107	0
85	MG	5	3542	1/1	0.89	0.30	57,57,57,57	0
86	OHX	m7	206	7/7	0.89	0.22	94,94,94,94	0
85	MG	2	1993	1/1	0.89	0.16	44,44,44,44	0
86	OHX	6	2163	7/7	0.89	0.21	99,99,99,99	0
85	MG	6	2021	1/1	0.89	0.08	45,45,45,45	0
85	MG	1	3513	1/1	0.90	0.27	16,16,16,16	0
85	MG	1	3682	1/1	0.90	0.20	34,34,34,34	0
85	MG	5	3707	1/1	0.90	0.29	35,35,35,35	0
85	MG	1	3777	1/1	0.90	0.24	46,46,46,46	0
85	MG	5	3899	1/1	0.90	0.10	24,24,24,24	0
85	MG	7	203	1/1	0.90	0.28	45,45,45,45	0
85	MG	5	3513	1/1	0.90	0.32	19,19,19,19	0
85	MG	5	3714	1/1	0.90	0.18	38,38,38,38	0
85	MG	5	3715	1/1	0.90	0.20	36,36,36,36	0
85	MG	1	3557	1/1	0.90	0.13	37,37,37,37	0
86	OHX	6	2205	7/7	0.90	0.18	123,123,123,123	0
85	MG	7	215	1/1	0.90	0.19	34,34,34,34	0
85	MG	5	3521	1/1	0.90	0.24	23,23,23,23	0
85	MG	1	3515	1/1	0.90	0.38	28,28,28,28	0
85	MG	5	3527	1/1	0.90	0.39	46,46,46,46	0
85	MG	5	3532	1/1	0.90	0.24	23,23,23,23	0
85	MG	2	1941	1/1	0.90	0.36	65,65,65,65	0
85	MG	5	3536	1/1	0.90	0.26	25,25,25,25	0
86	OHX	5	4015	7/7	0.90	0.15	126,126,126,126	0
85	MG	1	3790	1/1	0.90	0.23	49,49,49,49	0
86	OHX	5	4069	7/7	0.90	0.19	104,104,104,104	0
85	MG	8	207	1/1	0.90	0.17	53,53,53,53	0
85	MG	1	3692	1/1	0.90	0.12	25,25,25,25	0
85	MG	1	3564	1/1	0.90	0.18	26,26,26,26	0
86	OHX	5	4102	7/7	0.90	0.13	130,130,130,130	0
85	MG	1	3695	1/1	0.90	0.18	43,43,43,43	0
86	OHX	1	4157	7/7	0.90	0.20	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4138	7/7	0.90	0.23	95,95,95,95	0
86	OHX	1	4159	7/7	0.90	0.14	135,135,135,135	0
85	MG	1	3812	1/1	0.90	0.13	37,37,37,37	0
85	MG	2	2012	1/1	0.90	0.32	59,59,59,59	0
86	OHX	5	4144	7/7	0.90	0.20	108,108,108,108	0
85	MG	17	301	1/1	0.90	0.19	30,30,30,30	0
86	OHX	5	4148	7/7	0.90	0.19	99,99,99,99	0
85	MG	5	3750	1/1	0.90	0.20	31,31,31,31	0
85	MG	5	3754	1/1	0.90	0.10	35,35,35,35	0
85	MG	5	3756	1/1	0.90	0.15	37,37,37,37	0
86	OHX	5	4155	7/7	0.90	0.19	104,104,104,104	0
85	MG	6	1955	1/1	0.90	0.39	34,34,34,34	0
85	MG	6	2044	1/1	0.90	0.38	63,63,63,63	0
85	MG	1	3483	1/1	0.90	0.10	29,29,29,29	0
85	MG	L7	301	1/1	0.90	0.12	30,30,30,30	0
85	MG	6	1959	1/1	0.90	0.37	50,50,50,50	0
86	OHX	5	4165	7/7	0.90	0.20	104,104,104,104	0
85	MG	1	3819	1/1	0.90	0.16	27,27,27,27	0
85	MG	5	3771	1/1	0.90	0.10	57,57,57,57	0
86	OHX	5	4169	7/7	0.90	0.20	99,99,99,99	0
85	MG	1	3828	1/1	0.90	0.30	24,24,24,24	0
85	MG	5	3773	1/1	0.90	0.10	21,21,21,21	0
86	OHX	2	2103	7/7	0.90	0.18	117,117,117,117	0
85	MG	1	3829	1/1	0.90	0.29	15,15,15,15	0
85	MG	1	3698	1/1	0.90	0.11	28,28,28,28	0
86	OHX	2	2123	7/7	0.90	0.16	113,113,113,113	0
85	MG	5	3581	1/1	0.90	0.28	28,28,28,28	0
85	MG	1	3455	1/1	0.90	0.41	46,46,46,46	0
85	MG	1	3833	1/1	0.90	0.49	29,29,29,29	0
86	OHX	2	2137	7/7	0.90	0.20	102,102,102,102	0
85	MG	1	3582	1/1	0.90	0.22	28,28,28,28	0
86	OHX	2	2140	7/7	0.90	0.17	138,138,138,138	0
85	MG	5	3786	1/1	0.90	0.46	72,72,72,72	0
85	MG	d3	201	1/1	0.90	0.28	36,36,36,36	0
86	OHX	2	2144	7/7	0.90	0.21	96,96,96,96	0
85	MG	5	3612	1/1	0.90	0.09	25,25,25,25	0
85	MG	2	1923	1/1	0.90	0.37	49,49,49,49	0
86	OHX	1	4198	7/7	0.90	0.19	101,101,101,101	0
85	MG	1	3703	1/1	0.90	0.26	47,47,47,47	0
86	OHX	1	4200	7/7	0.90	0.20	104,104,104,104	0
85	MG	1	3586	1/1	0.90	0.24	18,18,18,18	0
85	MG	5	3799	1/1	0.90	0.23	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4214	7/7	0.90	0.34	91,91,91,91	0
85	MG	5	3800	1/1	0.90	0.07	29,29,29,29	0
86	OHX	1	4206	7/7	0.90	0.15	126,126,126,126	0
85	MG	1	3706	1/1	0.90	0.10	40,40,40,40	0
85	MG	5	3630	1/1	0.90	0.42	67,67,67,67	0
85	MG	2	1973	1/1	0.90	0.32	65,65,65,65	0
85	MG	6	1980	1/1	0.90	0.12	69,69,69,69	0
85	MG	5	3638	1/1	0.90	0.19	30,30,30,30	0
85	MG	1	3595	1/1	0.90	0.33	17,17,17,17	0
85	MG	1	3596	1/1	0.90	0.28	25,25,25,25	0
85	MG	1	3495	1/1	0.90	0.21	34,34,34,34	0
86	OHX	5	4227	7/7	0.90	0.19	108,108,108,108	0
86	OHX	2	2162	7/7	0.90	0.16	132,132,132,132	0
85	MG	5	3427	1/1	0.90	0.18	28,28,28,28	0
85	MG	1	3720	1/1	0.90	0.11	18,18,18,18	0
86	OHX	M8	202	7/7	0.90	0.21	103,103,103,103	0
85	MG	5	3433	1/1	0.90	0.25	38,38,38,38	0
86	OHX	6	2107	7/7	0.90	0.19	92,92,92,92	0
85	MG	1	3722	1/1	0.90	0.17	44,44,44,44	0
85	MG	1	3852	1/1	0.90	0.20	59,59,59,59	0
86	OHX	6	2136	7/7	0.90	0.16	129,129,129,129	0
85	MG	1	3727	1/1	0.90	0.19	43,43,43,43	0
85	MG	S8	301	1/1	0.90	0.13	47,47,47,47	0
85	MG	5	3835	1/1	0.90	0.17	29,29,29,29	0
85	MG	1	3536	1/1	0.90	0.33	34,34,34,34	0
85	MG	5	3665	1/1	0.90	0.20	40,40,40,40	0
86	OHX	6	2155	7/7	0.90	0.15	136,136,136,136	0
86	OHX	6	2157	7/7	0.90	0.15	114,114,114,114	0
85	MG	6	1992	1/1	0.90	0.30	62,62,62,62	0
85	MG	1	3463	1/1	0.90	0.19	36,36,36,36	0
86	OHX	6	2165	7/7	0.90	0.22	96,96,96,96	0
85	MG	1	3611	1/1	0.90	0.34	42,42,42,42	0
85	MG	1	3543	1/1	0.90	0.27	26,26,26,26	0
85	MG	5	3680	1/1	0.90	0.14	26,26,26,26	0
85	MG	2	2006	1/1	0.90	0.13	45,45,45,45	0
86	OHX	6	2172	7/7	0.90	0.15	132,132,132,132	0
85	MG	6	2004	1/1	0.90	0.14	65,65,65,65	0
85	MG	6	1927	1/1	0.90	0.24	45,45,45,45	0
85	MG	2	1910	1/1	0.90	0.34	41,41,41,41	0
85	MG	3	205	1/1	0.90	0.31	27,27,27,27	0
86	OHX	1	4079	7/7	0.90	0.14	115,115,115,115	0
86	OHX	1	4083	7/7	0.90	0.21	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3877	1/1	0.90	0.25	16,16,16,16	0
85	MG	5	3880	1/1	0.90	0.24	36,36,36,36	0
85	MG	1	3755	1/1	0.90	0.17	36,36,36,36	0
86	OHX	1	4098	7/7	0.90	0.17	115,115,115,115	0
86	OHX	1	4103	7/7	0.90	0.18	105,105,105,105	0
85	MG	5	3693	1/1	0.90	0.06	33,33,33,33	0
85	MG	5	3480	1/1	0.90	0.20	58,58,58,58	0
85	MG	6	1931	1/1	0.90	0.37	56,56,56,56	0
85	MG	1	3401	1/1	0.90	0.31	33,33,33,33	0
85	MG	1	3621	1/1	0.90	0.13	24,24,24,24	0
85	MG	2	1999	1/1	0.90	0.20	85,85,85,85	0
85	MG	5	3430	1/1	0.91	0.13	19,19,19,19	0
85	MG	1	3783	1/1	0.91	0.17	40,40,40,40	0
85	MG	6	1919	1/1	0.91	0.35	34,34,34,34	0
85	MG	5	3832	1/1	0.91	0.20	21,21,21,21	0
85	MG	3	202	1/1	0.91	0.15	36,36,36,36	0
85	MG	5	3656	1/1	0.91	0.25	39,39,39,39	0
85	MG	5	3659	1/1	0.91	0.09	32,32,32,32	0
85	MG	1	3785	1/1	0.91	0.12	26,26,26,26	0
86	OHX	1	3922	7/7	0.91	0.24	80,80,80,80	0
86	OHX	1	4037	7/7	0.91	0.18	97,97,97,97	0
86	OHX	1	4057	7/7	0.91	0.15	112,112,112,112	0
85	MG	1	3700	1/1	0.91	0.21	35,35,35,35	0
86	OHX	1	4066	7/7	0.91	0.17	102,102,102,102	0
86	OHX	1	4068	7/7	0.91	0.38	75,75,75,75	0
85	MG	6	1993	1/1	0.91	0.10	44,44,44,44	0
85	MG	5	3853	1/1	0.91	0.31	38,38,38,38	0
86	OHX	6	2193	7/7	0.91	0.17	110,110,110,110	0
86	OHX	1	4082	7/7	0.91	0.17	104,104,104,104	0
85	MG	6	1994	1/1	0.91	0.23	47,47,47,47	0
86	OHX	1	4085	7/7	0.91	0.17	109,109,109,109	0
86	OHX	1	4088	7/7	0.91	0.13	119,119,119,119	0
85	MG	3	206	1/1	0.91	0.34	26,26,26,26	0
85	MG	5	3667	1/1	0.91	0.08	19,19,19,19	0
86	OHX	1	4093	7/7	0.91	0.14	124,124,124,124	0
85	MG	1	3789	1/1	0.91	0.09	44,44,44,44	0
86	OHX	6	2202	7/7	0.91	0.17	114,114,114,114	0
85	MG	2	2022	1/1	0.91	0.10	70,70,70,70	0
85	MG	5	3871	1/1	0.91	0.40	51,51,51,51	0
85	MG	1	3800	1/1	0.91	0.28	53,53,53,53	0
85	MG	1	3656	1/1	0.91	0.22	19,19,19,19	0
85	MG	5	3678	1/1	0.91	0.17	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3559	1/1	0.91	0.20	16,16,16,16	0
85	MG	5	3879	1/1	0.91	0.13	26,26,26,26	0
86	OHX	1	4117	7/7	0.91	0.17	115,115,115,115	0
85	MG	3	214	1/1	0.91	0.30	50,50,50,50	0
85	MG	2	1949	1/1	0.91	0.23	43,43,43,43	0
85	MG	5	3884	1/1	0.91	0.29	49,49,49,49	0
86	OHX	5	4033	7/7	0.91	0.17	102,102,102,102	0
85	MG	2	1984	1/1	0.91	0.18	62,62,62,62	0
85	MG	5	3476	1/1	0.91	0.29	28,28,28,28	0
85	MG	6	2012	1/1	0.91	0.31	48,48,48,48	0
85	MG	2	1956	1/1	0.91	0.32	48,48,48,48	0
85	MG	6	2017	1/1	0.91	0.24	58,58,58,58	0
85	MG	4	210	1/1	0.91	0.26	34,34,34,34	0
86	OHX	5	4107	7/7	0.91	0.19	101,101,101,101	0
85	MG	2	2004	1/1	0.91	0.11	66,66,66,66	0
86	OHX	5	4115	7/7	0.91	0.15	109,109,109,109	0
86	OHX	5	4121	7/7	0.91	0.19	108,108,108,108	0
86	OHX	5	4133	7/7	0.91	0.19	101,101,101,101	0
86	OHX	5	4136	7/7	0.91	0.20	103,103,103,103	0
85	MG	5	3895	1/1	0.91	0.19	83,83,83,83	0
85	MG	5	3698	1/1	0.91	0.16	30,30,30,30	0
85	MG	1	3577	1/1	0.91	0.24	17,17,17,17	0
85	MG	1	3715	1/1	0.91	0.13	32,32,32,32	0
85	MG	5	3500	1/1	0.91	0.26	20,20,20,20	0
85	MG	6	2024	1/1	0.91	0.41	69,69,69,69	0
85	MG	7	204	1/1	0.91	0.42	57,57,57,57	0
85	MG	1	3666	1/1	0.91	0.22	35,35,35,35	0
85	MG	5	3505	1/1	0.91	0.20	21,21,21,21	0
85	MG	2	2013	1/1	0.91	0.22	41,41,41,41	0
85	MG	5	3514	1/1	0.91	0.26	27,27,27,27	0
85	MG	5	3712	1/1	0.91	0.12	53,53,53,53	0
85	MG	6	2028	1/1	0.91	0.16	76,76,76,76	0
85	MG	6	2030	1/1	0.91	0.40	61,61,61,61	0
86	OHX	1	4158	7/7	0.91	0.14	124,124,124,124	0
85	MG	1	3470	1/1	0.91	0.09	29,29,29,29	0
85	MG	1	3669	1/1	0.91	0.18	39,39,39,39	0
85	MG	5	3721	1/1	0.91	0.12	29,29,29,29	0
85	MG	1	3450	1/1	0.91	0.34	29,29,29,29	0
85	MG	5	3533	1/1	0.91	0.17	39,39,39,39	0
85	MG	6	1944	1/1	0.91	0.41	57,57,57,57	0
85	MG	5	3729	1/1	0.91	0.23	19,19,19,19	0
86	OHX	5	4175	7/7	0.91	0.20	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3730	1/1	0.91	0.21	40,40,40,40	0
85	MG	L2	301	1/1	0.91	0.29	20,20,20,20	0
85	MG	8	211	1/1	0.91	0.33	49,49,49,49	0
85	MG	1	3538	1/1	0.91	0.19	30,30,30,30	0
85	MG	l2	303	1/1	0.91	0.06	28,28,28,28	0
86	OHX	5	4185	7/7	0.91	0.19	94,94,94,94	0
85	MG	L5	301	1/1	0.91	0.34	52,52,52,52	0
86	OHX	5	4187	7/7	0.91	0.38	86,86,86,86	0
85	MG	1	3628	1/1	0.91	0.24	58,58,58,58	0
85	MG	5	3736	1/1	0.91	0.12	35,35,35,35	0
85	MG	L8	301	1/1	0.91	0.32	52,52,52,52	0
85	MG	5	3738	1/1	0.91	0.43	55,55,55,55	0
85	MG	1	3737	1/1	0.91	0.18	38,38,38,38	0
85	MG	1	3679	1/1	0.91	0.25	48,48,48,48	0
85	MG	5	3746	1/1	0.91	0.14	51,51,51,51	0
85	MG	n8	202	1/1	0.91	0.18	24,24,24,24	0
85	MG	1	3506	1/1	0.91	0.33	30,30,30,30	0
86	OHX	1	4186	7/7	0.91	0.15	120,120,120,120	0
85	MG	o1	201	1/1	0.91	0.15	33,33,33,33	0
85	MG	5	3555	1/1	0.91	0.27	38,38,38,38	0
86	OHX	5	4208	7/7	0.91	0.14	131,131,131,131	0
86	OHX	5	4210	7/7	0.91	0.18	110,110,110,110	0
85	MG	1	3843	1/1	0.91	0.36	41,41,41,41	0
85	MG	1	3588	1/1	0.91	0.43	31,31,31,31	0
86	OHX	2	2069	7/7	0.91	0.13	133,133,133,133	0
85	MG	N6	201	1/1	0.91	0.15	33,33,33,33	0
86	OHX	5	4215	7/7	0.91	0.10	179,179,179,179	0
85	MG	6	1964	1/1	0.91	0.29	48,48,48,48	0
85	MG	5	3760	1/1	0.91	0.06	36,36,36,36	0
85	MG	s1	301	1/1	0.91	0.26	67,67,67,67	0
85	MG	1	3633	1/1	0.91	0.10	43,43,43,43	0
85	MG	5	3766	1/1	0.91	0.07	29,29,29,29	0
86	OHX	2	2128	7/7	0.91	0.16	104,104,104,104	0
85	MG	N8	204	1/1	0.91	0.12	30,30,30,30	0
85	MG	1	3590	1/1	0.91	0.37	35,35,35,35	0
85	MG	1	3691	1/1	0.91	0.09	35,35,35,35	0
85	MG	1	3542	1/1	0.91	0.33	24,24,24,24	0
85	MG	5	3588	1/1	0.91	0.30	17,17,17,17	0
85	MG	5	3589	1/1	0.91	0.34	27,27,27,27	0
85	MG	5	3591	1/1	0.91	0.30	18,18,18,18	0
85	MG	5	3777	1/1	0.91	0.11	44,44,44,44	0
86	OHX	3	225	7/7	0.91	0.18	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3778	1/1	0.91	0.08	35,35,35,35	0
85	MG	1	3452	1/1	0.91	0.26	35,35,35,35	0
85	MG	5	3594	1/1	0.91	0.38	32,32,32,32	0
85	MG	5	3781	1/1	0.91	0.15	32,32,32,32	0
85	MG	5	3596	1/1	0.91	0.28	24,24,24,24	0
85	MG	5	3599	1/1	0.91	0.20	32,32,32,32	0
85	MG	d3	202	1/1	0.91	0.19	44,44,44,44	0
85	MG	5	3602	1/1	0.91	0.18	27,27,27,27	0
85	MG	1	3510	1/1	0.91	0.31	20,20,20,20	0
86	OHX	O9	101	7/7	0.91	0.38	82,82,82,82	0
86	OHX	2	2155	7/7	0.91	0.15	117,117,117,117	0
85	MG	5	3606	1/1	0.91	0.29	20,20,20,20	0
85	MG	5	3794	1/1	0.91	0.09	34,34,34,34	0
85	MG	6	1974	1/1	0.91	0.23	47,47,47,47	0
85	MG	1	3475	1/1	0.91	0.17	22,22,22,22	0
85	MG	1	3772	1/1	0.91	0.18	44,44,44,44	0
85	MG	5	3407	1/1	0.91	0.20	29,29,29,29	0
86	OHX	6	2144	7/7	0.91	0.12	147,147,147,147	0
85	MG	5	3627	1/1	0.91	0.23	52,52,52,52	0
85	MG	5	3415	1/1	0.91	0.18	39,39,39,39	0
86	OHX	6	2153	7/7	0.91	0.15	120,120,120,120	0
86	OHX	6	2154	7/7	0.91	0.21	91,91,91,91	0
85	MG	5	3416	1/1	0.91	0.10	22,22,22,22	0
86	OHX	6	2156	7/7	0.91	0.16	113,113,113,113	0
85	MG	5	3633	1/1	0.91	0.42	71,71,71,71	0
85	MG	1	3453	1/1	0.91	0.21	25,25,25,25	0
86	OHX	6	2161	7/7	0.91	0.17	111,111,111,111	0
86	OHX	2	2167	7/7	0.91	0.14	137,137,137,137	0
86	OHX	6	2164	7/7	0.91	0.17	101,101,101,101	0
86	OHX	2	2168	7/7	0.91	0.21	93,93,93,93	0
86	OHX	6	2166	7/7	0.91	0.18	102,102,102,102	0
85	MG	1	3435	1/1	0.91	0.22	29,29,29,29	0
85	MG	2	1982	1/1	0.91	0.41	59,59,59,59	0
85	MG	5	3639	1/1	0.91	0.26	28,28,28,28	0
85	MG	6	1913	1/1	0.91	0.29	31,31,31,31	0
85	MG	1	3861	1/1	0.91	0.30	40,40,40,40	0
85	MG	1	4211	1/1	0.91	0.25	51,51,51,51	0
85	MG	n8	203	1/1	0.92	0.07	16,16,16,16	0
85	MG	1	3601	1/1	0.92	0.14	24,24,24,24	0
85	MG	n9	101	1/1	0.92	0.07	20,20,20,20	0
85	MG	1	3831	1/1	0.92	0.20	20,20,20,20	0
85	MG	5	3503	1/1	0.92	0.30	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	6	2209	1/1	0.92	0.20	48,48,48,48	0
85	MG	4	207	1/1	0.92	0.24	22,22,22,22	0
85	MG	5	3508	1/1	0.92	0.25	30,30,30,30	0
86	OHX	2	2081	7/7	0.92	0.11	145,145,145,145	0
86	OHX	5	3974	7/7	0.92	0.33	76,76,76,76	0
85	MG	1	3556	1/1	0.92	0.32	25,25,25,25	0
86	OHX	5	4025	7/7	0.92	0.20	75,75,75,75	0
86	OHX	2	2097	7/7	0.92	0.14	140,140,140,140	0
85	MG	1	3432	1/1	0.92	0.10	23,23,23,23	0
85	MG	5	3518	1/1	0.92	0.19	17,17,17,17	0
86	OHX	5	4085	7/7	0.92	0.17	100,100,100,100	0
86	OHX	2	2108	7/7	0.92	0.16	105,105,105,105	0
86	OHX	5	4097	7/7	0.92	0.17	110,110,110,110	0
85	MG	s8	302	1/1	0.92	0.15	37,37,37,37	0
86	OHX	2	2118	7/7	0.92	0.13	134,134,134,134	0
85	MG	1	3606	1/1	0.92	0.32	56,56,56,56	0
86	OHX	5	4106	7/7	0.92	0.19	95,95,95,95	0
86	OHX	2	2122	7/7	0.92	0.15	116,116,116,116	0
85	MG	5	3524	1/1	0.92	0.31	20,20,20,20	0
85	MG	1	3688	1/1	0.92	0.10	24,24,24,24	0
86	OHX	5	4117	7/7	0.92	0.18	95,95,95,95	0
85	MG	1	3690	1/1	0.92	0.32	34,34,34,34	0
86	OHX	5	4122	7/7	0.92	0.17	108,108,108,108	0
85	MG	1	3643	1/1	0.92	0.24	51,51,51,51	0
86	OHX	5	4135	7/7	0.92	0.17	112,112,112,112	0
85	MG	1	3501	1/1	0.92	0.31	18,18,18,18	0
85	MG	2	1922	1/1	0.92	0.33	55,55,55,55	0
85	MG	1	3504	1/1	0.92	0.35	32,32,32,32	0
86	OHX	2	2139	7/7	0.92	0.15	110,110,110,110	0
85	MG	1	3481	1/1	0.92	0.24	24,24,24,24	0
85	MG	5	3403	1/1	0.92	0.34	38,38,38,38	0
85	MG	6	1996	1/1	0.92	0.09	35,35,35,35	0
86	OHX	5	4146	7/7	0.92	0.24	82,82,82,82	0
85	MG	5	3824	1/1	0.92	0.08	36,36,36,36	0
85	MG	5	3544	1/1	0.92	0.44	41,41,41,41	0
85	MG	5	3831	1/1	0.92	0.14	42,42,42,42	0
85	MG	5	3548	1/1	0.92	0.35	32,32,32,32	0
85	MG	1	3565	1/1	0.92	0.19	27,27,27,27	0
85	MG	5	3834	1/1	0.92	0.12	29,29,29,29	0
86	OHX	5	4156	7/7	0.92	0.16	110,110,110,110	0
85	MG	5	3550	1/1	0.92	0.21	20,20,20,20	0
85	MG	L4	401	1/1	0.92	0.18	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4193	7/7	0.92	0.17	104,104,104,104	0
85	MG	5	3409	1/1	0.92	0.28	32,32,32,32	0
85	MG	5	3411	1/1	0.92	0.31	27,27,27,27	0
85	MG	1	3482	1/1	0.92	0.25	39,39,39,39	0
86	OHX	5	4166	7/7	0.92	0.18	99,99,99,99	0
85	MG	5	3556	1/1	0.92	0.29	16,16,16,16	0
85	MG	1	3619	1/1	0.92	0.12	31,31,31,31	0
85	MG	5	3855	1/1	0.92	0.17	44,44,44,44	0
86	OHX	5	4170	7/7	0.92	0.10	163,163,163,163	0
85	MG	5	3559	1/1	0.92	0.21	26,26,26,26	0
85	MG	1	3509	1/1	0.92	0.21	33,33,33,33	0
85	MG	5	3859	1/1	0.92	0.15	46,46,46,46	0
85	MG	2	2008	1/1	0.92	0.38	39,39,39,39	0
85	MG	5	3711	1/1	0.92	0.11	28,28,28,28	0
85	MG	1	3416	1/1	0.92	0.22	20,20,20,20	0
85	MG	6	2009	1/1	0.92	0.27	46,46,46,46	0
85	MG	1	3782	1/1	0.92	0.11	35,35,35,35	0
85	MG	5	3426	1/1	0.92	0.21	31,31,31,31	0
85	MG	5	3717	1/1	0.92	0.16	38,38,38,38	0
86	OHX	4	232	7/7	0.92	0.13	121,121,121,121	0
86	OHX	5	4189	7/7	0.92	0.20	94,94,94,94	0
86	OHX	2	2170	7/7	0.92	0.16	116,116,116,116	0
85	MG	5	3878	1/1	0.92	0.16	23,23,23,23	0
86	OHX	5	4194	7/7	0.92	0.12	145,145,145,145	0
85	MG	6	1943	1/1	0.92	0.32	32,32,32,32	0
85	MG	M8	201	1/1	0.92	0.18	44,44,44,44	0
85	MG	2	1918	1/1	0.92	0.41	40,40,40,40	0
85	MG	5	3723	1/1	0.92	0.26	34,34,34,34	0
86	OHX	M7	204	7/7	0.92	0.39	74,74,74,74	0
85	MG	5	3725	1/1	0.92	0.23	26,26,26,26	0
85	MG	5	3587	1/1	0.92	0.44	42,42,42,42	0
85	MG	5	3887	1/1	0.92	0.22	39,39,39,39	0
85	MG	2	1911	1/1	0.92	0.32	45,45,45,45	0
86	OHX	6	2097	7/7	0.92	0.15	109,109,109,109	0
86	OHX	6	2102	7/7	0.92	0.13	147,147,147,147	0
85	MG	1	3472	1/1	0.92	0.28	20,20,20,20	0
86	OHX	S8	302	7/7	0.92	0.11	133,133,133,133	0
85	MG	5	3437	1/1	0.92	0.17	35,35,35,35	0
86	OHX	6	2134	7/7	0.92	0.14	125,125,125,125	0
85	MG	1	3518	1/1	0.92	0.35	17,17,17,17	0
86	OHX	6	2137	7/7	0.92	0.17	105,105,105,105	0
85	MG	5	3445	1/1	0.92	0.23	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	3595	1/1	0.92	0.24	14,14,14,14	0
86	OHX	1	4013	7/7	0.92	0.10	133,133,133,133	0
86	OHX	1	4015	7/7	0.92	0.15	105,105,105,105	0
86	OHX	1	4027	7/7	0.92	0.18	101,101,101,101	0
86	OHX	1	4031	7/7	0.92	0.18	95,95,95,95	0
85	MG	1	3709	1/1	0.92	0.14	26,26,26,26	0
86	OHX	1	4055	7/7	0.92	0.16	100,100,100,100	0
85	MG	1	3862	1/1	0.92	0.20	28,28,28,28	0
85	MG	5	3600	1/1	0.92	0.12	31,31,31,31	0
85	MG	5	3451	1/1	0.92	0.12	25,25,25,25	0
85	MG	7	201	1/1	0.92	0.38	32,32,32,32	0
86	OHX	1	4072	7/7	0.92	0.14	108,108,108,108	0
85	MG	1	3791	1/1	0.92	0.25	27,27,27,27	0
85	MG	O4	201	1/1	0.92	0.16	45,45,45,45	0
85	MG	1	3428	1/1	0.92	0.37	27,27,27,27	0
85	MG	1	3801	1/1	0.92	0.18	25,25,25,25	0
85	MG	1	3671	1/1	0.92	0.43	50,50,50,50	0
85	MG	7	211	1/1	0.92	0.10	23,23,23,23	0
86	OHX	6	2169	7/7	0.92	0.14	118,118,118,118	0
85	MG	3	204	1/1	0.92	0.40	41,41,41,41	0
85	MG	5	3755	1/1	0.92	0.17	52,52,52,52	0
85	MG	1	3713	1/1	0.92	0.07	22,22,22,22	0
85	MG	5	3618	1/1	0.92	0.14	33,33,33,33	0
85	MG	8	201	1/1	0.92	0.10	31,31,31,31	0
85	MG	5	3620	1/1	0.92	0.19	27,27,27,27	0
85	MG	5	3623	1/1	0.92	0.28	32,32,32,32	0
85	MG	5	3625	1/1	0.92	0.15	52,52,52,52	0
85	MG	1	3550	1/1	0.92	0.26	28,28,28,28	0
85	MG	3	207	1/1	0.92	0.32	56,56,56,56	0
86	OHX	1	4114	7/7	0.92	0.18	96,96,96,96	0
85	MG	1	3552	1/1	0.92	0.38	29,29,29,29	0
85	MG	1	3429	1/1	0.92	0.31	35,35,35,35	0
85	MG	5	3635	1/1	0.92	0.20	36,36,36,36	0
86	OHX	1	4122	7/7	0.92	0.15	116,116,116,116	0
85	MG	1	3599	1/1	0.92	0.22	17,17,17,17	0
85	MG	1	3724	1/1	0.92	0.12	32,32,32,32	0
85	MG	1	3821	1/1	0.92	0.13	31,31,31,31	0
85	MG	8	214	1/1	0.92	0.37	50,50,50,50	0
85	MG	6	2043	1/1	0.92	0.35	52,52,52,52	0
85	MG	5	3640	1/1	0.92	0.16	36,36,36,36	0
86	OHX	1	4133	7/7	0.92	0.20	95,95,95,95	0
85	MG	6	1918	1/1	0.92	0.37	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	l5	302	7/7	0.92	0.13	114,114,114,114	0
85	MG	5	3643	1/1	0.92	0.11	22,22,22,22	0
85	MG	5	3493	1/1	0.92	0.12	30,30,30,30	0
85	MG	5	3495	1/1	0.92	0.15	22,22,22,22	0
85	MG	1	3680	1/1	0.92	0.11	31,31,31,31	0
85	MG	1	3681	1/1	0.92	0.17	30,30,30,30	0
85	MG	m7	204	1/1	0.92	0.12	23,23,23,23	0
85	MG	5	3653	1/1	0.92	0.28	54,54,54,54	0
85	MG	5	3789	1/1	0.92	0.17	16,16,16,16	0
85	MG	5	3402	1/1	0.93	0.20	17,17,17,17	0
85	MG	1	3815	1/1	0.93	0.09	32,32,32,32	0
85	MG	1	3558	1/1	0.93	0.36	44,44,44,44	0
85	MG	1	3488	1/1	0.93	0.15	40,40,40,40	0
86	OHX	1	4132	7/7	0.93	0.15	85,85,85,85	0
85	MG	5	3801	1/1	0.93	0.20	36,36,36,36	0
85	MG	5	3406	1/1	0.93	0.09	33,33,33,33	0
86	OHX	1	4135	7/7	0.93	0.31	84,84,84,84	0
85	MG	1	3489	1/1	0.93	0.20	23,23,23,23	0
85	MG	5	3805	1/1	0.93	0.12	18,18,18,18	0
85	MG	4	205	1/1	0.93	0.31	42,42,42,42	0
86	OHX	2	2076	7/7	0.93	0.15	115,115,115,115	0
86	OHX	s4	301	7/7	0.93	0.14	119,119,119,119	0
85	MG	5	3546	1/1	0.93	0.32	40,40,40,40	0
86	OHX	2	2082	7/7	0.93	0.16	108,108,108,108	0
86	OHX	c5	201	7/7	0.93	0.11	130,130,130,130	0
86	OHX	2	2089	7/7	0.93	0.16	99,99,99,99	0
86	OHX	2	2092	7/7	0.93	0.16	112,112,112,112	0
85	MG	4	206	1/1	0.93	0.24	21,21,21,21	0
86	OHX	5	4004	7/7	0.93	0.16	93,93,93,93	0
85	MG	5	3413	1/1	0.93	0.15	32,32,32,32	0
85	MG	1	3687	1/1	0.93	0.29	38,38,38,38	0
85	MG	4	208	1/1	0.93	0.25	22,22,22,22	0
86	OHX	2	2104	7/7	0.93	0.10	185,185,185,185	0
86	OHX	5	4060	7/7	0.93	0.16	102,102,102,102	0
86	OHX	5	4061	7/7	0.93	0.15	99,99,99,99	0
85	MG	5	3417	1/1	0.93	0.21	20,20,20,20	0
86	OHX	5	4074	7/7	0.93	0.17	99,99,99,99	0
86	OHX	5	4082	7/7	0.93	0.12	112,112,112,112	0
86	OHX	2	2112	7/7	0.93	0.12	130,130,130,130	0
86	OHX	5	4094	7/7	0.93	0.14	98,98,98,98	0
85	MG	5	3683	1/1	0.93	0.12	24,24,24,24	0
85	MG	6	1997	1/1	0.93	0.23	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	2	2119	7/7	0.93	0.14	112,112,112,112	0
85	MG	4	209	1/1	0.93	0.22	17,17,17,17	0
86	OHX	2	2121	7/7	0.93	0.14	121,121,121,121	0
85	MG	5	3687	1/1	0.93	0.08	30,30,30,30	0
86	OHX	1	4164	7/7	0.93	0.29	91,91,91,91	0
85	MG	5	3823	1/1	0.93	0.20	49,49,49,49	0
86	OHX	2	2124	7/7	0.93	0.16	116,116,116,116	0
86	OHX	2	2125	7/7	0.93	0.14	114,114,114,114	0
86	OHX	2	2127	7/7	0.93	0.15	109,109,109,109	0
85	MG	1	3738	1/1	0.93	0.17	34,34,34,34	0
86	OHX	5	4123	7/7	0.93	0.13	121,121,121,121	0
86	OHX	5	4128	7/7	0.93	0.13	123,123,123,123	0
86	OHX	5	4129	7/7	0.93	0.13	118,118,118,118	0
86	OHX	5	4131	7/7	0.93	0.11	155,155,155,155	0
86	OHX	2	2129	7/7	0.93	0.15	125,125,125,125	0
86	OHX	2	2132	7/7	0.93	0.18	95,95,95,95	0
86	OHX	2	2133	7/7	0.93	0.13	123,123,123,123	0
85	MG	1	3646	1/1	0.93	0.15	33,33,33,33	0
85	MG	1	3744	1/1	0.93	0.18	18,18,18,18	0
85	MG	1	3465	1/1	0.93	0.25	42,42,42,42	0
85	MG	1	3491	1/1	0.93	0.21	19,19,19,19	0
85	MG	5	3565	1/1	0.93	0.33	40,40,40,40	0
85	MG	5	3568	1/1	0.93	0.28	24,24,24,24	0
85	MG	5	3701	1/1	0.93	0.15	26,26,26,26	0
85	MG	1	3537	1/1	0.93	0.38	26,26,26,26	0
85	MG	1	3476	1/1	0.93	0.15	38,38,38,38	0
85	MG	5	3432	1/1	0.93	0.11	24,24,24,24	0
85	MG	5	3849	1/1	0.93	0.25	48,48,48,48	0
86	OHX	5	4152	7/7	0.93	0.31	82,82,82,82	0
85	MG	5	3572	1/1	0.93	0.27	22,22,22,22	0
86	OHX	1	4188	7/7	0.93	0.12	153,153,153,153	0
85	MG	1	3756	1/1	0.93	0.10	19,19,19,19	0
86	OHX	2	2149	7/7	0.93	0.28	85,85,85,85	0
85	MG	1	3757	1/1	0.93	0.07	35,35,35,35	0
85	MG	5	3856	1/1	0.93	0.12	31,31,31,31	0
85	MG	5	3580	1/1	0.93	0.27	22,22,22,22	0
85	MG	5	3436	1/1	0.93	0.18	23,23,23,23	0
85	MG	1	3761	1/1	0.93	0.18	36,36,36,36	0
85	MG	5	3713	1/1	0.93	0.10	30,30,30,30	0
85	MG	5	3583	1/1	0.93	0.28	21,21,21,21	0
85	MG	5	3866	1/1	0.93	0.12	17,17,17,17	0
85	MG	5	3438	1/1	0.93	0.43	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	1	3763	1/1	0.93	0.07	30,30,30,30	0
86	OHX	1	4201	7/7	0.93	0.36	90,90,90,90	0
85	MG	1	3652	1/1	0.93	0.10	19,19,19,19	0
85	MG	5	3590	1/1	0.93	0.18	28,28,28,28	0
86	OHX	5	4177	7/7	0.93	0.17	100,100,100,100	0
85	MG	1	3655	1/1	0.93	0.26	29,29,29,29	0
85	MG	1	3571	1/1	0.93	0.22	23,23,23,23	0
85	MG	L7	302	1/1	0.93	0.14	30,30,30,30	0
85	MG	1	3574	1/1	0.93	0.28	12,12,12,12	0
86	OHX	3	222	7/7	0.93	0.12	120,120,120,120	0
85	MG	5	3726	1/1	0.93	0.07	43,43,43,43	0
85	MG	1	3512	1/1	0.93	0.29	17,17,17,17	0
85	MG	1	3771	1/1	0.93	0.15	38,38,38,38	0
85	MG	1	3851	1/1	0.93	0.17	13,13,13,13	0
85	MG	2	2009	1/1	0.93	0.36	44,44,44,44	0
85	MG	1	3773	1/1	0.93	0.23	46,46,46,46	0
86	OHX	5	4192	7/7	0.93	0.25	92,92,92,92	0
85	MG	5	3604	1/1	0.93	0.11	29,29,29,29	0
85	MG	5	3891	1/1	0.93	0.31	50,50,50,50	0
85	MG	N3	201	1/1	0.93	0.28	23,23,23,23	0
85	MG	1	3774	1/1	0.93	0.14	53,53,53,53	0
86	OHX	M0	303	7/7	0.93	0.16	92,92,92,92	0
85	MG	5	3609	1/1	0.93	0.17	26,26,26,26	0
85	MG	5	3610	1/1	0.93	0.19	37,37,37,37	0
85	MG	6	2035	1/1	0.93	0.11	43,43,43,43	0
85	MG	5	3474	1/1	0.93	0.23	42,42,42,42	0
85	MG	1	3514	1/1	0.93	0.28	18,18,18,18	0
86	OHX	6	2079	7/7	0.93	0.16	91,91,91,91	0
85	MG	1	3622	1/1	0.93	0.10	35,35,35,35	0
85	MG	5	4255	1/1	0.93	0.45	17,17,17,17	0
85	MG	5	4257	1/1	0.93	0.26	19,19,19,19	0
85	MG	5	3617	1/1	0.93	0.16	32,32,32,32	0
85	MG	2	1974	1/1	0.93	0.26	55,55,55,55	0
86	OHX	6	2127	7/7	0.93	0.16	105,105,105,105	0
86	OHX	6	2129	7/7	0.93	0.33	81,81,81,81	0
86	OHX	6	2130	7/7	0.93	0.17	94,94,94,94	0
86	OHX	1	3952	7/7	0.93	0.19	72,72,72,72	0
86	OHX	1	3965	7/7	0.93	0.15	90,90,90,90	0
85	MG	5	3753	1/1	0.93	0.09	38,38,38,38	0
85	MG	1	3498	1/1	0.93	0.31	23,23,23,23	0
86	OHX	1	4017	7/7	0.93	0.21	89,89,89,89	0
86	OHX	6	2141	7/7	0.93	0.16	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	6	2142	7/7	0.93	0.16	108,108,108,108	0
86	OHX	1	4019	7/7	0.93	0.14	111,111,111,111	0
86	OHX	1	4024	7/7	0.93	0.27	85,85,85,85	0
85	MG	5	3622	1/1	0.93	0.30	30,30,30,30	0
86	OHX	6	2149	7/7	0.93	0.14	112,112,112,112	0
85	MG	1	3705	1/1	0.93	0.11	28,28,28,28	0
85	MG	6	1965	1/1	0.93	0.15	60,60,60,60	0
85	MG	5	3626	1/1	0.93	0.22	44,44,44,44	0
85	MG	2	2181	1/1	0.93	0.25	56,56,56,56	0
85	MG	O7	102	1/1	0.93	0.16	27,27,27,27	0
86	OHX	1	4062	7/7	0.93	0.36	82,82,82,82	0
86	OHX	1	4065	7/7	0.93	0.28	87,87,87,87	0
85	MG	1	3447	1/1	0.93	0.12	21,21,21,21	0
86	OHX	1	4067	7/7	0.93	0.16	115,115,115,115	0
85	MG	5	3765	1/1	0.93	0.08	46,46,46,46	0
86	OHX	1	4070	7/7	0.93	0.18	93,93,93,93	0
85	MG	5	3632	1/1	0.93	0.08	23,23,23,23	0
86	OHX	1	4074	7/7	0.93	0.30	91,91,91,91	0
85	MG	1	3788	1/1	0.93	0.18	73,73,73,73	0
85	MG	5	3634	1/1	0.93	0.12	42,42,42,42	0
85	MG	6	1903	1/1	0.93	0.36	39,39,39,39	0
85	MG	6	1971	1/1	0.93	0.10	51,51,51,51	0
85	MG	1	3461	1/1	0.93	0.24	19,19,19,19	0
85	MG	1	3523	1/1	0.93	0.27	17,17,17,17	0
85	MG	1	3672	1/1	0.93	0.23	18,18,18,18	0
85	MG	6	1976	1/1	0.93	0.21	52,52,52,52	0
85	MG	5	3506	1/1	0.93	0.33	25,25,25,25	0
85	MG	1	3630	1/1	0.93	0.08	18,18,18,18	0
86	OHX	6	2179	7/7	0.93	0.26	83,83,83,83	0
86	OHX	1	4097	7/7	0.93	0.16	102,102,102,102	0
85	MG	5	3510	1/1	0.93	0.27	17,17,17,17	0
85	MG	6	1978	1/1	0.93	0.19	37,37,37,37	0
86	OHX	8	229	7/7	0.93	0.14	111,111,111,111	0
85	MG	l3	401	1/1	0.93	0.08	19,19,19,19	0
85	MG	6	1910	1/1	0.93	0.23	40,40,40,40	0
86	OHX	l3	404	7/7	0.93	0.15	106,106,106,106	0
85	MG	5	3783	1/1	0.93	0.11	48,48,48,48	0
85	MG	1	3594	1/1	0.93	0.32	13,13,13,13	0
85	MG	2	1965	1/1	0.93	0.30	48,48,48,48	0
86	OHX	1	4115	7/7	0.93	0.33	80,80,80,80	0
85	MG	1	3555	1/1	0.93	0.33	19,19,19,19	0
85	MG	1	3598	1/1	0.93	0.24	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	m5	304	1/1	0.93	0.12	70,70,70,70	0
86	OHX	1	4121	7/7	0.93	0.31	88,88,88,88	0
85	MG	1	3811	1/1	0.93	0.17	37,37,37,37	0
85	MG	1	3526	1/1	0.93	0.26	18,18,18,18	0
85	MG	1	3486	1/1	0.93	0.19	19,19,19,19	0
88	3J2	1	4209	26/26	0.93	0.11	19,19,19,19	0
85	MG	1	3653	1/1	0.94	0.19	36,36,36,36	0
86	OHX	2	2130	7/7	0.94	0.10	168,168,168,168	0
85	MG	5	3700	1/1	0.94	0.19	45,45,45,45	0
85	MG	1	3758	1/1	0.94	0.09	20,20,20,20	0
86	OHX	5	3975	7/7	0.94	0.13	83,83,83,83	0
86	OHX	5	3995	7/7	0.94	0.17	87,87,87,87	0
86	OHX	5	3999	7/7	0.94	0.14	84,84,84,84	0
85	MG	1	3760	1/1	0.94	0.08	33,33,33,33	0
85	MG	5	3703	1/1	0.94	0.34	59,59,59,59	0
85	MG	4	221	1/1	0.94	0.27	39,39,39,39	0
86	OHX	1	4163	7/7	0.94	0.24	86,86,86,86	0
86	OHX	5	4036	7/7	0.94	0.12	106,106,106,106	0
86	OHX	5	4039	7/7	0.94	0.14	138,138,138,138	0
85	MG	1	3462	1/1	0.94	0.20	18,18,18,18	0
85	MG	1	3434	1/1	0.94	0.18	30,30,30,30	0
85	MG	L2	302	1/1	0.94	0.07	23,23,23,23	0
86	OHX	5	4062	7/7	0.94	0.11	127,127,127,127	0
86	OHX	5	4065	7/7	0.94	0.13	96,96,96,96	0
86	OHX	5	4068	7/7	0.94	0.16	95,95,95,95	0
85	MG	5	3578	1/1	0.94	0.26	19,19,19,19	0
85	MG	L2	303	1/1	0.94	0.29	37,37,37,37	0
85	MG	5	3865	1/1	0.94	0.10	33,33,33,33	0
85	MG	1	3534	1/1	0.94	0.31	17,17,17,17	0
86	OHX	1	4172	7/7	0.94	0.29	89,89,89,89	0
85	MG	5	3868	1/1	0.94	0.20	19,19,19,19	0
85	MG	5	3869	1/1	0.94	0.36	23,23,23,23	0
86	OHX	5	4098	7/7	0.94	0.23	93,93,93,93	0
85	MG	5	3870	1/1	0.94	0.23	18,18,18,18	0
85	MG	1	3617	1/1	0.94	0.36	54,54,54,54	0
85	MG	1	3505	1/1	0.94	0.21	24,24,24,24	0
86	OHX	5	4103	7/7	0.94	0.15	107,107,107,107	0
86	OHX	5	4104	7/7	0.94	0.30	83,83,83,83	0
85	MG	5	3453	1/1	0.94	0.34	33,33,33,33	0
85	MG	SM	3401	1/1	0.94	0.11	41,41,41,41	0
85	MG	1	3436	1/1	0.94	0.22	21,21,21,21	0
86	OHX	5	4111	7/7	0.94	0.17	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3456	1/1	0.94	0.17	16,16,16,16	0
85	MG	1	3485	1/1	0.94	0.22	29,29,29,29	0
86	OHX	5	4118	7/7	0.94	0.21	89,89,89,89	0
85	MG	1	3849	1/1	0.94	0.20	48,48,48,48	0
85	MG	5	3463	1/1	0.94	0.31	32,32,32,32	0
85	MG	6	1947	1/1	0.94	0.38	48,48,48,48	0
86	OHX	5	4124	7/7	0.94	0.12	124,124,124,124	0
85	MG	5	3465	1/1	0.94	0.26	50,50,50,50	0
85	MG	5	3598	1/1	0.94	0.22	28,28,28,28	0
85	MG	6	1949	1/1	0.94	0.30	40,40,40,40	0
85	MG	5	3468	1/1	0.94	0.16	24,24,24,24	0
85	MG	M1	201	1/1	0.94	0.23	64,64,64,64	0
85	MG	M3	201	1/1	0.94	0.11	35,35,35,35	0
85	MG	5	3603	1/1	0.94	0.05	23,23,23,23	0
85	MG	1	3451	1/1	0.94	0.18	21,21,21,21	0
85	MG	6	1954	1/1	0.94	0.21	40,40,40,40	0
85	MG	M4	201	1/1	0.94	0.17	44,44,44,44	0
85	MG	5	3607	1/1	0.94	0.23	19,19,19,19	0
86	OHX	5	4142	7/7	0.94	0.15	97,97,97,97	0
85	MG	M5	303	1/1	0.94	0.26	39,39,39,39	0
85	MG	M6	201	1/1	0.94	0.09	36,36,36,36	0
85	MG	5	3740	1/1	0.94	0.18	52,52,52,52	0
85	MG	5	3742	1/1	0.94	0.29	26,26,26,26	0
85	MG	5	3611	1/1	0.94	0.07	25,25,25,25	0
85	MG	1	3487	1/1	0.94	0.17	24,24,24,24	0
85	MG	1	3585	1/1	0.94	0.32	29,29,29,29	0
85	MG	5	3484	1/1	0.94	0.11	32,32,32,32	0
85	MG	7	205	1/1	0.94	0.30	19,19,19,19	0
85	MG	1	3776	1/1	0.94	0.20	19,19,19,19	0
85	MG	5	3488	1/1	0.94	0.09	21,21,21,21	0
85	MG	1	3708	1/1	0.94	0.22	22,22,22,22	0
85	MG	7	210	1/1	0.94	0.26	31,31,31,31	0
86	OHX	5	4161	7/7	0.94	0.34	90,90,90,90	0
85	MG	5	3619	1/1	0.94	0.34	44,44,44,44	0
86	OHX	C5	201	7/7	0.94	0.11	137,137,137,137	0
86	OHX	4	234	7/7	0.94	0.24	88,88,88,88	0
85	MG	N3	203	1/1	0.94	0.22	39,39,39,39	0
85	MG	5	3494	1/1	0.94	0.18	17,17,17,17	0
86	OHX	1	3951	7/7	0.94	0.16	81,81,81,81	0
85	MG	1	3855	1/1	0.94	0.35	44,44,44,44	0
85	MG	1	3439	1/1	0.94	0.12	28,28,28,28	0
86	OHX	1	4001	7/7	0.94	0.21	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4005	7/7	0.94	0.16	96,96,96,96	0
85	MG	1	3587	1/1	0.94	0.24	21,21,21,21	0
85	MG	1	3781	1/1	0.94	0.29	50,50,50,50	0
86	OHX	5	4178	7/7	0.94	0.30	80,80,80,80	0
85	MG	1	3425	1/1	0.94	0.07	46,46,46,46	0
85	MG	2	1902	1/1	0.94	0.27	30,30,30,30	0
86	OHX	1	4020	7/7	0.94	0.13	115,115,115,115	0
85	MG	1	3675	1/1	0.94	0.08	31,31,31,31	0
85	MG	1	3473	1/1	0.94	0.28	15,15,15,15	0
85	MG	1	3592	1/1	0.94	0.24	19,19,19,19	0
86	OHX	1	4032	7/7	0.94	0.12	117,117,117,117	0
85	MG	6	1901	1/1	0.94	0.34	41,41,41,41	0
86	OHX	1	4041	7/7	0.94	0.32	82,82,82,82	0
86	OHX	6	2121	7/7	0.94	0.13	116,116,116,116	0
86	OHX	6	2124	7/7	0.94	0.12	119,119,119,119	0
86	OHX	6	2125	7/7	0.94	0.13	121,121,121,121	0
85	MG	5	3509	1/1	0.94	0.35	23,23,23,23	0
86	OHX	1	4056	7/7	0.94	0.10	125,125,125,125	0
85	MG	1	3403	1/1	0.94	0.20	24,24,24,24	0
85	MG	1	3517	1/1	0.94	0.22	22,22,22,22	0
86	OHX	6	2135	7/7	0.94	0.17	104,104,104,104	0
85	MG	1	3725	1/1	0.94	0.17	49,49,49,49	0
85	MG	5	3516	1/1	0.94	0.25	26,26,26,26	0
85	MG	8	215	1/1	0.94	0.27	23,23,23,23	0
85	MG	6	1905	1/1	0.94	0.32	47,47,47,47	0
85	MG	1	3794	1/1	0.94	0.14	18,18,18,18	0
85	MG	1	3494	1/1	0.94	0.19	32,32,32,32	0
85	MG	5	3401	1/1	0.94	0.22	42,42,42,42	0
86	OHX	1	4073	7/7	0.94	0.36	89,89,89,89	0
86	OHX	6	2146	7/7	0.94	0.14	116,116,116,116	0
85	MG	5	3647	1/1	0.94	0.15	33,33,33,33	0
86	OHX	1	4075	7/7	0.94	0.28	91,91,91,91	0
85	MG	19	201	1/1	0.94	0.09	27,27,27,27	0
86	OHX	1	4078	7/7	0.94	0.31	92,92,92,92	0
85	MG	1	3519	1/1	0.94	0.21	25,25,25,25	0
86	OHX	1	4081	7/7	0.94	0.10	179,179,179,179	0
85	MG	1	3733	1/1	0.94	0.14	28,28,28,28	0
85	MG	5	3787	1/1	0.94	0.10	31,31,31,31	0
85	MG	5	3652	1/1	0.94	0.19	15,15,15,15	0
86	OHX	6	2160	7/7	0.94	0.18	113,113,113,113	0
85	MG	1	3683	1/1	0.94	0.10	26,26,26,26	0
86	OHX	1	4089	7/7	0.94	0.12	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3804	1/1	0.94	0.11	37,37,37,37	0
85	MG	5	3534	1/1	0.94	0.23	29,29,29,29	0
86	OHX	1	4092	7/7	0.94	0.12	118,118,118,118	0
85	MG	5	3793	1/1	0.94	0.17	32,32,32,32	0
85	MG	2	1947	1/1	0.94	0.41	45,45,45,45	0
85	MG	5	3658	1/1	0.94	0.18	19,19,19,19	0
85	MG	1	3736	1/1	0.94	0.30	44,44,44,44	0
85	MG	1	3444	1/1	0.94	0.17	28,28,28,28	0
85	MG	1	3640	1/1	0.94	0.14	26,26,26,26	0
85	MG	5	3541	1/1	0.94	0.28	21,21,21,21	0
86	OHX	6	2174	7/7	0.94	0.34	85,85,85,85	0
86	OHX	1	4108	7/7	0.94	0.33	84,84,84,84	0
85	MG	q0	202	1/1	0.94	0.07	28,28,28,28	0
85	MG	1	3739	1/1	0.94	0.32	49,49,49,49	0
86	OHX	2	2041	7/7	0.94	0.15	80,80,80,80	0
86	OHX	2	2058	7/7	0.94	0.12	114,114,114,114	0
85	MG	5	3543	1/1	0.94	0.17	21,21,21,21	0
85	MG	5	3666	1/1	0.94	0.15	21,21,21,21	0
86	OHX	2	2078	7/7	0.94	0.14	95,95,95,95	0
85	MG	5	3414	1/1	0.94	0.28	22,22,22,22	0
85	MG	5	3668	1/1	0.94	0.10	29,29,29,29	0
85	MG	5	3545	1/1	0.94	0.26	33,33,33,33	0
85	MG	1	3816	1/1	0.94	0.13	44,44,44,44	0
85	MG	5	3675	1/1	0.94	0.13	34,34,34,34	0
85	MG	1	3741	1/1	0.94	0.10	26,26,26,26	0
86	OHX	1	4128	7/7	0.94	0.32	89,89,89,89	0
86	OHX	7	225	7/7	0.94	0.14	107,107,107,107	0
85	MG	2	1916	1/1	0.94	0.30	43,43,43,43	0
86	OHX	2	2101	7/7	0.94	0.14	117,117,117,117	0
85	MG	1	3743	1/1	0.94	0.24	42,42,42,42	0
86	OHX	8	225	7/7	0.94	0.12	119,119,119,119	0
85	MG	5	3679	1/1	0.94	0.20	33,33,33,33	0
86	OHX	2	2106	7/7	0.94	0.15	106,106,106,106	0
85	MG	1	3827	1/1	0.94	0.21	17,17,17,17	0
85	MG	1	3478	1/1	0.94	0.20	64,64,64,64	0
85	MG	5	3422	1/1	0.94	0.27	25,25,25,25	0
86	OHX	2	2117	7/7	0.94	0.15	113,113,113,113	0
85	MG	5	3554	1/1	0.94	0.32	34,34,34,34	0
85	MG	1	3525	1/1	0.94	0.21	17,17,17,17	0
85	MG	1	3433	1/1	0.94	0.12	37,37,37,37	0
85	MG	1	3527	1/1	0.94	0.29	19,19,19,19	0
85	MG	5	3558	1/1	0.94	0.25	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	m0	302	7/7	0.94	0.12	102,102,102,102	0
85	MG	1	3480	1/1	0.94	0.30	31,31,31,31	0
85	MG	5	3428	1/1	0.94	0.35	38,38,38,38	0
85	MG	1	3612	1/1	0.94	0.23	25,25,25,25	0
86	OHX	1	4150	7/7	0.94	0.18	98,98,98,98	0
86	OHX	2	2126	7/7	0.94	0.16	96,96,96,96	0
85	MG	6	2007	1/1	0.94	0.11	51,51,51,51	0
85	MG	5	3566	1/1	0.94	0.26	17,17,17,17	0
88	3J2	5	4254	26/26	0.94	0.10	19,19,19,19	0
85	MG	1	3575	1/1	0.95	0.21	17,17,17,17	0
85	MG	5	3597	1/1	0.95	0.29	23,23,23,23	0
85	MG	5	3487	1/1	0.95	0.27	16,16,16,16	0
85	MG	6	1984	1/1	0.95	0.08	37,37,37,37	0
86	OHX	1	4139	7/7	0.95	0.28	83,83,83,83	0
85	MG	5	3489	1/1	0.95	0.27	28,28,28,28	0
86	OHX	c8	203	7/7	0.95	0.11	119,119,119,119	0
85	MG	1	3784	1/1	0.95	0.14	27,27,27,27	0
85	MG	5	3492	1/1	0.95	0.08	30,30,30,30	0
86	OHX	sR	401	7/7	0.95	0.10	142,142,142,142	0
86	OHX	5	3967	7/7	0.95	0.12	85,85,85,85	0
85	MG	5	3719	1/1	0.95	0.08	41,41,41,41	0
85	MG	1	3676	1/1	0.95	0.18	35,35,35,35	0
86	OHX	5	3994	7/7	0.95	0.13	102,102,102,102	0
85	MG	1	3740	1/1	0.95	0.13	33,33,33,33	0
86	OHX	1	4147	7/7	0.95	0.14	107,107,107,107	0
85	MG	1	3414	1/1	0.95	0.16	21,21,21,21	0
85	MG	5	3496	1/1	0.95	0.29	23,23,23,23	0
86	OHX	5	4023	7/7	0.95	0.15	89,89,89,89	0
86	OHX	5	4024	7/7	0.95	0.23	80,80,80,80	0
85	MG	1	3578	1/1	0.95	0.33	25,25,25,25	0
85	MG	5	3608	1/1	0.95	0.19	22,22,22,22	0
86	OHX	5	4035	7/7	0.95	0.12	96,96,96,96	0
85	MG	1	3600	1/1	0.95	0.23	21,21,21,21	0
85	MG	1	3464	1/1	0.95	0.20	29,29,29,29	0
86	OHX	5	4040	7/7	0.95	0.12	100,100,100,100	0
86	OHX	5	4041	7/7	0.95	0.18	85,85,85,85	0
86	OHX	5	4043	7/7	0.95	0.14	97,97,97,97	0
86	OHX	5	4048	7/7	0.95	0.11	109,109,109,109	0
86	OHX	2	2142	7/7	0.95	0.11	146,146,146,146	0
86	OHX	5	4056	7/7	0.95	0.13	111,111,111,111	0
85	MG	5	3501	1/1	0.95	0.14	30,30,30,30	0
85	MG	1	3793	1/1	0.95	0.20	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3883	1/1	0.95	0.28	39,39,39,39	0
85	MG	1	3747	1/1	0.95	0.11	35,35,35,35	0
86	OHX	5	4067	7/7	0.95	0.12	114,114,114,114	0
85	MG	L7	303	1/1	0.95	0.22	32,32,32,32	0
85	MG	1	3797	1/1	0.95	0.14	76,76,76,76	0
85	MG	1	3430	1/1	0.95	0.22	30,30,30,30	0
86	OHX	5	4075	7/7	0.95	0.12	141,141,141,141	0
86	OHX	5	4077	7/7	0.95	0.15	97,97,97,97	0
86	OHX	5	4080	7/7	0.95	0.33	82,82,82,82	0
85	MG	5	3507	1/1	0.95	0.26	19,19,19,19	0
85	MG	1	3603	1/1	0.95	0.14	29,29,29,29	0
86	OHX	5	4089	7/7	0.95	0.26	80,80,80,80	0
86	OHX	5	4093	7/7	0.95	0.13	107,107,107,107	0
85	MG	6	1998	1/1	0.95	0.07	45,45,45,45	0
85	MG	5	3621	1/1	0.95	0.15	45,45,45,45	0
85	MG	1	3752	1/1	0.95	0.07	29,29,29,29	0
85	MG	5	3412	1/1	0.95	0.18	21,21,21,21	0
85	MG	5	3624	1/1	0.95	0.16	20,20,20,20	0
85	MG	1	3753	1/1	0.95	0.17	15,15,15,15	0
86	OHX	5	4101	7/7	0.95	0.23	74,74,74,74	0
85	MG	1	4210	1/1	0.95	0.17	20,20,20,20	0
85	MG	5	3752	1/1	0.95	0.16	31,31,31,31	0
85	MG	M5	301	1/1	0.95	0.17	26,26,26,26	0
86	OHX	5	4105	7/7	0.95	0.20	85,85,85,85	0
85	MG	M5	302	1/1	0.95	0.25	39,39,39,39	0
85	MG	5	3520	1/1	0.95	0.18	29,29,29,29	0
86	OHX	5	4108	7/7	0.95	0.20	85,85,85,85	0
85	MG	5	3631	1/1	0.95	0.11	34,34,34,34	0
85	MG	1	3415	1/1	0.95	0.11	32,32,32,32	0
86	OHX	5	4114	7/7	0.95	0.29	90,90,90,90	0
85	MG	5	3523	1/1	0.95	0.29	27,27,27,27	0
85	MG	1	4214	1/1	0.95	0.11	42,42,42,42	0
85	MG	5	3419	1/1	0.95	0.18	24,24,24,24	0
86	OHX	5	4120	7/7	0.95	0.11	112,112,112,112	0
85	MG	1	3468	1/1	0.95	0.29	48,48,48,48	0
85	MG	5	3528	1/1	0.95	0.13	16,16,16,16	0
85	MG	5	3529	1/1	0.95	0.21	20,20,20,20	0
85	MG	M7	203	1/1	0.95	0.11	27,27,27,27	0
85	MG	7	212	1/1	0.95	0.10	27,27,27,27	0
85	MG	7	213	1/1	0.95	0.19	50,50,50,50	0
85	MG	1	3658	1/1	0.95	0.11	22,22,22,22	0
85	MG	M9	201	1/1	0.95	0.25	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	5	4134	7/7	0.95	0.27	92,92,92,92	0
85	MG	6	2013	1/1	0.95	0.13	48,48,48,48	0
85	MG	2	2005	1/1	0.95	0.09	58,58,58,58	0
85	MG	1	3714	1/1	0.95	0.14	28,28,28,28	0
85	MG	5	3538	1/1	0.95	0.21	15,15,15,15	0
85	MG	6	1948	1/1	0.95	0.32	33,33,33,33	0
85	MG	6	2019	1/1	0.95	0.06	39,39,39,39	0
85	MG	N3	202	1/1	0.95	0.19	54,54,54,54	0
85	MG	1	3759	1/1	0.95	0.08	36,36,36,36	0
85	MG	1	3562	1/1	0.95	0.27	19,19,19,19	0
86	OHX	5	4145	7/7	0.95	0.32	89,89,89,89	0
86	OHX	1	3919	7/7	0.95	0.13	92,92,92,92	0
85	MG	6	2023	1/1	0.95	0.24	80,80,80,80	0
86	OHX	1	3934	7/7	0.95	0.15	78,78,78,78	0
86	OHX	1	3945	7/7	0.95	0.14	85,85,85,85	0
86	OHX	1	3949	7/7	0.95	0.13	98,98,98,98	0
85	MG	1	3817	1/1	0.95	0.14	31,31,31,31	0
85	MG	5	3547	1/1	0.95	0.24	39,39,39,39	0
86	OHX	3	221	7/7	0.95	0.14	98,98,98,98	0
86	OHX	1	3962	7/7	0.95	0.16	73,73,73,73	0
85	MG	6	1953	1/1	0.95	0.46	54,54,54,54	0
86	OHX	1	3989	7/7	0.95	0.24	80,80,80,80	0
85	MG	8	212	1/1	0.95	0.17	27,27,27,27	0
86	OHX	4	228	7/7	0.95	0.25	87,87,87,87	0
85	MG	1	3716	1/1	0.95	0.23	57,57,57,57	0
86	OHX	1	4007	7/7	0.95	0.14	100,100,100,100	0
86	OHX	1	4008	7/7	0.95	0.12	97,97,97,97	0
86	OHX	1	4009	7/7	0.95	0.12	112,112,112,112	0
85	MG	5	3440	1/1	0.95	0.28	25,25,25,25	0
85	MG	2	1967	1/1	0.95	0.32	49,49,49,49	0
85	MG	12	301	1/1	0.95	0.29	32,32,32,32	0
85	MG	5	3663	1/1	0.95	0.20	46,46,46,46	0
85	MG	5	3442	1/1	0.95	0.15	24,24,24,24	0
86	OHX	5	4172	7/7	0.95	0.33	77,77,77,77	0
86	OHX	1	4022	7/7	0.95	0.13	96,96,96,96	0
85	MG	6	2029	1/1	0.95	0.18	68,68,68,68	0
86	OHX	1	4025	7/7	0.95	0.14	105,105,105,105	0
85	MG	N9	101	1/1	0.95	0.16	19,19,19,19	0
85	MG	1	3820	1/1	0.95	0.20	47,47,47,47	0
86	OHX	5	4180	7/7	0.95	0.10	131,131,131,131	0
86	OHX	6	2066	7/7	0.95	0.14	76,76,76,76	0
85	MG	1	3689	1/1	0.95	0.11	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	6	2087	7/7	0.95	0.10	116,116,116,116	0
86	OHX	5	4184	7/7	0.95	0.29	94,94,94,94	0
85	MG	5	3797	1/1	0.95	0.12	25,25,25,25	0
85	MG	1	3822	1/1	0.95	0.06	31,31,31,31	0
86	OHX	6	2103	7/7	0.95	0.12	155,155,155,155	0
86	OHX	1	4044	7/7	0.95	0.23	91,91,91,91	0
86	OHX	6	2108	7/7	0.95	0.16	93,93,93,93	0
86	OHX	1	4046	7/7	0.95	0.12	104,104,104,104	0
86	OHX	6	2114	7/7	0.95	0.13	96,96,96,96	0
86	OHX	6	2115	7/7	0.95	0.31	85,85,85,85	0
86	OHX	6	2116	7/7	0.95	0.14	100,100,100,100	0
86	OHX	6	2117	7/7	0.95	0.13	94,94,94,94	0
86	OHX	1	4048	7/7	0.95	0.14	105,105,105,105	0
86	OHX	1	4050	7/7	0.95	0.11	121,121,121,121	0
86	OHX	5	4201	7/7	0.95	0.31	93,93,93,93	0
86	OHX	1	4052	7/7	0.95	0.29	90,90,90,90	0
85	MG	5	3671	1/1	0.95	0.24	42,42,42,42	0
85	MG	m5	303	1/1	0.95	0.14	46,46,46,46	0
85	MG	6	2034	1/1	0.95	0.23	53,53,53,53	0
85	MG	1	3825	1/1	0.95	0.20	35,35,35,35	0
86	OHX	6	2131	7/7	0.95	0.13	118,118,118,118	0
86	OHX	6	2132	7/7	0.95	0.12	117,117,117,117	0
86	OHX	5	4209	7/7	0.95	0.31	83,83,83,83	0
86	OHX	1	4059	7/7	0.95	0.28	94,94,94,94	0
85	MG	m7	203	1/1	0.95	0.09	35,35,35,35	0
86	OHX	1	4064	7/7	0.95	0.19	93,93,93,93	0
85	MG	5	3803	1/1	0.95	0.07	34,34,34,34	0
85	MG	n3	201	1/1	0.95	0.26	18,18,18,18	0
85	MG	1	3459	1/1	0.95	0.22	18,18,18,18	0
85	MG	n8	201	1/1	0.95	0.10	36,36,36,36	0
86	OHX	1	4069	7/7	0.95	0.13	93,93,93,93	0
85	MG	1	3723	1/1	0.95	0.06	33,33,33,33	0
86	OHX	1	4071	7/7	0.95	0.19	90,90,90,90	0
85	MG	4	203	1/1	0.95	0.36	38,38,38,38	0
85	MG	5	3461	1/1	0.95	0.15	29,29,29,29	0
85	MG	5	3567	1/1	0.95	0.22	19,19,19,19	0
86	OHX	6	2150	7/7	0.95	0.29	87,87,87,87	0
85	MG	1	3767	1/1	0.95	0.18	17,17,17,17	0
86	OHX	1	4076	7/7	0.95	0.29	88,88,88,88	0
85	MG	o3	201	1/1	0.95	0.18	21,21,21,21	0
85	MG	1	3589	1/1	0.95	0.26	27,27,27,27	0
85	MG	1	3460	1/1	0.95	0.26	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4080	7/7	0.95	0.14	96,96,96,96	0
85	MG	1	3726	1/1	0.95	0.19	24,24,24,24	0
85	MG	5	3467	1/1	0.95	0.10	21,21,21,21	0
86	OHX	2	2032	7/7	0.95	0.24	94,94,94,94	0
85	MG	1	3568	1/1	0.95	0.25	18,18,18,18	0
86	OHX	2	2056	7/7	0.95	0.18	91,91,91,91	0
85	MG	5	3575	1/1	0.95	0.22	30,30,30,30	0
85	MG	5	3576	1/1	0.95	0.19	26,26,26,26	0
85	MG	5	3691	1/1	0.95	0.21	39,39,39,39	0
86	OHX	2	2077	7/7	0.95	0.16	97,97,97,97	0
85	MG	1	3729	1/1	0.95	0.17	17,17,17,17	0
86	OHX	1	4095	7/7	0.95	0.24	90,90,90,90	0
85	MG	5	3826	1/1	0.95	0.06	30,30,30,30	0
85	MG	5	3470	1/1	0.95	0.23	27,27,27,27	0
86	OHX	2	2086	7/7	0.95	0.12	117,117,117,117	0
86	OHX	1	4099	7/7	0.95	0.15	93,93,93,93	0
86	OHX	1	4100	7/7	0.95	0.25	94,94,94,94	0
86	OHX	1	4101	7/7	0.95	0.10	123,123,123,123	0
85	MG	5	3830	1/1	0.95	0.18	63,63,63,63	0
85	MG	5	3579	1/1	0.95	0.28	29,29,29,29	0
86	OHX	1	4106	7/7	0.95	0.28	79,79,79,79	0
85	MG	1	3731	1/1	0.95	0.11	47,47,47,47	0
86	OHX	7	220	7/7	0.95	0.15	70,70,70,70	0
85	MG	5	3472	1/1	0.95	0.07	25,25,25,25	0
86	OHX	2	2098	7/7	0.95	0.10	122,122,122,122	0
86	OHX	1	4110	7/7	0.95	0.29	90,90,90,90	0
85	MG	1	3616	1/1	0.95	0.28	36,36,36,36	0
86	OHX	8	224	7/7	0.95	0.13	98,98,98,98	0
86	OHX	1	4112	7/7	0.95	0.14	97,97,97,97	0
86	OHX	8	226	7/7	0.95	0.15	96,96,96,96	0
86	OHX	1	4113	7/7	0.95	0.16	99,99,99,99	0
85	MG	1	3551	1/1	0.95	0.30	23,23,23,23	0
86	OHX	2	2102	7/7	0.95	0.13	112,112,112,112	0
85	MG	1	3778	1/1	0.95	0.08	30,30,30,30	0
85	MG	5	3843	1/1	0.95	0.21	35,35,35,35	0
85	MG	5	3844	1/1	0.95	0.22	40,40,40,40	0
86	OHX	1	4120	7/7	0.95	0.12	117,117,117,117	0
85	MG	1	3642	1/1	0.95	0.20	30,30,30,30	0
85	MG	5	3478	1/1	0.95	0.23	54,54,54,54	0
86	OHX	2	2114	7/7	0.95	0.11	136,136,136,136	0
85	MG	2	1934	1/1	0.95	0.33	37,37,37,37	0
86	OHX	19	202	7/7	0.95	0.18	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	3673	1/1	0.95	0.11	51,51,51,51	0
85	MG	5	3850	1/1	0.95	0.14	35,35,35,35	0
85	MG	5	3852	1/1	0.95	0.23	53,53,53,53	0
85	MG	5	3592	1/1	0.95	0.27	21,21,21,21	0
85	MG	6	1917	1/1	0.95	0.30	46,46,46,46	0
86	OHX	n6	202	7/7	0.95	0.13	105,105,105,105	0
86	OHX	1	4131	7/7	0.95	0.29	86,86,86,86	0
85	MG	5	3482	1/1	0.95	0.30	39,39,39,39	0
87	ZN	e1	501	1/1	0.95	0.07	143,143,143,143	0
85	MG	5	3710	1/1	0.95	0.17	77,77,77,77	0
85	MG	2	1906	1/1	0.95	0.26	39,39,39,39	0
85	MG	1	3508	1/1	0.96	0.31	16,16,16,16	0
86	OHX	1	4006	7/7	0.96	0.13	101,101,101,101	0
86	OHX	5	4045	7/7	0.96	0.12	97,97,97,97	0
86	OHX	5	4046	7/7	0.96	0.20	88,88,88,88	0
85	MG	1	3860	1/1	0.96	0.32	51,51,51,51	0
85	MG	1	3762	1/1	0.96	0.18	34,34,34,34	0
86	OHX	5	4055	7/7	0.96	0.11	105,105,105,105	0
86	OHX	2	2038	7/7	0.96	0.13	110,110,110,110	0
86	OHX	5	4058	7/7	0.96	0.10	119,119,119,119	0
86	OHX	5	4059	7/7	0.96	0.23	79,79,79,79	0
85	MG	1	3593	1/1	0.96	0.26	16,16,16,16	0
86	OHX	1	4014	7/7	0.96	0.17	90,90,90,90	0
86	OHX	2	2054	7/7	0.96	0.10	105,105,105,105	0
86	OHX	2	2055	7/7	0.96	0.11	106,106,106,106	0
86	OHX	1	4018	7/7	0.96	0.21	86,86,86,86	0
85	MG	M0	301	1/1	0.96	0.17	32,32,32,32	0
85	MG	5	3460	1/1	0.96	0.09	19,19,19,19	0
86	OHX	2	2062	7/7	0.96	0.11	106,106,106,106	0
86	OHX	2	2064	7/7	0.96	0.09	110,110,110,110	0
86	OHX	2	2067	7/7	0.96	0.11	109,109,109,109	0
86	OHX	5	4078	7/7	0.96	0.16	91,91,91,91	0
85	MG	1	3814	1/1	0.96	0.05	25,25,25,25	0
86	OHX	5	4081	7/7	0.96	0.20	88,88,88,88	0
86	OHX	1	4030	7/7	0.96	0.09	118,118,118,118	0
86	OHX	5	4084	7/7	0.96	0.23	91,91,91,91	0
86	OHX	2	2070	7/7	0.96	0.18	89,89,89,89	0
86	OHX	5	4087	7/7	0.96	0.30	76,76,76,76	0
86	OHX	1	4205	7/7	0.96	0.32	88,88,88,88	0
86	OHX	5	4090	7/7	0.96	0.23	83,83,83,83	0
86	OHX	2	2075	7/7	0.96	0.27	89,89,89,89	0
86	OHX	1	4034	7/7	0.96	0.21	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4036	7/7	0.96	0.13	102,102,102,102	0
86	OHX	5	4096	7/7	0.96	0.24	92,92,92,92	0
85	MG	1	3566	1/1	0.96	0.35	26,26,26,26	0
86	OHX	1	4040	7/7	0.96	0.29	82,82,82,82	0
85	MG	5	3735	1/1	0.96	0.08	27,27,27,27	0
86	OHX	1	4042	7/7	0.96	0.12	94,94,94,94	0
86	OHX	1	4043	7/7	0.96	0.12	109,109,109,109	0
85	MG	1	4213	1/1	0.96	0.13	31,31,31,31	0
86	OHX	4	230	7/7	0.96	0.19	89,89,89,89	0
86	OHX	2	2079	7/7	0.96	0.11	99,99,99,99	0
86	OHX	2	2080	7/7	0.96	0.28	93,93,93,93	0
85	MG	1	3659	1/1	0.96	0.12	30,30,30,30	0
85	MG	M3	203	1/1	0.96	0.07	22,22,22,22	0
86	OHX	1	4054	7/7	0.96	0.09	148,148,148,148	0
86	OHX	2	2083	7/7	0.96	0.10	120,120,120,120	0
85	MG	5	3863	1/1	0.96	0.28	45,45,45,45	0
86	OHX	5	4113	7/7	0.96	0.23	87,87,87,87	0
86	OHX	2	2087	7/7	0.96	0.18	90,90,90,90	0
86	OHX	2	2088	7/7	0.96	0.14	100,100,100,100	0
85	MG	5	3739	1/1	0.96	0.21	27,27,27,27	0
86	OHX	1	4061	7/7	0.96	0.09	123,123,123,123	0
86	OHX	5	4119	7/7	0.96	0.22	94,94,94,94	0
85	MG	1	3545	1/1	0.96	0.28	39,39,39,39	0
86	OHX	2	2093	7/7	0.96	0.25	91,91,91,91	0
86	OHX	O3	202	7/7	0.96	0.26	81,81,81,81	0
86	OHX	O7	104	7/7	0.96	0.16	77,77,77,77	0
85	MG	1	3569	1/1	0.96	0.20	15,15,15,15	0
86	OHX	2	2095	7/7	0.96	0.09	133,133,133,133	0
86	OHX	6	2068	7/7	0.96	0.15	107,107,107,107	0
86	OHX	5	4130	7/7	0.96	0.15	84,84,84,84	0
86	OHX	2	2096	7/7	0.96	0.10	121,121,121,121	0
86	OHX	5	4132	7/7	0.96	0.25	86,86,86,86	0
85	MG	5	3867	1/1	0.96	0.23	15,15,15,15	0
86	OHX	6	2088	7/7	0.96	0.13	82,82,82,82	0
86	OHX	6	2093	7/7	0.96	0.18	93,93,93,93	0
85	MG	5	3743	1/1	0.96	0.06	22,22,22,22	0
86	OHX	6	2099	7/7	0.96	0.09	125,125,125,125	0
86	OHX	6	2100	7/7	0.96	0.11	103,103,103,103	0
86	OHX	6	2101	7/7	0.96	0.09	141,141,141,141	0
85	MG	1	3693	1/1	0.96	0.12	31,31,31,31	0
85	MG	1	3730	1/1	0.96	0.13	31,31,31,31	0
86	OHX	6	2104	7/7	0.96	0.11	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	6	2106	7/7	0.96	0.11	101,101,101,101	0
85	MG	1	3431	1/1	0.96	0.24	29,29,29,29	0
85	MG	1	3421	1/1	0.96	0.19	24,24,24,24	0
85	MG	1	3824	1/1	0.96	0.20	17,17,17,17	0
86	OHX	6	2113	7/7	0.96	0.12	102,102,102,102	0
85	MG	1	3572	1/1	0.96	0.29	21,21,21,21	0
86	OHX	5	4150	7/7	0.96	0.33	85,85,85,85	0
85	MG	1	3573	1/1	0.96	0.30	27,27,27,27	0
86	OHX	2	2109	7/7	0.96	0.10	123,123,123,123	0
85	MG	sM	301	1/1	0.96	0.09	31,31,31,31	0
86	OHX	6	2118	7/7	0.96	0.12	101,101,101,101	0
86	OHX	2	2113	7/7	0.96	0.13	107,107,107,107	0
85	MG	5	3564	1/1	0.96	0.12	16,16,16,16	0
86	OHX	5	4158	7/7	0.96	0.25	79,79,79,79	0
86	OHX	6	2122	7/7	0.96	0.12	95,95,95,95	0
86	OHX	6	2123	7/7	0.96	0.29	84,84,84,84	0
85	MG	1	3775	1/1	0.96	0.07	36,36,36,36	0
85	MG	1	3548	1/1	0.96	0.28	30,30,30,30	0
86	OHX	6	2126	7/7	0.96	0.21	83,83,83,83	0
85	MG	5	3657	1/1	0.96	0.21	34,34,34,34	0
86	OHX	6	2128	7/7	0.96	0.13	115,115,115,115	0
85	MG	1	3445	1/1	0.96	0.05	32,32,32,32	0
86	OHX	1	4086	7/7	0.96	0.10	120,120,120,120	0
85	MG	6	2003	1/1	0.96	0.13	46,46,46,46	0
85	MG	1	3496	1/1	0.96	0.16	19,19,19,19	0
85	MG	5	3483	1/1	0.96	0.31	18,18,18,18	0
85	MG	1	3670	1/1	0.96	0.41	45,45,45,45	0
86	OHX	5	4174	7/7	0.96	0.24	91,91,91,91	0
85	MG	5	3767	1/1	0.96	0.09	28,28,28,28	0
85	MG	1	3605	1/1	0.96	0.24	43,43,43,43	0
86	OHX	1	4094	7/7	0.96	0.24	85,85,85,85	0
85	MG	1	3834	1/1	0.96	0.24	24,24,24,24	0
86	OHX	6	2140	7/7	0.96	0.14	97,97,97,97	0
85	MG	N8	202	1/1	0.96	0.10	40,40,40,40	0
85	MG	5	3410	1/1	0.96	0.23	33,33,33,33	0
85	MG	5	3490	1/1	0.96	0.06	39,39,39,39	0
85	MG	2	1985	1/1	0.96	0.19	49,49,49,49	0
86	OHX	6	2145	7/7	0.96	0.13	105,105,105,105	0
85	MG	6	2010	1/1	0.96	0.07	39,39,39,39	0
85	MG	N8	205	1/1	0.96	0.14	24,24,24,24	0
86	OHX	6	2148	7/7	0.96	0.13	109,109,109,109	0
85	MG	1	3579	1/1	0.96	0.31	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4104	7/7	0.96	0.22	94,94,94,94	0
85	MG	1	3837	1/1	0.96	0.22	20,20,20,20	0
85	MG	6	2014	1/1	0.96	0.21	55,55,55,55	0
85	MG	5	3584	1/1	0.96	0.33	23,23,23,23	0
86	OHX	5	4193	7/7	0.96	0.28	88,88,88,88	0
85	MG	5	3586	1/1	0.96	0.18	16,16,16,16	0
85	MG	1	3608	1/1	0.96	0.17	32,32,32,32	0
85	MG	5	3498	1/1	0.96	0.16	21,21,21,21	0
85	MG	7	206	1/1	0.96	0.14	33,33,33,33	0
86	OHX	5	4199	7/7	0.96	0.24	86,86,86,86	0
85	MG	5	3785	1/1	0.96	0.11	24,24,24,24	0
85	MG	6	2016	1/1	0.96	0.19	37,37,37,37	0
86	OHX	6	2162	7/7	0.96	0.19	89,89,89,89	0
85	MG	1	3423	1/1	0.96	0.19	28,28,28,28	0
85	MG	5	3788	1/1	0.96	0.12	35,35,35,35	0
85	MG	1	3533	1/1	0.96	0.12	19,19,19,19	0
85	MG	5	3684	1/1	0.96	0.12	36,36,36,36	0
85	MG	6	1956	1/1	0.96	0.34	40,40,40,40	0
85	MG	1	3746	1/1	0.96	0.17	36,36,36,36	0
85	MG	4	211	1/1	0.96	0.09	33,33,33,33	0
85	MG	5	3688	1/1	0.96	0.10	31,31,31,31	0
85	MG	2	2001	1/1	0.96	0.20	67,67,67,67	0
86	OHX	1	4124	7/7	0.96	0.20	95,95,95,95	0
85	MG	2	1925	1/1	0.96	0.42	56,56,56,56	0
85	MG	1	3749	1/1	0.96	0.23	43,43,43,43	0
85	MG	6	1962	1/1	0.96	0.14	42,42,42,42	0
85	MG	5	3694	1/1	0.96	0.09	34,34,34,34	0
85	MG	5	3429	1/1	0.96	0.19	18,18,18,18	0
85	MG	6	2026	1/1	0.96	0.26	40,40,40,40	0
85	MG	5	3697	1/1	0.96	0.11	43,43,43,43	0
86	OHX	6	2180	7/7	0.96	0.26	91,91,91,91	0
85	MG	1	3437	1/1	0.96	0.18	36,36,36,36	0
85	MG	2	2015	1/1	0.96	0.35	48,48,48,48	0
85	MG	5	3515	1/1	0.96	0.20	20,20,20,20	0
85	MG	4	217	1/1	0.96	0.26	51,51,51,51	0
85	MG	6	1908	1/1	0.96	0.21	38,38,38,38	0
85	MG	1	3409	1/1	0.96	0.18	22,22,22,22	0
85	MG	1	3795	1/1	0.96	0.13	40,40,40,40	0
85	MG	4	220	1/1	0.96	0.09	26,26,26,26	0
85	MG	5	3522	1/1	0.96	0.36	32,32,32,32	0
85	MG	5	3439	1/1	0.96	0.18	21,21,21,21	0
85	MG	5	3817	1/1	0.96	0.06	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3402	1/1	0.96	0.34	35,35,35,35	0
85	MG	1	3651	1/1	0.96	0.08	30,30,30,30	0
85	MG	5	3526	1/1	0.96	0.27	24,24,24,24	0
86	OHX	1	4146	7/7	0.96	0.22	85,85,85,85	0
85	MG	1	3541	1/1	0.96	0.17	17,17,17,17	0
85	MG	m0	301	1/1	0.96	0.10	21,21,21,21	0
85	MG	5	3615	1/1	0.96	0.18	18,18,18,18	0
85	MG	5	3443	1/1	0.96	0.22	16,16,16,16	0
85	MG	5	3827	1/1	0.96	0.12	28,28,28,28	0
85	MG	5	3828	1/1	0.96	0.17	18,18,18,18	0
85	MG	5	3444	1/1	0.96	0.07	21,21,21,21	0
85	MG	m7	201	1/1	0.96	0.23	20,20,20,20	0
85	MG	5	3531	1/1	0.96	0.27	37,37,37,37	0
85	MG	1	3718	1/1	0.96	0.27	38,38,38,38	0
85	MG	5	3447	1/1	0.96	0.08	26,26,26,26	0
86	OHX	SR	401	7/7	0.96	0.09	146,146,146,146	0
86	OHX	1	3909	7/7	0.96	0.16	66,66,66,66	0
85	MG	2	1942	1/1	0.96	0.19	54,54,54,54	0
85	MG	1	3492	1/1	0.96	0.17	37,37,37,37	0
86	OHX	1	3927	7/7	0.96	0.14	78,78,78,78	0
85	MG	5	3720	1/1	0.96	0.07	30,30,30,30	0
86	OHX	1	3939	7/7	0.96	0.14	75,75,75,75	0
85	MG	5	3836	1/1	0.96	0.11	28,28,28,28	0
86	OHX	8	221	7/7	0.96	0.11	108,108,108,108	0
86	OHX	8	222	7/7	0.96	0.13	92,92,92,92	0
86	OHX	1	3948	7/7	0.96	0.11	103,103,103,103	0
85	MG	5	3839	1/1	0.96	0.09	48,48,48,48	0
86	OHX	5	3928	7/7	0.96	0.14	54,54,54,54	0
86	OHX	5	3942	7/7	0.96	0.14	70,70,70,70	0
85	MG	5	3450	1/1	0.96	0.14	22,22,22,22	0
85	MG	1	3721	1/1	0.96	0.11	44,44,44,44	0
86	OHX	1	3961	7/7	0.96	0.10	101,101,101,101	0
86	OHX	5	3976	7/7	0.96	0.14	79,79,79,79	0
85	MG	5	3452	1/1	0.96	0.09	23,23,23,23	0
85	MG	5	3539	1/1	0.96	0.27	19,19,19,19	0
86	OHX	1	3978	7/7	0.96	0.16	81,81,81,81	0
86	OHX	5	4000	7/7	0.96	0.14	91,91,91,91	0
86	OHX	1	4177	7/7	0.96	0.27	73,73,73,73	0
86	OHX	5	4011	7/7	0.96	0.10	135,135,135,135	0
86	OHX	1	3986	7/7	0.96	0.13	95,95,95,95	0
85	MG	5	3846	1/1	0.96	0.14	21,21,21,21	0
86	OHX	1	3990	7/7	0.96	0.11	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	3992	7/7	0.96	0.11	101,101,101,101	0
86	OHX	m5	305	7/7	0.96	0.12	97,97,97,97	0
86	OHX	5	4028	7/7	0.96	0.18	90,90,90,90	0
86	OHX	5	4029	7/7	0.96	0.10	113,113,113,113	0
86	OHX	1	3993	7/7	0.96	0.22	72,72,72,72	0
86	OHX	5	4034	7/7	0.96	0.11	100,100,100,100	0
86	OHX	1	3994	7/7	0.96	0.10	141,141,141,141	0
86	OHX	1	3996	7/7	0.96	0.25	81,81,81,81	0
86	OHX	1	3998	7/7	0.96	0.20	71,71,71,71	0
85	MG	1	3809	1/1	0.96	0.18	41,41,41,41	0
85	MG	5	3749	1/1	0.97	0.13	35,35,35,35	0
85	MG	5	3810	1/1	0.97	0.10	20,20,20,20	0
86	OHX	5	4091	7/7	0.97	0.21	84,84,84,84	0
86	OHX	5	4092	7/7	0.97	0.21	89,89,89,89	0
85	MG	6	1945	1/1	0.97	0.32	29,29,29,29	0
85	MG	1	3810	1/1	0.97	0.24	42,42,42,42	0
86	OHX	1	3999	7/7	0.97	0.11	92,92,92,92	0
85	MG	m5	302	1/1	0.97	0.07	31,31,31,31	0
85	MG	5	3882	1/1	0.97	0.13	16,16,16,16	0
85	MG	1	3610	1/1	0.97	0.09	33,33,33,33	0
85	MG	5	3651	1/1	0.97	0.16	21,21,21,21	0
85	MG	M7	202	1/1	0.97	0.21	23,23,23,23	0
85	MG	1	4216	1/1	0.97	0.17	16,16,16,16	0
85	MG	1	3641	1/1	0.97	0.14	31,31,31,31	0
85	MG	m7	205	1/1	0.97	0.04	27,27,27,27	0
85	MG	n0	201	1/1	0.97	0.06	32,32,32,32	0
85	MG	1	3661	1/1	0.97	0.05	37,37,37,37	0
86	OHX	6	2133	7/7	0.97	0.13	94,94,94,94	0
85	MG	5	3889	1/1	0.97	0.22	15,15,15,15	0
85	MG	1	3841	1/1	0.97	0.23	24,24,24,24	0
85	MG	1	3466	1/1	0.97	0.17	37,37,37,37	0
85	MG	1	3786	1/1	0.97	0.25	15,15,15,15	0
86	OHX	1	4023	7/7	0.97	0.10	96,96,96,96	0
85	MG	5	3825	1/1	0.97	0.09	26,26,26,26	0
85	MG	n8	205	1/1	0.97	0.08	24,24,24,24	0
86	OHX	5	4116	7/7	0.97	0.22	78,78,78,78	0
86	OHX	1	4151	7/7	0.97	0.20	77,77,77,77	0
86	OHX	1	4026	7/7	0.97	0.21	76,76,76,76	0
85	MG	5	3764	1/1	0.97	0.08	27,27,27,27	0
86	OHX	1	4029	7/7	0.97	0.24	80,80,80,80	0
85	MG	1	3844	1/1	0.97	0.16	30,30,30,30	0
85	MG	6	1921	1/1	0.97	0.31	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3530	1/1	0.97	0.28	15,15,15,15	0
86	OHX	1	4033	7/7	0.97	0.22	88,88,88,88	0
86	OHX	5	4125	7/7	0.97	0.10	111,111,111,111	0
86	OHX	5	4126	7/7	0.97	0.19	89,89,89,89	0
86	OHX	5	4127	7/7	0.97	0.24	92,92,92,92	0
85	MG	1	3553	1/1	0.97	0.25	33,33,33,33	0
86	OHX	1	4035	7/7	0.97	0.18	83,83,83,83	0
85	MG	5	3574	1/1	0.97	0.25	18,18,18,18	0
86	OHX	6	2152	7/7	0.97	0.20	84,84,84,84	0
85	MG	1	3644	1/1	0.97	0.10	23,23,23,23	0
86	OHX	1	4038	7/7	0.97	0.23	70,70,70,70	0
86	OHX	1	4039	7/7	0.97	0.14	85,85,85,85	0
85	MG	5	4256	1/1	0.97	0.11	23,23,23,23	0
85	MG	1	3576	1/1	0.97	0.14	17,17,17,17	0
86	OHX	1	4168	7/7	0.97	0.24	79,79,79,79	0
86	OHX	2	2147	7/7	0.97	0.10	97,97,97,97	0
85	MG	L3	401	1/1	0.97	0.25	22,22,22,22	0
86	OHX	2	2044	7/7	0.97	0.12	94,94,94,94	0
86	OHX	1	4045	7/7	0.97	0.19	87,87,87,87	0
86	OHX	2	2050	7/7	0.97	0.09	95,95,95,95	0
86	OHX	5	4143	7/7	0.97	0.18	90,90,90,90	0
86	OHX	1	4047	7/7	0.97	0.10	111,111,111,111	0
86	OHX	2	2051	7/7	0.97	0.12	91,91,91,91	0
86	OHX	1	4049	7/7	0.97	0.20	76,76,76,76	0
85	MG	7	202	1/1	0.97	0.26	15,15,15,15	0
86	OHX	1	4051	7/7	0.97	0.23	72,72,72,72	0
85	MG	5	3774	1/1	0.97	0.15	19,19,19,19	0
86	OHX	1	4053	7/7	0.97	0.27	89,89,89,89	0
85	MG	N8	203	1/1	0.97	0.12	23,23,23,23	0
86	OHX	2	2057	7/7	0.97	0.09	104,104,104,104	0
85	MG	5	3838	1/1	0.97	0.15	23,23,23,23	0
86	OHX	5	4154	7/7	0.97	0.26	89,89,89,89	0
85	MG	6	1999	1/1	0.97	0.25	51,51,51,51	0
86	OHX	2	2063	7/7	0.97	0.11	96,96,96,96	0
85	MG	1	3503	1/1	0.97	0.20	17,17,17,17	0
86	OHX	2	2065	7/7	0.97	0.20	85,85,85,85	0
85	MG	5	3670	1/1	0.97	0.10	22,22,22,22	0
86	OHX	1	4063	7/7	0.97	0.19	89,89,89,89	0
86	OHX	2	2068	7/7	0.97	0.10	112,112,112,112	0
86	OHX	5	4162	7/7	0.97	0.23	87,87,87,87	0
85	MG	1	3629	1/1	0.97	0.16	27,27,27,27	0
85	MG	5	3672	1/1	0.97	0.24	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	2	2072	7/7	0.97	0.11	102,102,102,102	0
86	OHX	2	2074	7/7	0.97	0.09	116,116,116,116	0
85	MG	L4	402	1/1	0.97	0.06	18,18,18,18	0
85	MG	5	3674	1/1	0.97	0.27	29,29,29,29	0
85	MG	5	3724	1/1	0.97	0.09	30,30,30,30	0
85	MG	1	3792	1/1	0.97	0.12	16,16,16,16	0
85	MG	5	3457	1/1	0.97	0.25	25,25,25,25	0
85	MG	5	3585	1/1	0.97	0.32	15,15,15,15	0
85	MG	5	3628	1/1	0.97	0.09	29,29,29,29	0
85	MG	1	3412	1/1	0.97	0.23	28,28,28,28	0
85	MG	1	3406	1/1	0.97	0.14	26,26,26,26	0
86	OHX	2	2085	7/7	0.97	0.19	93,93,93,93	0
85	MG	1	3438	1/1	0.97	0.28	20,20,20,20	0
85	MG	1	3826	1/1	0.97	0.18	15,15,15,15	0
85	MG	5	3462	1/1	0.97	0.25	23,23,23,23	0
85	MG	1	3796	1/1	0.97	0.10	33,33,33,33	0
86	OHX	3	217	7/7	0.97	0.12	81,81,81,81	0
86	OHX	3	219	7/7	0.97	0.10	95,95,95,95	0
86	OHX	3	220	7/7	0.97	0.10	98,98,98,98	0
86	OHX	2	2090	7/7	0.97	0.15	86,86,86,86	0
86	OHX	2	2091	7/7	0.97	0.13	93,93,93,93	0
86	OHX	C1	201	7/7	0.97	0.12	106,106,106,106	0
86	OHX	6	2206	7/7	0.97	0.07	184,184,184,184	0
86	OHX	1	4087	7/7	0.97	0.22	85,85,85,85	0
85	MG	1	3618	1/1	0.97	0.14	54,54,54,54	0
86	OHX	4	226	7/7	0.97	0.10	86,86,86,86	0
85	MG	5	3862	1/1	0.97	0.13	30,30,30,30	0
86	OHX	4	229	7/7	0.97	0.21	79,79,79,79	0
86	OHX	C8	201	7/7	0.97	0.10	95,95,95,95	0
86	OHX	4	231	7/7	0.97	0.25	75,75,75,75	0
85	MG	1	3798	1/1	0.97	0.08	40,40,40,40	0
86	OHX	4	233	7/7	0.97	0.12	105,105,105,105	0
85	MG	1	3529	1/1	0.97	0.36	27,27,27,27	0
86	OHX	5	4200	7/7	0.97	0.24	89,89,89,89	0
86	OHX	1	3895	7/7	0.97	0.15	60,60,60,60	0
86	OHX	5	3902	7/7	0.97	0.10	47,47,47,47	0
85	MG	1	3654	1/1	0.97	0.18	22,22,22,22	0
86	OHX	1	3915	7/7	0.97	0.13	64,64,64,64	0
86	OHX	5	3953	7/7	0.97	0.14	95,95,95,95	0
86	OHX	5	3956	7/7	0.97	0.08	73,73,73,73	0
86	OHX	5	3957	7/7	0.97	0.12	70,70,70,70	0
86	OHX	5	3961	7/7	0.97	0.10	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	3964	7/7	0.97	0.10	71,71,71,71	0
86	OHX	1	3916	7/7	0.97	0.10	77,77,77,77	0
86	OHX	5	3970	7/7	0.97	0.12	78,78,78,78	0
86	OHX	L3	403	7/7	0.97	0.19	90,90,90,90	0
86	OHX	L3	404	7/7	0.97	0.15	83,83,83,83	0
85	MG	5	3798	1/1	0.97	0.12	32,32,32,32	0
86	OHX	5	3978	7/7	0.97	0.11	75,75,75,75	0
86	OHX	5	3981	7/7	0.97	0.14	80,80,80,80	0
86	OHX	5	4217	7/7	0.97	0.26	74,74,74,74	0
86	OHX	5	3989	7/7	0.97	0.09	93,93,93,93	0
86	OHX	5	3992	7/7	0.97	0.14	78,78,78,78	0
85	MG	6	1975	1/1	0.97	0.21	41,41,41,41	0
86	OHX	1	3923	7/7	0.97	0.10	66,66,66,66	0
86	OHX	M5	304	7/7	0.97	0.17	85,85,85,85	0
86	OHX	2	2099	7/7	0.97	0.22	90,90,90,90	0
86	OHX	5	4002	7/7	0.97	0.11	82,82,82,82	0
85	MG	1	3411	1/1	0.97	0.11	20,20,20,20	0
86	OHX	1	3936	7/7	0.97	0.12	67,67,67,67	0
86	OHX	5	4012	7/7	0.97	0.18	69,69,69,69	0
85	MG	5	3741	1/1	0.97	0.20	17,17,17,17	0
86	OHX	5	4016	7/7	0.97	0.10	101,101,101,101	0
86	OHX	5	4021	7/7	0.97	0.22	80,80,80,80	0
86	OHX	O2	201	7/7	0.97	0.24	70,70,70,70	0
85	MG	1	3427	1/1	0.97	0.14	41,41,41,41	0
86	OHX	1	3946	7/7	0.97	0.11	60,60,60,60	0
86	OHX	5	4234	7/7	0.97	0.20	76,76,76,76	0
86	OHX	5	4026	7/7	0.97	0.14	62,62,62,62	0
86	OHX	5	4027	7/7	0.97	0.19	68,68,68,68	0
86	OHX	1	3947	7/7	0.97	0.14	89,89,89,89	0
85	MG	12	302	1/1	0.97	0.32	28,28,28,28	0
86	OHX	5	4030	7/7	0.97	0.15	75,75,75,75	0
86	OHX	5	4031	7/7	0.97	0.21	79,79,79,79	0
85	MG	5	3692	1/1	0.97	0.09	34,34,34,34	0
86	OHX	6	2071	7/7	0.97	0.10	83,83,83,83	0
86	OHX	6	2073	7/7	0.97	0.10	93,93,93,93	0
86	OHX	6	2076	7/7	0.97	0.09	123,123,123,123	0
86	OHX	5	4037	7/7	0.97	0.30	64,64,64,64	0
86	OHX	5	4038	7/7	0.97	0.13	96,96,96,96	0
86	OHX	2	2105	7/7	0.97	0.23	89,89,89,89	0
86	OHX	6	2085	7/7	0.97	0.10	96,96,96,96	0
86	OHX	6	2086	7/7	0.97	0.10	96,96,96,96	0
85	MG	1	3532	1/1	0.97	0.29	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4044	7/7	0.97	0.19	72,72,72,72	0
86	OHX	2	2107	7/7	0.97	0.17	86,86,86,86	0
86	OHX	7	218	7/7	0.97	0.11	70,70,70,70	0
86	OHX	6	2090	7/7	0.97	0.10	99,99,99,99	0
85	MG	13	402	1/1	0.97	0.30	17,17,17,17	0
86	OHX	7	226	7/7	0.97	0.23	84,84,84,84	0
86	OHX	5	4049	7/7	0.97	0.22	79,79,79,79	0
86	OHX	5	4050	7/7	0.97	0.18	74,74,74,74	0
86	OHX	5	4051	7/7	0.97	0.21	74,74,74,74	0
86	OHX	8	219	7/7	0.97	0.15	81,81,81,81	0
86	OHX	6	2094	7/7	0.97	0.09	96,96,96,96	0
86	OHX	5	4054	7/7	0.97	0.25	83,83,83,83	0
86	OHX	8	223	7/7	0.97	0.22	87,87,87,87	0
86	OHX	6	2095	7/7	0.97	0.17	84,84,84,84	0
86	OHX	6	2096	7/7	0.97	0.09	110,110,110,110	0
86	OHX	5	4057	7/7	0.97	0.22	92,92,92,92	0
85	MG	14	401	1/1	0.97	0.06	22,22,22,22	0
86	OHX	6	2098	7/7	0.97	0.10	105,105,105,105	0
86	OHX	1	3967	7/7	0.97	0.10	98,98,98,98	0
86	OHX	1	3972	7/7	0.97	0.11	92,92,92,92	0
86	OHX	1	3975	7/7	0.97	0.17	66,66,66,66	0
86	OHX	1	4118	7/7	0.97	0.27	73,73,73,73	0
86	OHX	5	4066	7/7	0.97	0.20	79,79,79,79	0
86	OHX	1	3977	7/7	0.97	0.16	79,79,79,79	0
86	OHX	2	2111	7/7	0.97	0.17	91,91,91,91	0
86	OHX	6	2105	7/7	0.97	0.17	92,92,92,92	0
86	OHX	5	4073	7/7	0.97	0.20	86,86,86,86	0
86	OHX	1	3981	7/7	0.97	0.18	83,83,83,83	0
86	OHX	1	3984	7/7	0.97	0.11	93,93,93,93	0
86	OHX	1	3985	7/7	0.97	0.14	89,89,89,89	0
85	MG	1	3597	1/1	0.97	0.38	12,12,12,12	0
86	OHX	5	4079	7/7	0.97	0.23	79,79,79,79	0
86	OHX	6	2110	7/7	0.97	0.17	87,87,87,87	0
86	OHX	6	2111	7/7	0.97	0.10	98,98,98,98	0
85	MG	5	3874	1/1	0.97	0.35	31,31,31,31	0
86	OHX	5	4083	7/7	0.97	0.16	89,89,89,89	0
87	ZN	E1	501	1/1	0.97	0.05	104,104,104,104	0
87	ZN	Q2	501	1/1	0.97	0.12	56,56,56,56	0
85	MG	5	3645	1/1	0.97	0.21	26,26,26,26	0
86	OHX	1	3991	7/7	0.97	0.11	94,94,94,94	0
86	OHX	5	4086	7/7	0.97	0.23	82,82,82,82	0
85	MG	1	3717	1/1	0.97	0.04	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	2	2047	7/7	0.98	0.09	87,87,87,87	0
86	OHX	5	3933	7/7	0.98	0.08	53,53,53,53	0
86	OHX	5	3934	7/7	0.98	0.12	75,75,75,75	0
86	OHX	1	3966	7/7	0.98	0.19	67,67,67,67	0
86	OHX	5	3945	7/7	0.98	0.10	63,63,63,63	0
86	OHX	5	3946	7/7	0.98	0.10	68,68,68,68	0
86	OHX	5	3948	7/7	0.98	0.08	54,54,54,54	0
86	OHX	5	3949	7/7	0.98	0.08	65,65,65,65	0
86	OHX	5	3950	7/7	0.98	0.12	77,77,77,77	0
86	OHX	5	3951	7/7	0.98	0.10	80,80,80,80	0
85	MG	1	3539	1/1	0.98	0.27	15,15,15,15	0
86	OHX	5	3954	7/7	0.98	0.09	82,82,82,82	0
86	OHX	1	3968	7/7	0.98	0.09	84,84,84,84	0
86	OHX	1	3969	7/7	0.98	0.17	81,81,81,81	0
86	OHX	5	3959	7/7	0.98	0.10	63,63,63,63	0
86	OHX	1	3970	7/7	0.98	0.18	73,73,73,73	0
86	OHX	1	3971	7/7	0.98	0.17	78,78,78,78	0
85	MG	1	3805	1/1	0.98	0.13	27,27,27,27	0
86	OHX	5	3968	7/7	0.98	0.15	70,70,70,70	0
86	OHX	1	3973	7/7	0.98	0.10	81,81,81,81	0
86	OHX	1	3974	7/7	0.98	0.17	77,77,77,77	0
86	OHX	2	2052	7/7	0.98	0.12	79,79,79,79	0
86	OHX	1	3976	7/7	0.98	0.25	62,62,62,62	0
85	MG	5	3837	1/1	0.98	0.09	46,46,46,46	0
86	OHX	5	3980	7/7	0.98	0.10	70,70,70,70	0
86	OHX	6	2112	7/7	0.98	0.17	85,85,85,85	0
86	OHX	5	3982	7/7	0.98	0.12	59,59,59,59	0
86	OHX	5	3984	7/7	0.98	0.19	71,71,71,71	0
86	OHX	5	3988	7/7	0.98	0.11	71,71,71,71	0
85	MG	3	210	1/1	0.98	0.20	49,49,49,49	0
85	MG	5	3648	1/1	0.98	0.16	33,33,33,33	0
86	OHX	5	3993	7/7	0.98	0.22	65,65,65,65	0
86	OHX	1	3982	7/7	0.98	0.17	68,68,68,68	0
86	OHX	1	3983	7/7	0.98	0.21	76,76,76,76	0
86	OHX	5	3996	7/7	0.98	0.15	72,72,72,72	0
86	OHX	5	3997	7/7	0.98	0.07	97,97,97,97	0
86	OHX	2	2110	7/7	0.98	0.08	107,107,107,107	0
85	MG	5	3876	1/1	0.98	0.29	32,32,32,32	0
86	OHX	5	4001	7/7	0.98	0.23	51,51,51,51	0
85	MG	5	3840	1/1	0.98	0.07	51,51,51,51	0
86	OHX	5	4003	7/7	0.98	0.16	72,72,72,72	0
86	OHX	6	2120	7/7	0.98	0.17	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4005	7/7	0.98	0.07	105,105,105,105	0
86	OHX	5	4173	7/7	0.98	0.24	64,64,64,64	0
86	OHX	5	4008	7/7	0.98	0.09	81,81,81,81	0
86	OHX	5	4009	7/7	0.98	0.21	78,78,78,78	0
86	OHX	5	4010	7/7	0.98	0.15	78,78,78,78	0
86	OHX	1	4084	7/7	0.98	0.26	62,62,62,62	0
86	OHX	1	3987	7/7	0.98	0.12	72,72,72,72	0
86	OHX	5	4013	7/7	0.98	0.19	75,75,75,75	0
86	OHX	5	4014	7/7	0.98	0.13	79,79,79,79	0
86	OHX	2	2059	7/7	0.98	0.11	89,89,89,89	0
86	OHX	2	2060	7/7	0.98	0.09	96,96,96,96	0
86	OHX	5	4017	7/7	0.98	0.18	76,76,76,76	0
86	OHX	5	4018	7/7	0.98	0.16	87,87,87,87	0
86	OHX	5	4019	7/7	0.98	0.23	71,71,71,71	0
86	OHX	5	4020	7/7	0.98	0.12	84,84,84,84	0
86	OHX	2	2115	7/7	0.98	0.12	95,95,95,95	0
86	OHX	5	4022	7/7	0.98	0.09	97,97,97,97	0
85	MG	5	3841	1/1	0.98	0.08	23,23,23,23	0
85	MG	5	3807	1/1	0.98	0.15	24,24,24,24	0
85	MG	1	4212	1/1	0.98	0.30	22,22,22,22	0
86	OHX	1	3995	7/7	0.98	0.07	123,123,123,123	0
85	MG	5	3751	1/1	0.98	0.27	34,34,34,34	0
85	MG	m6	201	1/1	0.98	0.06	21,21,21,21	0
85	MG	1	3806	1/1	0.98	0.11	24,24,24,24	0
86	OHX	1	4000	7/7	0.98	0.18	80,80,80,80	0
85	MG	5	3511	1/1	0.98	0.19	19,19,19,19	0
86	OHX	5	4032	7/7	0.98	0.10	84,84,84,84	0
86	OHX	1	4002	7/7	0.98	0.17	88,88,88,88	0
86	OHX	1	4003	7/7	0.98	0.14	74,74,74,74	0
86	OHX	1	4004	7/7	0.98	0.16	79,79,79,79	0
85	MG	5	3512	1/1	0.98	0.25	45,45,45,45	0
86	OHX	1	4102	7/7	0.98	0.22	88,88,88,88	0
86	OHX	2	2071	7/7	0.98	0.09	102,102,102,102	0
85	MG	1	3807	1/1	0.98	0.08	36,36,36,36	0
85	MG	5	3435	1/1	0.98	0.17	17,17,17,17	0
85	MG	5	3815	1/1	0.98	0.05	29,29,29,29	0
86	OHX	5	4042	7/7	0.98	0.20	70,70,70,70	0
86	OHX	1	4010	7/7	0.98	0.15	87,87,87,87	0
86	OHX	1	4011	7/7	0.98	0.13	90,90,90,90	0
86	OHX	1	4012	7/7	0.98	0.16	85,85,85,85	0
85	MG	6	1983	1/1	0.98	0.11	37,37,37,37	0
86	OHX	5	4047	7/7	0.98	0.18	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	3	215	7/7	0.98	0.09	77,77,77,77	0
86	OHX	3	216	7/7	0.98	0.13	79,79,79,79	0
85	MG	5	3562	1/1	0.98	0.39	27,27,27,27	0
86	OHX	3	218	7/7	0.98	0.17	74,74,74,74	0
85	MG	5	3759	1/1	0.98	0.07	30,30,30,30	0
86	OHX	1	4016	7/7	0.98	0.16	84,84,84,84	0
86	OHX	2	2131	7/7	0.98	0.20	92,92,92,92	0
85	MG	5	3819	1/1	0.98	0.18	46,46,46,46	0
85	MG	1	4215	1/1	0.98	0.30	18,18,18,18	0
85	MG	1	3728	1/1	0.98	0.06	21,21,21,21	0
86	OHX	6	2158	7/7	0.98	0.17	91,91,91,91	0
86	OHX	1	4021	7/7	0.98	0.16	77,77,77,77	0
86	OHX	4	225	7/7	0.98	0.14	75,75,75,75	0
85	MG	1	3567	1/1	0.98	0.20	20,20,20,20	0
86	OHX	5	4063	7/7	0.98	0.22	87,87,87,87	0
86	OHX	5	4064	7/7	0.98	0.18	89,89,89,89	0
86	OHX	4	227	7/7	0.98	0.12	93,93,93,93	0
86	OHX	1	3889	7/7	0.98	0.13	63,63,63,63	0
85	MG	5	3763	1/1	0.98	0.17	25,25,25,25	0
86	OHX	1	3898	7/7	0.98	0.10	65,65,65,65	0
86	OHX	1	3899	7/7	0.98	0.10	63,63,63,63	0
86	OHX	5	4070	7/7	0.98	0.15	89,89,89,89	0
86	OHX	5	4071	7/7	0.98	0.18	86,86,86,86	0
86	OHX	5	4072	7/7	0.98	0.20	87,87,87,87	0
86	OHX	1	3903	7/7	0.98	0.10	65,65,65,65	0
86	OHX	1	4028	7/7	0.98	0.16	77,77,77,77	0
86	OHX	1	3907	7/7	0.98	0.10	70,70,70,70	0
86	OHX	2	2084	7/7	0.98	0.09	110,110,110,110	0
86	OHX	1	3910	7/7	0.98	0.09	72,72,72,72	0
86	OHX	5	4244	7/7	0.98	0.13	62,62,62,62	0
86	OHX	1	3913	7/7	0.98	0.07	63,63,63,63	0
85	MG	5	3477	1/1	0.98	0.20	16,16,16,16	0
85	MG	1	3799	1/1	0.98	0.06	42,42,42,42	0
85	MG	1	3645	1/1	0.98	0.19	24,24,24,24	0
86	OHX	1	3920	7/7	0.98	0.12	67,67,67,67	0
86	OHX	1	3921	7/7	0.98	0.07	69,69,69,69	0
85	MG	1	3823	1/1	0.98	0.07	44,44,44,44	0
85	MG	5	3425	1/1	0.98	0.17	27,27,27,27	0
86	OHX	1	3925	7/7	0.98	0.12	89,89,89,89	0
85	MG	1	3561	1/1	0.98	0.30	25,25,25,25	0
86	OHX	7	219	7/7	0.98	0.12	66,66,66,66	0
86	OHX	1	3928	7/7	0.98	0.09	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	7	224	7/7	0.98	0.13	81,81,81,81	0
86	OHX	1	3931	7/7	0.98	0.10	76,76,76,76	0
86	OHX	1	3932	7/7	0.98	0.11	79,79,79,79	0
86	OHX	2	2026	7/7	0.98	0.14	71,71,71,71	0
86	OHX	2	2029	7/7	0.98	0.10	77,77,77,77	0
86	OHX	1	3938	7/7	0.98	0.10	93,93,93,93	0
86	OHX	8	218	7/7	0.98	0.11	89,89,89,89	0
86	OHX	Q2	502	7/7	0.98	0.17	56,56,56,56	0
86	OHX	8	220	7/7	0.98	0.16	81,81,81,81	0
86	OHX	6	2053	7/7	0.98	0.12	64,64,64,64	0
86	OHX	6	2056	7/7	0.98	0.12	64,64,64,64	0
86	OHX	6	2057	7/7	0.98	0.12	70,70,70,70	0
86	OHX	6	2061	7/7	0.98	0.12	79,79,79,79	0
86	OHX	2	2030	7/7	0.98	0.10	79,79,79,79	0
86	OHX	6	2067	7/7	0.98	0.09	87,87,87,87	0
86	OHX	1	3943	7/7	0.98	0.08	82,82,82,82	0
86	OHX	6	2070	7/7	0.98	0.12	67,67,67,67	0
86	OHX	1	3944	7/7	0.98	0.09	68,68,68,68	0
86	OHX	2	2031	7/7	0.98	0.11	77,77,77,77	0
86	OHX	6	2075	7/7	0.98	0.10	103,103,103,103	0
86	OHX	l3	403	7/7	0.98	0.11	73,73,73,73	0
85	MG	5	3641	1/1	0.98	0.06	25,25,25,25	0
86	OHX	2	2034	7/7	0.98	0.14	88,88,88,88	0
86	OHX	6	2080	7/7	0.98	0.12	74,74,74,74	0
86	OHX	5	4112	7/7	0.98	0.23	74,74,74,74	0
86	OHX	6	2081	7/7	0.98	0.10	85,85,85,85	0
86	OHX	6	2082	7/7	0.98	0.11	80,80,80,80	0
86	OHX	2	2035	7/7	0.98	0.11	79,79,79,79	0
86	OHX	1	4152	7/7	0.98	0.18	84,84,84,84	0
86	OHX	2	2036	7/7	0.98	0.12	80,80,80,80	0
85	MG	1	3751	1/1	0.98	0.11	45,45,45,45	0
86	OHX	s1	302	7/7	0.98	0.12	71,71,71,71	0
86	OHX	m6	202	7/7	0.98	0.12	67,67,67,67	0
86	OHX	6	2089	7/7	0.98	0.14	88,88,88,88	0
86	OHX	2	2039	7/7	0.98	0.09	78,78,78,78	0
86	OHX	m9	201	7/7	0.98	0.17	78,78,78,78	0
86	OHX	6	2091	7/7	0.98	0.08	107,107,107,107	0
86	OHX	o3	202	7/7	0.98	0.17	79,79,79,79	0
86	OHX	6	2092	7/7	0.98	0.12	85,85,85,85	0
87	ZN	D9	101	1/1	0.98	0.04	60,60,60,60	0
86	OHX	1	3956	7/7	0.98	0.17	68,68,68,68	0
86	OHX	1	3959	7/7	0.98	0.12	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	1	4060	7/7	0.98	0.20	75,75,75,75	0
85	MG	1	3711	1/1	0.98	0.12	40,40,40,40	0
87	ZN	q2	501	1/1	0.98	0.09	51,51,51,51	0
85	MG	5	3485	1/1	0.98	0.17	30,30,30,30	0
86	OHX	1	3964	7/7	0.98	0.10	74,74,74,74	0
86	OHX	1	3908	7/7	0.99	0.08	54,54,54,54	0
85	MG	5	3860	1/1	0.99	0.08	49,49,49,49	0
86	OHX	5	3983	7/7	0.99	0.10	58,58,58,58	0
86	OHX	2	2024	7/7	0.99	0.15	57,57,57,57	0
86	OHX	5	3985	7/7	0.99	0.13	67,67,67,67	0
86	OHX	5	3986	7/7	0.99	0.09	60,60,60,60	0
86	OHX	5	3987	7/7	0.99	0.08	56,56,56,56	0
86	OHX	1	3911	7/7	0.99	0.07	61,61,61,61	0
86	OHX	M6	202	7/7	0.99	0.11	80,80,80,80	0
86	OHX	5	3990	7/7	0.99	0.08	60,60,60,60	0
86	OHX	5	3991	7/7	0.99	0.10	72,72,72,72	0
86	OHX	1	3912	7/7	0.99	0.07	60,60,60,60	0
86	OHX	2	2025	7/7	0.99	0.10	65,65,65,65	0
86	OHX	1	3914	7/7	0.99	0.07	73,73,73,73	0
86	OHX	1	3997	7/7	0.99	0.10	60,60,60,60	0
86	OHX	N9	102	7/7	0.99	0.09	44,44,44,44	0
86	OHX	2	2053	7/7	0.99	0.07	85,85,85,85	0
86	OHX	5	3998	7/7	0.99	0.07	82,82,82,82	0
85	MG	1	3520	1/1	0.99	0.06	22,22,22,22	0
86	OHX	1	3917	7/7	0.99	0.08	77,77,77,77	0
86	OHX	O7	105	7/7	0.99	0.11	68,68,68,68	0
86	OHX	1	3918	7/7	0.99	0.08	61,61,61,61	0
86	OHX	2	2027	7/7	0.99	0.09	66,66,66,66	0
86	OHX	6	2050	7/7	0.99	0.13	59,59,59,59	0
86	OHX	6	2052	7/7	0.99	0.11	60,60,60,60	0
86	OHX	5	4006	7/7	0.99	0.07	43,43,43,43	0
86	OHX	5	4007	7/7	0.99	0.14	67,67,67,67	0
86	OHX	2	2028	7/7	0.99	0.08	56,56,56,56	0
86	OHX	6	2054	7/7	0.99	0.09	53,53,53,53	0
86	OHX	6	2055	7/7	0.99	0.11	64,64,64,64	0
85	MG	5	3768	1/1	0.99	0.06	33,33,33,33	0
85	MG	5	3748	1/1	0.99	0.23	37,37,37,37	0
86	OHX	6	2058	7/7	0.99	0.08	54,54,54,54	0
86	OHX	6	2059	7/7	0.99	0.09	59,59,59,59	0
86	OHX	6	2060	7/7	0.99	0.08	72,72,72,72	0
85	MG	1	3584	1/1	0.99	0.24	30,30,30,30	0
86	OHX	6	2062	7/7	0.99	0.06	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	6	2063	7/7	0.99	0.08	65,65,65,65	0
86	OHX	6	2064	7/7	0.99	0.07	69,69,69,69	0
86	OHX	6	2065	7/7	0.99	0.07	68,68,68,68	0
86	OHX	1	3924	7/7	0.99	0.09	51,51,51,51	0
85	MG	5	3851	1/1	0.99	0.13	37,37,37,37	0
86	OHX	1	3926	7/7	0.99	0.08	61,61,61,61	0
86	OHX	6	2069	7/7	0.99	0.15	73,73,73,73	0
86	OHX	2	2061	7/7	0.99	0.13	80,80,80,80	0
86	OHX	2	2033	7/7	0.99	0.09	79,79,79,79	0
86	OHX	6	2072	7/7	0.99	0.11	68,68,68,68	0
86	OHX	1	3930	7/7	0.99	0.07	63,63,63,63	0
86	OHX	6	2074	7/7	0.99	0.15	69,69,69,69	0
85	MG	1	3768	1/1	0.99	0.10	48,48,48,48	0
85	MG	5	3561	1/1	0.99	0.34	21,21,21,21	0
86	OHX	6	2077	7/7	0.99	0.09	67,67,67,67	0
86	OHX	6	2078	7/7	0.99	0.09	81,81,81,81	0
86	OHX	1	3933	7/7	0.99	0.08	57,57,57,57	0
85	MG	1	3639	1/1	0.99	0.12	25,25,25,25	0
86	OHX	1	3935	7/7	0.99	0.07	71,71,71,71	0
86	OHX	5	4198	7/7	0.99	0.18	64,64,64,64	0
86	OHX	2	2066	7/7	0.99	0.15	85,85,85,85	0
86	OHX	6	2083	7/7	0.99	0.08	72,72,72,72	0
86	OHX	6	2084	7/7	0.99	0.07	81,81,81,81	0
86	OHX	1	3937	7/7	0.99	0.09	63,63,63,63	0
85	MG	5	3408	1/1	0.99	0.11	18,18,18,18	0
85	MG	1	3745	1/1	0.99	0.04	29,29,29,29	0
86	OHX	1	3940	7/7	0.99	0.07	74,74,74,74	0
86	OHX	1	3941	7/7	0.99	0.14	66,66,66,66	0
86	OHX	1	3942	7/7	0.99	0.13	60,60,60,60	0
86	OHX	2	2040	7/7	0.99	0.07	74,74,74,74	0
85	MG	5	3820	1/1	0.99	0.06	42,42,42,42	0
86	OHX	2	2042	7/7	0.99	0.07	78,78,78,78	0
85	MG	5	3446	1/1	0.99	0.14	23,23,23,23	0
86	OHX	1	3865	7/7	0.99	0.08	43,43,43,43	0
86	OHX	1	3867	7/7	0.99	0.14	44,44,44,44	0
86	OHX	1	3868	7/7	0.99	0.10	40,40,40,40	0
86	OHX	5	4053	7/7	0.99	0.10	75,75,75,75	0
86	OHX	1	3950	7/7	0.99	0.06	75,75,75,75	0
86	OHX	1	3869	7/7	0.99	0.11	43,43,43,43	0
86	OHX	1	3872	7/7	0.99	0.09	43,43,43,43	0
86	OHX	1	3953	7/7	0.99	0.08	60,60,60,60	0
86	OHX	1	3954	7/7	0.99	0.13	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	3955	7/7	0.99	0.10	75,75,75,75	0
86	OHX	1	3873	7/7	0.99	0.07	42,42,42,42	0
86	OHX	1	3957	7/7	0.99	0.17	52,52,52,52	0
86	OHX	1	3958	7/7	0.99	0.09	81,81,81,81	0
86	OHX	1	3878	7/7	0.99	0.11	49,49,49,49	0
86	OHX	1	3960	7/7	0.99	0.09	74,74,74,74	0
86	OHX	1	3879	7/7	0.99	0.05	44,44,44,44	0
86	OHX	1	3880	7/7	0.99	0.08	53,53,53,53	0
86	OHX	1	3963	7/7	0.99	0.06	46,46,46,46	0
86	OHX	1	3881	7/7	0.99	0.09	46,46,46,46	0
86	OHX	1	3883	7/7	0.99	0.09	53,53,53,53	0
86	OHX	5	3900	7/7	0.99	0.12	36,36,36,36	0
86	OHX	1	3884	7/7	0.99	0.08	51,51,51,51	0
86	OHX	5	3903	7/7	0.99	0.10	38,38,38,38	0
86	OHX	5	3904	7/7	0.99	0.11	39,39,39,39	0
86	OHX	5	3905	7/7	0.99	0.12	43,43,43,43	0
86	OHX	5	3907	7/7	0.99	0.10	45,45,45,45	0
86	OHX	5	4076	7/7	0.99	0.13	67,67,67,67	0
86	OHX	5	3908	7/7	0.99	0.13	47,47,47,47	0
86	OHX	5	3909	7/7	0.99	0.10	42,42,42,42	0
86	OHX	5	3911	7/7	0.99	0.12	50,50,50,50	0
86	OHX	5	3912	7/7	0.99	0.10	40,40,40,40	0
86	OHX	5	3914	7/7	0.99	0.10	46,46,46,46	0
86	OHX	5	3915	7/7	0.99	0.10	47,47,47,47	0
86	OHX	5	3916	7/7	0.99	0.09	45,45,45,45	0
86	OHX	5	3917	7/7	0.99	0.07	53,53,53,53	0
86	OHX	5	3918	7/7	0.99	0.06	45,45,45,45	0
86	OHX	5	3919	7/7	0.99	0.07	44,44,44,44	0
86	OHX	5	3922	7/7	0.99	0.07	46,46,46,46	0
86	OHX	5	4088	7/7	0.99	0.19	68,68,68,68	0
86	OHX	5	3924	7/7	0.99	0.08	53,53,53,53	0
86	OHX	5	3925	7/7	0.99	0.11	55,55,55,55	0
86	OHX	1	3886	7/7	0.99	0.10	62,62,62,62	0
86	OHX	5	3929	7/7	0.99	0.07	56,56,56,56	0
86	OHX	5	3930	7/7	0.99	0.09	68,68,68,68	0
86	OHX	5	3931	7/7	0.99	0.12	62,62,62,62	0
86	OHX	7	221	7/7	0.99	0.13	66,66,66,66	0
86	OHX	7	222	7/7	0.99	0.12	65,65,65,65	0
86	OHX	7	223	7/7	0.99	0.08	73,73,73,73	0
86	OHX	1	3888	7/7	0.99	0.07	47,47,47,47	0
86	OHX	2	2073	7/7	0.99	0.09	85,85,85,85	0
86	OHX	5	3936	7/7	0.99	0.07	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	3937	7/7	0.99	0.07	56,56,56,56	0
86	OHX	5	3939	7/7	0.99	0.06	52,52,52,52	0
86	OHX	5	3940	7/7	0.99	0.10	66,66,66,66	0
86	OHX	8	217	7/7	0.99	0.11	67,67,67,67	0
86	OHX	5	3941	7/7	0.99	0.09	72,72,72,72	0
86	OHX	1	3890	7/7	0.99	0.06	49,49,49,49	0
86	OHX	5	3943	7/7	0.99	0.08	62,62,62,62	0
86	OHX	5	3944	7/7	0.99	0.12	74,74,74,74	0
86	OHX	1	3892	7/7	0.99	0.09	54,54,54,54	0
86	OHX	1	3893	7/7	0.99	0.09	53,53,53,53	0
86	OHX	5	3947	7/7	0.99	0.08	54,54,54,54	0
86	OHX	1	3894	7/7	0.99	0.11	60,60,60,60	0
86	OHX	5	4109	7/7	0.99	0.19	67,67,67,67	0
86	OHX	4	223	7/7	0.99	0.10	41,41,41,41	0
86	OHX	4	224	7/7	0.99	0.12	72,72,72,72	0
86	OHX	2	2045	7/7	0.99	0.10	78,78,78,78	0
86	OHX	5	3952	7/7	0.99	0.08	62,62,62,62	0
86	OHX	1	3896	7/7	0.99	0.10	57,57,57,57	0
86	OHX	1	3897	7/7	0.99	0.07	55,55,55,55	0
86	OHX	5	3955	7/7	0.99	0.07	72,72,72,72	0
86	OHX	2	2046	7/7	0.99	0.10	78,78,78,78	0
85	MG	5	3517	1/1	0.99	0.32	18,18,18,18	0
86	OHX	5	3958	7/7	0.99	0.08	59,59,59,59	0
86	OHX	1	3979	7/7	0.99	0.14	56,56,56,56	0
86	OHX	5	3960	7/7	0.99	0.07	49,49,49,49	0
86	OHX	1	3980	7/7	0.99	0.08	86,86,86,86	0
86	OHX	5	3962	7/7	0.99	0.10	71,71,71,71	0
86	OHX	5	3963	7/7	0.99	0.06	71,71,71,71	0
86	OHX	1	3900	7/7	0.99	0.06	48,48,48,48	0
86	OHX	5	3965	7/7	0.99	0.12	56,56,56,56	0
86	OHX	5	3966	7/7	0.99	0.08	80,80,80,80	0
86	OHX	1	3901	7/7	0.99	0.05	57,57,57,57	0
86	OHX	1	3902	7/7	0.99	0.08	58,58,58,58	0
86	OHX	5	3969	7/7	0.99	0.08	64,64,64,64	0
86	OHX	n3	202	7/7	0.99	0.08	64,64,64,64	0
86	OHX	2	2048	7/7	0.99	0.04	102,102,102,102	0
86	OHX	n9	102	7/7	0.99	0.10	46,46,46,46	0
86	OHX	5	3971	7/7	0.99	0.08	76,76,76,76	0
86	OHX	o7	502	7/7	0.99	0.10	74,74,74,74	0
86	OHX	q1	101	7/7	0.99	0.15	74,74,74,74	0
86	OHX	q2	502	7/7	0.99	0.13	57,57,57,57	0
87	ZN	D6	500	1/1	0.99	0.02	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	3972	7/7	0.99	0.16	64,64,64,64	0
86	OHX	5	3973	7/7	0.99	0.09	56,56,56,56	0
86	OHX	1	3904	7/7	0.99	0.05	54,54,54,54	0
87	ZN	Q0	500	1/1	0.99	0.03	31,31,31,31	0
86	OHX	1	3905	7/7	0.99	0.07	66,66,66,66	0
87	ZN	Q3	501	1/1	0.99	0.02	43,43,43,43	0
87	ZN	d6	101	1/1	0.99	0.03	49,49,49,49	0
86	OHX	1	3906	7/7	0.99	0.08	62,62,62,62	0
87	ZN	d9	101	1/1	0.99	0.04	67,67,67,67	0
86	OHX	5	3977	7/7	0.99	0.07	79,79,79,79	0
86	OHX	1	3988	7/7	0.99	0.16	82,82,82,82	0
87	ZN	q3	501	1/1	0.99	0.02	48,48,48,48	0
86	OHX	5	3979	7/7	0.99	0.12	60,60,60,60	0
86	OHX	2	2049	7/7	0.99	0.08	90,90,90,90	0
86	OHX	5	3901	7/7	1.00	0.11	33,33,33,33	0
86	OHX	1	3864	7/7	1.00	0.12	39,39,39,39	0
86	OHX	1	3870	7/7	1.00	0.05	44,44,44,44	0
86	OHX	1	3882	7/7	1.00	0.05	42,42,42,42	0
86	OHX	5	3932	7/7	1.00	0.05	43,43,43,43	0
86	OHX	1	3871	7/7	1.00	0.11	46,46,46,46	0
86	OHX	5	3906	7/7	1.00	0.09	42,42,42,42	0
86	OHX	5	3935	7/7	1.00	0.04	52,52,52,52	0
86	OHX	8	216	7/7	1.00	0.09	43,43,43,43	0
86	OHX	1	3929	7/7	1.00	0.08	56,56,56,56	0
86	OHX	2	2043	7/7	1.00	0.05	75,75,75,75	0
86	OHX	5	3938	7/7	1.00	0.05	48,48,48,48	0
86	OHX	1	3885	7/7	1.00	0.06	50,50,50,50	0
86	OHX	5	3910	7/7	1.00	0.04	42,42,42,42	0
86	OHX	1	3866	7/7	1.00	0.09	39,39,39,39	0
86	OHX	1	3887	7/7	1.00	0.06	50,50,50,50	0
86	OHX	5	3913	7/7	1.00	0.06	42,42,42,42	0
86	OHX	6	2049	7/7	1.00	0.13	45,45,45,45	0
86	OHX	1	3874	7/7	1.00	0.08	47,47,47,47	0
86	OHX	6	2051	7/7	1.00	0.08	51,51,51,51	0
87	ZN	O7	101	1/1	1.00	0.01	22,22,22,22	0
86	OHX	1	3875	7/7	1.00	0.07	43,43,43,43	0
86	OHX	1	3876	7/7	1.00	0.04	41,41,41,41	0
86	OHX	1	3891	7/7	1.00	0.03	47,47,47,47	0
86	OHX	5	3920	7/7	1.00	0.06	52,52,52,52	0
86	OHX	5	3921	7/7	1.00	0.07	52,52,52,52	0
86	OHX	1	3877	7/7	1.00	0.08	48,48,48,48	0
86	OHX	5	3923	7/7	1.00	0.07	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	ZN	o7	501	1/1	1.00	0.03	31,31,31,31	0
87	ZN	q0	201	1/1	1.00	0.01	21,21,21,21	0
86	OHX	2	2037	7/7	1.00	0.06	72,72,72,72	0
86	OHX	1	3863	7/7	1.00	0.11	32,32,32,32	0
86	OHX	5	3926	7/7	1.00	0.05	47,47,47,47	0
86	OHX	5	3927	7/7	1.00	0.05	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.