



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 03:28 AM UTC

PDB ID : 4U4Y / pdb_00004u4y
Title : Crystal structure of Pactamycin bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 3.20 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

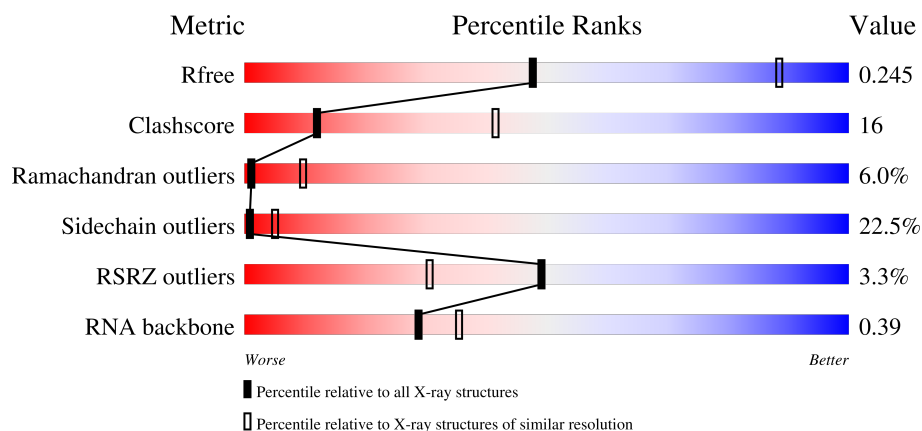
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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	3% 37% 43% 17% .
1	6	1800	3% 41% 45% 14%
2	S0	251	4% 30% 38% 13% . 18%
2	s0	251	2% 37% 33% 11% . 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	

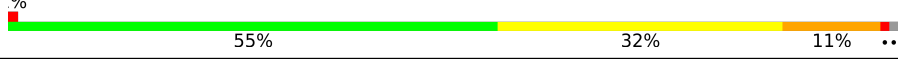
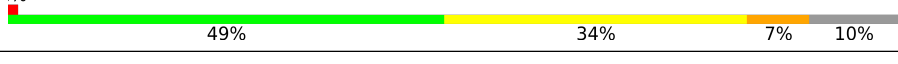
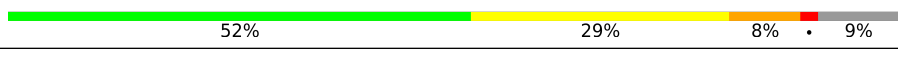
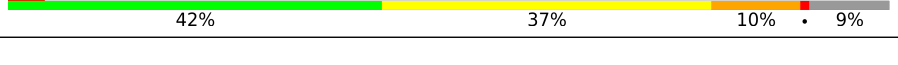
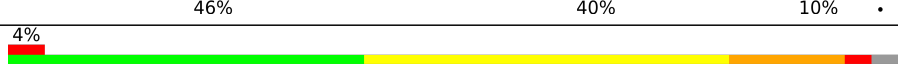
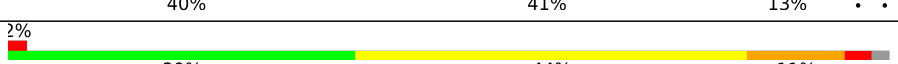
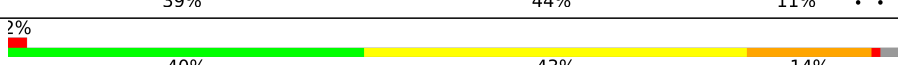
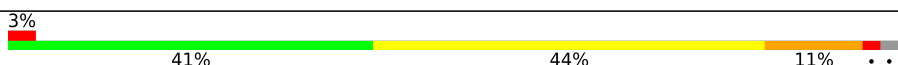
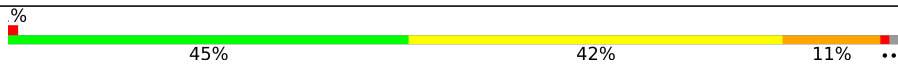
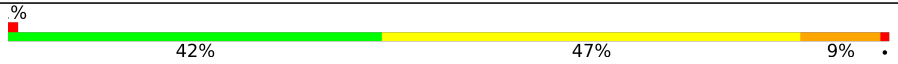
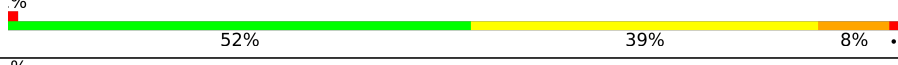
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Mol	Chain	Length	Quality of chain
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158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

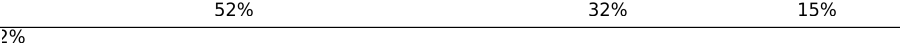
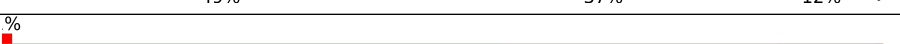
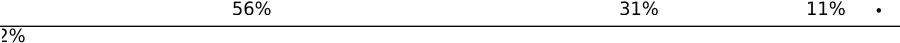
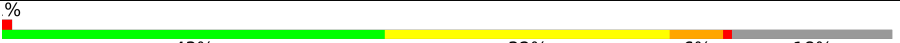
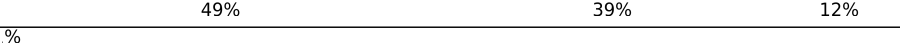
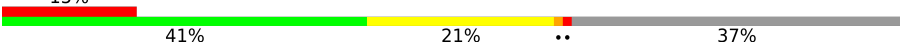
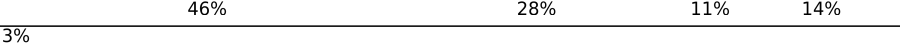
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Mol	Chain	Length	Quality of chain
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4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

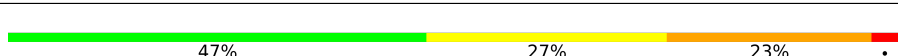
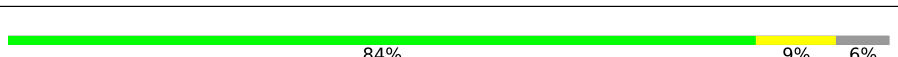
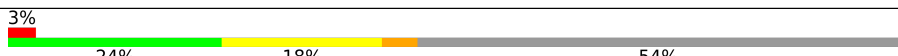
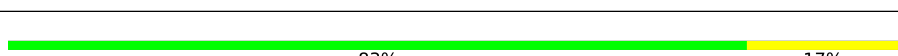
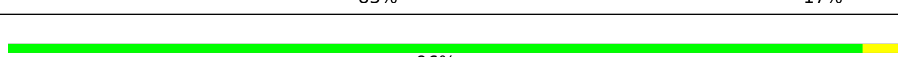
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Mol	Chain	Length	Quality of chain
66	O0	104	
66	o0	104	
67	O1	112	
67	o1	112	
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	120	
70	o4	120	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	

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Mol	Chain	Length	Quality of chain
78	q2	105	
79	Q3	91	
79	q3	91	
80	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	3635	-	-	-	X
85	MG	1	3665	-	-	-	X
85	MG	1	3815	-	-	-	X
85	MG	2	1910	-	-	-	X
85	MG	2	1914	-	-	-	X
85	MG	2	1915	-	-	-	X
85	MG	2	1937	-	-	-	X
85	MG	2	1949	-	-	-	X
85	MG	2	1958	-	-	-	X
85	MG	2	1967	-	-	-	X
85	MG	2	1974	-	-	-	X
85	MG	2	1986	-	-	-	X
85	MG	2	1994	-	-	-	X
85	MG	2	2003	-	-	-	X
85	MG	2	2010	-	-	-	X
85	MG	4	220	-	-	-	X
85	MG	5	3464	-	-	-	X
85	MG	5	3635	-	-	-	X
85	MG	5	3682	-	-	-	X
85	MG	5	3686	-	-	-	X
85	MG	5	3884	-	-	-	X
85	MG	6	1909	-	-	-	X
85	MG	6	1924	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	6	1966	-	-	-	X
85	MG	6	2028	-	-	-	X
85	MG	6	2039	-	-	-	X
85	MG	O3	201	-	-	-	X
86	OHX	1	3936	-	-	X	-
86	OHX	1	3955	-	-	X	-
86	OHX	1	3969	-	-	X	-
86	OHX	1	3973	-	-	X	-
86	OHX	1	4001	-	-	X	-
86	OHX	1	4026	-	-	X	-
86	OHX	1	4030	-	-	X	-
86	OHX	1	4043	-	-	X	-
86	OHX	1	4054	-	-	X	-
86	OHX	1	4083	-	-	X	-
86	OHX	1	4146	-	-	X	-
86	OHX	1	4154	-	-	X	-
86	OHX	1	4155	-	-	X	-
86	OHX	1	4162	-	-	X	-
86	OHX	1	4171	-	-	X	-
86	OHX	1	4197	-	-	X	-
86	OHX	2	2032	-	-	X	-
86	OHX	2	2045	-	-	X	-
86	OHX	2	2090	-	-	X	-
86	OHX	2	2096	-	-	X	-
86	OHX	2	2100	-	-	X	-
86	OHX	2	2110	-	-	X	-
86	OHX	2	2145	-	-	X	-
86	OHX	5	3943	-	-	X	-
86	OHX	5	3963	-	-	X	-
86	OHX	5	3974	-	-	X	-
86	OHX	5	3979	-	-	X	-
86	OHX	5	4002	-	-	X	-
86	OHX	5	4011	-	-	X	-
86	OHX	5	4021	-	-	X	-
86	OHX	5	4035	-	-	X	-
86	OHX	5	4055	-	-	X	-
86	OHX	5	4066	-	-	X	-
86	OHX	5	4090	-	-	X	-
86	OHX	5	4143	-	-	X	-
86	OHX	5	4199	-	-	X	-
86	OHX	5	4200	-	-	X	-
86	OHX	5	4201	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	5	4217	-	-	X	-
86	OHX	5	4233	-	-	X	-
86	OHX	5	4237	-	-	X	-
86	OHX	5	4242	-	-	X	-
86	OHX	6	2059	-	-	X	-
86	OHX	6	2120	-	-	X	-
86	OHX	6	2125	-	-	X	-
86	OHX	6	2146	-	-	X	-
86	OHX	6	2149	-	-	X	-
86	OHX	6	2170	-	-	X	-
86	OHX	7	217	-	-	X	-
86	OHX	7	225	-	-	X	-
86	OHX	8	219	-	-	X	-
86	OHX	8	227	-	-	X	-
86	OHX	8	228	-	-	X	-
86	OHX	O7	104	-	-	X	-
86	OHX	q1	102	-	-	X	-

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411223 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
			1214	775	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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			

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

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

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

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

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

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

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

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

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

- 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
			679	402	140	137				

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	M3	193	Total	C	N	O	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				

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	O0	97	Total	C	N	O	S	0	0	0
			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 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O4	121	LYS	-	expression tag	UNP P87262
o4	121	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			
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			

- Molecule 81 is a protein called unknown protein chain 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
			1076	686	192	195	3			

- Molecule 83 is a protein called unknown protein chain 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 chain 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	124	Total	Mg	0	0
			124	124		
85	S2	2	Total	Mg	0	0
			2	2		
85	S8	1	Total	Mg	0	0
			1	1		
85	D0	1	Total	Mg	0	0
			1	1		
85	D3	1	Total	Mg	0	0
			1	1		
85	SM	1	Total	Mg	0	0
			1	1		
85	1	471	Total	Mg	0	0
			471	471		
85	3	14	Total	Mg	0	0
			14	14		
85	4	21	Total	Mg	0	0
			21	21		
85	L2	1	Total	Mg	0	0
			1	1		
85	L3	2	Total	Mg	0	0
			2	2		
85	L4	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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	M5	2	Total 2	Mg 2	0	0
85	M6	2	Total 2	Mg 2	0	0
85	M7	4	Total 4	Mg 4	0	0
85	M9	3	Total 3	Mg 3	0	0
85	N0	1	Total 1	Mg 1	0	0
85	N3	2	Total 2	Mg 2	0	0
85	N5	1	Total 1	Mg 1	0	0
85	N6	1	Total 1	Mg 1	0	0
85	N8	4	Total 4	Mg 4	0	0
85	N9	1	Total 1	Mg 1	0	0
85	O2	1	Total 1	Mg 1	0	0
85	O3	1	Total 1	Mg 1	0	0
85	O7	2	Total 2	Mg 2	0	0
85	Q2	1	Total 1	Mg 1	0	0
85	6	147	Total 147	Mg 147	0	0

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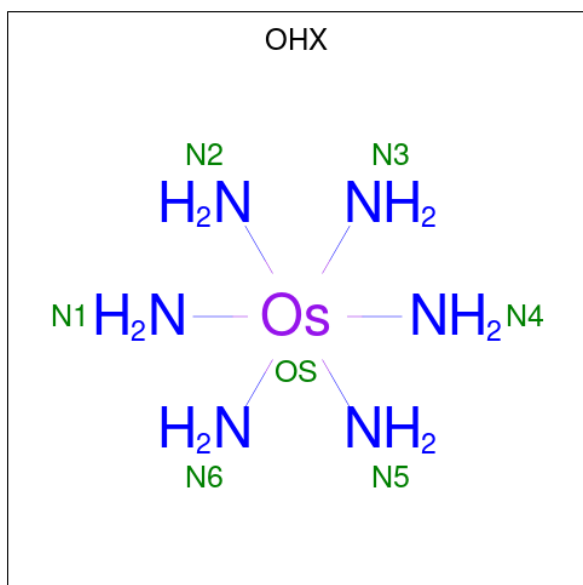
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	s1	1	Total 1	Mg 1	0	0
85	s2	1	Total 1	Mg 1	0	0
85	s8	2	Total 2	Mg 2	0	0
85	c1	1	Total 1	Mg 1	0	0
85	c7	1	Total 1	Mg 1	0	0
85	c8	2	Total 2	Mg 2	0	0
85	d3	2	Total 2	Mg 2	0	0
85	d6	1	Total 1	Mg 1	0	0
85	sM	2	Total 2	Mg 2	0	0
85	5	504	Total 504	Mg 504	0	0
85	7	14	Total 14	Mg 14	0	0
85	8	16	Total 16	Mg 16	0	0
85	l2	1	Total 1	Mg 1	0	0
85	l3	2	Total 2	Mg 2	0	0
85	l4	1	Total 1	Mg 1	0	0
85	l5	2	Total 2	Mg 2	0	0
85	l7	2	Total 2	Mg 2	0	0
85	l8	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	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	m7	5	Total 5	Mg 5	0	0
85	n0	2	Total 2	Mg 2	0	0
85	n3	2	Total 2	Mg 2	0	0
85	n6	1	Total 1	Mg 1	0	0
85	n8	4	Total 4	Mg 4	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	q0	1	Total 1	Mg 1	0	0
85	q1	1	Total 1	Mg 1	0	0
85	q3	2	Total 2	Mg 2	0	0

- 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		
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		
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		

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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
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86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
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
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86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
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	S6	1	Total	N	Os	0	0
			7	6	1		
86	S8	1	Total	N	Os	0	0
			7	6	1		
86	C3	1	Total	N	Os	0	0
			7	6	1		
86	C5	1	Total	N	Os	0	0
			7	6	1		
86	C8	1	Total	N	Os	0	0
			7	6	1		
86	D3	1	Total	N	Os	0	0
			7	6	1		
86	D9	1	Total	N	Os	0	0
			7	6	1		
86	SR	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
			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
			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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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			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
			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
			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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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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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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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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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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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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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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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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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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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	L3	1	Total	N	Os	0	0
			7	6	1		
86	L3	1	Total	N	Os	0	0
			7	6	1		
86	L3	1	Total	N	Os	0	0
			7	6	1		
86	L4	1	Total	N	Os	0	0
			7	6	1		
86	M0	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	M5	1	Total	N	Os	0	0
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86	M7	1	Total	N	Os	0	0
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86	M7	1	Total	N	Os	0	0
			7	6	1		
86	M9	1	Total	N	Os	0	0
			7	6	1		
86	N1	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	Q2	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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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	s9	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			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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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		
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		
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		
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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		
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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86	5	1	Total	N	Os	0	0
			7	6	1		
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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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		
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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		
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
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86	5	1	Total	N	Os	0	0
			7	6	1		
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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		

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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
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86	5	1	Total	N	Os	0	0
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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		
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86	7	1	Total	N	Os	0	0
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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	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
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86	7	1	Total	N	Os	0	0
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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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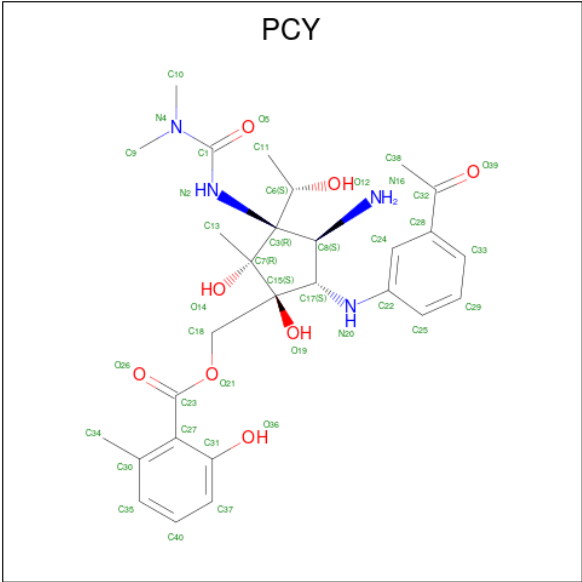
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	8	1	Total	N	Os	0	0
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86	13	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	14	1	Total	N	Os	0	0
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86	14	1	Total	N	Os	0	0
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86	15	1	Total	N	Os	0	0
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86	15	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		
86	19	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m1	1	Total	N	Os	0	0
			7	6	1		
86	m4	1	Total	N	Os	0	0
			7	6	1		
86	m5	1	Total	N	Os	0	0
			7	6	1		
86	m6	1	Total	N	Os	0	0
			7	6	1		
86	m7	1	Total	N	Os	0	0
			7	6	1		
86	m8	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o2	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	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 Pactamycin (CCD ID: PCY) (formula: $C_{28}H_{38}N_4O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
87	2	1	Total	C	N	O	0	0
			40	28	4	8		
87	6	1	Total	C	N	O	0	0
			40	28	4	8		

- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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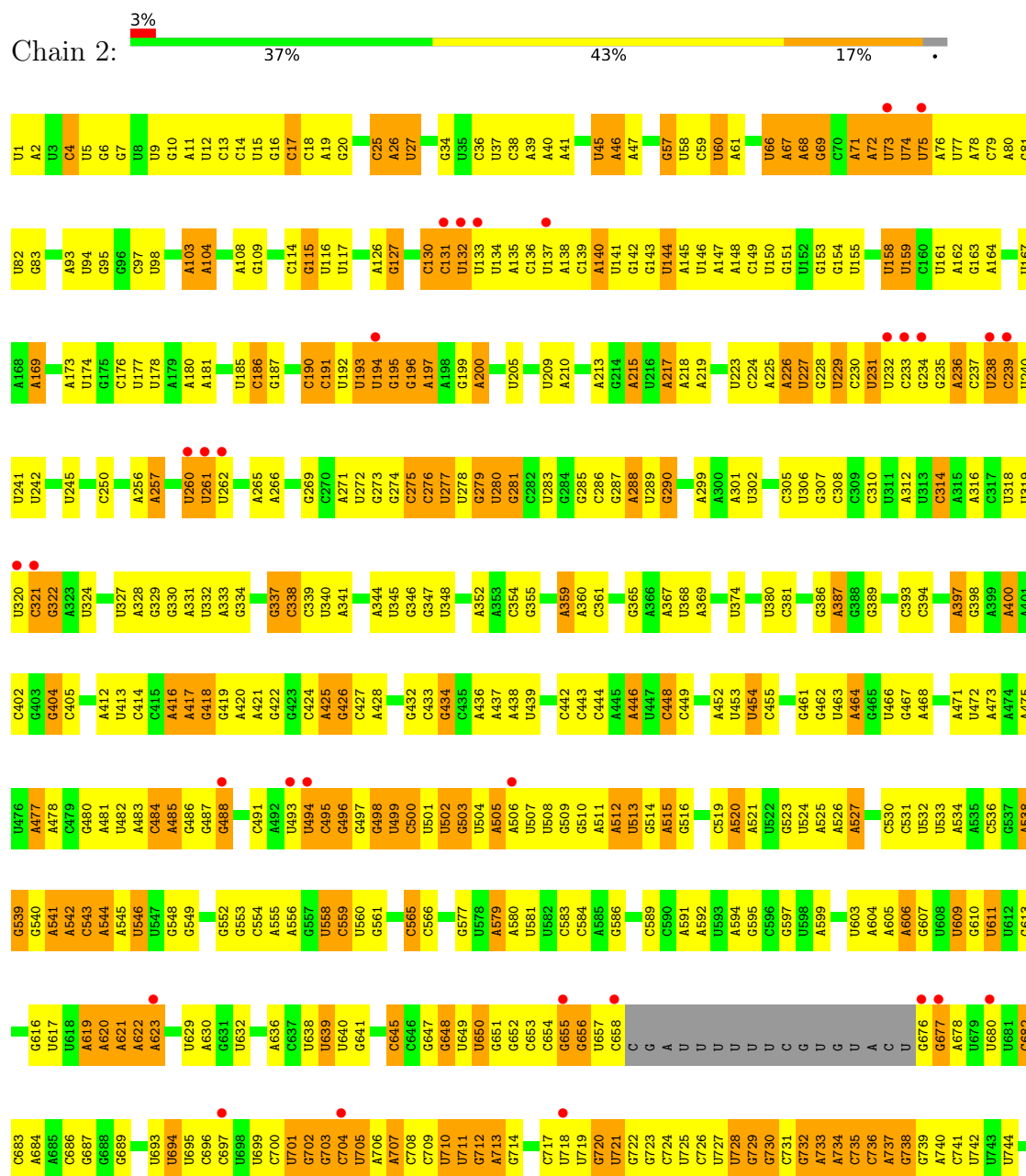
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	d9	1	Total 1	Zn 1	0	0
88	e1	1	Total 1	Zn 1	0	0
88	o7	1	Total 1	Zn 1	0	0
88	q0	1	Total 1	Zn 1	0	0
88	q2	1	Total 1	Zn 1	0	0
88	q3	1	Total 1	Zn 1	0	0

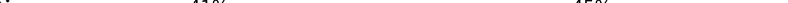
3 Residue-property plots

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

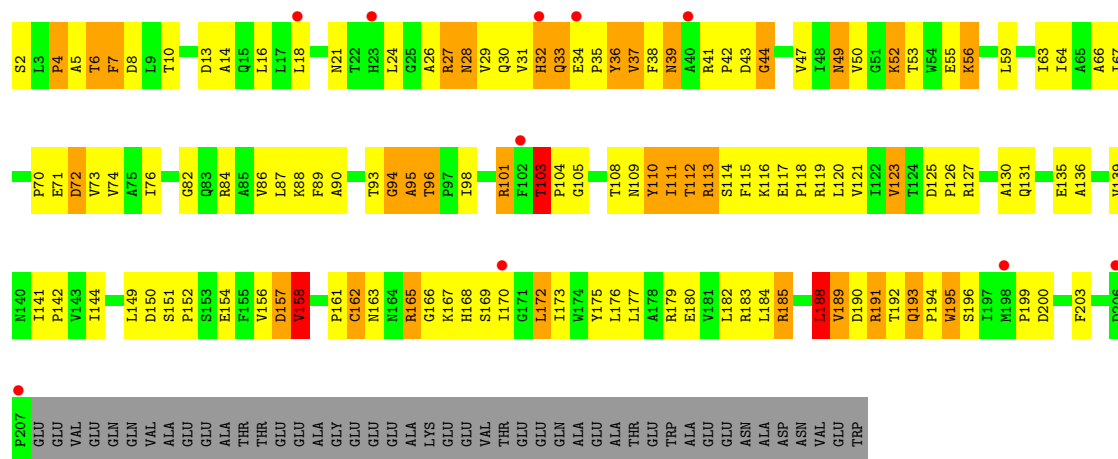


G1717	U1650	A1583	U1511	A1446	U1372	C1309	G1228	G1149	G1064	A978	A887	U820	U749
G1718	A1651	G1584	G1512	U1449	A1376	U1310	G1229	G1150	A1065	A979	U888	U821	A753
A1719	C1652	U1585	G1513	U1450	C1376	U1311	A1230	A1151	C1066	G984	A892	U822	A754
G1720	G1654	A1586	U1514	U1451	U1377	U1312	U1231	A1152	C1067	G985	U893	G824	A755
G1727	U1657	G1588	A1516	U1452	U1378	U1314	G1233	G1153	C1068	G986	U894	G825	A756
A1728	U1658	C1589	U1517	G1453	C1379	U1315	A1234	A1157	C1075	G987	U895	U826	
	G1658	G1590	G1518	U1454	U1380	G1316	C1235	C1158	A1076	C990	U896	C827	U759
A1731	U1659	C1591	U1519	G1455	U1381	G1317	A1236	C1159	U1079	G991	U897	C828	A760
	A1660	A1592	U1520	C1456	A1382		G1237	A1160	A898	G992	A898	A829	A761
U1735	U1661	G1593	G1521	C1457	C1383	U1320	A1238	C1161	U1080	A993	U899	U830	A762
G1736	G1662	G1594	U1522	G1458	A1384	A1321	U1239	G1162	A1081	G994	A900	U831	G763
G1737	G1663	U1595	G1523	C1459	G1385	A1322	U1240	A1163	C1082	G995	G901	U832	U764
U1738	A1524	A1460	A1524	A1460	G1385	C1383	G1241	G1164		A995	G902	U833	G765
C1739	A1525	C1461	A1525	C1461	A1388	G1324	A1242	G1165	G1085	C1000	U903	U834	U766
	U1598	G1466	A1526		C1389	A1325	G1243	A1166	A1086	G1001	U904	U835	U767
U1742	U1599		U1527	G1466	U1390	A1326	A1244	G1167	A1087	G1002	U911	U836	C768
U1743	A1600	G1601	C1528		G1393	A1329	C1246	U1174	A1091	U1004	U912	U837	A769
A1744	G1602	U1603	C1530	A1470	G1394	G1330	U1247	C1173	A1092	A1005	U913	U838	A770
G1745	U1604	G1605	C1533	C1471	U1397	A1331	C1248	U1175	C1096	U1009	U914	U839	C773
A1746	G1606	G1607	U1535	C1472	U1398	C1332	U1249	G1176	A915	G914	U915	U841	A774
G1747	G1608	G1609	U1536	G1474	C1399	U1334	U1250	C1177	U1097	C1010	U916	C842	G775
G1748	U1680	U1610	C1537	C1476	A1401	A1336	U1253	G1178	G1100	G1011	U917	U844	G778
A1756	U1681	G1611	G1541	G1477	C1404	A1337	U1254	C1179	G1101	U1012	U918	U845	U779
	U1682	U1612	G1542	G1478	G1405	C1338	G1255	U1181	U1104	G1013	A919	G846	U780
G1760	G1683	G1613	U1543	C1481	U1409	U1340	U1256	A1182	U1105	U1014	U920	U847	U781
A1766	A1614	A1615	G1544	C1482	G1410	A1341	U1257	A1183	C1105	U1015	U921	U848	U782
G1767	G1616	G1617	G1546	A1483	A1411	C1342	U1258	A1184	U1106	U1017	C927	U850	G784
U1768	G1619	C1620	U1553	G1484	U1412	U1343	U1266	U1191	G1111	U1018	U928	U851	U785
A1769	G1621	U1621	G1554	C1486	U1413	A1344	G1267	U1194	A1026	C931	U932	C852	A788
U1770	G1622	G1623	A1555	G1487	U1414	A1346	C1274	C1195	A1027	U933	U854	G853	A789
	G1624	G1625	U1557	G1488	U1415	U1347	G1277	A1196	C1028	A933	A855	A856	U792
G1773	U1629	U1630	A1558	U1489	G1416	A1348	U1280	C1197	U1029	C934	A856	U857	A793
G1774	A1631	A1632	U1560	C1490	A1417	U1349	G1281	G1198	A1030	U935	U858	G858	U794
U1775	C1633	C1634	U1561	G1491	C1420	U1350	U1282	G1199	U1031	G936			A796
A1776	U1635	U1636	U1562	U1492	G1424	U1351	U1283	G1200	C1032	C942	U861	U862	U800
G1777	C1637	C1638	C1563	C1494	A1424	U1352	C1284	G1201	A1039	C943	A863	A862	G801
	U1639	U1640	G1564	C1495	A1427	C1354	U1285	A1202	G1040	A944	A864	U864	G802
A1780	A1631	A1632	U1565	C1496	G1428	U1356	U1286	A1203	G1041	A951	A865	G866	A806
A1781	C1633	C1634	U1566	U1497	G1429	A1357	A1287	C1207	G1042	A952	G867	G867	U807
U1782	U1635	U1636	U1567	G1498	U1430	G1358	G1288	A1211	U1043	G953	G868		A808
C1784	C1637	C1638	C1568	C1500	U1431	C1359	U1289	G1218	C1044	G954			U809
U1785	A1639	A1640	U1569	C1501	U1432	U1360	U1290	A1219	C1045				A810
	U1641	U1642	G1570	G1502	G1433	U1361	G1291	G1214	U1052	G957	G871	G872	G811
G1788	C1639	C1640	U1571	G1503	U1434	U1362	G1294	C1215	G1053	U958	U873	U873	A812
	U1641	U1642	U1572	G1504	G1435	U1363	G1295	C1216	U1057	U959			U813
G1792	A1643	A1644	G1573	U1505	A1436	G1364	G1296	A1217	U1058	U960	G876		A814
A1793	C1645	C1646	U1574	G1506	U1437	G1367	A1296	G1218	U1059	U961			G815
U1794	U1647	U1648	U1575	G1507	U1442	G1368	U1301	A1219	U1060	A966	U882	C883	G816
C1796	A1649	A1650	U1576	U1508	U1443	U1369	U1302	G1220	U1061	A967	U884	A884	A817
U1798	U1651	U1652	U1577	C1509	A1444	U1370	A1226	A1227	A1062	C969	C885	C818	C819
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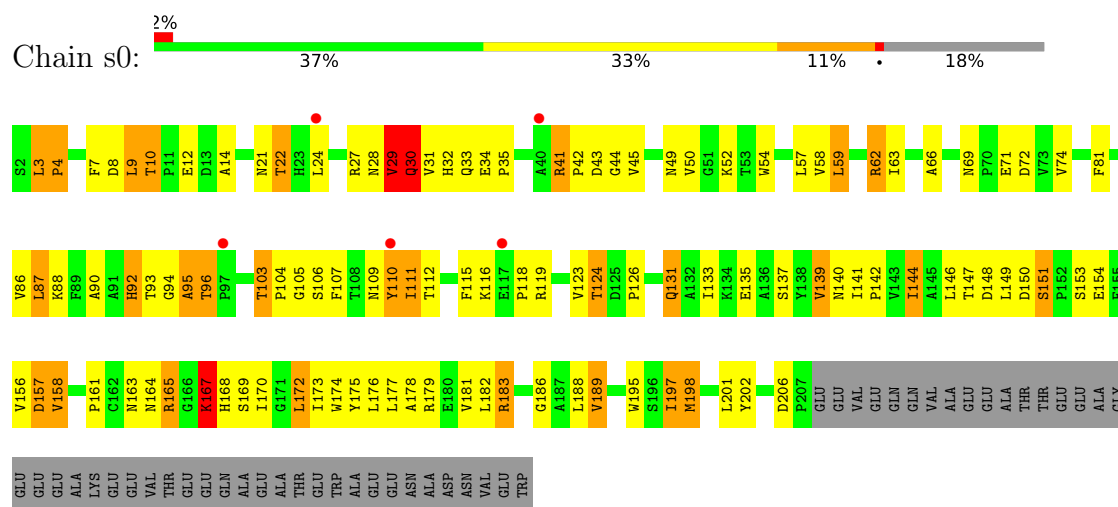
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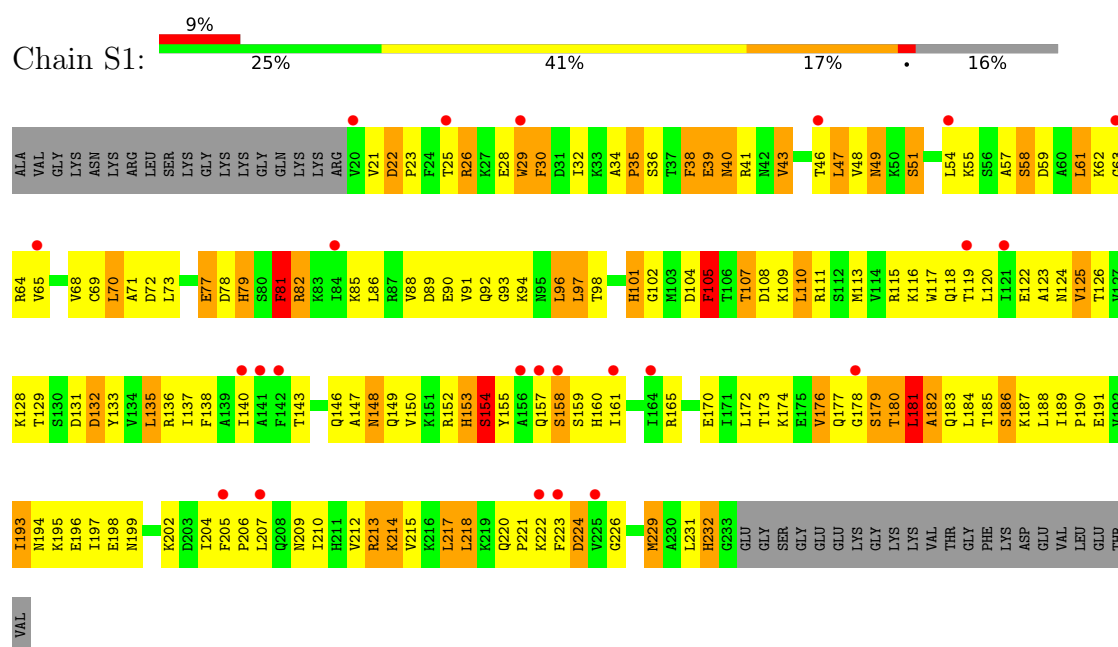




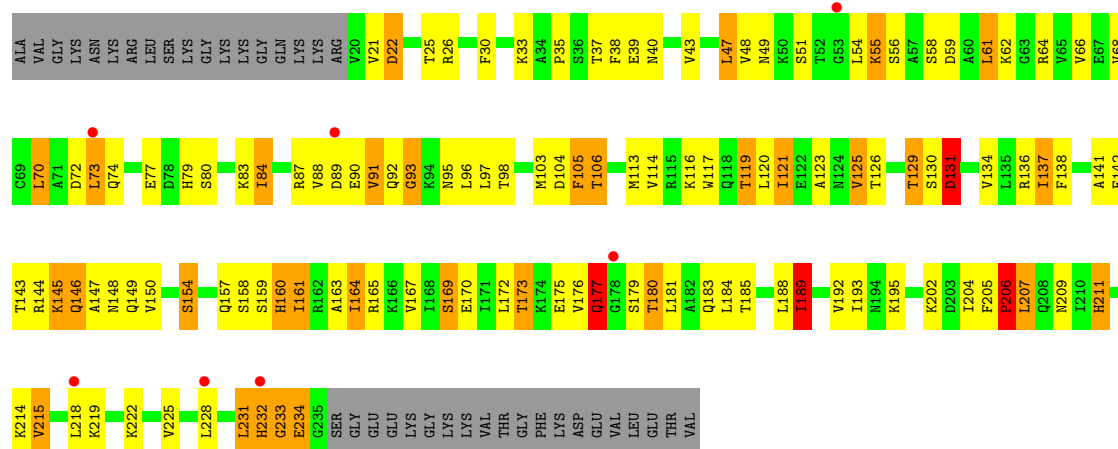
• Molecule 2: 40S ribosomal protein S0-A



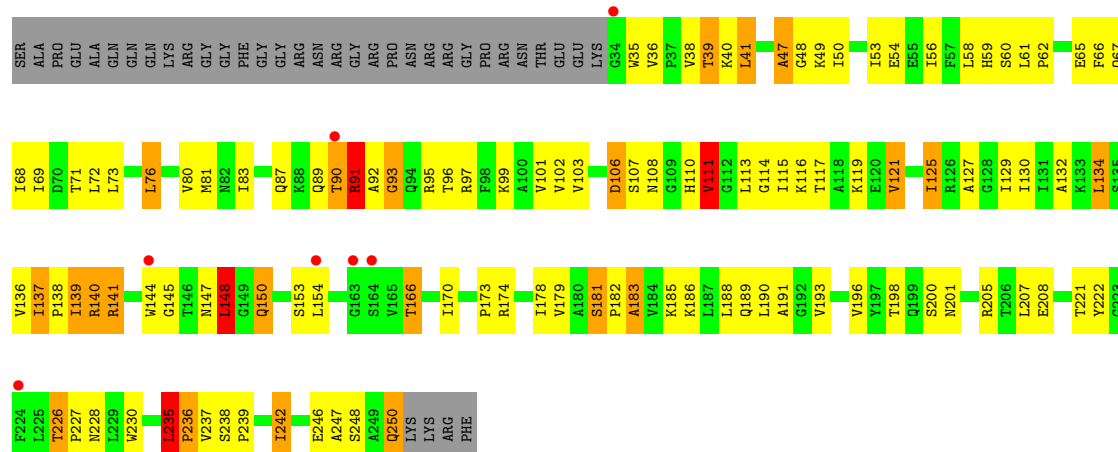
• Molecule 3: 40S ribosomal protein S1-A



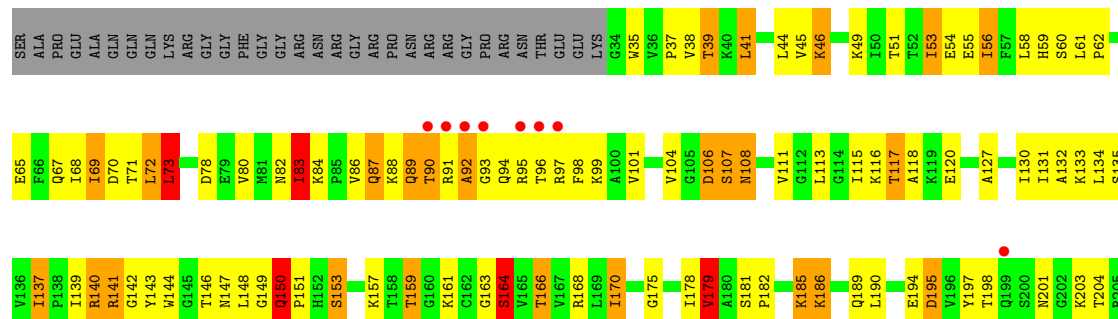
Chain s1:



Chain S2:

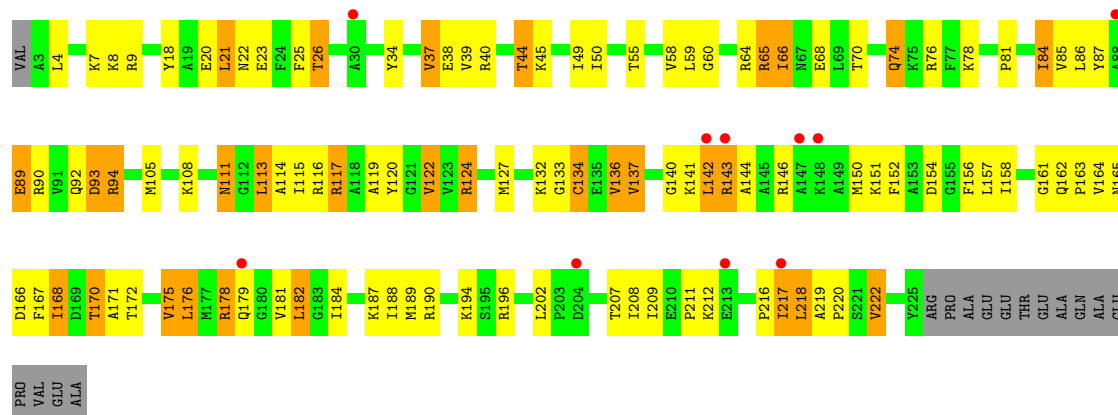


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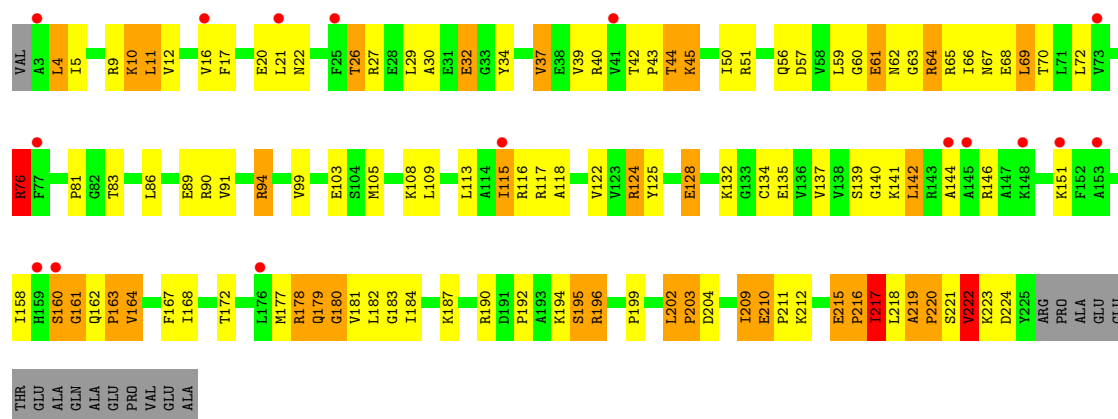




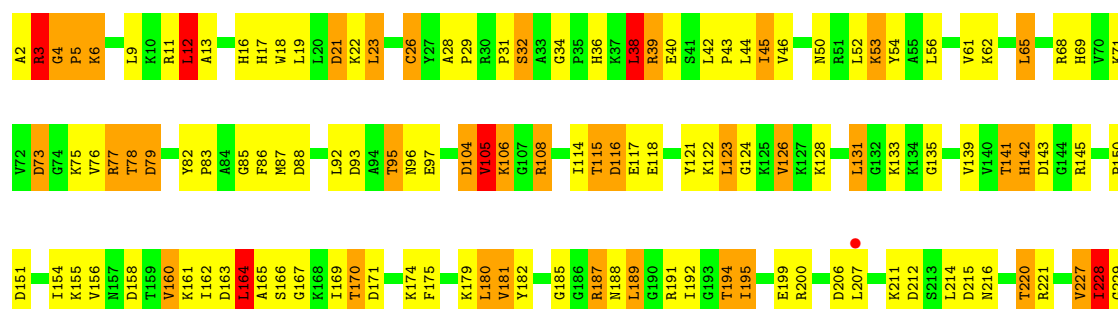
• Molecule 5: 40S ribosomal protein S3



• Molecule 5: 40S ribosomal protein S3

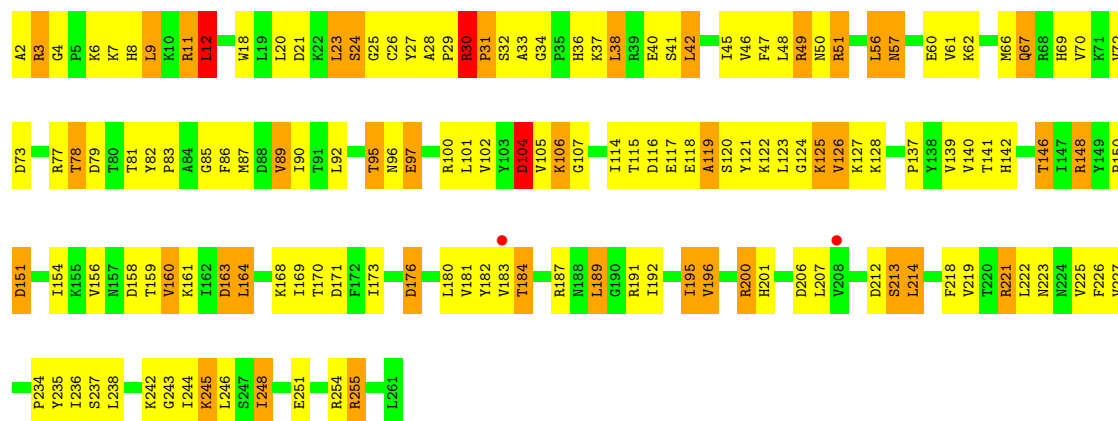
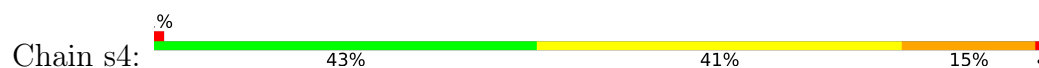


• Molecule 6: 40S ribosomal protein S4-A

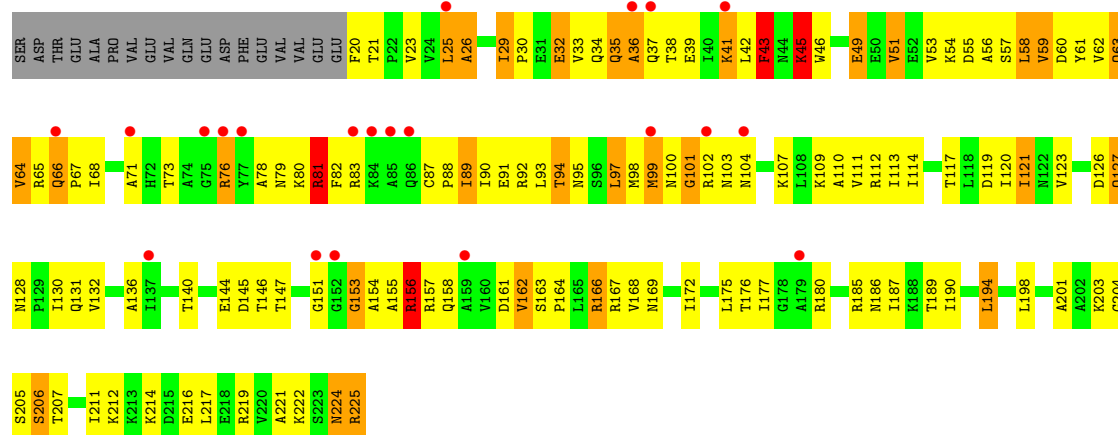




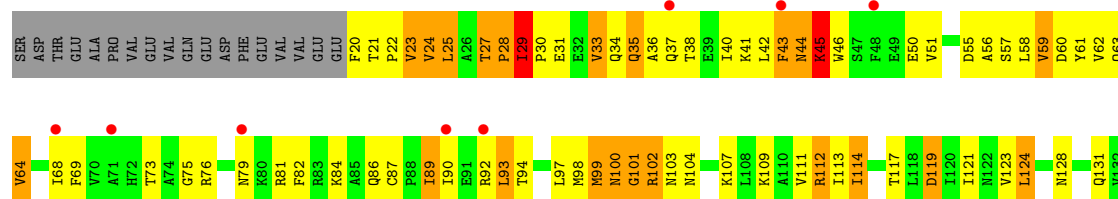
• Molecule 6: 40S ribosomal protein S4-A

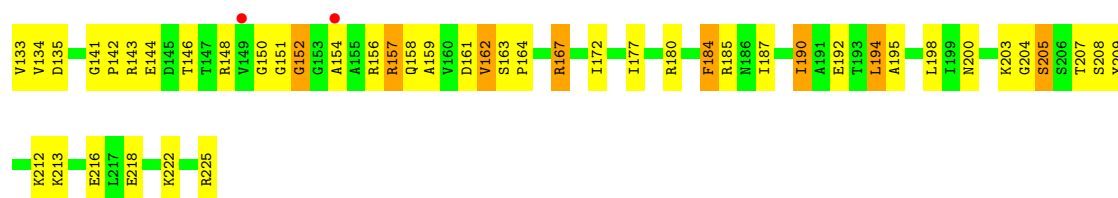


• Molecule 7: 40S ribosomal protein S5

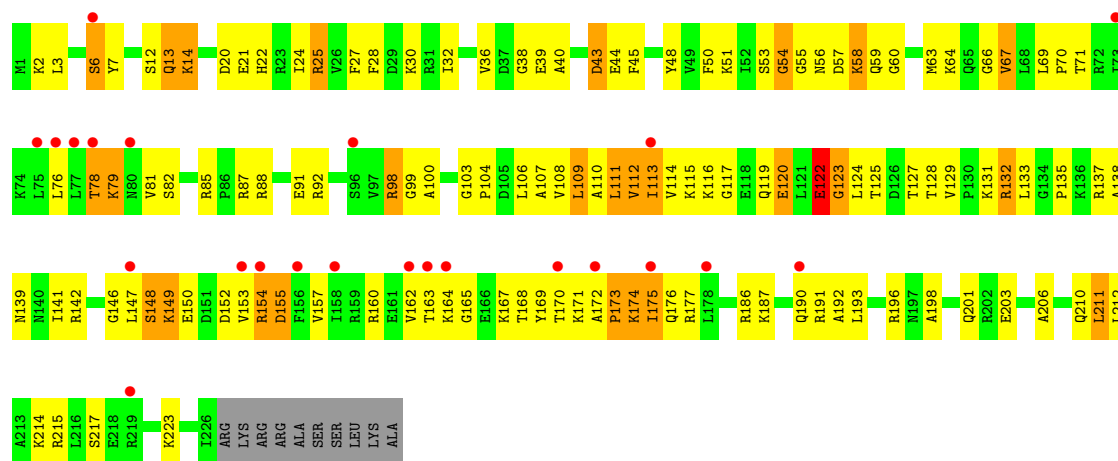
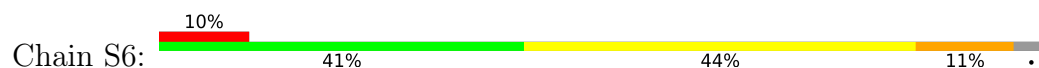


• Molecule 7: 40S ribosomal protein S5

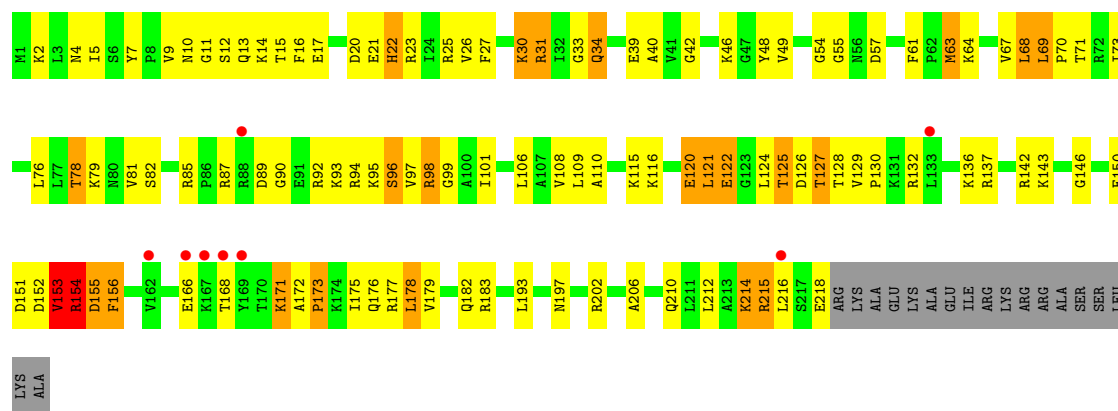




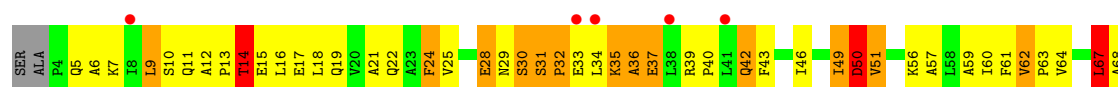
• Molecule 8: 40S ribosomal protein S6-A

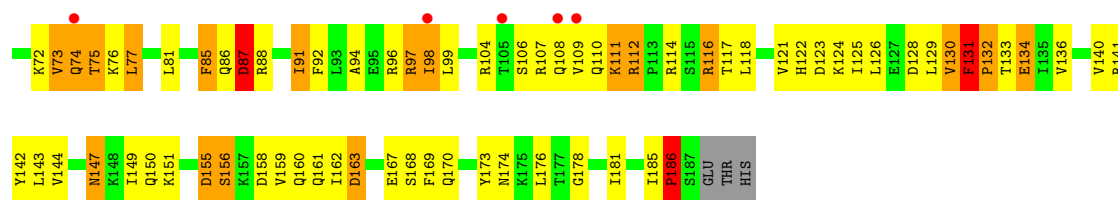


• Molecule 8: 40S ribosomal protein S6-A

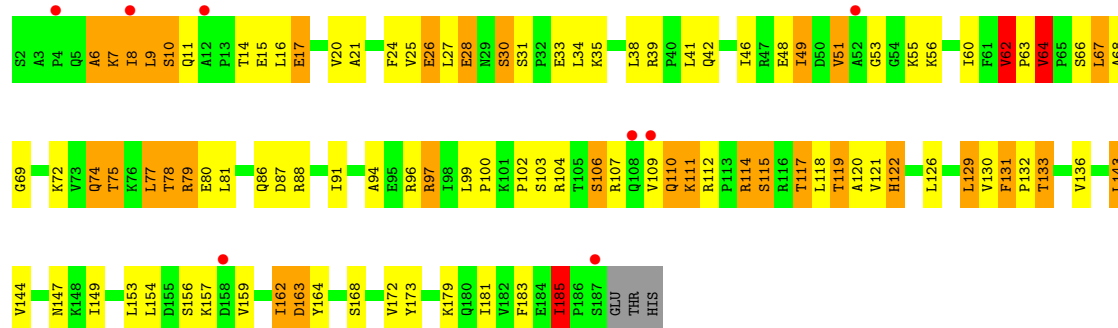


• Molecule 9: 40S ribosomal protein S7-A

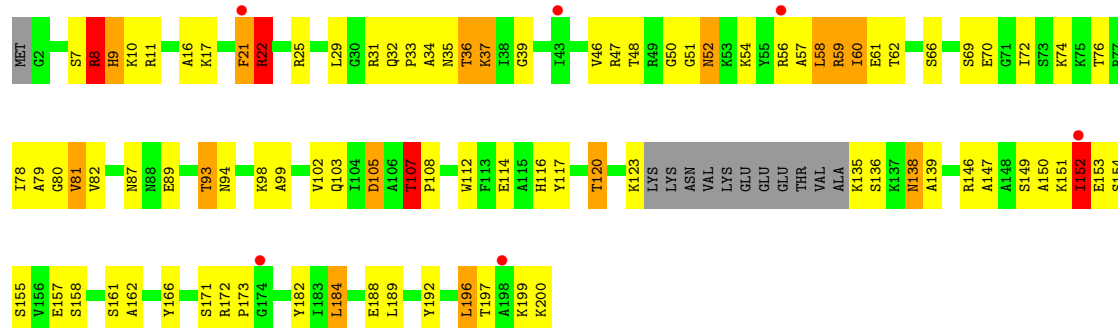




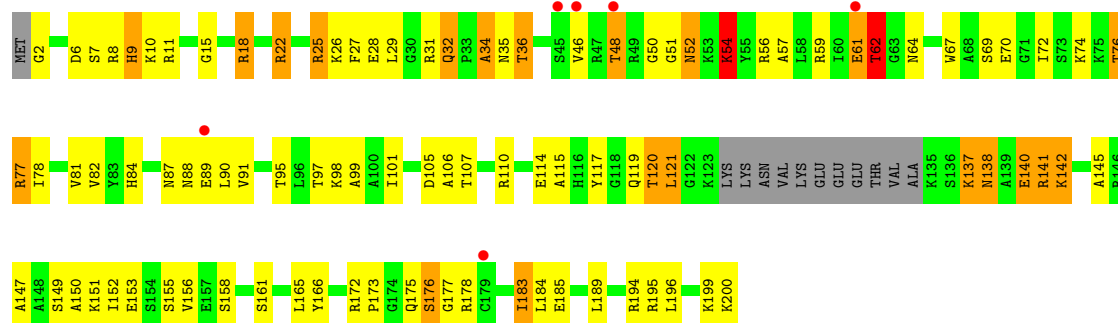
• Molecule 9: 40S ribosomal protein S7-A



• Molecule 10: 40S ribosomal protein S8-A

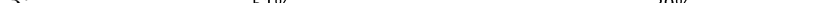


• Molecule 10: 40S ribosomal protein S8-A



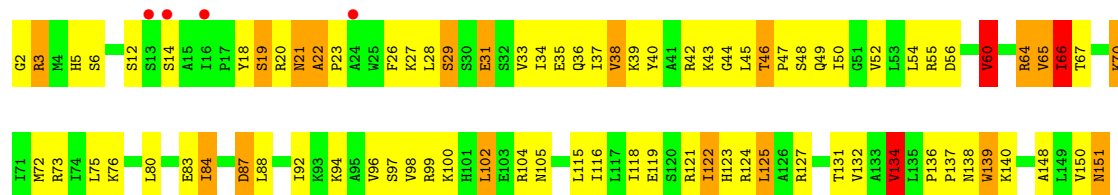
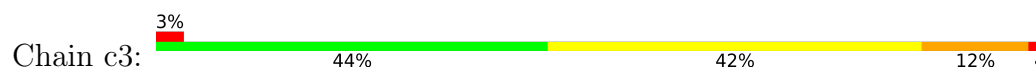
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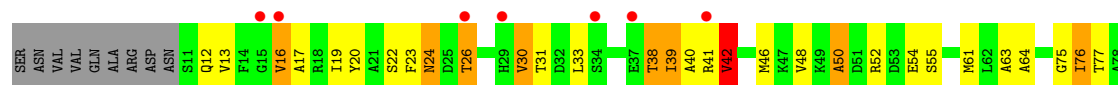
- Chain C3: 



• Molecule 15: 40S ribosomal protein S13



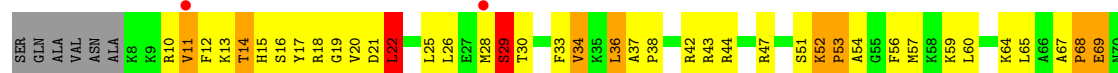
• Molecule 16: 40S ribosomal protein S14-A



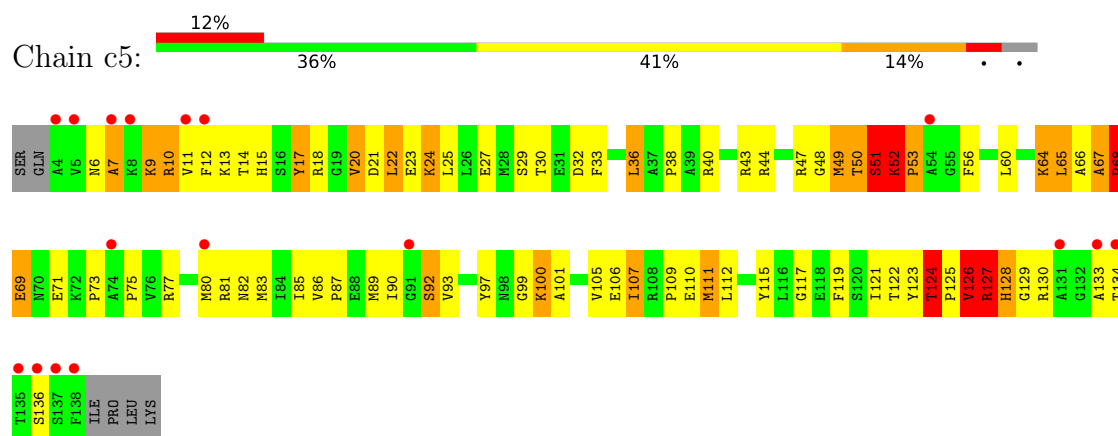
• Molecule 16: 40S ribosomal protein S14-A



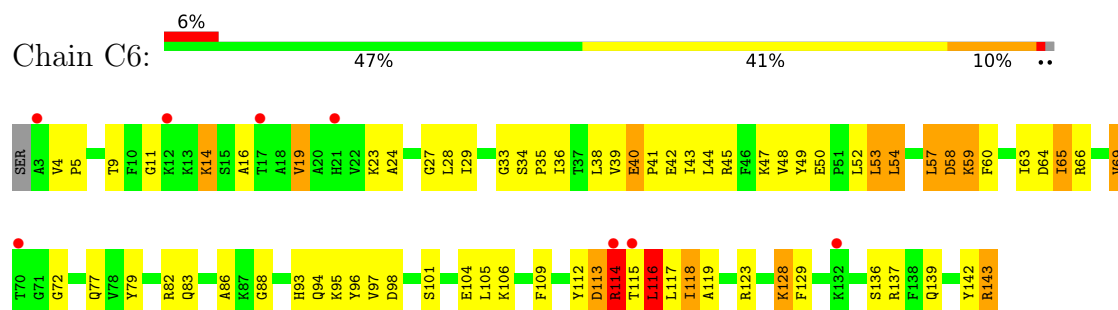
• Molecule 17: 40S ribosomal protein S15



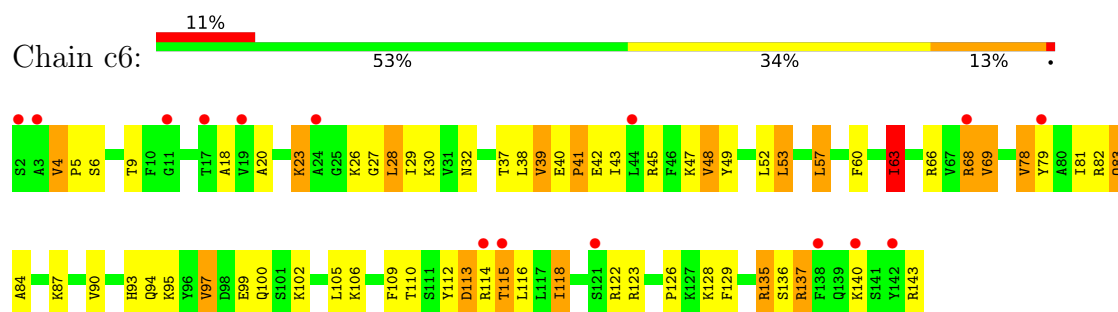
- Molecule 17: 40S ribosomal protein S15



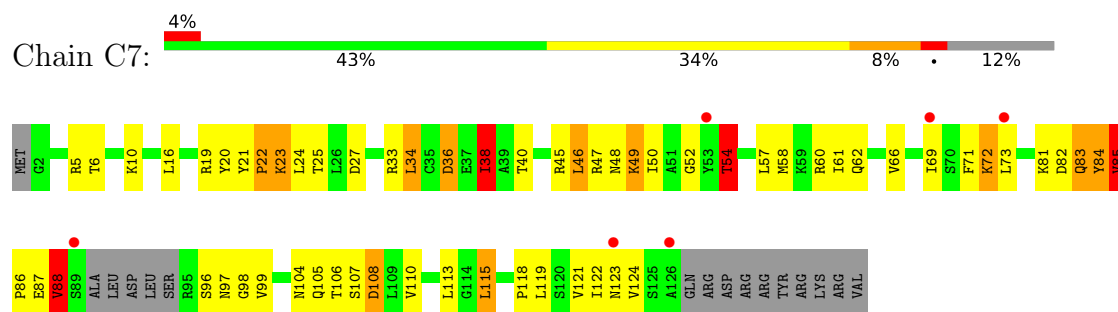
- Molecule 18: 40S ribosomal protein S16-A



- Molecule 18: 40S ribosomal protein S16-A

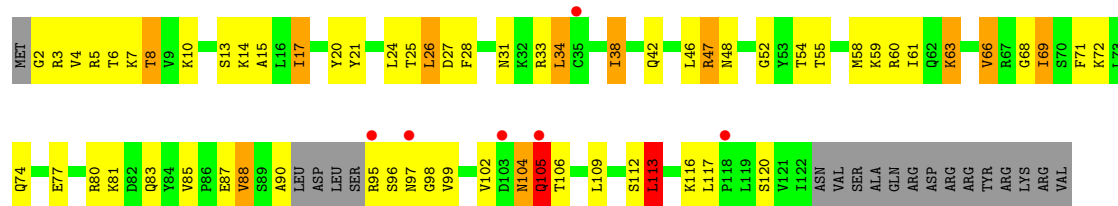


- Molecule 19: 40S ribosomal protein S17-A

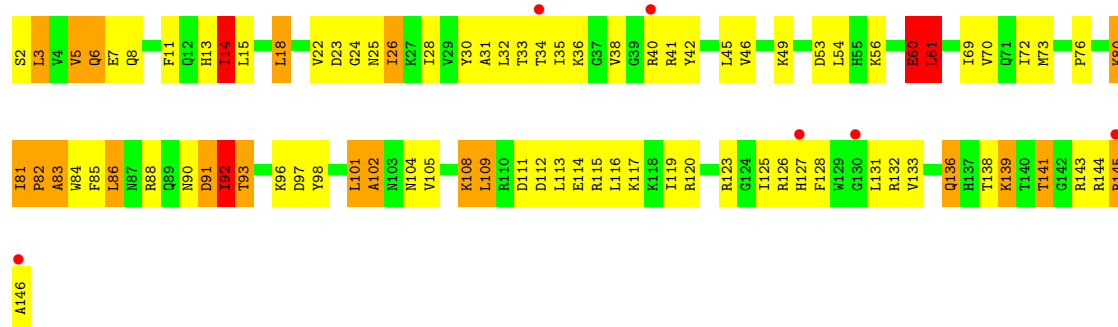


- Molecule 19: 40S ribosomal protein S17-A

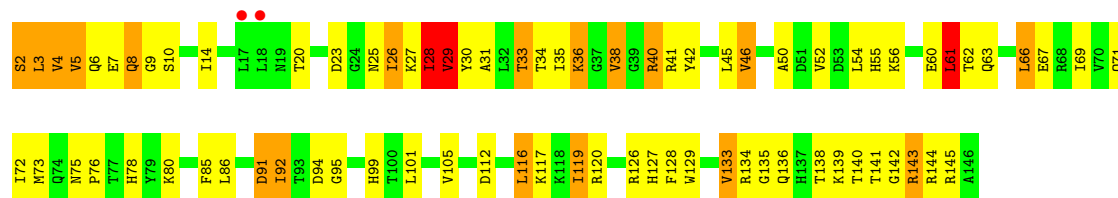




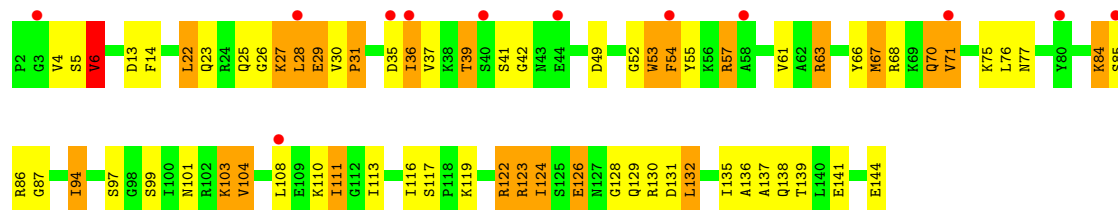
• Molecule 20: 40S ribosomal protein S18-A



• Molecule 20: 40S ribosomal protein S18-A



• Molecule 21: 40S ribosomal protein S19-A

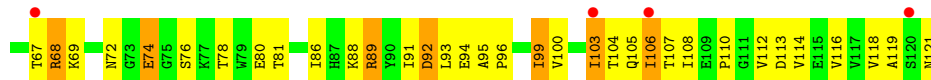
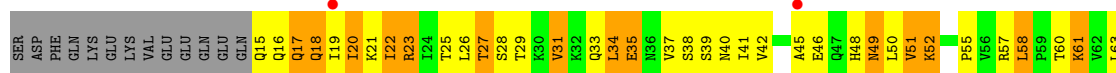


• Molecule 21: 40S ribosomal protein S19-A

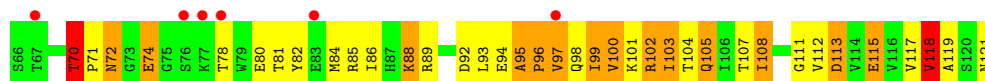
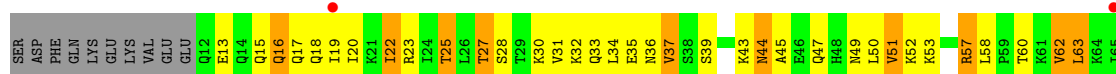




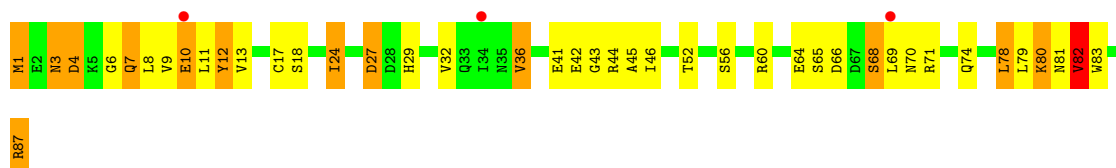
- Molecule 22: 40S ribosomal protein S20



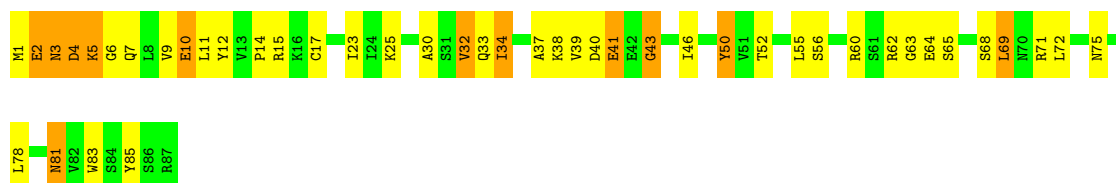
- Molecule 22: 40S ribosomal protein S20



- Molecule 23: 40S ribosomal protein S21-A

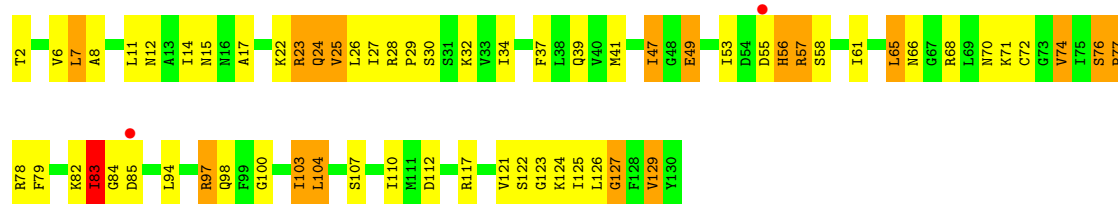


- Molecule 23: 40S ribosomal protein S21-A

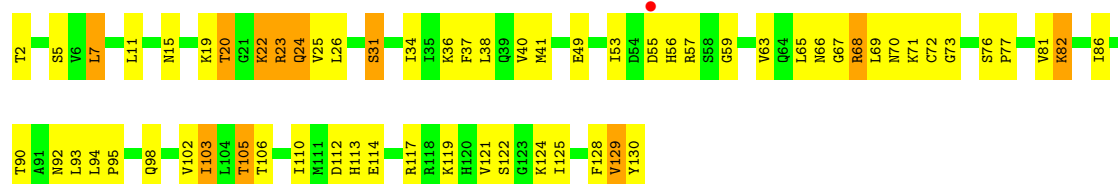


- Molecule 24: 40S ribosomal protein S22-A

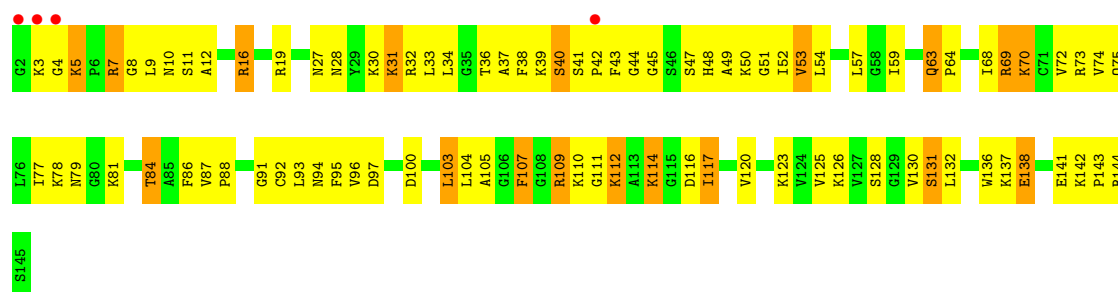




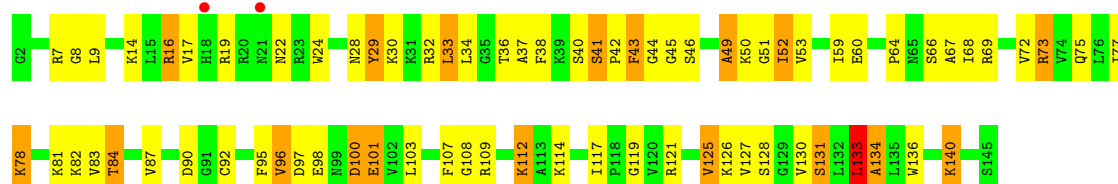
• Molecule 24: 40S ribosomal protein S22-A



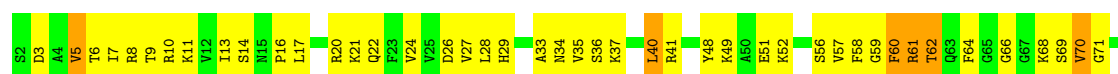
• Molecule 25: 40S ribosomal protein S23-A



• Molecule 25: 40S ribosomal protein S23-A

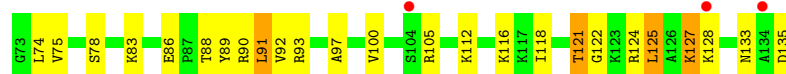
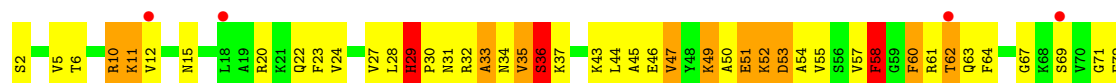


• Molecule 26: 40S ribosomal protein S24-A

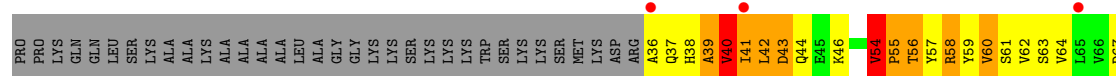




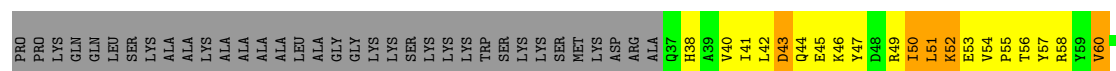
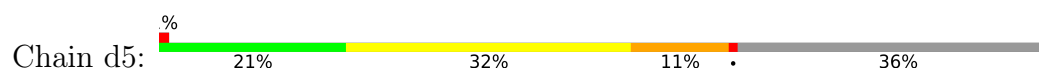
- Molecule 26: 40S ribosomal protein S24-A



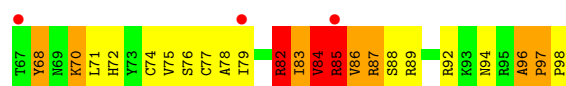
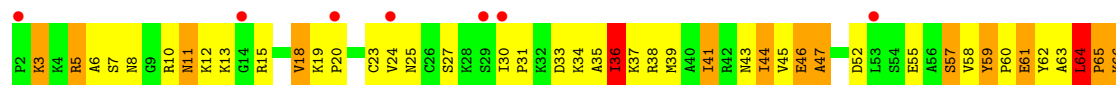
- Molecule 27: 40S ribosomal protein S25-A



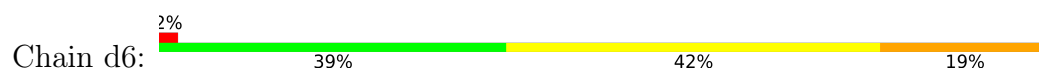
- Molecule 27: 40S ribosomal protein S25-A



- Molecule 28: 40S ribosomal protein S26-B

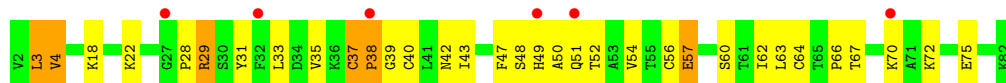


- Molecule 28: 40S ribosomal protein S26-B

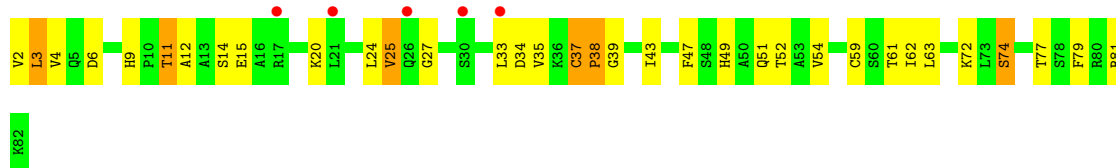




- Molecule 29: 40S ribosomal protein S27-A



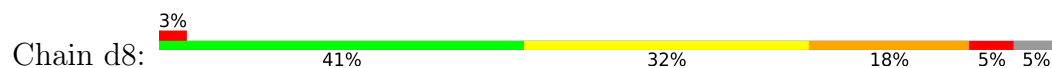
- Molecule 29: 40S ribosomal protein S27-A



- Molecule 30: 40S ribosomal protein S28-A



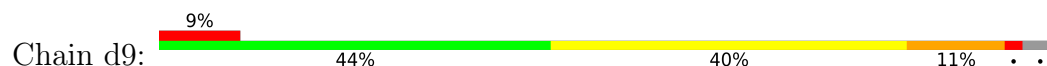
- Molecule 30: 40S ribosomal protein S28-A

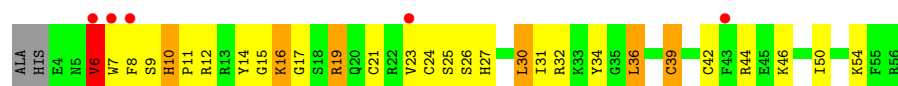


- Molecule 31: 40S ribosomal protein S29-A



- Molecule 31: 40S ribosomal protein S29-A

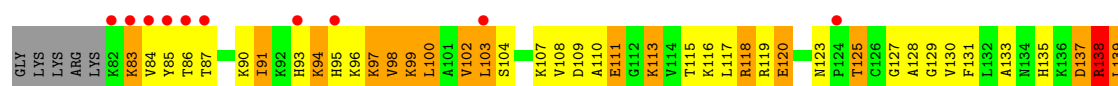




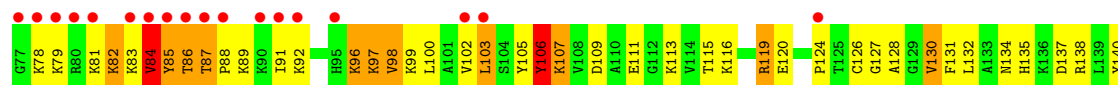
- Molecule 32: 40S ribosomal protein S30-A



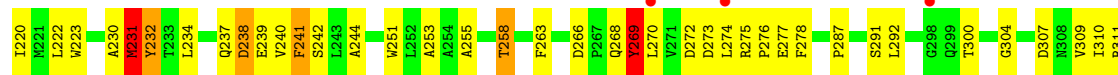
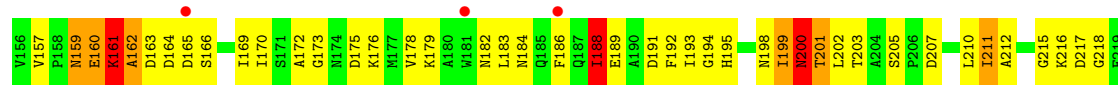
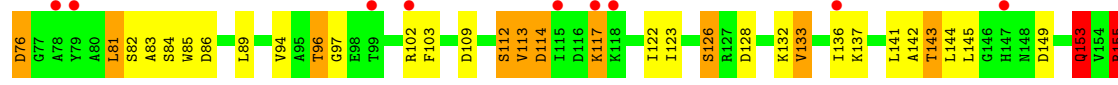
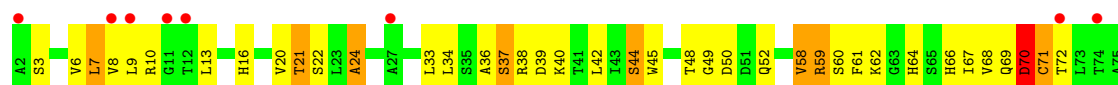
- Molecule 33: Ubiquitin-40S ribosomal protein S31



- Molecule 33: Ubiquitin-40S ribosomal protein S31

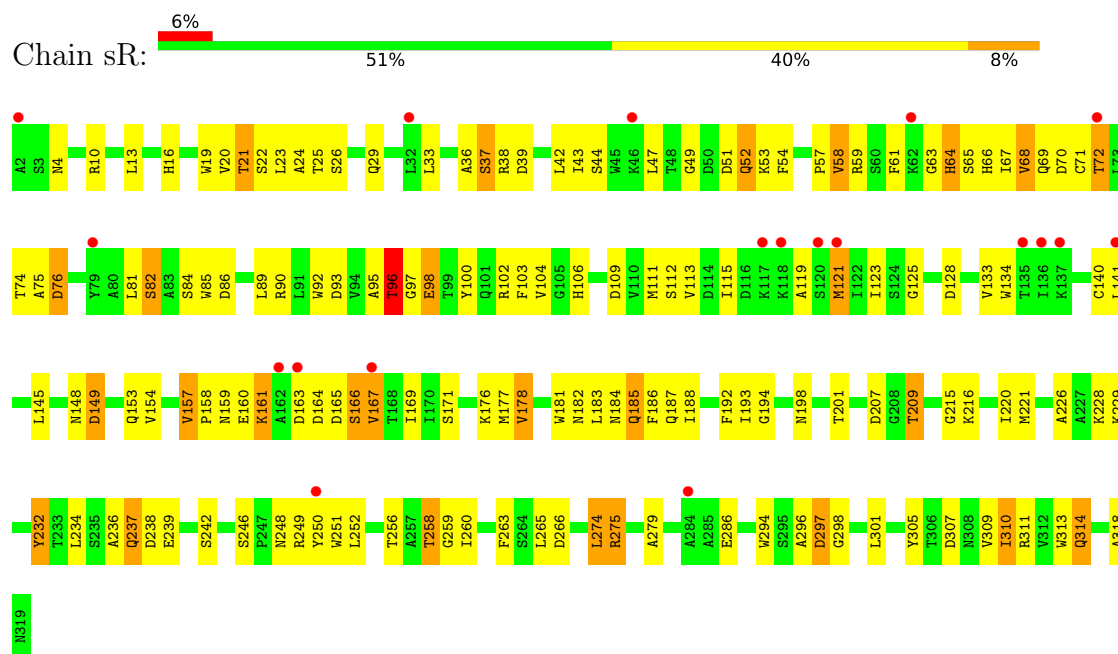


- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

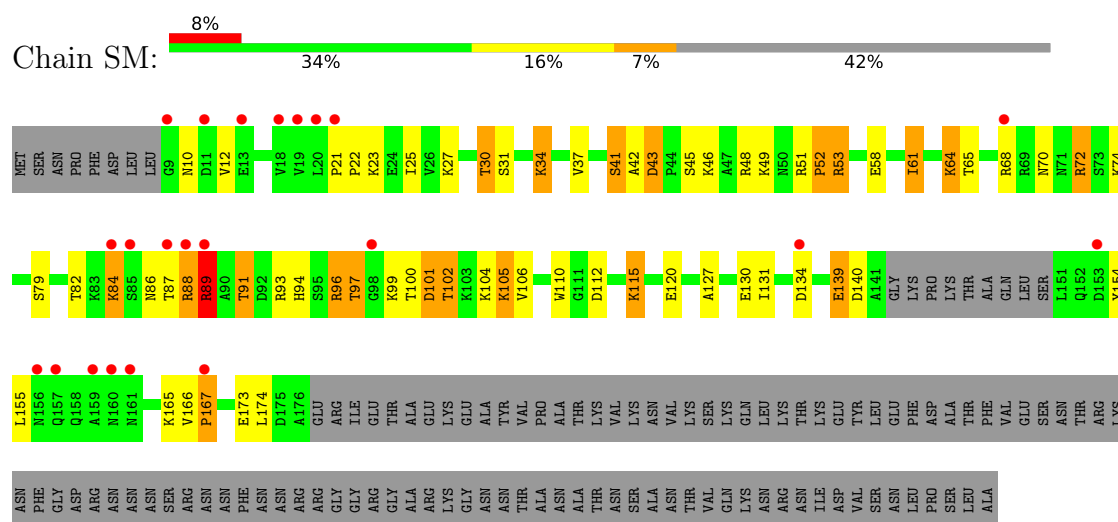


V312
W313
Q314
V315
M316
T317
A318
N319

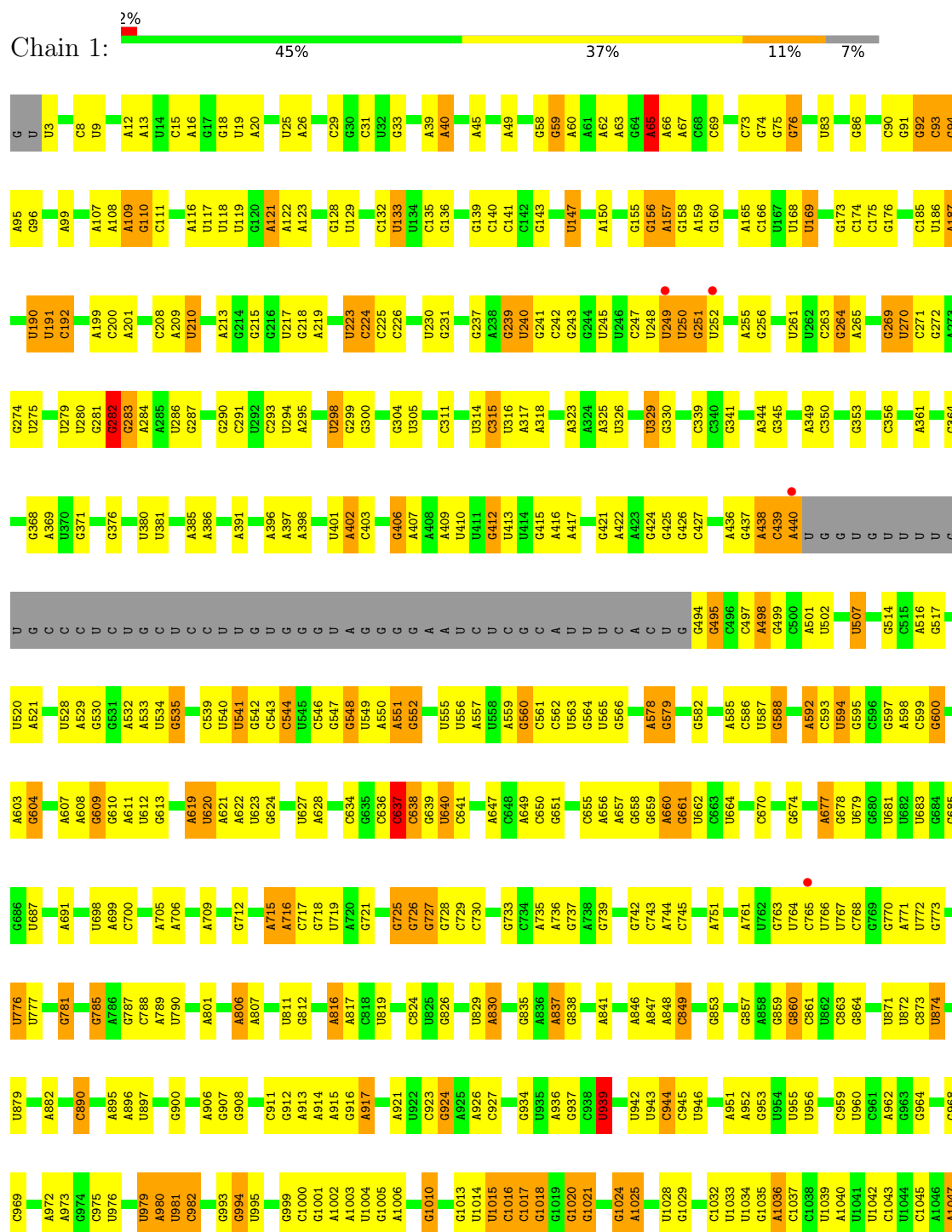
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



• Molecule 35: Suppressor protein STM1

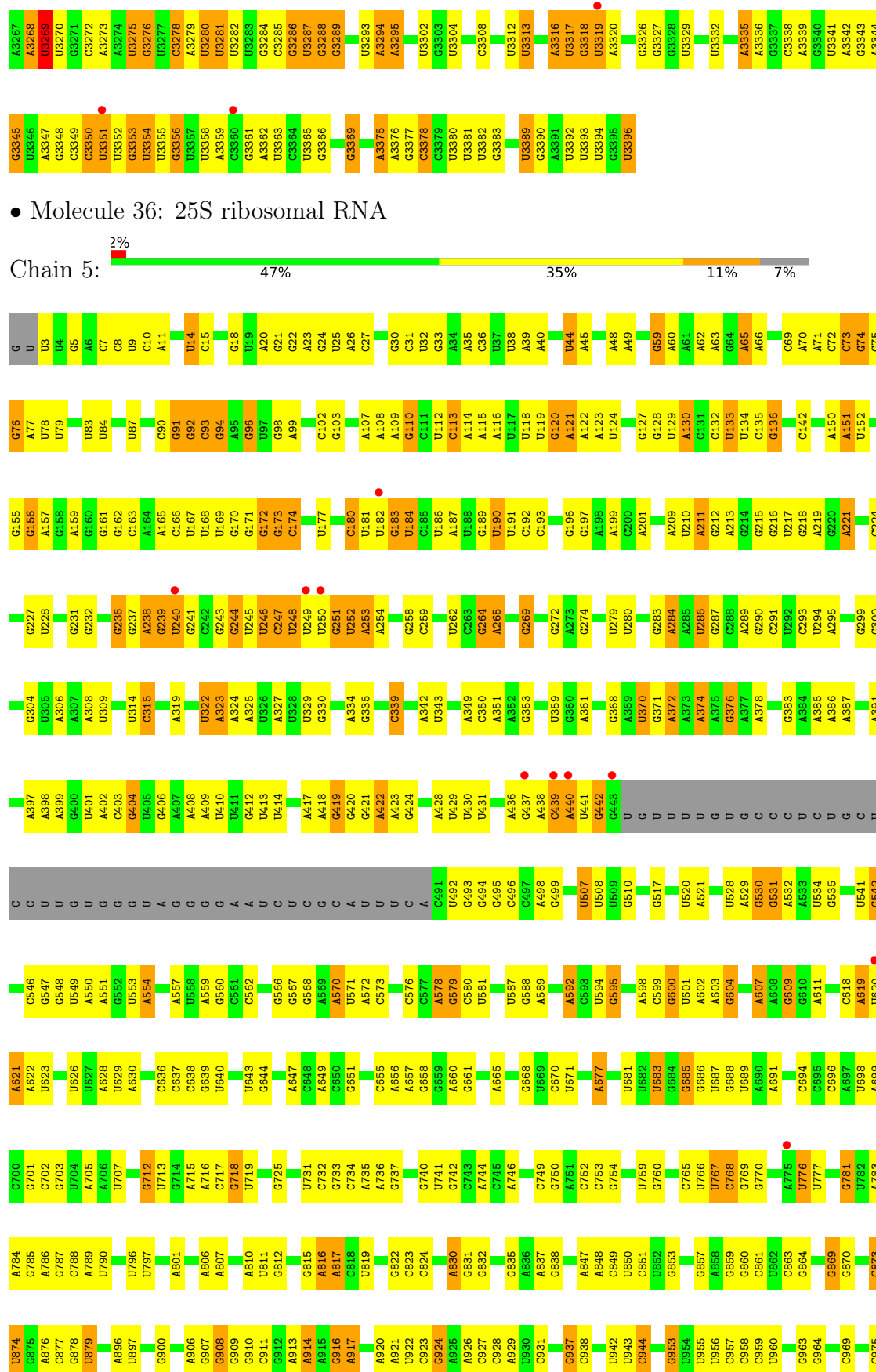


- Molecule 36: 25S ribosomal RNA





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A3180	U3107	A3032	U2795	G2700	C2622	A2540	U	A2401	U2310	G2234	U2194
G3181	A3033	G2871	G2796	A2703	U2541	U2542	C	G2402	A2313	G2155	C2156
A3182	C3034	A2872	G2799	A2705	G2623	U2543	G	G2403	U2314	G2235	G2157
A3183	A3035	G2873	G2800	A2706	G2624	U2544	C	A2404	G2315	G2236	A2158
A3184	U2954	G2874	A2801	G2707	A2628	C2545	G	G2406	G2316	G2239	U2159
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A3186	A2956	G2878	A2803	C2709	U2630	A2547	C	U2408	U2318	G2241	G2161
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U3192	G3043	U2880	A2808	U2713	U2634	C2549	U	G2412	A2324	A2244	A2168
A3193	G3044	U2881	C2809	G2714	A2635	U2550	A	G2413	A2333	C2248	G2169
G3194	A3045	U2882	C2808	G2715	A2636	U2551	A	G2414	U2334	G2249	U2170
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G3197	A3049	C2885	G2812	U2720	G2640	C2554	U	C2420	U2337	G2250	G2173
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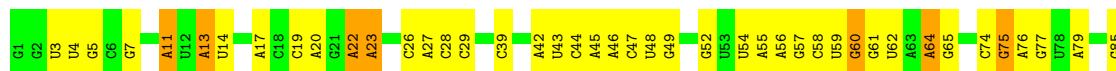


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U	U	U	U	U1760	U1760	G1833	G1833	A1914	U1754	A1648	G1578	U1483	U1389	C1297	U1118	U1052	U1052
U	U	U	U	U1761	U1761	G1834	G1834	A1915	U1755	A1649	G1579	U1484	U1390	C1298	U1119	U1053	U1053
U	U	U	U	U1762	U1762	G1835	G1835	A1916	U1756	A1650	G1580	U1485	U1391	C1299	U1120	U1054	U1054
U	U	U	U	U1763	U1763	G1836	G1836	A1917	U1757	A1651	G1581	U1486	U1392	C1300	U1121	U1055	U1055
U	U	U	U	U1764	U1764	G1837	G1837	A1918	U1758	A1652	G1582	U1487	U1393	C1301	U1122	U1056	U1056
U	U	U	U	U1765	U1765	G1838	G1838	A1919	U1759	A1653	G1583	U1488	U1394	C1302	U1123	U1057	U1057
U	U	U	U	U1766	U1766	G1839	G1839	A1920	U1760	A1654	G1584	U1489	U1395	C1303	U1124	U1058	U1058
U	U	U	U	U1767	U1767	G1840	G1840	A1921	U1761	A1655	G1585	U1490	U1396	C1304	U1125	U1059	U1059
U	U	U	U	U1768	U1768	G1841	G1841	A1922	U1762	A1656	G1586	U1491	U1397	C1305	U1126	U1060	U1060
U	U	U	U	U1769	U1769	G1842	G1842	A1923	U1763	A1657	G1587	U1492	U1398	C1306	U1127	U1061	U1061
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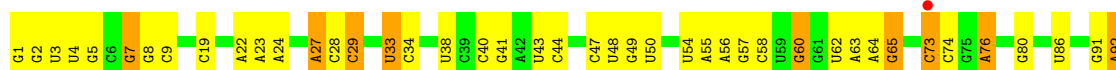




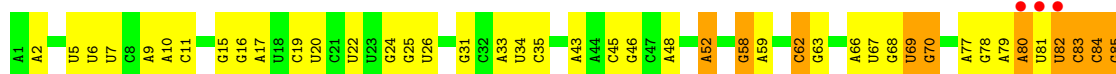
• Molecule 37: 5S ribosomal RNA



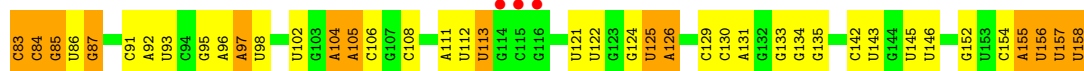
• Molecule 37: 5S ribosomal RNA



• Molecule 38: 5.8S ribosomal RNA

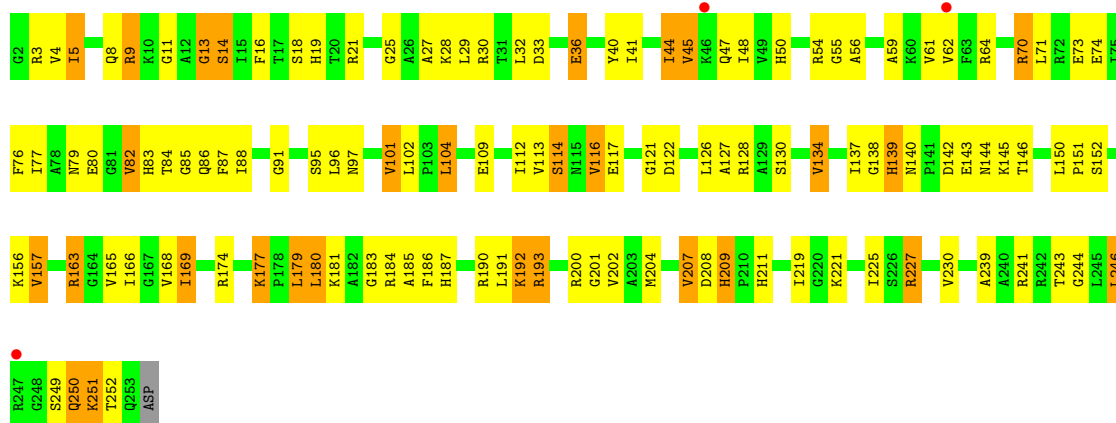


• Molecule 38: 5.8S ribosomal RNA

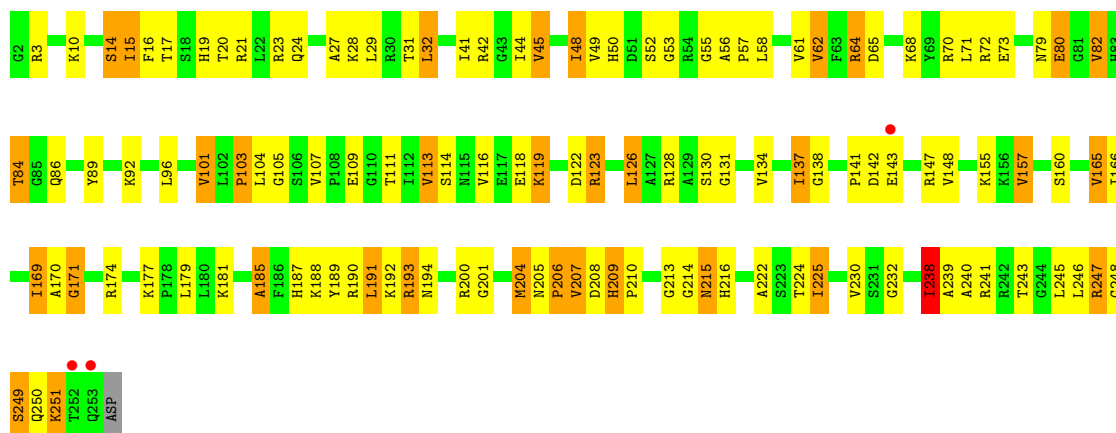


• Molecule 39: 60S ribosomal protein L2-A

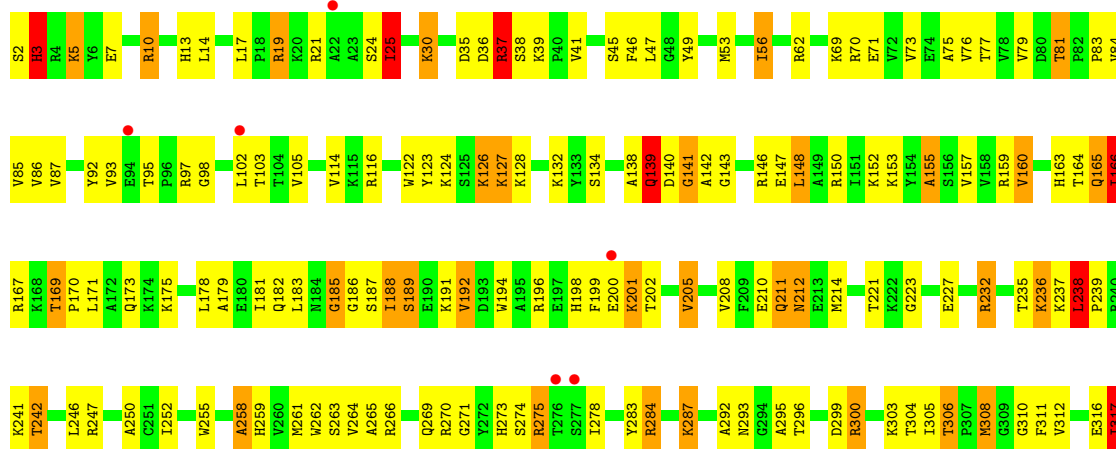




• Molecule 39: 60S ribosomal protein L2-A

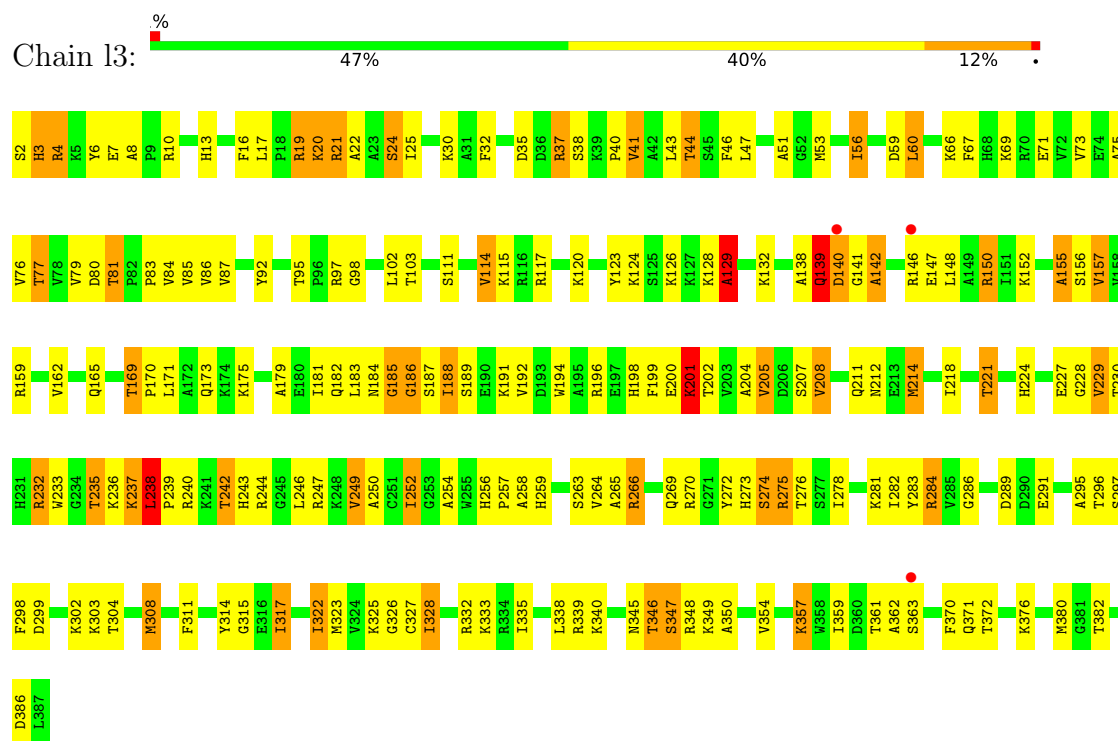


• Molecule 40: 60S ribosomal protein L3

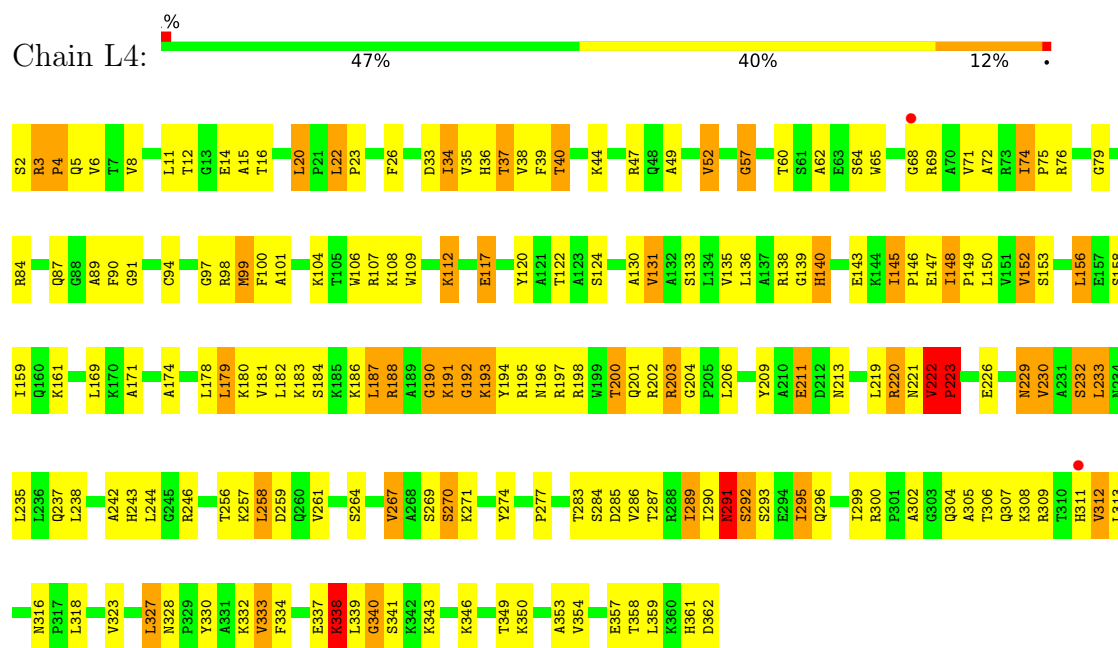




• Molecule 40: 60S ribosomal protein L3

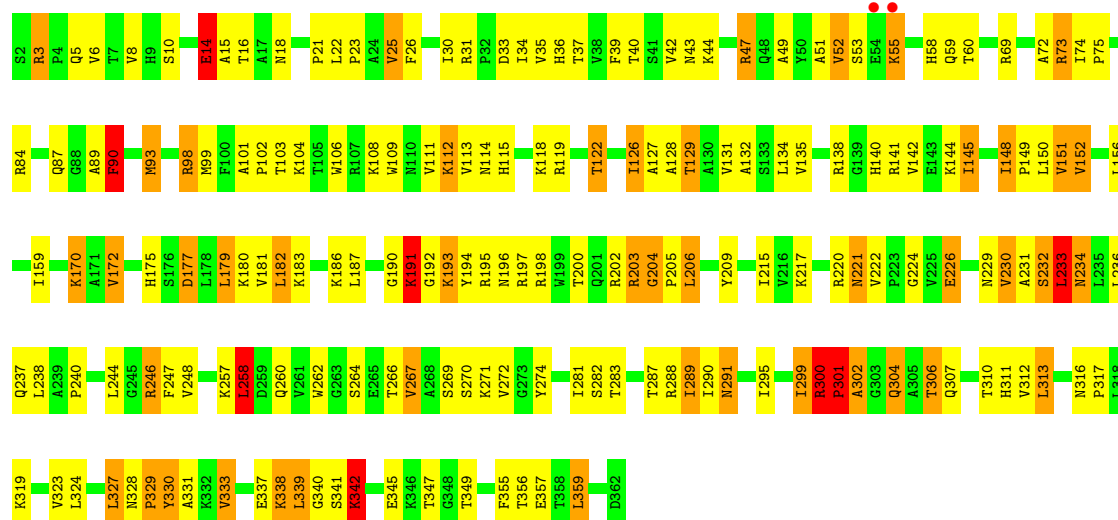


• Molecule 41: 60S ribosomal protein L4-A

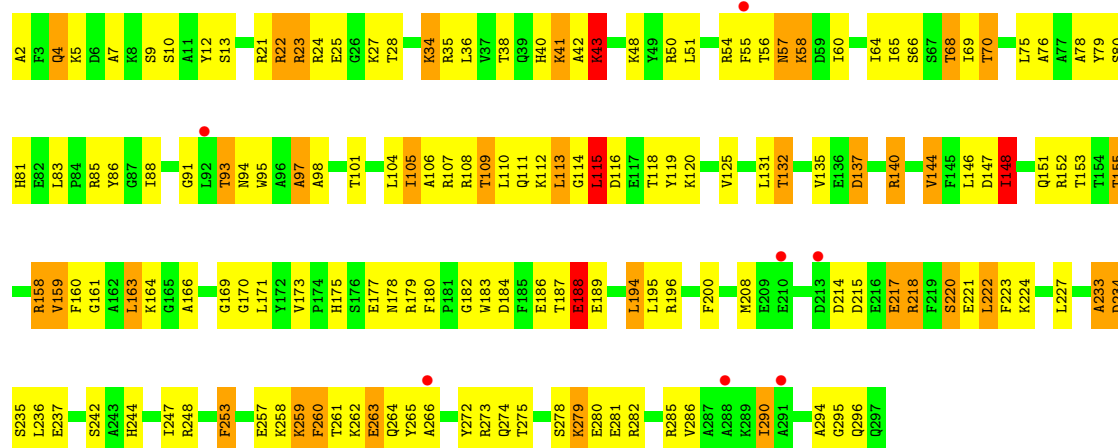


• Molecule 41: 60S ribosomal protein L4-A

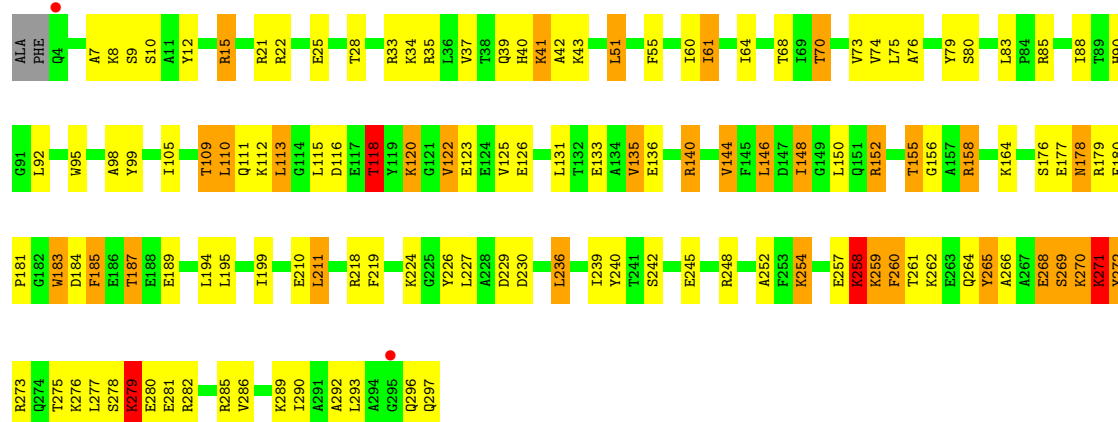




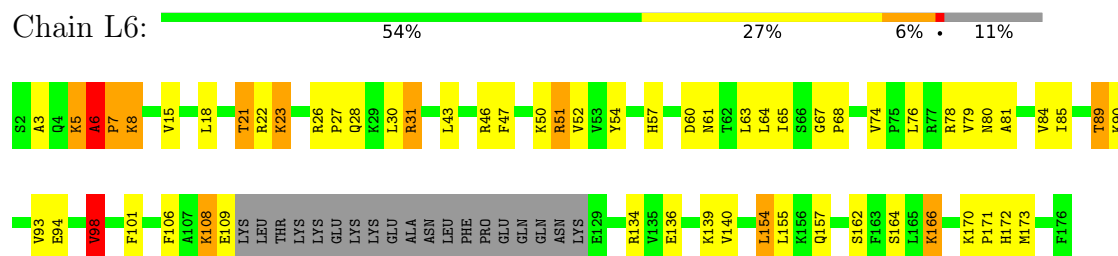
• Molecule 42: 60S ribosomal protein L5



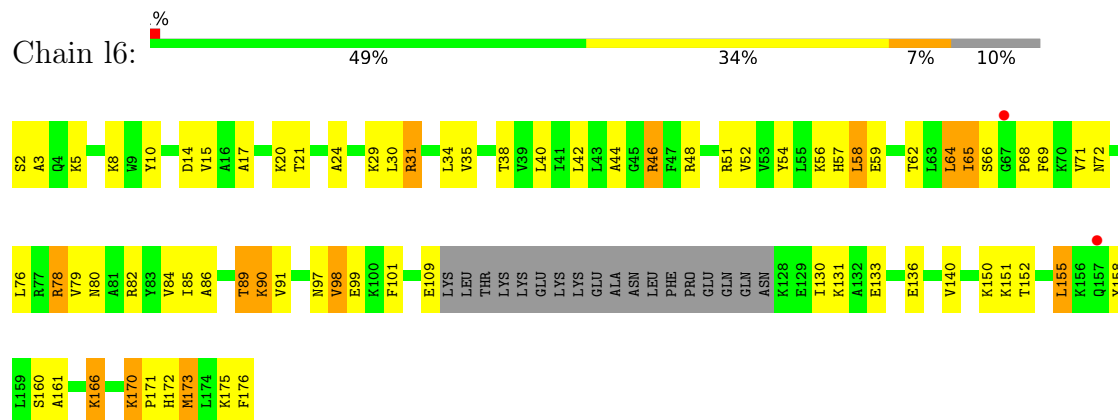
• Molecule 42: 60S ribosomal protein L5



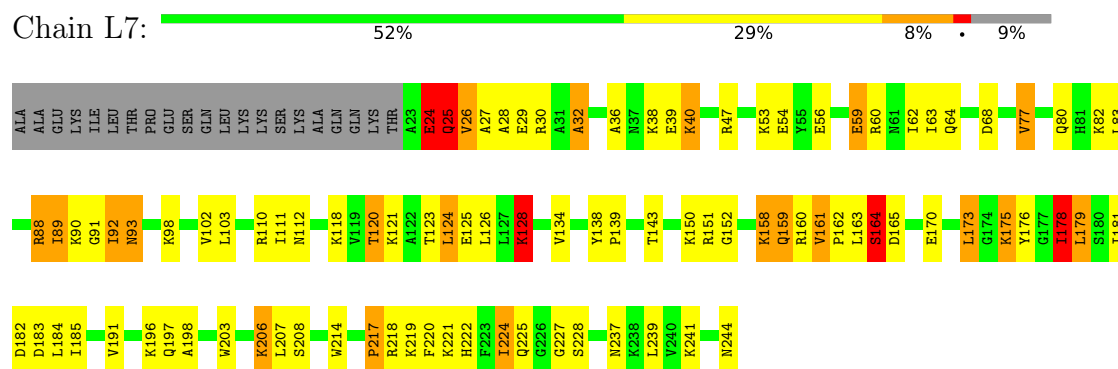
- Molecule 43: 60S ribosomal protein L6-A



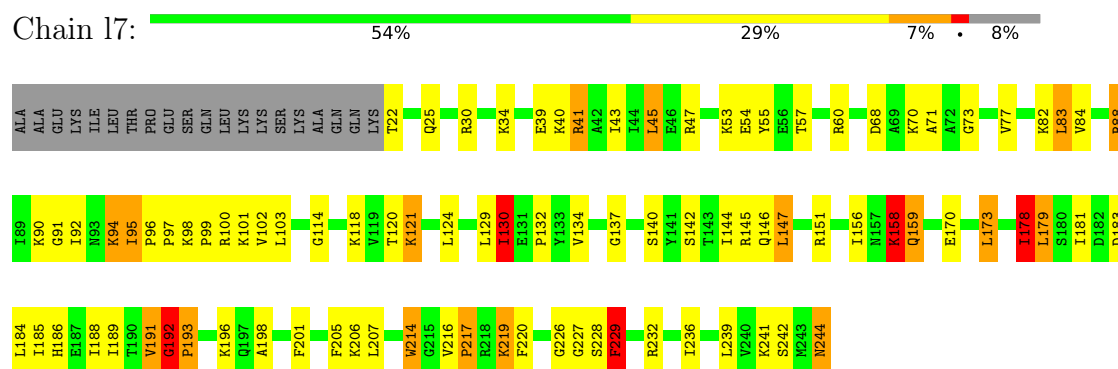
- Molecule 43: 60S ribosomal protein L6-A



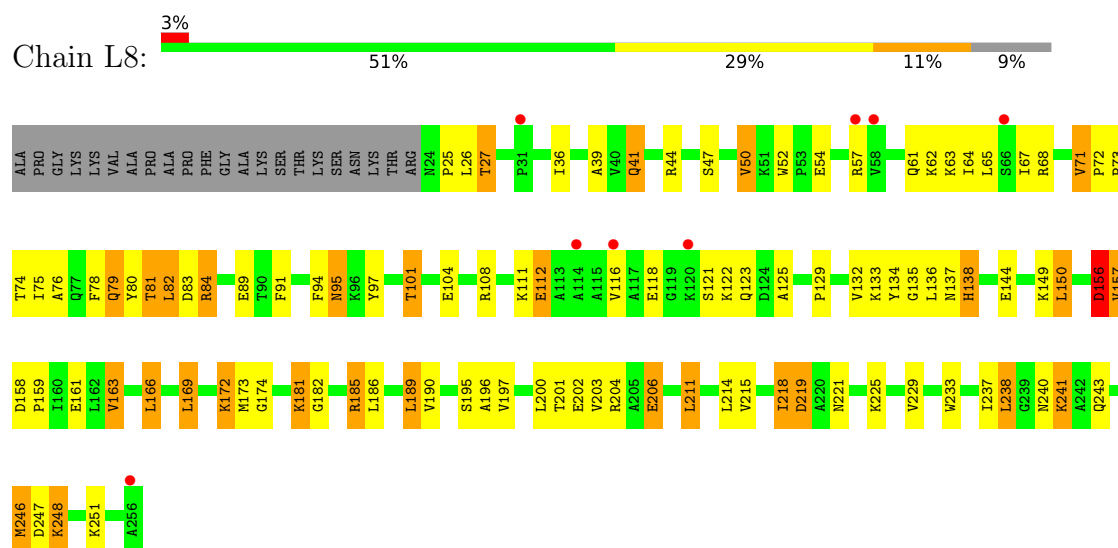
- Molecule 44: 60S ribosomal protein L7-A



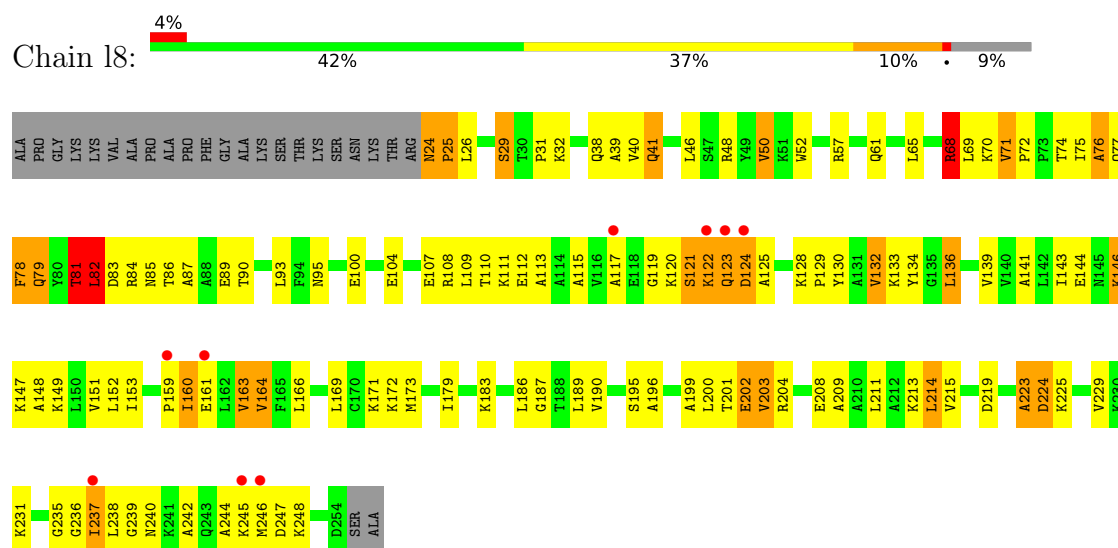
- Molecule 44: 60S ribosomal protein L7-A



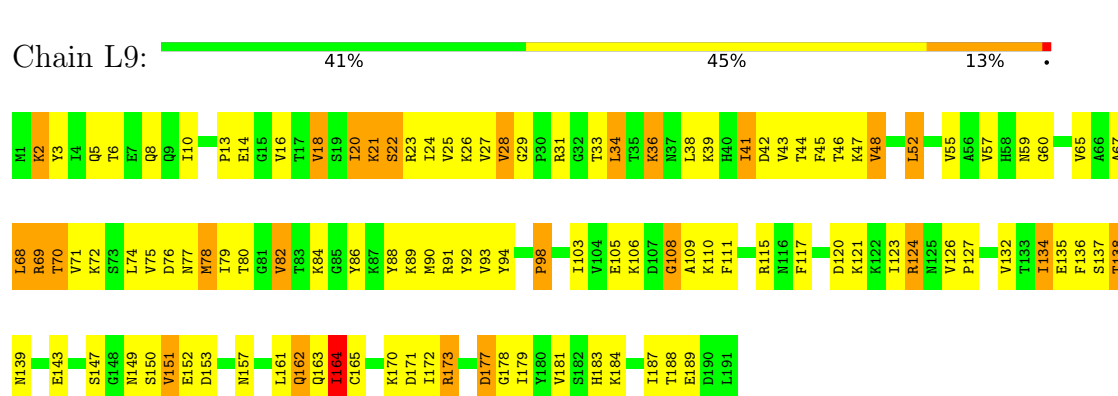
- Molecule 45: 60S ribosomal protein L8-A



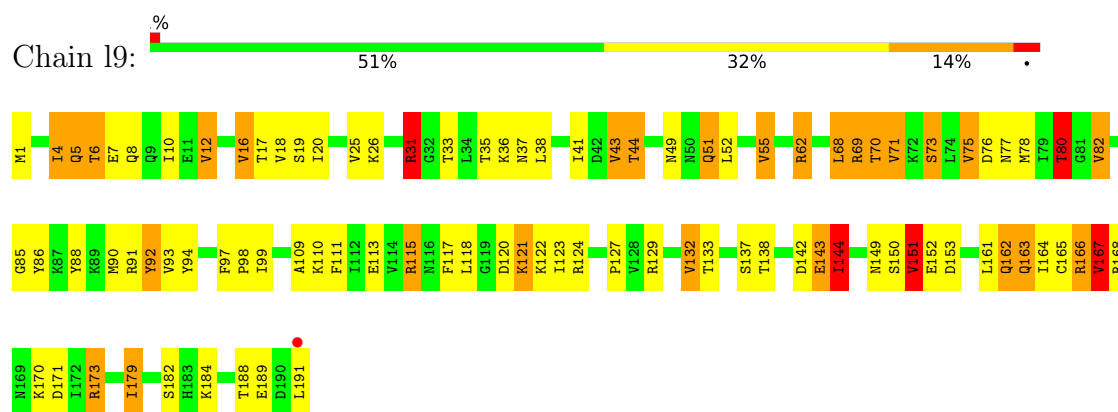
- Molecule 45: 60S ribosomal protein L8-A



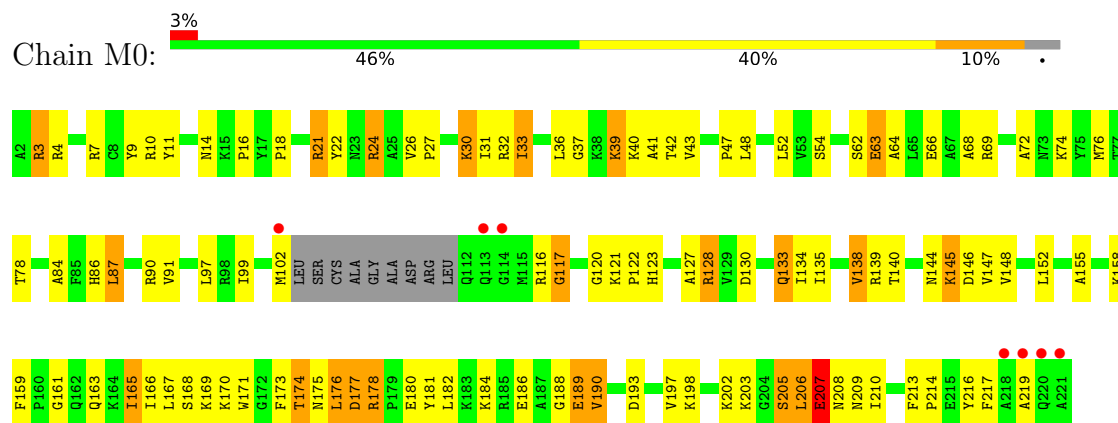
- Molecule 46: 60S ribosomal protein L9-A



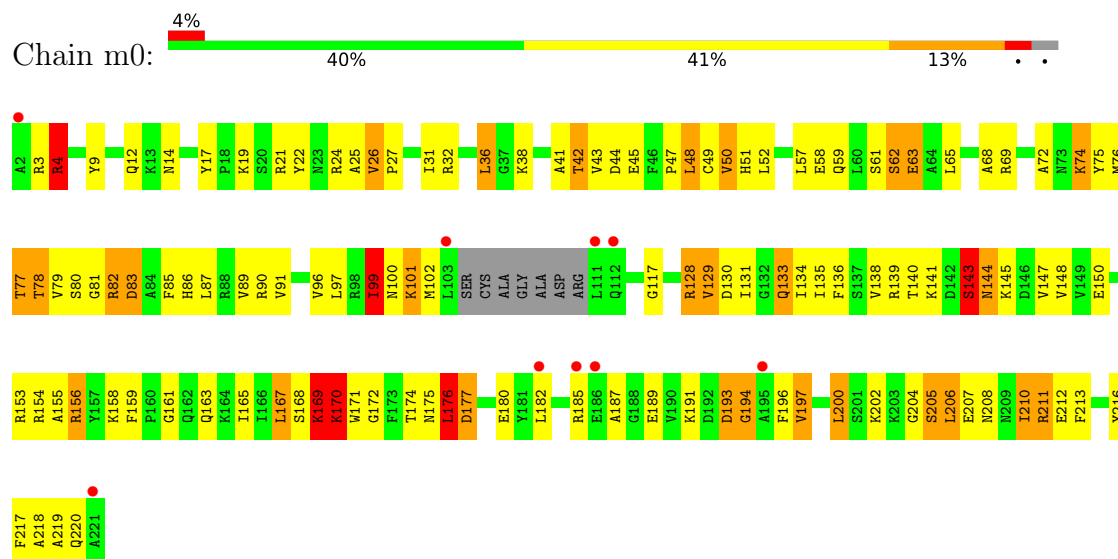
- Molecule 46: 60S ribosomal protein L9-A



• Molecule 47: 60S ribosomal protein L10

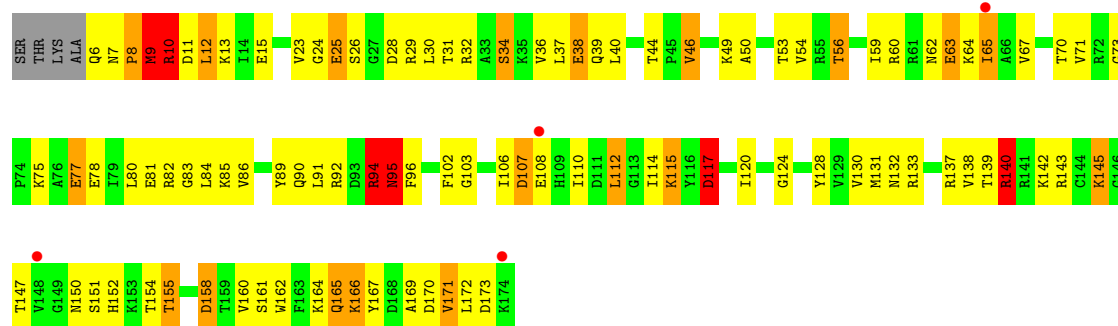


• Molecule 47: 60S ribosomal protein L10

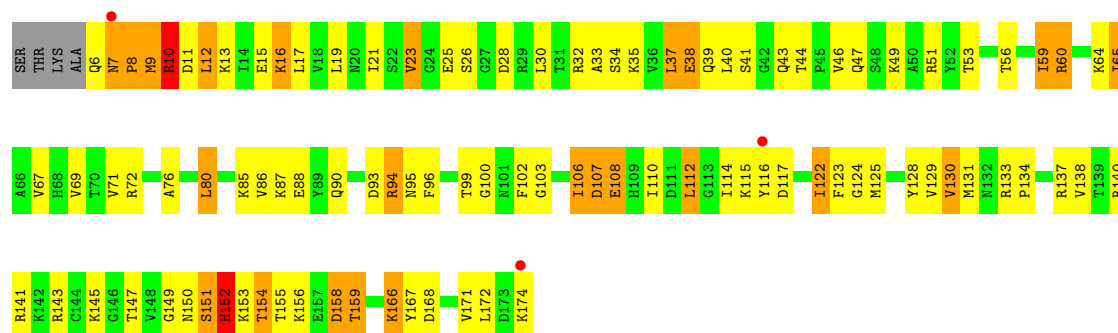
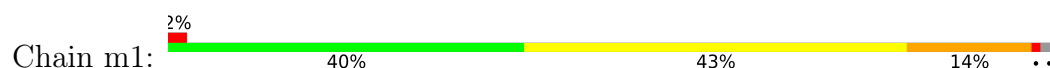


• Molecule 48: 60S ribosomal protein L11-B

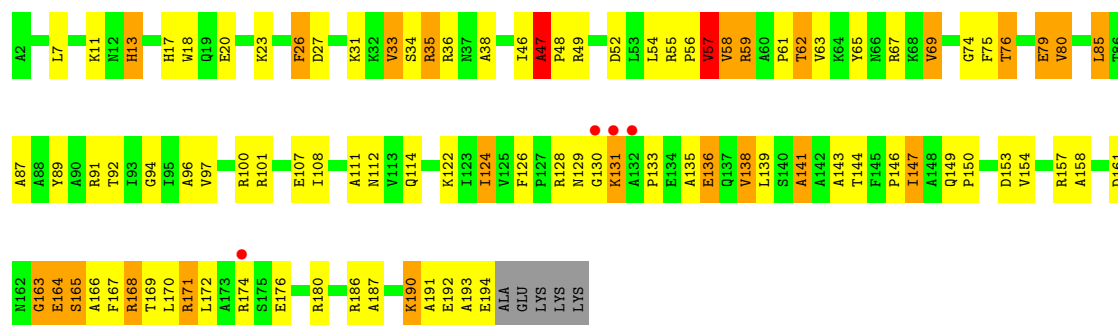




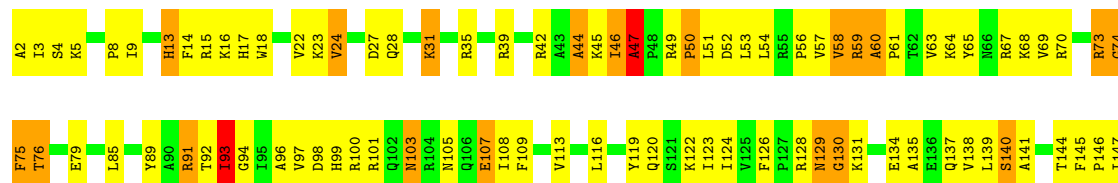
• Molecule 48: 60S ribosomal protein L11-B

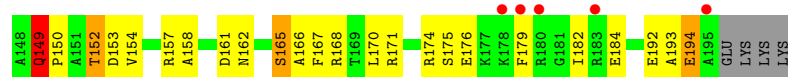


• Molecule 49: 60S ribosomal protein L13-A

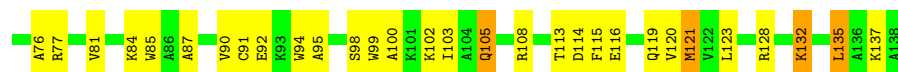
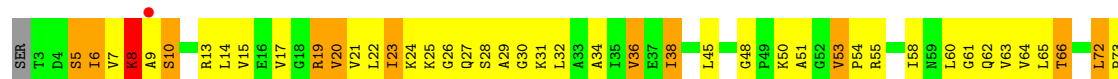


• Molecule 49: 60S ribosomal protein L13-A

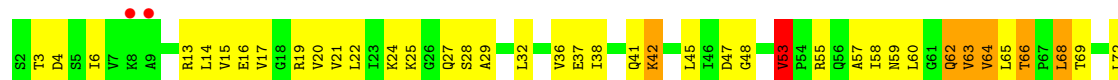
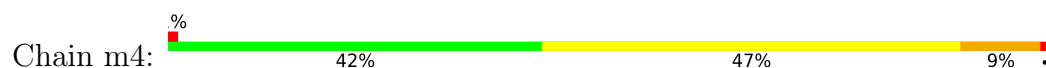




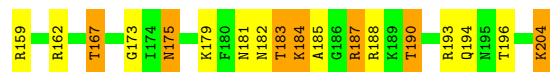
- Molecule 50: 60S ribosomal protein L14-A



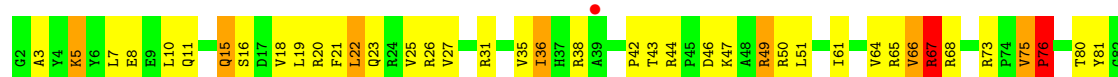
- Molecule 50: 60S ribosomal protein L14-A

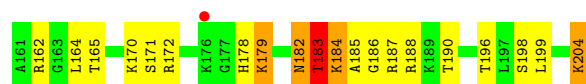


- Molecule 51: 60S ribosomal protein L15-A

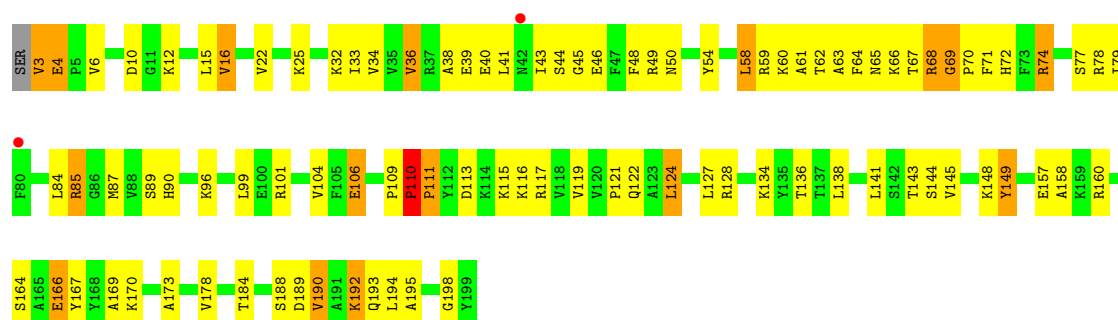


- Molecule 51: 60S ribosomal protein L15-A

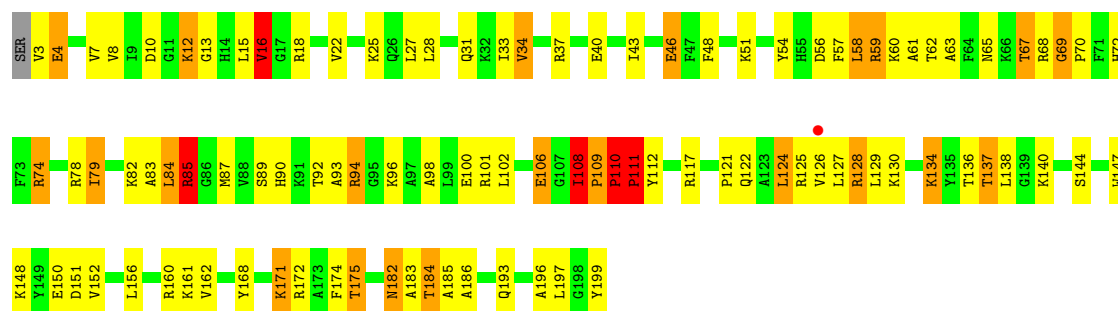




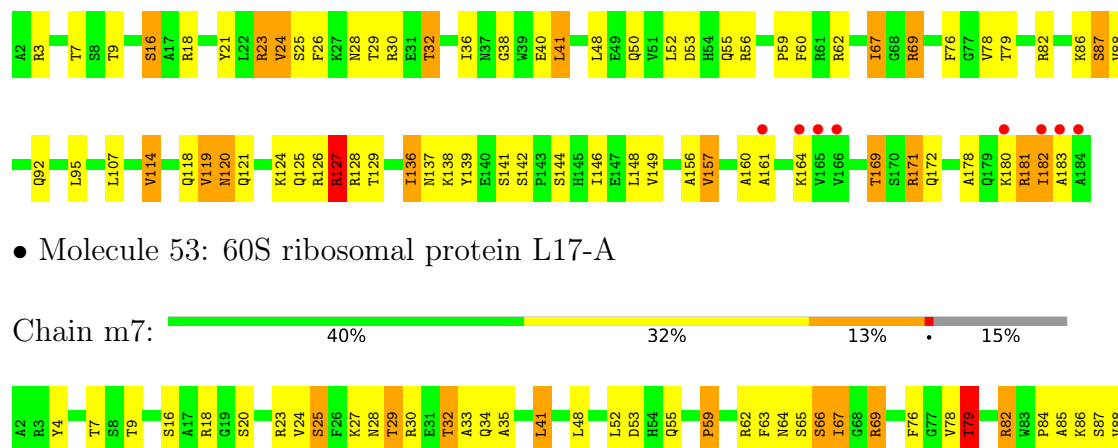
- Molecule 52: 60S ribosomal protein L16-A



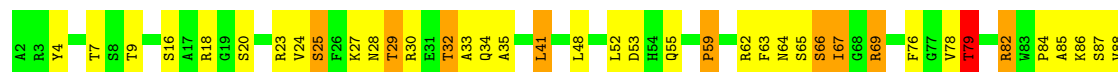
- Molecule 52: 60S ribosomal protein L16-A

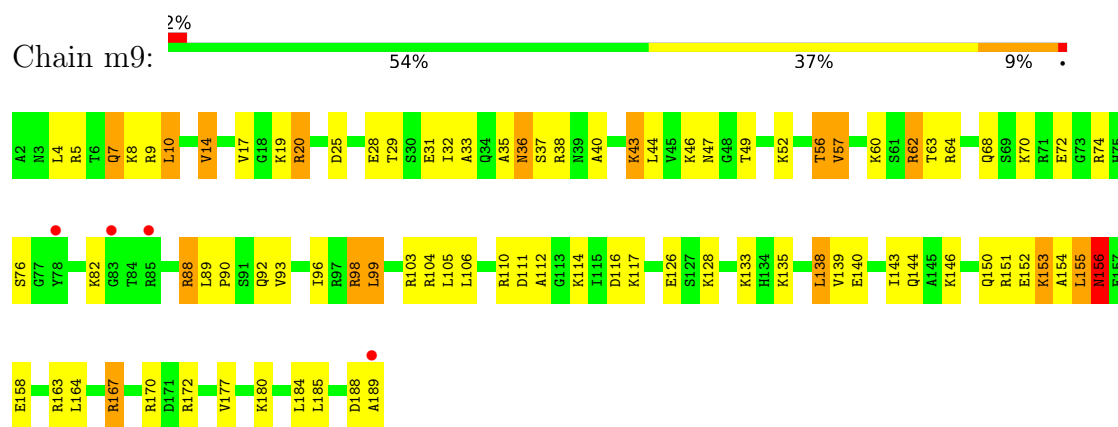


- Molecule 53: 60S ribosomal protein L17-A

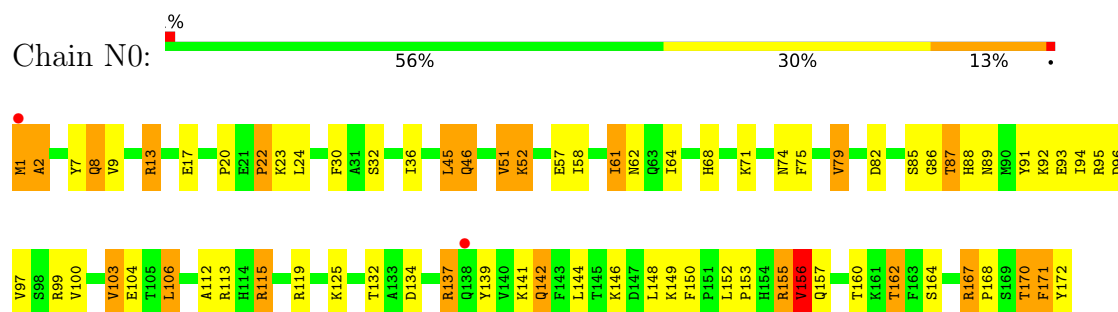


- Molecule 53: 60S ribosomal protein L17-A

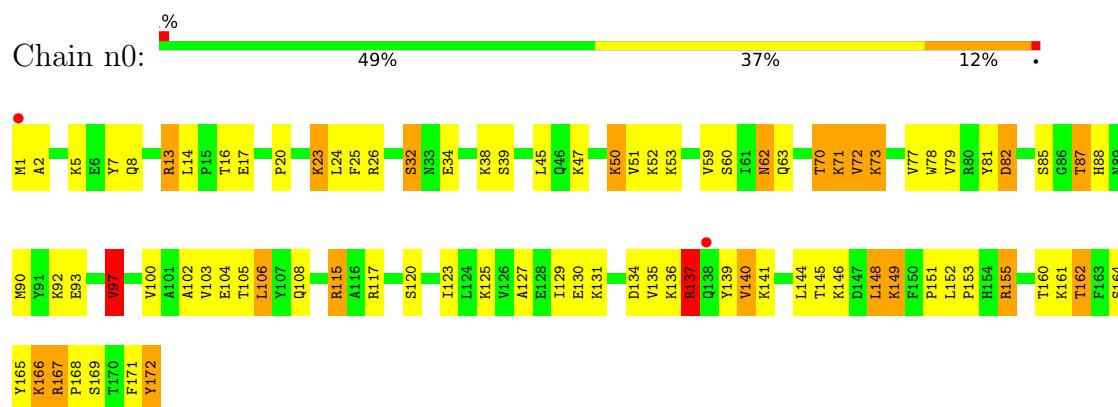




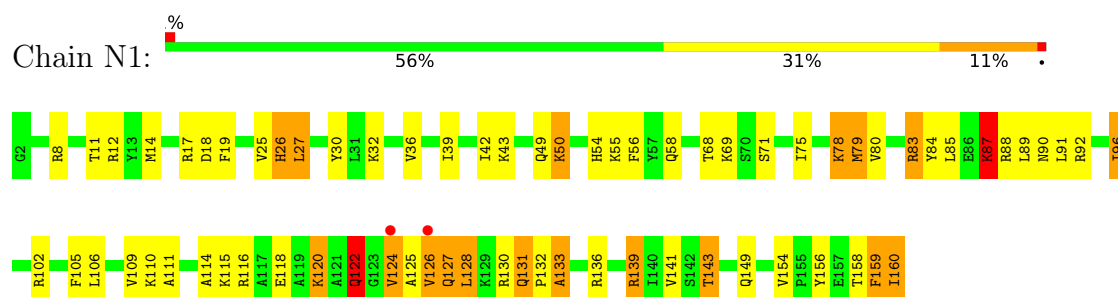
- Molecule 56: 60S ribosomal protein L20-A



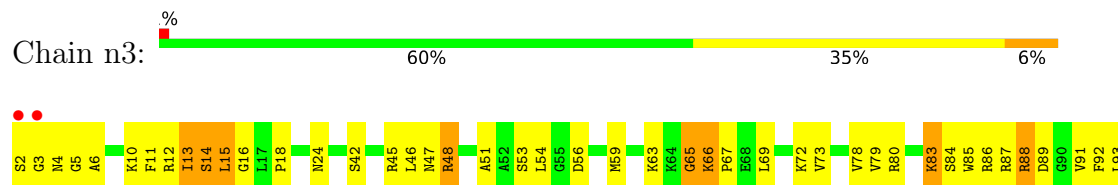
- Molecule 56: 60S ribosomal protein L20-A

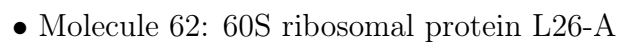


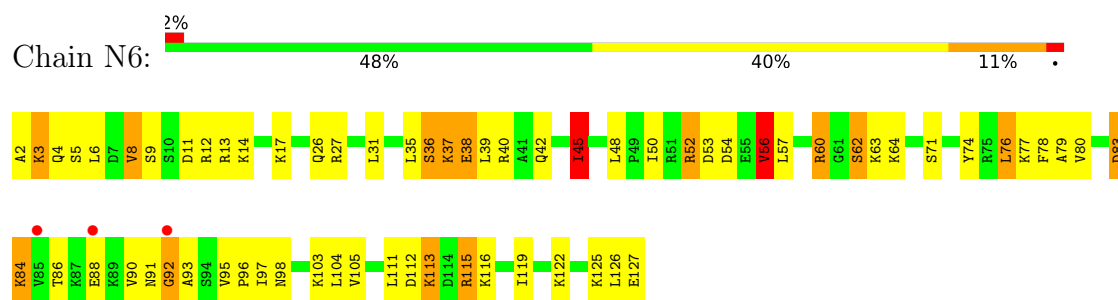
- Molecule 57: 60S ribosomal protein L21-A



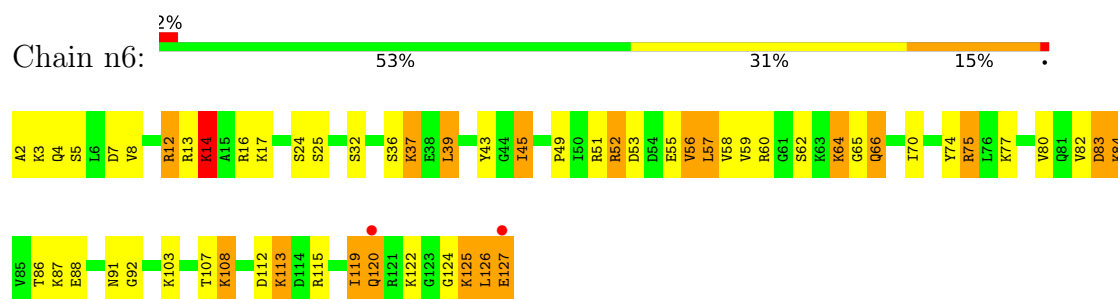
- Molecule 57: 60S ribosomal protein L21-A



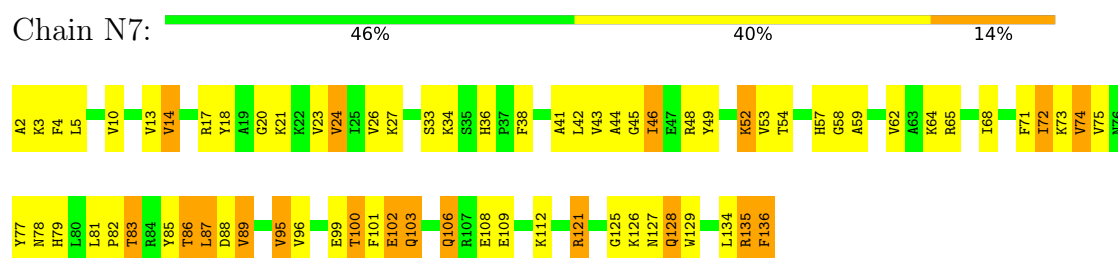




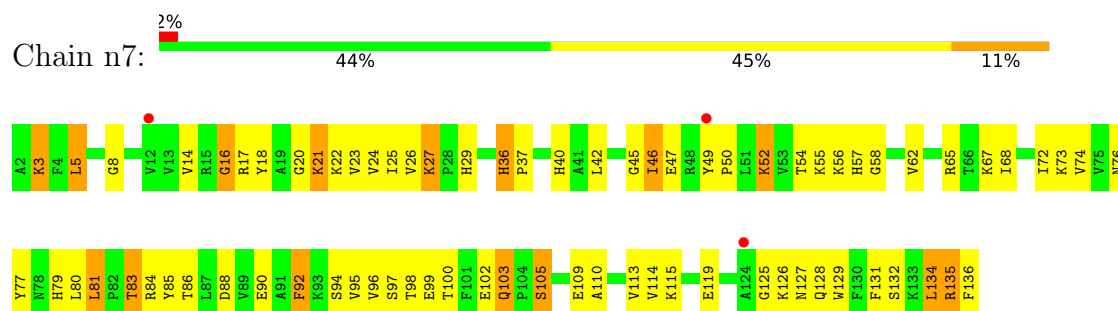
• Molecule 62: 60S ribosomal protein L26-A



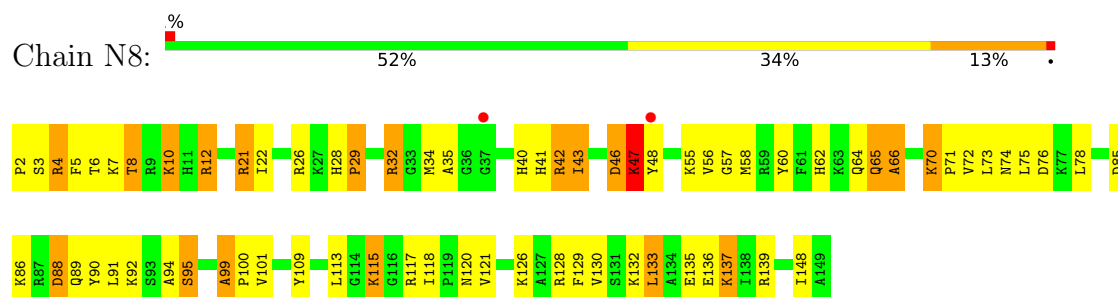
• Molecule 63: 60S ribosomal protein L27-A



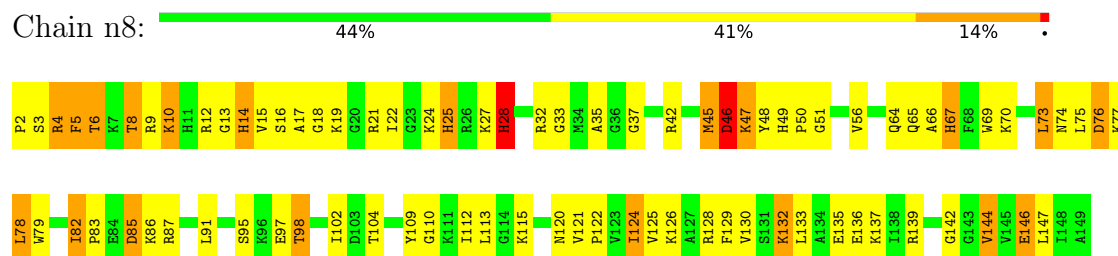
• Molecule 63: 60S ribosomal protein L27-A



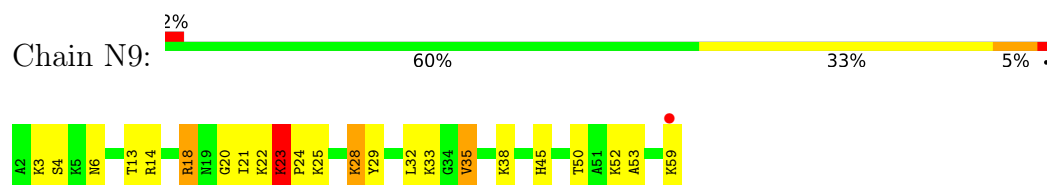
• Molecule 64: 60S ribosomal protein L28



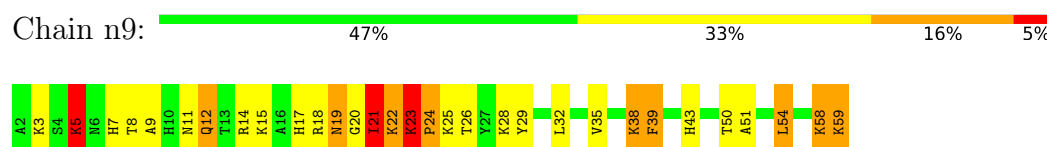
- Molecule 64: 60S ribosomal protein L28



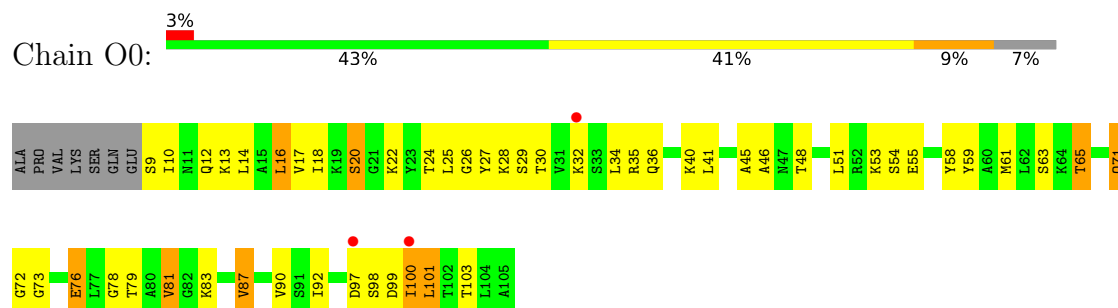
- Molecule 65: 60S ribosomal protein L29



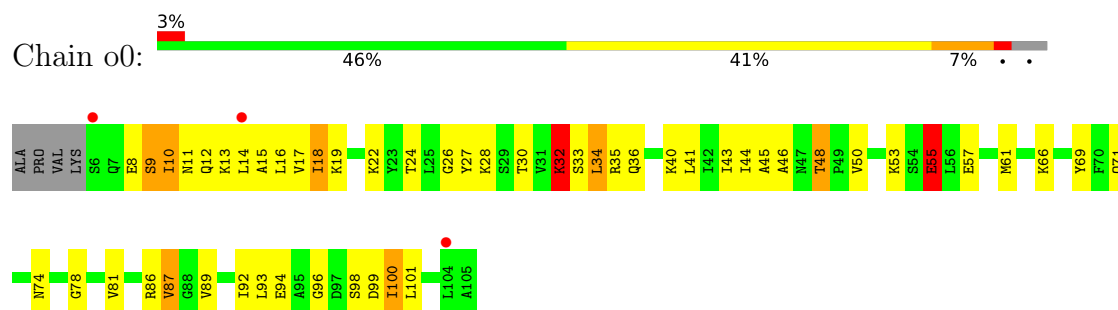
- Molecule 65: 60S ribosomal protein L29



- Molecule 66: 60S ribosomal protein L30



- Molecule 66: 60S ribosomal protein L30



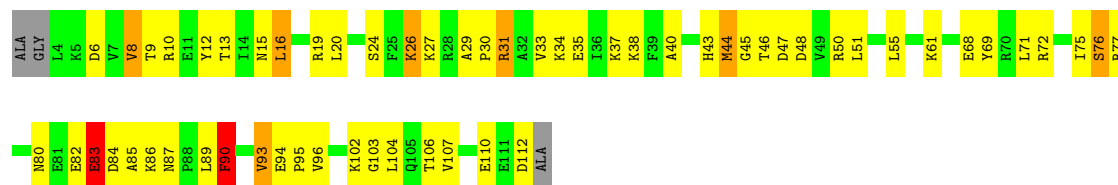
- Molecule 67: 60S ribosomal protein L31-A





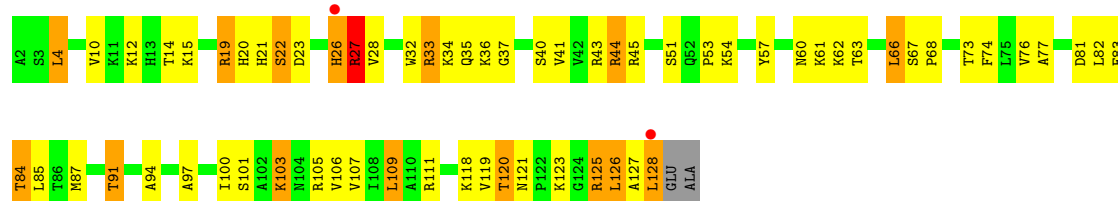
• Molecule 67: 60S ribosomal protein L31-A

Chain o1: 45% 45% 6% ..



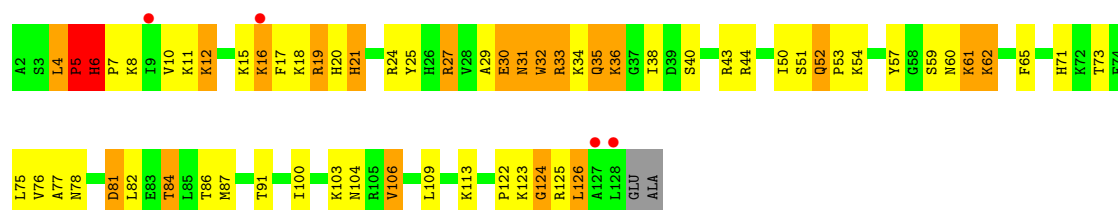
• Molecule 68: 60S ribosomal protein L32

Chain O2: 2% 48% 38% 12% ..



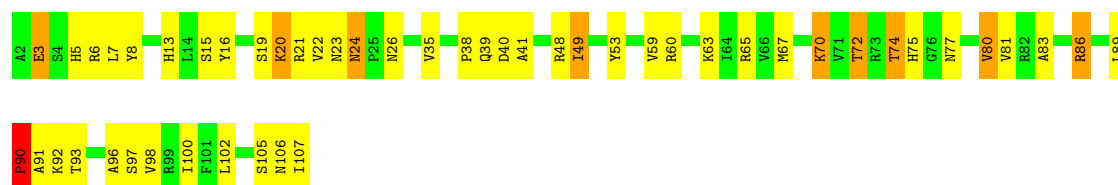
• Molecule 68: 60S ribosomal protein L32

Chain o2: 3% 49% 33% 16% ..

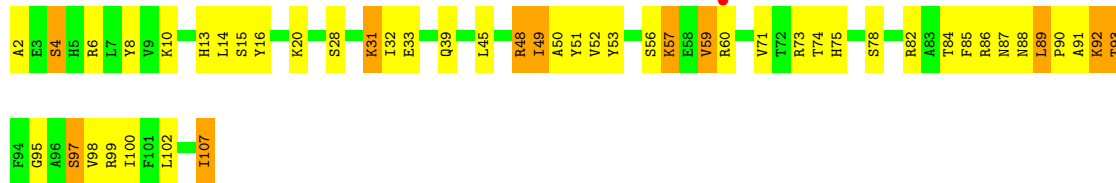


• Molecule 69: 60S ribosomal protein L33-A

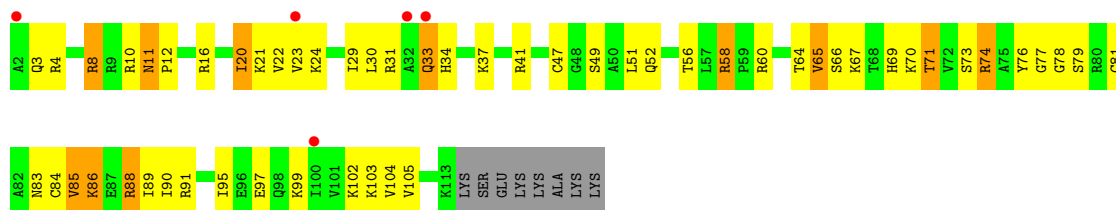
Chain O3: 53% 38% 8% ..



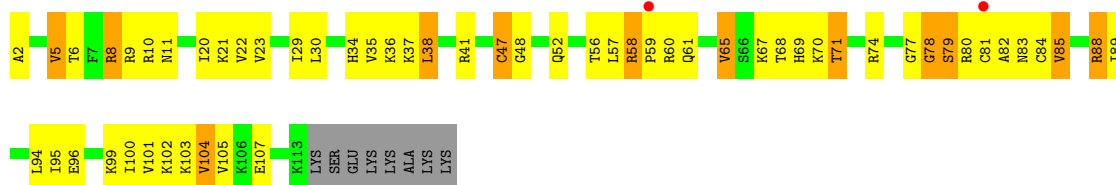
• Molecule 69: 60S ribosomal protein L33-A



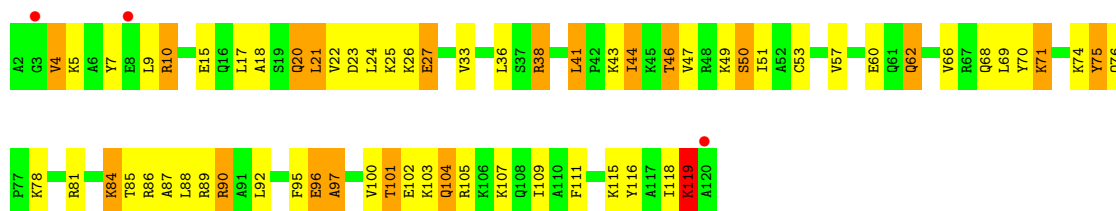
• Molecule 70: 60S ribosomal protein L34-A



• Molecule 70: 60S ribosomal protein L34-A

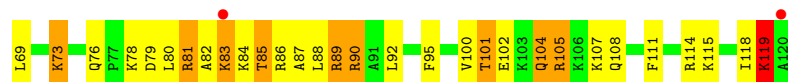


• Molecule 71: 60S ribosomal protein L35-A

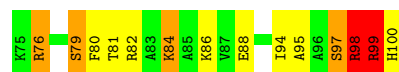


• Molecule 71: 60S ribosomal protein L35-A

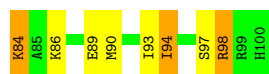




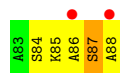
• Molecule 72: 60S ribosomal protein L36-A



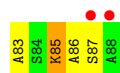
• Molecule 72: 60S ribosomal protein L36-A



• Molecule 73: 60S ribosomal protein L37-A

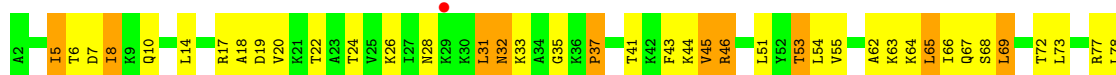


• Molecule 73: 60S ribosomal protein L37-A



• Molecule 74: 60S ribosomal protein L38

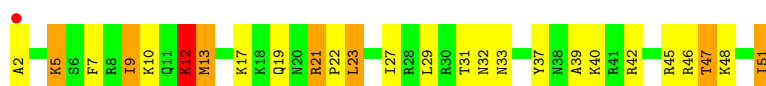




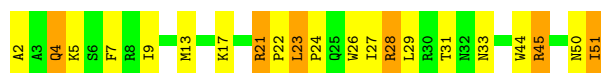
- Molecule 74: 60S ribosomal protein L38



- Molecule 75: 60S ribosomal protein L39



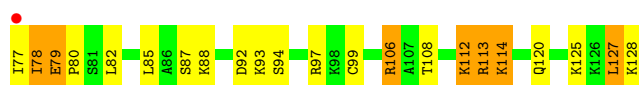
- Molecule 75: 60S ribosomal protein L39



- Molecule 76: Ubiquitin-60S ribosomal protein L40



- Molecule 76: Ubiquitin-60S ribosomal protein L40



- Molecule 77: 60S ribosomal protein L41-A

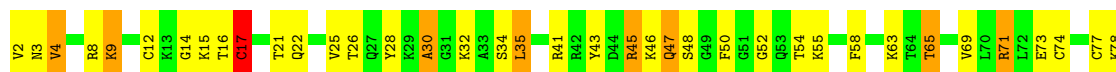


- Molecule 77: 60S ribosomal protein L41-A





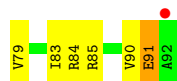
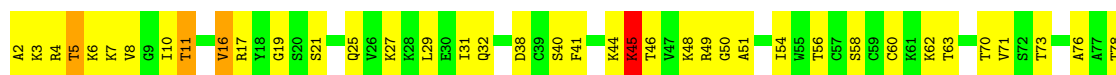
- Molecule 78: 60S ribosomal protein L42-A



- Molecule 78: 60S ribosomal protein L42-A



- Molecule 79: 60S ribosomal protein L43-A

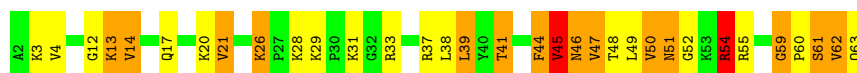


- Molecule 79: 60S ribosomal protein L43-A



- Molecule 80: 40S ribosomal protein S30-A





- Molecule 81: unknown protein chain m2

Chain m2: 84% 9% 6%



- Molecule 82: 60S acidic ribosomal protein P0

Chain p0: 3% 24% 18% 54%



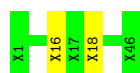
- Molecule 83: unknown protein chain p1

Chain p1: 83% 17%



- Molecule 84: unknown protein chain 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	436.92Å 288.52Å 305.75Å 90.00° 99.04° 90.00°	Depositor
Resolution (Å)	267.96 – 3.20 267.96 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (267.96-3.20) 99.9 (267.96-3.20)	Depositor EDS
R_{merge}	0.39	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.193 , 0.245 0.195 , 0.245	Depositor DCC
R_{free} test set	24529 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	81.5	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 169.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	411223	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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: PCY, MG, OHX, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.43	0/41698	0.63	4/64972 (0.0%)
1	6	0.51	0/42765	0.68	8/66634 (0.0%)
2	S0	0.64	0/1617	1.12	11/2215 (0.5%)
2	s0	0.70	0/1623	1.13	6/2222 (0.3%)
3	S1	0.53	0/1735	0.95	7/2335 (0.3%)
3	s1	0.63	0/1748	1.03	10/2352 (0.4%)
4	S2	0.69	0/1665	1.10	11/2263 (0.5%)
4	s2	0.82	0/1665	1.23	12/2263 (0.5%)
5	S3	0.63	0/1759	1.05	4/2368 (0.2%)
5	s3	0.60	0/1759	1.02	9/2368 (0.4%)
6	S4	0.64	0/2109	1.09	15/2839 (0.5%)
6	s4	0.75	0/2109	1.11	7/2839 (0.2%)
7	S5	0.54	0/1629	1.04	4/2202 (0.2%)
7	s5	0.64	0/1629	1.06	6/2202 (0.3%)
8	S6	0.61	0/1823	1.04	9/2439 (0.4%)
8	s6	0.75	0/1779	1.07	7/2379 (0.3%)
9	S7	0.58	0/1506	1.05	5/2028 (0.2%)
9	s7	0.65	0/1516	1.13	10/2043 (0.5%)
10	S8	0.75	0/1514	1.09	5/2021 (0.2%)
10	s8	0.85	1/1514 (0.1%)	1.15	6/2021 (0.3%)
11	S9	0.65	0/1519	1.05	4/2035 (0.2%)
11	s9	0.75	0/1519	1.22	15/2035 (0.7%)
12	C0	0.55	0/790	1.02	3/1069 (0.3%)
12	c0	0.52	0/777	0.94	3/1049 (0.3%)
13	C1	0.81	1/1240 (0.1%)	1.16	8/1675 (0.5%)
13	c1	0.86	1/1194 (0.1%)	1.20	6/1610 (0.4%)
14	C2	0.54	0/900	0.94	0/1224
14	c2	0.43	0/900	0.91	1/1224 (0.1%)
15	C3	0.68	0/1215	1.03	4/1638 (0.2%)
15	c3	0.77	0/1215	1.17	5/1638 (0.3%)
16	C4	0.65	0/901	1.05	3/1217 (0.2%)
16	c4	0.71	0/960	1.15	7/1290 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.62	0/998	1.00	0/1341
17	c5	0.64	0/1060	1.13	9/1426 (0.6%)
18	C6	0.60	0/1125	1.04	6/1510 (0.4%)
18	c6	0.68	0/1131	1.10	6/1518 (0.4%)
19	C7	0.62	0/935	1.04	6/1254 (0.5%)
19	c7	0.66	0/914	1.09	1/1224 (0.1%)
20	C8	0.61	0/1211	1.09	7/1628 (0.4%)
20	c8	0.66	0/1211	1.02	0/1628
21	C9	0.56	0/1130	0.96	2/1517 (0.1%)
21	c9	0.66	0/1130	1.02	1/1517 (0.1%)
22	D0	0.62	0/865	1.04	3/1169 (0.3%)
22	d0	0.67	0/892	1.06	6/1205 (0.5%)
23	D1	0.63	0/693	1.00	3/935 (0.3%)
23	d1	0.74	0/693	1.00	0/935
24	D2	0.70	0/1038	1.12	4/1395 (0.3%)
24	d2	0.84	0/1038	1.11	6/1395 (0.4%)
25	D3	0.81	0/1139	1.19	8/1518 (0.5%)
25	d3	0.90	2/1139 (0.2%)	1.19	4/1518 (0.3%)
26	D4	0.58	0/1087	0.99	1/1449 (0.1%)
26	d4	0.73	0/1087	1.13	4/1449 (0.3%)
27	D5	0.57	0/571	1.05	5/768 (0.7%)
27	d5	0.65	0/566	1.09	4/761 (0.5%)
28	D6	0.70	0/782	1.13	4/1047 (0.4%)
28	d6	0.75	0/782	1.10	3/1047 (0.3%)
29	D7	0.57	0/620	1.12	4/838 (0.5%)
29	d7	0.63	0/620	1.17	4/838 (0.5%)
30	D8	0.49	0/499	0.94	0/670
30	d8	0.59	0/499	1.08	3/670 (0.4%)
31	D9	0.68	0/452	1.05	1/600 (0.2%)
31	d9	0.66	0/452	1.04	4/600 (0.7%)
32	E0	0.61	0/483	1.04	1/643 (0.2%)
33	E1	0.64	0/577	1.10	3/770 (0.4%)
33	e1	0.59	0/619	1.03	3/822 (0.4%)
34	SR	0.59	0/2494	0.98	8/3393 (0.2%)
34	sR	0.54	0/2495	0.91	1/3395 (0.0%)
35	SM	0.75	0/1113	1.18	4/1502 (0.3%)
35	sM	0.67	0/682	1.34	10/921 (1.1%)
36	1	0.64	0/75394	0.78	17/117545 (0.0%)
36	5	0.66	0/75414	0.78	8/117575 (0.0%)
37	3	0.54	0/2883	0.69	1/4491 (0.0%)
37	7	0.64	0/2883	0.79	0/4491
38	4	0.63	0/3746	0.75	0/5832
38	8	0.56	0/3746	0.69	0/5832

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	1.00	3/1948 (0.2%)	1.28	15/2617 (0.6%)
39	l2	0.98	1/1946 (0.1%)	1.30	18/2614 (0.7%)
40	L3	0.93	2/3146 (0.1%)	1.21	12/4228 (0.3%)
40	l3	1.09	4/3146 (0.1%)	1.30	23/4228 (0.5%)
41	L4	1.04	3/2800 (0.1%)	1.35	17/3790 (0.4%)
41	l4	0.96	2/2800 (0.1%)	1.28	15/3790 (0.4%)
42	L5	0.72	0/2425	1.01	3/3271 (0.1%)
42	l5	0.89	0/2408	1.16	10/3248 (0.3%)
43	L6	0.98	0/1260	1.28	4/1694 (0.2%)
43	l6	0.94	0/1269	1.18	5/1705 (0.3%)
44	L7	1.02	1/1821 (0.1%)	1.23	7/2451 (0.3%)
44	l7	1.05	0/1828	1.30	14/2461 (0.6%)
45	L8	0.73	0/1836	1.06	7/2481 (0.3%)
45	l8	0.70	0/1795	1.12	10/2429 (0.4%)
46	L9	0.80	0/1539	1.10	0/2073
46	l9	1.04	1/1539 (0.1%)	1.21	9/2073 (0.4%)
47	M0	0.94	2/1741 (0.1%)	1.15	10/2335 (0.4%)
47	m0	0.99	0/1758	1.30	12/2358 (0.5%)
48	M1	0.64	0/1374	1.06	5/1842 (0.3%)
48	m1	0.85	0/1374	1.14	5/1842 (0.3%)
49	M3	1.00	3/1568 (0.2%)	1.25	6/2106 (0.3%)
49	m3	0.94	1/1573 (0.1%)	1.26	8/2113 (0.4%)
50	M4	0.98	0/1068	1.20	2/1438 (0.1%)
50	m4	1.10	2/1074 (0.2%)	1.28	5/1446 (0.3%)
51	M5	0.95	1/1757 (0.1%)	1.17	7/2354 (0.3%)
51	m5	0.83	0/1757	1.23	9/2354 (0.4%)
52	M6	1.03	0/1585	1.26	10/2128 (0.5%)
52	m6	1.22	1/1585 (0.1%)	1.40	13/2128 (0.6%)
53	M7	1.02	0/1443	1.16	3/1944 (0.2%)
53	m7	1.11	2/1250 (0.2%)	1.20	3/1683 (0.2%)
54	M8	1.03	2/1465 (0.1%)	1.37	15/1965 (0.8%)
54	m8	0.97	0/1465	1.26	9/1965 (0.5%)
55	M9	0.73	0/1538	1.08	3/2050 (0.1%)
55	m9	0.82	0/1538	1.01	1/2050 (0.0%)
56	N0	0.95	0/1481	1.23	6/1990 (0.3%)
56	n0	1.15	2/1481 (0.1%)	1.31	10/1990 (0.5%)
57	N1	0.96	0/1300	1.20	2/1743 (0.1%)
57	n1	1.00	0/1300	1.20	1/1743 (0.1%)
58	N2	0.55	0/812	0.95	3/1099 (0.3%)
58	n2	0.60	0/794	1.10	5/1076 (0.5%)
59	N3	0.93	0/1018	1.20	7/1369 (0.5%)
59	n3	1.13	0/1018	1.34	6/1369 (0.4%)
60	N4	0.76	0/712	1.25	3/958 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.95	0/1052	1.19	4/1398 (0.3%)
61	N5	0.82	0/979	1.19	4/1321 (0.3%)
61	n5	0.84	0/974	1.19	8/1314 (0.6%)
62	N6	0.91	0/1004	1.21	2/1341 (0.1%)
62	n6	0.87	0/1004	1.15	2/1341 (0.1%)
63	N7	0.67	0/1118	1.09	2/1497 (0.1%)
63	n7	0.62	0/1118	1.02	4/1497 (0.3%)
64	N8	1.06	1/1204 (0.1%)	1.33	9/1612 (0.6%)
64	n8	0.96	0/1204	1.34	12/1612 (0.7%)
65	N9	0.94	0/473	1.37	2/629 (0.3%)
65	n9	1.00	0/473	1.49	5/629 (0.8%)
66	O0	0.61	0/751	1.01	1/1008 (0.1%)
66	o0	0.64	0/775	0.99	2/1040 (0.2%)
67	O1	0.83	1/890 (0.1%)	1.16	4/1196 (0.3%)
67	o1	0.96	0/897	1.25	4/1205 (0.3%)
68	O2	1.11	1/1041 (0.1%)	1.31	4/1394 (0.3%)
68	o2	1.01	1/1041 (0.1%)	1.29	6/1394 (0.4%)
69	O3	1.06	0/868	1.27	7/1168 (0.6%)
69	o3	1.12	2/868 (0.2%)	1.33	7/1168 (0.6%)
70	O4	0.87	0/890	1.25	4/1189 (0.3%)
70	o4	0.80	0/890	1.20	6/1189 (0.5%)
71	O5	0.89	0/978	1.17	3/1301 (0.2%)
71	o5	0.76	0/974	1.04	1/1297 (0.1%)
72	O6	0.82	0/778	1.16	3/1034 (0.3%)
72	o6	0.74	0/777	1.16	4/1033 (0.4%)
73	O7	1.03	0/696	1.44	5/923 (0.5%)
73	o7	0.91	0/696	1.16	2/923 (0.2%)
74	O8	0.63	0/618	1.07	2/826 (0.2%)
74	o8	0.62	0/614	0.99	0/822
75	O9	1.02	0/443	1.21	2/588 (0.3%)
75	o9	0.86	0/443	1.19	2/588 (0.3%)
76	Q0	0.78	0/423	1.07	2/562 (0.4%)
76	q0	1.11	0/423	1.30	3/562 (0.5%)
77	Q1	0.79	0/234	0.99	0/300
77	q1	0.92	0/234	1.07	1/300 (0.3%)
78	Q2	0.95	1/860 (0.1%)	1.20	6/1136 (0.5%)
78	q2	0.86	2/860 (0.2%)	1.05	2/1136 (0.2%)
79	Q3	0.93	0/701	1.17	4/934 (0.4%)
79	q3	0.86	0/701	1.19	2/934 (0.2%)
80	e0	0.74	0/499	1.24	4/665 (0.6%)
82	p0	0.58	0/1091	0.99	2/1472 (0.1%)
All	All	0.70	47/430072 (0.0%)	0.92	867/631360 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	s5	0	2
9	S7	0	1
9	s7	0	2
10	S8	0	2
16	C4	0	2
16	c4	0	1
17	c5	0	1
18	c6	0	1
19	C7	0	2
19	c7	0	2
22	d0	0	1
25	d3	0	1
26	d4	0	1
27	D5	0	2
27	d5	0	1
28	D6	0	1
31	D9	0	1
34	SR	0	1
39	L2	0	1
39	l2	0	2
43	L6	0	1
44	l7	0	2
47	m0	0	1
51	m5	0	1
52	M6	0	1
52	m6	0	1
56	N0	0	1
64	n8	0	2
65	N9	0	1
65	n9	0	1
67	O1	0	1
67	o1	0	1
68	o2	0	2
73	o7	0	1
81	m2	0	1
All	All	0	46

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	M0	127	ALA	CA-CB	-9.53	1.38	1.53
54	M8	18	ALA	CA-CB	-7.22	1.45	1.54
78	Q2	17	CYS	CB-SG	7.03	2.04	1.81
39	L2	192	LYS	CA-C	6.68	1.56	1.52
40	l3	295	ALA	CA-CB	-6.43	1.43	1.53

The worst 5 of 867 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	m5	75	VAL	CA-C-N	14.78	138.31	119.84
51	m5	75	VAL	C-N-CA	14.78	138.31	119.84
65	n9	23	LYS	CA-C-N	-13.68	102.74	119.84
65	n9	23	LYS	C-N-CA	-13.68	102.74	119.84
60	N4	80	ARG	CA-C-N	13.67	136.93	119.84

There are no chirality outliers.

5 of 46 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
16	C4	124	ASP	Peptide
9	S7	131	PHE	Peptide
10	S8	79	ALA	Peptide
10	S8	8	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37283	0	18757	966	1
1	6	38238	0	19240	863	0
2	S0	1577	0	1567	86	0
2	s0	1583	0	1578	70	0
3	S1	1709	0	1784	114	0
3	s1	1722	0	1793	86	0
4	S2	1635	0	1723	73	0
4	s2	1635	0	1723	74	0
5	S3	1734	0	1817	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	s3	1734	0	1817	73	0
6	S4	2068	0	2154	91	0
6	s4	2068	0	2154	98	0
7	S5	1609	0	1675	106	0
7	s5	1609	0	1675	90	0
8	S6	1799	0	1878	103	0
8	s6	1755	0	1846	73	0
9	S7	1481	0	1572	73	0
9	s7	1491	0	1578	79	0
10	S8	1489	0	1525	56	0
10	s8	1489	0	1525	72	0
11	S9	1494	0	1573	76	0
11	s9	1494	0	1573	88	0
12	C0	773	0	729	40	0
12	c0	762	0	699	39	0
13	C1	1214	0	1259	59	0
13	c1	1168	0	1231	55	0
14	C2	892	0	891	29	0
14	c2	892	0	891	23	0
15	C3	1192	0	1255	50	0
15	c3	1192	0	1255	57	0
16	C4	891	0	883	58	0
16	c4	949	0	985	48	0
17	C5	977	0	1002	52	0
17	c5	1039	0	1050	65	0
18	C6	1105	0	1166	59	0
18	c6	1111	0	1171	48	0
19	C7	926	0	930	43	0
19	c7	906	0	909	37	0
20	C8	1192	0	1222	65	0
20	c8	1192	0	1222	61	0
21	C9	1112	0	1124	57	0
21	c9	1112	0	1124	41	0
22	D0	855	0	917	51	0
22	d0	882	0	939	38	0
23	D1	684	0	672	36	0
23	d1	684	0	672	34	0
24	D2	1021	0	1060	48	0
24	d2	1021	0	1060	40	0
25	D3	1121	0	1196	61	0
25	d3	1121	0	1196	42	0
26	D4	1073	0	1132	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	d4	1073	0	1132	48	0
27	D5	563	0	603	34	0
27	d5	558	0	598	38	0
28	D6	769	0	814	81	0
28	d6	769	0	814	47	0
29	D7	610	0	631	19	0
29	d7	610	0	632	19	0
30	D8	497	0	535	26	0
30	d8	497	0	535	25	0
31	D9	442	0	428	20	0
31	d9	442	0	428	20	0
32	E0	475	0	525	19	0
33	E1	566	0	602	35	0
33	e1	608	0	656	34	0
34	SR	2441	0	2397	109	0
34	sR	2442	0	2392	93	0
35	SM	1104	0	996	50	0
35	sM	679	0	603	31	0
36	1	67355	0	33845	1220	0
36	5	67376	0	33856	1198	0
37	3	2579	0	1304	55	0
37	7	2579	0	1303	50	0
38	4	3353	0	1695	65	1
38	8	3353	0	1695	72	0
39	L2	1914	0	1981	81	0
39	l2	1912	0	1976	86	0
40	L3	3075	0	3142	128	0
40	l3	3075	0	3142	134	0
41	L4	2748	0	2859	120	0
41	l4	2748	0	2859	133	0
42	L5	2375	0	2325	119	0
42	l5	2359	0	2311	91	0
43	L6	1239	0	1326	35	0
43	l6	1248	0	1339	50	0
44	L7	1784	0	1862	74	0
44	l7	1791	0	1869	57	0
45	L8	1804	0	1877	68	0
45	l8	1763	0	1819	68	0
46	L9	1518	0	1587	93	0
46	l9	1518	0	1587	71	0
47	M0	1705	0	1735	75	0
47	m0	1722	0	1755	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	M1	1353	0	1383	66	0
48	m1	1353	0	1383	56	0
49	M3	1543	0	1608	72	0
49	m3	1548	0	1613	86	0
50	M4	1053	0	1149	51	0
50	m4	1059	0	1154	50	0
51	M5	1720	0	1779	73	0
51	m5	1720	0	1779	74	0
52	M6	1555	0	1659	66	0
52	m6	1555	0	1659	67	0
53	M7	1420	0	1437	44	0
53	m7	1227	0	1236	56	0
54	M8	1441	0	1543	63	0
54	m8	1441	0	1543	45	0
55	M9	1521	0	1617	68	0
55	m9	1521	0	1617	58	0
56	N0	1445	0	1487	51	0
56	n0	1445	0	1487	54	0
57	N1	1276	0	1323	48	0
57	n1	1276	0	1323	61	0
58	N2	796	0	812	23	0
58	n2	778	0	791	19	0
59	N3	1003	0	1048	44	0
59	n3	1003	0	1048	39	0
60	N4	699	0	640	14	0
60	n4	1038	0	1071	23	1
61	N5	964	0	1025	33	0
61	n5	959	0	1023	43	0
62	N6	993	0	1081	34	0
62	n6	993	0	1081	37	0
63	N7	1092	0	1155	52	0
63	n7	1092	0	1155	54	0
64	N8	1173	0	1215	57	0
64	n8	1173	0	1215	65	0
65	N9	462	0	491	10	0
65	n9	462	0	491	31	0
66	O0	743	0	797	27	0
66	o0	767	0	816	35	0
67	O1	876	0	912	23	0
67	o1	883	0	918	28	0
68	O2	1020	0	1090	38	0
68	o2	1020	0	1090	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	O3	850	0	880	32	0
69	o3	850	0	880	37	0
70	O4	880	0	945	45	0
70	o4	880	0	945	34	0
71	O5	969	0	1078	42	0
71	o5	965	0	1067	60	0
72	O6	771	0	849	44	0
72	o6	770	0	846	30	0
73	O7	681	0	683	27	0
73	o7	681	0	683	25	0
74	O8	612	0	682	20	0
74	o8	608	0	671	31	0
75	O9	436	0	475	22	0
75	o9	436	0	475	18	0
76	Q0	417	0	455	13	0
76	q0	417	0	455	13	0
77	Q1	233	0	284	15	0
77	q1	233	0	284	11	0
78	Q2	847	0	917	33	0
78	q2	847	0	918	36	0
79	Q3	694	0	734	28	0
79	q3	694	0	734	27	0
80	e0	491	0	542	23	0
81	m2	750	0	174	8	0
82	p0	1076	0	1040	40	1
83	p1	235	0	51	4	0
84	p2	230	0	54	1	0
85	1	471	0	0	0	0
85	2	124	0	0	0	0
85	3	14	0	0	0	0
85	4	21	0	0	0	0
85	5	504	0	0	0	0
85	6	147	0	0	0	0
85	7	14	0	0	0	0
85	8	16	0	0	0	0
85	D0	1	0	0	0	0
85	D3	1	0	0	0	0
85	L2	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	M5	2	0	0	0	0
85	M6	2	0	0	0	0
85	M7	4	0	0	0	0
85	M9	3	0	0	0	0
85	N0	1	0	0	0	0
85	N3	2	0	0	0	0
85	N5	1	0	0	0	0
85	N6	1	0	0	0	0
85	N8	4	0	0	0	0
85	N9	1	0	0	0	0
85	O2	1	0	0	0	0
85	O3	1	0	0	0	0
85	O7	2	0	0	0	0
85	Q2	1	0	0	0	0
85	S2	2	0	0	0	0
85	S8	1	0	0	0	0
85	SM	1	0	0	0	0
85	c1	1	0	0	0	0
85	c7	1	0	0	0	0
85	c8	2	0	0	0	0
85	d3	2	0	0	0	0
85	d6	1	0	0	0	0
85	l2	1	0	0	0	0
85	l3	2	0	0	0	0
85	l4	1	0	0	0	0
85	l5	2	0	0	0	0
85	l7	2	0	0	0	0
85	l8	1	0	0	0	0
85	m1	2	0	0	0	0
85	m5	4	0	0	0	0
85	m6	2	0	0	0	0
85	m7	5	0	0	0	0
85	n0	2	0	0	0	0
85	n3	2	0	0	0	0
85	n6	1	0	0	0	0
85	n8	4	0	0	0	0
85	o1	1	0	0	0	0
85	o3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	o4	1	0	0	0	0
85	q0	1	0	0	0	0
85	q1	1	0	0	0	0
85	q3	2	0	0	0	0
85	s1	1	0	0	0	0
85	s2	1	0	0	0	0
85	s8	2	0	0	0	0
85	sM	2	0	0	0	0
86	1	2457	0	0	209	0
86	2	1078	0	0	113	0
86	3	84	0	0	2	0
86	4	119	0	0	13	0
86	5	2464	0	0	210	0
86	6	1106	0	0	111	0
86	7	84	0	0	8	0
86	8	112	0	0	18	0
86	C3	7	0	0	0	0
86	C5	7	0	0	2	0
86	C8	7	0	0	0	0
86	D3	7	0	0	0	0
86	D9	7	0	0	1	0
86	L3	21	0	0	1	0
86	L4	7	0	0	1	0
86	M0	7	0	0	0	0
86	M5	7	0	0	1	0
86	M7	14	0	0	2	0
86	M9	7	0	0	0	0
86	N1	7	0	0	1	0
86	N9	7	0	0	0	0
86	O3	7	0	0	1	0
86	O7	7	0	0	7	0
86	Q2	7	0	0	2	0
86	S6	7	0	0	0	0
86	S8	7	0	0	0	0
86	SR	7	0	0	0	0
86	c3	7	0	0	2	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	0	0
86	l4	14	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	l5	21	0	0	1	0
86	l9	7	0	0	0	0
86	m0	14	0	0	3	0
86	m1	7	0	0	0	0
86	m4	7	0	0	0	0
86	m5	7	0	0	0	0
86	m6	7	0	0	0	0
86	m7	7	0	0	1	0
86	m8	7	0	0	0	0
86	n3	7	0	0	0	0
86	n9	14	0	0	2	0
86	o2	7	0	0	0	0
86	o3	7	0	0	1	0
86	o7	14	0	0	4	0
86	q1	7	0	0	6	0
86	q2	7	0	0	3	0
86	s1	14	0	0	2	0
86	s4	7	0	0	0	0
86	s8	7	0	0	1	0
86	s9	7	0	0	2	0
86	sR	7	0	0	0	0
87	2	40	0	37	5	0
87	6	40	0	37	1	0
88	D6	1	0	0	0	0
88	D7	1	0	0	0	0
88	D9	1	0	0	0	0
88	E1	1	0	0	0	0
88	O7	1	0	0	0	0
88	Q0	1	0	0	0	0
88	Q2	1	0	0	0	0
88	Q3	1	0	0	0	0
88	d6	1	0	0	0	0
88	d7	1	0	0	0	0
88	d9	1	0	0	0	0
88	e1	1	0	0	0	0
88	o7	1	0	0	0	0
88	q0	1	0	0	0	0
88	q2	1	0	0	0	0
88	q3	1	0	0	0	0
All	All	411223	0	297358	10941	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 10941 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:q2:17:CYS:SG	78:q2:17:CYS:CB	2.01	1.48
78:Q2:17:CYS:SG	78:Q2:17:CYS:CB	2.04	1.43
40:l3:296:THR:HG22	40:l3:298:PHE:H	1.20	1.05
1:6:1011:G:OP2	86:6:2120:OHX:N3	1.90	1.03
1:2:1339:C:O2'	1:2:1341:A:N7	1.94	1.01

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:236:A:O2'	38:4:158:U:O2'[2_556]	2.13	0.07
60:n4:106:GLU:OE2	82:p0:16:ARG:NH2[2_657]	2.16	0.04

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%)	148 (72%)	34 (17%)	22 (11%)	0	2
2	s0	204/251 (81%)	155 (76%)	31 (15%)	18 (9%)	0	3
3	S1	212/254 (84%)	143 (68%)	36 (17%)	33 (16%)	0	0
3	s1	214/254 (84%)	168 (78%)	30 (14%)	16 (8%)	1	5
4	S2	215/253 (85%)	176 (82%)	24 (11%)	15 (7%)	1	6
4	s2	215/253 (85%)	178 (83%)	24 (11%)	13 (6%)	1	10
5	S3	221/239 (92%)	182 (82%)	31 (14%)	8 (4%)	2	19
5	s3	221/239 (92%)	172 (78%)	31 (14%)	18 (8%)	1	4
6	S4	258/260 (99%)	208 (81%)	27 (10%)	23 (9%)	0	3
6	s4	258/260 (99%)	200 (78%)	36 (14%)	22 (8%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	S5	204/224 (91%)	154 (76%)	29 (14%)	21 (10%)	0	2
7	s5	204/224 (91%)	158 (78%)	26 (13%)	20 (10%)	0	2
8	S6	224/236 (95%)	185 (83%)	22 (10%)	17 (8%)	1	5
8	s6	216/236 (92%)	187 (87%)	19 (9%)	10 (5%)	2	15
9	S7	182/189 (96%)	134 (74%)	23 (13%)	25 (14%)	0	1
9	s7	184/189 (97%)	145 (79%)	27 (15%)	12 (6%)	1	8
10	S8	184/200 (92%)	149 (81%)	24 (13%)	11 (6%)	1	10
10	s8	184/200 (92%)	159 (86%)	19 (10%)	6 (3%)	3	21
11	S9	183/196 (93%)	143 (78%)	29 (16%)	11 (6%)	1	10
11	s9	183/196 (93%)	148 (81%)	25 (14%)	10 (6%)	1	11
12	C0	94/105 (90%)	74 (79%)	10 (11%)	10 (11%)	0	2
12	c0	92/105 (88%)	63 (68%)	15 (16%)	14 (15%)	0	0
13	C1	153/155 (99%)	118 (77%)	20 (13%)	15 (10%)	0	2
13	c1	144/155 (93%)	117 (81%)	19 (13%)	8 (6%)	1	11
14	C2	122/142 (86%)	75 (62%)	26 (21%)	21 (17%)	0	0
14	c2	122/142 (86%)	69 (57%)	34 (28%)	19 (16%)	0	0
15	C3	148/150 (99%)	120 (81%)	20 (14%)	8 (5%)	1	12
15	c3	148/150 (99%)	120 (81%)	18 (12%)	10 (7%)	1	7
16	C4	125/136 (92%)	94 (75%)	21 (17%)	10 (8%)	1	4
16	c4	126/136 (93%)	92 (73%)	22 (18%)	12 (10%)	0	3
17	C5	122/141 (86%)	90 (74%)	18 (15%)	14 (12%)	0	1
17	c5	133/141 (94%)	86 (65%)	23 (17%)	24 (18%)	0	0
18	C6	139/142 (98%)	116 (84%)	13 (9%)	10 (7%)	1	6
18	c6	140/142 (99%)	115 (82%)	18 (13%)	7 (5%)	1	13
19	C7	116/136 (85%)	86 (74%)	18 (16%)	12 (10%)	0	2
19	c7	113/136 (83%)	87 (77%)	12 (11%)	14 (12%)	0	1
20	C8	143/145 (99%)	110 (77%)	22 (15%)	11 (8%)	1	5
20	c8	143/145 (99%)	111 (78%)	22 (15%)	10 (7%)	1	6
21	C9	141/143 (99%)	113 (80%)	25 (18%)	3 (2%)	5	31
21	c9	141/143 (99%)	116 (82%)	18 (13%)	7 (5%)	1	13
22	D0	105/120 (88%)	83 (79%)	19 (18%)	3 (3%)	3	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	d0	108/120 (90%)	82 (76%)	16 (15%)	10 (9%)	0	3
23	D1	85/87 (98%)	65 (76%)	14 (16%)	6 (7%)	1	6
23	d1	85/87 (98%)	74 (87%)	7 (8%)	4 (5%)	2	14
24	D2	127/129 (98%)	108 (85%)	12 (9%)	7 (6%)	1	11
24	d2	127/129 (98%)	114 (90%)	9 (7%)	4 (3%)	3	22
25	D3	142/144 (99%)	107 (75%)	22 (16%)	13 (9%)	0	3
25	d3	142/144 (99%)	116 (82%)	19 (13%)	7 (5%)	1	13
26	D4	132/134 (98%)	102 (77%)	23 (17%)	7 (5%)	1	12
26	d4	132/134 (98%)	101 (76%)	21 (16%)	10 (8%)	1	5
27	D5	68/107 (64%)	43 (63%)	14 (21%)	11 (16%)	0	0
27	d5	67/107 (63%)	50 (75%)	14 (21%)	3 (4%)	2	15
28	D6	95/97 (98%)	56 (59%)	19 (20%)	20 (21%)	0	0
28	d6	95/97 (98%)	73 (77%)	13 (14%)	9 (10%)	0	3
29	D7	79/81 (98%)	61 (77%)	15 (19%)	3 (4%)	2	18
29	d7	79/81 (98%)	60 (76%)	15 (19%)	4 (5%)	1	13
30	D8	61/66 (92%)	50 (82%)	7 (12%)	4 (7%)	1	7
30	d8	61/66 (92%)	44 (72%)	10 (16%)	7 (12%)	0	1
31	D9	51/55 (93%)	43 (84%)	7 (14%)	1 (2%)	6	31
31	d9	51/55 (93%)	39 (76%)	8 (16%)	4 (8%)	1	5
32	E0	58/60 (97%)	49 (84%)	6 (10%)	3 (5%)	1	12
33	E1	69/76 (91%)	33 (48%)	15 (22%)	21 (30%)	0	0
33	e1	74/76 (97%)	33 (45%)	24 (32%)	17 (23%)	0	0
34	SR	316/318 (99%)	244 (77%)	52 (16%)	20 (6%)	1	8
34	sR	316/318 (99%)	259 (82%)	43 (14%)	14 (4%)	2	15
35	SM	155/273 (57%)	114 (74%)	23 (15%)	18 (12%)	0	1
35	sM	98/273 (36%)	61 (62%)	21 (21%)	16 (16%)	0	0
39	L2	250/253 (99%)	218 (87%)	26 (10%)	6 (2%)	4	28
39	l2	250/253 (99%)	203 (81%)	36 (14%)	11 (4%)	2	15
40	L3	384/386 (100%)	336 (88%)	30 (8%)	18 (5%)	2	14
40	l3	384/386 (100%)	329 (86%)	42 (11%)	13 (3%)	3	20
41	L4	359/361 (99%)	303 (84%)	37 (10%)	19 (5%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	l4	359/361 (99%)	297 (83%)	43 (12%)	19 (5%)	1	12
42	L5	294/296 (99%)	244 (83%)	31 (10%)	19 (6%)	1	8
42	l5	292/296 (99%)	250 (86%)	30 (10%)	12 (4%)	2	17
43	L6	152/175 (87%)	129 (85%)	19 (12%)	4 (3%)	4	26
43	l6	153/175 (87%)	125 (82%)	24 (16%)	4 (3%)	4	26
44	L7	220/243 (90%)	183 (83%)	28 (13%)	9 (4%)	2	17
44	l7	221/243 (91%)	191 (86%)	24 (11%)	6 (3%)	4	25
45	L8	231/255 (91%)	185 (80%)	37 (16%)	9 (4%)	2	18
45	l8	229/255 (90%)	175 (76%)	32 (14%)	22 (10%)	0	3
46	L9	189/191 (99%)	161 (85%)	24 (13%)	4 (2%)	5	31
46	l9	189/191 (99%)	165 (87%)	18 (10%)	6 (3%)	3	21
47	M0	207/220 (94%)	168 (81%)	33 (16%)	6 (3%)	3	24
47	m0	209/220 (95%)	175 (84%)	20 (10%)	14 (7%)	1	7
48	M1	167/173 (96%)	135 (81%)	18 (11%)	14 (8%)	0	4
48	m1	167/173 (96%)	132 (79%)	20 (12%)	15 (9%)	0	3
49	M3	191/198 (96%)	161 (84%)	21 (11%)	9 (5%)	2	14
49	m3	192/198 (97%)	154 (80%)	19 (10%)	19 (10%)	0	2
50	M4	134/137 (98%)	119 (89%)	8 (6%)	7 (5%)	1	12
50	m4	135/137 (98%)	118 (87%)	15 (11%)	2 (2%)	8	37
51	M5	201/203 (99%)	184 (92%)	11 (6%)	6 (3%)	3	23
51	m5	201/203 (99%)	181 (90%)	15 (8%)	5 (2%)	4	27
52	M6	195/198 (98%)	176 (90%)	16 (8%)	3 (2%)	8	37
52	m6	195/198 (98%)	175 (90%)	15 (8%)	5 (3%)	4	26
53	M7	181/183 (99%)	154 (85%)	22 (12%)	5 (3%)	4	25
53	m7	153/183 (84%)	131 (86%)	19 (12%)	3 (2%)	6	31
54	M8	183/185 (99%)	157 (86%)	19 (10%)	7 (4%)	2	18
54	m8	183/185 (99%)	148 (81%)	29 (16%)	6 (3%)	3	21
55	M9	186/188 (99%)	165 (89%)	17 (9%)	4 (2%)	5	29
55	m9	186/188 (99%)	162 (87%)	20 (11%)	4 (2%)	5	29
56	N0	170/172 (99%)	152 (89%)	15 (9%)	3 (2%)	6	34
56	n0	170/172 (99%)	154 (91%)	13 (8%)	3 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	N1	157/159 (99%)	136 (87%)	13 (8%)	8 (5%)	1	13
57	n1	157/159 (99%)	139 (88%)	16 (10%)	2 (1%)	9	40
58	N2	98/120 (82%)	77 (79%)	15 (15%)	6 (6%)	1	9
58	n2	96/120 (80%)	75 (78%)	19 (20%)	2 (2%)	5	31
59	N3	134/136 (98%)	119 (89%)	15 (11%)	0	100	100
59	n3	134/136 (98%)	122 (91%)	10 (8%)	2 (2%)	8	37
60	N4	96/155 (62%)	72 (75%)	18 (19%)	6 (6%)	1	8
60	n4	133/155 (86%)	111 (84%)	15 (11%)	7 (5%)	1	12
61	N5	119/141 (84%)	106 (89%)	9 (8%)	4 (3%)	3	20
61	n5	118/141 (84%)	96 (81%)	15 (13%)	7 (6%)	1	10
62	N6	124/126 (98%)	110 (89%)	8 (6%)	6 (5%)	2	14
62	n6	124/126 (98%)	108 (87%)	11 (9%)	5 (4%)	2	17
63	N7	133/135 (98%)	112 (84%)	14 (10%)	7 (5%)	1	12
63	n7	133/135 (98%)	108 (81%)	20 (15%)	5 (4%)	2	18
64	N8	146/148 (99%)	124 (85%)	18 (12%)	4 (3%)	4	25
64	n8	146/148 (99%)	120 (82%)	16 (11%)	10 (7%)	1	7
65	N9	56/58 (97%)	44 (79%)	10 (18%)	2 (4%)	2	19
65	n9	56/58 (97%)	41 (73%)	10 (18%)	5 (9%)	0	3
66	O0	95/104 (91%)	83 (87%)	10 (10%)	2 (2%)	5	31
66	o0	98/104 (94%)	86 (88%)	9 (9%)	3 (3%)	3	22
67	O1	107/112 (96%)	95 (89%)	7 (6%)	5 (5%)	2	14
67	o1	107/112 (96%)	91 (85%)	12 (11%)	4 (4%)	2	18
68	O2	125/129 (97%)	109 (87%)	13 (10%)	3 (2%)	4	28
68	o2	125/129 (97%)	102 (82%)	18 (14%)	5 (4%)	2	17
69	O3	104/106 (98%)	93 (89%)	10 (10%)	1 (1%)	12	45
69	o3	104/106 (98%)	90 (86%)	11 (11%)	3 (3%)	3	24
70	O4	110/120 (92%)	92 (84%)	16 (14%)	2 (2%)	6	34
70	o4	110/120 (92%)	92 (84%)	12 (11%)	6 (6%)	1	11
71	O5	117/119 (98%)	103 (88%)	8 (7%)	6 (5%)	1	13
71	o5	117/119 (98%)	97 (83%)	13 (11%)	7 (6%)	1	10
72	O6	97/99 (98%)	76 (78%)	11 (11%)	10 (10%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	o6	97/99 (98%)	74 (76%)	16 (16%)	7 (7%)	1	6
73	O7	85/87 (98%)	73 (86%)	10 (12%)	2 (2%)	4	28
73	o7	85/87 (98%)	69 (81%)	13 (15%)	3 (4%)	3	20
74	O8	75/77 (97%)	61 (81%)	9 (12%)	5 (7%)	1	7
74	o8	75/77 (97%)	59 (79%)	11 (15%)	5 (7%)	1	7
75	O9	48/50 (96%)	41 (85%)	7 (15%)	0	100	100
75	o9	48/50 (96%)	41 (85%)	5 (10%)	2 (4%)	2	16
76	Q0	50/52 (96%)	43 (86%)	5 (10%)	2 (4%)	2	17
76	q0	50/52 (96%)	45 (90%)	4 (8%)	1 (2%)	6	31
77	Q1	23/25 (92%)	23 (100%)	0	0	100	100
77	q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	2	16
78	Q2	103/105 (98%)	78 (76%)	16 (16%)	9 (9%)	0	3
78	q2	103/105 (98%)	90 (87%)	11 (11%)	2 (2%)	6	33
79	Q3	89/91 (98%)	75 (84%)	10 (11%)	4 (4%)	2	15
79	q3	89/91 (98%)	76 (85%)	12 (14%)	1 (1%)	11	43
80	e0	60/62 (97%)	48 (80%)	5 (8%)	7 (12%)	0	1
82	p0	139/311 (45%)	111 (80%)	23 (16%)	5 (4%)	2	19
All	All	22333/24143 (92%)	18179 (81%)	2816 (13%)	1338 (6%)	1	10

5 of 1338 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	66	ALA
2	S0	158	VAL
2	S0	191	ARG
2	S0	194	PRO
3	S1	40	ASN

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%)	127 (77%)	37 (23%)	1	5
2	s0	165/209 (79%)	128 (78%)	37 (22%)	1	5
3	S1	191/223 (86%)	142 (74%)	49 (26%)	0	3
3	s1	192/223 (86%)	145 (76%)	47 (24%)	1	3
4	S2	176/204 (86%)	136 (77%)	40 (23%)	1	5
4	s2	176/204 (86%)	115 (65%)	61 (35%)	0	0
5	S3	182/194 (94%)	138 (76%)	44 (24%)	1	4
5	s3	182/194 (94%)	142 (78%)	40 (22%)	1	6
6	S4	221/221 (100%)	168 (76%)	53 (24%)	1	4
6	s4	221/221 (100%)	170 (77%)	51 (23%)	1	5
7	S5	173/190 (91%)	142 (82%)	31 (18%)	2	9
7	s5	173/190 (91%)	135 (78%)	38 (22%)	1	6
8	S6	188/201 (94%)	156 (83%)	32 (17%)	2	11
8	s6	187/201 (93%)	143 (76%)	44 (24%)	1	4
9	S7	165/169 (98%)	127 (77%)	38 (23%)	1	5
9	s7	165/169 (98%)	137 (83%)	28 (17%)	2	11
10	S8	150/161 (93%)	124 (83%)	26 (17%)	2	10
10	s8	150/161 (93%)	116 (77%)	34 (23%)	1	5
11	S9	158/165 (96%)	121 (77%)	37 (23%)	1	4
11	s9	158/165 (96%)	115 (73%)	43 (27%)	0	2
12	C0	77/98 (79%)	60 (78%)	17 (22%)	1	5
12	c0	73/98 (74%)	63 (86%)	10 (14%)	3	18
13	C1	129/136 (95%)	107 (83%)	22 (17%)	2	11
13	c1	129/136 (95%)	104 (81%)	25 (19%)	1	8
14	C2	88/118 (75%)	65 (74%)	23 (26%)	0	3
14	c2	88/118 (75%)	63 (72%)	25 (28%)	0	2
15	C3	127/127 (100%)	103 (81%)	24 (19%)	1	9
15	c3	127/127 (100%)	93 (73%)	34 (27%)	0	2
16	C4	81/104 (78%)	54 (67%)	27 (33%)	0	1
16	c4	97/104 (93%)	75 (77%)	22 (23%)	1	5
17	C5	101/117 (86%)	80 (79%)	21 (21%)	1	7
17	c5	103/117 (88%)	81 (79%)	22 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	C6	117/118 (99%)	93 (80%)	24 (20%)	1	7
18	c6	118/118 (100%)	98 (83%)	20 (17%)	2	11
19	C7	94/124 (76%)	75 (80%)	19 (20%)	1	7
19	c7	92/124 (74%)	73 (79%)	19 (21%)	1	7
20	C8	128/128 (100%)	97 (76%)	31 (24%)	1	4
20	c8	128/128 (100%)	98 (77%)	30 (23%)	1	4
21	C9	115/115 (100%)	84 (73%)	31 (27%)	0	2
21	c9	115/115 (100%)	92 (80%)	23 (20%)	1	7
22	D0	100/113 (88%)	70 (70%)	30 (30%)	0	1
22	d0	103/113 (91%)	71 (69%)	32 (31%)	0	1
23	D1	74/74 (100%)	54 (73%)	20 (27%)	0	2
23	d1	74/74 (100%)	56 (76%)	18 (24%)	1	4
24	D2	110/110 (100%)	84 (76%)	26 (24%)	1	4
24	d2	110/110 (100%)	93 (84%)	17 (16%)	2	14
25	D3	119/119 (100%)	94 (79%)	25 (21%)	1	6
25	d3	119/119 (100%)	92 (77%)	27 (23%)	1	5
26	D4	112/112 (100%)	87 (78%)	25 (22%)	1	5
26	d4	112/112 (100%)	88 (79%)	24 (21%)	1	6
27	D5	61/88 (69%)	44 (72%)	17 (28%)	0	2
27	d5	61/88 (69%)	49 (80%)	12 (20%)	1	8
28	D6	83/83 (100%)	68 (82%)	15 (18%)	2	9
28	d6	83/83 (100%)	66 (80%)	17 (20%)	1	7
29	D7	70/70 (100%)	61 (87%)	9 (13%)	4	20
29	d7	70/70 (100%)	59 (84%)	11 (16%)	2	13
30	D8	56/59 (95%)	43 (77%)	13 (23%)	1	5
30	d8	56/59 (95%)	41 (73%)	15 (27%)	0	2
31	D9	47/48 (98%)	40 (85%)	7 (15%)	3	15
31	d9	47/48 (98%)	35 (74%)	12 (26%)	0	3
32	E0	51/51 (100%)	37 (72%)	14 (28%)	0	2
33	E1	62/66 (94%)	48 (77%)	14 (23%)	1	5
33	e1	66/66 (100%)	46 (70%)	20 (30%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	SR	260/261 (100%)	211 (81%)	49 (19%)	1	9
34	sR	260/261 (100%)	225 (86%)	35 (14%)	4	19
35	SM	97/228 (42%)	72 (74%)	25 (26%)	0	3
35	sM	54/228 (24%)	40 (74%)	14 (26%)	0	3
39	L2	193/195 (99%)	147 (76%)	46 (24%)	1	4
39	l2	192/195 (98%)	154 (80%)	38 (20%)	1	8
40	L3	321/322 (100%)	235 (73%)	86 (27%)	0	2
40	l3	321/322 (100%)	245 (76%)	76 (24%)	1	4
41	L4	288/288 (100%)	225 (78%)	63 (22%)	1	5
41	l4	288/288 (100%)	220 (76%)	68 (24%)	1	4
42	L5	244/244 (100%)	188 (77%)	56 (23%)	1	5
42	l5	243/244 (100%)	188 (77%)	55 (23%)	1	5
43	L6	134/152 (88%)	113 (84%)	21 (16%)	2	13
43	l6	135/152 (89%)	109 (81%)	26 (19%)	1	8
44	L7	186/204 (91%)	151 (81%)	35 (19%)	1	9
44	l7	187/204 (92%)	158 (84%)	29 (16%)	2	14
45	L8	187/207 (90%)	146 (78%)	41 (22%)	1	5
45	l8	177/207 (86%)	138 (78%)	39 (22%)	1	6
46	L9	171/171 (100%)	130 (76%)	41 (24%)	1	4
46	l9	171/171 (100%)	129 (75%)	42 (25%)	1	3
47	M0	177/186 (95%)	141 (80%)	36 (20%)	1	7
47	m0	179/186 (96%)	137 (76%)	42 (24%)	1	4
48	M1	147/150 (98%)	108 (74%)	39 (26%)	0	3
48	m1	147/150 (98%)	111 (76%)	36 (24%)	1	3
49	M3	154/158 (98%)	125 (81%)	29 (19%)	1	9
49	m3	154/158 (98%)	123 (80%)	31 (20%)	1	7
50	M4	107/108 (99%)	86 (80%)	21 (20%)	1	8
50	m4	108/108 (100%)	78 (72%)	30 (28%)	0	2
51	M5	175/175 (100%)	144 (82%)	31 (18%)	2	10
51	m5	175/175 (100%)	142 (81%)	33 (19%)	1	9
52	M6	160/161 (99%)	130 (81%)	30 (19%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	m6	160/161 (99%)	119 (74%)	41 (26%)	0	3
53	M7	140/145 (97%)	103 (74%)	37 (26%)	0	3
53	m7	125/145 (86%)	93 (74%)	32 (26%)	0	3
54	M8	150/150 (100%)	122 (81%)	28 (19%)	1	9
54	m8	150/150 (100%)	110 (73%)	40 (27%)	0	3
55	M9	153/153 (100%)	115 (75%)	38 (25%)	1	3
55	m9	153/153 (100%)	115 (75%)	38 (25%)	1	3
56	N0	156/156 (100%)	123 (79%)	33 (21%)	1	6
56	n0	156/156 (100%)	113 (72%)	43 (28%)	0	2
57	N1	136/136 (100%)	103 (76%)	33 (24%)	1	4
57	n1	136/136 (100%)	103 (76%)	33 (24%)	1	4
58	N2	87/106 (82%)	72 (83%)	15 (17%)	2	10
58	n2	85/106 (80%)	65 (76%)	20 (24%)	1	4
59	N3	104/104 (100%)	80 (77%)	24 (23%)	1	5
59	n3	104/104 (100%)	90 (86%)	14 (14%)	4	19
60	N4	57/129 (44%)	49 (86%)	8 (14%)	3	17
60	n4	100/129 (78%)	85 (85%)	15 (15%)	3	15
61	N5	104/117 (89%)	77 (74%)	27 (26%)	0	3
61	n5	104/117 (89%)	82 (79%)	22 (21%)	1	6
62	N6	109/109 (100%)	80 (73%)	29 (27%)	0	3
62	n6	109/109 (100%)	81 (74%)	28 (26%)	0	3
63	N7	115/115 (100%)	88 (76%)	27 (24%)	1	4
63	n7	115/115 (100%)	90 (78%)	25 (22%)	1	6
64	N8	118/118 (100%)	94 (80%)	24 (20%)	1	7
64	n8	118/118 (100%)	93 (79%)	25 (21%)	1	6
65	N9	46/46 (100%)	33 (72%)	13 (28%)	0	2
65	n9	46/46 (100%)	33 (72%)	13 (28%)	0	2
66	O0	81/87 (93%)	62 (76%)	19 (24%)	1	4
66	o0	84/87 (97%)	67 (80%)	17 (20%)	1	7
67	O1	92/96 (96%)	63 (68%)	29 (32%)	0	1
67	o1	94/96 (98%)	67 (71%)	27 (29%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	O2	109/110 (99%)	82 (75%)	27 (25%)	1	3
68	o2	109/110 (99%)	80 (73%)	29 (27%)	0	3
69	O3	90/90 (100%)	75 (83%)	15 (17%)	2	11
69	o3	90/90 (100%)	74 (82%)	16 (18%)	2	10
70	O4	95/102 (93%)	77 (81%)	18 (19%)	1	9
70	o4	95/102 (93%)	75 (79%)	20 (21%)	1	6
71	O5	104/104 (100%)	77 (74%)	27 (26%)	0	3
71	o5	103/104 (99%)	75 (73%)	28 (27%)	0	2
72	O6	81/81 (100%)	59 (73%)	22 (27%)	0	2
72	o6	80/81 (99%)	56 (70%)	24 (30%)	0	1
73	O7	70/70 (100%)	55 (79%)	15 (21%)	1	6
73	o7	70/70 (100%)	54 (77%)	16 (23%)	1	5
74	O8	68/68 (100%)	53 (78%)	15 (22%)	1	5
74	o8	67/68 (98%)	53 (79%)	14 (21%)	1	6
75	O9	45/45 (100%)	30 (67%)	15 (33%)	0	1
75	o9	45/45 (100%)	38 (84%)	7 (16%)	2	13
76	Q0	47/47 (100%)	36 (77%)	11 (23%)	1	4
76	q0	47/47 (100%)	36 (77%)	11 (23%)	1	4
77	Q1	23/23 (100%)	12 (52%)	11 (48%)	0	0
77	q1	23/23 (100%)	17 (74%)	6 (26%)	0	3
78	Q2	90/90 (100%)	69 (77%)	21 (23%)	1	5
78	q2	90/90 (100%)	70 (78%)	20 (22%)	1	5
79	Q3	71/71 (100%)	54 (76%)	17 (24%)	1	4
79	q3	71/71 (100%)	51 (72%)	20 (28%)	0	2
80	e0	53/53 (100%)	37 (70%)	16 (30%)	0	1
82	p0	105/253 (42%)	84 (80%)	21 (20%)	1	7
All	All	18730/20241 (92%)	14509 (78%)	4221 (22%)	1	5

5 of 4221 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
55	m9	177	VAL
59	n3	88	ARG

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Mol	Chain	Res	Type
55	m9	158	GLU
78	q2	2	VAL
55	M9	10	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 184 such sidechains are listed below:

Mol	Chain	Res	Type
18	c6	100	GLN
47	m0	23	ASN
20	c8	78	HIS
34	sR	101	GLN
52	m6	31	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	483 (27%)	50 (2%)
1	6	1792/1800 (99%)	484 (27%)	49 (2%)
36	1	3145/3396 (92%)	696 (22%)	93 (2%)
36	5	3145/3396 (92%)	698 (22%)	78 (2%)
37	3	120/121 (99%)	17 (14%)	1 (0%)
37	7	120/121 (99%)	20 (16%)	1 (0%)
38	4	157/158 (99%)	41 (26%)	6 (3%)
38	8	157/158 (99%)	38 (24%)	1 (0%)
All	All	10383/10950 (94%)	2477 (23%)	279 (2%)

5 of 2477 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 279 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	5	1355	A
36	5	1580	A

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Mol	Chain	Res	Type
36	5	2682	C
36	1	1751	G
36	1	1589	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2558 ligands modelled in this entry, 1426 are monoatomic - leaving 1132 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	5	4035	-	0,6,6	-	-	-		
86	OHX	1	3899	-	0,6,6	-	-	-		
86	OHX	1	4137	-	0,6,6	-	-	-		
86	OHX	5	4186	-	0,6,6	-	-	-		
86	OHX	1	4104	-	0,6,6	-	-	-		
86	OHX	1	4030	-	0,6,6	-	-	-		
86	OHX	8	229	-	0,6,6	-	-	-		
86	OHX	6	2174	-	0,6,6	-	-	-		
86	OHX	2	2026	-	0,6,6	-	-	-		
86	OHX	1	4043	-	0,6,6	-	-	-		
86	OHX	5	4198	-	0,6,6	-	-	-		
86	OHX	5	4141	-	0,6,6	-	-	-		
86	OHX	1	3955	-	0,6,6	-	-	-		
86	OHX	1	3892	-	0,6,6	-	-	-		
86	OHX	19	600	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4038	-	0,6,6	-	-	-		
86	OHX	5	3961	-	0,6,6	-	-	-		
86	OHX	2	2084	-	0,6,6	-	-	-		
86	OHX	5	4175	-	0,6,6	-	-	-		
86	OHX	2	2067	-	0,6,6	-	-	-		
86	OHX	2	2061	-	0,6,6	-	-	-		
86	OHX	1	3932	-	0,6,6	-	-	-		
86	OHX	5	3920	-	0,6,6	-	-	-		
86	OHX	1	4153	-	0,6,6	-	-	-		
86	OHX	5	4040	-	0,6,6	-	-	-		
86	OHX	5	4232	-	0,6,6	-	-	-		
86	OHX	5	4162	-	0,6,6	-	-	-		
86	OHX	5	4089	-	0,6,6	-	-	-		
86	OHX	2	2056	-	0,6,6	-	-	-		
86	OHX	5	4122	-	0,6,6	-	-	-		
86	OHX	5	3963	-	0,6,6	-	-	-		
86	OHX	1	4037	-	0,6,6	-	-	-		
86	OHX	5	3931	-	0,6,6	-	-	-		
86	OHX	5	4075	-	0,6,6	-	-	-		
86	OHX	1	3896	-	0,6,6	-	-	-		
86	OHX	2	2133	-	0,6,6	-	-	-		
86	OHX	1	4202	-	0,6,6	-	-	-		
86	OHX	5	3912	-	0,6,6	-	-	-		
86	OHX	1	4045	-	0,6,6	-	-	-		
86	OHX	1	3970	-	0,6,6	-	-	-		
86	OHX	1	4180	-	0,6,6	-	-	-		
86	OHX	2	2117	-	0,6,6	-	-	-		
86	OHX	6	2118	-	0,6,6	-	-	-		
86	OHX	1	4101	-	0,6,6	-	-	-		
86	OHX	5	3910	-	0,6,6	-	-	-		
86	OHX	1	3869	-	0,6,6	-	-	-		
86	OHX	1	4157	-	0,6,6	-	-	-		
86	OHX	2	2130	-	0,6,6	-	-	-		
86	OHX	6	2046	-	0,6,6	-	-	-		
86	OHX	6	2095	-	0,6,6	-	-	-		
86	OHX	1	4203	-	0,6,6	-	-	-		
86	OHX	5	4072	-	0,6,6	-	-	-		
86	OHX	7	225	-	0,6,6	-	-	-		
86	OHX	5	4087	-	0,6,6	-	-	-		
86	OHX	5	4117	-	0,6,6	-	-	-		
86	OHX	5	4225	-	0,6,6	-	-	-		
86	OHX	1	4050	-	0,6,6	-	-	-		
86	OHX	6	2178	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4081	-	0,6,6	-	-	-		
86	OHX	5	4050	-	0,6,6	-	-	-		
86	OHX	5	3921	-	0,6,6	-	-	-		
86	OHX	5	4213	-	0,6,6	-	-	-		
86	OHX	6	2200	-	0,6,6	-	-	-		
86	OHX	1	3979	-	0,6,6	-	-	-		
86	OHX	1	3875	-	0,6,6	-	-	-		
86	OHX	d9	102	-	0,6,6	-	-	-		
86	OHX	1	3888	-	0,6,6	-	-	-		
86	OHX	1	3972	-	0,6,6	-	-	-		
86	OHX	1	4035	-	0,6,6	-	-	-		
86	OHX	2	2127	-	0,6,6	-	-	-		
86	OHX	2	2177	-	0,6,6	-	-	-		
86	OHX	1	4036	-	0,6,6	-	-	-		
86	OHX	1	4039	-	0,6,6	-	-	-		
86	OHX	1	4007	-	0,6,6	-	-	-		
86	OHX	1	4061	-	0,6,6	-	-	-		
86	OHX	2	2154	-	0,6,6	-	-	-		
86	OHX	1	4140	-	0,6,6	-	-	-		
86	OHX	5	4231	-	0,6,6	-	-	-		
86	OHX	m6	203	-	0,6,6	-	-	-		
86	OHX	5	4012	-	0,6,6	-	-	-		
86	OHX	5	4017	-	0,6,6	-	-	-		
86	OHX	2	2106	-	0,6,6	-	-	-		
86	OHX	1	3978	-	0,6,6	-	-	-		
86	OHX	1	3940	-	0,6,6	-	-	-		
86	OHX	5	4188	-	0,6,6	-	-	-		
86	OHX	5	4245	-	0,6,6	-	-	-		
86	OHX	2	2119	-	0,6,6	-	-	-		
86	OHX	1	3879	-	0,6,6	-	-	-		
86	OHX	1	4156	-	0,6,6	-	-	-		
86	OHX	1	3969	-	0,6,6	-	-	-		
86	OHX	5	4170	-	0,6,6	-	-	-		
86	OHX	2	2064	-	0,6,6	-	-	-		
86	OHX	5	4064	-	0,6,6	-	-	-		
86	OHX	6	2188	-	0,6,6	-	-	-		
86	OHX	6	2198	-	0,6,6	-	-	-		
86	OHX	6	2104	-	0,6,6	-	-	-		
86	OHX	L4	403	-	0,6,6	-	-	-		
86	OHX	5	4169	-	0,6,6	-	-	-		
86	OHX	6	2094	-	0,6,6	-	-	-		
86	OHX	5	3985	-	0,6,6	-	-	-		
86	OHX	5	4109	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2090	-	0,6,6	-	-	-		
86	OHX	2	2167	-	0,6,6	-	-	-		
86	OHX	M7	206	-	0,6,6	-	-	-		
86	OHX	5	3991	-	0,6,6	-	-	-		
86	OHX	2	2111	-	0,6,6	-	-	-		
86	OHX	5	4120	-	0,6,6	-	-	-		
86	OHX	3	219	-	0,6,6	-	-	-		
86	OHX	5	4097	-	0,6,6	-	-	-		
86	OHX	2	2038	-	0,6,6	-	-	-		
86	OHX	M0	303	-	0,6,6	-	-	-		
86	OHX	1	3881	-	0,6,6	-	-	-		
86	OHX	2	2151	-	0,6,6	-	-	-		
86	OHX	5	4026	-	0,6,6	-	-	-		
86	OHX	8	219	-	0,6,6	-	-	-		
86	OHX	6	2180	-	0,6,6	-	-	-		
86	OHX	C8	201	-	0,6,6	-	-	-		
86	OHX	1	4075	-	0,6,6	-	-	-		
86	OHX	s4	301	-	0,6,6	-	-	-		
86	OHX	1	4021	-	0,6,6	-	-	-		
86	OHX	1	4058	-	0,6,6	-	-	-		
86	OHX	5	4049	-	0,6,6	-	-	-		
86	OHX	5	4129	-	0,6,6	-	-	-		
86	OHX	6	2061	-	0,6,6	-	-	-		
86	OHX	5	3917	-	0,6,6	-	-	-		
86	OHX	1	4086	-	0,6,6	-	-	-		
86	OHX	1	3952	-	0,6,6	-	-	-		
86	OHX	1	3971	-	0,6,6	-	-	-		
86	OHX	1	3982	-	0,6,6	-	-	-		
86	OHX	1	4107	-	0,6,6	-	-	-		
86	OHX	5	3970	-	0,6,6	-	-	-		
86	OHX	m5	305	-	0,6,6	-	-	-		
86	OHX	1	3993	-	0,6,6	-	-	-		
86	OHX	1	3998	-	0,6,6	-	-	-		
86	OHX	1	3919	-	0,6,6	-	-	-		
86	OHX	1	3865	-	0,6,6	-	-	-		
86	OHX	1	4029	-	0,6,6	-	-	-		
86	OHX	5	4233	86	0,6,6	-	-	-		
86	OHX	SR	401	-	0,6,6	-	-	-		
86	OHX	1	4149	-	0,6,6	-	-	-		
86	OHX	6	2115	-	0,6,6	-	-	-		
86	OHX	5	4048	-	0,6,6	-	-	-		
86	OHX	1	4001	-	0,6,6	-	-	-		
86	OHX	1	3895	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3939	-	0,6,6	-	-	-		
86	OHX	1	4154	-	0,6,6	-	-	-		
86	OHX	8	221	-	0,6,6	-	-	-		
86	OHX	o2	201	-	0,6,6	-	-	-		
86	OHX	2	2153	-	0,6,6	-	-	-		
86	OHX	1	3964	-	0,6,6	-	-	-		
86	OHX	1	4102	-	0,6,6	-	-	-		
86	OHX	3	222	-	0,6,6	-	-	-		
86	OHX	5	4187	-	0,6,6	-	-	-		
86	OHX	4	224	-	0,6,6	-	-	-		
86	OHX	1	4196	-	0,6,6	-	-	-		
86	OHX	6	2103	-	0,6,6	-	-	-		
86	OHX	s8	303	-	0,6,6	-	-	-		
86	OHX	5	4085	-	0,6,6	-	-	-		
86	OHX	1	4066	-	0,6,6	-	-	-		
86	OHX	1	3980	-	0,6,6	-	-	-		
86	OHX	4	237	-	0,6,6	-	-	-		
86	OHX	5	3939	-	0,6,6	-	-	-		
86	OHX	5	4046	-	0,6,6	-	-	-		
86	OHX	6	2105	-	0,6,6	-	-	-		
86	OHX	5	3978	-	0,6,6	-	-	-		
86	OHX	2	2166	-	0,6,6	-	-	-		
86	OHX	1	3933	-	0,6,6	-	-	-		
86	OHX	5	4016	-	0,6,6	-	-	-		
86	OHX	1	4141	-	0,6,6	-	-	-		
86	OHX	5	4024	-	0,6,6	-	-	-		
86	OHX	5	4018	-	0,6,6	-	-	-		
86	OHX	2	2144	-	0,6,6	-	-	-		
86	OHX	6	2106	-	0,6,6	-	-	-		
86	OHX	5	4044	-	0,6,6	-	-	-		
86	OHX	6	2131	-	0,6,6	-	-	-		
86	OHX	6	2119	-	0,6,6	-	-	-		
86	OHX	1	3945	-	0,6,6	-	-	-		
86	OHX	6	2062	-	0,6,6	-	-	-		
86	OHX	2	2160	-	0,6,6	-	-	-		
86	OHX	6	2186	-	0,6,6	-	-	-		
86	OHX	5	4166	-	0,6,6	-	-	-		
86	OHX	2	2175	-	0,6,6	-	-	-		
86	OHX	6	2064	-	0,6,6	-	-	-		
86	OHX	6	2203	-	0,6,6	-	-	-		
86	OHX	5	4094	-	0,6,6	-	-	-		
86	OHX	1	3877	-	0,6,6	-	-	-		
86	OHX	5	4036	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2081	-	0,6,6	-	-	-		
86	OHX	6	2056	-	0,6,6	-	-	-		
86	OHX	6	2170	-	0,6,6	-	-	-		
86	OHX	2	2155	-	0,6,6	-	-	-		
86	OHX	4	226	-	0,6,6	-	-	-		
86	OHX	5	4124	-	0,6,6	-	-	-		
86	OHX	1	4002	-	0,6,6	-	-	-		
86	OHX	q2	502	-	0,6,6	-	-	-		
86	OHX	2	2116	-	0,6,6	-	-	-		
86	OHX	2	2126	-	0,6,6	-	-	-		
86	OHX	1	3916	-	0,6,6	-	-	-		
86	OHX	6	2111	-	0,6,6	-	-	-		
86	OHX	2	2075	-	0,6,6	-	-	-		
86	OHX	1	4099	-	0,6,6	-	-	-		
86	OHX	2	2135	-	0,6,6	-	-	-		
86	OHX	1	3977	-	0,6,6	-	-	-		
86	OHX	5	4179	-	0,6,6	-	-	-		
86	OHX	15	305	-	0,6,6	-	-	-		
86	OHX	5	4224	-	0,6,6	-	-	-		
86	OHX	1	4082	-	0,6,6	-	-	-		
86	OHX	5	3990	-	0,6,6	-	-	-		
86	OHX	15	304	-	0,6,6	-	-	-		
86	OHX	1	4169	-	0,6,6	-	-	-		
86	OHX	2	2041	-	0,6,6	-	-	-		
86	OHX	5	4093	-	0,6,6	-	-	-		
86	OHX	5	4114	-	0,6,6	-	-	-		
86	OHX	5	4034	-	0,6,6	-	-	-		
86	OHX	1	4023	-	0,6,6	-	-	-		
86	OHX	6	2177	-	0,6,6	-	-	-		
86	OHX	M5	303	-	0,6,6	-	-	-		
86	OHX	1	3924	-	0,6,6	-	-	-		
86	OHX	6	2134	-	0,6,6	-	-	-		
86	OHX	5	4116	-	0,6,6	-	-	-		
86	OHX	1	3921	-	0,6,6	-	-	-		
86	OHX	1	3935	-	0,6,6	-	-	-		
86	OHX	5	3924	-	0,6,6	-	-	-		
86	OHX	6	2120	-	0,6,6	-	-	-		
86	OHX	5	4142	-	0,6,6	-	-	-		
86	OHX	2	2162	-	0,6,6	-	-	-		
86	OHX	5	4157	-	0,6,6	-	-	-		
86	OHX	5	4196	-	0,6,6	-	-	-		
86	OHX	1	3947	-	0,6,6	-	-	-		
86	OHX	5	4209	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3947	-	0,6,6	-	-	-		
86	OHX	5	3979	-	0,6,6	-	-	-		
86	OHX	5	4069	-	0,6,6	-	-	-		
86	OHX	o7	502	-	0,6,6	-	-	-		
86	OHX	5	4029	-	0,6,6	-	-	-		
86	OHX	5	4135	-	0,6,6	-	-	-		
86	OHX	1	4189	-	0,6,6	-	-	-		
86	OHX	1	4109	-	0,6,6	-	-	-		
86	OHX	1	4017	-	0,6,6	-	-	-		
86	OHX	6	2169	-	0,6,6	-	-	-		
86	OHX	6	2107	-	0,6,6	-	-	-		
86	OHX	5	4148	-	0,6,6	-	-	-		
86	OHX	1	4040	-	0,6,6	-	-	-		
86	OHX	6	2087	-	0,6,6	-	-	-		
86	OHX	1	4026	-	0,6,6	-	-	-		
86	OHX	6	2114	-	0,6,6	-	-	-		
86	OHX	14	403	-	0,6,6	-	-	-		
86	OHX	8	218	-	0,6,6	-	-	-		
86	OHX	1	4000	-	0,6,6	-	-	-		
86	OHX	1	4174	-	0,6,6	-	-	-		
86	OHX	2	2047	-	0,6,6	-	-	-		
86	OHX	1	3949	-	0,6,6	-	-	-		
86	OHX	1	3902	-	0,6,6	-	-	-		
86	OHX	1	3910	-	0,6,6	-	-	-		
86	OHX	5	4132	-	0,6,6	-	-	-		
86	OHX	5	4164	-	0,6,6	-	-	-		
86	OHX	13	403	-	0,6,6	-	-	-		
86	OHX	6	2149	-	0,6,6	-	-	-		
86	OHX	1	4126	-	0,6,6	-	-	-		
86	OHX	1	3959	-	0,6,6	-	-	-		
86	OHX	2	2157	-	0,6,6	-	-	-		
86	OHX	5	4063	-	0,6,6	-	-	-		
86	OHX	6	2201	-	0,6,6	-	-	-		
86	OHX	5	3953	-	0,6,6	-	-	-		
86	OHX	6	2047	-	0,6,6	-	-	-		
86	OHX	6	2092	-	0,6,6	-	-	-		
86	OHX	7	219	-	0,6,6	-	-	-		
86	OHX	1	4028	-	0,6,6	-	-	-		
86	OHX	1	4103	-	0,6,6	-	-	-		
86	OHX	1	3887	-	0,6,6	-	-	-		
86	OHX	2	2057	-	0,6,6	-	-	-		
86	OHX	4	223	-	0,6,6	-	-	-		
86	OHX	2	2040	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2079	-	0,6,6	-	-	-		
86	OHX	6	2175	-	0,6,6	-	-	-		
86	OHX	5	3922	-	0,6,6	-	-	-		
86	OHX	6	2112	-	0,6,6	-	-	-		
86	OHX	6	2100	-	0,6,6	-	-	-		
86	OHX	1	4178	-	0,6,6	-	-	-		
86	OHX	2	2108	-	0,6,6	-	-	-		
86	OHX	6	2193	-	0,6,6	-	-	-		
86	OHX	5	4178	-	0,6,6	-	-	-		
86	OHX	8	226	-	0,6,6	-	-	-		
86	OHX	6	2073	-	0,6,6	-	-	-		
86	OHX	1	3889	-	0,6,6	-	-	-		
86	OHX	6	2052	-	0,6,6	-	-	-		
86	OHX	6	2058	-	0,6,6	-	-	-		
86	OHX	1	3942	-	0,6,6	-	-	-		
86	OHX	1	4072	-	0,6,6	-	-	-		
86	OHX	1	4024	-	0,6,6	-	-	-		
86	OHX	1	4186	-	0,6,6	-	-	-		
86	OHX	7	215	-	0,6,6	-	-	-		
86	OHX	6	2128	-	0,6,6	-	-	-		
86	OHX	5	4042	-	0,6,6	-	-	-		
86	OHX	5	4106	-	0,6,6	-	-	-		
86	OHX	1	4085	-	0,6,6	-	-	-		
86	OHX	2	2132	-	0,6,6	-	-	-		
86	OHX	6	2075	-	0,6,6	-	-	-		
86	OHX	6	2158	-	0,6,6	-	-	-		
86	OHX	1	4211	-	0,6,6	-	-	-		
86	OHX	6	2184	-	0,6,6	-	-	-		
86	OHX	6	2117	-	0,6,6	-	-	-		
86	OHX	5	3926	-	0,6,6	-	-	-		
86	OHX	5	3966	-	0,6,6	-	-	-		
86	OHX	5	4103	-	0,6,6	-	-	-		
86	OHX	6	2191	-	0,6,6	-	-	-		
86	OHX	5	4228	-	0,6,6	-	-	-		
86	OHX	1	3961	-	0,6,6	-	-	-		
86	OHX	1	4185	-	0,6,6	-	-	-		
86	OHX	6	2144	-	0,6,6	-	-	-		
86	OHX	sR	401	-	0,6,6	-	-	-		
86	OHX	5	4240	-	0,6,6	-	-	-		
86	OHX	1	4175	-	0,6,6	-	-	-		
86	OHX	5	4210	-	0,6,6	-	-	-		
86	OHX	5	4236	-	0,6,6	-	-	-		
86	OHX	1	3938	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2091	-	0,6,6	-	-	-		
86	OHX	5	4199	-	0,6,6	-	-	-		
86	OHX	2	2150	-	0,6,6	-	-	-		
86	OHX	1	3920	-	0,6,6	-	-	-		
86	OHX	1	3898	-	0,6,6	-	-	-		
86	OHX	5	4104	-	0,6,6	-	-	-		
86	OHX	1	4090	-	0,6,6	-	-	-		
86	OHX	5	4019	-	0,6,6	-	-	-		
86	OHX	1	3922	-	0,6,6	-	-	-		
86	OHX	5	4062	-	0,6,6	-	-	-		
86	OHX	1	3967	-	0,6,6	-	-	-		
86	OHX	2	2114	-	0,6,6	-	-	-		
86	OHX	1	3990	-	0,6,6	-	-	-		
86	OHX	1	3912	-	0,6,6	-	-	-		
86	OHX	2	2101	-	0,6,6	-	-	-		
86	OHX	1	4078	-	0,6,6	-	-	-		
86	OHX	6	2136	-	0,6,6	-	-	-		
86	OHX	5	4176	-	0,6,6	-	-	-		
86	OHX	5	4171	-	0,6,6	-	-	-		
86	OHX	1	4200	-	0,6,6	-	-	-		
86	OHX	6	2051	-	0,6,6	-	-	-		
86	OHX	5	4125	-	0,6,6	-	-	-		
86	OHX	5	4032	-	0,6,6	-	-	-		
86	OHX	5	4217	-	0,6,6	-	-	-		
86	OHX	5	3909	-	0,6,6	-	-	-		
86	OHX	6	2143	-	0,6,6	-	-	-		
86	OHX	5	3916	-	0,6,6	-	-	-		
86	OHX	1	3874	-	0,6,6	-	-	-		
86	OHX	6	2113	-	0,6,6	-	-	-		
86	OHX	5	4248	-	0,6,6	-	-	-		
86	OHX	5	4194	-	0,6,6	-	-	-		
86	OHX	6	2190	-	0,6,6	-	-	-		
86	OHX	5	4136	-	0,6,6	-	-	-		
86	OHX	2	2027	-	0,6,6	-	-	-		
86	OHX	1	3996	-	0,6,6	-	-	-		
86	OHX	5	4237	-	0,6,6	-	-	-		
86	OHX	1	3962	-	0,6,6	-	-	-		
86	OHX	2	2129	-	0,6,6	-	-	-		
86	OHX	1	4205	-	0,6,6	-	-	-		
86	OHX	5	4083	-	0,6,6	-	-	-		
86	OHX	1	4204	-	0,6,6	-	-	-		
86	OHX	5	4041	-	0,6,6	-	-	-		
86	OHX	1	4209	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3981	-	0,6,6	-	-	-		
86	OHX	2	2043	-	0,6,6	-	-	-		
86	OHX	5	4084	-	0,6,6	-	-	-		
86	OHX	1	4191	-	0,6,6	-	-	-		
86	OHX	1	4046	-	0,6,6	-	-	-		
86	OHX	1	4160	-	0,6,6	-	-	-		
86	OHX	6	2129	-	0,6,6	-	-	-		
86	OHX	5	3914	-	0,6,6	-	-	-		
86	OHX	1	4089	-	0,6,6	-	-	-		
86	OHX	5	3982	-	0,6,6	-	-	-		
86	OHX	8	225	-	0,6,6	-	-	-		
86	OHX	2	2118	-	0,6,6	-	-	-		
86	OHX	2	2156	-	0,6,6	-	-	-		
86	OHX	2	2090	-	0,6,6	-	-	-		
86	OHX	1	3893	-	0,6,6	-	-	-		
86	OHX	2	2063	-	0,6,6	-	-	-		
86	OHX	3	216	-	0,6,6	-	-	-		
86	OHX	1	3985	-	0,6,6	-	-	-		
86	OHX	6	2048	-	0,6,6	-	-	-		
86	OHX	5	3999	-	0,6,6	-	-	-		
86	OHX	5	4067	-	0,6,6	-	-	-		
86	OHX	5	4100	-	0,6,6	-	-	-		
86	OHX	5	4204	-	0,6,6	-	-	-		
86	OHX	2	2053	-	0,6,6	-	-	-		
86	OHX	2	2089	-	0,6,6	-	-	-		
86	OHX	O7	104	-	0,6,6	-	-	-		
86	OHX	1	4120	-	0,6,6	-	-	-		
86	OHX	1	4097	-	0,6,6	-	-	-		
86	OHX	5	3940	-	0,6,6	-	-	-		
86	OHX	1	4147	-	0,6,6	-	-	-		
86	OHX	3	221	-	0,6,6	-	-	-		
86	OHX	5	4147	-	0,6,6	-	-	-		
86	OHX	1	4130	-	0,6,6	-	-	-		
86	OHX	5	3954	-	0,6,6	-	-	-		
86	OHX	1	3911	-	0,6,6	-	-	-		
86	OHX	1	4161	-	0,6,6	-	-	-		
86	OHX	5	4014	-	0,6,6	-	-	-		
86	OHX	1	4049	-	0,6,6	-	-	-		
86	OHX	2	2115	-	0,6,6	-	-	-		
86	OHX	1	3973	-	0,6,6	-	-	-		
86	OHX	2	2159	-	0,6,6	-	-	-		
86	OHX	2	2172	-	0,6,6	-	-	-		
86	OHX	D3	202	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3863	-	0,6,6	-	-	-		
86	OHX	1	3917	-	0,6,6	-	-	-		
86	OHX	1	4167	-	0,6,6	-	-	-		
86	OHX	1	3866	-	0,6,6	-	-	-		
86	OHX	6	2072	-	0,6,6	-	-	-		
86	OHX	6	2122	-	0,6,6	-	-	-		
86	OHX	1	4190	-	0,6,6	-	-	-		
86	OHX	5	4230	-	0,6,6	-	-	-		
86	OHX	4	232	-	0,6,6	-	-	-		
86	OHX	7	223	-	0,6,6	-	-	-		
86	OHX	5	4249	-	0,6,6	-	-	-		
86	OHX	1	3989	-	0,6,6	-	-	-		
86	OHX	6	2097	-	0,6,6	-	-	-		
86	OHX	1	4112	-	0,6,6	-	-	-		
86	OHX	5	4177	-	0,6,6	-	-	-		
86	OHX	4	238	-	0,6,6	-	-	-		
86	OHX	5	4201	-	0,6,6	-	-	-		
86	OHX	8	224	-	0,6,6	-	-	-		
86	OHX	5	3929	-	0,6,6	-	-	-		
86	OHX	1	4048	-	0,6,6	-	-	-		
86	OHX	6	2066	-	0,6,6	-	-	-		
86	OHX	5	4165	-	0,6,6	-	-	-		
86	OHX	1	4034	-	0,6,6	-	-	-		
86	OHX	5	4110	-	0,6,6	-	-	-		
86	OHX	1	3951	-	0,6,6	-	-	-		
86	OHX	5	4031	-	0,6,6	-	-	-		
86	OHX	2	2142	-	0,6,6	-	-	-		
86	OHX	s1	302	-	0,6,6	-	-	-		
86	OHX	5	4251	-	0,6,6	-	-	-		
86	OHX	2	2077	-	0,6,6	-	-	-		
86	OHX	5	4163	-	0,6,6	-	-	-		
86	OHX	1	4170	-	0,6,6	-	-	-		
86	OHX	5	3995	-	0,6,6	-	-	-		
86	OHX	5	4207	-	0,6,6	-	-	-		
86	OHX	5	4212	-	0,6,6	-	-	-		
86	OHX	6	2096	-	0,6,6	-	-	-		
86	OHX	1	4155	-	0,6,6	-	-	-		
86	OHX	6	2109	-	0,6,6	-	-	-		
86	OHX	2	2123	-	0,6,6	-	-	-		
86	OHX	6	2101	-	0,6,6	-	-	-		
86	OHX	5	4221	-	0,6,6	-	-	-		
86	OHX	5	4123	-	0,6,6	-	-	-		
86	OHX	5	4250	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4167	-	0,6,6	-	-	-		
86	OHX	5	3923	-	0,6,6	-	-	-		
86	OHX	5	4011	-	0,6,6	-	-	-		
86	OHX	q1	102	-	0,6,6	-	-	-		
86	OHX	1	3991	-	0,6,6	-	-	-		
86	OHX	2	2098	-	0,6,6	-	-	-		
86	OHX	1	4199	-	0,6,6	-	-	-		
86	OHX	1	4042	-	0,6,6	-	-	-		
86	OHX	5	4158	-	0,6,6	-	-	-		
86	OHX	1	4106	-	0,6,6	-	-	-		
86	OHX	2	2086	-	0,6,6	-	-	-		
86	OHX	6	2099	-	0,6,6	-	-	-		
86	OHX	5	4052	-	0,6,6	-	-	-		
86	OHX	7	222	-	0,6,6	-	-	-		
86	OHX	1	4152	-	0,6,6	-	-	-		
86	OHX	1	3897	-	0,6,6	-	-	-		
86	OHX	1	4018	-	0,6,6	-	-	-		
86	OHX	5	4208	-	0,6,6	-	-	-		
86	OHX	8	228	-	0,6,6	-	-	-		
86	OHX	6	2140	-	0,6,6	-	-	-		
86	OHX	c8	203	-	0,6,6	-	-	-		
86	OHX	6	2067	-	0,6,6	-	-	-		
86	OHX	1	4060	-	0,6,6	-	-	-		
86	OHX	2	2148	-	0,6,6	-	-	-		
86	OHX	1	3986	-	0,6,6	-	-	-		
86	OHX	1	4129	-	0,6,6	-	-	-		
86	OHX	2	2102	-	0,6,6	-	-	-		
86	OHX	1	4171	-	0,6,6	-	-	-		
86	OHX	6	2088	-	0,6,6	-	-	-		
86	OHX	6	2187	-	0,6,6	-	-	-		
86	OHX	5	3933	-	0,6,6	-	-	-		
86	OHX	5	3965	-	0,6,6	-	-	-		
86	OHX	1	4151	-	0,6,6	-	-	-		
86	OHX	8	217	-	0,6,6	-	-	-		
86	OHX	5	4138	-	0,6,6	-	-	-		
86	OHX	1	4124	-	0,6,6	-	-	-		
86	OHX	6	2054	-	0,6,6	-	-	-		
86	OHX	3	223	-	0,6,6	-	-	-		
86	OHX	5	4242	-	0,6,6	-	-	-		
86	OHX	2	2059	-	0,6,6	-	-	-		
86	OHX	m1	203	-	0,6,6	-	-	-		
86	OHX	1	4150	-	0,6,6	-	-	-		
86	OHX	M9	204	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2053	-	0,6,6	-	-	-		
86	OHX	6	2055	-	0,6,6	-	-	-		
86	OHX	5	3905	-	0,6,6	-	-	-		
86	OHX	1	4125	-	0,6,6	-	-	-		
86	OHX	1	4132	-	0,6,6	-	-	-		
86	OHX	1	4032	-	0,6,6	-	-	-		
86	OHX	1	3894	-	0,6,6	-	-	-		
86	OHX	6	2199	-	0,6,6	-	-	-		
86	OHX	3	217	-	0,6,6	-	-	-		
86	OHX	5	4000	-	0,6,6	-	-	-		
86	OHX	1	4172	-	0,6,6	-	-	-		
86	OHX	5	4195	-	0,6,6	-	-	-		
86	OHX	1	4114	-	0,6,6	-	-	-		
86	OHX	5	4005	-	0,6,6	-	-	-		
86	OHX	5	3946	-	0,6,6	-	-	-		
86	OHX	5	3952	-	0,6,6	-	-	-		
86	OHX	6	2069	-	0,6,6	-	-	-		
86	OHX	1	3906	-	0,6,6	-	-	-		
86	OHX	5	4139	-	0,6,6	-	-	-		
86	OHX	1	4074	-	0,6,6	-	-	-		
86	OHX	2	2131	-	0,6,6	-	-	-		
86	OHX	1	3884	-	0,6,6	-	-	-		
86	OHX	6	2063	-	0,6,6	-	-	-		
86	OHX	1	3981	-	0,6,6	-	-	-		
86	OHX	5	4080	-	0,6,6	-	-	-		
86	OHX	5	4020	-	0,6,6	-	-	-		
86	OHX	1	3957	-	0,6,6	-	-	-		
86	OHX	1	4168	-	0,6,6	-	-	-		
86	OHX	1	4016	-	0,6,6	-	-	-		
86	OHX	2	2032	-	0,6,6	-	-	-		
86	OHX	5	4118	-	0,6,6	-	-	-		
86	OHX	1	3929	-	0,6,6	-	-	-		
86	OHX	6	2155	-	0,6,6	-	-	-		
86	OHX	1	4143	-	0,6,6	-	-	-		
86	OHX	1	4133	-	0,6,6	-	-	-		
86	OHX	1	4131	-	0,6,6	-	-	-		
86	OHX	5	4127	-	0,6,6	-	-	-		
86	OHX	5	4134	-	0,6,6	-	-	-		
86	OHX	8	220	-	0,6,6	-	-	-		
86	OHX	1	4068	-	0,6,6	-	-	-		
86	OHX	1	4062	-	0,6,6	-	-	-		
86	OHX	5	4068	-	0,6,6	-	-	-		
86	OHX	5	3951	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4010	-	0,6,6	-	-	-		
86	OHX	6	2085	-	0,6,6	-	-	-		
86	OHX	1	4094	-	0,6,6	-	-	-		
86	OHX	3	220	-	0,6,6	-	-	-		
86	OHX	5	4197	-	0,6,6	-	-	-		
86	OHX	1	3926	-	0,6,6	-	-	-		
86	OHX	L3	404	-	0,6,6	-	-	-		
86	OHX	6	2145	-	0,6,6	-	-	-		
86	OHX	1	4070	-	0,6,6	-	-	-		
86	OHX	1	3918	-	0,6,6	-	-	-		
86	OHX	5	4023	-	0,6,6	-	-	-		
86	OHX	5	4081	-	0,6,6	-	-	-		
86	OHX	5	4130	-	0,6,6	-	-	-		
86	OHX	2	2163	-	0,6,6	-	-	-		
86	OHX	2	2171	-	0,6,6	-	-	-		
86	OHX	1	4164	-	0,6,6	-	-	-		
86	OHX	1	4184	-	0,6,6	-	-	-		
86	OHX	3	225	-	0,6,6	-	-	-		
86	OHX	2	2128	-	0,6,6	-	-	-		
86	OHX	1	3891	-	0,6,6	-	-	-		
86	OHX	2	2092	-	0,6,6	-	-	-		
86	OHX	5	4133	-	0,6,6	-	-	-		
86	OHX	1	4163	-	0,6,6	-	-	-		
86	OHX	5	4220	-	0,6,6	-	-	-		
86	OHX	6	2077	-	0,6,6	-	-	-		
86	OHX	7	216	-	0,6,6	-	-	-		
86	OHX	6	2197	-	0,6,6	-	-	-		
86	OHX	1	4128	-	0,6,6	-	-	-		
86	OHX	2	2168	-	0,6,6	-	-	-		
86	OHX	1	4194	-	0,6,6	-	-	-		
86	OHX	2	2146	-	0,6,6	-	-	-		
86	OHX	5	4155	-	0,6,6	-	-	-		
86	OHX	1	4113	-	0,6,6	-	-	-		
86	OHX	5	4235	-	0,6,6	-	-	-		
86	OHX	5	3902	-	0,6,6	-	-	-		
86	OHX	1	3876	-	0,6,6	-	-	-		
86	OHX	2	2039	-	0,6,6	-	-	-		
86	OHX	6	2148	-	0,6,6	-	-	-		
86	OHX	6	2160	-	0,6,6	-	-	-		
86	OHX	2	2124	-	0,6,6	-	-	-		
86	OHX	s1	303	-	0,6,6	-	-	-		
86	OHX	6	2065	-	0,6,6	-	-	-		
86	OHX	2	2080	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4076	-	0,6,6	-	-	-		
86	OHX	6	2194	-	0,6,6	-	-	-		
86	OHX	5	4008	-	0,6,6	-	-	-		
86	OHX	6	2150	-	0,6,6	-	-	-		
86	OHX	2	2037	-	0,6,6	-	-	-		
86	OHX	5	3928	-	0,6,6	-	-	-		
86	OHX	5	4203	-	0,6,6	-	-	-		
86	OHX	1	3995	-	0,6,6	-	-	-		
86	OHX	6	2168	-	0,6,6	-	-	-		
86	OHX	1	4071	-	0,6,6	-	-	-		
86	OHX	1	4146	-	0,6,6	-	-	-		
86	OHX	6	2133	-	0,6,6	-	-	-		
86	OHX	2	2103	-	0,6,6	-	-	-		
86	OHX	1	4033	-	0,6,6	-	-	-		
86	OHX	1	3997	-	0,6,6	-	-	-		
86	OHX	6	2157	-	0,6,6	-	-	-		
86	OHX	2	2145	-	0,6,6	-	-	-		
86	OHX	5	3906	-	0,6,6	-	-	-		
86	OHX	2	2044	-	0,6,6	-	-	-		
86	OHX	2	2093	-	0,6,6	-	-	-		
86	OHX	1	4031	-	0,6,6	-	-	-		
86	OHX	1	4123	-	0,6,6	-	-	-		
86	OHX	S8	302	-	0,6,6	-	-	-		
86	OHX	2	2051	-	0,6,6	-	-	-		
86	OHX	2	2065	-	0,6,6	-	-	-		
86	OHX	2	2105	-	0,6,6	-	-	-		
86	OHX	5	3989	-	0,6,6	-	-	-		
86	OHX	7	217	-	0,6,6	-	-	-		
86	OHX	5	3936	-	0,6,6	-	-	-		
86	OHX	2	2143	-	0,6,6	-	-	-		
86	OHX	2	2164	-	0,6,6	-	-	-		
86	OHX	n3	203	-	0,6,6	-	-	-		
86	OHX	2	2025	-	0,6,6	-	-	-		
86	OHX	2	2104	-	0,6,6	-	-	-		
86	OHX	2	2045	-	0,6,6	-	-	-		
86	OHX	6	2102	-	0,6,6	-	-	-		
86	OHX	1	4192	-	0,6,6	-	-	-		
86	OHX	2	2173	-	0,6,6	-	-	-		
86	OHX	2	2036	-	0,6,6	-	-	-		
86	OHX	1	4019	-	0,6,6	-	-	-		
86	OHX	5	3996	-	0,6,6	-	-	-		
86	OHX	1	4011	-	0,6,6	-	-	-		
86	OHX	1	4188	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2049	-	0,6,6	-	-	-		
86	OHX	8	227	-	0,6,6	-	-	-		
86	OHX	1	4144	-	0,6,6	-	-	-		
86	OHX	1	3953	-	0,6,6	-	-	-		
86	OHX	2	2152	-	0,6,6	-	-	-		
86	OHX	1	4176	-	0,6,6	-	-	-		
86	OHX	1	3937	-	0,6,6	-	-	-		
86	OHX	5	3957	-	0,6,6	-	-	-		
86	OHX	5	4054	-	0,6,6	-	-	-		
86	OHX	5	3984	-	0,6,6	-	-	-		
86	OHX	1	4122	-	0,6,6	-	-	-		
86	OHX	5	4239	-	0,6,6	-	-	-		
86	OHX	7	226	-	0,6,6	-	-	-		
86	OHX	2	2121	-	0,6,6	-	-	-		
86	OHX	6	2153	-	0,6,6	-	-	-		
86	OHX	5	4160	-	0,6,6	-	-	-		
86	OHX	5	3976	-	0,6,6	-	-	-		
86	OHX	1	4080	-	0,6,6	-	-	-		
86	OHX	5	4185	-	0,6,6	-	-	-		
86	OHX	6	2152	-	0,6,6	-	-	-		
86	OHX	5	4003	-	0,6,6	-	-	-		
86	OHX	6	2082	-	0,6,6	-	-	-		
86	OHX	5	4096	-	0,6,6	-	-	-		
86	OHX	5	4077	-	0,6,6	-	-	-		
86	OHX	5	4079	-	0,6,6	-	-	-		
86	OHX	5	3937	-	0,6,6	-	-	-		
86	OHX	1	4095	-	0,6,6	-	-	-		
86	OHX	5	4214	-	0,6,6	-	-	-		
86	OHX	5	4047	-	0,6,6	-	-	-		
86	OHX	1	4083	-	0,6,6	-	-	-		
86	OHX	5	3958	-	0,6,6	-	-	-		
86	OHX	1	4010	-	0,6,6	-	-	-		
86	OHX	1	4041	-	0,6,6	-	-	-		
86	OHX	5	4013	-	0,6,6	-	-	-		
86	OHX	6	2078	-	0,6,6	-	-	-		
86	OHX	1	3956	-	0,6,6	-	-	-		
86	OHX	2	2138	-	0,6,6	-	-	-		
86	OHX	1	4020	-	0,6,6	-	-	-		
86	OHX	2	2076	-	0,6,6	-	-	-		
86	OHX	1	3908	-	0,6,6	-	-	-		
86	OHX	6	2146	-	0,6,6	-	-	-		
86	OHX	5	4161	-	0,6,6	-	-	-		
86	OHX	4	228	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3901	-	0,6,6	-	-	-		
86	OHX	5	3960	-	0,6,6	-	-	-		
86	OHX	1	3900	-	0,6,6	-	-	-		
86	OHX	5	4216	-	0,6,6	-	-	-		
86	OHX	5	4146	-	0,6,6	-	-	-		
86	OHX	4	231	-	0,6,6	-	-	-		
86	OHX	5	4073	-	0,6,6	-	-	-		
86	OHX	5	3944	-	0,6,6	-	-	-		
86	OHX	2	2134	-	0,6,6	-	-	-		
86	OHX	5	4193	-	0,6,6	-	-	-		
86	OHX	1	3999	-	0,6,6	-	-	-		
86	OHX	5	3948	-	0,6,6	-	-	-		
86	OHX	1	3934	-	0,6,6	-	-	-		
86	OHX	1	3988	-	0,6,6	-	-	-		
86	OHX	1	4159	-	0,6,6	-	-	-		
86	OHX	5	3974	-	0,6,6	-	-	-		
86	OHX	n9	101	-	0,6,6	-	-	-		
86	OHX	5	3983	-	0,6,6	-	-	-		
86	OHX	5	4222	-	0,6,6	-	-	-		
86	OHX	1	4067	-	0,6,6	-	-	-		
86	OHX	5	3950	-	0,6,6	-	-	-		
86	OHX	2	2071	-	0,6,6	-	-	-		
86	OHX	5	4172	-	0,6,6	-	-	-		
86	OHX	5	4241	-	0,6,6	-	-	-		
86	OHX	2	2024	-	0,6,6	-	-	-		
86	OHX	8	230	-	0,6,6	-	-	-		
86	OHX	m0	301	-	0,6,6	-	-	-		
86	OHX	6	2126	-	0,6,6	-	-	-		
86	OHX	5	4056	-	0,6,6	-	-	-		
86	OHX	2	2046	-	0,6,6	-	-	-		
86	OHX	5	3997	-	0,6,6	-	-	-		
86	OHX	4	222	-	0,6,6	-	-	-		
86	OHX	6	2176	-	0,6,6	-	-	-		
86	OHX	1	4119	-	0,6,6	-	-	-		
86	OHX	C3	201	-	0,6,6	-	-	-		
86	OHX	1	3954	-	0,6,6	-	-	-		
86	OHX	1	3885	-	0,6,6	-	-	-		
86	OHX	1	4014	-	0,6,6	-	-	-		
86	OHX	6	2071	-	0,6,6	-	-	-		
86	OHX	6	2132	-	0,6,6	-	-	-		
86	OHX	5	4156	-	0,6,6	-	-	-		
86	OHX	5	4182	-	0,6,6	-	-	-		
86	OHX	1	3883	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4152	-	0,6,6	-	-	-		
86	OHX	D9	102	-	0,6,6	-	-	-		
86	OHX	1	4052	-	0,6,6	-	-	-		
86	OHX	1	4117	-	0,6,6	-	-	-		
86	OHX	4	225	-	0,6,6	-	-	-		
86	OHX	6	2080	-	0,6,6	-	-	-		
86	OHX	6	2123	-	0,6,6	-	-	-		
86	OHX	5	4144	-	0,6,6	-	-	-		
86	OHX	5	4183	-	0,6,6	-	-	-		
86	OHX	6	2135	-	0,6,6	-	-	-		
86	OHX	6	2202	-	0,6,6	-	-	-		
86	OHX	5	3934	-	0,6,6	-	-	-		
86	OHX	1	4177	-	0,6,6	-	-	-		
86	OHX	6	2098	-	0,6,6	-	-	-		
86	OHX	6	2139	-	0,6,6	-	-	-		
86	OHX	6	2049	-	0,6,6	-	-	-		
86	OHX	2	2100	-	0,6,6	-	-	-		
86	OHX	1	3928	-	0,6,6	-	-	-		
86	OHX	6	2196	-	0,6,6	-	-	-		
86	OHX	1	3941	-	0,6,6	-	-	-		
86	OHX	5	4009	-	0,6,6	-	-	-		
86	OHX	5	4108	-	0,6,6	-	-	-		
86	OHX	6	2070	-	0,6,6	-	-	-		
86	OHX	5	4200	-	0,6,6	-	-	-		
86	OHX	7	221	-	0,6,6	-	-	-		
86	OHX	2	2099	-	0,6,6	-	-	-		
86	OHX	5	4025	-	0,6,6	-	-	-		
86	OHX	1	4084	-	0,6,6	-	-	-		
86	OHX	6	2141	-	0,6,6	-	-	-		
86	OHX	4	229	-	0,6,6	-	-	-		
86	OHX	o3	202	-	0,6,6	-	-	-		
86	OHX	2	2170	-	0,6,6	-	-	-		
86	OHX	5	4037	-	0,6,6	-	-	-		
86	OHX	1	4121	-	0,6,6	-	-	-		
86	OHX	6	2089	-	0,6,6	-	-	-		
86	OHX	4	236	-	0,6,6	-	-	-		
86	OHX	5	4015	-	0,6,6	-	-	-		
86	OHX	5	4006	-	0,6,6	-	-	-		
86	OHX	5	3903	-	0,6,6	-	-	-		
86	OHX	5	4060	-	0,6,6	-	-	-		
86	OHX	2	2096	-	0,6,6	-	-	-		
86	OHX	3	224	-	0,6,6	-	-	-		
86	OHX	5	4091	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2088	-	0,6,6	-	-	-		
86	OHX	2	2109	-	0,6,6	-	-	-		
86	OHX	6	2192	-	0,6,6	-	-	-		
86	OHX	5	4107	-	0,6,6	-	-	-		
86	OHX	5	3964	-	0,6,6	-	-	-		
86	OHX	1	4100	-	0,6,6	-	-	-		
86	OHX	4	233	-	0,6,6	-	-	-		
86	OHX	5	4111	-	0,6,6	-	-	-		
86	OHX	2	2054	-	0,6,6	-	-	-		
86	OHX	S6	301	-	0,6,6	-	-	-		
86	OHX	5	4113	-	0,6,6	-	-	-		
86	OHX	5	3913	-	0,6,6	-	-	-		
86	OHX	1	4093	-	0,6,6	-	-	-		
86	OHX	1	4158	-	0,6,6	-	-	-		
86	OHX	5	3962	-	0,6,6	-	-	-		
86	OHX	5	4191	-	0,6,6	-	-	-		
86	OHX	1	4098	-	0,6,6	-	-	-		
86	OHX	6	2068	-	0,6,6	-	-	-		
86	OHX	5	4022	-	0,6,6	-	-	-		
86	OHX	7	220	-	0,6,6	-	-	-		
86	OHX	5	4098	-	0,6,6	-	-	-		
86	OHX	5	4102	-	0,6,6	-	-	-		
86	OHX	5	4145	-	0,6,6	-	-	-		
86	OHX	6	2138	-	0,6,6	-	-	-		
86	OHX	L3	403	-	0,6,6	-	-	-		
86	OHX	1	4208	-	0,6,6	-	-	-		
86	OHX	6	2173	-	0,6,6	-	-	-		
86	OHX	5	4115	-	0,6,6	-	-	-		
86	OHX	1	3966	-	0,6,6	-	-	-		
86	OHX	2	2029	-	0,6,6	-	-	-		
86	OHX	5	4159	-	0,6,6	-	-	-		
86	OHX	2	2060	-	0,6,6	-	-	-		
86	OHX	5	4173	-	0,6,6	-	-	-		
86	OHX	5	3968	-	0,6,6	-	-	-		
86	OHX	1	4069	-	0,6,6	-	-	-		
86	OHX	2	2028	-	0,6,6	-	-	-		
86	OHX	d4	201	-	0,6,6	-	-	-		
86	OHX	2	2042	-	0,6,6	-	-	-		
86	OHX	5	4223	-	0,6,6	-	-	-		
86	OHX	1	4210	-	0,6,6	-	-	-		
86	OHX	7	218	-	0,6,6	-	-	-		
86	OHX	5	4192	-	0,6,6	-	-	-		
86	OHX	5	4229	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	m8	201	-	0,6,6	-	-	-		
86	OHX	1	4053	-	0,6,6	-	-	-		
86	OHX	1	4201	-	0,6,6	-	-	-		
86	OHX	2	2074	-	0,6,6	-	-	-		
86	OHX	1	4165	-	0,6,6	-	-	-		
86	OHX	1	4187	-	0,6,6	-	-	-		
86	OHX	c5	201	-	0,6,6	-	-	-		
86	OHX	6	2137	-	0,6,6	-	-	-		
86	OHX	1	3905	-	0,6,6	-	-	-		
86	OHX	1	3930	-	0,6,6	-	-	-		
86	OHX	1	3880	-	0,6,6	-	-	-		
86	OHX	5	3945	-	0,6,6	-	-	-		
86	OHX	5	4038	-	0,6,6	-	-	-		
86	OHX	1	3944	-	0,6,6	-	-	-		
86	OHX	1	4212	-	0,6,6	-	-	-		
86	OHX	Q2	503	-	0,6,6	-	-	-		
86	OHX	6	2076	-	0,6,6	-	-	-		
86	OHX	1	3871	-	0,6,6	-	-	-		
86	OHX	1	3868	-	0,6,6	-	-	-		
86	OHX	6	2164	-	0,6,6	-	-	-		
86	OHX	6	2167	-	0,6,6	-	-	-		
86	OHX	5	4218	-	0,6,6	-	-	-		
86	OHX	6	2074	-	0,6,6	-	-	-		
86	OHX	1	3976	-	0,6,6	-	-	-		
86	OHX	5	3943	86	0,6,6	-	-	-		
86	OHX	1	3909	-	0,6,6	-	-	-		
86	OHX	5	4206	-	0,6,6	-	-	-		
86	OHX	5	4053	-	0,6,6	-	-	-		
86	OHX	5	3986	-	0,6,6	-	-	-		
86	OHX	6	2091	-	0,6,6	-	-	-		
86	OHX	6	2050	-	0,6,6	-	-	-		
86	OHX	1	3960	-	0,6,6	-	-	-		
86	OHX	5	4078	-	0,6,6	-	-	-		
86	OHX	m7	206	-	0,6,6	-	-	-		
86	OHX	2	2140	-	0,6,6	-	-	-		
86	OHX	5	4150	-	0,6,6	-	-	-		
86	OHX	2	2107	-	0,6,6	-	-	-		
86	OHX	5	4181	-	0,6,6	-	-	-		
86	OHX	1	4073	-	0,6,6	-	-	-		
86	OHX	1	4022	-	0,6,6	-	-	-		
86	OHX	5	4180	-	0,6,6	-	-	-		
86	OHX	5	4090	-	0,6,6	-	-	-		
86	OHX	1	3925	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4118	-	0,6,6	-	-	-		
86	OHX	2	2176	-	0,6,6	-	-	-		
86	OHX	2	2087	-	0,6,6	-	-	-		
86	OHX	5	4128	-	0,6,6	-	-	-		
86	OHX	1	4127	-	0,6,6	-	-	-		
86	OHX	1	4206	-	0,6,6	-	-	-		
86	OHX	6	2142	-	0,6,6	-	-	-		
86	OHX	1	3913	-	0,6,6	-	-	-		
86	OHX	6	2183	-	0,6,6	-	-	-		
86	OHX	5	3927	-	0,6,6	-	-	-		
86	OHX	1	3882	-	0,6,6	-	-	-		
86	OHX	1	3873	-	0,6,6	-	-	-		
86	OHX	5	4184	-	0,6,6	-	-	-		
86	OHX	4	235	-	0,6,6	-	-	-		
86	OHX	6	2108	-	0,6,6	-	-	-		
86	OHX	2	2033	-	0,6,6	-	-	-		
86	OHX	5	4168	-	0,6,6	-	-	-		
86	OHX	8	223	-	0,6,6	-	-	-		
86	OHX	5	4226	-	0,6,6	-	-	-		
86	OHX	6	2156	-	0,6,6	-	-	-		
86	OHX	1	4148	-	0,6,6	-	-	-		
86	OHX	1	4197	-	0,6,6	-	-	-		
86	OHX	5	4030	-	0,6,6	-	-	-		
86	OHX	1	4108	-	0,6,6	-	-	-		
86	OHX	1	3948	-	0,6,6	-	-	-		
86	OHX	1	3870	-	0,6,6	-	-	-		
86	OHX	1	3963	-	0,6,6	-	-	-		
86	OHX	1	4051	-	0,6,6	-	-	-		
86	OHX	6	2161	-	0,6,6	-	-	-		
86	OHX	2	2136	-	0,6,6	-	-	-		
86	OHX	1	3890	-	0,6,6	-	-	-		
86	OHX	8	231	-	0,6,6	-	-	-		
86	OHX	1	4056	-	0,6,6	-	-	-		
86	OHX	2	2069	-	0,6,6	-	-	-		
86	OHX	1	4179	-	0,6,6	-	-	-		
86	OHX	N1	201	-	0,6,6	-	-	-		
86	OHX	5	3915	-	0,6,6	-	-	-		
86	OHX	6	2127	-	0,6,6	-	-	-		
86	OHX	5	3969	-	0,6,6	-	-	-		
86	OHX	6	2179	-	0,6,6	-	-	-		
86	OHX	1	4115	-	0,6,6	-	-	-		
86	OHX	1	4162	-	0,6,6	-	-	-		
86	OHX	2	2125	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4002	-	0,6,6	-	-	-		
86	OHX	5	4153	-	0,6,6	-	-	-		
86	OHX	1	4076	-	0,6,6	-	-	-		
86	OHX	5	4070	-	0,6,6	-	-	-		
86	OHX	5	3918	-	0,6,6	-	-	-		
86	OHX	2	2070	-	0,6,6	-	-	-		
86	OHX	1	4013	-	0,6,6	-	-	-		
86	OHX	1	3984	-	0,6,6	-	-	-		
86	OHX	1	4065	-	0,6,6	-	-	-		
86	OHX	1	3878	-	0,6,6	-	-	-		
86	OHX	5	4202	-	0,6,6	-	-	-		
86	OHX	2	2058	-	0,6,6	-	-	-		
86	OHX	5	3977	-	0,6,6	-	-	-		
86	OHX	1	3992	-	0,6,6	-	-	-		
86	OHX	2	2068	-	0,6,6	-	-	-		
86	OHX	1	4136	-	0,6,6	-	-	-		
86	OHX	5	4045	-	0,6,6	-	-	-		
86	OHX	2	2085	-	0,6,6	-	-	-		
86	OHX	5	4119	-	0,6,6	-	-	-		
86	OHX	5	4057	-	0,6,6	-	-	-		
86	OHX	6	2125	-	0,6,6	-	-	-		
86	OHX	5	4101	-	0,6,6	-	-	-		
86	OHX	8	222	-	0,6,6	-	-	-		
86	OHX	5	4028	-	0,6,6	-	-	-		
86	OHX	5	4058	-	0,6,6	-	-	-		
86	OHX	6	2185	-	0,6,6	-	-	-		
86	OHX	6	2195	-	0,6,6	-	-	-		
86	OHX	5	4065	-	0,6,6	-	-	-		
86	OHX	6	2181	-	0,6,6	-	-	-		
86	OHX	5	3941	-	0,6,6	-	-	-		
86	OHX	1	4207	-	0,6,6	-	-	-		
86	OHX	5	3992	-	0,6,6	-	-	-		
86	OHX	2	2031	-	0,6,6	-	-	-		
86	OHX	2	2034	-	0,6,6	-	-	-		
86	OHX	1	3914	-	0,6,6	-	-	-		
86	OHX	6	2130	-	0,6,6	-	-	-		
86	OHX	6	2151	-	0,6,6	-	-	-		
86	OHX	2	2120	-	0,6,6	-	-	-		
86	OHX	2	2147	-	0,6,6	-	-	-		
86	OHX	5	3972	-	0,6,6	-	-	-		
86	OHX	5	3987	-	0,6,6	-	-	-		
86	OHX	5	4140	-	0,6,6	-	-	-		
86	OHX	1	3931	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4039	-	0,6,6	-	-	-		
86	OHX	5	4247	-	0,6,6	-	-	-		
86	OHX	1	3968	-	0,6,6	-	-	-		
87	PCY	2	2178	-	34,42,42	0.47	0	41,65,65	1.40	3 (7%)
86	OHX	5	4126	-	0,6,6	-	-	-		
86	OHX	1	3923	-	0,6,6	-	-	-		
86	OHX	5	4211	-	0,6,6	-	-	-		
86	OHX	5	4227	-	0,6,6	-	-	-		
86	OHX	6	2086	-	0,6,6	-	-	-		
86	OHX	c3	201	-	0,6,6	-	-	-		
86	OHX	1	4054	-	0,6,6	-	-	-		
86	OHX	2	2122	-	0,6,6	-	-	-		
86	OHX	1	3994	-	0,6,6	-	-	-		
86	OHX	6	2110	-	0,6,6	-	-	-		
86	OHX	2	2113	-	0,6,6	-	-	-		
86	OHX	L3	405	-	0,6,6	-	-	-		
86	OHX	1	4166	-	0,6,6	-	-	-		
86	OHX	5	3942	-	0,6,6	-	-	-		
86	OHX	1	4088	-	0,6,6	-	-	-		
86	OHX	2	2073	-	0,6,6	-	-	-		
86	OHX	2	2052	-	0,6,6	-	-	-		
86	OHX	O3	202	-	0,6,6	-	-	-		
86	OHX	l5	303	-	0,6,6	-	-	-		
86	OHX	o7	503	-	0,6,6	-	-	-		
86	OHX	5	4238	-	0,6,6	-	-	-		
86	OHX	5	4066	-	0,6,6	-	-	-		
86	OHX	1	4003	-	0,6,6	-	-	-		
86	OHX	14	402	-	0,6,6	-	-	-		
86	OHX	2	2030	-	0,6,6	-	-	-		
86	OHX	1	4096	-	0,6,6	-	-	-		
86	OHX	2	2158	-	0,6,6	-	-	-		
86	OHX	1	3886	-	0,6,6	-	-	-		
86	OHX	1	4077	-	0,6,6	-	-	-		
86	OHX	1	4079	-	0,6,6	-	-	-		
86	OHX	2	2149	-	0,6,6	-	-	-		
86	OHX	1	4213	-	0,6,6	-	-	-		
86	OHX	4	230	-	0,6,6	-	-	-		
86	OHX	1	3903	-	0,6,6	-	-	-		
86	OHX	1	4047	-	0,6,6	-	-	-		
86	OHX	1	4091	-	0,6,6	-	-	-		
86	OHX	6	2154	-	0,6,6	-	-	-		
86	OHX	5	4131	-	0,6,6	-	-	-		
86	OHX	5	4055	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4092	-	0,6,6	-	-	-		
86	OHX	1	4004	-	0,6,6	-	-	-		
86	OHX	5	4051	-	0,6,6	-	-	-		
86	OHX	6	2084	-	0,6,6	-	-	-		
86	OHX	6	2121	-	0,6,6	-	-	-		
86	OHX	5	4021	-	0,6,6	-	-	-		
86	OHX	6	2171	-	0,6,6	-	-	-		
86	OHX	1	4008	-	0,6,6	-	-	-		
86	OHX	1	3907	-	0,6,6	-	-	-		
86	OHX	1	4198	-	0,6,6	-	-	-		
86	OHX	5	3971	-	0,6,6	-	-	-		
86	OHX	2	2079	-	0,6,6	-	-	-		
86	OHX	6	2083	-	0,6,6	-	-	-		
86	OHX	1	3904	-	0,6,6	-	-	-		
86	OHX	6	2159	-	0,6,6	-	-	-		
86	OHX	2	2112	-	0,6,6	-	-	-		
86	OHX	5	4234	-	0,6,6	-	-	-		
86	OHX	5	3993	-	0,6,6	-	-	-		
86	OHX	5	3919	-	0,6,6	-	-	-		
86	OHX	1	3927	-	0,6,6	-	-	-		
86	OHX	5	4121	-	0,6,6	-	-	-		
86	OHX	5	4137	-	0,6,6	-	-	-		
86	OHX	1	3946	-	0,6,6	-	-	-		
86	OHX	5	4095	-	0,6,6	-	-	-		
86	OHX	1	3974	-	0,6,6	-	-	-		
86	OHX	2	2161	-	0,6,6	-	-	-		
86	OHX	5	4001	-	0,6,6	-	-	-		
86	OHX	6	2189	-	0,6,6	-	-	-		
86	OHX	5	4043	-	0,6,6	-	-	-		
86	OHX	5	3904	-	0,6,6	-	-	-		
86	OHX	2	2062	-	0,6,6	-	-	-		
86	OHX	2	2139	-	0,6,6	-	-	-		
86	OHX	1	3915	-	0,6,6	-	-	-		
86	OHX	1	3950	-	0,6,6	-	-	-		
86	OHX	1	4059	-	0,6,6	-	-	-		
86	OHX	5	4071	-	0,6,6	-	-	-		
86	OHX	5	4143	-	0,6,6	-	-	-		
86	OHX	6	2081	-	0,6,6	-	-	-		
86	OHX	1	3936	-	0,6,6	-	-	-		
86	OHX	7	224	-	0,6,6	-	-	-		
86	OHX	m4	201	-	0,6,6	-	-	-		
86	OHX	4	227	-	0,6,6	-	-	-		
86	OHX	6	2059	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3867	-	0,6,6	-	-	-		
86	OHX	2	2141	-	0,6,6	-	-	-		
86	OHX	5	3901	-	0,6,6	-	-	-		
86	OHX	5	3900	-	0,6,6	-	-	-		
86	OHX	5	3930	-	0,6,6	-	-	-		
86	OHX	5	3938	-	0,6,6	-	-	-		
86	OHX	5	4007	-	0,6,6	-	-	-		
86	OHX	8	232	-	0,6,6	-	-	-		
86	OHX	1	4134	-	0,6,6	-	-	-		
86	OHX	4	234	-	0,6,6	-	-	-		
86	OHX	5	3932	-	0,6,6	-	-	-		
86	OHX	1	4182	-	0,6,6	-	-	-		
86	OHX	5	4243	-	0,6,6	-	-	-		
86	OHX	5	3980	-	0,6,6	-	-	-		
86	OHX	5	3988	-	0,6,6	-	-	-		
86	OHX	2	2078	-	0,6,6	-	-	-		
86	OHX	1	4027	-	0,6,6	-	-	-		
86	OHX	1	4183	-	0,6,6	-	-	-		
86	OHX	5	3956	-	0,6,6	-	-	-		
86	OHX	1	4195	-	0,6,6	-	-	-		
86	OHX	6	2147	-	0,6,6	-	-	-		
86	OHX	5	3955	-	0,6,6	-	-	-		
86	OHX	6	2163	-	0,6,6	-	-	-		
86	OHX	5	4033	-	0,6,6	-	-	-		
86	OHX	1	4110	-	0,6,6	-	-	-		
86	OHX	1	4087	-	0,6,6	-	-	-		
86	OHX	1	4012	-	0,6,6	-	-	-		
86	OHX	M7	205	-	0,6,6	-	-	-		
86	OHX	m0	302	-	0,6,6	-	-	-		
86	OHX	1	4193	-	0,6,6	-	-	-		
86	OHX	2	2165	-	0,6,6	-	-	-		
86	OHX	C5	201	-	0,6,6	-	-	-		
86	OHX	1	3958	-	0,6,6	-	-	-		
86	OHX	1	4009	-	0,6,6	-	-	-		
86	OHX	5	4086	-	0,6,6	-	-	-		
86	OHX	2	2137	-	0,6,6	-	-	-		
86	OHX	5	4074	-	0,6,6	-	-	-		
86	OHX	N9	102	-	0,6,6	-	-	-		
86	OHX	1	4055	-	0,6,6	-	-	-		
86	OHX	1	4135	-	0,6,6	-	-	-		
86	OHX	1	4006	-	0,6,6	-	-	-		
86	OHX	5	4244	-	0,6,6	-	-	-		
86	OHX	6	2172	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4044	-	0,6,6	-	-	-		
86	OHX	1	4005	-	0,6,6	-	-	-		
86	OHX	5	4205	-	0,6,6	-	-	-		
86	OHX	5	4112	-	0,6,6	-	-	-		
86	OHX	1	4111	-	0,6,6	-	-	-		
86	OHX	5	4088	-	0,6,6	-	-	-		
86	OHX	1	3983	-	0,6,6	-	-	-		
86	OHX	3	218	-	0,6,6	-	-	-		
86	OHX	2	2174	-	0,6,6	-	-	-		
86	OHX	5	4099	-	0,6,6	-	-	-		
86	OHX	5	3911	-	0,6,6	-	-	-		
86	OHX	6	2093	-	0,6,6	-	-	-		
86	OHX	1	3987	-	0,6,6	-	-	-		
86	OHX	2	2095	-	0,6,6	-	-	-		
86	OHX	2	2169	-	0,6,6	-	-	-		
86	OHX	5	4082	-	0,6,6	-	-	-		
86	OHX	1	4145	-	0,6,6	-	-	-		
86	OHX	5	4246	-	0,6,6	-	-	-		
86	OHX	3	226	-	0,6,6	-	-	-		
86	OHX	2	2072	-	0,6,6	-	-	-		
86	OHX	5	4061	-	0,6,6	-	-	-		
87	PCY	6	2204	-	34,42,42	0.60	1 (2%)	41,65,65	1.39	2 (4%)
86	OHX	1	4173	-	0,6,6	-	-	-		
86	OHX	5	3935	-	0,6,6	-	-	-		
86	OHX	2	2097	-	0,6,6	-	-	-		
86	OHX	6	2124	-	0,6,6	-	-	-		
86	OHX	2	2048	-	0,6,6	-	-	-		
86	OHX	5	3907	-	0,6,6	-	-	-		
86	OHX	6	2182	-	0,6,6	-	-	-		
86	OHX	6	2116	-	0,6,6	-	-	-		
86	OHX	13	404	-	0,6,6	-	-	-		
86	OHX	1	3864	-	0,6,6	-	-	-		
86	OHX	1	4142	-	0,6,6	-	-	-		
86	OHX	6	2057	-	0,6,6	-	-	-		
86	OHX	2	2082	-	0,6,6	-	-	-		
86	OHX	5	4189	-	0,6,6	-	-	-		
86	OHX	1	3965	-	0,6,6	-	-	-		
86	OHX	5	3925	-	0,6,6	-	-	-		
86	OHX	5	4154	-	0,6,6	-	-	-		
86	OHX	3	215	-	0,6,6	-	-	-		
86	OHX	1	4025	-	0,6,6	-	-	-		
86	OHX	1	4064	-	0,6,6	-	-	-		
86	OHX	1	4138	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	n9	102	-	0,6,6	-	-	-		
86	OHX	5	3973	-	0,6,6	-	-	-		
86	OHX	2	2083	-	0,6,6	-	-	-		
86	OHX	1	4015	-	0,6,6	-	-	-		
86	OHX	6	2060	-	0,6,6	-	-	-		
86	OHX	1	4063	-	0,6,6	-	-	-		
86	OHX	5	4215	-	0,6,6	-	-	-		
86	OHX	1	4139	-	0,6,6	-	-	-		
86	OHX	5	3994	-	0,6,6	-	-	-		
86	OHX	2	2094	-	0,6,6	-	-	-		
86	OHX	1	3943	-	0,6,6	-	-	-		
86	OHX	2	2050	-	0,6,6	-	-	-		
86	OHX	1	4057	-	0,6,6	-	-	-		
86	OHX	1	4116	-	0,6,6	-	-	-		
86	OHX	5	3949	-	0,6,6	-	-	-		
86	OHX	1	4105	-	0,6,6	-	-	-		
86	OHX	6	2162	-	0,6,6	-	-	-		
86	OHX	5	3998	-	0,6,6	-	-	-		
86	OHX	5	4174	-	0,6,6	-	-	-		
86	OHX	5	4219	-	0,6,6	-	-	-		
86	OHX	5	3967	-	0,6,6	-	-	-		
86	OHX	5	4105	-	0,6,6	-	-	-		
86	OHX	5	4151	-	0,6,6	-	-	-		
86	OHX	5	3959	-	0,6,6	-	-	-		
86	OHX	1	4181	-	0,6,6	-	-	-		
86	OHX	5	4027	-	0,6,6	-	-	-		
86	OHX	5	4190	-	0,6,6	-	-	-		
86	OHX	2	2066	-	0,6,6	-	-	-		
86	OHX	s9	201	-	0,6,6	-	-	-		
86	OHX	5	3908	-	0,6,6	-	-	-		
86	OHX	1	3872	-	0,6,6	-	-	-		
86	OHX	1	4092	-	0,6,6	-	-	-		
86	OHX	2	2055	-	0,6,6	-	-	-		
86	OHX	6	2166	-	0,6,6	-	-	-		
86	OHX	1	3975	-	0,6,6	-	-	-		
86	OHX	5	4004	-	0,6,6	-	-	-		
86	OHX	5	4059	-	0,6,6	-	-	-		
86	OHX	5	3975	-	0,6,6	-	-	-		
86	OHX	6	2165	-	0,6,6	-	-	-		
86	OHX	2	2110	-	0,6,6	-	-	-		
86	OHX	5	4149	-	0,6,6	-	-	-		
86	OHX	2	2035	-	0,6,6	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	PCY	6	2204	-	-	10/33/67/67	0/3/3/3
87	PCY	2	2178	-	-	6/33/67/67	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	6	2204	PCY	C24-C28	2.05	1.42	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	2	2178	PCY	N2-C1-N4	-7.12	111.41	116.74
87	6	2204	PCY	N2-C1-N4	-6.81	111.64	116.74
87	2	2178	PCY	O14-C7-C13	-2.91	102.82	109.17
87	2	2178	PCY	O5-C1-N2	2.23	126.12	121.36
87	6	2204	PCY	O5-C1-N2	2.20	126.04	121.36

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	2	2178	PCY	N2-C3-C6-C11
87	2	2178	PCY	N2-C3-C6-O12
87	2	2178	PCY	C7-C3-C6-C11
87	2	2178	PCY	C8-C3-C6-C11
87	6	2204	PCY	N2-C3-C6-C11

There are no ring outliers.

488 monomers are involved in 732 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	4035	OHX	4	0
86	1	4137	OHX	1	0
86	5	4186	OHX	1	0
86	1	4030	OHX	6	0
86	8	229	OHX	2	0
86	6	2174	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	4043	OHX	6	0
86	5	4198	OHX	3	0
86	5	4141	OHX	1	0
86	1	3955	OHX	5	0
86	1	4038	OHX	2	0
86	5	3961	OHX	1	0
86	2	2084	OHX	1	0
86	2	2067	OHX	1	0
86	5	3920	OHX	1	0
86	1	4153	OHX	2	0
86	5	4162	OHX	1	0
86	5	4089	OHX	1	0
86	5	3963	OHX	4	0
86	1	4037	OHX	2	0
86	1	3896	OHX	1	0
86	1	3970	OHX	1	0
86	1	4180	OHX	3	0
86	2	2117	OHX	2	0
86	5	3910	OHX	1	0
86	2	2130	OHX	1	0
86	6	2046	OHX	1	0
86	6	2095	OHX	1	0
86	5	4072	OHX	1	0
86	7	225	OHX	7	0
86	6	2178	OHX	1	0
86	1	4081	OHX	1	0
86	5	4050	OHX	1	0
86	1	3979	OHX	1	0
86	1	3888	OHX	1	0
86	1	3972	OHX	1	0
86	2	2127	OHX	1	0
86	1	4036	OHX	2	0
86	1	4039	OHX	2	0
86	2	2154	OHX	1	0
86	5	4231	OHX	1	0
86	5	4017	OHX	1	0
86	2	2106	OHX	1	0
86	1	3978	OHX	1	0
86	1	3879	OHX	1	0
86	1	3969	OHX	6	0
86	6	2188	OHX	2	0
86	L4	403	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	3985	OHX	1	0
86	2	2167	OHX	1	0
86	M7	206	OHX	1	0
86	2	2111	OHX	1	0
86	5	4120	OHX	1	0
86	5	4097	OHX	1	0
86	2	2038	OHX	1	0
86	1	3881	OHX	1	0
86	2	2151	OHX	1	0
86	8	219	OHX	6	0
86	5	4049	OHX	1	0
86	6	2061	OHX	1	0
86	5	3917	OHX	2	0
86	5	3970	OHX	1	0
86	1	3865	OHX	1	0
86	5	4233	OHX	6	0
86	1	4001	OHX	6	0
86	1	4154	OHX	4	0
86	2	2153	OHX	1	0
86	1	3964	OHX	1	0
86	4	224	OHX	1	0
86	1	4196	OHX	1	0
86	6	2103	OHX	1	0
86	s8	303	OHX	1	0
86	1	4066	OHX	1	0
86	1	3980	OHX	1	0
86	4	237	OHX	1	0
86	2	2166	OHX	1	0
86	1	4141	OHX	1	0
86	5	4024	OHX	1	0
86	2	2144	OHX	1	0
86	6	2106	OHX	1	0
86	5	4044	OHX	1	0
86	6	2119	OHX	1	0
86	1	3945	OHX	1	0
86	6	2062	OHX	2	0
86	2	2160	OHX	1	0
86	6	2203	OHX	1	0
86	6	2170	OHX	9	0
86	4	226	OHX	1	0
86	q2	502	OHX	3	0
86	2	2126	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	6	2111	OHX	2	0
86	2	2075	OHX	1	0
86	15	305	OHX	1	0
86	5	4224	OHX	2	0
86	5	3990	OHX	1	0
86	5	4093	OHX	3	0
86	5	4114	OHX	1	0
86	6	2177	OHX	1	0
86	M5	303	OHX	1	0
86	1	3924	OHX	2	0
86	6	2120	OHX	8	0
86	5	4196	OHX	1	0
86	5	3979	OHX	8	0
86	o7	502	OHX	1	0
86	5	4029	OHX	1	0
86	1	4017	OHX	1	0
86	6	2169	OHX	1	0
86	6	2107	OHX	2	0
86	1	4026	OHX	5	0
86	6	2114	OHX	1	0
86	8	218	OHX	1	0
86	1	4000	OHX	1	0
86	1	4174	OHX	1	0
86	2	2047	OHX	1	0
86	6	2149	OHX	5	0
86	6	2201	OHX	2	0
86	6	2092	OHX	1	0
86	1	4028	OHX	1	0
86	2	2040	OHX	2	0
86	6	2079	OHX	1	0
86	6	2112	OHX	1	0
86	6	2100	OHX	3	0
86	1	4178	OHX	1	0
86	8	226	OHX	1	0
86	6	2073	OHX	2	0
86	1	3889	OHX	1	0
86	1	4072	OHX	1	0
86	6	2128	OHX	1	0
86	2	2132	OHX	1	0
86	6	2075	OHX	1	0
86	6	2158	OHX	2	0
86	6	2117	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	3926	OHX	1	0
86	6	2191	OHX	1	0
86	5	4228	OHX	1	0
86	1	3961	OHX	1	0
86	5	4236	OHX	1	0
86	1	3938	OHX	2	0
86	2	2091	OHX	1	0
86	5	4199	OHX	10	0
86	1	3898	OHX	1	0
86	1	3922	OHX	1	0
86	1	4078	OHX	1	0
86	6	2136	OHX	1	0
86	1	4200	OHX	1	0
86	5	4217	OHX	7	0
86	5	3916	OHX	1	0
86	5	4248	OHX	1	0
86	5	4194	OHX	1	0
86	2	2027	OHX	2	0
86	5	4237	OHX	4	0
86	2	2043	OHX	1	0
86	1	4046	OHX	2	0
86	8	225	OHX	1	0
86	2	2156	OHX	3	0
86	2	2090	OHX	4	0
86	3	216	OHX	1	0
86	O7	104	OHX	7	0
86	1	4097	OHX	1	0
86	1	4147	OHX	1	0
86	5	4147	OHX	1	0
86	1	4130	OHX	1	0
86	1	3911	OHX	1	0
86	5	4014	OHX	1	0
86	1	3973	OHX	4	0
86	2	2159	OHX	2	0
86	1	3917	OHX	1	0
86	1	4167	OHX	2	0
86	6	2122	OHX	1	0
86	4	232	OHX	1	0
86	6	2097	OHX	2	0
86	4	238	OHX	1	0
86	5	4201	OHX	7	0
86	5	4110	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	s1	302	OHX	2	0
86	2	2077	OHX	1	0
86	5	4163	OHX	1	0
86	6	2096	OHX	1	0
86	1	4155	OHX	6	0
86	6	2109	OHX	1	0
86	5	4250	OHX	1	0
86	5	3923	OHX	2	0
86	5	4011	OHX	6	0
86	q1	102	OHX	6	0
86	1	3991	OHX	1	0
86	2	2098	OHX	2	0
86	1	4042	OHX	3	0
86	1	4106	OHX	1	0
86	5	4052	OHX	1	0
86	5	4208	OHX	1	0
86	8	228	OHX	4	0
86	2	2148	OHX	1	0
86	1	4171	OHX	7	0
86	6	2088	OHX	1	0
86	6	2187	OHX	1	0
86	5	3933	OHX	1	0
86	5	3965	OHX	1	0
86	8	217	OHX	2	0
86	5	4138	OHX	1	0
86	1	4124	OHX	1	0
86	6	2054	OHX	1	0
86	5	4242	OHX	5	0
86	1	4150	OHX	1	0
86	6	2055	OHX	1	0
86	1	4132	OHX	1	0
86	1	4032	OHX	1	0
86	5	4195	OHX	1	0
86	1	4074	OHX	1	0
86	1	3884	OHX	2	0
86	1	3981	OHX	1	0
86	1	3957	OHX	2	0
86	1	4168	OHX	1	0
86	2	2032	OHX	8	0
86	1	4143	OHX	2	0
86	1	4131	OHX	2	0
86	1	4094	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	L3	404	OHX	1	0
86	6	2145	OHX	1	0
86	5	4023	OHX	3	0
86	5	4081	OHX	1	0
86	5	4130	OHX	1	0
86	2	2163	OHX	2	0
86	1	4164	OHX	1	0
86	2	2128	OHX	1	0
86	2	2092	OHX	1	0
86	1	4163	OHX	1	0
86	1	4194	OHX	1	0
86	1	4113	OHX	1	0
86	5	3902	OHX	2	0
86	1	3876	OHX	1	0
86	2	2039	OHX	1	0
86	6	2148	OHX	1	0
86	6	2160	OHX	1	0
86	2	2124	OHX	1	0
86	6	2065	OHX	1	0
86	5	4008	OHX	1	0
86	6	2150	OHX	1	0
86	2	2037	OHX	2	0
86	5	4203	OHX	1	0
86	1	3995	OHX	1	0
86	1	4071	OHX	1	0
86	1	4146	OHX	6	0
86	2	2145	OHX	7	0
86	5	3906	OHX	1	0
86	2	2065	OHX	1	0
86	2	2105	OHX	1	0
86	7	217	OHX	6	0
86	2	2164	OHX	1	0
86	2	2025	OHX	1	0
86	2	2045	OHX	6	0
86	6	2102	OHX	1	0
86	1	4192	OHX	1	0
86	2	2036	OHX	1	0
86	5	3996	OHX	1	0
86	1	4011	OHX	1	0
86	2	2049	OHX	1	0
86	8	227	OHX	6	0
86	1	3937	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	3957	OHX	1	0
86	5	4054	OHX	1	0
86	5	3984	OHX	2	0
86	5	4239	OHX	1	0
86	6	2153	OHX	2	0
86	5	4160	OHX	1	0
86	5	4185	OHX	1	0
86	5	4003	OHX	1	0
86	5	4096	OHX	1	0
86	5	4079	OHX	1	0
86	1	4095	OHX	1	0
86	5	4214	OHX	1	0
86	1	4083	OHX	4	0
86	5	3958	OHX	3	0
86	1	4041	OHX	2	0
86	5	4013	OHX	1	0
86	2	2138	OHX	1	0
86	2	2076	OHX	1	0
86	6	2146	OHX	7	0
86	4	228	OHX	1	0
86	5	3960	OHX	1	0
86	4	231	OHX	1	0
86	2	2134	OHX	1	0
86	5	4193	OHX	1	0
86	1	3999	OHX	1	0
86	5	3948	OHX	1	0
86	1	4159	OHX	1	0
86	5	3974	OHX	4	0
86	n9	101	OHX	1	0
86	5	3983	OHX	1	0
86	2	2071	OHX	1	0
86	2	2024	OHX	1	0
86	m0	301	OHX	2	0
86	6	2126	OHX	3	0
86	2	2046	OHX	1	0
86	4	222	OHX	1	0
86	1	3954	OHX	1	0
86	6	2071	OHX	1	0
86	5	4182	OHX	1	0
86	D9	102	OHX	1	0
86	1	4117	OHX	1	0
86	4	225	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	6	2123	OHX	2	0
86	5	4144	OHX	1	0
86	6	2135	OHX	1	0
86	6	2049	OHX	1	0
86	2	2100	OHX	6	0
86	1	3928	OHX	1	0
86	6	2070	OHX	1	0
86	5	4200	OHX	7	0
86	1	4084	OHX	3	0
86	o3	202	OHX	1	0
86	2	2170	OHX	1	0
86	1	4121	OHX	1	0
86	4	236	OHX	1	0
86	2	2096	OHX	7	0
86	2	2109	OHX	1	0
86	5	4111	OHX	1	0
86	2	2054	OHX	1	0
86	1	4098	OHX	2	0
86	6	2068	OHX	1	0
86	5	4102	OHX	2	0
86	6	2138	OHX	1	0
86	1	4208	OHX	1	0
86	1	3966	OHX	1	0
86	5	4159	OHX	2	0
86	2	2060	OHX	1	0
86	5	4173	OHX	1	0
86	1	4069	OHX	1	0
86	d4	201	OHX	1	0
86	5	4223	OHX	1	0
86	7	218	OHX	1	0
86	5	4192	OHX	3	0
86	2	2074	OHX	1	0
86	1	4187	OHX	1	0
86	c5	201	OHX	1	0
86	6	2137	OHX	2	0
86	1	3930	OHX	2	0
86	1	3880	OHX	1	0
86	1	3944	OHX	1	0
86	Q2	503	OHX	2	0
86	1	3868	OHX	2	0
86	6	2074	OHX	1	0
86	5	3943	OHX	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3909	OHX	2	0
86	1	3960	OHX	1	0
86	5	4078	OHX	1	0
86	m7	206	OHX	1	0
86	2	2140	OHX	1	0
86	2	2107	OHX	1	0
86	5	4181	OHX	1	0
86	1	4073	OHX	1	0
86	5	4090	OHX	7	0
86	2	2176	OHX	1	0
86	2	2087	OHX	1	0
86	1	4206	OHX	1	0
86	6	2142	OHX	1	0
86	1	3913	OHX	1	0
86	6	2183	OHX	1	0
86	1	3882	OHX	2	0
86	5	4184	OHX	1	0
86	6	2108	OHX	2	0
86	5	4168	OHX	1	0
86	8	223	OHX	1	0
86	5	4226	OHX	2	0
86	6	2156	OHX	1	0
86	1	4197	OHX	6	0
86	1	4108	OHX	1	0
86	1	3948	OHX	1	0
86	1	3870	OHX	1	0
86	1	3963	OHX	1	0
86	2	2136	OHX	2	0
86	1	3890	OHX	1	0
86	1	4179	OHX	1	0
86	N1	201	OHX	1	0
86	6	2179	OHX	2	0
86	1	4162	OHX	6	0
86	5	4002	OHX	4	0
86	1	4065	OHX	1	0
86	1	3878	OHX	1	0
86	5	4202	OHX	3	0
86	2	2058	OHX	1	0
86	2	2068	OHX	1	0
86	2	2085	OHX	2	0
86	5	4119	OHX	1	0
86	6	2125	OHX	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	4101	OHX	1	0
86	6	2185	OHX	1	0
86	6	2181	OHX	1	0
86	5	3992	OHX	3	0
86	6	2130	OHX	2	0
86	2	2147	OHX	1	0
86	5	3987	OHX	1	0
86	5	4140	OHX	1	0
86	1	3931	OHX	1	0
87	2	2178	PCY	5	0
86	1	3923	OHX	1	0
86	6	2086	OHX	1	0
86	c3	201	OHX	2	0
86	1	4054	OHX	6	0
86	2	2122	OHX	3	0
86	1	3994	OHX	1	0
86	6	2110	OHX	1	0
86	1	4166	OHX	2	0
86	5	3942	OHX	1	0
86	2	2052	OHX	1	0
86	O3	202	OHX	1	0
86	o7	503	OHX	3	0
86	5	4066	OHX	7	0
86	14	402	OHX	1	0
86	1	4079	OHX	3	0
86	4	230	OHX	1	0
86	1	3903	OHX	1	0
86	1	4047	OHX	1	0
86	5	4131	OHX	1	0
86	5	4055	OHX	6	0
86	5	4092	OHX	1	0
86	1	4004	OHX	2	0
86	5	4051	OHX	1	0
86	6	2121	OHX	1	0
86	5	4021	OHX	6	0
86	1	4008	OHX	1	0
86	1	4198	OHX	1	0
86	1	3904	OHX	1	0
86	2	2112	OHX	2	0
86	5	4137	OHX	1	0
86	1	3974	OHX	1	0
86	6	2189	OHX	1	0

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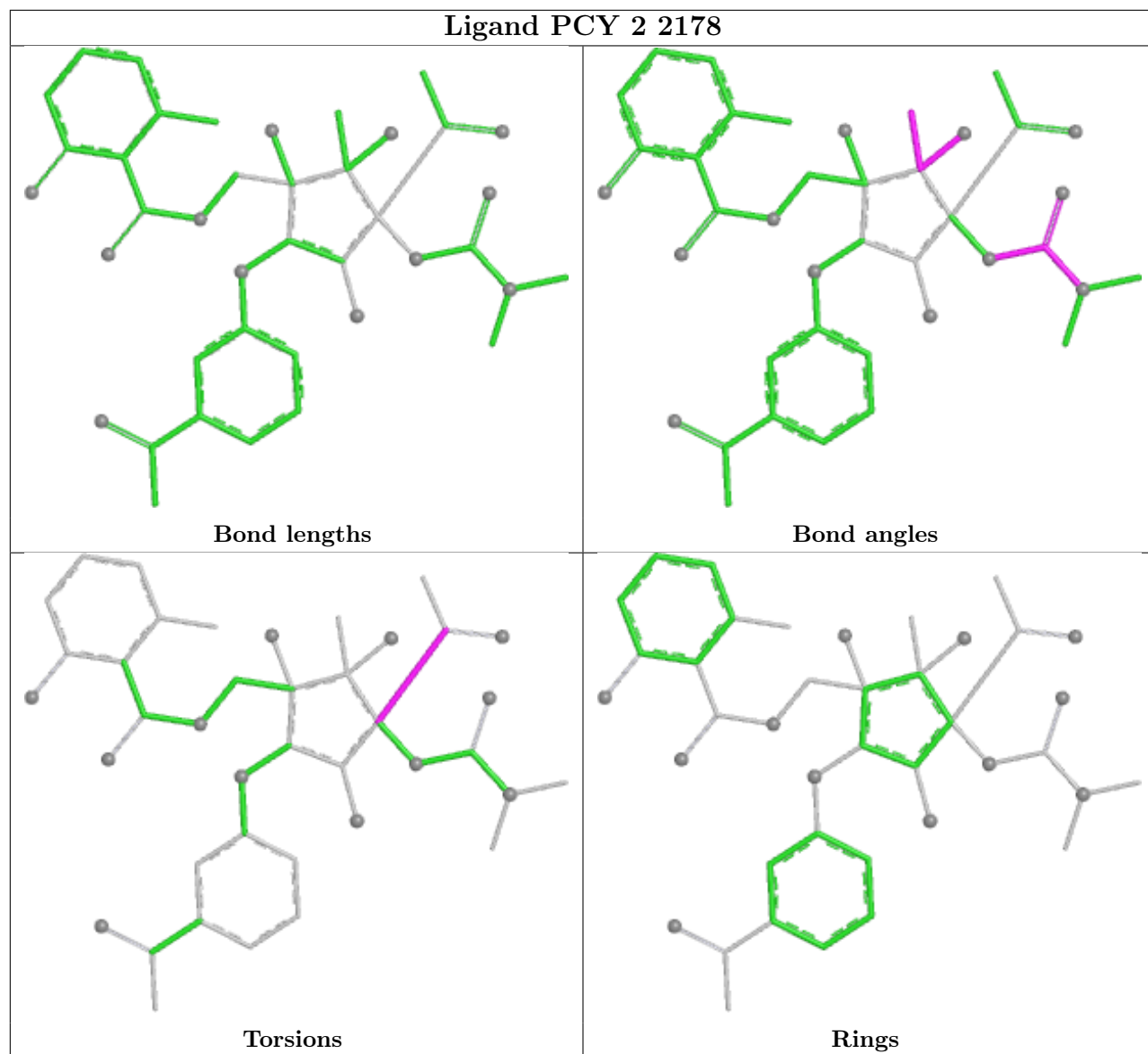
Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3915	OHX	1	0
86	1	4059	OHX	1	0
86	5	4143	OHX	6	0
86	1	3936	OHX	6	0
86	6	2059	OHX	6	0
86	2	2141	OHX	1	0
86	5	3938	OHX	1	0
86	5	4007	OHX	1	0
86	1	4134	OHX	1	0
86	4	234	OHX	2	0
86	1	4182	OHX	1	0
86	5	3980	OHX	1	0
86	2	2078	OHX	1	0
86	1	4195	OHX	1	0
86	5	4033	OHX	1	0
86	1	4087	OHX	1	0
86	M7	205	OHX	1	0
86	m0	302	OHX	1	0
86	1	4193	OHX	1	0
86	C5	201	OHX	2	0
86	5	4086	OHX	1	0
86	5	4074	OHX	1	0
86	1	4055	OHX	3	0
86	1	4006	OHX	1	0
86	1	4044	OHX	1	0
86	5	4205	OHX	1	0
86	1	3983	OHX	1	0
86	5	4099	OHX	1	0
86	5	3911	OHX	2	0
86	1	4145	OHX	1	0
86	5	4246	OHX	1	0
86	3	226	OHX	1	0
86	2	2072	OHX	1	0
86	5	4061	OHX	1	0
87	6	2204	PCY	1	0
86	2	2097	OHX	2	0
86	6	2124	OHX	1	0
86	2	2048	OHX	2	0
86	5	3907	OHX	3	0
86	5	3925	OHX	1	0
86	1	4025	OHX	1	0
86	1	4138	OHX	3	0

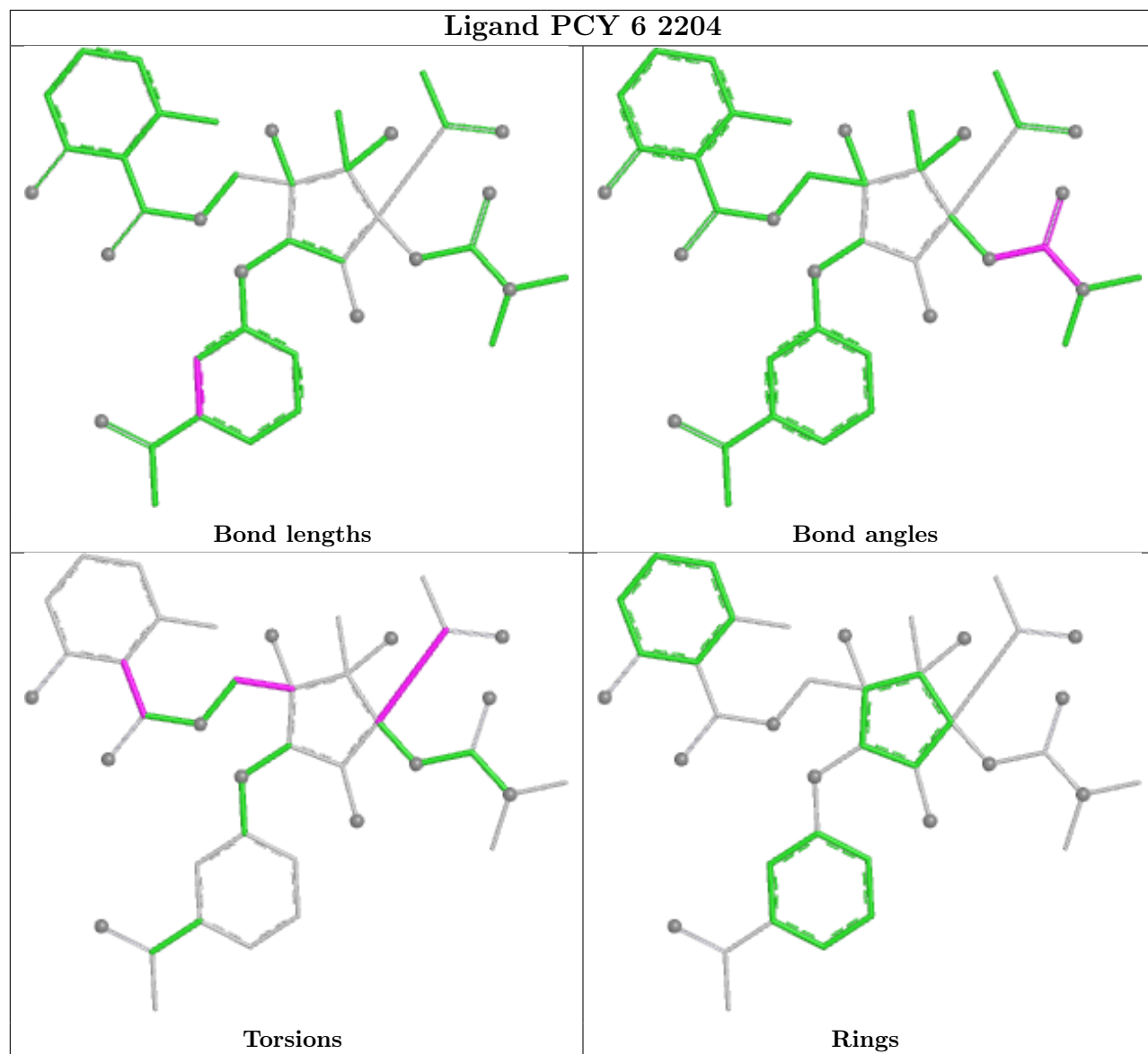
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	n9	102	OHX	1	0
86	5	3973	OHX	2	0
86	2	2083	OHX	1	0
86	1	4015	OHX	1	0
86	1	4139	OHX	2	0
86	2	2094	OHX	1	0
86	1	3943	OHX	1	0
86	5	3949	OHX	1	0
86	6	2162	OHX	1	0
86	5	4174	OHX	1	0
86	5	4219	OHX	1	0
86	5	4105	OHX	2	0
86	5	3959	OHX	2	0
86	5	4027	OHX	1	0
86	5	4190	OHX	3	0
86	2	2066	OHX	1	0
86	s9	201	OHX	2	0
86	5	3908	OHX	1	0
86	1	3872	OHX	1	0
86	2	2110	OHX	7	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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%)	0.25	55 (3%)	51	32	54, 88, 172, 274	0
1	6	1795/1800 (99%)	0.11	58 (3%)	50	31	41, 74, 181, 278	0
2	S0	206/251 (82%)	0.60	10 (4%)	35	22	90, 107, 123, 157	0
2	s0	206/251 (82%)	0.36	5 (2%)	59	40	71, 91, 109, 115	0
3	S1	214/254 (84%)	0.93	24 (11%)	10	7	92, 120, 146, 154	0
3	s1	216/254 (85%)	0.24	7 (3%)	50	31	67, 85, 111, 126	0
4	S2	217/253 (85%)	0.37	7 (3%)	50	31	68, 86, 104, 124	0
4	s2	217/253 (85%)	0.32	9 (4%)	41	25	54, 71, 92, 113	0
5	S3	223/239 (93%)	0.45	10 (4%)	38	24	77, 90, 128, 147	0
5	s3	223/239 (93%)	0.67	16 (7%)	21	14	73, 105, 129, 136	0
6	S4	260/260 (100%)	0.24	2 (0%)	82	67	63, 87, 102, 127	0
6	s4	260/260 (100%)	0.06	2 (0%)	82	67	54, 71, 90, 129	0
7	S5	206/224 (91%)	0.90	21 (10%)	12	8	94, 115, 135, 147	0
7	s5	206/224 (91%)	0.48	10 (4%)	35	22	65, 91, 121, 140	0
8	S6	226/236 (95%)	0.71	23 (10%)	12	8	64, 103, 123, 151	0
8	s6	218/236 (92%)	0.23	8 (3%)	45	28	50, 78, 105, 136	0
9	S7	184/189 (97%)	0.58	10 (5%)	31	20	86, 115, 149, 159	0
9	s7	186/189 (98%)	0.47	8 (4%)	40	24	68, 100, 138, 150	0
10	S8	188/200 (94%)	0.33	6 (3%)	50	31	56, 71, 112, 133	0
10	s8	188/200 (94%)	0.43	6 (3%)	50	31	45, 64, 107, 123	0
11	S9	185/196 (94%)	0.55	8 (4%)	40	24	80, 96, 132, 165	0
11	s9	185/196 (94%)	0.39	6 (3%)	50	31	63, 77, 116, 147	0
12	C0	96/105 (91%)	0.48	6 (6%)	26	17	82, 105, 138, 158	0
12	c0	96/105 (91%)	1.03	17 (17%)	4	3	96, 131, 153, 178	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	C1	155/155 (100%)	0.31	8 (5%) 33 21	56, 70, 131, 141	0
13	c1	146/155 (94%)	0.38	11 (7%) 20 13	47, 61, 100, 114	0
14	C2	124/142 (87%)	0.89	12 (9%) 13 9	134, 149, 169, 186	0
14	c2	124/142 (87%)	1.48	28 (22%) 2 2	177, 199, 225, 235	0
15	C3	150/150 (100%)	0.37	5 (3%) 49 30	64, 84, 102, 111	0
15	c3	150/150 (100%)	0.28	4 (2%) 56 36	56, 72, 91, 114	0
16	C4	127/136 (93%)	0.82	11 (8%) 16 11	66, 109, 128, 132	0
16	c4	128/136 (94%)	0.19	2 (1%) 70 51	51, 80, 92, 103	0
17	C5	124/141 (87%)	0.54	3 (2%) 59 40	81, 100, 142, 154	0
17	c5	135/141 (95%)	0.75	17 (12%) 8 6	73, 102, 139, 202	0
18	C6	141/142 (99%)	0.63	8 (5%) 29 19	80, 104, 112, 117	0
18	c6	142/142 (100%)	0.79	15 (10%) 11 8	64, 85, 104, 132	0
19	C7	120/136 (88%)	0.66	6 (5%) 34 22	89, 106, 134, 140	0
19	c7	117/136 (86%)	0.60	6 (5%) 33 21	77, 93, 118, 122	0
20	C8	145/145 (100%)	0.72	6 (4%) 41 25	79, 106, 131, 142	0
20	c8	145/145 (100%)	0.18	2 (1%) 73 54	70, 85, 110, 129	0
21	C9	143/143 (100%)	0.74	12 (8%) 17 11	88, 106, 124, 137	0
21	c9	143/143 (100%)	0.12	0 100 100	61, 77, 100, 124	0
22	D0	107/120 (89%)	0.77	6 (5%) 30 19	73, 108, 153, 160	0
22	d0	110/120 (91%)	0.85	8 (7%) 21 13	67, 107, 155, 192	0
23	D1	87/87 (100%)	0.35	3 (3%) 48 30	87, 94, 114, 129	0
23	d1	87/87 (100%)	-0.04	0 100 100	65, 76, 101, 116	0
24	D2	129/129 (100%)	0.25	2 (1%) 70 51	67, 80, 88, 100	0
24	d2	129/129 (100%)	-0.10	1 (0%) 82 67	52, 61, 69, 78	0
25	D3	144/144 (100%)	0.38	4 (2%) 55 35	57, 66, 77, 93	0
25	d3	144/144 (100%)	-0.09	2 (1%) 73 54	45, 50, 65, 83	0
26	D4	134/134 (100%)	0.51	4 (2%) 52 33	75, 104, 123, 135	0
26	d4	134/134 (100%)	0.25	7 (5%) 33 21	56, 81, 98, 127	0
27	D5	70/107 (65%)	0.76	4 (5%) 29 19	110, 127, 137, 141	0
27	d5	69/107 (64%)	0.41	1 (1%) 73 54	80, 107, 126, 134	0
28	D6	97/97 (100%)	0.91	10 (10%) 12 8	72, 88, 136, 142	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	d6	97/97 (100%)	0.22	2 (2%) 63 43	56, 68, 99, 109	0
29	D7	81/81 (100%)	0.67	6 (7%) 20 13	81, 95, 140, 146	0
29	d7	81/81 (100%)	0.61	5 (6%) 26 17	66, 84, 135, 138	0
30	D8	63/66 (95%)	0.92	6 (9%) 14 9	105, 126, 146, 166	0
30	d8	63/66 (95%)	0.40	2 (3%) 50 31	82, 101, 121, 130	0
31	D9	53/55 (96%)	0.39	1 (1%) 66 46	74, 81, 107, 116	0
31	d9	53/55 (96%)	0.78	5 (9%) 14 9	73, 81, 128, 144	0
32	E0	60/60 (100%)	0.39	1 (1%) 69 49	64, 96, 136, 145	0
33	E1	71/76 (93%)	1.32	12 (16%) 4 3	108, 129, 150, 160	0
33	e1	76/76 (100%)	1.81	21 (27%) 1 1	134, 164, 176, 179	0
34	SR	318/318 (100%)	0.71	23 (7%) 21 14	69, 113, 140, 159	0
34	sR	318/318 (100%)	0.58	19 (5%) 27 17	91, 113, 135, 158	0
35	SM	159/273 (58%)	0.83	22 (13%) 6 5	63, 90, 144, 149	0
35	sM	104/273 (38%)	1.13	22 (21%) 2 2	71, 102, 185, 195	0
36	1	3149/3396 (92%)	-0.17	77 (2%) 59 40	29, 53, 141, 267	0
36	5	3150/3396 (92%)	-0.23	66 (2%) 63 43	28, 52, 128, 273	0
37	3	121/121 (100%)	-0.24	0 100 100	42, 72, 90, 96	0
37	7	121/121 (100%)	-0.45	1 (0%) 82 67	34, 55, 67, 75	0
38	4	158/158 (100%)	-0.25	5 (3%) 50 31	37, 54, 98, 137	0
38	8	158/158 (100%)	-0.17	6 (3%) 44 27	41, 64, 108, 133	0
39	L2	252/253 (99%)	-0.12	3 (1%) 76 58	33, 48, 67, 74	0
39	l2	252/253 (99%)	0.01	3 (1%) 76 58	36, 54, 76, 89	0
40	L3	386/386 (100%)	-0.01	7 (1%) 67 48	34, 57, 72, 117	0
40	l3	386/386 (100%)	-0.31	3 (0%) 82 67	28, 41, 56, 99	0
41	L4	361/361 (100%)	-0.20	2 (0%) 85 73	30, 45, 63, 77	0
41	l4	361/361 (100%)	-0.04	2 (0%) 85 73	36, 53, 74, 91	0
42	L5	296/296 (100%)	0.27	7 (2%) 59 40	52, 80, 102, 126	0
42	l5	294/296 (99%)	-0.06	2 (0%) 84 69	42, 59, 88, 138	0
43	L6	156/175 (89%)	-0.11	0 100 100	39, 48, 71, 93	0
43	l6	157/175 (89%)	0.02	2 (1%) 75 55	42, 51, 73, 90	0
44	L7	222/243 (91%)	-0.26	0 100 100	34, 42, 79, 127	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	l7	223/243 (91%)	-0.30	0	100	100	30, 40, 85, 136	0
45	L8	233/255 (91%)	0.23	8 (3%)	48	30	54, 70, 111, 124	0
45	l8	231/255 (90%)	0.40	9 (3%)	43	27	69, 84, 113, 121	0
46	L9	191/191 (100%)	0.07	0	100	100	52, 66, 82, 100	0
46	l9	191/191 (100%)	-0.25	1 (0%)	87	76	38, 45, 69, 107	0
47	M0	211/220 (95%)	-0.01	7 (3%)	49	30	40, 58, 93, 116	0
47	m0	213/220 (96%)	-0.02	9 (4%)	40	25	36, 54, 82, 100	0
48	M1	169/173 (97%)	0.27	4 (2%)	59	40	61, 85, 101, 114	0
48	m1	169/173 (97%)	0.03	3 (1%)	67	48	44, 65, 77, 93	0
49	M3	193/198 (97%)	-0.13	4 (2%)	63	43	34, 54, 100, 125	0
49	m3	194/198 (97%)	0.26	5 (2%)	57	37	45, 66, 110, 137	0
50	M4	136/137 (99%)	-0.19	1 (0%)	84	69	45, 53, 68, 80	0
50	m4	137/137 (100%)	-0.23	2 (1%)	72	52	36, 44, 65, 79	0
51	M5	203/203 (100%)	0.02	2 (0%)	79	63	33, 46, 58, 65	0
51	m5	203/203 (100%)	0.15	2 (0%)	79	63	43, 58, 72, 77	0
52	M6	197/198 (99%)	-0.21	2 (1%)	79	63	35, 44, 65, 69	0
52	m6	197/198 (99%)	-0.24	1 (0%)	87	76	28, 33, 62, 70	0
53	M7	183/183 (100%)	0.07	8 (4%)	39	24	37, 45, 123, 148	0
53	m7	155/183 (84%)	-0.27	0	100	100	32, 41, 57, 87	0
54	M8	185/185 (100%)	0.05	11 (5%)	28	18	36, 45, 59, 72	0
54	m8	185/185 (100%)	0.11	7 (3%)	44	27	39, 51, 60, 67	0
55	M9	188/188 (100%)	0.40	11 (5%)	28	18	50, 67, 157, 165	0
55	m9	188/188 (100%)	0.26	4 (2%)	63	43	46, 62, 130, 144	0
56	N0	172/172 (100%)	-0.27	2 (1%)	76	58	43, 51, 66, 73	0
56	n0	172/172 (100%)	-0.32	2 (1%)	76	58	32, 40, 50, 67	0
57	N1	159/159 (100%)	-0.10	2 (1%)	75	55	41, 51, 93, 101	0
57	n1	159/159 (100%)	-0.06	3 (1%)	66	46	36, 44, 86, 97	0
58	N2	100/120 (83%)	0.61	6 (6%)	27	17	81, 100, 116, 131	0
58	n2	98/120 (81%)	0.22	1 (1%)	79	63	72, 88, 103, 109	0
59	N3	136/136 (100%)	-0.00	2 (1%)	72	52	40, 51, 67, 82	0
59	n3	136/136 (100%)	-0.26	2 (1%)	72	52	28, 40, 56, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	N4	98/155 (63%)	1.01	24 (24%) 2 2	52, 68, 167, 180	0
60	n4	135/155 (87%)	0.58	8 (5%) 28 18	40, 87, 138, 158	0
61	N5	121/141 (85%)	0.12	4 (3%) 49 30	46, 61, 81, 115	0
61	n5	120/141 (85%)	0.17	4 (3%) 49 30	52, 67, 89, 96	0
62	N6	126/126 (100%)	-0.05	3 (2%) 59 40	40, 55, 68, 85	0
62	n6	126/126 (100%)	0.10	2 (1%) 70 51	49, 64, 81, 89	0
63	N7	135/135 (100%)	0.17	0 100 100	70, 85, 99, 108	0
63	n7	135/135 (100%)	0.38	3 (2%) 62 42	78, 96, 117, 126	0
64	N8	148/148 (100%)	-0.04	2 (1%) 73 54	27, 44, 72, 84	0
64	n8	148/148 (100%)	-0.18	0 100 100	33, 53, 76, 80	0
65	N9	58/58 (100%)	0.10	1 (1%) 69 49	39, 55, 105, 116	0
65	n9	58/58 (100%)	0.14	0 100 100	37, 56, 83, 92	0
66	O0	97/104 (93%)	0.08	3 (3%) 51 32	68, 78, 111, 117	0
66	o0	100/104 (96%)	0.26	3 (3%) 52 33	74, 85, 115, 124	0
67	O1	109/112 (97%)	0.07	1 (0%) 81 64	47, 61, 102, 118	0
67	o1	109/112 (97%)	-0.07	0 100 100	39, 52, 94, 118	0
68	O2	127/129 (98%)	-0.23	2 (1%) 70 51	28, 42, 55, 76	0
68	o2	127/129 (98%)	-0.04	4 (3%) 51 32	30, 49, 66, 88	0
69	O3	106/106 (100%)	-0.27	0 100 100	34, 41, 67, 78	0
69	o3	106/106 (100%)	-0.12	1 (0%) 81 64	31, 39, 71, 87	0
70	O4	112/120 (93%)	0.52	5 (4%) 38 24	47, 66, 111, 123	0
70	o4	112/120 (93%)	0.34	2 (1%) 67 48	46, 70, 116, 128	0
71	O5	119/119 (100%)	0.07	3 (2%) 58 39	43, 65, 71, 75	0
71	o5	119/119 (100%)	0.05	2 (1%) 69 49	56, 71, 83, 88	0
72	O6	99/99 (100%)	0.08	2 (2%) 65 45	49, 63, 97, 118	0
72	o6	99/99 (100%)	0.23	2 (2%) 65 45	61, 75, 99, 124	0
73	O7	87/87 (100%)	0.19	2 (2%) 61 41	33, 41, 79, 106	0
73	o7	87/87 (100%)	0.09	2 (2%) 61 41	41, 46, 85, 122	0
74	O8	77/77 (100%)	0.26	1 (1%) 75 55	72, 88, 110, 122	0
74	o8	77/77 (100%)	0.42	1 (1%) 75 55	75, 92, 108, 113	0
75	O9	50/50 (100%)	-0.06	1 (2%) 65 45	43, 49, 55, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	o9	50/50 (100%)	-0.08	0 100 100	51, 54, 66, 72	0
76	Q0	52/52 (100%)	-0.11	0 100 100	49, 59, 85, 96	0
76	q0	52/52 (100%)	-0.44	1 (1%) 66 46	34, 40, 54, 66	0
77	Q1	25/25 (100%)	-0.05	0 100 100	52, 55, 59, 67	0
77	q1	25/25 (100%)	-0.23	0 100 100	43, 48, 62, 69	0
78	Q2	105/105 (100%)	-0.01	1 (0%) 79 63	39, 56, 86, 124	0
78	q2	105/105 (100%)	-0.08	1 (0%) 79 63	45, 57, 87, 120	0
79	Q3	91/91 (100%)	0.03	1 (1%) 78 61	42, 54, 74, 89	0
79	q3	91/91 (100%)	-0.01	1 (1%) 78 61	40, 55, 74, 84	0
80	e0	62/62 (100%)	0.26	0 100 100	59, 77, 119, 141	0
81	m2	0/160	-	-	-	-
82	p0	143/311 (45%)	0.66	8 (5%) 30 19	88, 107, 193, 202	0
83	p1	0/47	-	-	-	-
84	p2	0/46	-	-	-	-
All	All	33063/35346 (93%)	0.14	1097 (3%) 49 30	27, 68, 134, 278	0

The worst 5 of 1097 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	5	2873	U	11.4
33	e1	77	GLY	8.8
33	e1	85	TYR	8.6
1	2	261	U	8.2
33	e1	80	ARG	8.1

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	3805	1/1	-0.58	0.38	190,190,190,190	0
85	MG	1	3815	1/1	-0.33	0.49	128,128,128,128	0
85	MG	6	2013	1/1	0.18	0.32	150,150,150,150	0
85	MG	2	2003	1/1	0.23	0.43	118,118,118,118	0
85	MG	2	1988	1/1	0.24	0.27	96,96,96,96	0
85	MG	5	3773	1/1	0.34	0.33	111,111,111,111	0
85	MG	2	1958	1/1	0.37	0.50	98,98,98,98	0
85	MG	5	3807	1/1	0.41	0.20	163,163,163,163	0
85	MG	5	3898	1/1	0.47	0.33	154,154,154,154	0
85	MG	5	3780	1/1	0.50	0.39	83,83,83,83	0
85	MG	2	1994	1/1	0.52	0.42	98,98,98,98	0
85	MG	5	3793	1/1	0.53	0.32	89,89,89,89	0
85	MG	5	3464	1/1	0.56	0.41	88,88,88,88	0
85	MG	6	1909	1/1	0.58	0.45	107,107,107,107	0
85	MG	1	3406	1/1	0.59	0.36	96,96,96,96	0
85	MG	5	3888	1/1	0.61	0.39	90,90,90,90	0
85	MG	2	1978	1/1	0.62	0.40	93,93,93,93	0
85	MG	2	1962	1/1	0.62	0.24	130,130,130,130	0
85	MG	o1	201	1/1	0.62	0.15	85,85,85,85	0
85	MG	1	3480	1/1	0.63	0.33	78,78,78,78	0
85	MG	3	201	1/1	0.63	0.32	78,78,78,78	0
85	MG	5	3678	1/1	0.63	0.28	97,97,97,97	0
85	MG	2	2018	1/1	0.63	0.30	80,80,80,80	0
85	MG	6	1963	1/1	0.63	0.38	96,96,96,96	0
85	MG	2	1949	1/1	0.64	0.43	82,82,82,82	0
85	MG	6	1924	1/1	0.64	0.45	95,95,95,95	0
85	MG	5	3884	1/1	0.64	0.40	83,83,83,83	0
85	MG	5	3710	1/1	0.64	0.37	91,91,91,91	0
85	MG	2	2019	1/1	0.64	0.33	73,73,73,73	0
85	MG	1	3650	1/1	0.64	0.37	100,100,100,100	0
85	MG	6	1966	1/1	0.65	0.46	82,82,82,82	0
85	MG	5	3651	1/1	0.65	0.27	111,111,111,111	0
85	MG	6	1940	1/1	0.66	0.40	85,85,85,85	0
85	MG	1	3635	1/1	0.67	0.42	72,72,72,72	0
85	MG	2	1974	1/1	0.67	0.50	86,86,86,86	0
85	MG	2	1976	1/1	0.67	0.34	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	2	1915	1/1	0.67	0.41	74,74,74,74	0
85	MG	2	2017	1/1	0.67	0.38	85,85,85,85	0
85	MG	6	1904	1/1	0.67	0.33	68,68,68,68	0
85	MG	2	1986	1/1	0.68	0.41	103,103,103,103	0
85	MG	2	1953	1/1	0.68	0.28	104,104,104,104	0
85	MG	15	302	1/1	0.68	0.25	64,64,64,64	0
85	MG	2	1945	1/1	0.68	0.26	89,89,89,89	0
85	MG	M1	201	1/1	0.69	0.24	78,78,78,78	0
85	MG	2	2023	1/1	0.69	0.21	121,121,121,121	0
85	MG	2	1990	1/1	0.69	0.32	106,106,106,106	0
85	MG	5	3815	1/1	0.70	0.16	89,89,89,89	0
86	OHX	1	4185	7/7	0.70	0.19	190,190,190,190	0
85	MG	5	3809	1/1	0.71	0.33	100,100,100,100	0
85	MG	2	1937	1/1	0.71	0.40	61,61,61,61	0
85	MG	2	1967	1/1	0.71	0.47	106,106,106,106	0
85	MG	6	1988	1/1	0.71	0.23	84,84,84,84	0
85	MG	2	2010	1/1	0.71	0.42	73,73,73,73	0
85	MG	6	2028	1/1	0.71	0.44	80,80,80,80	0
85	MG	6	2045	1/1	0.71	0.24	78,78,78,78	0
85	MG	O7	102	1/1	0.71	0.33	81,81,81,81	0
85	MG	6	2039	1/1	0.72	0.43	94,94,94,94	0
85	MG	2	1971	1/1	0.72	0.34	81,81,81,81	0
85	MG	1	3665	1/1	0.72	0.44	75,75,75,75	0
85	MG	2	1952	1/1	0.73	0.39	95,95,95,95	0
85	MG	M9	202	1/1	0.73	0.28	68,68,68,68	0
85	MG	5	3860	1/1	0.73	0.18	88,88,88,88	0
85	MG	2	1914	1/1	0.73	0.40	71,71,71,71	0
85	MG	6	1998	1/1	0.73	0.32	95,95,95,95	0
85	MG	1	3730	1/1	0.73	0.21	86,86,86,86	0
85	MG	1	3408	1/1	0.73	0.28	44,44,44,44	0
85	MG	2	1968	1/1	0.73	0.29	79,79,79,79	0
86	OHX	1	4174	7/7	0.73	0.20	162,162,162,162	0
85	MG	2	1951	1/1	0.73	0.30	97,97,97,97	0
85	MG	1	3624	1/1	0.74	0.38	82,82,82,82	0
85	MG	5	3462	1/1	0.74	0.18	42,42,42,42	0
85	MG	2	1965	1/1	0.74	0.31	86,86,86,86	0
85	MG	1	3711	1/1	0.74	0.39	81,81,81,81	0
85	MG	6	2044	1/1	0.74	0.38	81,81,81,81	0
86	OHX	14	403	7/7	0.74	0.21	156,156,156,156	0
85	MG	5	3742	1/1	0.75	0.34	35,35,35,35	0
85	MG	2	1928	1/1	0.75	0.39	79,79,79,79	0
85	MG	Q2	502	1/1	0.75	0.34	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	5	3474	1/1	0.75	0.28	79,79,79,79	0
85	MG	M9	201	1/1	0.75	0.13	68,68,68,68	0
85	MG	4	220	1/1	0.75	0.41	82,82,82,82	0
85	MG	5	3682	1/1	0.75	0.40	81,81,81,81	0
86	OHX	1	4188	7/7	0.75	0.26	146,146,146,146	0
85	MG	N5	201	1/1	0.75	0.24	70,70,70,70	0
85	MG	1	3649	1/1	0.76	0.28	69,69,69,69	0
85	MG	M3	202	1/1	0.76	0.34	91,91,91,91	0
85	MG	3	209	1/1	0.76	0.28	69,69,69,69	0
86	OHX	5	4222	7/7	0.76	0.18	186,186,186,186	0
86	OHX	5	4228	7/7	0.76	0.29	130,130,130,130	0
86	OHX	5	4235	7/7	0.76	0.22	154,154,154,154	0
85	MG	1	3747	1/1	0.76	0.14	50,50,50,50	0
85	MG	2	1970	1/1	0.77	0.34	69,69,69,69	0
85	MG	5	3570	1/1	0.77	0.38	29,29,29,29	0
85	MG	5	3897	1/1	0.77	0.17	66,66,66,66	0
85	MG	5	3686	1/1	0.77	0.41	63,63,63,63	0
85	MG	8	213	1/1	0.77	0.17	59,59,59,59	0
85	MG	5	3823	1/1	0.77	0.34	45,45,45,45	0
85	MG	5	3415	1/1	0.77	0.16	55,55,55,55	0
85	MG	6	1928	1/1	0.78	0.37	74,74,74,74	0
86	OHX	2	2161	7/7	0.78	0.16	181,181,181,181	0
86	OHX	2	2162	7/7	0.78	0.23	159,159,159,159	0
86	OHX	1	4141	7/7	0.78	0.24	133,133,133,133	0
85	MG	1	3616	1/1	0.78	0.16	67,67,67,67	0
85	MG	6	1961	1/1	0.78	0.30	80,80,80,80	0
85	MG	6	2034	1/1	0.78	0.26	73,73,73,73	0
86	OHX	6	2169	7/7	0.78	0.18	163,163,163,163	0
86	OHX	6	2184	7/7	0.78	0.16	179,179,179,179	0
85	MG	6	1906	1/1	0.78	0.32	47,47,47,47	0
85	MG	2	1961	1/1	0.78	0.40	81,81,81,81	0
86	OHX	5	4234	7/7	0.78	0.21	162,162,162,162	0
85	MG	6	1983	1/1	0.78	0.17	80,80,80,80	0
86	OHX	5	4237	7/7	0.78	0.20	168,168,168,168	0
86	OHX	5	4239	7/7	0.78	0.20	158,158,158,158	0
86	OHX	5	4240	7/7	0.78	0.17	194,194,194,194	0
86	OHX	5	4241	7/7	0.78	0.14	239,239,239,239	0
86	OHX	14	402	7/7	0.78	0.18	155,155,155,155	0
85	MG	3	208	1/1	0.78	0.17	60,60,60,60	0
85	MG	6	1911	1/1	0.79	0.39	82,82,82,82	0
86	OHX	1	4168	7/7	0.79	0.18	165,165,165,165	0
86	OHX	1	4170	7/7	0.79	0.23	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	6	2003	1/1	0.79	0.24	96,96,96,96	0
85	MG	5	3635	1/1	0.79	0.41	81,81,81,81	0
85	MG	5	3824	1/1	0.79	0.23	94,94,94,94	0
86	OHX	1	4193	7/7	0.79	0.19	150,150,150,150	0
86	OHX	1	4199	7/7	0.79	0.20	150,150,150,150	0
86	OHX	6	2147	7/7	0.79	0.20	147,147,147,147	0
85	MG	1	3471	1/1	0.79	0.13	40,40,40,40	0
85	MG	5	3878	1/1	0.79	0.29	51,51,51,51	0
86	OHX	6	2187	7/7	0.79	0.20	161,161,161,161	0
86	OHX	6	2189	7/7	0.79	0.20	150,150,150,150	0
85	MG	2	1904	1/1	0.79	0.38	74,74,74,74	0
85	MG	6	1930	1/1	0.79	0.19	56,56,56,56	0
85	MG	5	3893	1/1	0.79	0.13	73,73,73,73	0
85	MG	O3	201	1/1	0.79	0.41	74,74,74,74	0
85	MG	1	3562	1/1	0.79	0.31	48,48,48,48	0
85	MG	2	1908	1/1	0.79	0.34	73,73,73,73	0
85	MG	2	1910	1/1	0.79	0.43	60,60,60,60	0
85	MG	5	3420	1/1	0.79	0.21	96,96,96,96	0
85	MG	2	1950	1/1	0.79	0.29	97,97,97,97	0
85	MG	2	1930	1/1	0.79	0.26	64,64,64,64	0
86	OHX	15	305	7/7	0.79	0.20	149,149,149,149	0
85	MG	2	1926	1/1	0.80	0.38	91,91,91,91	0
85	MG	6	1984	1/1	0.80	0.20	78,78,78,78	0
85	MG	6	1986	1/1	0.80	0.15	69,69,69,69	0
85	MG	1	3705	1/1	0.80	0.18	43,43,43,43	0
85	MG	5	3425	1/1	0.80	0.20	46,46,46,46	0
85	MG	7	204	1/1	0.80	0.27	63,63,63,63	0
85	MG	7	213	1/1	0.80	0.21	52,52,52,52	0
85	MG	6	1991	1/1	0.80	0.15	54,54,54,54	0
86	OHX	6	2190	7/7	0.80	0.19	179,179,179,179	0
85	MG	5	3781	1/1	0.80	0.31	82,82,82,82	0
85	MG	6	1935	1/1	0.80	0.21	52,52,52,52	0
85	MG	5	3467	1/1	0.80	0.19	114,114,114,114	0
85	MG	1	3629	1/1	0.80	0.13	41,41,41,41	0
85	MG	5	3478	1/1	0.80	0.30	64,64,64,64	0
86	OHX	1	4158	7/7	0.80	0.17	162,162,162,162	0
85	MG	2	1991	1/1	0.80	0.22	101,101,101,101	0
85	MG	1	3592	1/1	0.80	0.25	53,53,53,53	0
85	MG	2	1963	1/1	0.80	0.26	94,94,94,94	0
86	OHX	1	4176	7/7	0.80	0.19	163,163,163,163	0
85	MG	6	1968	1/1	0.80	0.34	58,58,58,58	0
85	MG	6	2030	1/1	0.81	0.22	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	3573	1/1	0.81	0.29	39,39,39,39	0
86	OHX	1	4169	7/7	0.81	0.18	181,181,181,181	0
85	MG	2	1924	1/1	0.81	0.45	83,83,83,83	0
86	OHX	s1	303	7/7	0.81	0.16	184,184,184,184	0
85	MG	2	2006	1/1	0.81	0.13	64,64,64,64	0
85	MG	1	3495	1/1	0.81	0.22	50,50,50,50	0
86	OHX	5	4231	7/7	0.81	0.23	136,136,136,136	0
85	MG	5	3769	1/1	0.81	0.16	111,111,111,111	0
86	OHX	1	4186	7/7	0.81	0.20	146,146,146,146	0
85	MG	1	3528	1/1	0.81	0.32	46,46,46,46	0
86	OHX	2	2158	7/7	0.81	0.18	167,167,167,167	0
85	MG	1	3545	1/1	0.81	0.26	52,52,52,52	0
86	OHX	4	238	7/7	0.81	0.25	145,145,145,145	0
85	MG	2	1999	1/1	0.81	0.29	71,71,71,71	0
85	MG	5	3657	1/1	0.81	0.16	47,47,47,47	0
86	OHX	6	2183	7/7	0.81	0.22	147,147,147,147	0
85	MG	1	3456	1/1	0.82	0.38	62,62,62,62	0
86	OHX	1	4164	7/7	0.82	0.12	219,219,219,219	0
85	MG	6	1965	1/1	0.82	0.28	66,66,66,66	0
85	MG	1	3586	1/1	0.82	0.34	38,38,38,38	0
85	MG	6	2206	1/1	0.82	0.18	68,68,68,68	0
85	MG	6	1907	1/1	0.82	0.31	70,70,70,70	0
85	MG	5	3797	1/1	0.82	0.18	93,93,93,93	0
85	MG	5	3798	1/1	0.82	0.17	59,59,59,59	0
85	MG	6	1970	1/1	0.82	0.21	65,65,65,65	0
85	MG	6	1971	1/1	0.82	0.34	65,65,65,65	0
85	MG	2	1977	1/1	0.82	0.21	72,72,72,72	0
85	MG	5	3463	1/1	0.82	0.19	62,62,62,62	0
85	MG	2	1941	1/1	0.82	0.24	68,68,68,68	0
86	OHX	L4	403	7/7	0.82	0.18	147,147,147,147	0
86	OHX	M7	205	7/7	0.82	0.28	124,124,124,124	0
85	MG	6	1923	1/1	0.82	0.31	68,68,68,68	0
86	OHX	6	2155	7/7	0.82	0.15	187,187,187,187	0
85	MG	2	1982	1/1	0.82	0.26	79,79,79,79	0
85	MG	6	1926	1/1	0.82	0.32	52,52,52,52	0
85	MG	5	3554	1/1	0.82	0.31	35,35,35,35	0
86	OHX	6	2185	7/7	0.82	0.19	152,152,152,152	0
85	MG	6	1995	1/1	0.82	0.30	72,72,72,72	0
85	MG	5	3632	1/1	0.82	0.39	86,86,86,86	0
85	MG	1	3521	1/1	0.82	0.24	74,74,74,74	0
86	OHX	6	2192	7/7	0.82	0.15	188,188,188,188	0
85	MG	6	2001	1/1	0.82	0.25	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4165	7/7	0.82	0.17	194,194,194,194	0
86	OHX	5	4189	7/7	0.82	0.17	164,164,164,164	0
86	OHX	5	4197	7/7	0.82	0.17	165,165,165,165	0
86	OHX	5	4204	7/7	0.82	0.20	151,151,151,151	0
86	OHX	5	4206	7/7	0.82	0.21	158,158,158,158	0
86	OHX	5	4207	7/7	0.82	0.22	146,146,146,146	0
86	OHX	5	4219	7/7	0.82	0.20	140,140,140,140	0
85	MG	2	1993	1/1	0.82	0.20	67,67,67,67	0
85	MG	8	211	1/1	0.82	0.09	68,68,68,68	0
85	MG	5	3676	1/1	0.82	0.13	47,47,47,47	0
85	MG	l3	402	1/1	0.82	0.36	37,37,37,37	0
85	MG	1	3846	1/1	0.82	0.18	45,45,45,45	0
85	MG	2	1940	1/1	0.82	0.20	69,69,69,69	0
85	MG	q3	502	1/1	0.82	0.14	62,62,62,62	0
86	OHX	2	2148	7/7	0.82	0.15	166,166,166,166	0
85	MG	6	1946	1/1	0.82	0.44	64,64,64,64	0
85	MG	1	3411	1/1	0.82	0.30	44,44,44,44	0
85	MG	6	2038	1/1	0.82	0.41	81,81,81,81	0
85	MG	5	3747	1/1	0.82	0.28	39,39,39,39	0
86	OHX	n9	102	7/7	0.82	0.16	173,173,173,173	0
86	OHX	2	2177	7/7	0.83	0.17	184,184,184,184	0
85	MG	5	3457	1/1	0.83	0.28	31,31,31,31	0
85	MG	2	1907	1/1	0.83	0.40	61,61,61,61	0
85	MG	1	3709	1/1	0.83	0.23	66,66,66,66	0
85	MG	6	1922	1/1	0.83	0.30	52,52,52,52	0
85	MG	2	1939	1/1	0.83	0.25	68,68,68,68	0
86	OHX	5	4154	7/7	0.83	0.23	130,130,130,130	0
85	MG	2	1923	1/1	0.83	0.31	58,58,58,58	0
85	MG	2	1973	1/1	0.83	0.29	73,73,73,73	0
85	MG	5	3486	1/1	0.83	0.28	56,56,56,56	0
85	MG	1	3749	1/1	0.83	0.19	55,55,55,55	0
85	MG	5	3786	1/1	0.83	0.23	89,89,89,89	0
85	MG	2	1905	1/1	0.83	0.41	62,62,62,62	0
85	MG	5	3574	1/1	0.83	0.40	35,35,35,35	0
86	OHX	5	4220	7/7	0.83	0.14	185,185,185,185	0
86	OHX	5	4221	7/7	0.83	0.19	157,157,157,157	0
86	OHX	1	4194	7/7	0.83	0.18	146,146,146,146	0
86	OHX	1	4195	7/7	0.83	0.16	174,174,174,174	0
86	OHX	5	4230	7/7	0.83	0.18	165,165,165,165	0
86	OHX	1	4196	7/7	0.83	0.23	139,139,139,139	0
85	MG	1	3420	1/1	0.83	0.30	83,83,83,83	0
86	OHX	1	4203	7/7	0.83	0.20	150,150,150,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	n8	201	1/1	0.83	0.15	37,37,37,37	0
85	MG	1	3548	1/1	0.83	0.32	54,54,54,54	0
85	MG	5	3401	1/1	0.83	0.25	63,63,63,63	0
85	MG	5	3811	1/1	0.83	0.15	45,45,45,45	0
86	OHX	5	4247	7/7	0.83	0.19	152,152,152,152	0
86	OHX	7	226	7/7	0.83	0.16	157,157,157,157	0
85	MG	1	3421	1/1	0.83	0.46	77,77,77,77	0
86	OHX	2	2159	7/7	0.83	0.21	145,145,145,145	0
85	MG	2	1996	1/1	0.83	0.27	96,96,96,96	0
85	MG	1	3697	1/1	0.83	0.31	74,74,74,74	0
85	MG	1	3632	1/1	0.84	0.40	75,75,75,75	0
85	MG	6	2005	1/1	0.84	0.21	62,62,62,62	0
86	OHX	1	4200	7/7	0.84	0.20	148,148,148,148	0
85	MG	1	3500	1/1	0.84	0.27	75,75,75,75	0
85	MG	5	3615	1/1	0.84	0.20	53,53,53,53	0
85	MG	1	3513	1/1	0.84	0.20	26,26,26,26	0
85	MG	M9	203	1/1	0.84	0.19	61,61,61,61	0
86	OHX	M7	206	7/7	0.84	0.20	142,142,142,142	0
86	OHX	6	2136	7/7	0.84	0.19	138,138,138,138	0
85	MG	6	1954	1/1	0.84	0.36	45,45,45,45	0
85	MG	1	3760	1/1	0.84	0.17	47,47,47,47	0
85	MG	1	3780	1/1	0.84	0.31	48,48,48,48	0
85	MG	6	1964	1/1	0.84	0.24	55,55,55,55	0
85	MG	1	3802	1/1	0.84	0.19	64,64,64,64	0
85	MG	1	3409	1/1	0.84	0.33	31,31,31,31	0
85	MG	c7	201	1/1	0.84	0.29	73,73,73,73	0
86	OHX	6	2188	7/7	0.84	0.18	148,148,148,148	0
85	MG	5	3728	1/1	0.84	0.23	102,102,102,102	0
85	MG	5	3732	1/1	0.84	0.39	69,69,69,69	0
85	MG	sM	302	1/1	0.84	0.17	51,51,51,51	0
86	OHX	6	2195	7/7	0.84	0.14	186,186,186,186	0
86	OHX	6	2203	7/7	0.84	0.18	157,157,157,157	0
86	OHX	2	2137	7/7	0.84	0.14	176,176,176,176	0
85	MG	1	3657	1/1	0.84	0.28	47,47,47,47	0
85	MG	5	3756	1/1	0.84	0.11	49,49,49,49	0
86	OHX	5	4180	7/7	0.84	0.16	161,161,161,161	0
85	MG	5	3757	1/1	0.84	0.20	60,60,60,60	0
85	MG	1	3842	1/1	0.84	0.31	59,59,59,59	0
85	MG	2	1989	1/1	0.84	0.28	57,57,57,57	0
86	OHX	2	2174	7/7	0.84	0.14	187,187,187,187	0
85	MG	1	3667	1/1	0.84	0.14	53,53,53,53	0
86	OHX	1	4110	7/7	0.84	0.19	155,155,155,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4126	7/7	0.84	0.16	155,155,155,155	0
86	OHX	1	4140	7/7	0.84	0.21	147,147,147,147	0
85	MG	5	3431	1/1	0.84	0.11	35,35,35,35	0
85	MG	1	3535	1/1	0.84	0.25	45,45,45,45	0
85	MG	5	3790	1/1	0.84	0.28	58,58,58,58	0
85	MG	6	1920	1/1	0.84	0.31	61,61,61,61	0
85	MG	1	3619	1/1	0.84	0.26	70,70,70,70	0
85	MG	3	211	1/1	0.84	0.13	85,85,85,85	0
85	MG	6	1993	1/1	0.84	0.24	57,57,57,57	0
85	MG	3	214	1/1	0.84	0.20	64,64,64,64	0
86	OHX	1	4178	7/7	0.84	0.21	145,145,145,145	0
85	MG	2	2007	1/1	0.84	0.40	74,74,74,74	0
86	OHX	5	4245	7/7	0.84	0.19	167,167,167,167	0
85	MG	5	3479	1/1	0.84	0.23	70,70,70,70	0
85	MG	5	3816	1/1	0.84	0.12	57,57,57,57	0
86	OHX	1	4191	7/7	0.84	0.16	154,154,154,154	0
85	MG	2	1960	1/1	0.84	0.26	57,57,57,57	0
85	MG	5	3491	1/1	0.84	0.30	62,62,62,62	0
85	MG	5	3859	1/1	0.84	0.32	77,77,77,77	0
85	MG	5	3502	1/1	0.85	0.26	45,45,45,45	0
85	MG	5	3520	1/1	0.85	0.32	42,42,42,42	0
85	MG	2	1947	1/1	0.85	0.23	88,88,88,88	0
85	MG	6	1932	1/1	0.85	0.27	46,46,46,46	0
85	MG	1	3530	1/1	0.85	0.32	61,61,61,61	0
85	MG	1	3470	1/1	0.85	0.24	51,51,51,51	0
86	OHX	1	4201	7/7	0.85	0.22	148,148,148,148	0
85	MG	5	3626	1/1	0.85	0.21	34,34,34,34	0
85	MG	6	2035	1/1	0.85	0.16	71,71,71,71	0
85	MG	6	2037	1/1	0.85	0.41	58,58,58,58	0
85	MG	5	3644	1/1	0.85	0.28	57,57,57,57	0
85	MG	L5	301	1/1	0.85	0.25	56,56,56,56	0
86	OHX	M9	204	7/7	0.85	0.14	175,175,175,175	0
85	MG	5	3653	1/1	0.85	0.23	31,31,31,31	0
85	MG	6	1952	1/1	0.85	0.27	62,62,62,62	0
85	MG	1	3719	1/1	0.85	0.14	47,47,47,47	0
85	MG	1	3729	1/1	0.85	0.14	57,57,57,57	0
86	OHX	6	2182	7/7	0.85	0.18	154,154,154,154	0
85	MG	2	1933	1/1	0.85	0.33	75,75,75,75	0
85	MG	1	3733	1/1	0.85	0.22	52,52,52,52	0
85	MG	5	3687	1/1	0.85	0.31	79,79,79,79	0
86	OHX	6	2186	7/7	0.85	0.15	172,172,172,172	0
86	OHX	2	2146	7/7	0.85	0.13	183,183,183,183	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3734	1/1	0.85	0.14	34,34,34,34	0
85	MG	1	3475	1/1	0.85	0.32	74,74,74,74	0
85	MG	5	3404	1/1	0.85	0.09	52,52,52,52	0
85	MG	2	1957	1/1	0.85	0.42	80,80,80,80	0
85	MG	2	1943	1/1	0.85	0.33	67,67,67,67	0
86	OHX	2	2163	7/7	0.85	0.14	180,180,180,180	0
86	OHX	2	2171	7/7	0.85	0.15	177,177,177,177	0
86	OHX	2	2172	7/7	0.85	0.17	172,172,172,172	0
85	MG	5	3421	1/1	0.85	0.34	35,35,35,35	0
86	OHX	2	2175	7/7	0.85	0.16	178,178,178,178	0
85	MG	1	3764	1/1	0.85	0.12	58,58,58,58	0
86	OHX	S6	301	7/7	0.85	0.15	164,164,164,164	0
86	OHX	1	4061	7/7	0.85	0.20	141,141,141,141	0
86	OHX	1	4099	7/7	0.85	0.15	170,170,170,170	0
85	MG	5	3430	1/1	0.85	0.23	66,66,66,66	0
85	MG	2	2005	1/1	0.85	0.17	64,64,64,64	0
85	MG	5	3433	1/1	0.85	0.27	85,85,85,85	0
85	MG	5	3447	1/1	0.85	0.21	66,66,66,66	0
86	OHX	1	4146	7/7	0.85	0.20	144,144,144,144	0
86	OHX	5	4226	7/7	0.85	0.16	155,155,155,155	0
85	MG	5	3452	1/1	0.85	0.21	47,47,47,47	0
86	OHX	1	4163	7/7	0.85	0.20	137,137,137,137	0
85	MG	1	3659	1/1	0.85	0.23	63,63,63,63	0
86	OHX	1	4165	7/7	0.85	0.25	127,127,127,127	0
86	OHX	1	4167	7/7	0.85	0.22	124,124,124,124	0
85	MG	2	1901	1/1	0.85	0.19	82,82,82,82	0
85	MG	1	3608	1/1	0.85	0.39	67,67,67,67	0
85	MG	1	3668	1/1	0.85	0.21	82,82,82,82	0
85	MG	1	3844	1/1	0.85	0.30	59,59,59,59	0
85	MG	5	3471	1/1	0.85	0.14	39,39,39,39	0
85	MG	1	3669	1/1	0.85	0.29	63,63,63,63	0
85	MG	1	3847	1/1	0.85	0.25	54,54,54,54	0
85	MG	1	3678	1/1	0.85	0.13	36,36,36,36	0
86	OHX	1	4187	7/7	0.85	0.20	138,138,138,138	0
85	MG	1	3444	1/1	0.85	0.40	67,67,67,67	0
86	OHX	m1	203	7/7	0.85	0.15	162,162,162,162	0
86	OHX	m4	201	7/7	0.85	0.11	219,219,219,219	0
85	MG	1	3698	1/1	0.85	0.28	42,42,42,42	0
85	MG	1	3437	1/1	0.86	0.24	35,35,35,35	0
85	MG	5	3652	1/1	0.86	0.32	63,63,63,63	0
85	MG	1	3748	1/1	0.86	0.24	57,57,57,57	0
85	MG	2	1942	1/1	0.86	0.25	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3664	1/1	0.86	0.49	57,57,57,57	0
85	MG	m7	204	1/1	0.86	0.15	32,32,32,32	0
85	MG	1	3753	1/1	0.86	0.21	100,100,100,100	0
86	OHX	1	4206	7/7	0.86	0.22	137,137,137,137	0
86	OHX	1	4212	7/7	0.86	0.20	146,146,146,146	0
86	OHX	4	235	7/7	0.86	0.17	161,161,161,161	0
85	MG	1	3451	1/1	0.86	0.27	47,47,47,47	0
85	MG	5	3681	1/1	0.86	0.11	39,39,39,39	0
86	OHX	2	2135	7/7	0.86	0.16	147,147,147,147	0
85	MG	S8	301	1/1	0.86	0.18	56,56,56,56	0
85	MG	1	3556	1/1	0.86	0.20	53,53,53,53	0
86	OHX	6	2106	7/7	0.86	0.17	139,139,139,139	0
85	MG	D0	201	1/1	0.86	0.28	68,68,68,68	0
86	OHX	2	2155	7/7	0.86	0.11	247,247,247,247	0
86	OHX	2	2157	7/7	0.86	0.10	289,289,289,289	0
85	MG	D3	201	1/1	0.86	0.14	55,55,55,55	0
86	OHX	6	2174	7/7	0.86	0.15	168,168,168,168	0
86	OHX	6	2177	7/7	0.86	0.17	149,149,149,149	0
85	MG	5	3718	1/1	0.86	0.19	61,61,61,61	0
86	OHX	2	2160	7/7	0.86	0.15	181,181,181,181	0
85	MG	1	3583	1/1	0.86	0.30	43,43,43,43	0
85	MG	1	3817	1/1	0.86	0.15	50,50,50,50	0
85	MG	2	1948	1/1	0.86	0.18	62,62,62,62	0
85	MG	1	3589	1/1	0.86	0.39	40,40,40,40	0
85	MG	5	3453	1/1	0.86	0.24	102,102,102,102	0
85	MG	2	1931	1/1	0.86	0.44	59,59,59,59	0
85	MG	6	1914	1/1	0.86	0.17	70,70,70,70	0
85	MG	5	3770	1/1	0.86	0.22	71,71,71,71	0
85	MG	1	3485	1/1	0.86	0.30	43,43,43,43	0
86	OHX	6	2199	7/7	0.86	0.17	160,160,160,160	0
85	MG	1	3858	1/1	0.86	0.43	74,74,74,74	0
86	OHX	1	4091	7/7	0.86	0.15	160,160,160,160	0
86	OHX	5	4142	7/7	0.86	0.18	142,142,142,142	0
85	MG	1	4215	1/1	0.86	0.12	42,42,42,42	0
86	OHX	1	4108	7/7	0.86	0.17	148,148,148,148	0
86	OHX	5	4172	7/7	0.86	0.15	179,179,179,179	0
85	MG	2	1920	1/1	0.86	0.19	56,56,56,56	0
86	OHX	1	4124	7/7	0.86	0.23	127,127,127,127	0
85	MG	6	1925	1/1	0.86	0.42	36,36,36,36	0
86	OHX	5	4203	7/7	0.86	0.17	147,147,147,147	0
86	OHX	1	4128	7/7	0.86	0.14	179,179,179,179	0
86	OHX	1	4130	7/7	0.86	0.16	167,167,167,167	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	6	2004	1/1	0.86	0.39	69,69,69,69	0
86	OHX	5	4211	7/7	0.86	0.23	124,124,124,124	0
85	MG	2	1985	1/1	0.86	0.21	67,67,67,67	0
85	MG	1	3507	1/1	0.86	0.38	33,33,33,33	0
86	OHX	1	4149	7/7	0.86	0.15	155,155,155,155	0
85	MG	5	3488	1/1	0.86	0.12	33,33,33,33	0
86	OHX	5	4225	7/7	0.86	0.19	157,157,157,157	0
86	OHX	1	4159	7/7	0.86	0.16	164,164,164,164	0
85	MG	6	1929	1/1	0.86	0.30	57,57,57,57	0
85	MG	1	3414	1/1	0.86	0.38	59,59,59,59	0
85	MG	5	3504	1/1	0.86	0.30	52,52,52,52	0
85	MG	5	3508	1/1	0.86	0.32	41,41,41,41	0
85	MG	2	1992	1/1	0.86	0.14	56,56,56,56	0
85	MG	5	3542	1/1	0.86	0.24	31,31,31,31	0
85	MG	6	1934	1/1	0.86	0.28	72,72,72,72	0
85	MG	6	2036	1/1	0.86	0.20	56,56,56,56	0
85	MG	2	2020	1/1	0.86	0.35	65,65,65,65	0
85	MG	6	1936	1/1	0.86	0.35	72,72,72,72	0
86	OHX	1	4179	7/7	0.86	0.20	144,144,144,144	0
86	OHX	5	4248	7/7	0.86	0.18	142,142,142,142	0
86	OHX	1	4181	7/7	0.86	0.18	149,149,149,149	0
86	OHX	8	229	7/7	0.86	0.17	138,138,138,138	0
85	MG	L3	402	1/1	0.86	0.14	43,43,43,43	0
85	MG	6	1941	1/1	0.86	0.31	53,53,53,53	0
85	MG	5	3633	1/1	0.86	0.15	39,39,39,39	0
86	OHX	m0	302	7/7	0.86	0.20	139,139,139,139	0
85	MG	1	3637	1/1	0.86	0.29	62,62,62,62	0
85	MG	5	4253	1/1	0.86	0.27	45,45,45,45	0
86	OHX	m7	206	7/7	0.86	0.20	131,131,131,131	0
85	MG	6	1950	1/1	0.86	0.20	44,44,44,44	0
85	MG	1	3789	1/1	0.87	0.19	84,84,84,84	0
86	OHX	6	2173	7/7	0.87	0.22	138,138,138,138	0
85	MG	5	3475	1/1	0.87	0.28	37,37,37,37	0
86	OHX	1	4131	7/7	0.87	0.20	132,132,132,132	0
86	OHX	6	2180	7/7	0.87	0.20	147,147,147,147	0
86	OHX	1	4133	7/7	0.87	0.19	125,125,125,125	0
85	MG	1	3799	1/1	0.87	0.22	86,86,86,86	0
85	MG	6	2041	1/1	0.87	0.31	68,68,68,68	0
86	OHX	1	4145	7/7	0.87	0.17	154,154,154,154	0
85	MG	5	3480	1/1	0.87	0.25	41,41,41,41	0
85	MG	8	202	1/1	0.87	0.23	71,71,71,71	0
85	MG	5	3481	1/1	0.87	0.26	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	2	1917	1/1	0.87	0.37	55,55,55,55	0
85	MG	2	1975	1/1	0.87	0.36	62,62,62,62	0
85	MG	1	3498	1/1	0.87	0.42	36,36,36,36	0
85	MG	m1	201	1/1	0.87	0.26	64,64,64,64	0
85	MG	s8	301	1/1	0.87	0.14	50,50,50,50	0
85	MG	M7	202	1/1	0.87	0.12	35,35,35,35	0
85	MG	1	3618	1/1	0.87	0.32	59,59,59,59	0
86	OHX	s9	201	7/7	0.87	0.19	138,138,138,138	0
86	OHX	d9	102	7/7	0.87	0.15	181,181,181,181	0
86	OHX	5	4139	7/7	0.87	0.21	137,137,137,137	0
86	OHX	5	4141	7/7	0.87	0.18	139,139,139,139	0
85	MG	1	3818	1/1	0.87	0.18	64,64,64,64	0
86	OHX	2	2101	7/7	0.87	0.16	159,159,159,159	0
86	OHX	5	4161	7/7	0.87	0.19	134,134,134,134	0
85	MG	5	3778	1/1	0.87	0.16	81,81,81,81	0
86	OHX	5	4170	7/7	0.87	0.19	142,142,142,142	0
85	MG	6	1931	1/1	0.87	0.47	65,65,65,65	0
86	OHX	2	2144	7/7	0.87	0.13	179,179,179,179	0
86	OHX	5	4184	7/7	0.87	0.17	140,140,140,140	0
86	OHX	5	4185	7/7	0.87	0.18	132,132,132,132	0
85	MG	5	3406	1/1	0.87	0.14	41,41,41,41	0
86	OHX	1	4183	7/7	0.87	0.22	140,140,140,140	0
86	OHX	1	4184	7/7	0.87	0.19	158,158,158,158	0
86	OHX	2	2147	7/7	0.87	0.20	130,130,130,130	0
85	MG	5	3782	1/1	0.87	0.16	84,84,84,84	0
86	OHX	2	2153	7/7	0.87	0.14	157,157,157,157	0
85	MG	1	3555	1/1	0.87	0.36	36,36,36,36	0
86	OHX	1	4189	7/7	0.87	0.16	151,151,151,151	0
85	MG	6	1933	1/1	0.87	0.43	65,65,65,65	0
85	MG	5	3791	1/1	0.87	0.29	55,55,55,55	0
85	MG	2	1909	1/1	0.87	0.31	65,65,65,65	0
86	OHX	5	4223	7/7	0.87	0.16	153,153,153,153	0
85	MG	5	3423	1/1	0.87	0.26	60,60,60,60	0
85	MG	2	1921	1/1	0.87	0.39	54,54,54,54	0
85	MG	6	1999	1/1	0.87	0.14	102,102,102,102	0
85	MG	1	3670	1/1	0.87	0.16	54,54,54,54	0
85	MG	5	3637	1/1	0.87	0.26	49,49,49,49	0
85	MG	2	1912	1/1	0.87	0.26	66,66,66,66	0
86	OHX	2	2173	7/7	0.87	0.17	151,151,151,151	0
86	OHX	5	4236	7/7	0.87	0.21	144,144,144,144	0
86	OHX	1	4209	7/7	0.87	0.21	133,133,133,133	0
86	OHX	5	4238	7/7	0.87	0.15	154,154,154,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3687	1/1	0.87	0.14	53,53,53,53	0
86	OHX	3	223	7/7	0.87	0.15	175,175,175,175	0
85	MG	2	2012	1/1	0.87	0.33	67,67,67,67	0
86	OHX	4	237	7/7	0.87	0.18	144,144,144,144	0
85	MG	2	1979	1/1	0.87	0.35	53,53,53,53	0
85	MG	1	3703	1/1	0.87	0.36	64,64,64,64	0
86	OHX	5	4249	7/7	0.87	0.18	163,163,163,163	0
85	MG	1	3765	1/1	0.87	0.23	54,54,54,54	0
85	MG	6	1958	1/1	0.87	0.34	61,61,61,61	0
86	OHX	8	232	7/7	0.87	0.18	152,152,152,152	0
85	MG	5	3880	1/1	0.87	0.25	26,26,26,26	0
85	MG	1	3430	1/1	0.87	0.28	47,47,47,47	0
85	MG	6	1917	1/1	0.87	0.29	57,57,57,57	0
85	MG	4	211	1/1	0.87	0.25	54,54,54,54	0
86	OHX	6	2151	7/7	0.87	0.15	169,169,169,169	0
85	MG	5	3894	1/1	0.87	0.20	61,61,61,61	0
86	OHX	6	2163	7/7	0.87	0.13	198,198,198,198	0
86	OHX	6	2164	7/7	0.87	0.16	160,160,160,160	0
88	ZN	d7	101	1/1	0.87	0.14	156,156,156,156	0
85	MG	1	3527	1/1	0.88	0.35	32,32,32,32	0
85	MG	5	3754	1/1	0.88	0.19	56,56,56,56	0
85	MG	1	3417	1/1	0.88	0.22	35,35,35,35	0
85	MG	1	3610	1/1	0.88	0.10	41,41,41,41	0
85	MG	1	3686	1/1	0.88	0.22	96,96,96,96	0
85	MG	1	3483	1/1	0.88	0.23	53,53,53,53	0
85	MG	N8	204	1/1	0.88	0.42	38,38,38,38	0
85	MG	5	3776	1/1	0.88	0.28	66,66,66,66	0
86	OHX	2	2169	7/7	0.88	0.17	150,150,150,150	0
85	MG	1	3696	1/1	0.88	0.12	64,64,64,64	0
86	OHX	6	2171	7/7	0.88	0.15	149,149,149,149	0
85	MG	5	3494	1/1	0.88	0.24	29,29,29,29	0
85	MG	1	3418	1/1	0.88	0.23	44,44,44,44	0
85	MG	1	3494	1/1	0.88	0.23	45,45,45,45	0
86	OHX	6	2179	7/7	0.88	0.20	139,139,139,139	0
85	MG	1	3547	1/1	0.88	0.23	50,50,50,50	0
86	OHX	6	2181	7/7	0.88	0.18	143,143,143,143	0
85	MG	5	3513	1/1	0.88	0.31	34,34,34,34	0
85	MG	s2	301	1/1	0.88	0.13	53,53,53,53	0
85	MG	5	3524	1/1	0.88	0.32	31,31,31,31	0
85	MG	5	3533	1/1	0.88	0.25	54,54,54,54	0
86	OHX	1	4094	7/7	0.88	0.14	152,152,152,152	0
85	MG	5	3537	1/1	0.88	0.28	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3540	1/1	0.88	0.34	28,28,28,28	0
85	MG	1	3837	1/1	0.88	0.25	44,44,44,44	0
85	MG	5	3551	1/1	0.88	0.29	33,33,33,33	0
86	OHX	6	2191	7/7	0.88	0.16	165,165,165,165	0
85	MG	2	1938	1/1	0.88	0.31	66,66,66,66	0
85	MG	6	1967	1/1	0.88	0.22	81,81,81,81	0
86	OHX	1	4129	7/7	0.88	0.16	158,158,158,158	0
86	OHX	6	2202	7/7	0.88	0.19	155,155,155,155	0
85	MG	5	3572	1/1	0.88	0.29	41,41,41,41	0
85	MG	1	3497	1/1	0.88	0.30	41,41,41,41	0
85	MG	5	3845	1/1	0.88	0.28	50,50,50,50	0
86	OHX	1	4137	7/7	0.88	0.17	146,146,146,146	0
85	MG	5	3846	1/1	0.88	0.33	55,55,55,55	0
85	MG	5	3858	1/1	0.88	0.19	53,53,53,53	0
86	OHX	1	4142	7/7	0.88	0.14	153,153,153,153	0
86	OHX	1	4144	7/7	0.88	0.15	166,166,166,166	0
86	OHX	5	4160	7/7	0.88	0.19	137,137,137,137	0
85	MG	5	3583	1/1	0.88	0.27	45,45,45,45	0
86	OHX	5	4164	7/7	0.88	0.17	159,159,159,159	0
85	MG	5	3588	1/1	0.88	0.41	51,51,51,51	0
85	MG	5	3867	1/1	0.88	0.23	67,67,67,67	0
85	MG	5	3876	1/1	0.88	0.35	63,63,63,63	0
85	MG	5	3602	1/1	0.88	0.14	64,64,64,64	0
86	OHX	1	4161	7/7	0.88	0.14	160,160,160,160	0
85	MG	1	3458	1/1	0.88	0.26	40,40,40,40	0
86	OHX	5	4188	7/7	0.88	0.23	126,126,126,126	0
85	MG	5	3618	1/1	0.88	0.21	52,52,52,52	0
86	OHX	5	4196	7/7	0.88	0.19	143,143,143,143	0
85	MG	1	3714	1/1	0.88	0.13	49,49,49,49	0
86	OHX	1	4166	7/7	0.88	0.19	132,132,132,132	0
85	MG	6	1977	1/1	0.88	0.23	48,48,48,48	0
85	MG	5	3416	1/1	0.88	0.11	36,36,36,36	0
85	MG	5	3896	1/1	0.88	0.29	54,54,54,54	0
85	MG	6	1979	1/1	0.88	0.34	63,63,63,63	0
86	OHX	1	4173	7/7	0.88	0.15	151,151,151,151	0
85	MG	2	1954	1/1	0.88	0.24	64,64,64,64	0
86	OHX	1	4175	7/7	0.88	0.22	134,134,134,134	0
85	MG	5	3638	1/1	0.88	0.21	50,50,50,50	0
85	MG	5	4256	1/1	0.88	0.27	35,35,35,35	0
86	OHX	5	4224	7/7	0.88	0.21	136,136,136,136	0
85	MG	5	3643	1/1	0.88	0.12	46,46,46,46	0
85	MG	1	3725	1/1	0.88	0.40	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	4222	1/1	0.88	0.28	34,34,34,34	0
86	OHX	5	4229	7/7	0.88	0.11	194,194,194,194	0
85	MG	1	3647	1/1	0.88	0.11	51,51,51,51	0
85	MG	1	3563	1/1	0.88	0.24	42,42,42,42	0
85	MG	1	3405	1/1	0.88	0.28	70,70,70,70	0
85	MG	5	3440	1/1	0.88	0.26	34,34,34,34	0
85	MG	5	3674	1/1	0.88	0.13	69,69,69,69	0
85	MG	2	2015	1/1	0.88	0.29	61,61,61,61	0
85	MG	1	3584	1/1	0.88	0.34	51,51,51,51	0
85	MG	4	205	1/1	0.88	0.23	29,29,29,29	0
85	MG	q1	101	1/1	0.88	0.19	40,40,40,40	0
85	MG	4	208	1/1	0.88	0.28	46,46,46,46	0
86	OHX	5	4243	7/7	0.88	0.14	178,178,178,178	0
86	OHX	2	2094	7/7	0.88	0.14	151,151,151,151	0
86	OHX	5	4246	7/7	0.88	0.17	154,154,154,154	0
85	MG	1	3660	1/1	0.88	0.12	34,34,34,34	0
86	OHX	2	2117	7/7	0.88	0.17	148,148,148,148	0
86	OHX	2	2134	7/7	0.88	0.16	148,148,148,148	0
86	OHX	7	224	7/7	0.88	0.17	150,150,150,150	0
85	MG	1	3663	1/1	0.88	0.20	53,53,53,53	0
85	MG	5	3697	1/1	0.88	0.12	45,45,45,45	0
86	OHX	2	2139	7/7	0.88	0.17	171,171,171,171	0
86	OHX	1	4211	7/7	0.88	0.13	169,169,169,169	0
85	MG	1	3479	1/1	0.88	0.19	84,84,84,84	0
86	OHX	1	4213	7/7	0.88	0.19	159,159,159,159	0
85	MG	1	3754	1/1	0.88	0.11	44,44,44,44	0
85	MG	6	2020	1/1	0.88	0.33	91,91,91,91	0
85	MG	1	3523	1/1	0.88	0.26	26,26,26,26	0
86	OHX	2	2149	7/7	0.88	0.14	181,181,181,181	0
86	OHX	2	2150	7/7	0.88	0.12	197,197,197,197	0
88	ZN	D7	101	1/1	0.88	0.10	162,162,162,162	0
85	MG	1	3591	1/1	0.88	0.40	53,53,53,53	0
85	MG	6	1910	1/1	0.89	0.30	46,46,46,46	0
86	OHX	6	2178	7/7	0.89	0.14	163,163,163,163	0
85	MG	1	3515	1/1	0.89	0.30	34,34,34,34	0
85	MG	5	3499	1/1	0.89	0.30	40,40,40,40	0
85	MG	5	3500	1/1	0.89	0.21	31,31,31,31	0
85	MG	5	3694	1/1	0.89	0.21	51,51,51,51	0
85	MG	1	3593	1/1	0.89	0.23	29,29,29,29	0
86	OHX	1	4138	7/7	0.89	0.24	124,124,124,124	0
86	OHX	1	4139	7/7	0.89	0.17	137,137,137,137	0
85	MG	5	4255	1/1	0.89	0.28	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3651	1/1	0.89	0.14	74,74,74,74	0
85	MG	5	3715	1/1	0.89	0.15	52,52,52,52	0
85	MG	c8	201	1/1	0.89	0.39	69,69,69,69	0
85	MG	7	214	1/1	0.89	0.23	51,51,51,51	0
85	MG	5	3720	1/1	0.89	0.34	63,63,63,63	0
86	OHX	1	4148	7/7	0.89	0.14	148,148,148,148	0
86	OHX	6	2194	7/7	0.89	0.14	173,173,173,173	0
85	MG	8	207	1/1	0.89	0.15	44,44,44,44	0
86	OHX	6	2198	7/7	0.89	0.17	153,153,153,153	0
85	MG	5	3722	1/1	0.89	0.19	49,49,49,49	0
85	MG	5	3512	1/1	0.89	0.31	58,58,58,58	0
85	MG	5	3731	1/1	0.89	0.11	47,47,47,47	0
85	MG	d3	202	1/1	0.89	0.21	54,54,54,54	0
85	MG	l7	302	1/1	0.89	0.18	40,40,40,40	0
86	OHX	c3	201	7/7	0.89	0.13	162,162,162,162	0
86	OHX	c5	201	7/7	0.89	0.11	176,176,176,176	0
86	OHX	d4	201	7/7	0.89	0.13	162,162,162,162	0
85	MG	1	3478	1/1	0.89	0.33	47,47,47,47	0
86	OHX	5	4096	7/7	0.89	0.15	152,152,152,152	0
85	MG	m1	202	1/1	0.89	0.34	64,64,64,64	0
85	MG	6	1978	1/1	0.89	0.19	77,77,77,77	0
85	MG	5	3527	1/1	0.89	0.43	55,55,55,55	0
86	OHX	5	4147	7/7	0.89	0.20	126,126,126,126	0
86	OHX	5	4153	7/7	0.89	0.22	124,124,124,124	0
85	MG	1	3773	1/1	0.89	0.20	57,57,57,57	0
86	OHX	5	4158	7/7	0.89	0.16	144,144,144,144	0
85	MG	o4	201	1/1	0.89	0.28	69,69,69,69	0
85	MG	3	212	1/1	0.89	0.12	80,80,80,80	0
85	MG	1	3778	1/1	0.89	0.13	46,46,46,46	0
85	MG	2	1934	1/1	0.89	0.34	58,58,58,58	0
86	OHX	5	4169	7/7	0.89	0.17	148,148,148,148	0
85	MG	5	3545	1/1	0.89	0.37	51,51,51,51	0
85	MG	1	3784	1/1	0.89	0.18	59,59,59,59	0
86	OHX	5	4177	7/7	0.89	0.17	144,144,144,144	0
86	OHX	5	4178	7/7	0.89	0.17	136,136,136,136	0
86	OHX	2	2121	7/7	0.89	0.17	146,146,146,146	0
86	OHX	5	4183	7/7	0.89	0.14	153,153,153,153	0
86	OHX	2	2130	7/7	0.89	0.13	207,207,207,207	0
86	OHX	1	4182	7/7	0.89	0.15	153,153,153,153	0
85	MG	6	1990	1/1	0.89	0.25	74,74,74,74	0
85	MG	5	3564	1/1	0.89	0.34	31,31,31,31	0
86	OHX	2	2136	7/7	0.89	0.16	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3785	1/1	0.89	0.31	43,43,43,43	0
86	OHX	5	4198	7/7	0.89	0.19	128,128,128,128	0
85	MG	1	3615	1/1	0.89	0.16	36,36,36,36	0
85	MG	1	3798	1/1	0.89	0.12	60,60,60,60	0
85	MG	1	3450	1/1	0.89	0.25	39,39,39,39	0
85	MG	1	3664	1/1	0.89	0.19	45,45,45,45	0
86	OHX	5	4209	7/7	0.89	0.20	131,131,131,131	0
86	OHX	5	4210	7/7	0.89	0.17	157,157,157,157	0
85	MG	5	3590	1/1	0.89	0.28	32,32,32,32	0
86	OHX	5	4212	7/7	0.89	0.15	146,146,146,146	0
86	OHX	5	4213	7/7	0.89	0.17	152,152,152,152	0
85	MG	6	2000	1/1	0.89	0.20	57,57,57,57	0
85	MG	2	1944	1/1	0.89	0.14	67,67,67,67	0
85	MG	1	3502	1/1	0.89	0.44	41,41,41,41	0
85	MG	5	3808	1/1	0.89	0.08	29,29,29,29	0
85	MG	2	1969	1/1	0.89	0.19	66,66,66,66	0
85	MG	1	3536	1/1	0.89	0.39	55,55,55,55	0
86	OHX	1	4202	7/7	0.89	0.17	144,144,144,144	0
85	MG	5	3814	1/1	0.89	0.12	50,50,50,50	0
86	OHX	5	4227	7/7	0.89	0.16	142,142,142,142	0
86	OHX	1	4204	7/7	0.89	0.17	148,148,148,148	0
85	MG	6	1939	1/1	0.89	0.30	62,62,62,62	0
86	OHX	1	4207	7/7	0.89	0.18	144,144,144,144	0
85	MG	1	3539	1/1	0.89	0.28	25,25,25,25	0
85	MG	1	3540	1/1	0.89	0.28	54,54,54,54	0
85	MG	1	3735	1/1	0.89	0.26	64,64,64,64	0
86	OHX	2	2167	7/7	0.89	0.16	163,163,163,163	0
85	MG	5	3831	1/1	0.89	0.22	49,49,49,49	0
85	MG	5	3639	1/1	0.89	0.12	55,55,55,55	0
85	MG	N9	101	1/1	0.89	0.14	31,31,31,31	0
85	MG	5	3848	1/1	0.89	0.10	37,37,37,37	0
85	MG	1	3476	1/1	0.89	0.24	37,37,37,37	0
85	MG	1	3546	1/1	0.89	0.28	68,68,68,68	0
86	OHX	5	4244	7/7	0.89	0.18	143,143,143,143	0
85	MG	1	3855	1/1	0.89	0.27	44,44,44,44	0
85	MG	6	1902	1/1	0.89	0.21	55,55,55,55	0
85	MG	5	3868	1/1	0.89	0.14	49,49,49,49	0
86	OHX	1	4066	7/7	0.89	0.17	143,143,143,143	0
86	OHX	6	2138	7/7	0.89	0.16	130,130,130,130	0
86	OHX	1	4079	7/7	0.89	0.18	126,126,126,126	0
86	OHX	6	2149	7/7	0.89	0.16	149,149,149,149	0
86	OHX	8	228	7/7	0.89	0.16	156,156,156,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3872	1/1	0.89	0.34	40,40,40,40	0
85	MG	5	3875	1/1	0.89	0.25	45,45,45,45	0
86	OHX	6	2159	7/7	0.89	0.18	140,140,140,140	0
85	MG	1	3856	1/1	0.89	0.32	67,67,67,67	0
85	MG	1	3689	1/1	0.89	0.34	60,60,60,60	0
86	OHX	19	600	7/7	0.89	0.18	134,134,134,134	0
86	OHX	6	2167	7/7	0.89	0.22	128,128,128,128	0
86	OHX	6	2168	7/7	0.89	0.15	162,162,162,162	0
85	MG	5	3483	1/1	0.89	0.22	69,69,69,69	0
86	OHX	1	4111	7/7	0.89	0.23	128,128,128,128	0
86	OHX	m8	201	7/7	0.89	0.18	145,145,145,145	0
85	MG	1	3861	1/1	0.89	0.20	53,53,53,53	0
86	OHX	o7	503	7/7	0.89	0.22	142,142,142,142	0
87	PCY	2	2178	40/40	0.89	0.15	77,77,77,77	0
85	MG	1	3692	1/1	0.89	0.34	43,43,43,43	0
86	OHX	6	2175	7/7	0.89	0.20	119,119,119,119	0
85	MG	1	3638	1/1	0.90	0.19	64,64,64,64	0
85	MG	5	3516	1/1	0.90	0.21	42,42,42,42	0
85	MG	5	3517	1/1	0.90	0.27	23,23,23,23	0
85	MG	1	3642	1/1	0.90	0.20	44,44,44,44	0
85	MG	3	203	1/1	0.90	0.14	97,97,97,97	0
85	MG	5	3525	1/1	0.90	0.27	47,47,47,47	0
85	MG	1	3643	1/1	0.90	0.20	44,44,44,44	0
86	OHX	2	2170	7/7	0.90	0.15	154,154,154,154	0
85	MG	1	3646	1/1	0.90	0.23	40,40,40,40	0
85	MG	5	3796	1/1	0.90	0.09	50,50,50,50	0
85	MG	1	3505	1/1	0.90	0.18	35,35,35,35	0
85	MG	5	3538	1/1	0.90	0.41	42,42,42,42	0
85	MG	1	3648	1/1	0.90	0.13	46,46,46,46	0
85	MG	1	3559	1/1	0.90	0.23	39,39,39,39	0
85	MG	2	1946	1/1	0.90	0.14	60,60,60,60	0
86	OHX	S8	302	7/7	0.90	0.12	173,173,173,173	0
85	MG	5	3810	1/1	0.90	0.14	43,43,43,43	0
86	OHX	1	4062	7/7	0.90	0.17	130,130,130,130	0
85	MG	5	3550	1/1	0.90	0.36	50,50,50,50	0
86	OHX	1	4068	7/7	0.90	0.18	127,127,127,127	0
86	OHX	1	4075	7/7	0.90	0.13	143,143,143,143	0
85	MG	2	2021	1/1	0.90	0.42	66,66,66,66	0
85	MG	2	1964	1/1	0.90	0.24	56,56,56,56	0
86	OHX	1	4093	7/7	0.90	0.17	138,138,138,138	0
85	MG	5	3555	1/1	0.90	0.31	46,46,46,46	0
85	MG	5	3817	1/1	0.90	0.20	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4101	7/7	0.90	0.14	149,149,149,149	0
86	OHX	6	2193	7/7	0.90	0.12	195,195,195,195	0
85	MG	5	3559	1/1	0.90	0.23	34,34,34,34	0
85	MG	4	212	1/1	0.90	0.13	39,39,39,39	0
85	MG	5	3830	1/1	0.90	0.25	26,26,26,26	0
86	OHX	1	4112	7/7	0.90	0.11	181,181,181,181	0
86	OHX	1	4114	7/7	0.90	0.17	138,138,138,138	0
86	OHX	1	4117	7/7	0.90	0.16	138,138,138,138	0
86	OHX	1	4119	7/7	0.90	0.16	142,142,142,142	0
86	OHX	s8	303	7/7	0.90	0.13	167,167,167,167	0
85	MG	5	3568	1/1	0.90	0.26	30,30,30,30	0
85	MG	5	3569	1/1	0.90	0.30	32,32,32,32	0
85	MG	c1	201	1/1	0.90	0.25	47,47,47,47	0
85	MG	5	3847	1/1	0.90	0.13	42,42,42,42	0
85	MG	1	3580	1/1	0.90	0.25	43,43,43,43	0
86	OHX	5	4062	7/7	0.90	0.15	132,132,132,132	0
85	MG	6	1951	1/1	0.90	0.29	68,68,68,68	0
86	OHX	5	4099	7/7	0.90	0.18	129,129,129,129	0
86	OHX	5	4109	7/7	0.90	0.19	128,128,128,128	0
86	OHX	5	4138	7/7	0.90	0.14	135,135,135,135	0
86	OHX	1	4132	7/7	0.90	0.18	148,148,148,148	0
86	OHX	5	4140	7/7	0.90	0.14	146,146,146,146	0
85	MG	5	3582	1/1	0.90	0.21	34,34,34,34	0
85	MG	1	3516	1/1	0.90	0.33	39,39,39,39	0
85	MG	2	1906	1/1	0.90	0.20	53,53,53,53	0
86	OHX	5	4148	7/7	0.90	0.19	137,137,137,137	0
85	MG	6	1955	1/1	0.90	0.31	40,40,40,40	0
85	MG	5	3595	1/1	0.90	0.32	37,37,37,37	0
86	OHX	5	4157	7/7	0.90	0.15	143,143,143,143	0
85	MG	5	3600	1/1	0.90	0.20	44,44,44,44	0
86	OHX	5	4159	7/7	0.90	0.18	125,125,125,125	0
85	MG	L8	301	1/1	0.90	0.23	63,63,63,63	0
85	MG	5	3608	1/1	0.90	0.29	31,31,31,31	0
85	MG	2	1918	1/1	0.90	0.41	55,55,55,55	0
85	MG	1	3767	1/1	0.90	0.17	89,89,89,89	0
86	OHX	5	4168	7/7	0.90	0.12	159,159,159,159	0
85	MG	5	3621	1/1	0.90	0.32	49,49,49,49	0
85	MG	M6	202	1/1	0.90	0.10	65,65,65,65	0
86	OHX	1	4156	7/7	0.90	0.14	150,150,150,150	0
85	MG	5	3629	1/1	0.90	0.21	66,66,66,66	0
85	MG	5	3895	1/1	0.90	0.09	119,119,119,119	0
85	MG	5	3631	1/1	0.90	0.22	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4182	7/7	0.90	0.16	145,145,145,145	0
85	MG	1	3524	1/1	0.90	0.12	43,43,43,43	0
85	MG	1	3590	1/1	0.90	0.21	38,38,38,38	0
85	MG	1	3435	1/1	0.90	0.09	50,50,50,50	0
85	MG	1	3482	1/1	0.90	0.21	34,34,34,34	0
85	MG	N0	201	1/1	0.90	0.25	45,45,45,45	0
86	OHX	5	4190	7/7	0.90	0.18	134,134,134,134	0
86	OHX	5	4193	7/7	0.90	0.20	135,135,135,135	0
86	OHX	5	4194	7/7	0.90	0.18	132,132,132,132	0
85	MG	7	201	1/1	0.90	0.31	40,40,40,40	0
85	MG	7	203	1/1	0.90	0.31	57,57,57,57	0
85	MG	2	1936	1/1	0.90	0.26	55,55,55,55	0
85	MG	6	1976	1/1	0.90	0.22	48,48,48,48	0
85	MG	5	3437	1/1	0.90	0.35	61,61,61,61	0
86	OHX	5	4205	7/7	0.90	0.17	145,145,145,145	0
85	MG	1	3673	1/1	0.90	0.19	28,28,28,28	0
85	MG	8	205	1/1	0.90	0.18	54,54,54,54	0
85	MG	1	3597	1/1	0.90	0.34	44,44,44,44	0
85	MG	1	3679	1/1	0.90	0.17	65,65,65,65	0
86	OHX	1	4180	7/7	0.90	0.21	114,114,114,114	0
85	MG	5	3654	1/1	0.90	0.12	43,43,43,43	0
85	MG	2	1959	1/1	0.90	0.21	66,66,66,66	0
86	OHX	5	4218	7/7	0.90	0.15	145,145,145,145	0
85	MG	1	3804	1/1	0.90	0.16	42,42,42,42	0
85	MG	1	3487	1/1	0.90	0.28	45,45,45,45	0
85	MG	1	3612	1/1	0.90	0.30	46,46,46,46	0
85	MG	1	3489	1/1	0.90	0.36	54,54,54,54	0
85	MG	2	1929	1/1	0.90	0.33	66,66,66,66	0
85	MG	1	3543	1/1	0.90	0.30	39,39,39,39	0
85	MG	n8	203	1/1	0.90	0.20	47,47,47,47	0
85	MG	5	3472	1/1	0.90	0.16	47,47,47,47	0
85	MG	1	3838	1/1	0.90	0.23	42,42,42,42	0
85	MG	6	1997	1/1	0.90	0.31	59,59,59,59	0
85	MG	2	2016	1/1	0.90	0.33	63,63,63,63	0
86	OHX	2	2092	7/7	0.90	0.15	150,150,150,150	0
86	OHX	1	4198	7/7	0.90	0.17	137,137,137,137	0
85	MG	2	1913	1/1	0.90	0.32	79,79,79,79	0
85	MG	1	3625	1/1	0.90	0.21	37,37,37,37	0
85	MG	2	1997	1/1	0.90	0.10	80,80,80,80	0
86	OHX	2	2120	7/7	0.90	0.13	158,158,158,158	0
85	MG	6	1921	1/1	0.90	0.29	43,43,43,43	0
85	MG	1	3467	1/1	0.90	0.22	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4205	7/7	0.90	0.16	155,155,155,155	0
85	MG	1	3551	1/1	0.90	0.34	35,35,35,35	0
86	OHX	5	4242	7/7	0.90	0.22	116,116,116,116	0
85	MG	5	3489	1/1	0.90	0.25	56,56,56,56	0
86	OHX	1	4208	7/7	0.90	0.19	137,137,137,137	0
85	MG	6	2006	1/1	0.90	0.12	54,54,54,54	0
85	MG	6	2012	1/1	0.90	0.13	70,70,70,70	0
86	OHX	2	2138	7/7	0.90	0.14	147,147,147,147	0
85	MG	5	3745	1/1	0.90	0.20	64,64,64,64	0
86	OHX	2	2140	7/7	0.90	0.14	167,167,167,167	0
86	OHX	5	4250	7/7	0.90	0.16	143,143,143,143	0
86	OHX	3	224	7/7	0.90	0.17	148,148,148,148	0
86	OHX	4	234	7/7	0.90	0.18	126,126,126,126	0
85	MG	5	3498	1/1	0.90	0.24	36,36,36,36	0
86	OHX	4	236	7/7	0.90	0.16	153,153,153,153	0
85	MG	2	1925	1/1	0.90	0.41	65,65,65,65	0
85	MG	6	2019	1/1	0.90	0.14	110,110,110,110	0
85	MG	1	3721	1/1	0.90	0.09	55,55,55,55	0
85	MG	5	3761	1/1	0.90	0.22	77,77,77,77	0
85	MG	5	3762	1/1	0.90	0.18	39,39,39,39	0
86	OHX	2	2152	7/7	0.90	0.13	178,178,178,178	0
85	MG	5	3503	1/1	0.90	0.33	32,32,32,32	0
86	OHX	6	2120	7/7	0.90	0.18	122,122,122,122	0
86	OHX	6	2126	7/7	0.90	0.25	116,116,116,116	0
86	OHX	2	2154	7/7	0.90	0.15	149,149,149,149	0
85	MG	1	3722	1/1	0.90	0.12	48,48,48,48	0
86	OHX	2	2156	7/7	0.90	0.20	129,129,129,129	0
85	MG	6	2029	1/1	0.90	0.20	105,105,105,105	0
85	MG	1	4220	1/1	0.90	0.11	48,48,48,48	0
86	OHX	6	2152	7/7	0.90	0.14	151,151,151,151	0
85	MG	1	3443	1/1	0.91	0.17	82,82,82,82	0
86	OHX	1	4120	7/7	0.91	0.14	161,161,161,161	0
85	MG	sM	301	1/1	0.91	0.17	48,48,48,48	0
85	MG	1	3415	1/1	0.91	0.28	37,37,37,37	0
86	OHX	1	4127	7/7	0.91	0.17	135,135,135,135	0
85	MG	6	1975	1/1	0.91	0.16	59,59,59,59	0
85	MG	7	207	1/1	0.91	0.08	56,56,56,56	0
85	MG	7	208	1/1	0.91	0.31	52,52,52,52	0
85	MG	7	211	1/1	0.91	0.09	72,72,72,72	0
85	MG	7	212	1/1	0.91	0.07	51,51,51,51	0
85	MG	5	3723	1/1	0.91	0.17	53,53,53,53	0
86	OHX	1	4134	7/7	0.91	0.17	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3724	1/1	0.91	0.14	40,40,40,40	0
86	OHX	6	2196	7/7	0.91	0.15	149,149,149,149	0
85	MG	5	3725	1/1	0.91	0.14	37,37,37,37	0
85	MG	8	203	1/1	0.91	0.28	40,40,40,40	0
85	MG	5	3726	1/1	0.91	0.18	59,59,59,59	0
85	MG	5	3403	1/1	0.91	0.27	54,54,54,54	0
85	MG	1	3402	1/1	0.91	0.34	56,56,56,56	0
85	MG	2	1927	1/1	0.91	0.31	51,51,51,51	0
85	MG	5	3734	1/1	0.91	0.38	71,71,71,71	0
85	MG	15	301	1/1	0.91	0.29	67,67,67,67	0
85	MG	5	3738	1/1	0.91	0.30	67,67,67,67	0
85	MG	5	3543	1/1	0.91	0.33	66,66,66,66	0
85	MG	5	3411	1/1	0.91	0.29	42,42,42,42	0
86	OHX	5	4017	7/7	0.91	0.15	161,161,161,161	0
86	OHX	1	4157	7/7	0.91	0.16	143,143,143,143	0
85	MG	1	3452	1/1	0.91	0.21	36,36,36,36	0
86	OHX	5	4097	7/7	0.91	0.16	132,132,132,132	0
85	MG	2	1980	1/1	0.91	0.23	68,68,68,68	0
86	OHX	5	4101	7/7	0.91	0.14	150,150,150,150	0
86	OHX	1	4160	7/7	0.91	0.17	147,147,147,147	0
86	OHX	5	4111	7/7	0.91	0.14	145,145,145,145	0
86	OHX	5	4118	7/7	0.91	0.16	139,139,139,139	0
86	OHX	5	4120	7/7	0.91	0.16	133,133,133,133	0
86	OHX	5	4129	7/7	0.91	0.12	150,150,150,150	0
86	OHX	5	4132	7/7	0.91	0.11	192,192,192,192	0
86	OHX	5	4133	7/7	0.91	0.17	132,132,132,132	0
85	MG	5	3418	1/1	0.91	0.28	28,28,28,28	0
86	OHX	1	4162	7/7	0.91	0.13	166,166,166,166	0
85	MG	1	3770	1/1	0.91	0.10	53,53,53,53	0
85	MG	1	3550	1/1	0.91	0.26	43,43,43,43	0
85	MG	1	3702	1/1	0.91	0.28	51,51,51,51	0
85	MG	1	3779	1/1	0.91	0.10	50,50,50,50	0
85	MG	1	3599	1/1	0.91	0.28	39,39,39,39	0
85	MG	1	3782	1/1	0.91	0.31	64,64,64,64	0
85	MG	1	3603	1/1	0.91	0.20	39,39,39,39	0
86	OHX	5	4156	7/7	0.91	0.15	142,142,142,142	0
85	MG	1	3707	1/1	0.91	0.15	55,55,55,55	0
86	OHX	1	4172	7/7	0.91	0.11	174,174,174,174	0
86	OHX	2	2109	7/7	0.91	0.15	140,140,140,140	0
86	OHX	2	2113	7/7	0.91	0.12	167,167,167,167	0
85	MG	4	209	1/1	0.91	0.10	53,53,53,53	0
86	OHX	5	4162	7/7	0.91	0.18	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	2	1919	1/1	0.91	0.42	76,76,76,76	0
86	OHX	1	4177	7/7	0.91	0.08	238,238,238,238	0
86	OHX	5	4166	7/7	0.91	0.16	149,149,149,149	0
85	MG	1	3654	1/1	0.91	0.23	34,34,34,34	0
86	OHX	2	2125	7/7	0.91	0.16	151,151,151,151	0
86	OHX	2	2128	7/7	0.91	0.14	143,143,143,143	0
85	MG	4	213	1/1	0.91	0.17	63,63,63,63	0
86	OHX	5	4176	7/7	0.91	0.18	148,148,148,148	0
86	OHX	2	2132	7/7	0.91	0.13	159,159,159,159	0
85	MG	5	3594	1/1	0.91	0.32	41,41,41,41	0
85	MG	4	214	1/1	0.91	0.09	47,47,47,47	0
85	MG	5	3792	1/1	0.91	0.14	36,36,36,36	0
85	MG	4	217	1/1	0.91	0.15	41,41,41,41	0
85	MG	2	2001	1/1	0.91	0.20	78,78,78,78	0
85	MG	1	3717	1/1	0.91	0.37	57,57,57,57	0
86	OHX	5	4187	7/7	0.91	0.18	133,133,133,133	0
85	MG	5	3614	1/1	0.91	0.10	34,34,34,34	0
86	OHX	2	2142	7/7	0.91	0.15	140,140,140,140	0
86	OHX	2	2143	7/7	0.91	0.21	138,138,138,138	0
86	OHX	5	4191	7/7	0.91	0.14	148,148,148,148	0
85	MG	5	3805	1/1	0.91	0.12	65,65,65,65	0
85	MG	1	3493	1/1	0.91	0.37	74,74,74,74	0
85	MG	5	3470	1/1	0.91	0.18	44,44,44,44	0
85	MG	6	2009	1/1	0.91	0.16	55,55,55,55	0
85	MG	6	2011	1/1	0.91	0.12	51,51,51,51	0
85	MG	1	3557	1/1	0.91	0.30	49,49,49,49	0
85	MG	1	3814	1/1	0.91	0.13	53,53,53,53	0
85	MG	1	3468	1/1	0.91	0.30	48,48,48,48	0
85	MG	1	3432	1/1	0.91	0.25	39,39,39,39	0
85	MG	6	2026	1/1	0.91	0.16	86,86,86,86	0
85	MG	6	1943	1/1	0.91	0.33	38,38,38,38	0
85	MG	1	3728	1/1	0.91	0.19	38,38,38,38	0
85	MG	6	1949	1/1	0.91	0.35	56,56,56,56	0
85	MG	6	2031	1/1	0.91	0.27	70,70,70,70	0
85	MG	5	3837	1/1	0.91	0.13	50,50,50,50	0
86	OHX	5	4214	7/7	0.91	0.18	133,133,133,133	0
85	MG	5	3844	1/1	0.91	0.16	59,59,59,59	0
85	MG	1	3824	1/1	0.91	0.12	45,45,45,45	0
85	MG	1	3826	1/1	0.91	0.17	29,29,29,29	0
85	MG	1	3827	1/1	0.91	0.19	52,52,52,52	0
85	MG	5	3495	1/1	0.91	0.13	36,36,36,36	0
85	MG	5	3855	1/1	0.91	0.25	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3857	1/1	0.91	0.19	65,65,65,65	0
85	MG	2	2008	1/1	0.91	0.40	48,48,48,48	0
85	MG	5	3656	1/1	0.91	0.10	59,59,59,59	0
85	MG	1	3570	1/1	0.91	0.34	42,42,42,42	0
85	MG	5	3866	1/1	0.91	0.31	54,54,54,54	0
86	OHX	2	2176	7/7	0.91	0.17	153,153,153,153	0
85	MG	5	3662	1/1	0.91	0.23	36,36,36,36	0
85	MG	N6	201	1/1	0.91	0.30	51,51,51,51	0
86	OHX	5	4232	7/7	0.91	0.11	179,179,179,179	0
85	MG	5	3668	1/1	0.91	0.15	34,34,34,34	0
86	OHX	6	2116	7/7	0.91	0.15	145,145,145,145	0
86	OHX	1	4060	7/7	0.91	0.13	158,158,158,158	0
85	MG	6	1959	1/1	0.91	0.36	51,51,51,51	0
86	OHX	6	2131	7/7	0.91	0.13	149,149,149,149	0
86	OHX	6	2133	7/7	0.91	0.14	161,161,161,161	0
86	OHX	6	2134	7/7	0.91	0.15	134,134,134,134	0
85	MG	6	1960	1/1	0.91	0.30	40,40,40,40	0
85	MG	1	3533	1/1	0.91	0.13	38,38,38,38	0
86	OHX	6	2141	7/7	0.91	0.11	174,174,174,174	0
85	MG	2	2002	1/1	0.91	0.24	80,80,80,80	0
86	OHX	1	4071	7/7	0.91	0.23	113,113,113,113	0
85	MG	1	3499	1/1	0.91	0.30	63,63,63,63	0
85	MG	5	3886	1/1	0.91	0.30	57,57,57,57	0
86	OHX	6	2153	7/7	0.91	0.13	145,145,145,145	0
86	OHX	1	4080	7/7	0.91	0.14	144,144,144,144	0
86	OHX	6	2157	7/7	0.91	0.14	145,145,145,145	0
86	OHX	1	4086	7/7	0.91	0.18	133,133,133,133	0
86	OHX	7	225	7/7	0.91	0.20	127,127,127,127	0
85	MG	5	3684	1/1	0.91	0.08	35,35,35,35	0
85	MG	5	3889	1/1	0.91	0.29	65,65,65,65	0
86	OHX	6	2165	7/7	0.91	0.14	157,157,157,157	0
86	OHX	8	231	7/7	0.91	0.17	138,138,138,138	0
86	OHX	6	2166	7/7	0.91	0.11	189,189,189,189	0
85	MG	5	3891	1/1	0.91	0.17	38,38,38,38	0
86	OHX	1	4095	7/7	0.91	0.13	153,153,153,153	0
86	OHX	l5	304	7/7	0.91	0.15	148,148,148,148	0
86	OHX	1	4098	7/7	0.91	0.15	128,128,128,128	0
85	MG	1	3633	1/1	0.91	0.14	59,59,59,59	0
86	OHX	6	2172	7/7	0.91	0.17	155,155,155,155	0
85	MG	1	3442	1/1	0.91	0.24	30,30,30,30	0
86	OHX	1	4106	7/7	0.91	0.15	142,142,142,142	0
85	MG	5	3689	1/1	0.91	0.15	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3690	1/1	0.91	0.15	62,62,62,62	0
85	MG	5	3692	1/1	0.91	0.19	52,52,52,52	0
85	MG	1	3636	1/1	0.91	0.12	46,46,46,46	0
85	MG	6	1903	1/1	0.91	0.33	47,47,47,47	0
85	MG	c8	202	1/1	0.91	0.30	66,66,66,66	0
86	OHX	1	4118	7/7	0.91	0.19	123,123,123,123	0
85	MG	1	3681	1/1	0.92	0.11	50,50,50,50	0
85	MG	1	3829	1/1	0.92	0.30	37,37,37,37	0
85	MG	5	3729	1/1	0.92	0.26	31,31,31,31	0
85	MG	8	212	1/1	0.92	0.17	43,43,43,43	0
85	MG	1	3831	1/1	0.92	0.26	24,24,24,24	0
86	OHX	1	4136	7/7	0.92	0.17	133,133,133,133	0
85	MG	1	3832	1/1	0.92	0.29	62,62,62,62	0
85	MG	1	3542	1/1	0.92	0.23	35,35,35,35	0
85	MG	1	3419	1/1	0.92	0.22	48,48,48,48	0
85	MG	1	3841	1/1	0.92	0.23	45,45,45,45	0
86	OHX	6	2200	7/7	0.92	0.16	156,156,156,156	0
85	MG	1	3639	1/1	0.92	0.13	70,70,70,70	0
85	MG	5	3546	1/1	0.92	0.29	45,45,45,45	0
86	OHX	1	4143	7/7	0.92	0.18	122,122,122,122	0
85	MG	m7	201	1/1	0.92	0.30	32,32,32,32	0
85	MG	5	3751	1/1	0.92	0.21	48,48,48,48	0
85	MG	5	3547	1/1	0.92	0.30	46,46,46,46	0
86	OHX	1	4147	7/7	0.92	0.13	152,152,152,152	0
85	MG	6	1974	1/1	0.92	0.20	58,58,58,58	0
85	MG	n8	204	1/1	0.92	0.16	43,43,43,43	0
86	OHX	1	4152	7/7	0.92	0.18	137,137,137,137	0
86	OHX	5	4027	7/7	0.92	0.16	112,112,112,112	0
85	MG	2	1983	1/1	0.92	0.19	71,71,71,71	0
85	MG	2	2014	1/1	0.92	0.29	61,61,61,61	0
85	MG	1	3422	1/1	0.92	0.27	32,32,32,32	0
85	MG	1	3849	1/1	0.92	0.32	58,58,58,58	0
86	OHX	2	2089	7/7	0.92	0.15	138,138,138,138	0
86	OHX	5	4108	7/7	0.92	0.15	135,135,135,135	0
85	MG	1	3850	1/1	0.92	0.18	45,45,45,45	0
85	MG	5	3567	1/1	0.92	0.28	28,28,28,28	0
86	OHX	5	4116	7/7	0.92	0.12	159,159,159,159	0
85	MG	6	1980	1/1	0.92	0.22	71,71,71,71	0
86	OHX	5	4119	7/7	0.92	0.17	125,125,125,125	0
86	OHX	2	2104	7/7	0.92	0.13	156,156,156,156	0
86	OHX	5	4121	7/7	0.92	0.12	154,154,154,154	0
86	OHX	5	4128	7/7	0.92	0.15	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3425	1/1	0.92	0.14	49,49,49,49	0
85	MG	5	3779	1/1	0.92	0.21	53,53,53,53	0
85	MG	1	3766	1/1	0.92	0.24	61,61,61,61	0
85	MG	1	3857	1/1	0.92	0.27	46,46,46,46	0
85	MG	5	3573	1/1	0.92	0.24	31,31,31,31	0
86	OHX	2	2123	7/7	0.92	0.13	151,151,151,151	0
85	MG	5	3784	1/1	0.92	0.16	33,33,33,33	0
86	OHX	2	2126	7/7	0.92	0.15	135,135,135,135	0
86	OHX	5	4145	7/7	0.92	0.17	142,142,142,142	0
85	MG	6	1908	1/1	0.92	0.28	49,49,49,49	0
85	MG	5	3789	1/1	0.92	0.09	36,36,36,36	0
86	OHX	5	4151	7/7	0.92	0.19	125,125,125,125	0
85	MG	1	3701	1/1	0.92	0.26	50,50,50,50	0
86	OHX	2	2133	7/7	0.92	0.11	163,163,163,163	0
85	MG	5	3432	1/1	0.92	0.22	42,42,42,42	0
85	MG	1	3517	1/1	0.92	0.27	33,33,33,33	0
85	MG	5	3589	1/1	0.92	0.28	28,28,28,28	0
85	MG	5	3794	1/1	0.92	0.14	36,36,36,36	0
85	MG	6	1992	1/1	0.92	0.13	54,54,54,54	0
85	MG	1	3772	1/1	0.92	0.12	62,62,62,62	0
85	MG	5	3442	1/1	0.92	0.18	30,30,30,30	0
85	MG	5	3444	1/1	0.92	0.27	40,40,40,40	0
85	MG	6	1994	1/1	0.92	0.30	46,46,46,46	0
85	MG	5	3604	1/1	0.92	0.14	38,38,38,38	0
86	OHX	5	4167	7/7	0.92	0.16	134,134,134,134	0
85	MG	5	3606	1/1	0.92	0.14	38,38,38,38	0
85	MG	5	3449	1/1	0.92	0.22	33,33,33,33	0
86	OHX	1	4190	7/7	0.92	0.13	157,157,157,157	0
86	OHX	5	4171	7/7	0.92	0.10	190,190,190,190	0
85	MG	1	4218	1/1	0.92	0.15	74,74,74,74	0
86	OHX	5	4173	7/7	0.92	0.23	111,111,111,111	0
85	MG	1	3518	1/1	0.92	0.31	29,29,29,29	0
85	MG	1	3776	1/1	0.92	0.21	35,35,35,35	0
85	MG	1	3605	1/1	0.92	0.09	57,57,57,57	0
86	OHX	5	4179	7/7	0.92	0.18	119,119,119,119	0
85	MG	1	3607	1/1	0.92	0.29	78,78,78,78	0
86	OHX	1	4197	7/7	0.92	0.15	140,140,140,140	0
85	MG	3	207	1/1	0.92	0.28	70,70,70,70	0
85	MG	5	3465	1/1	0.92	0.14	36,36,36,36	0
85	MG	6	2002	1/1	0.92	0.13	75,75,75,75	0
86	OHX	5	4186	7/7	0.92	0.17	131,131,131,131	0
85	MG	5	3469	1/1	0.92	0.25	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3834	1/1	0.92	0.12	68,68,68,68	0
85	MG	1	3519	1/1	0.92	0.25	41,41,41,41	0
85	MG	1	3460	1/1	0.92	0.27	35,35,35,35	0
85	MG	1	3490	1/1	0.92	0.07	47,47,47,47	0
85	MG	1	3715	1/1	0.92	0.34	70,70,70,70	0
85	MG	5	3641	1/1	0.92	0.17	37,37,37,37	0
85	MG	1	3787	1/1	0.92	0.18	28,28,28,28	0
85	MG	2	2000	1/1	0.92	0.21	91,91,91,91	0
86	OHX	1	4210	7/7	0.92	0.20	135,135,135,135	0
85	MG	5	3646	1/1	0.92	0.14	55,55,55,55	0
85	MG	5	3647	1/1	0.92	0.25	38,38,38,38	0
85	MG	5	3648	1/1	0.92	0.34	54,54,54,54	0
86	OHX	3	221	7/7	0.92	0.12	150,150,150,150	0
86	OHX	3	222	7/7	0.92	0.18	131,131,131,131	0
86	OHX	5	4208	7/7	0.92	0.12	160,160,160,160	0
85	MG	1	3795	1/1	0.92	0.20	54,54,54,54	0
85	MG	1	3718	1/1	0.92	0.21	56,56,56,56	0
86	OHX	3	225	7/7	0.92	0.18	139,139,139,139	0
85	MG	6	2015	1/1	0.92	0.15	78,78,78,78	0
85	MG	4	210	1/1	0.92	0.22	58,58,58,58	0
85	MG	S2	302	1/1	0.92	0.32	66,66,66,66	0
86	OHX	5	4215	7/7	0.92	0.09	204,204,204,204	0
86	OHX	5	4216	7/7	0.92	0.17	152,152,152,152	0
85	MG	6	2022	1/1	0.92	0.12	57,57,57,57	0
85	MG	5	3660	1/1	0.92	0.17	30,30,30,30	0
86	OHX	L3	405	7/7	0.92	0.12	162,162,162,162	0
86	OHX	C5	201	7/7	0.92	0.11	179,179,179,179	0
86	OHX	D3	202	7/7	0.92	0.13	145,145,145,145	0
86	OHX	D9	102	7/7	0.92	0.14	153,153,153,153	0
86	OHX	1	4014	7/7	0.92	0.10	165,165,165,165	0
86	OHX	O3	202	7/7	0.92	0.17	126,126,126,126	0
86	OHX	6	2104	7/7	0.92	0.15	123,123,123,123	0
86	OHX	1	4025	7/7	0.92	0.17	125,125,125,125	0
86	OHX	1	4034	7/7	0.92	0.15	134,134,134,134	0
85	MG	2	1902	1/1	0.92	0.21	39,39,39,39	0
85	MG	1	3803	1/1	0.92	0.14	38,38,38,38	0
86	OHX	6	2127	7/7	0.92	0.14	132,132,132,132	0
85	MG	5	3882	1/1	0.92	0.18	32,32,32,32	0
85	MG	1	3436	1/1	0.92	0.23	43,43,43,43	0
85	MG	5	3885	1/1	0.92	0.21	34,34,34,34	0
85	MG	4	216	1/1	0.92	0.20	61,61,61,61	0
85	MG	5	3496	1/1	0.92	0.27	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4078	7/7	0.92	0.17	138,138,138,138	0
85	MG	5	3497	1/1	0.92	0.10	43,43,43,43	0
85	MG	5	3890	1/1	0.92	0.23	53,53,53,53	0
86	OHX	1	4081	7/7	0.92	0.17	136,136,136,136	0
86	OHX	1	4082	7/7	0.92	0.13	144,144,144,144	0
85	MG	2	1911	1/1	0.92	0.29	55,55,55,55	0
86	OHX	1	4088	7/7	0.92	0.14	141,141,141,141	0
85	MG	4	219	1/1	0.92	0.16	50,50,50,50	0
85	MG	1	3811	1/1	0.92	0.12	51,51,51,51	0
86	OHX	6	2162	7/7	0.92	0.14	137,137,137,137	0
85	MG	6	1947	1/1	0.92	0.29	52,52,52,52	0
85	MG	1	3579	1/1	0.92	0.33	40,40,40,40	0
85	MG	2	1935	1/1	0.92	0.36	50,50,50,50	0
86	OHX	5	4251	7/7	0.92	0.12	168,168,168,168	0
85	MG	L7	303	1/1	0.92	0.26	56,56,56,56	0
85	MG	1	3581	1/1	0.92	0.24	34,34,34,34	0
86	OHX	1	4103	7/7	0.92	0.17	133,133,133,133	0
85	MG	SM	301	1/1	0.92	0.15	57,57,57,57	0
85	MG	5	3514	1/1	0.92	0.20	39,39,39,39	0
85	MG	5	3700	1/1	0.92	0.09	40,40,40,40	0
85	MG	5	3705	1/1	0.92	0.05	41,41,41,41	0
85	MG	5	3708	1/1	0.92	0.29	48,48,48,48	0
85	MG	5	3515	1/1	0.92	0.23	32,32,32,32	0
86	OHX	6	2176	7/7	0.92	0.19	127,127,127,127	0
86	OHX	1	4115	7/7	0.92	0.14	144,144,144,144	0
85	MG	1	3819	1/1	0.92	0.11	45,45,45,45	0
85	MG	7	209	1/1	0.92	0.22	42,42,42,42	0
85	MG	7	210	1/1	0.92	0.17	64,64,64,64	0
85	MG	M5	301	1/1	0.92	0.10	48,48,48,48	0
86	OHX	1	4121	7/7	0.92	0.20	117,117,117,117	0
85	MG	5	3519	1/1	0.92	0.33	31,31,31,31	0
86	OHX	1	4125	7/7	0.92	0.14	156,156,156,156	0
85	MG	1	3501	1/1	0.92	0.33	27,27,27,27	0
85	MG	5	3521	1/1	0.92	0.28	35,35,35,35	0
85	MG	2	2011	1/1	0.92	0.30	63,63,63,63	0
85	MG	M7	203	1/1	0.92	0.09	40,40,40,40	0
85	MG	5	3851	1/1	0.93	0.27	58,58,58,58	0
85	MG	2	1987	1/1	0.93	0.25	72,72,72,72	0
86	OHX	sR	401	7/7	0.93	0.10	169,169,169,169	0
85	MG	5	3856	1/1	0.93	0.13	76,76,76,76	0
85	MG	5	3532	1/1	0.93	0.26	36,36,36,36	0
86	OHX	5	4036	7/7	0.93	0.12	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3683	1/1	0.93	0.12	36,36,36,36	0
86	OHX	5	4063	7/7	0.93	0.13	136,136,136,136	0
86	OHX	5	4075	7/7	0.93	0.18	128,128,128,128	0
86	OHX	5	4076	7/7	0.93	0.14	131,131,131,131	0
86	OHX	5	4087	7/7	0.93	0.14	131,131,131,131	0
86	OHX	5	4088	7/7	0.93	0.17	123,123,123,123	0
86	OHX	5	4089	7/7	0.93	0.21	120,120,120,120	0
86	OHX	5	4092	7/7	0.93	0.16	125,125,125,125	0
85	MG	4	202	1/1	0.93	0.30	49,49,49,49	0
85	MG	S2	301	1/1	0.93	0.33	52,52,52,52	0
85	MG	1	3429	1/1	0.93	0.42	42,42,42,42	0
85	MG	5	3688	1/1	0.93	0.16	46,46,46,46	0
86	OHX	5	4102	7/7	0.93	0.17	113,113,113,113	0
86	OHX	5	4103	7/7	0.93	0.10	158,158,158,158	0
86	OHX	5	4106	7/7	0.93	0.16	120,120,120,120	0
85	MG	1	3807	1/1	0.93	0.17	41,41,41,41	0
85	MG	1	3525	1/1	0.93	0.24	26,26,26,26	0
85	MG	5	3691	1/1	0.93	0.27	40,40,40,40	0
85	MG	1	3813	1/1	0.93	0.17	52,52,52,52	0
85	MG	1	3736	1/1	0.93	0.18	56,56,56,56	0
85	MG	1	3738	1/1	0.93	0.30	67,67,67,67	0
86	OHX	2	2164	7/7	0.93	0.12	172,172,172,172	0
86	OHX	2	2166	7/7	0.93	0.17	129,129,129,129	0
86	OHX	5	4123	7/7	0.93	0.13	141,141,141,141	0
85	MG	1	3745	1/1	0.93	0.12	56,56,56,56	0
86	OHX	2	2168	7/7	0.93	0.14	145,145,145,145	0
85	MG	5	3704	1/1	0.93	0.22	64,64,64,64	0
85	MG	5	3548	1/1	0.93	0.25	50,50,50,50	0
86	OHX	5	4134	7/7	0.93	0.14	136,136,136,136	0
86	OHX	5	4135	7/7	0.93	0.16	128,128,128,128	0
86	OHX	5	4137	7/7	0.93	0.18	135,135,135,135	0
85	MG	5	3439	1/1	0.93	0.24	41,41,41,41	0
85	MG	1	3683	1/1	0.93	0.17	52,52,52,52	0
85	MG	5	3713	1/1	0.93	0.12	43,43,43,43	0
85	MG	1	3553	1/1	0.93	0.27	36,36,36,36	0
85	MG	1	3554	1/1	0.93	0.31	25,25,25,25	0
85	MG	5	3445	1/1	0.93	0.07	40,40,40,40	0
85	MG	5	3721	1/1	0.93	0.12	56,56,56,56	0
85	MG	1	3641	1/1	0.93	0.19	44,44,44,44	0
86	OHX	5	4149	7/7	0.93	0.13	136,136,136,136	0
86	OHX	5	4150	7/7	0.93	0.13	153,153,153,153	0
85	MG	1	3469	1/1	0.93	0.30	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4152	7/7	0.93	0.12	158,158,158,158	0
86	OHX	C3	201	7/7	0.93	0.10	179,179,179,179	0
85	MG	1	3756	1/1	0.93	0.09	52,52,52,52	0
85	MG	1	3830	1/1	0.93	0.24	37,37,37,37	0
85	MG	1	3695	1/1	0.93	0.19	47,47,47,47	0
86	OHX	1	3950	7/7	0.93	0.18	109,109,109,109	0
86	OHX	1	3963	7/7	0.93	0.13	124,124,124,124	0
86	OHX	1	3994	7/7	0.93	0.14	171,171,171,171	0
85	MG	5	3458	1/1	0.93	0.14	35,35,35,35	0
86	OHX	1	4016	7/7	0.93	0.14	140,140,140,140	0
86	OHX	1	4018	7/7	0.93	0.14	129,129,129,129	0
85	MG	5	3461	1/1	0.93	0.30	53,53,53,53	0
85	MG	1	3763	1/1	0.93	0.12	43,43,43,43	0
86	OHX	1	4044	7/7	0.93	0.17	120,120,120,120	0
86	OHX	1	4056	7/7	0.93	0.17	125,125,125,125	0
85	MG	5	3577	1/1	0.93	0.25	38,38,38,38	0
85	MG	1	3407	1/1	0.93	0.24	39,39,39,39	0
85	MG	6	2016	1/1	0.93	0.17	30,30,30,30	0
86	OHX	1	4065	7/7	0.93	0.17	123,123,123,123	0
85	MG	6	2018	1/1	0.93	0.11	59,59,59,59	0
85	MG	M3	203	1/1	0.93	0.13	33,33,33,33	0
86	OHX	1	4069	7/7	0.93	0.13	140,140,140,140	0
85	MG	5	3746	1/1	0.93	0.12	66,66,66,66	0
86	OHX	3	226	7/7	0.93	0.15	149,149,149,149	0
86	OHX	1	4073	7/7	0.93	0.14	135,135,135,135	0
85	MG	1	3645	1/1	0.93	0.23	42,42,42,42	0
86	OHX	1	4076	7/7	0.93	0.17	129,129,129,129	0
85	MG	6	2021	1/1	0.93	0.25	62,62,62,62	0
85	MG	2	1916	1/1	0.93	0.23	54,54,54,54	0
85	MG	5	3599	1/1	0.93	0.15	46,46,46,46	0
85	MG	8	201	1/1	0.93	0.13	52,52,52,52	0
86	OHX	M0	303	7/7	0.93	0.13	124,124,124,124	0
85	MG	6	2023	1/1	0.93	0.28	48,48,48,48	0
86	OHX	1	4083	7/7	0.93	0.14	137,137,137,137	0
86	OHX	1	4085	7/7	0.93	0.14	142,142,142,142	0
86	OHX	5	4192	7/7	0.93	0.15	132,132,132,132	0
85	MG	5	3760	1/1	0.93	0.14	57,57,57,57	0
85	MG	1	3488	1/1	0.93	0.17	35,35,35,35	0
86	OHX	5	4195	7/7	0.93	0.11	176,176,176,176	0
86	OHX	1	4090	7/7	0.93	0.17	128,128,128,128	0
85	MG	1	3561	1/1	0.93	0.29	25,25,25,25	0
85	MG	8	209	1/1	0.93	0.17	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4200	7/7	0.93	0.15	124,124,124,124	0
86	OHX	5	4202	7/7	0.93	0.17	129,129,129,129	0
86	OHX	6	2124	7/7	0.93	0.15	141,141,141,141	0
85	MG	5	3764	1/1	0.93	0.31	45,45,45,45	0
85	MG	5	3477	1/1	0.93	0.24	56,56,56,56	0
86	OHX	1	4096	7/7	0.93	0.12	159,159,159,159	0
86	OHX	6	2132	7/7	0.93	0.16	133,133,133,133	0
85	MG	1	3510	1/1	0.93	0.25	34,34,34,34	0
85	MG	5	3609	1/1	0.93	0.25	31,31,31,31	0
86	OHX	6	2135	7/7	0.93	0.12	145,145,145,145	0
86	OHX	1	4100	7/7	0.93	0.14	145,145,145,145	0
85	MG	5	3775	1/1	0.93	0.23	30,30,30,30	0
86	OHX	6	2140	7/7	0.93	0.15	138,138,138,138	0
85	MG	1	3473	1/1	0.93	0.27	32,32,32,32	0
86	OHX	6	2143	7/7	0.93	0.12	154,154,154,154	0
85	MG	1	3775	1/1	0.93	0.11	55,55,55,55	0
86	OHX	1	4107	7/7	0.93	0.14	132,132,132,132	0
86	OHX	6	2150	7/7	0.93	0.17	125,125,125,125	0
85	MG	6	2033	1/1	0.93	0.33	64,64,64,64	0
86	OHX	1	4109	7/7	0.93	0.18	123,123,123,123	0
85	MG	5	3620	1/1	0.93	0.10	41,41,41,41	0
85	MG	m5	303	1/1	0.93	0.20	57,57,57,57	0
86	OHX	6	2156	7/7	0.93	0.18	144,144,144,144	0
85	MG	m5	304	1/1	0.93	0.19	108,108,108,108	0
85	MG	5	3482	1/1	0.93	0.28	29,29,29,29	0
86	OHX	6	2160	7/7	0.93	0.15	133,133,133,133	0
85	MG	5	3625	1/1	0.93	0.23	39,39,39,39	0
85	MG	1	3564	1/1	0.93	0.18	38,38,38,38	0
85	MG	1	3777	1/1	0.93	0.15	66,66,66,66	0
85	MG	1	3569	1/1	0.93	0.21	26,26,26,26	0
85	MG	N8	201	1/1	0.93	0.09	31,31,31,31	0
85	MG	1	3514	1/1	0.93	0.29	37,37,37,37	0
86	OHX	1	4122	7/7	0.93	0.14	146,146,146,146	0
86	OHX	1	4123	7/7	0.93	0.12	153,153,153,153	0
85	MG	1	3617	1/1	0.93	0.21	45,45,45,45	0
85	MG	5	3636	1/1	0.93	0.13	54,54,54,54	0
85	MG	1	3474	1/1	0.93	0.22	23,23,23,23	0
85	MG	1	3401	1/1	0.93	0.27	38,38,38,38	0
85	MG	1	4216	1/1	0.93	0.17	48,48,48,48	0
85	MG	6	1901	1/1	0.93	0.32	42,42,42,42	0
85	MG	5	3804	1/1	0.93	0.14	42,42,42,42	0
86	OHX	2	2105	7/7	0.93	0.10	206,206,206,206	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3621	1/1	0.93	0.11	43,43,43,43	0
85	MG	1	3786	1/1	0.93	0.16	36,36,36,36	0
85	MG	6	1972	1/1	0.93	0.18	53,53,53,53	0
86	OHX	2	2118	7/7	0.93	0.14	149,149,149,149	0
86	OHX	2	2119	7/7	0.93	0.12	165,165,165,165	0
85	MG	1	3622	1/1	0.93	0.23	49,49,49,49	0
85	MG	2	1932	1/1	0.93	0.20	59,59,59,59	0
85	MG	5	3505	1/1	0.93	0.26	26,26,26,26	0
85	MG	5	3813	1/1	0.93	0.18	42,42,42,42	0
85	MG	1	3790	1/1	0.93	0.16	60,60,60,60	0
86	OHX	2	2127	7/7	0.93	0.14	142,142,142,142	0
85	MG	3	206	1/1	0.93	0.28	36,36,36,36	0
85	MG	1	3544	1/1	0.93	0.27	34,34,34,34	0
85	MG	1	3796	1/1	0.93	0.30	39,39,39,39	0
85	MG	1	3477	1/1	0.93	0.32	52,52,52,52	0
85	MG	1	3413	1/1	0.93	0.24	47,47,47,47	0
86	OHX	l5	303	7/7	0.93	0.11	147,147,147,147	0
85	MG	5	3661	1/1	0.93	0.14	46,46,46,46	0
86	OHX	1	4151	7/7	0.93	0.15	139,139,139,139	0
85	MG	6	1916	1/1	0.93	0.21	52,52,52,52	0
85	MG	1	3672	1/1	0.93	0.26	49,49,49,49	0
85	MG	6	1987	1/1	0.93	0.09	48,48,48,48	0
85	MG	5	3839	1/1	0.93	0.20	39,39,39,39	0
85	MG	5	3843	1/1	0.93	0.11	42,42,42,42	0
85	MG	5	3669	1/1	0.93	0.09	33,33,33,33	0
86	OHX	s4	301	7/7	0.93	0.13	149,149,149,149	0
85	MG	6	1918	1/1	0.93	0.34	64,64,64,64	0
85	MG	6	1919	1/1	0.93	0.30	43,43,43,43	0
85	MG	5	3417	1/1	0.93	0.24	29,29,29,29	0
88	ZN	Q2	501	1/1	0.93	0.24	92,92,92,92	0
85	MG	5	3680	1/1	0.93	0.22	52,52,52,52	0
85	MG	6	1942	1/1	0.94	0.20	32,32,32,32	0
85	MG	L7	302	1/1	0.94	0.09	42,42,42,42	0
86	OHX	2	2115	7/7	0.94	0.12	164,164,164,164	0
86	OHX	c8	203	7/7	0.94	0.10	153,153,153,153	0
85	MG	6	2024	1/1	0.94	0.17	66,66,66,66	0
85	MG	1	3541	1/1	0.94	0.24	27,27,27,27	0
85	MG	5	3617	1/1	0.94	0.17	35,35,35,35	0
86	OHX	5	3996	7/7	0.94	0.13	115,115,115,115	0
86	OHX	5	4000	7/7	0.94	0.14	117,117,117,117	0
85	MG	1	3426	1/1	0.94	0.15	59,59,59,59	0
85	MG	5	3619	1/1	0.94	0.26	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4032	7/7	0.94	0.15	119,119,119,119	0
85	MG	1	3565	1/1	0.94	0.32	29,29,29,29	0
86	OHX	5	4037	7/7	0.94	0.12	125,125,125,125	0
86	OHX	5	4041	7/7	0.94	0.13	164,164,164,164	0
86	OHX	5	4042	7/7	0.94	0.12	138,138,138,138	0
86	OHX	5	4051	7/7	0.94	0.14	117,117,117,117	0
86	OHX	1	4150	7/7	0.94	0.14	120,120,120,120	0
86	OHX	2	2124	7/7	0.94	0.14	145,145,145,145	0
86	OHX	5	4070	7/7	0.94	0.14	135,135,135,135	0
86	OHX	5	4071	7/7	0.94	0.14	137,137,137,137	0
86	OHX	5	4073	7/7	0.94	0.14	122,122,122,122	0
85	MG	1	3611	1/1	0.94	0.07	43,43,43,43	0
85	MG	5	3624	1/1	0.94	0.26	46,46,46,46	0
86	OHX	5	4079	7/7	0.94	0.14	139,139,139,139	0
86	OHX	5	4084	7/7	0.94	0.11	144,144,144,144	0
85	MG	1	3833	1/1	0.94	0.25	30,30,30,30	0
85	MG	6	2032	1/1	0.94	0.11	51,51,51,51	0
86	OHX	2	2129	7/7	0.94	0.12	149,149,149,149	0
85	MG	1	3457	1/1	0.94	0.13	27,27,27,27	0
86	OHX	5	4095	7/7	0.94	0.13	128,128,128,128	0
85	MG	5	3801	1/1	0.94	0.17	78,78,78,78	0
85	MG	5	3803	1/1	0.94	0.06	40,40,40,40	0
86	OHX	5	4098	7/7	0.94	0.13	144,144,144,144	0
85	MG	1	3441	1/1	0.94	0.23	46,46,46,46	0
86	OHX	5	4100	7/7	0.94	0.13	136,136,136,136	0
85	MG	1	3706	1/1	0.94	0.14	63,63,63,63	0
85	MG	5	3806	1/1	0.94	0.11	53,53,53,53	0
85	MG	5	3484	1/1	0.94	0.11	51,51,51,51	0
86	OHX	5	4105	7/7	0.94	0.18	111,111,111,111	0
85	MG	1	3771	1/1	0.94	0.20	52,52,52,52	0
85	MG	M7	204	1/1	0.94	0.10	66,66,66,66	0
85	MG	1	3459	1/1	0.94	0.31	62,62,62,62	0
85	MG	1	3845	1/1	0.94	0.31	53,53,53,53	0
86	OHX	5	4114	7/7	0.94	0.16	124,124,124,124	0
86	OHX	5	4115	7/7	0.94	0.16	125,125,125,125	0
85	MG	5	3492	1/1	0.94	0.16	47,47,47,47	0
85	MG	5	3493	1/1	0.94	0.10	45,45,45,45	0
85	MG	5	3642	1/1	0.94	0.24	54,54,54,54	0
85	MG	1	3655	1/1	0.94	0.17	41,41,41,41	0
85	MG	1	3577	1/1	0.94	0.29	25,25,25,25	0
85	MG	N3	201	1/1	0.94	0.19	33,33,33,33	0
86	OHX	5	4124	7/7	0.94	0.12	157,157,157,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4125	7/7	0.94	0.11	154,154,154,154	0
85	MG	1	3713	1/1	0.94	0.10	46,46,46,46	0
86	OHX	2	2151	7/7	0.94	0.14	154,154,154,154	0
85	MG	5	3829	1/1	0.94	0.26	36,36,36,36	0
85	MG	s1	301	1/1	0.94	0.20	78,78,78,78	0
85	MG	1	3522	1/1	0.94	0.30	33,33,33,33	0
85	MG	2	1981	1/1	0.94	0.34	62,62,62,62	0
86	OHX	5	4136	7/7	0.94	0.12	140,140,140,140	0
85	MG	5	3836	1/1	0.94	0.08	39,39,39,39	0
85	MG	5	3501	1/1	0.94	0.16	44,44,44,44	0
85	MG	6	1969	1/1	0.94	0.20	54,54,54,54	0
85	MG	5	3841	1/1	0.94	0.08	59,59,59,59	0
85	MG	5	3655	1/1	0.94	0.25	66,66,66,66	0
85	MG	N8	202	1/1	0.94	0.17	32,32,32,32	0
86	OHX	5	4144	7/7	0.94	0.15	123,123,123,123	0
85	MG	1	3463	1/1	0.94	0.29	25,25,25,25	0
85	MG	5	3658	1/1	0.94	0.21	47,47,47,47	0
85	MG	5	3659	1/1	0.94	0.18	49,49,49,49	0
86	OHX	2	2165	7/7	0.94	0.10	167,167,167,167	0
85	MG	1	3549	1/1	0.94	0.16	29,29,29,29	0
85	MG	5	3849	1/1	0.94	0.10	54,54,54,54	0
85	MG	5	3507	1/1	0.94	0.29	27,27,27,27	0
85	MG	2	2009	1/1	0.94	0.28	50,50,50,50	0
85	MG	5	3663	1/1	0.94	0.32	48,48,48,48	0
85	MG	5	3511	1/1	0.94	0.18	34,34,34,34	0
85	MG	5	3665	1/1	0.94	0.12	58,58,58,58	0
85	MG	1	3859	1/1	0.94	0.22	131,131,131,131	0
85	MG	1	3783	1/1	0.94	0.13	51,51,51,51	0
85	MG	2	1955	1/1	0.94	0.25	54,54,54,54	0
85	MG	1	3588	1/1	0.94	0.25	31,31,31,31	0
85	MG	1	3723	1/1	0.94	0.08	43,43,43,43	0
86	OHX	5	4163	7/7	0.94	0.16	123,123,123,123	0
85	MG	5	3870	1/1	0.94	0.22	39,39,39,39	0
85	MG	5	3405	1/1	0.94	0.18	32,32,32,32	0
85	MG	5	3874	1/1	0.94	0.40	54,54,54,54	0
85	MG	5	3518	1/1	0.94	0.23	26,26,26,26	0
85	MG	1	3630	1/1	0.94	0.15	36,36,36,36	0
85	MG	5	3408	1/1	0.94	0.13	33,33,33,33	0
85	MG	5	3879	1/1	0.94	0.18	42,42,42,42	0
85	MG	1	3788	1/1	0.94	0.12	68,68,68,68	0
86	OHX	1	3980	7/7	0.94	0.14	112,112,112,112	0
85	MG	5	3881	1/1	0.94	0.15	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4175	7/7	0.94	0.16	133,133,133,133	0
86	OHX	1	3998	7/7	0.94	0.16	120,120,120,120	0
86	OHX	1	4006	7/7	0.94	0.15	128,128,128,128	0
86	OHX	1	4009	7/7	0.94	0.12	136,136,136,136	0
86	OHX	4	231	7/7	0.94	0.12	124,124,124,124	0
86	OHX	4	232	7/7	0.94	0.11	147,147,147,147	0
85	MG	1	3631	1/1	0.94	0.07	40,40,40,40	0
85	MG	3	202	1/1	0.94	0.11	46,46,46,46	0
85	MG	1	3552	1/1	0.94	0.37	31,31,31,31	0
86	OHX	1	4021	7/7	0.94	0.10	153,153,153,153	0
85	MG	5	3529	1/1	0.94	0.24	29,29,29,29	0
86	OHX	1	4027	7/7	0.94	0.12	141,141,141,141	0
86	OHX	1	4029	7/7	0.94	0.14	138,138,138,138	0
85	MG	3	204	1/1	0.94	0.37	57,57,57,57	0
86	OHX	1	4042	7/7	0.94	0.15	117,117,117,117	0
86	OHX	1	4043	7/7	0.94	0.14	117,117,117,117	0
85	MG	1	3445	1/1	0.94	0.20	46,46,46,46	0
86	OHX	1	4048	7/7	0.94	0.15	125,125,125,125	0
86	OHX	6	2094	7/7	0.94	0.13	135,135,135,135	0
86	OHX	1	4053	7/7	0.94	0.19	119,119,119,119	0
85	MG	5	3534	1/1	0.94	0.23	36,36,36,36	0
86	OHX	6	2107	7/7	0.94	0.14	120,120,120,120	0
85	MG	5	3536	1/1	0.94	0.30	41,41,41,41	0
86	OHX	6	2118	7/7	0.94	0.12	143,143,143,143	0
85	MG	1	3731	1/1	0.94	0.19	59,59,59,59	0
85	MG	6	1915	1/1	0.94	0.24	53,53,53,53	0
86	OHX	6	2125	7/7	0.94	0.14	142,142,142,142	0
85	MG	5	3701	1/1	0.94	0.12	63,63,63,63	0
85	MG	5	3703	1/1	0.94	0.10	65,65,65,65	0
85	MG	1	3675	1/1	0.94	0.29	60,60,60,60	0
85	MG	5	3541	1/1	0.94	0.27	34,34,34,34	0
86	OHX	1	4070	7/7	0.94	0.13	152,152,152,152	0
85	MG	5	3426	1/1	0.94	0.16	38,38,38,38	0
85	MG	1	3447	1/1	0.94	0.25	47,47,47,47	0
86	OHX	1	4074	7/7	0.94	0.14	134,134,134,134	0
85	MG	5	3712	1/1	0.94	0.17	90,90,90,90	0
85	MG	1	3800	1/1	0.94	0.11	56,56,56,56	0
85	MG	1	3531	1/1	0.94	0.21	24,24,24,24	0
85	MG	5	3717	1/1	0.94	0.19	52,52,52,52	0
86	OHX	6	2145	7/7	0.94	0.12	139,139,139,139	0
85	MG	3	213	1/1	0.94	0.31	58,58,58,58	0
85	MG	5	3434	1/1	0.94	0.16	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3434	1/1	0.94	0.08	49,49,49,49	0
85	MG	1	3472	1/1	0.94	0.07	38,38,38,38	0
85	MG	5	3552	1/1	0.94	0.17	45,45,45,45	0
85	MG	1	3739	1/1	0.94	0.13	49,49,49,49	0
85	MG	4	206	1/1	0.94	0.30	36,36,36,36	0
85	MG	5	3556	1/1	0.94	0.22	42,42,42,42	0
85	MG	1	3744	1/1	0.94	0.13	39,39,39,39	0
85	MG	5	3560	1/1	0.94	0.30	36,36,36,36	0
85	MG	5	3730	1/1	0.94	0.13	52,52,52,52	0
86	OHX	6	2161	7/7	0.94	0.15	129,129,129,129	0
85	MG	1	3810	1/1	0.94	0.24	44,44,44,44	0
85	MG	2	2004	1/1	0.94	0.20	87,87,87,87	0
85	MG	8	208	1/1	0.94	0.15	45,45,45,45	0
85	MG	5	3448	1/1	0.94	0.23	52,52,52,52	0
85	MG	5	3735	1/1	0.94	0.09	42,42,42,42	0
85	MG	1	3640	1/1	0.94	0.24	42,42,42,42	0
86	OHX	1	4102	7/7	0.94	0.14	130,130,130,130	0
85	MG	5	3450	1/1	0.94	0.24	38,38,38,38	0
86	OHX	6	2170	7/7	0.94	0.18	119,119,119,119	0
85	MG	13	401	1/1	0.94	0.35	27,27,27,27	0
85	MG	5	3744	1/1	0.94	0.25	42,42,42,42	0
85	MG	5	3451	1/1	0.94	0.12	33,33,33,33	0
85	MG	1	3600	1/1	0.94	0.20	30,30,30,30	0
85	MG	17	301	1/1	0.94	0.24	47,47,47,47	0
85	MG	1	3690	1/1	0.94	0.13	40,40,40,40	0
85	MG	18	301	1/1	0.94	0.33	73,73,73,73	0
86	OHX	1	4113	7/7	0.94	0.15	131,131,131,131	0
85	MG	5	3455	1/1	0.94	0.20	43,43,43,43	0
85	MG	5	3578	1/1	0.94	0.36	37,37,37,37	0
85	MG	m5	302	1/1	0.94	0.13	60,60,60,60	0
86	OHX	7	222	7/7	0.94	0.12	140,140,140,140	0
86	OHX	7	223	7/7	0.94	0.15	122,122,122,122	0
85	MG	5	3755	1/1	0.94	0.20	58,58,58,58	0
85	MG	1	3750	1/1	0.94	0.16	60,60,60,60	0
85	MG	m6	201	1/1	0.94	0.14	36,36,36,36	0
85	MG	1	3751	1/1	0.94	0.09	44,44,44,44	0
85	MG	5	3459	1/1	0.94	0.20	41,41,41,41	0
86	OHX	8	230	7/7	0.94	0.12	150,150,150,150	0
85	MG	5	3460	1/1	0.94	0.22	33,33,33,33	0
85	MG	1	3752	1/1	0.94	0.17	31,31,31,31	0
86	OHX	13	404	7/7	0.94	0.13	143,143,143,143	0
85	MG	5	3592	1/1	0.94	0.21	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	5	3765	1/1	0.94	0.07	60,60,60,60	0
85	MG	5	3767	1/1	0.94	0.11	45,45,45,45	0
85	MG	5	3593	1/1	0.94	0.26	29,29,29,29	0
85	MG	1	3823	1/1	0.94	0.11	45,45,45,45	0
86	OHX	2	2076	7/7	0.94	0.13	152,152,152,152	0
86	OHX	2	2081	7/7	0.94	0.12	161,161,161,161	0
86	OHX	2	2082	7/7	0.94	0.14	138,138,138,138	0
86	OHX	6	2197	7/7	0.94	0.14	148,148,148,148	0
85	MG	6	2017	1/1	0.94	0.28	47,47,47,47	0
85	MG	1	3601	1/1	0.94	0.25	31,31,31,31	0
86	OHX	1	4135	7/7	0.94	0.14	115,115,115,115	0
85	MG	1	3492	1/1	0.94	0.20	69,69,69,69	0
85	MG	L4	401	1/1	0.94	0.13	68,68,68,68	0
87	PCY	6	2204	40/40	0.94	0.11	59,59,59,59	0
85	MG	5	3468	1/1	0.94	0.33	46,46,46,46	0
85	MG	1	3412	1/1	0.94	0.14	36,36,36,36	0
86	OHX	2	2107	7/7	0.94	0.13	140,140,140,140	0
88	ZN	q2	501	1/1	0.94	0.26	95,95,95,95	0
85	MG	1	3575	1/1	0.95	0.24	28,28,28,28	0
85	MG	1	4219	1/1	0.95	0.26	39,39,39,39	0
85	MG	1	3576	1/1	0.95	0.19	28,28,28,28	0
85	MG	o3	201	1/1	0.95	0.17	37,37,37,37	0
85	MG	5	3771	1/1	0.95	0.18	71,71,71,71	0
85	MG	1	4221	1/1	0.95	0.23	40,40,40,40	0
85	MG	5	3603	1/1	0.95	0.17	42,42,42,42	0
85	MG	q3	503	1/1	0.95	0.11	63,63,63,63	0
86	OHX	2	2041	7/7	0.95	0.14	103,103,103,103	0
86	OHX	2	2064	7/7	0.95	0.10	137,137,137,137	0
85	MG	1	3440	1/1	0.95	0.24	41,41,41,41	0
86	OHX	5	3994	7/7	0.95	0.31	105,105,105,105	0
86	OHX	2	2077	7/7	0.95	0.14	141,141,141,141	0
86	OHX	2	2079	7/7	0.95	0.11	135,135,135,135	0
86	OHX	2	2080	7/7	0.95	0.14	130,130,130,130	0
86	OHX	5	4021	7/7	0.95	0.14	107,107,107,107	0
86	OHX	5	4023	7/7	0.95	0.12	115,115,115,115	0
86	OHX	5	4026	7/7	0.95	0.15	116,116,116,116	0
85	MG	5	3777	1/1	0.95	0.23	61,61,61,61	0
85	MG	5	3605	1/1	0.95	0.07	31,31,31,31	0
85	MG	5	3466	1/1	0.95	0.10	37,37,37,37	0
85	MG	5	3607	1/1	0.95	0.22	51,51,51,51	0
86	OHX	5	4040	7/7	0.95	0.12	132,132,132,132	0
85	MG	6	2010	1/1	0.95	0.26	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	2	2098	7/7	0.95	0.09	174,174,174,174	0
86	OHX	5	4043	7/7	0.95	0.14	122,122,122,122	0
86	OHX	5	4045	7/7	0.95	0.13	130,130,130,130	0
85	MG	6	1913	1/1	0.95	0.26	36,36,36,36	0
86	OHX	5	4052	7/7	0.95	0.14	115,115,115,115	0
86	OHX	5	4054	7/7	0.95	0.12	115,115,115,115	0
86	OHX	5	4057	7/7	0.95	0.11	137,137,137,137	0
86	OHX	5	4061	7/7	0.95	0.14	116,116,116,116	0
86	OHX	2	2102	7/7	0.95	0.11	148,148,148,148	0
85	MG	5	3783	1/1	0.95	0.20	60,60,60,60	0
86	OHX	5	4068	7/7	0.95	0.14	117,117,117,117	0
86	OHX	5	4069	7/7	0.95	0.10	143,143,143,143	0
85	MG	1	3578	1/1	0.95	0.33	34,34,34,34	0
86	OHX	2	2106	7/7	0.95	0.12	127,127,127,127	0
85	MG	5	3785	1/1	0.95	0.08	35,35,35,35	0
86	OHX	5	4074	7/7	0.95	0.12	125,125,125,125	0
85	MG	1	3620	1/1	0.95	0.32	45,45,45,45	0
85	MG	5	3616	1/1	0.95	0.13	49,49,49,49	0
86	OHX	2	2114	7/7	0.95	0.12	138,138,138,138	0
86	OHX	5	4080	7/7	0.95	0.12	122,122,122,122	0
86	OHX	5	4082	7/7	0.95	0.15	114,114,114,114	0
85	MG	6	2014	1/1	0.95	0.15	48,48,48,48	0
86	OHX	5	4086	7/7	0.95	0.13	132,132,132,132	0
85	MG	1	3496	1/1	0.95	0.15	38,38,38,38	0
85	MG	5	3473	1/1	0.95	0.19	43,43,43,43	0
85	MG	2	1995	1/1	0.95	0.27	49,49,49,49	0
85	MG	3	205	1/1	0.95	0.21	37,37,37,37	0
85	MG	5	3795	1/1	0.95	0.16	43,43,43,43	0
86	OHX	1	4153	7/7	0.95	0.15	139,139,139,139	0
86	OHX	2	2122	7/7	0.95	0.11	156,156,156,156	0
85	MG	5	3623	1/1	0.95	0.15	66,66,66,66	0
85	MG	5	3476	1/1	0.95	0.14	32,32,32,32	0
85	MG	1	3671	1/1	0.95	0.30	50,50,50,50	0
85	MG	1	3737	1/1	0.95	0.15	52,52,52,52	0
85	MG	5	3802	1/1	0.95	0.07	47,47,47,47	0
85	MG	5	3627	1/1	0.95	0.23	64,64,64,64	0
86	OHX	5	4104	7/7	0.95	0.12	140,140,140,140	0
85	MG	1	3623	1/1	0.95	0.23	56,56,56,56	0
85	MG	5	3630	1/1	0.95	0.10	41,41,41,41	0
86	OHX	5	4107	7/7	0.95	0.14	130,130,130,130	0
85	MG	1	3427	1/1	0.95	0.17	43,43,43,43	0
85	MG	2	2013	1/1	0.95	0.15	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3806	1/1	0.95	0.10	56,56,56,56	0
86	OHX	5	4112	7/7	0.95	0.14	135,135,135,135	0
86	OHX	5	4113	7/7	0.95	0.18	117,117,117,117	0
85	MG	1	3627	1/1	0.95	0.09	41,41,41,41	0
85	MG	6	2025	1/1	0.95	0.11	88,88,88,88	0
85	MG	1	3403	1/1	0.95	0.26	37,37,37,37	0
86	OHX	5	4117	7/7	0.95	0.16	110,110,110,110	0
85	MG	4	201	1/1	0.95	0.30	43,43,43,43	0
85	MG	1	3585	1/1	0.95	0.35	51,51,51,51	0
85	MG	4	203	1/1	0.95	0.30	45,45,45,45	0
86	OHX	2	2141	7/7	0.95	0.10	169,169,169,169	0
86	OHX	5	4122	7/7	0.95	0.12	150,150,150,150	0
85	MG	4	204	1/1	0.95	0.25	37,37,37,37	0
85	MG	1	3465	1/1	0.95	0.27	57,57,57,57	0
85	MG	1	3526	1/1	0.95	0.24	26,26,26,26	0
86	OHX	5	4127	7/7	0.95	0.12	134,134,134,134	0
85	MG	5	3645	1/1	0.95	0.14	40,40,40,40	0
85	MG	4	207	1/1	0.95	0.23	41,41,41,41	0
86	OHX	5	4131	7/7	0.95	0.13	121,121,121,121	0
85	MG	1	3404	1/1	0.95	0.35	54,54,54,54	0
85	MG	1	3816	1/1	0.95	0.09	38,38,38,38	0
85	MG	5	3833	1/1	0.95	0.17	52,52,52,52	0
85	MG	6	1937	1/1	0.95	0.31	41,41,41,41	0
85	MG	6	1938	1/1	0.95	0.16	45,45,45,45	0
85	MG	1	3503	1/1	0.95	0.27	30,30,30,30	0
85	MG	6	2040	1/1	0.95	0.28	53,53,53,53	0
85	MG	5	3840	1/1	0.95	0.19	47,47,47,47	0
85	MG	1	3504	1/1	0.95	0.29	36,36,36,36	0
85	MG	6	2043	1/1	0.95	0.26	50,50,50,50	0
85	MG	2	1998	1/1	0.95	0.16	109,109,109,109	0
86	OHX	5	4143	7/7	0.95	0.13	140,140,140,140	0
86	OHX	1	4192	7/7	0.95	0.10	178,178,178,178	0
85	MG	1	3820	1/1	0.95	0.09	53,53,53,53	0
86	OHX	5	4146	7/7	0.95	0.15	126,126,126,126	0
85	MG	1	3821	1/1	0.95	0.09	40,40,40,40	0
85	MG	6	1944	1/1	0.95	0.34	59,59,59,59	0
85	MG	5	3510	1/1	0.95	0.25	26,26,26,26	0
85	MG	1	3532	1/1	0.95	0.26	37,37,37,37	0
85	MG	1	3758	1/1	0.95	0.19	61,61,61,61	0
85	MG	5	3854	1/1	0.95	0.14	66,66,66,66	0
85	MG	1	3594	1/1	0.95	0.27	24,24,24,24	0
85	MG	1	3596	1/1	0.95	0.31	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	5	4155	7/7	0.95	0.14	128,128,128,128	0
85	MG	5	3667	1/1	0.95	0.14	51,51,51,51	0
85	MG	4	221	1/1	0.95	0.14	67,67,67,67	0
85	MG	L3	401	1/1	0.95	0.18	39,39,39,39	0
85	MG	5	3673	1/1	0.95	0.29	32,32,32,32	0
85	MG	5	3861	1/1	0.95	0.33	60,60,60,60	0
85	MG	5	3863	1/1	0.95	0.09	42,42,42,42	0
85	MG	1	3828	1/1	0.95	0.06	37,37,37,37	0
85	MG	d6	102	1/1	0.95	0.13	53,53,53,53	0
85	MG	1	3558	1/1	0.95	0.26	27,27,27,27	0
85	MG	L4	402	1/1	0.95	0.08	36,36,36,36	0
85	MG	5	3871	1/1	0.95	0.12	48,48,48,48	0
85	MG	1	3449	1/1	0.95	0.11	43,43,43,43	0
86	OHX	3	216	7/7	0.95	0.14	117,117,117,117	0
86	OHX	3	220	7/7	0.95	0.12	138,138,138,138	0
85	MG	1	3508	1/1	0.95	0.25	20,20,20,20	0
85	MG	1	3644	1/1	0.95	0.13	70,70,70,70	0
85	MG	1	3768	1/1	0.95	0.10	43,43,43,43	0
85	MG	5	3528	1/1	0.95	0.20	33,33,33,33	0
86	OHX	1	3925	7/7	0.95	0.15	104,104,104,104	0
86	OHX	1	3949	7/7	0.95	0.13	115,115,115,115	0
85	MG	M0	301	1/1	0.95	0.17	48,48,48,48	0
86	OHX	1	3960	7/7	0.95	0.14	103,103,103,103	0
85	MG	1	3834	1/1	0.95	0.26	43,43,43,43	0
86	OHX	1	3974	7/7	0.95	0.20	99,99,99,99	0
86	OHX	1	3977	7/7	0.95	0.13	117,117,117,117	0
85	MG	5	3410	1/1	0.95	0.24	54,54,54,54	0
86	OHX	1	3982	7/7	0.95	0.15	113,113,113,113	0
86	OHX	L3	404	7/7	0.95	0.12	118,118,118,118	0
85	MG	M3	201	1/1	0.95	0.06	48,48,48,48	0
85	MG	5	3535	1/1	0.95	0.28	33,33,33,33	0
86	OHX	1	4001	7/7	0.95	0.14	115,115,115,115	0
86	OHX	1	4004	7/7	0.95	0.15	111,111,111,111	0
85	MG	1	3835	1/1	0.95	0.26	52,52,52,52	0
86	OHX	1	4007	7/7	0.95	0.12	140,140,140,140	0
86	OHX	1	4008	7/7	0.95	0.13	134,134,134,134	0
86	OHX	6	2063	7/7	0.95	0.14	101,101,101,101	0
86	OHX	6	2076	7/7	0.95	0.15	115,115,115,115	0
86	OHX	6	2084	7/7	0.95	0.13	131,131,131,131	0
85	MG	5	3693	1/1	0.95	0.07	44,44,44,44	0
86	OHX	6	2099	7/7	0.95	0.11	164,164,164,164	0
86	OHX	6	2102	7/7	0.95	0.15	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3836	1/1	0.95	0.26	34,34,34,34	0
86	OHX	5	4201	7/7	0.95	0.12	130,130,130,130	0
86	OHX	6	2105	7/7	0.95	0.14	121,121,121,121	0
85	MG	5	3695	1/1	0.95	0.08	42,42,42,42	0
85	MG	1	3704	1/1	0.95	0.18	63,63,63,63	0
86	OHX	6	2111	7/7	0.95	0.11	128,128,128,128	0
85	MG	5	3698	1/1	0.95	0.13	51,51,51,51	0
86	OHX	1	4023	7/7	0.95	0.11	138,138,138,138	0
85	MG	5	3699	1/1	0.95	0.19	50,50,50,50	0
86	OHX	6	2121	7/7	0.95	0.11	147,147,147,147	0
85	MG	M6	201	1/1	0.95	0.08	47,47,47,47	0
85	MG	5	3419	1/1	0.95	0.10	39,39,39,39	0
85	MG	1	3509	1/1	0.95	0.33	44,44,44,44	0
86	OHX	1	4035	7/7	0.95	0.12	149,149,149,149	0
85	MG	M7	201	1/1	0.95	0.22	36,36,36,36	0
85	MG	5	3422	1/1	0.95	0.15	43,43,43,43	0
85	MG	2	2179	1/1	0.95	0.09	69,69,69,69	0
86	OHX	5	4217	7/7	0.95	0.13	109,109,109,109	0
86	OHX	1	4045	7/7	0.95	0.13	119,119,119,119	0
85	MG	5	4254	1/1	0.95	0.28	29,29,29,29	0
86	OHX	1	4049	7/7	0.95	0.13	126,126,126,126	0
85	MG	5	3709	1/1	0.95	0.27	45,45,45,45	0
86	OHX	6	2139	7/7	0.95	0.14	140,140,140,140	0
86	OHX	1	4055	7/7	0.95	0.21	106,106,106,106	0
85	MG	1	3424	1/1	0.95	0.27	45,45,45,45	0
86	OHX	1	4057	7/7	0.95	0.09	189,189,189,189	0
86	OHX	1	4058	7/7	0.95	0.12	135,135,135,135	0
86	OHX	6	2146	7/7	0.95	0.16	119,119,119,119	0
86	OHX	1	4059	7/7	0.95	0.09	156,156,156,156	0
85	MG	1	3774	1/1	0.95	0.14	66,66,66,66	0
85	MG	5	3549	1/1	0.95	0.38	44,44,44,44	0
85	MG	5	3428	1/1	0.95	0.22	29,29,29,29	0
85	MG	7	205	1/1	0.95	0.26	30,30,30,30	0
86	OHX	5	4233	7/7	0.95	0.20	109,109,109,109	0
85	MG	2	1966	1/1	0.95	0.25	52,52,52,52	0
85	MG	1	3567	1/1	0.95	0.24	35,35,35,35	0
85	MG	1	3609	1/1	0.95	0.12	45,45,45,45	0
85	MG	1	3848	1/1	0.95	0.20	52,52,52,52	0
86	OHX	6	2158	7/7	0.95	0.13	119,119,119,119	0
85	MG	6	1981	1/1	0.95	0.16	50,50,50,50	0
86	OHX	1	4072	7/7	0.95	0.11	131,131,131,131	0
85	MG	5	3558	1/1	0.95	0.13	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3436	1/1	0.95	0.32	48,48,48,48	0
85	MG	1	3453	1/1	0.95	0.29	45,45,45,45	0
85	MG	5	3561	1/1	0.95	0.27	26,26,26,26	0
86	OHX	1	4077	7/7	0.95	0.14	130,130,130,130	0
85	MG	N3	202	1/1	0.95	0.13	46,46,46,46	0
85	MG	5	3566	1/1	0.95	0.31	37,37,37,37	0
85	MG	1	3455	1/1	0.95	0.26	55,55,55,55	0
85	MG	8	206	1/1	0.95	0.30	51,51,51,51	0
85	MG	1	3853	1/1	0.95	0.05	28,28,28,28	0
85	MG	5	3443	1/1	0.95	0.17	37,37,37,37	0
85	MG	1	3854	1/1	0.95	0.32	93,93,93,93	0
85	MG	5	3571	1/1	0.95	0.30	21,21,21,21	0
85	MG	6	1989	1/1	0.95	0.18	68,68,68,68	0
85	MG	1	3571	1/1	0.95	0.26	32,32,32,32	0
85	MG	8	214	1/1	0.95	0.07	50,50,50,50	0
86	OHX	1	4092	7/7	0.95	0.10	145,145,145,145	0
85	MG	8	216	1/1	0.95	0.25	33,33,33,33	0
85	MG	N8	203	1/1	0.95	0.07	50,50,50,50	0
85	MG	1	3781	1/1	0.95	0.09	42,42,42,42	0
85	MG	1	3656	1/1	0.95	0.17	45,45,45,45	0
86	OHX	1	4097	7/7	0.95	0.15	120,120,120,120	0
85	MG	5	3580	1/1	0.95	0.24	38,38,38,38	0
85	MG	5	3749	1/1	0.95	0.07	52,52,52,52	0
85	MG	5	3581	1/1	0.95	0.29	36,36,36,36	0
85	MG	1	3613	1/1	0.95	0.23	35,35,35,35	0
85	MG	1	3658	1/1	0.95	0.08	47,47,47,47	0
85	MG	1	3860	1/1	0.95	0.16	43,43,43,43	0
86	OHX	m0	301	7/7	0.95	0.11	126,126,126,126	0
86	OHX	1	4105	7/7	0.95	0.13	126,126,126,126	0
85	MG	1	3614	1/1	0.95	0.23	43,43,43,43	0
85	MG	1	3862	1/1	0.95	0.13	55,55,55,55	0
85	MG	5	3591	1/1	0.95	0.29	44,44,44,44	0
85	MG	1	4214	1/1	0.95	0.23	30,30,30,30	0
85	MG	1	3438	1/1	0.95	0.22	43,43,43,43	0
85	MG	1	3662	1/1	0.95	0.11	53,53,53,53	0
85	MG	n0	201	1/1	0.95	0.13	42,42,42,42	0
85	MG	n3	201	1/1	0.95	0.23	26,26,26,26	0
85	MG	n3	202	1/1	0.95	0.06	45,45,45,45	0
85	MG	n6	201	1/1	0.95	0.26	49,49,49,49	0
86	OHX	1	4116	7/7	0.95	0.14	132,132,132,132	0
85	MG	5	3766	1/1	0.95	0.09	42,42,42,42	0
85	MG	5	3752	1/1	0.96	0.15	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	2	2044	7/7	0.96	0.13	118,118,118,118	0
86	OHX	1	4024	7/7	0.96	0.09	132,132,132,132	0
86	OHX	2	2054	7/7	0.96	0.10	134,134,134,134	0
86	OHX	5	4072	7/7	0.96	0.13	122,122,122,122	0
86	OHX	1	4026	7/7	0.96	0.11	137,137,137,137	0
86	OHX	2	2055	7/7	0.96	0.10	135,135,135,135	0
86	OHX	1	4028	7/7	0.96	0.11	116,116,116,116	0
86	OHX	2	2056	7/7	0.96	0.11	124,124,124,124	0
86	OHX	5	4077	7/7	0.96	0.10	163,163,163,163	0
86	OHX	1	4031	7/7	0.96	0.13	115,115,115,115	0
86	OHX	2	2057	7/7	0.96	0.09	135,135,135,135	0
86	OHX	2	2058	7/7	0.96	0.10	144,144,144,144	0
86	OHX	5	4083	7/7	0.96	0.10	117,117,117,117	0
86	OHX	1	4036	7/7	0.96	0.12	122,122,122,122	0
86	OHX	5	4085	7/7	0.96	0.12	121,121,121,121	0
86	OHX	1	4037	7/7	0.96	0.12	128,128,128,128	0
86	OHX	1	4038	7/7	0.96	0.13	120,120,120,120	0
86	OHX	1	4040	7/7	0.96	0.12	123,123,123,123	0
86	OHX	1	4041	7/7	0.96	0.14	112,112,112,112	0
86	OHX	5	4090	7/7	0.96	0.23	109,109,109,109	0
86	OHX	5	4091	7/7	0.96	0.14	117,117,117,117	0
85	MG	5	3753	1/1	0.96	0.17	52,52,52,52	0
86	OHX	5	4094	7/7	0.96	0.11	138,138,138,138	0
86	OHX	2	2068	7/7	0.96	0.09	146,146,146,146	0
86	OHX	2	2069	7/7	0.96	0.10	150,150,150,150	0
86	OHX	3	219	7/7	0.96	0.10	130,130,130,130	0
85	MG	1	3761	1/1	0.96	0.10	51,51,51,51	0
86	OHX	1	4047	7/7	0.96	0.10	144,144,144,144	0
85	MG	5	3666	1/1	0.96	0.21	46,46,46,46	0
85	MG	5	3598	1/1	0.96	0.45	28,28,28,28	0
86	OHX	1	4050	7/7	0.96	0.10	147,147,147,147	0
86	OHX	1	4052	7/7	0.96	0.11	142,142,142,142	0
85	MG	1	3428	1/1	0.96	0.14	57,57,57,57	0
85	MG	2	1972	1/1	0.96	0.26	72,72,72,72	0
85	MG	5	3670	1/1	0.96	0.17	49,49,49,49	0
86	OHX	2	2083	7/7	0.96	0.08	157,157,157,157	0
86	OHX	2	2085	7/7	0.96	0.13	130,130,130,130	0
86	OHX	2	2087	7/7	0.96	0.12	122,122,122,122	0
85	MG	5	3671	1/1	0.96	0.07	34,34,34,34	0
86	OHX	2	2090	7/7	0.96	0.13	117,117,117,117	0
86	OHX	L3	403	7/7	0.96	0.12	126,126,126,126	0
86	OHX	2	2091	7/7	0.96	0.11	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3672	1/1	0.96	0.21	48,48,48,48	0
85	MG	5	3601	1/1	0.96	0.17	42,42,42,42	0
86	OHX	1	4067	7/7	0.96	0.15	126,126,126,126	0
86	OHX	2	2097	7/7	0.96	0.12	138,138,138,138	0
85	MG	5	3531	1/1	0.96	0.20	33,33,33,33	0
86	OHX	2	2099	7/7	0.96	0.10	156,156,156,156	0
85	MG	5	3873	1/1	0.96	0.16	38,38,38,38	0
85	MG	5	3675	1/1	0.96	0.27	39,39,39,39	0
86	OHX	6	2072	7/7	0.96	0.11	135,135,135,135	0
86	OHX	2	2103	7/7	0.96	0.10	147,147,147,147	0
85	MG	2	2022	1/1	0.96	0.23	102,102,102,102	0
86	OHX	5	4126	7/7	0.96	0.10	146,146,146,146	0
86	OHX	6	2085	7/7	0.96	0.11	109,109,109,109	0
85	MG	L2	301	1/1	0.96	0.11	38,38,38,38	0
85	MG	5	3877	1/1	0.96	0.38	46,46,46,46	0
85	MG	1	3732	1/1	0.96	0.19	36,36,36,36	0
86	OHX	2	2108	7/7	0.96	0.11	123,123,123,123	0
85	MG	1	3634	1/1	0.96	0.10	48,48,48,48	0
86	OHX	2	2110	7/7	0.96	0.09	161,161,161,161	0
85	MG	5	3774	1/1	0.96	0.09	39,39,39,39	0
86	OHX	6	2110	7/7	0.96	0.11	134,134,134,134	0
85	MG	1	3481	1/1	0.96	0.34	41,41,41,41	0
86	OHX	6	2113	7/7	0.96	0.11	130,130,130,130	0
86	OHX	6	2114	7/7	0.96	0.10	129,129,129,129	0
86	OHX	6	2115	7/7	0.96	0.10	130,130,130,130	0
85	MG	5	3424	1/1	0.96	0.17	41,41,41,41	0
86	OHX	6	2117	7/7	0.96	0.13	115,115,115,115	0
85	MG	1	3462	1/1	0.96	0.20	28,28,28,28	0
85	MG	1	3677	1/1	0.96	0.21	46,46,46,46	0
85	MG	1	3506	1/1	0.96	0.34	32,32,32,32	0
86	OHX	6	2122	7/7	0.96	0.11	138,138,138,138	0
86	OHX	6	2123	7/7	0.96	0.13	111,111,111,111	0
85	MG	5	3887	1/1	0.96	0.28	58,58,58,58	0
85	MG	5	3429	1/1	0.96	0.11	33,33,33,33	0
85	MG	1	3843	1/1	0.96	0.24	37,37,37,37	0
85	MG	5	3544	1/1	0.96	0.14	37,37,37,37	0
86	OHX	6	2128	7/7	0.96	0.12	157,157,157,157	0
86	OHX	6	2129	7/7	0.96	0.10	141,141,141,141	0
85	MG	1	3431	1/1	0.96	0.21	43,43,43,43	0
85	MG	5	3892	1/1	0.96	0.04	31,31,31,31	0
85	MG	1	3534	1/1	0.96	0.24	29,29,29,29	0
85	MG	6	1996	1/1	0.96	0.08	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3741	1/1	0.96	0.12	44,44,44,44	0
85	MG	5	3788	1/1	0.96	0.11	45,45,45,45	0
86	OHX	6	2137	7/7	0.96	0.14	129,129,129,129	0
85	MG	5	3435	1/1	0.96	0.18	35,35,35,35	0
85	MG	6	1953	1/1	0.96	0.49	62,62,62,62	0
85	MG	5	3899	1/1	0.96	0.22	47,47,47,47	0
85	MG	5	4252	1/1	0.96	0.12	40,40,40,40	0
86	OHX	1	4104	7/7	0.96	0.09	147,147,147,147	0
86	OHX	6	2144	7/7	0.96	0.12	133,133,133,133	0
85	MG	6	2042	1/1	0.96	0.14	52,52,52,52	0
85	MG	3	210	1/1	0.96	0.23	60,60,60,60	0
85	MG	5	3628	1/1	0.96	0.19	58,58,58,58	0
85	MG	5	3553	1/1	0.96	0.37	47,47,47,47	0
85	MG	1	3742	1/1	0.96	0.18	51,51,51,51	0
85	MG	7	202	1/1	0.96	0.22	27,27,27,27	0
85	MG	6	1957	1/1	0.96	0.32	49,49,49,49	0
85	MG	6	2205	1/1	0.96	0.25	54,54,54,54	0
86	OHX	6	2154	7/7	0.96	0.12	121,121,121,121	0
85	MG	5	3706	1/1	0.96	0.05	37,37,37,37	0
85	MG	7	206	1/1	0.96	0.07	43,43,43,43	0
85	MG	5	3799	1/1	0.96	0.11	42,42,42,42	0
85	MG	5	3800	1/1	0.96	0.15	40,40,40,40	0
86	OHX	5	4181	7/7	0.96	0.08	163,163,163,163	0
85	MG	1	3712	1/1	0.96	0.07	36,36,36,36	0
85	MG	5	3634	1/1	0.96	0.07	36,36,36,36	0
85	MG	1	3464	1/1	0.96	0.11	37,37,37,37	0
85	MG	5	3711	1/1	0.96	0.20	47,47,47,47	0
85	MG	M5	302	1/1	0.96	0.19	54,54,54,54	0
85	MG	1	3446	1/1	0.96	0.10	45,45,45,45	0
85	MG	5	3714	1/1	0.96	0.10	61,61,61,61	0
85	MG	1	3852	1/1	0.96	0.22	60,60,60,60	0
85	MG	6	2007	1/1	0.96	0.23	55,55,55,55	0
85	MG	8	204	1/1	0.96	0.29	40,40,40,40	0
85	MG	5	3640	1/1	0.96	0.23	49,49,49,49	0
85	MG	5	3719	1/1	0.96	0.09	52,52,52,52	0
85	MG	1	3566	1/1	0.96	0.26	30,30,30,30	0
85	MG	1	3537	1/1	0.96	0.36	31,31,31,31	0
85	MG	d3	201	1/1	0.96	0.24	48,48,48,48	0
85	MG	8	210	1/1	0.96	0.09	54,54,54,54	0
85	MG	1	3538	1/1	0.96	0.12	40,40,40,40	0
85	MG	5	3509	1/1	0.96	0.29	27,27,27,27	0
85	MG	5	3818	1/1	0.96	0.17	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3820	1/1	0.96	0.08	75,75,75,75	0
85	MG	8	215	1/1	0.96	0.25	51,51,51,51	0
85	MG	5	3821	1/1	0.96	0.12	60,60,60,60	0
85	MG	12	301	1/1	0.96	0.23	38,38,38,38	0
85	MG	5	3456	1/1	0.96	0.12	61,61,61,61	0
85	MG	2	1984	1/1	0.96	0.13	60,60,60,60	0
85	MG	5	3825	1/1	0.96	0.20	63,63,63,63	0
85	MG	1	3693	1/1	0.96	0.14	39,39,39,39	0
85	MG	5	3576	1/1	0.96	0.33	42,42,42,42	0
85	MG	1	3822	1/1	0.96	0.13	58,58,58,58	0
85	MG	5	3832	1/1	0.96	0.17	73,73,73,73	0
85	MG	1	3694	1/1	0.96	0.19	52,52,52,52	0
85	MG	1	3666	1/1	0.96	0.09	56,56,56,56	0
85	MG	m5	301	1/1	0.96	0.11	43,43,43,43	0
85	MG	5	3835	1/1	0.96	0.08	42,42,42,42	0
85	MG	5	3733	1/1	0.96	0.04	43,43,43,43	0
85	MG	1	3755	1/1	0.96	0.13	33,33,33,33	0
86	OHX	SR	401	7/7	0.96	0.09	175,175,175,175	0
86	OHX	1	4155	7/7	0.96	0.10	120,120,120,120	0
86	OHX	1	3907	7/7	0.96	0.20	90,90,90,90	0
86	OHX	1	3917	7/7	0.96	0.14	118,118,118,118	0
85	MG	1	3724	1/1	0.96	0.11	65,65,65,65	0
86	OHX	1	3937	7/7	0.96	0.13	106,106,106,106	0
86	OHX	1	3943	7/7	0.96	0.12	95,95,95,95	0
85	MG	5	3737	1/1	0.96	0.17	36,36,36,36	0
85	MG	m7	202	1/1	0.96	0.10	32,32,32,32	0
86	OHX	1	3959	7/7	0.96	0.10	123,123,123,123	0
85	MG	m7	203	1/1	0.96	0.16	51,51,51,51	0
85	MG	1	3423	1/1	0.96	0.10	35,35,35,35	0
85	MG	5	3842	1/1	0.96	0.09	68,68,68,68	0
86	OHX	1	3976	7/7	0.96	0.12	116,116,116,116	0
85	MG	5	3739	1/1	0.96	0.21	29,29,29,29	0
85	MG	5	3740	1/1	0.96	0.06	57,57,57,57	0
85	MG	5	3741	1/1	0.96	0.14	40,40,40,40	0
86	OHX	1	3987	7/7	0.96	0.12	122,122,122,122	0
86	OHX	5	3967	7/7	0.96	0.14	106,106,106,106	0
86	OHX	5	3975	7/7	0.96	0.12	112,112,112,112	0
86	OHX	5	3978	7/7	0.96	0.12	100,100,100,100	0
86	OHX	5	3984	7/7	0.96	0.20	103,103,103,103	0
86	OHX	5	3991	7/7	0.96	0.11	115,115,115,115	0
86	OHX	1	3988	7/7	0.96	0.12	112,112,112,112	0
86	OHX	5	3995	7/7	0.96	0.10	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	3993	7/7	0.96	0.20	103,103,103,103	0
85	MG	1	3572	1/1	0.96	0.33	27,27,27,27	0
86	OHX	5	4003	7/7	0.96	0.11	122,122,122,122	0
86	OHX	5	4006	7/7	0.96	0.11	121,121,121,121	0
86	OHX	5	4012	7/7	0.96	0.12	119,119,119,119	0
86	OHX	1	3996	7/7	0.96	0.13	121,121,121,121	0
85	MG	n8	202	1/1	0.96	0.07	33,33,33,33	0
86	OHX	1	3999	7/7	0.96	0.19	106,106,106,106	0
86	OHX	1	4000	7/7	0.96	0.10	133,133,133,133	0
85	MG	5	3743	1/1	0.96	0.06	35,35,35,35	0
86	OHX	5	4029	7/7	0.96	0.20	101,101,101,101	0
86	OHX	5	4030	7/7	0.96	0.12	124,124,124,124	0
86	OHX	5	4031	7/7	0.96	0.10	143,143,143,143	0
86	OHX	8	221	7/7	0.96	0.12	119,119,119,119	0
86	OHX	8	223	7/7	0.96	0.10	128,128,128,128	0
86	OHX	8	225	7/7	0.96	0.10	129,129,129,129	0
86	OHX	8	227	7/7	0.96	0.12	134,134,134,134	0
86	OHX	1	4002	7/7	0.96	0.11	128,128,128,128	0
86	OHX	5	4033	7/7	0.96	0.14	114,114,114,114	0
86	OHX	1	4003	7/7	0.96	0.11	124,124,124,124	0
85	MG	1	3792	1/1	0.96	0.21	67,67,67,67	0
86	OHX	5	4038	7/7	0.96	0.09	135,135,135,135	0
85	MG	4	215	1/1	0.96	0.15	70,70,70,70	0
85	MG	5	3850	1/1	0.96	0.22	47,47,47,47	0
85	MG	5	3522	1/1	0.96	0.38	41,41,41,41	0
85	MG	q0	202	1/1	0.96	0.08	52,52,52,52	0
86	OHX	1	4010	7/7	0.96	0.09	140,140,140,140	0
86	OHX	5	4048	7/7	0.96	0.11	120,120,120,120	0
86	OHX	5	4049	7/7	0.96	0.13	116,116,116,116	0
86	OHX	1	4011	7/7	0.96	0.11	126,126,126,126	0
86	OHX	1	4012	7/7	0.96	0.11	125,125,125,125	0
86	OHX	5	4053	7/7	0.96	0.20	108,108,108,108	0
86	OHX	1	4013	7/7	0.96	0.12	123,123,123,123	0
85	MG	5	3413	1/1	0.96	0.20	39,39,39,39	0
86	OHX	5	4058	7/7	0.96	0.10	143,143,143,143	0
86	OHX	5	4059	7/7	0.96	0.11	119,119,119,119	0
86	OHX	5	4060	7/7	0.96	0.10	154,154,154,154	0
86	OHX	1	4015	7/7	0.96	0.10	128,128,128,128	0
85	MG	1	4217	1/1	0.96	0.11	32,32,32,32	0
85	MG	5	3526	1/1	0.96	0.29	32,32,32,32	0
86	OHX	5	4064	7/7	0.96	0.08	160,160,160,160	0
86	OHX	5	4065	7/7	0.96	0.12	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	5	4067	7/7	0.96	0.10	135,135,135,135	0
85	MG	1	3604	1/1	0.97	0.16	42,42,42,42	0
85	MG	5	3506	1/1	0.97	0.38	36,36,36,36	0
86	OHX	2	2063	7/7	0.97	0.10	135,135,135,135	0
85	MG	6	2008	1/1	0.97	0.08	49,49,49,49	0
86	OHX	2	2066	7/7	0.97	0.13	114,114,114,114	0
86	OHX	2	2067	7/7	0.97	0.10	140,140,140,140	0
86	OHX	6	2108	7/7	0.97	0.09	128,128,128,128	0
86	OHX	6	2109	7/7	0.97	0.11	116,116,116,116	0
86	OHX	C8	201	7/7	0.97	0.11	117,117,117,117	0
85	MG	1	3680	1/1	0.97	0.11	58,58,58,58	0
86	OHX	6	2112	7/7	0.97	0.11	110,110,110,110	0
85	MG	1	3466	1/1	0.97	0.11	48,48,48,48	0
86	OHX	2	2070	7/7	0.97	0.13	117,117,117,117	0
86	OHX	1	3893	7/7	0.97	0.14	81,81,81,81	0
86	OHX	2	2074	7/7	0.97	0.08	148,148,148,148	0
86	OHX	2	2075	7/7	0.97	0.10	124,124,124,124	0
85	MG	1	3682	1/1	0.97	0.19	40,40,40,40	0
86	OHX	1	3929	7/7	0.97	0.10	106,106,106,106	0
86	OHX	1	3932	7/7	0.97	0.12	108,108,108,108	0
86	OHX	1	3934	7/7	0.97	0.11	96,96,96,96	0
86	OHX	1	3936	7/7	0.97	0.10	116,116,116,116	0
85	MG	1	3582	1/1	0.97	0.24	32,32,32,32	0
86	OHX	1	3942	7/7	0.97	0.11	106,106,106,106	0
86	OHX	2	2078	7/7	0.97	0.10	119,119,119,119	0
86	OHX	1	3944	7/7	0.97	0.09	112,112,112,112	0
86	OHX	1	3947	7/7	0.97	0.12	118,118,118,118	0
85	MG	5	3716	1/1	0.97	0.12	51,51,51,51	0
86	OHX	6	2130	7/7	0.97	0.10	128,128,128,128	0
85	MG	1	3684	1/1	0.97	0.21	49,49,49,49	0
86	OHX	1	3952	7/7	0.97	0.17	104,104,104,104	0
86	OHX	1	3954	7/7	0.97	0.17	99,99,99,99	0
85	MG	1	3809	1/1	0.97	0.08	49,49,49,49	0
85	MG	5	3402	1/1	0.97	0.22	30,30,30,30	0
85	MG	1	3710	1/1	0.97	0.07	53,53,53,53	0
86	OHX	1	3964	7/7	0.97	0.12	106,106,106,106	0
86	OHX	1	3965	7/7	0.97	0.10	131,131,131,131	0
86	OHX	1	3968	7/7	0.97	0.11	118,118,118,118	0
86	OHX	1	3970	7/7	0.97	0.12	110,110,110,110	0
86	OHX	1	3971	7/7	0.97	0.09	132,132,132,132	0
86	OHX	6	2142	7/7	0.97	0.11	132,132,132,132	0
86	OHX	1	3973	7/7	0.97	0.11	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	2	2084	7/7	0.97	0.09	138,138,138,138	0
86	OHX	5	4130	7/7	0.97	0.08	145,145,145,145	0
86	OHX	1	3975	7/7	0.97	0.22	100,100,100,100	0
85	MG	1	3685	1/1	0.97	0.06	38,38,38,38	0
86	OHX	2	2086	7/7	0.97	0.09	146,146,146,146	0
85	MG	1	3812	1/1	0.97	0.23	49,49,49,49	0
86	OHX	2	2088	7/7	0.97	0.10	130,130,130,130	0
86	OHX	1	3983	7/7	0.97	0.10	125,125,125,125	0
86	OHX	1	3984	7/7	0.97	0.10	119,119,119,119	0
86	OHX	1	3985	7/7	0.97	0.11	124,124,124,124	0
86	OHX	1	3986	7/7	0.97	0.11	112,112,112,112	0
85	MG	5	3649	1/1	0.97	0.18	43,43,43,43	0
85	MG	5	3650	1/1	0.97	0.13	43,43,43,43	0
86	OHX	1	3989	7/7	0.97	0.10	135,135,135,135	0
86	OHX	1	3990	7/7	0.97	0.09	131,131,131,131	0
86	OHX	1	3992	7/7	0.97	0.09	137,137,137,137	0
85	MG	1	3740	1/1	0.97	0.12	40,40,40,40	0
85	MG	1	3461	1/1	0.97	0.20	25,25,25,25	0
86	OHX	2	2093	7/7	0.97	0.17	123,123,123,123	0
85	MG	5	3727	1/1	0.97	0.08	36,36,36,36	0
86	OHX	2	2096	7/7	0.97	0.08	156,156,156,156	0
85	MG	5	3409	1/1	0.97	0.34	44,44,44,44	0
85	MG	5	3812	1/1	0.97	0.07	90,90,90,90	0
85	MG	5	3584	1/1	0.97	0.28	29,29,29,29	0
86	OHX	2	2100	7/7	0.97	0.11	128,128,128,128	0
85	MG	5	3585	1/1	0.97	0.37	31,31,31,31	0
86	OHX	1	4005	7/7	0.97	0.10	112,112,112,112	0
85	MG	5	3587	1/1	0.97	0.19	26,26,26,26	0
85	MG	1	3439	1/1	0.97	0.28	34,34,34,34	0
85	MG	1	3743	1/1	0.97	0.14	32,32,32,32	0
85	MG	5	3523	1/1	0.97	0.30	38,38,38,38	0
85	MG	5	3819	1/1	0.97	0.05	36,36,36,36	0
85	MG	5	3412	1/1	0.97	0.16	33,33,33,33	0
85	MG	5	3736	1/1	0.97	0.12	53,53,53,53	0
85	MG	1	3688	1/1	0.97	0.12	39,39,39,39	0
85	MG	1	3595	1/1	0.97	0.34	25,25,25,25	0
86	OHX	2	2111	7/7	0.97	0.08	147,147,147,147	0
86	OHX	2	2112	7/7	0.97	0.12	128,128,128,128	0
86	OHX	1	4017	7/7	0.97	0.10	120,120,120,120	0
85	MG	1	3746	1/1	0.97	0.07	49,49,49,49	0
86	OHX	1	4171	7/7	0.97	0.12	112,112,112,112	0
86	OHX	1	4019	7/7	0.97	0.10	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4020	7/7	0.97	0.09	143,143,143,143	0
85	MG	5	3828	1/1	0.97	0.08	43,43,43,43	0
86	OHX	1	4022	7/7	0.97	0.10	117,117,117,117	0
85	MG	1	3433	1/1	0.97	0.22	37,37,37,37	0
85	MG	1	3653	1/1	0.97	0.34	47,47,47,47	0
85	MG	2	1956	1/1	0.97	0.37	65,65,65,65	0
85	MG	1	3720	1/1	0.97	0.10	61,61,61,61	0
85	MG	1	3587	1/1	0.97	0.22	25,25,25,25	0
85	MG	6	1985	1/1	0.97	0.07	48,48,48,48	0
85	MG	1	3626	1/1	0.97	0.17	34,34,34,34	0
85	MG	1	3491	1/1	0.97	0.17	34,34,34,34	0
86	OHX	1	4033	7/7	0.97	0.23	104,104,104,104	0
85	MG	5	3748	1/1	0.97	0.19	48,48,48,48	0
85	MG	4	218	1/1	0.97	0.12	40,40,40,40	0
85	MG	5	3750	1/1	0.97	0.20	43,43,43,43	0
86	OHX	6	2201	7/7	0.97	0.07	193,193,193,193	0
85	MG	1	3674	1/1	0.97	0.08	76,76,76,76	0
85	MG	5	3539	1/1	0.97	0.21	23,23,23,23	0
86	OHX	1	4039	7/7	0.97	0.09	137,137,137,137	0
85	MG	5	3427	1/1	0.97	0.22	48,48,48,48	0
85	MG	1	3628	1/1	0.97	0.15	70,70,70,70	0
86	OHX	2	2131	7/7	0.97	0.12	125,125,125,125	0
85	MG	5	3677	1/1	0.97	0.05	43,43,43,43	0
85	MG	5	3610	1/1	0.97	0.17	31,31,31,31	0
85	MG	5	3611	1/1	0.97	0.15	39,39,39,39	0
85	MG	5	3758	1/1	0.97	0.10	56,56,56,56	0
85	MG	5	3612	1/1	0.97	0.23	51,51,51,51	0
85	MG	5	3613	1/1	0.97	0.04	34,34,34,34	0
86	OHX	5	3950	7/7	0.97	0.12	103,103,103,103	0
86	OHX	5	3956	7/7	0.97	0.12	102,102,102,102	0
86	OHX	5	3964	7/7	0.97	0.10	99,99,99,99	0
85	MG	1	3727	1/1	0.97	0.08	35,35,35,35	0
86	OHX	1	4051	7/7	0.97	0.08	149,149,149,149	0
86	OHX	5	3976	7/7	0.97	0.12	100,100,100,100	0
85	MG	5	3852	1/1	0.97	0.27	59,59,59,59	0
85	MG	5	3763	1/1	0.97	0.12	41,41,41,41	0
86	OHX	1	4054	7/7	0.97	0.09	154,154,154,154	0
86	OHX	5	3993	7/7	0.97	0.11	108,108,108,108	0
85	MG	1	3757	1/1	0.97	0.17	39,39,39,39	0
85	MG	5	3685	1/1	0.97	0.18	52,52,52,52	0
85	MG	6	1945	1/1	0.97	0.28	32,32,32,32	0
86	OHX	5	3997	7/7	0.97	0.21	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3699	1/1	0.97	0.27	46,46,46,46	0
86	OHX	5	4001	7/7	0.97	0.10	119,119,119,119	0
86	OHX	5	4002	7/7	0.97	0.21	80,80,80,80	0
86	OHX	2	2145	7/7	0.97	0.10	127,127,127,127	0
85	MG	5	3768	1/1	0.97	0.14	55,55,55,55	0
86	OHX	5	4011	7/7	0.97	0.11	113,113,113,113	0
85	MG	1	3794	1/1	0.97	0.10	29,29,29,29	0
86	OHX	5	4013	7/7	0.97	0.09	149,149,149,149	0
86	OHX	5	4015	7/7	0.97	0.11	111,111,111,111	0
86	OHX	5	4016	7/7	0.97	0.10	111,111,111,111	0
85	MG	5	3490	1/1	0.97	0.07	50,50,50,50	0
86	OHX	5	4018	7/7	0.97	0.10	128,128,128,128	0
86	OHX	5	4019	7/7	0.97	0.10	114,114,114,114	0
86	OHX	5	4020	7/7	0.97	0.11	125,125,125,125	0
86	OHX	1	4063	7/7	0.97	0.16	111,111,111,111	0
86	OHX	5	4022	7/7	0.97	0.09	123,123,123,123	0
86	OHX	1	4064	7/7	0.97	0.08	151,151,151,151	0
86	OHX	5	4025	7/7	0.97	0.11	113,113,113,113	0
86	OHX	3	217	7/7	0.97	0.10	113,113,113,113	0
86	OHX	3	218	7/7	0.97	0.09	123,123,123,123	0
85	MG	1	3759	1/1	0.97	0.08	37,37,37,37	0
85	MG	5	3865	1/1	0.97	0.15	38,38,38,38	0
85	MG	1	3700	1/1	0.97	0.14	50,50,50,50	0
85	MG	n0	202	1/1	0.97	0.13	41,41,41,41	0
85	MG	5	3622	1/1	0.97	0.14	37,37,37,37	0
86	OHX	5	4035	7/7	0.97	0.10	130,130,130,130	0
85	MG	1	3416	1/1	0.97	0.07	51,51,51,51	0
85	MG	5	3869	1/1	0.97	0.07	40,40,40,40	0
85	MG	L7	301	1/1	0.97	0.15	39,39,39,39	0
86	OHX	5	4039	7/7	0.97	0.23	103,103,103,103	0
86	OHX	4	227	7/7	0.97	0.10	108,108,108,108	0
86	OHX	4	230	7/7	0.97	0.13	115,115,115,115	0
85	MG	5	3438	1/1	0.97	0.22	32,32,32,32	0
85	MG	5	3696	1/1	0.97	0.17	76,76,76,76	0
86	OHX	5	4044	7/7	0.97	0.20	106,106,106,106	0
86	OHX	4	233	7/7	0.97	0.10	136,136,136,136	0
86	OHX	5	4046	7/7	0.97	0.15	110,110,110,110	0
86	OHX	7	216	7/7	0.97	0.12	97,97,97,97	0
86	OHX	7	221	7/7	0.97	0.10	112,112,112,112	0
86	OHX	5	4047	7/7	0.97	0.11	128,128,128,128	0
85	MG	1	3762	1/1	0.97	0.24	51,51,51,51	0
85	MG	1	3484	1/1	0.97	0.10	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4050	7/7	0.97	0.08	133,133,133,133	0
85	MG	1	3839	1/1	0.97	0.21	31,31,31,31	0
86	OHX	8	219	7/7	0.97	0.09	119,119,119,119	0
86	OHX	8	220	7/7	0.97	0.11	116,116,116,116	0
85	MG	6	1956	1/1	0.97	0.33	43,43,43,43	0
86	OHX	8	222	7/7	0.97	0.10	129,129,129,129	0
85	MG	5	3557	1/1	0.97	0.26	28,28,28,28	0
86	OHX	8	224	7/7	0.97	0.14	126,126,126,126	0
85	MG	5	3702	1/1	0.97	0.08	32,32,32,32	0
86	OHX	8	226	7/7	0.97	0.08	145,145,145,145	0
86	OHX	5	4056	7/7	0.97	0.12	111,111,111,111	0
85	MG	6	1912	1/1	0.97	0.28	52,52,52,52	0
85	MG	s8	302	1/1	0.97	0.12	45,45,45,45	0
86	OHX	2	2038	7/7	0.97	0.12	120,120,120,120	0
86	OHX	1	4084	7/7	0.97	0.07	195,195,195,195	0
86	OHX	M5	303	7/7	0.97	0.10	116,116,116,116	0
85	MG	5	3787	1/1	0.97	0.08	47,47,47,47	0
85	MG	5	3446	1/1	0.97	0.12	43,43,43,43	0
86	OHX	1	4087	7/7	0.97	0.26	94,94,94,94	0
86	OHX	2	2050	7/7	0.97	0.09	127,127,127,127	0
86	OHX	1	4089	7/7	0.97	0.07	162,162,162,162	0
86	OHX	6	2064	7/7	0.97	0.11	104,104,104,104	0
86	OHX	6	2065	7/7	0.97	0.15	112,112,112,112	0
86	OHX	2	2051	7/7	0.97	0.09	121,121,121,121	0
86	OHX	2	2053	7/7	0.97	0.09	116,116,116,116	0
86	OHX	6	2077	7/7	0.97	0.14	99,99,99,99	0
86	OHX	6	2080	7/7	0.97	0.17	107,107,107,107	0
86	OHX	m5	305	7/7	0.97	0.10	133,133,133,133	0
85	MG	1	3840	1/1	0.97	0.17	66,66,66,66	0
85	MG	5	3707	1/1	0.97	0.10	57,57,57,57	0
86	OHX	6	2087	7/7	0.97	0.09	126,126,126,126	0
86	OHX	o3	202	7/7	0.97	0.13	111,111,111,111	0
86	OHX	6	2088	7/7	0.97	0.10	133,133,133,133	0
86	OHX	6	2090	7/7	0.97	0.13	125,125,125,125	0
86	OHX	6	2093	7/7	0.97	0.09	135,135,135,135	0
85	MG	M0	302	1/1	0.97	0.18	55,55,55,55	0
86	OHX	6	2096	7/7	0.97	0.08	157,157,157,157	0
86	OHX	6	2097	7/7	0.97	0.08	126,126,126,126	0
88	ZN	e1	501	1/1	0.97	0.05	169,169,169,169	0
86	OHX	6	2098	7/7	0.97	0.08	157,157,157,157	0
86	OHX	1	3914	7/7	0.98	0.10	100,100,100,100	0
86	OHX	6	2073	7/7	0.98	0.09	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	6	2075	7/7	0.98	0.08	115,115,115,115	0
86	OHX	2	2045	7/7	0.98	0.10	109,109,109,109	0
86	OHX	1	3918	7/7	0.98	0.10	92,92,92,92	0
86	OHX	6	2078	7/7	0.98	0.10	107,107,107,107	0
86	OHX	1	3921	7/7	0.98	0.10	94,94,94,94	0
86	OHX	6	2081	7/7	0.98	0.08	109,109,109,109	0
86	OHX	5	3927	7/7	0.98	0.13	72,72,72,72	0
86	OHX	5	3930	7/7	0.98	0.12	84,84,84,84	0
86	OHX	5	3933	7/7	0.98	0.12	94,94,94,94	0
86	OHX	5	3941	7/7	0.98	0.10	85,85,85,85	0
86	OHX	5	3942	7/7	0.98	0.09	87,87,87,87	0
86	OHX	5	3945	7/7	0.98	0.10	90,90,90,90	0
86	OHX	5	3947	7/7	0.98	0.09	75,75,75,75	0
86	OHX	5	3948	7/7	0.98	0.09	92,92,92,92	0
86	OHX	6	2082	7/7	0.98	0.08	119,119,119,119	0
86	OHX	5	3951	7/7	0.98	0.10	85,85,85,85	0
86	OHX	5	3952	7/7	0.98	0.14	109,109,109,109	0
86	OHX	5	3953	7/7	0.98	0.09	104,104,104,104	0
86	OHX	6	2083	7/7	0.98	0.08	119,119,119,119	0
86	OHX	5	3957	7/7	0.98	0.10	96,96,96,96	0
86	OHX	5	3959	7/7	0.98	0.10	89,89,89,89	0
86	OHX	5	3961	7/7	0.98	0.09	77,77,77,77	0
86	OHX	1	3923	7/7	0.98	0.11	111,111,111,111	0
86	OHX	5	3965	7/7	0.98	0.15	88,88,88,88	0
86	OHX	2	2046	7/7	0.98	0.10	107,107,107,107	0
86	OHX	5	3968	7/7	0.98	0.10	97,97,97,97	0
86	OHX	5	3970	7/7	0.98	0.09	100,100,100,100	0
86	OHX	5	3973	7/7	0.98	0.13	87,87,87,87	0
86	OHX	1	3926	7/7	0.98	0.09	111,111,111,111	0
86	OHX	2	2047	7/7	0.98	0.07	117,117,117,117	0
86	OHX	6	2089	7/7	0.98	0.09	113,113,113,113	0
86	OHX	5	3980	7/7	0.98	0.10	100,100,100,100	0
86	OHX	5	3981	7/7	0.98	0.09	112,112,112,112	0
86	OHX	5	3982	7/7	0.98	0.12	95,95,95,95	0
86	OHX	1	3930	7/7	0.98	0.11	107,107,107,107	0
86	OHX	5	3985	7/7	0.98	0.15	98,98,98,98	0
86	OHX	5	3987	7/7	0.98	0.15	95,95,95,95	0
86	OHX	5	3988	7/7	0.98	0.09	107,107,107,107	0
86	OHX	5	3989	7/7	0.98	0.08	121,121,121,121	0
86	OHX	6	2091	7/7	0.98	0.09	116,116,116,116	0
86	OHX	5	3992	7/7	0.98	0.14	97,97,97,97	0
86	OHX	6	2092	7/7	0.98	0.10	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
85	MG	1	3574	1/1	0.98	0.23	24,24,24,24	0
86	OHX	1	3933	7/7	0.98	0.10	101,101,101,101	0
86	OHX	6	2095	7/7	0.98	0.08	129,129,129,129	0
86	OHX	1	4046	7/7	0.98	0.09	126,126,126,126	0
86	OHX	5	3998	7/7	0.98	0.08	120,120,120,120	0
86	OHX	5	3999	7/7	0.98	0.07	108,108,108,108	0
85	MG	6	1973	1/1	0.98	0.08	50,50,50,50	0
86	OHX	1	4154	7/7	0.98	0.10	110,110,110,110	0
86	OHX	1	3935	7/7	0.98	0.11	98,98,98,98	0
86	OHX	6	2100	7/7	0.98	0.08	158,158,158,158	0
86	OHX	5	4004	7/7	0.98	0.14	102,102,102,102	0
86	OHX	5	4005	7/7	0.98	0.10	111,111,111,111	0
86	OHX	6	2101	7/7	0.98	0.07	116,116,116,116	0
86	OHX	5	4007	7/7	0.98	0.07	126,126,126,126	0
86	OHX	5	4010	7/7	0.98	0.08	112,112,112,112	0
86	OHX	2	2052	7/7	0.98	0.08	109,109,109,109	0
86	OHX	6	2103	7/7	0.98	0.07	129,129,129,129	0
85	MG	1	3797	1/1	0.98	0.15	54,54,54,54	0
86	OHX	5	4014	7/7	0.98	0.12	100,100,100,100	0
86	OHX	1	3938	7/7	0.98	0.10	102,102,102,102	0
86	OHX	1	3939	7/7	0.98	0.11	102,102,102,102	0
86	OHX	1	3940	7/7	0.98	0.10	112,112,112,112	0
85	MG	5	3838	1/1	0.98	0.12	74,74,74,74	0
85	MG	5	3407	1/1	0.98	0.10	39,39,39,39	0
85	MG	5	3441	1/1	0.98	0.19	33,33,33,33	0
86	OHX	1	3945	7/7	0.98	0.09	110,110,110,110	0
86	OHX	1	3946	7/7	0.98	0.10	127,127,127,127	0
85	MG	1	3529	1/1	0.98	0.30	33,33,33,33	0
85	MG	5	3597	1/1	0.98	0.35	32,32,32,32	0
86	OHX	5	4199	7/7	0.98	0.17	94,94,94,94	0
86	OHX	2	2059	7/7	0.98	0.09	115,115,115,115	0
86	OHX	1	3951	7/7	0.98	0.14	103,103,103,103	0
86	OHX	5	4028	7/7	0.98	0.12	94,94,94,94	0
86	OHX	2	2060	7/7	0.98	0.09	124,124,124,124	0
86	OHX	1	3953	7/7	0.98	0.12	102,102,102,102	0
86	OHX	6	2119	7/7	0.98	0.09	127,127,127,127	0
86	OHX	2	2062	7/7	0.98	0.07	133,133,133,133	0
86	OHX	1	3956	7/7	0.98	0.09	111,111,111,111	0
86	OHX	5	4034	7/7	0.98	0.09	114,114,114,114	0
86	OHX	1	3957	7/7	0.98	0.07	113,113,113,113	0
86	OHX	1	3958	7/7	0.98	0.10	102,102,102,102	0
85	MG	1	3410	1/1	0.98	0.14	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	1948	1/1	0.98	0.26	41,41,41,41	0
86	OHX	1	3962	7/7	0.98	0.12	103,103,103,103	0
86	OHX	2	2065	7/7	0.98	0.10	118,118,118,118	0
85	MG	14	401	1/1	0.98	0.05	38,38,38,38	0
85	MG	1	3511	1/1	0.98	0.27	38,38,38,38	0
86	OHX	1	3966	7/7	0.98	0.12	104,104,104,104	0
86	OHX	1	3967	7/7	0.98	0.08	109,109,109,109	0
85	MG	5	3679	1/1	0.98	0.18	43,43,43,43	0
86	OHX	1	3969	7/7	0.98	0.15	108,108,108,108	0
85	MG	1	3568	1/1	0.98	0.29	27,27,27,27	0
85	MG	O2	201	1/1	0.98	0.09	34,34,34,34	0
86	OHX	1	3972	7/7	0.98	0.09	112,112,112,112	0
86	OHX	2	2071	7/7	0.98	0.08	130,130,130,130	0
86	OHX	2	2072	7/7	0.98	0.09	132,132,132,132	0
86	OHX	2	2073	7/7	0.98	0.09	128,128,128,128	0
85	MG	5	3414	1/1	0.98	0.28	31,31,31,31	0
85	MG	1	3825	1/1	0.98	0.09	62,62,62,62	0
86	OHX	1	3978	7/7	0.98	0.13	86,86,86,86	0
85	MG	5	3485	1/1	0.98	0.29	47,47,47,47	0
85	MG	6	1982	1/1	0.98	0.12	54,54,54,54	0
85	MG	5	3487	1/1	0.98	0.23	28,28,28,28	0
85	MG	5	3565	1/1	0.98	0.12	28,28,28,28	0
85	MG	1	3661	1/1	0.98	0.25	50,50,50,50	0
86	OHX	6	2148	7/7	0.98	0.13	115,115,115,115	0
85	MG	O7	103	1/1	0.98	0.19	41,41,41,41	0
85	MG	m6	202	1/1	0.98	0.06	32,32,32,32	0
85	MG	1	3691	1/1	0.98	0.20	42,42,42,42	0
86	OHX	5	4066	7/7	0.98	0.07	120,120,120,120	0
85	MG	5	3772	1/1	0.98	0.09	31,31,31,31	0
85	MG	5	3454	1/1	0.98	0.14	30,30,30,30	0
86	OHX	1	3991	7/7	0.98	0.15	108,108,108,108	0
85	MG	1	3851	1/1	0.98	0.10	66,66,66,66	0
85	MG	m7	205	1/1	0.98	0.08	34,34,34,34	0
85	MG	1	3708	1/1	0.98	0.24	35,35,35,35	0
86	OHX	1	3995	7/7	0.98	0.07	148,148,148,148	0
85	MG	5	3864	1/1	0.98	0.06	47,47,47,47	0
85	MG	1	3676	1/1	0.98	0.24	43,43,43,43	0
85	MG	1	3560	1/1	0.98	0.30	36,36,36,36	0
85	MG	1	3808	1/1	0.98	0.10	43,43,43,43	0
86	OHX	3	215	7/7	0.98	0.09	108,108,108,108	0
85	MG	1	3512	1/1	0.98	0.31	25,25,25,25	0
86	OHX	7	217	7/7	0.98	0.10	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	7	218	7/7	0.98	0.14	101,101,101,101	0
86	OHX	7	219	7/7	0.98	0.17	104,104,104,104	0
86	OHX	5	4081	7/7	0.98	0.10	115,115,115,115	0
85	MG	6	1962	1/1	0.98	0.12	41,41,41,41	0
86	OHX	2	2095	7/7	0.98	0.08	140,140,140,140	0
85	MG	1	3602	1/1	0.98	0.05	39,39,39,39	0
85	MG	1	3454	1/1	0.98	0.17	43,43,43,43	0
85	MG	1	3769	1/1	0.98	0.10	69,69,69,69	0
85	MG	5	3826	1/1	0.98	0.19	46,46,46,46	0
85	MG	5	3827	1/1	0.98	0.07	36,36,36,36	0
85	MG	1	3652	1/1	0.98	0.15	50,50,50,50	0
85	MG	6	2027	1/1	0.98	0.32	55,55,55,55	0
85	MG	2	1922	1/1	0.98	0.25	55,55,55,55	0
86	OHX	4	226	7/7	0.98	0.13	104,104,104,104	0
86	OHX	5	4093	7/7	0.98	0.10	119,119,119,119	0
85	MG	1	3791	1/1	0.98	0.10	31,31,31,31	0
86	OHX	4	228	7/7	0.98	0.08	123,123,123,123	0
86	OHX	4	229	7/7	0.98	0.08	125,125,125,125	0
86	OHX	2	2026	7/7	0.98	0.13	86,86,86,86	0
86	OHX	2	2029	7/7	0.98	0.10	98,98,98,98	0
86	OHX	2	2030	7/7	0.98	0.11	107,107,107,107	0
86	OHX	2	2031	7/7	0.98	0.14	97,97,97,97	0
86	OHX	13	403	7/7	0.98	0.11	106,106,106,106	0
86	OHX	2	2032	7/7	0.98	0.08	117,117,117,117	0
86	OHX	2	2034	7/7	0.98	0.13	110,110,110,110	0
86	OHX	2	2036	7/7	0.98	0.12	103,103,103,103	0
85	MG	1	3716	1/1	0.98	0.07	36,36,36,36	0
86	OHX	2	2039	7/7	0.98	0.10	106,106,106,106	0
86	OHX	2	2040	7/7	0.98	0.10	103,103,103,103	0
85	MG	2	1903	1/1	0.98	0.27	41,41,41,41	0
86	OHX	1	3887	7/7	0.98	0.12	79,79,79,79	0
86	OHX	2	2116	7/7	0.98	0.10	125,125,125,125	0
86	OHX	5	4110	7/7	0.98	0.19	98,98,98,98	0
86	OHX	1	3896	7/7	0.98	0.11	89,89,89,89	0
86	OHX	1	3897	7/7	0.98	0.10	88,88,88,88	0
86	OHX	m6	203	7/7	0.98	0.12	100,100,100,100	0
86	OHX	1	3902	7/7	0.98	0.10	88,88,88,88	0
85	MG	1	3606	1/1	0.98	0.27	52,52,52,52	0
86	OHX	1	4030	7/7	0.98	0.14	106,106,106,106	0
86	OHX	o2	201	7/7	0.98	0.19	105,105,105,105	0
86	OHX	1	3908	7/7	0.98	0.10	100,100,100,100	0
86	OHX	o7	502	7/7	0.98	0.09	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	O7	104	7/7	0.98	0.10	102,102,102,102	0
86	OHX	q1	102	7/7	0.98	0.19	103,103,103,103	0
86	OHX	6	2050	7/7	0.98	0.11	73,73,73,73	0
86	OHX	6	2054	7/7	0.98	0.11	85,85,85,85	0
86	OHX	1	4032	7/7	0.98	0.06	150,150,150,150	0
88	ZN	E1	501	1/1	0.98	0.05	123,123,123,123	0
86	OHX	1	3912	7/7	0.98	0.09	105,105,105,105	0
86	OHX	1	3913	7/7	0.98	0.10	92,92,92,92	0
86	OHX	6	2069	7/7	0.98	0.12	90,90,90,90	0
86	OHX	6	2070	7/7	0.98	0.09	111,111,111,111	0
86	OHX	1	3927	7/7	0.99	0.12	92,92,92,92	0
86	OHX	5	3986	7/7	0.99	0.10	91,91,91,91	0
86	OHX	1	3928	7/7	0.99	0.06	87,87,87,87	0
86	OHX	2	2042	7/7	0.99	0.07	99,99,99,99	0
86	OHX	2	2043	7/7	0.99	0.07	104,104,104,104	0
86	OHX	5	3990	7/7	0.99	0.07	88,88,88,88	0
86	OHX	1	3931	7/7	0.99	0.06	84,84,84,84	0
85	MG	5	3759	1/1	0.99	0.08	46,46,46,46	0
85	MG	1	3448	1/1	0.99	0.07	27,27,27,27	0
85	MG	6	1927	1/1	0.99	0.36	47,47,47,47	0
85	MG	1	3726	1/1	0.99	0.07	70,70,70,70	0
86	OHX	N1	201	7/7	0.99	0.06	70,70,70,70	0
86	OHX	N9	102	7/7	0.99	0.11	68,68,68,68	0
86	OHX	2	2048	7/7	0.99	0.06	136,136,136,136	0
86	OHX	2	2049	7/7	0.99	0.06	118,118,118,118	0
86	OHX	Q2	503	7/7	0.99	0.14	86,86,86,86	0
86	OHX	6	2046	7/7	0.99	0.11	61,61,61,61	0
86	OHX	6	2047	7/7	0.99	0.13	75,75,75,75	0
86	OHX	6	2048	7/7	0.99	0.10	69,69,69,69	0
86	OHX	6	2049	7/7	0.99	0.08	75,75,75,75	0
85	MG	5	3586	1/1	0.99	0.29	24,24,24,24	0
86	OHX	6	2051	7/7	0.99	0.08	70,70,70,70	0
86	OHX	6	2052	7/7	0.99	0.10	78,78,78,78	0
86	OHX	5	4008	7/7	0.99	0.08	80,80,80,80	0
86	OHX	5	4009	7/7	0.99	0.11	105,105,105,105	0
86	OHX	6	2053	7/7	0.99	0.11	89,89,89,89	0
85	MG	5	3530	1/1	0.99	0.31	28,28,28,28	0
86	OHX	6	2056	7/7	0.99	0.07	77,77,77,77	0
86	OHX	6	2057	7/7	0.99	0.06	89,89,89,89	0
86	OHX	5	4174	7/7	0.99	0.17	93,93,93,93	0
86	OHX	6	2058	7/7	0.99	0.09	94,94,94,94	0
86	OHX	6	2059	7/7	0.99	0.06	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	6	2060	7/7	0.99	0.07	87,87,87,87	0
86	OHX	6	2061	7/7	0.99	0.07	88,88,88,88	0
86	OHX	6	2062	7/7	0.99	0.07	86,86,86,86	0
85	MG	1	3598	1/1	0.99	0.37	14,14,14,14	0
86	OHX	1	3941	7/7	0.99	0.07	99,99,99,99	0
85	MG	5	3562	1/1	0.99	0.24	20,20,20,20	0
86	OHX	6	2066	7/7	0.99	0.12	99,99,99,99	0
86	OHX	6	2067	7/7	0.99	0.09	94,94,94,94	0
86	OHX	5	4024	7/7	0.99	0.07	119,119,119,119	0
86	OHX	6	2068	7/7	0.99	0.07	102,102,102,102	0
85	MG	5	3853	1/1	0.99	0.10	51,51,51,51	0
86	OHX	2	2024	7/7	0.99	0.12	76,76,76,76	0
86	OHX	6	2071	7/7	0.99	0.14	94,94,94,94	0
86	OHX	2	2025	7/7	0.99	0.11	82,82,82,82	0
85	MG	5	3575	1/1	0.99	0.25	26,26,26,26	0
86	OHX	6	2074	7/7	0.99	0.08	90,90,90,90	0
86	OHX	1	3867	7/7	0.99	0.13	62,62,62,62	0
86	OHX	1	3948	7/7	0.99	0.07	103,103,103,103	0
86	OHX	1	3869	7/7	0.99	0.12	60,60,60,60	0
86	OHX	1	3870	7/7	0.99	0.08	59,59,59,59	0
86	OHX	6	2079	7/7	0.99	0.06	106,106,106,106	0
86	OHX	1	3871	7/7	0.99	0.10	68,68,68,68	0
86	OHX	1	3872	7/7	0.99	0.10	61,61,61,61	0
86	OHX	1	3873	7/7	0.99	0.08	66,66,66,66	0
86	OHX	1	3876	7/7	0.99	0.09	67,67,67,67	0
86	OHX	1	3955	7/7	0.99	0.15	81,81,81,81	0
86	OHX	1	3877	7/7	0.99	0.11	70,70,70,70	0
86	OHX	6	2086	7/7	0.99	0.07	118,118,118,118	0
86	OHX	1	3879	7/7	0.99	0.08	75,75,75,75	0
86	OHX	1	3880	7/7	0.99	0.11	68,68,68,68	0
86	OHX	1	3882	7/7	0.99	0.09	74,74,74,74	0
86	OHX	1	3883	7/7	0.99	0.08	70,70,70,70	0
86	OHX	1	3961	7/7	0.99	0.12	79,79,79,79	0
86	OHX	1	3884	7/7	0.99	0.09	74,74,74,74	0
86	OHX	1	3885	7/7	0.99	0.09	80,80,80,80	0
86	OHX	2	2027	7/7	0.99	0.08	86,86,86,86	0
86	OHX	1	3888	7/7	0.99	0.07	75,75,75,75	0
86	OHX	1	3890	7/7	0.99	0.08	74,74,74,74	0
86	OHX	1	3891	7/7	0.99	0.07	75,75,75,75	0
86	OHX	5	4055	7/7	0.99	0.07	107,107,107,107	0
86	OHX	1	3892	7/7	0.99	0.10	83,83,83,83	0
86	OHX	s1	302	7/7	0.99	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	2	2028	7/7	0.99	0.08	78,78,78,78	0
86	OHX	1	3894	7/7	0.99	0.10	81,81,81,81	0
86	OHX	1	3895	7/7	0.99	0.08	79,79,79,79	0
85	MG	5	3563	1/1	0.99	0.41	35,35,35,35	0
86	OHX	2	2061	7/7	0.99	0.08	108,108,108,108	0
86	OHX	1	3898	7/7	0.99	0.08	72,72,72,72	0
86	OHX	1	3899	7/7	0.99	0.06	85,85,85,85	0
86	OHX	1	3900	7/7	0.99	0.09	84,84,84,84	0
86	OHX	1	3901	7/7	0.99	0.09	77,77,77,77	0
85	MG	6	1905	1/1	0.99	0.26	54,54,54,54	0
86	OHX	5	3900	7/7	0.99	0.12	51,51,51,51	0
86	OHX	5	3901	7/7	0.99	0.12	49,49,49,49	0
86	OHX	5	3903	7/7	0.99	0.10	55,55,55,55	0
86	OHX	5	3904	7/7	0.99	0.14	58,58,58,58	0
86	OHX	5	3905	7/7	0.99	0.11	58,58,58,58	0
86	OHX	5	3906	7/7	0.99	0.11	62,62,62,62	0
86	OHX	5	3907	7/7	0.99	0.11	65,65,65,65	0
86	OHX	5	3908	7/7	0.99	0.10	62,62,62,62	0
86	OHX	5	3910	7/7	0.99	0.13	71,71,71,71	0
86	OHX	5	3911	7/7	0.99	0.08	62,62,62,62	0
86	OHX	5	4078	7/7	0.99	0.13	100,100,100,100	0
86	OHX	5	3913	7/7	0.99	0.12	65,65,65,65	0
86	OHX	5	3915	7/7	0.99	0.12	66,66,66,66	0
86	OHX	5	3916	7/7	0.99	0.07	70,70,70,70	0
86	OHX	5	3918	7/7	0.99	0.07	63,63,63,63	0
86	OHX	5	3919	7/7	0.99	0.07	72,72,72,72	0
86	OHX	5	3921	7/7	0.99	0.06	65,65,65,65	0
86	OHX	5	3922	7/7	0.99	0.07	69,69,69,69	0
86	OHX	5	3923	7/7	0.99	0.07	66,66,66,66	0
86	OHX	5	3924	7/7	0.99	0.10	74,74,74,74	0
86	OHX	5	3925	7/7	0.99	0.07	72,72,72,72	0
86	OHX	1	3979	7/7	0.99	0.06	119,119,119,119	0
86	OHX	5	3928	7/7	0.99	0.07	78,78,78,78	0
86	OHX	7	215	7/7	0.99	0.09	91,91,91,91	0
86	OHX	5	3929	7/7	0.99	0.06	77,77,77,77	0
86	OHX	1	3903	7/7	0.99	0.07	94,94,94,94	0
86	OHX	5	3932	7/7	0.99	0.08	75,75,75,75	0
86	OHX	1	3981	7/7	0.99	0.12	100,100,100,100	0
86	OHX	7	220	7/7	0.99	0.07	106,106,106,106	0
86	OHX	5	3934	7/7	0.99	0.06	73,73,73,73	0
86	OHX	5	3935	7/7	0.99	0.07	83,83,83,83	0
86	OHX	5	3936	7/7	0.99	0.05	81,81,81,81	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	0.06	76,76,76,76	0
86	OHX	5	3938	7/7	0.99	0.08	78,78,78,78	0
86	OHX	5	3939	7/7	0.99	0.09	86,86,86,86	0
86	OHX	8	217	7/7	0.99	0.09	60,60,60,60	0
86	OHX	5	3940	7/7	0.99	0.12	88,88,88,88	0
86	OHX	1	3904	7/7	0.99	0.07	87,87,87,87	0
86	OHX	1	3905	7/7	0.99	0.10	91,91,91,91	0
86	OHX	5	3943	7/7	0.99	0.11	98,98,98,98	0
86	OHX	5	3944	7/7	0.99	0.09	83,83,83,83	0
85	MG	1	3793	1/1	0.99	0.16	41,41,41,41	0
86	OHX	5	3946	7/7	0.99	0.06	80,80,80,80	0
85	MG	5	3579	1/1	0.99	0.27	32,32,32,32	0
86	OHX	1	3909	7/7	0.99	0.06	86,86,86,86	0
86	OHX	5	3949	7/7	0.99	0.12	100,100,100,100	0
86	OHX	1	3910	7/7	0.99	0.07	87,87,87,87	0
86	OHX	1	3911	7/7	0.99	0.07	91,91,91,91	0
86	OHX	2	2033	7/7	0.99	0.07	104,104,104,104	0
85	MG	1	3520	1/1	0.99	0.06	39,39,39,39	0
86	OHX	5	3955	7/7	0.99	0.06	99,99,99,99	0
86	OHX	2	2035	7/7	0.99	0.09	103,103,103,103	0
86	OHX	4	222	7/7	0.99	0.09	59,59,59,59	0
86	OHX	5	3958	7/7	0.99	0.08	91,91,91,91	0
86	OHX	4	224	7/7	0.99	0.09	81,81,81,81	0
86	OHX	5	3960	7/7	0.99	0.08	75,75,75,75	0
86	OHX	4	225	7/7	0.99	0.14	94,94,94,94	0
86	OHX	5	3962	7/7	0.99	0.08	98,98,98,98	0
86	OHX	5	3963	7/7	0.99	0.06	92,92,92,92	0
86	OHX	1	3915	7/7	0.99	0.09	98,98,98,98	0
86	OHX	1	3916	7/7	0.99	0.07	92,92,92,92	0
86	OHX	5	3966	7/7	0.99	0.10	103,103,103,103	0
85	MG	5	3596	1/1	0.99	0.31	21,21,21,21	0
86	OHX	2	2037	7/7	0.99	0.06	97,97,97,97	0
86	OHX	5	3969	7/7	0.99	0.07	93,93,93,93	0
86	OHX	1	3919	7/7	0.99	0.08	98,98,98,98	0
86	OHX	n3	203	7/7	0.99	0.09	92,92,92,92	0
86	OHX	n9	101	7/7	0.99	0.09	70,70,70,70	0
86	OHX	5	3971	7/7	0.99	0.07	103,103,103,103	0
86	OHX	5	3972	7/7	0.99	0.08	91,91,91,91	0
86	OHX	1	3997	7/7	0.99	0.12	95,95,95,95	0
86	OHX	5	3974	7/7	0.99	0.08	87,87,87,87	0
86	OHX	1	3920	7/7	0.99	0.08	85,85,85,85	0
85	MG	1	3801	1/1	0.99	0.08	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	q2	502	7/7	0.99	0.10	87,87,87,87	0
86	OHX	5	3977	7/7	0.99	0.07	102,102,102,102	0
86	OHX	1	3922	7/7	0.99	0.14	80,80,80,80	0
86	OHX	5	3979	7/7	0.99	0.11	86,86,86,86	0
85	MG	5	3862	1/1	0.99	0.08	63,63,63,63	0
86	OHX	1	3924	7/7	0.99	0.06	92,92,92,92	0
85	MG	1	3486	1/1	0.99	0.35	41,41,41,41	0
86	OHX	5	3983	7/7	0.99	0.13	91,91,91,91	0
85	MG	5	3883	1/1	0.99	0.25	58,58,58,58	0
86	OHX	6	2055	7/7	1.00	0.07	76,76,76,76	0
86	OHX	1	3868	7/7	1.00	0.10	55,55,55,55	0
86	OHX	8	218	7/7	1.00	0.08	60,60,60,60	0
86	OHX	1	3863	7/7	1.00	0.11	47,47,47,47	0
86	OHX	5	3954	7/7	1.00	0.06	78,78,78,78	0
86	OHX	5	3931	7/7	1.00	0.05	68,68,68,68	0
86	OHX	5	3909	7/7	1.00	0.07	52,52,52,52	0
86	OHX	1	3889	7/7	1.00	0.05	70,70,70,70	0
86	OHX	4	223	7/7	1.00	0.10	67,67,67,67	0
86	OHX	5	3912	7/7	1.00	0.06	59,59,59,59	0
86	OHX	1	3878	7/7	1.00	0.04	69,69,69,69	0
86	OHX	5	3914	7/7	1.00	0.07	67,67,67,67	0
86	OHX	1	3864	7/7	1.00	0.10	50,50,50,50	0
86	OHX	1	3865	7/7	1.00	0.08	52,52,52,52	0
86	OHX	5	3917	7/7	1.00	0.06	67,67,67,67	0
86	OHX	1	3881	7/7	1.00	0.05	64,64,64,64	0
86	OHX	1	3906	7/7	1.00	0.05	78,78,78,78	0
86	OHX	5	3920	7/7	1.00	0.08	70,70,70,70	0
86	OHX	1	3866	7/7	1.00	0.10	59,59,59,59	0
88	ZN	D6	500	1/1	1.00	0.02	80,80,80,80	0
85	MG	5	3822	1/1	1.00	0.06	55,55,55,55	0
88	ZN	D9	101	1/1	1.00	0.05	81,81,81,81	0
86	OHX	5	3902	7/7	1.00	0.09	47,47,47,47	0
88	ZN	O7	101	1/1	1.00	0.01	41,41,41,41	0
88	ZN	Q0	500	1/1	1.00	0.02	56,56,56,56	0
86	OHX	1	3874	7/7	1.00	0.06	64,64,64,64	0
88	ZN	Q3	501	1/1	1.00	0.02	68,68,68,68	0
88	ZN	d6	101	1/1	1.00	0.02	62,62,62,62	0
86	OHX	1	3875	7/7	1.00	0.06	60,60,60,60	0
88	ZN	d9	101	1/1	1.00	0.02	78,78,78,78	0
86	OHX	5	3926	7/7	1.00	0.05	63,63,63,63	0
88	ZN	o7	501	1/1	1.00	0.01	44,44,44,44	0
88	ZN	q0	201	1/1	1.00	0.02	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	3886	7/7	1.00	0.07	73,73,73,73	0
88	ZN	q3	501	1/1	1.00	0.03	75,75,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.