wwPDB X-ray Structure Validation Summary Report (i)

Jan 4, 2024 – 03:26 pm GMT

PDB ID	:	5FCJ
Title	:	Structure of the anisomycin-containing uL3 W255C mutant 80S yeast ribosome
Authors	:	Mailliot, J.; Garreau de Loubresse, N.; Yusupova, G.; Dinman, J.D.; Yusupov, M.
Deposited on	:	2015-12-15
Resolution	:	3.10 Å(reported)

This is a 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 (i) 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 (i)) were used in the production of this report:

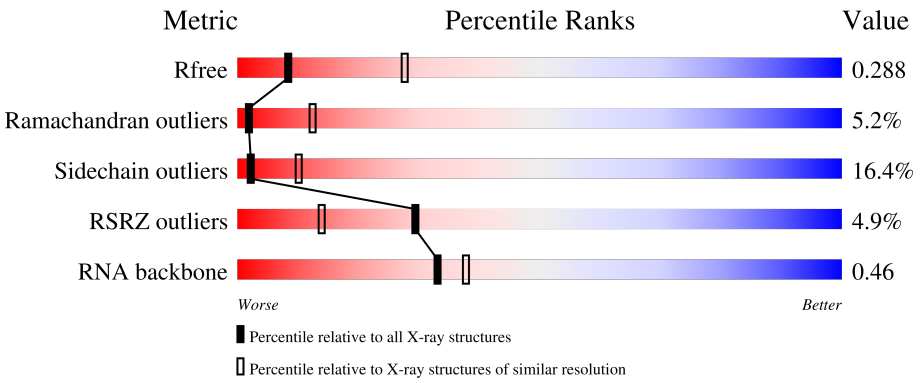
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1800	8% 72% 26% • •
1	6	1800	7% 72% 26% •
2	S0	251	6% 67% 14% • 18%
2	s0	251	2% 66% 16% • 18%
3	S1	254	17% 65% 19% • 16%

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

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Mol	Chain	Length	Quality of chain
16	C4	136	18% 75% 15% 7%
16	c4	136	% 74% 18% 6%
17	C5	141	2% 73% 14% 12%
17	c5	141	7% 77% 16%
18	C6	142	4% 82% 15%
18	c6	142	13% 82% 18%
19	C7	136	8% 71% 15% 12%
19	c7	136	12% 71% 14% 14%
20	C8	145	12% 77% 20%
20	c8	145	6% 77% 21%
21	C9	143	5% 80% 20%
21	c9	143	86% 13%
22	D0	120	22% 70% 19% 11%
22	d0	120	25% 67% 24% 8%
23	D1	87	6% 75% 25%
23	d1	87	2% 85% 15%
24	D2	129	2% 84% 14%
24	d2	129	87% 12%
25	D3	144	% 81% 19%
25	d3	144	86% 14%
26	D4	134	9% 80% 19%
26	d4	134	4% 81% 19%
27	D5	107	2% 45% 21% 35%
27	d5	107	9% 56% 8% 36%
28	D6	97	4% 71% 23% 6%

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

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Mol	Chain	Length	Quality of chain
41	L4	361	81% 18%
41	l4	361	.% 83% 15%
42	L5	296	2% 81% 18%
42	l5	296	2% 82% 17%
43	L6	175	78% 11% 11%
43	l6	175	.% 74% 14% 10%
44	L7	243	82% 9% 9%
44	l7	243	2% 80% 10% 8%
45	L8	255	3% 76% 15% 9%
45	l8	255	6% 74% 16% 9%
46	L9	191	.% 79% 20%
46	l9	191	.% 80% 20%
47	M0	220	.% 78% 18%
47	m0	220	2% 79% 17%
48	M1	173	4% 73% 21%
48	m1	173	.% 77% 18%
49	M3	198	3% 80% 17%
49	m3	198	3% 80% 17%
50	M4	137	.% 83% 15%
50	m4	137	.% 88% 11%
51	M5	203	82% 18%
51	m5	203	86% 13%
52	M6	198	.% 86% 13%
52	m6	198	87% 12%
53	M7	183	9% 85% 14%

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Mol	Chain	Length	Quality of chain
53	m7	183	75% 10% 15%
54	M8	185	85% 14% •
54	m8	185	.% 84% 15% •
55	M9	188	5% 89% 11%
55	m9	188	4% 82% 18%
56	N0	172	.% 83% 17% •
56	n0	172	82% 18%
57	N1	159	2% 82% 18%
57	n1	159	2% 82% 17% •
58	N2	120	9% 73% 10% 17%
58	n2	120	9% 68% 12% • 18%
59	N3	136	3% 86% 14%
59	n3	136	.% 91% 9%
60	N4	155	14% 55% 8% 37%
60	n4	155	12% 74% 13% • 13%
61	N5	141	.% 69% 15% • 14%
61	n5	141	4% 69% 15% • 15%
62	N6	126	3% 84% 15% •
62	n6	126	.% 83% 15% •
63	N7	135	2% 84% 14% •
63	n7	135	3% 79% 17% •
64	N8	148	.% 81% 14% 5%
64	n8	148	80% 19% •
65	N9	58	3% 83% 16% •
65	n9	58	78% 19% •

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Mol	Chain	Length	Quality of chain
66	O0	104	8% 76% 17% 7%
66	o0	104	5% 76% 19%
67	O1	112	79% 17%
67	o1	112	79% 19%
68	O2	129	82% 15%
68	o2	129	81% 16%
69	O3	106	91% 9%
69	o3	106	90% 10%
70	O4	120	5% 79% 14% 7%
70	o4	120	78% 15% 7%
71	O5	119	81% 18%
71	o5	119	82% 18%
72	O6	99	5% 76% 23%
72	o6	99	3% 71% 27%
73	O7	87	84% 15%
73	o7	87	83% 16%
74	O8	77	4% 82% 18%
74	o8	77	8% 84% 16%
75	O9	50	4% 86% 12%
75	o9	50	90% 10%
76	Q0	52	85% 13%
76	q0	52	77% 21%
77	Q1	25	4% 84% 16%
77	q1	25	68% 32%
78	Q2	105	3% 79% 19%

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Mol	Chain	Length	Quality of chain
78	q2	105	4% 84% 16%
79	Q3	91	80% 19%
79	q3	91	% 86% 11%
80	m2	150	100%
81	p0	311	4% 40% 6% 54%
82	p1	47	100%
83	p2	46	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	MG	1	3414	-	-	-	X
84	MG	1	3435	-	-	-	X
84	MG	1	3487	-	-	-	X
84	MG	1	3496	-	-	-	X
84	MG	1	3568	-	-	-	X
84	MG	1	3570	-	-	-	X
84	MG	1	3599	-	-	-	X
84	MG	1	3630	-	-	-	X
84	MG	1	3639	-	-	-	X
84	MG	1	3667	-	-	-	X
84	MG	1	3673	-	-	-	X
84	MG	1	3694	-	-	-	X
84	MG	1	3709	-	-	-	X
84	MG	1	3715	-	-	-	X
84	MG	1	4043	-	-	-	X
84	MG	2	1904	-	-	-	X
84	MG	2	1909	-	-	-	X
84	MG	2	1911	-	-	-	X
84	MG	2	1912	-	-	-	X
84	MG	2	1915	-	-	-	X
84	MG	2	1923	-	-	-	X
84	MG	2	1941	-	-	-	X
84	MG	2	1946	-	-	-	X
84	MG	2	1956	-	-	-	X
84	MG	2	1962	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	MG	2	1969	-	-	-	X
84	MG	2	1970	-	-	-	X
84	MG	2	1972	-	-	-	X
84	MG	2	1978	-	-	-	X
84	MG	4	202	-	-	-	X
84	MG	5	3457	-	-	-	X
84	MG	5	3476	-	-	-	X
84	MG	5	3542	-	-	-	X
84	MG	5	3617	-	-	-	X
84	MG	5	3632	-	-	-	X
84	MG	5	3636	-	-	-	X
84	MG	5	3641	-	-	-	X
84	MG	5	3643	-	-	-	X
84	MG	5	3655	-	-	-	X
84	MG	5	3709	-	-	-	X
84	MG	5	3731	-	-	-	X
84	MG	6	1917	-	-	-	X
84	MG	6	1930	-	-	-	X
84	MG	6	1938	-	-	-	X
84	MG	6	1961	-	-	-	X
84	MG	6	1965	-	-	-	X
84	MG	6	1969	-	-	-	X
84	MG	6	1971	-	-	-	X
84	MG	6	1984	-	-	-	X
84	MG	6	2001	-	-	-	X
84	MG	6	2002	-	-	-	X
84	MG	6	2008	-	-	-	X
84	MG	8	207	-	-	-	X
84	MG	O7	103	-	-	-	X
84	MG	SM	201	-	-	-	X
84	MG	l6	201	-	-	-	X
87	ANM	1	3401	X	-	-	X

2 Entry composition (i)

There are 87 unique types of molecules in this entry. The entry contains 410912 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	S0	206	1577	1014	278	283	2	0	0	0
2	s0	206	1612	1034	285	291	2	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	S7	184	1481	951	265	265	0	0	0
9	s7	186	1492	957	267	268	0	0	0

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

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

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

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

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

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

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

- Molecule 13 is a protein called 40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A (uS17).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	C1	155	1214	775	230	206	3	0	0	0
			Total	C	N	O	S			
13	c1	146	1169	748	221	197	3	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	C7	120	926	577	177	170	2	0	0	0
			Total	C	N	O	S			
19	c7	117	944	591	179	172	2	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	d9	53	443	275	92	72	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	E0	60	475	299	98	77	1	0	0	0
			Total	C	N	O	S			
32	e0	62	491	309	101	80	1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	SR	318	2437	1541	418	470	8	0	0	0
			Total	C	N	O	S			
34	sR	318	2445	1546	419	472	8	0	0	0

- Molecule 35 is a protein called Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1.

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
36	5	3150	67377	30095	12145	21987	3150	0	0	0

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L3	255	CYS	TRP	engineered mutation	UNP P14126
l3	255	CYS	TRP	engineered mutation	UNP P14126

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	L4	361	2748	1729	522	494	3	0	0	0
41	l4	361	2749	1730	522	494	3	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
60	N4	98	699	443	137	118	1	0	0	0
60	n4	135	1089	682	219	187	1	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
70	O4	112	880	545	179	152	4	0	0	0
70	o4	112	881	546	179	152	4	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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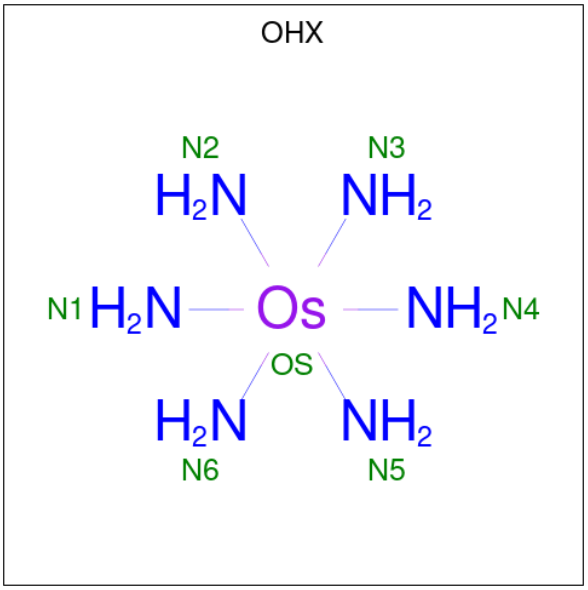
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	n6	2	Total Mg 2 2	0	0
84	n8	2	Total Mg 2 2	0	0
84	n9	1	Total Mg 1 1	0	0
84	o1	1	Total Mg 1 1	0	0
84	o3	1	Total Mg 1 1	0	0
84	o4	1	Total Mg 1 1	0	0
84	q0	1	Total Mg 1 1	0	0
84	q1	1	Total Mg 1 1	0	0

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



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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	S8	1	7	6	1	0	0
85	C3	1	7	6	1	0	0
85	C5	1	7	6	1	0	0
85	C8	1	7	6	1	0	0
85	D9	1	7	6	1	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	1	1	7	6	1	0	0
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85	1	1	7	6	1	0	0
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85	3	1	7	6	1	0	0
85	3	1	7	6	1	0	0
85	3	1	7	6	1	0	0
85	3	1	7	6	1	0	0
85	3	1	7	6	1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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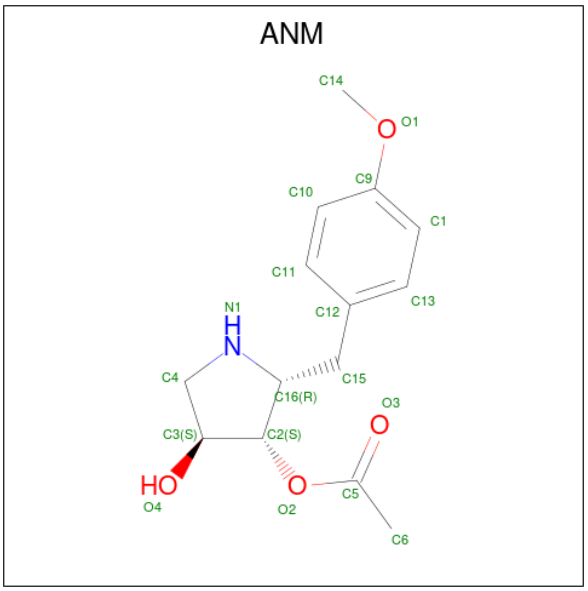
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	o9	1	7	6	1	0	0
			Total	N	Os		
85	q2	1	7	6	1	0	0

- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
86	D6	1	1	1	0	0
			Total	Zn		
86	D7	1	1	1	0	0
			Total	Zn		
86	D9	1	1	1	0	0
			Total	Zn		
86	E1	1	1	1	0	0
			Total	Zn		
86	O7	1	1	1	0	0
			Total	Zn		
86	Q0	1	1	1	0	0
			Total	Zn		
86	Q2	1	1	1	0	0
			Total	Zn		
86	Q3	1	1	1	0	0
			Total	Zn		
86	d6	1	1	1	0	0
			Total	Zn		
86	d7	1	1	1	0	0
			Total	Zn		
86	d9	1	1	1	0	0
			Total	Zn		
86	e1	1	1	1	0	0
			Total	Zn		
86	o7	1	1	1	0	0
			Total	Zn		
86	q0	1	1	1	0	0
			Total	Zn		
86	q2	1	1	1	0	0
			Total	Zn		
86	q3	1	1	1	0	0

- Molecule 87 is ANISOMYCIN (three-letter code: ANM) (formula: $C_{14}H_{19}NO_4$).



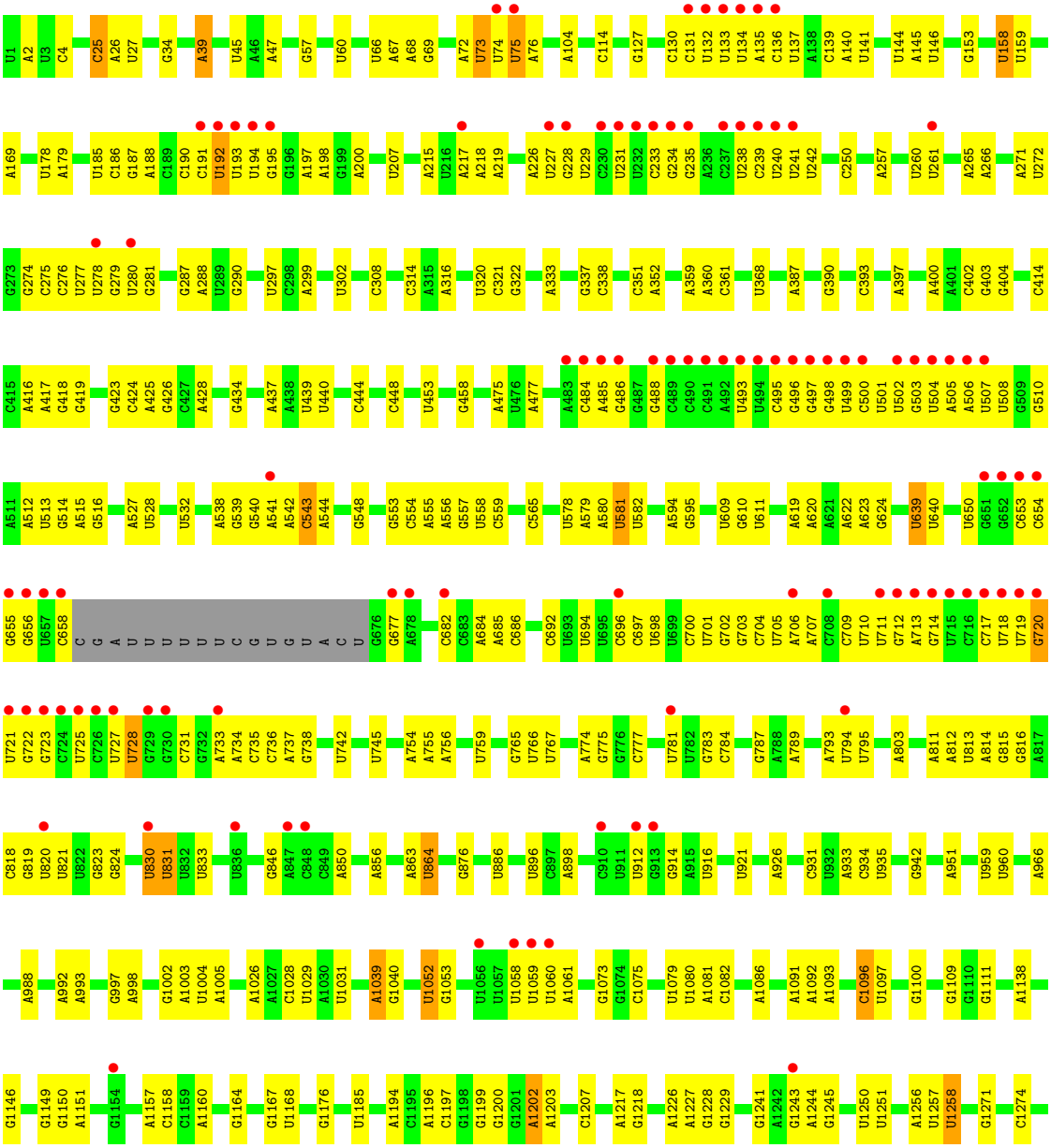
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
87	1	1	19	14	1	4	0	0

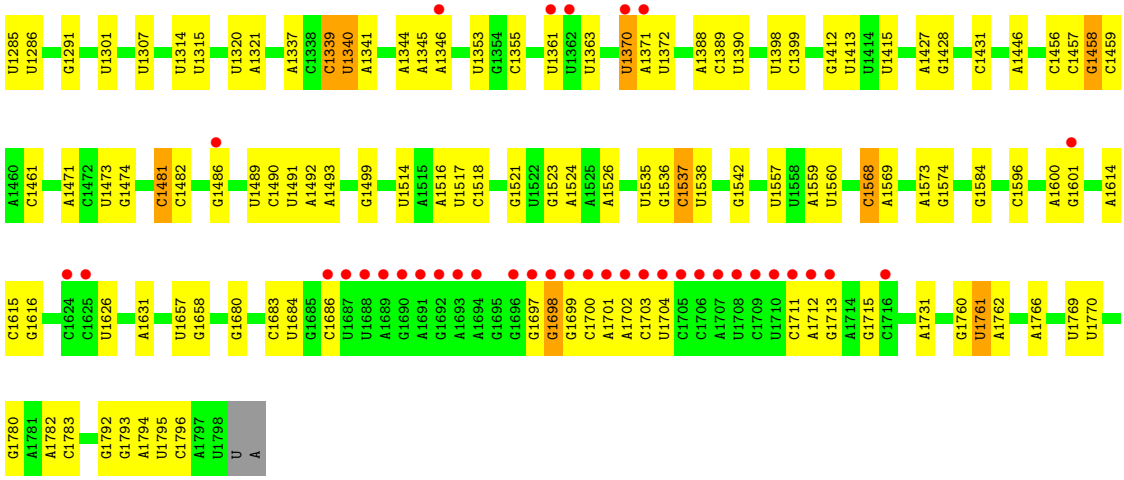
3 Residue-property plots (i)

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

- Molecule 1: 18S ribosomal RNA

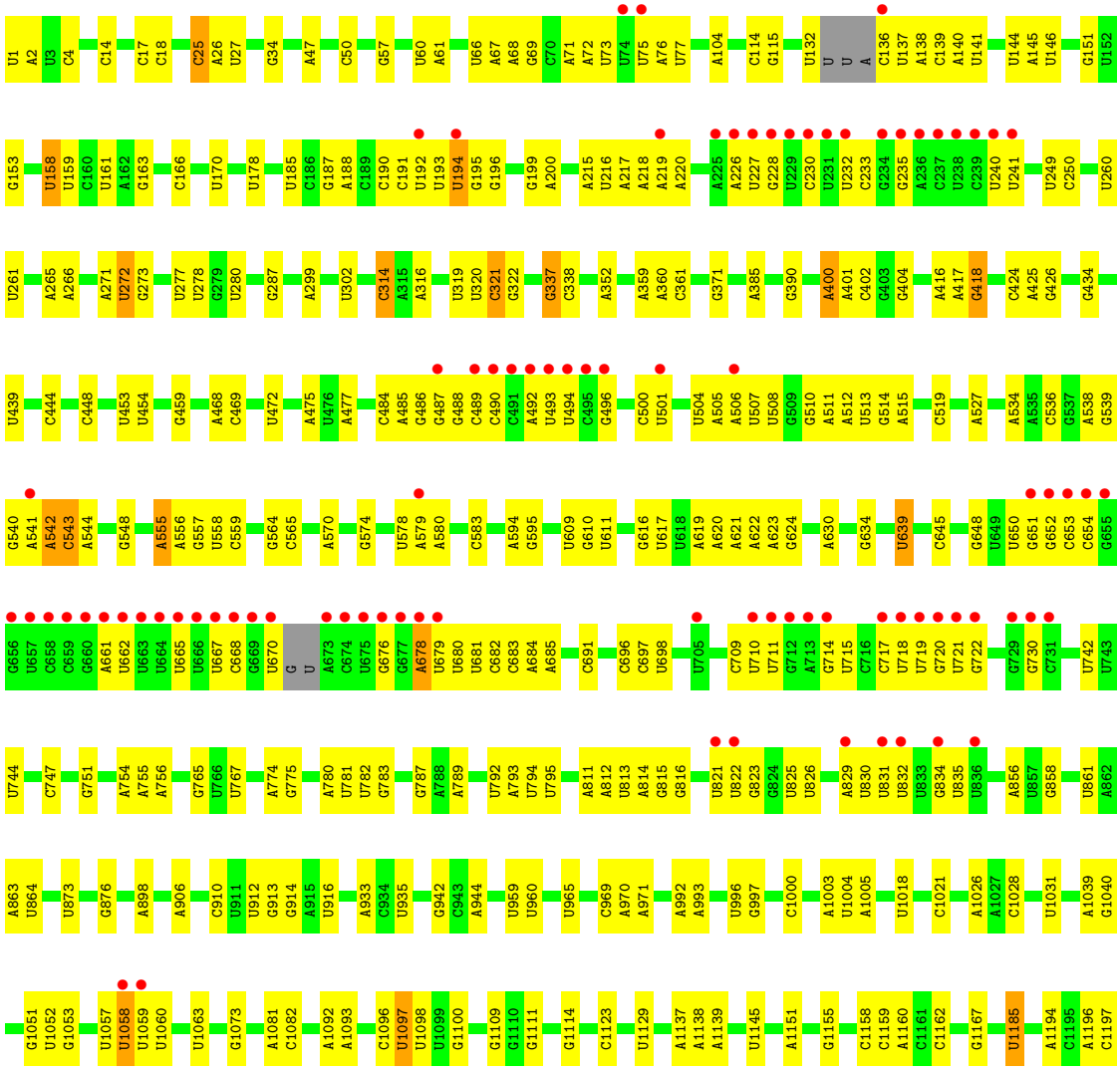
Chain 2:

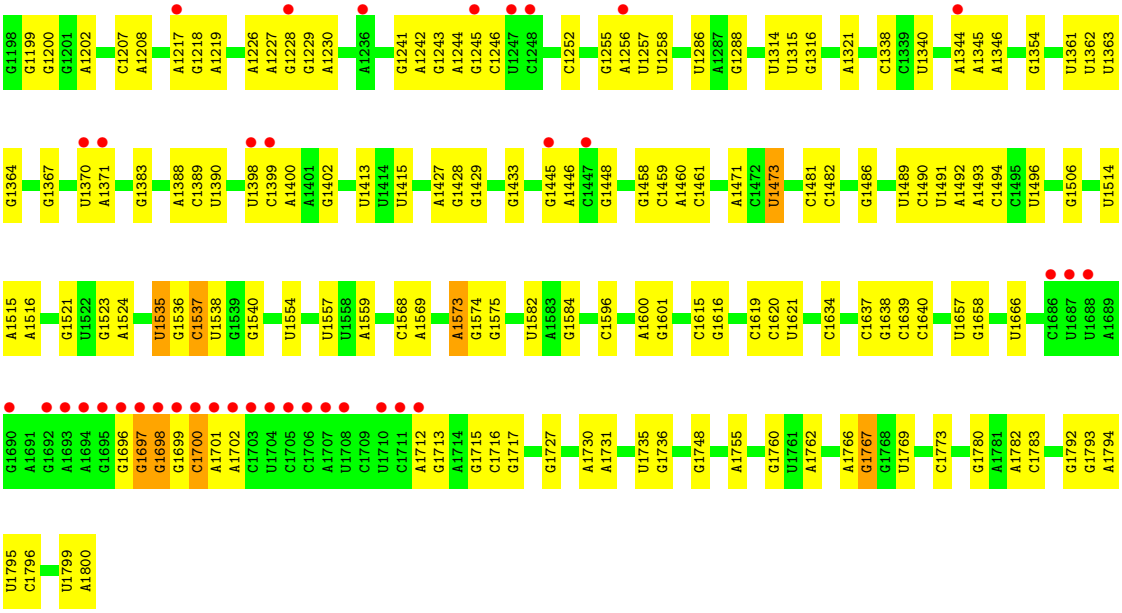




- Molecule 1: 18S ribosomal RNA

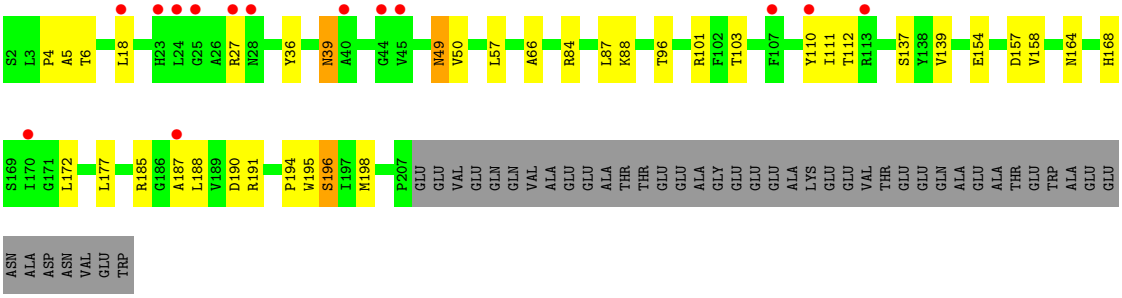
Chain 6:





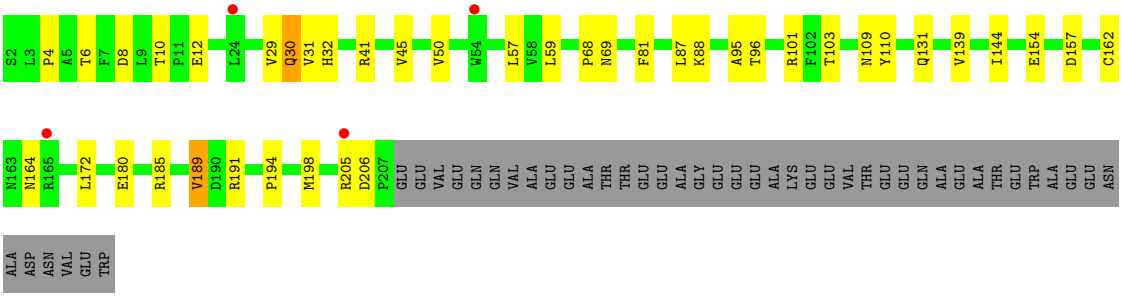
- Molecule 2: 40S ribosomal protein S0-A

Chain S0:



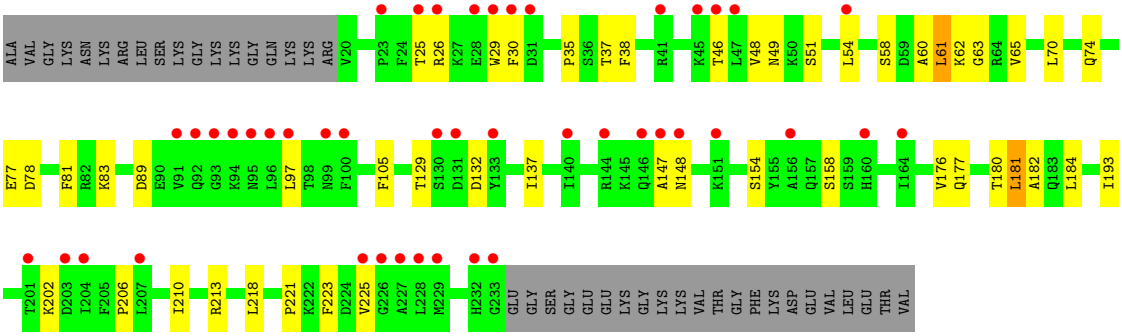
- Molecule 2: 40S ribosomal protein S0-A

Chain s0:



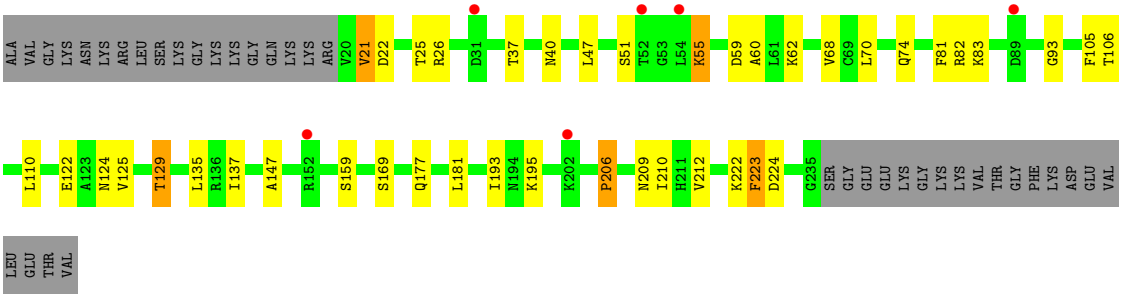
- Molecule 3: 40S ribosomal protein S1-A

Chain S1:



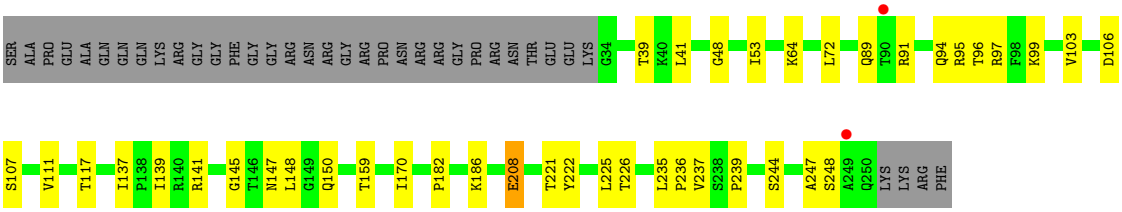
- Molecule 3: 40S ribosomal protein S1-A

Chain s1:



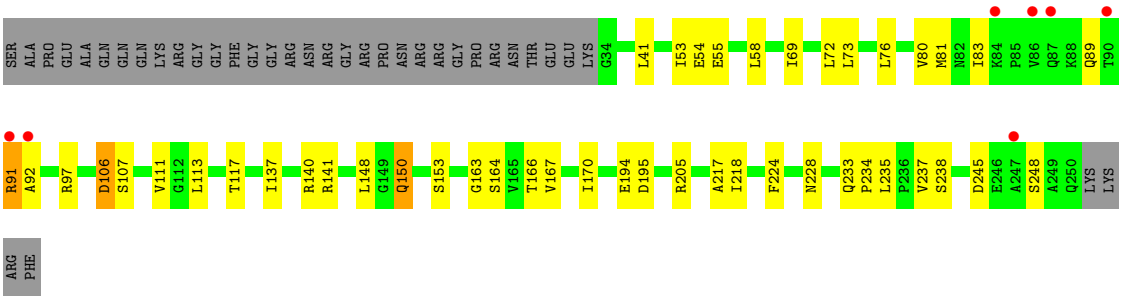
- Molecule 4: 40S ribosomal protein S2

Chain S2:



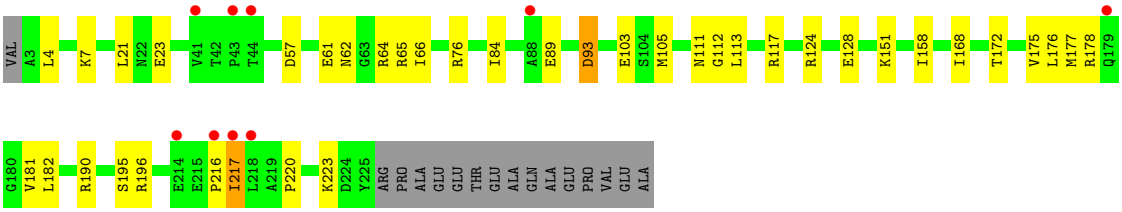
- Molecule 4: 40S ribosomal protein S2

Chain s2:



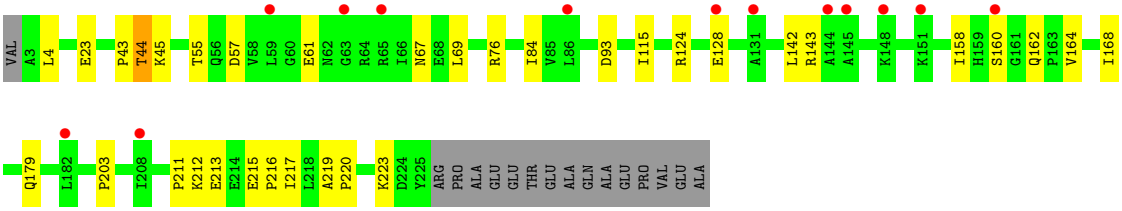
- Molecule 5: 40S ribosomal protein S3

Chain S3:



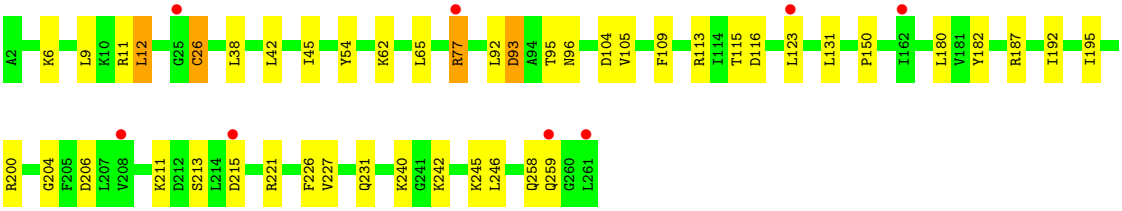
- Molecule 5: 40S ribosomal protein S3

Chain s3:



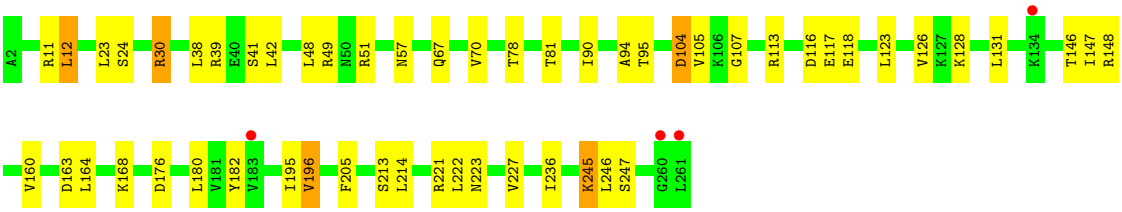
- Molecule 6: 40S ribosomal protein S4-A

Chain S4:



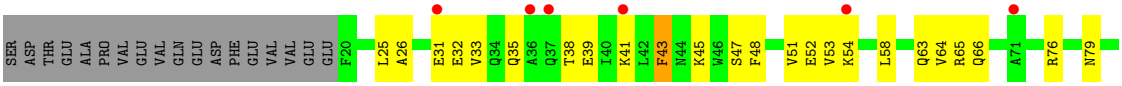
- Molecule 6: 40S ribosomal protein S4-A

Chain s4:



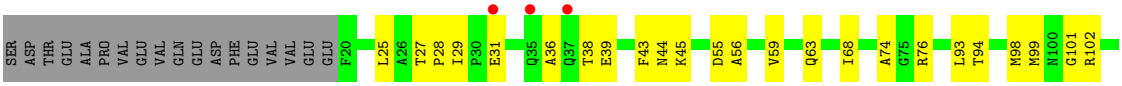
- Molecule 7: 40S ribosomal protein S5

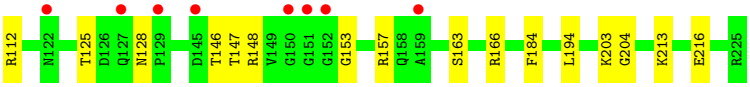
Chain S5:



• Molecule 7: 40S ribosomal protein S5

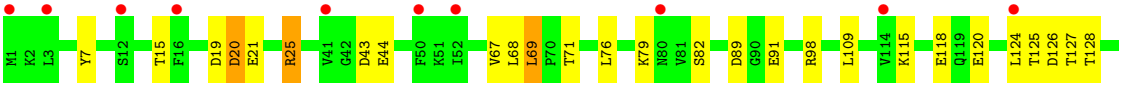
Chain s5:

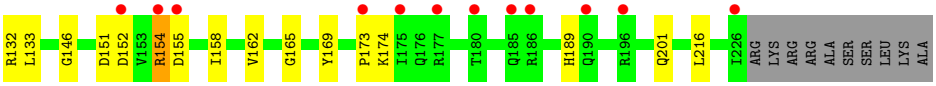




• Molecule 8: 40S ribosomal protein S6-A

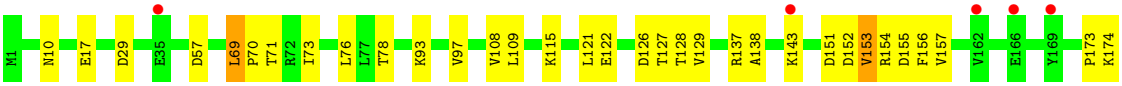
Chain S6:

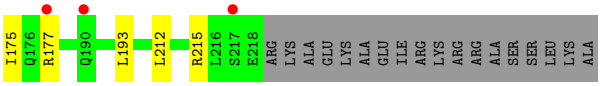




• Molecule 8: 40S ribosomal protein S6-A

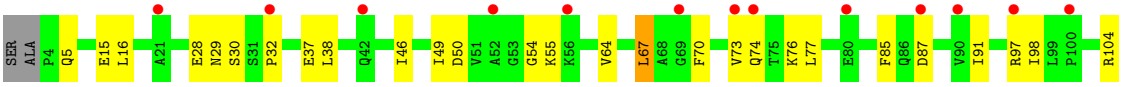
Chain s6:





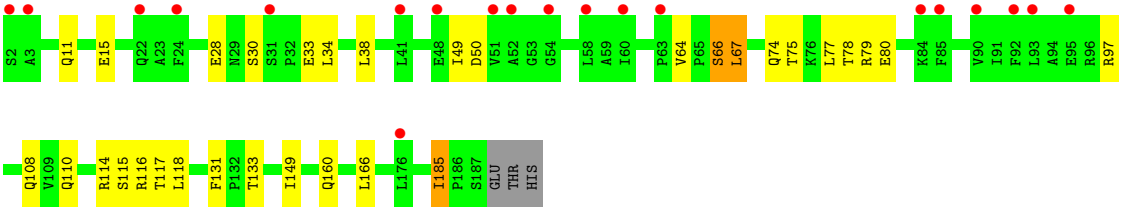
• Molecule 9: 40S ribosomal protein S7-A

Chain S7:



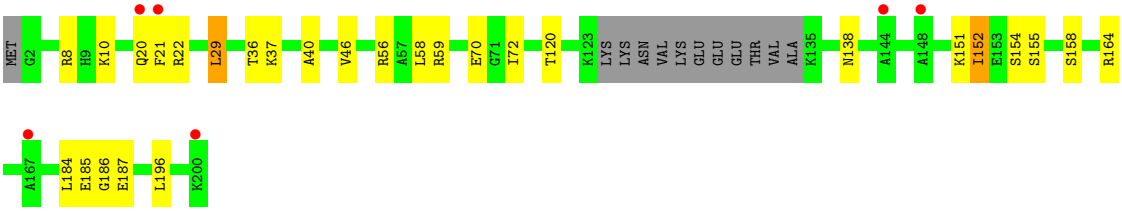
• Molecule 9: 40S ribosomal protein S7-A

Chain s7:



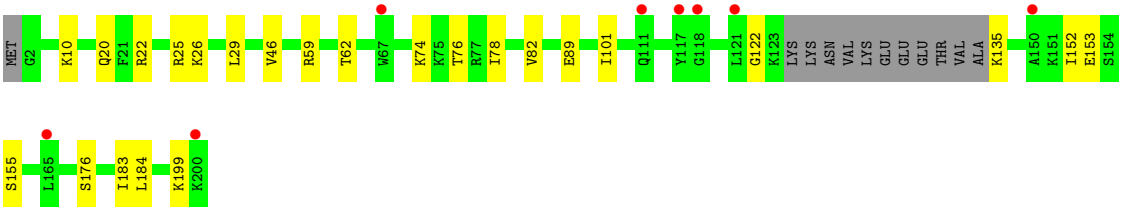
• Molecule 10: 40S ribosomal protein S8-A

Chain S8:



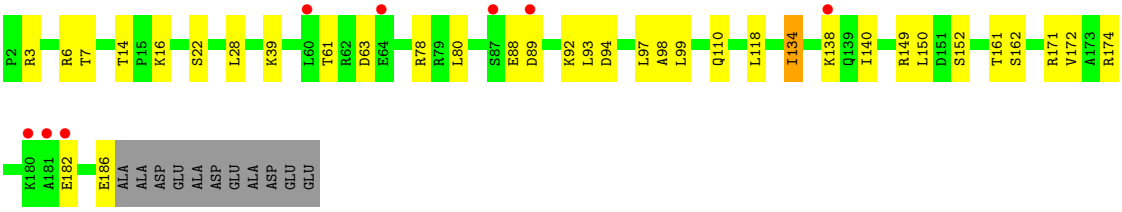
• Molecule 10: 40S ribosomal protein S8-A

Chain s8:



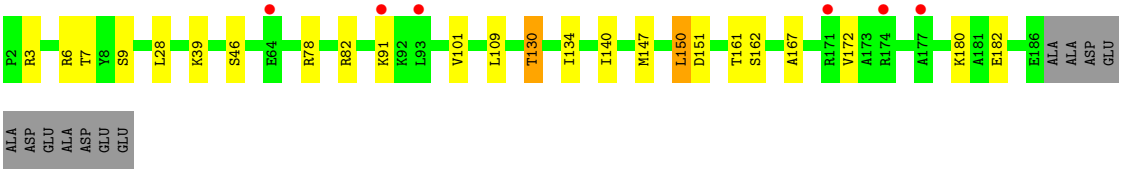
• Molecule 11: 40S ribosomal protein S9-A

Chain S9:



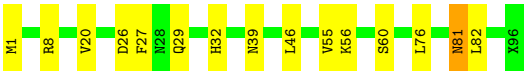
• Molecule 11: 40S ribosomal protein S9-A

Chain s9:



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

Chain C0:

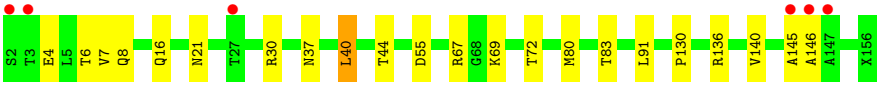


• Molecule 12: 40S ribosomal protein S10-A,40S ribosomal protein S10-A,40S ribosomal protein S10-A,40S ribosomal protein S10-A

Chain c0:

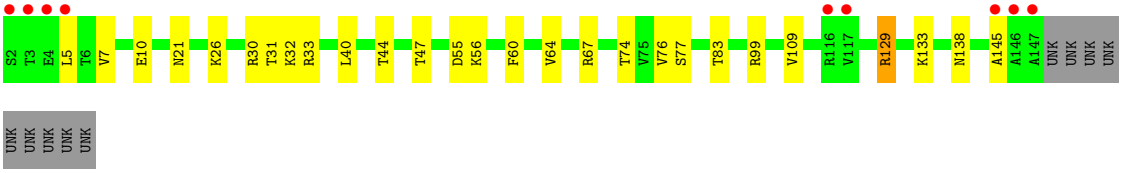
• Molecule 13: 40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A (uS17)

Chain C1:



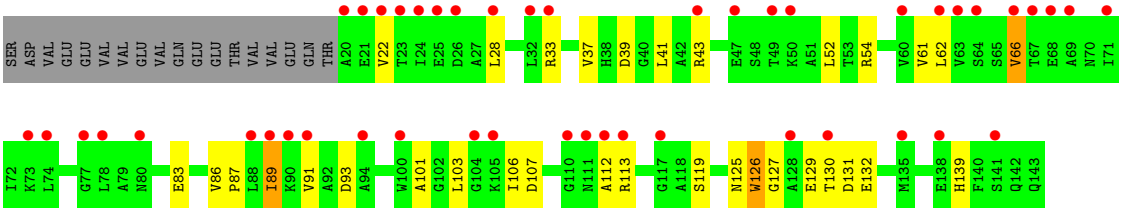
• Molecule 13: 40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A (uS17)

Chain c1:



• Molecule 14: 40S ribosomal protein S12

Chain C2:



• Molecule 14: 40S ribosomal protein S12

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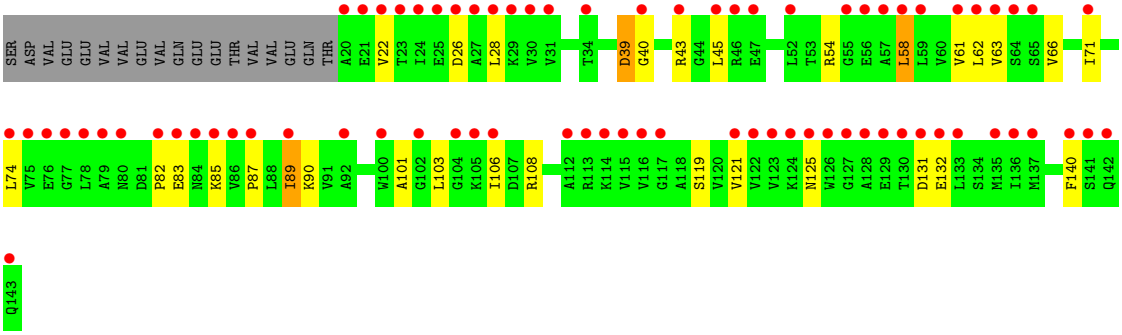
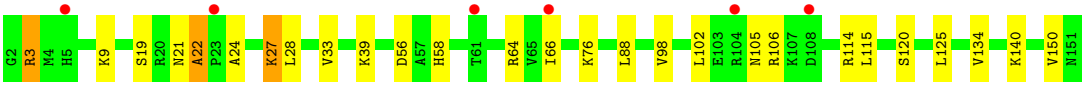


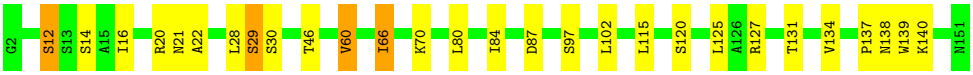
- Molecule 15: 40S ribosomal protein S13

Chain C3:



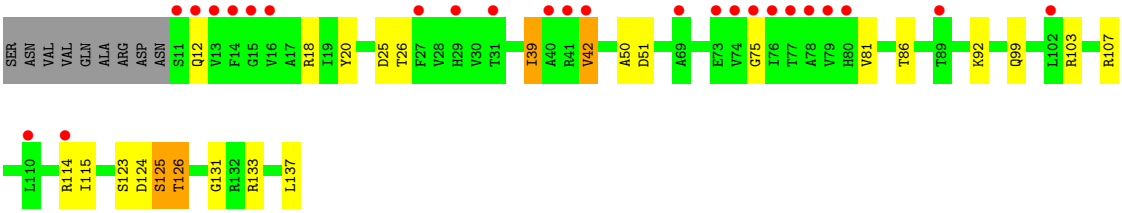
- Molecule 15: 40S ribosomal protein S13

Chain c3:



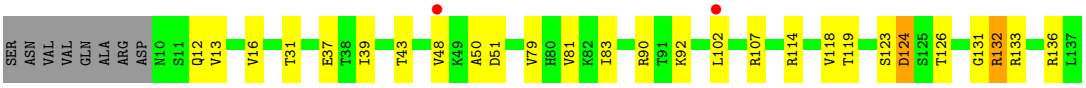
- Molecule 16: 40S ribosomal protein S14-A

Chain C4:



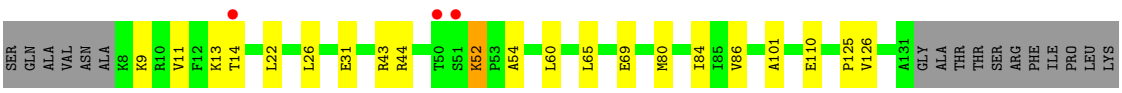
- Molecule 16: 40S ribosomal protein S14-A

Chain c4:



- Molecule 17: 40S ribosomal protein S15

Chain C5:

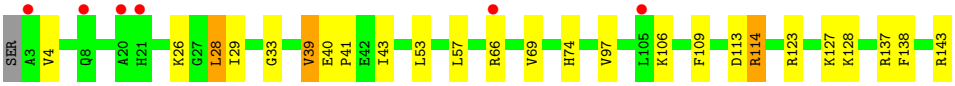


• Molecule 17: 40S ribosomal protein S15

Chain c5:

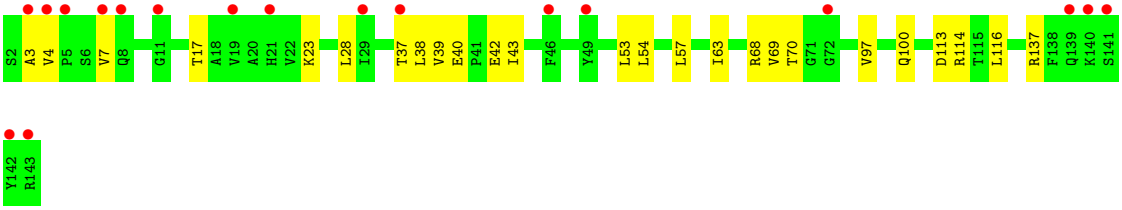
• Molecule 18: 40S ribosomal protein S16-A

Chain C6:



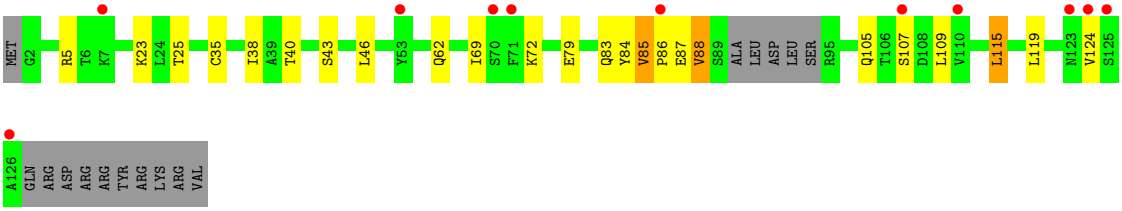
• Molecule 18: 40S ribosomal protein S16-A

Chain c6:



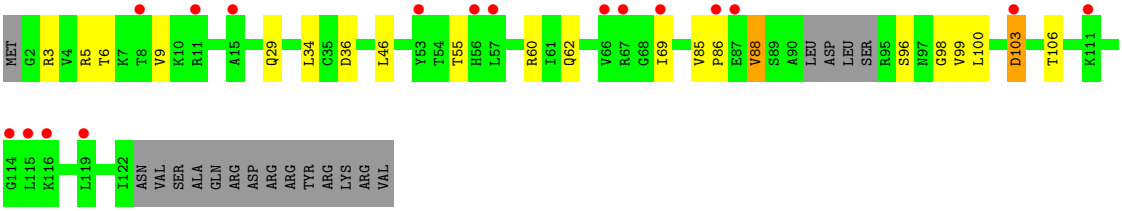
• Molecule 19: 40S ribosomal protein S17-A

Chain C7:



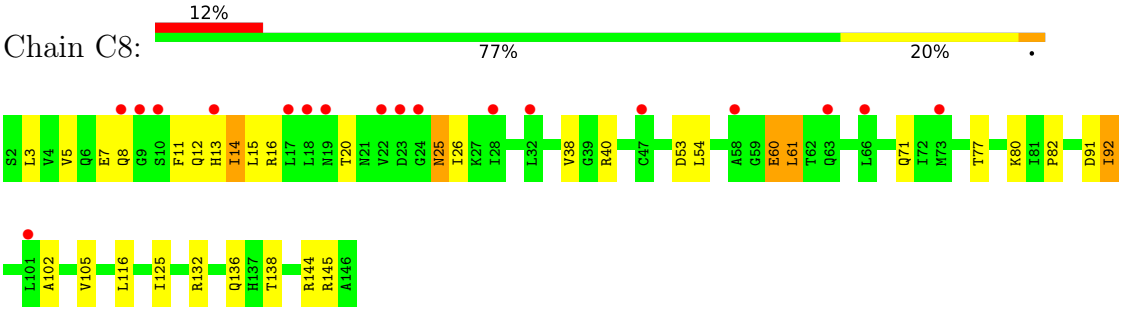
• Molecule 19: 40S ribosomal protein S17-A

Chain c7:



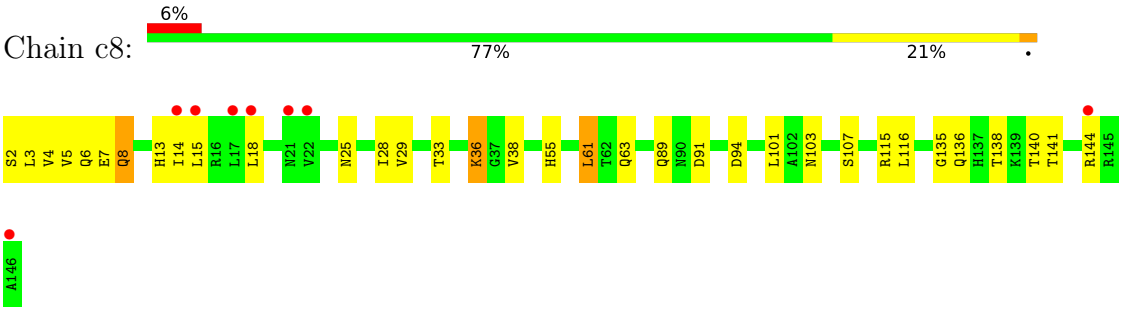
• Molecule 20: 40S ribosomal protein S18-A

Chain C8:



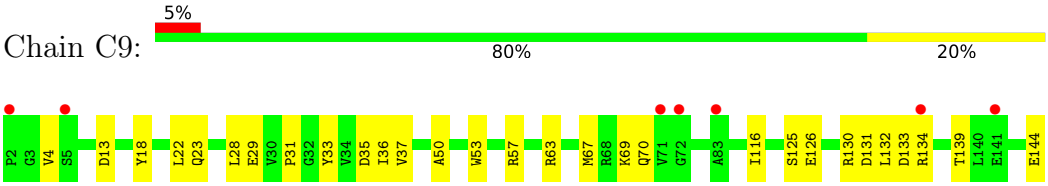
- Molecule 20: 40S ribosomal protein S18-A

Chain c8:



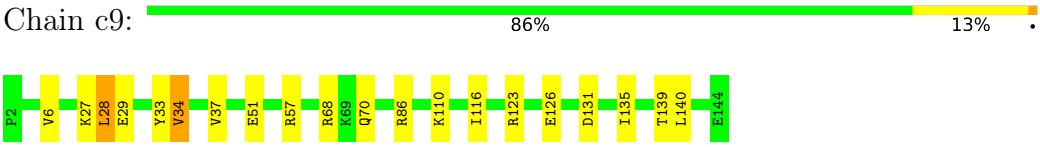
- Molecule 21: 40S ribosomal protein S19-A

Chain C9:



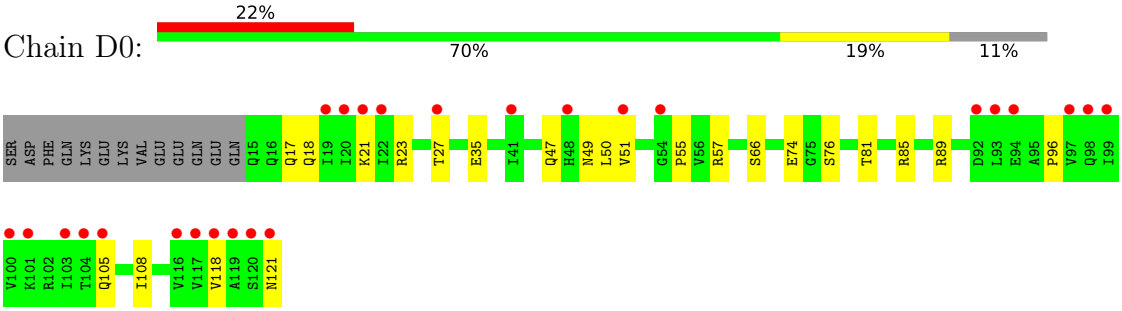
- Molecule 21: 40S ribosomal protein S19-A

Chain c9:



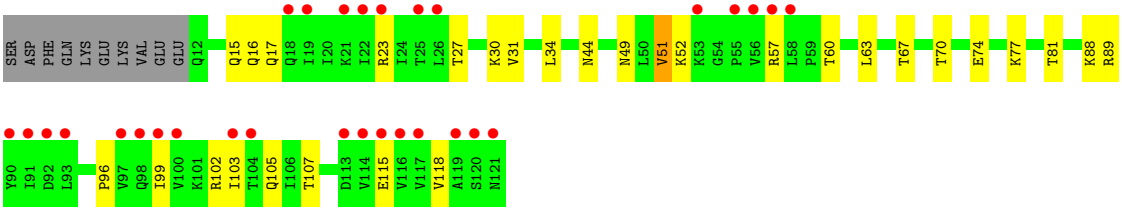
- Molecule 22: 40S ribosomal protein S20

Chain D0:



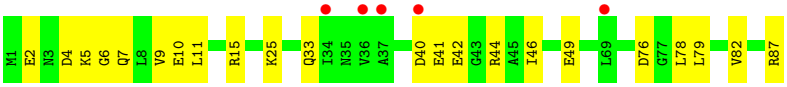
- Molecule 22: 40S ribosomal protein S20

Chain d0:



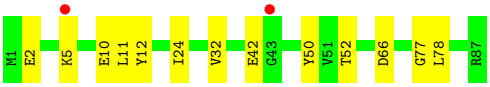
• Molecule 23: 40S ribosomal protein S21-A

Chain D1:



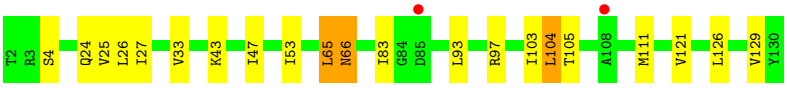
• Molecule 23: 40S ribosomal protein S21-A

Chain d1:



• Molecule 24: 40S ribosomal protein S22-A

Chain D2:

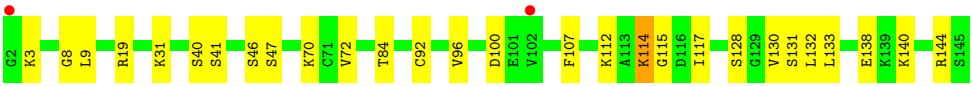


• Molecule 24: 40S ribosomal protein S22-A

Chain d2:

• Molecule 25: 40S ribosomal protein S23-A

Chain D3:

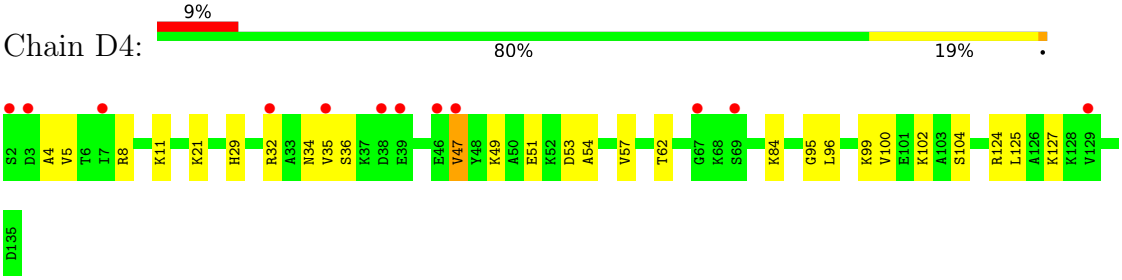


• Molecule 25: 40S ribosomal protein S23-A

Chain d3:

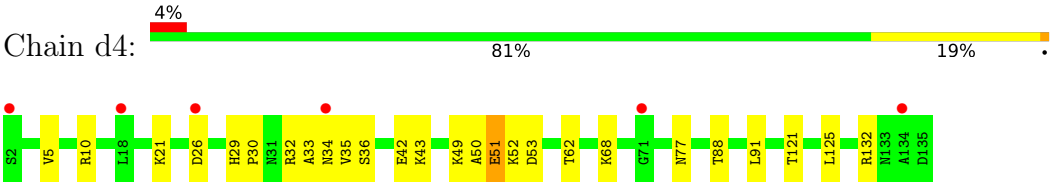
• Molecule 26: 40S ribosomal protein S24-A

Chain D4:



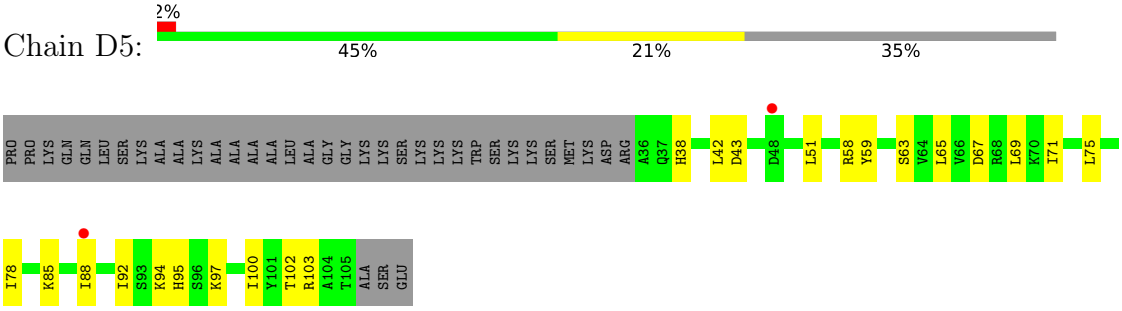
• Molecule 26: 40S ribosomal protein S24-A

Chain d4:



• Molecule 27: 40S ribosomal protein S25-A

Chain D5:



• Molecule 27: 40S ribosomal protein S25-A

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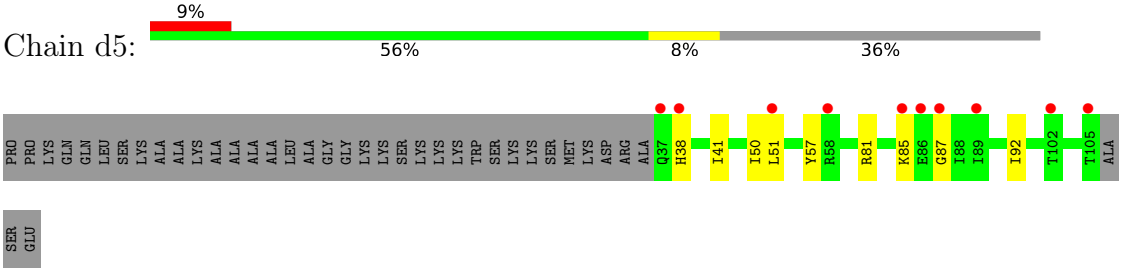
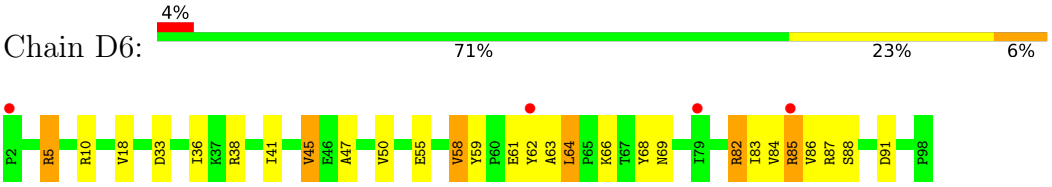


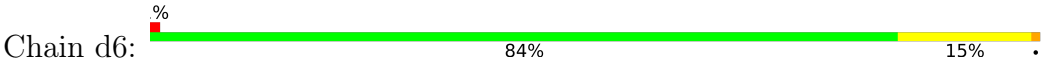
• Molecule 28: 40S ribosomal protein S26-B

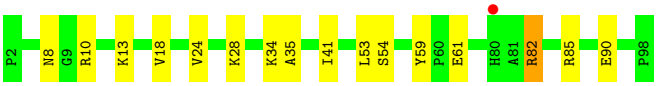
Chain D6:



• Molecule 28: 40S ribosomal protein S26-B

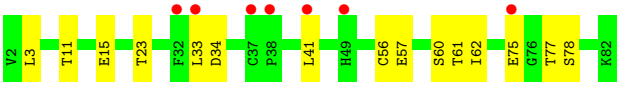
Chain d6:





• Molecule 29: 40S ribosomal protein S27-A

Chain D7:

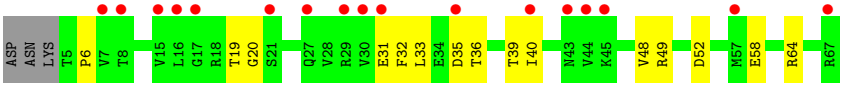


• Molecule 29: 40S ribosomal protein S27-A

Chain d7:

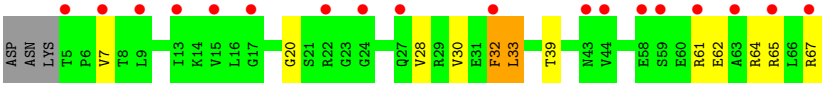
• Molecule 30: 40S ribosomal protein S28-A

Chain D8:



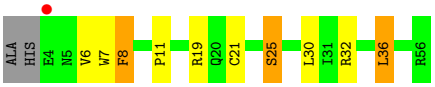
• Molecule 30: 40S ribosomal protein S28-A

Chain d8:



• Molecule 31: 40S ribosomal protein S29-A

Chain D9:



• Molecule 31: 40S ribosomal protein S29-A

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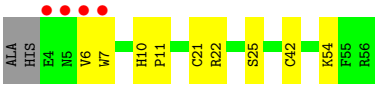
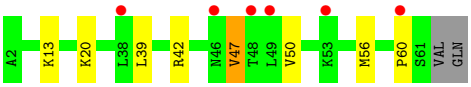


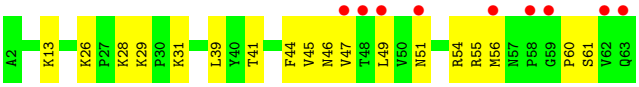
• Molecule 32: 40S ribosomal protein S30-A

Chain E0:



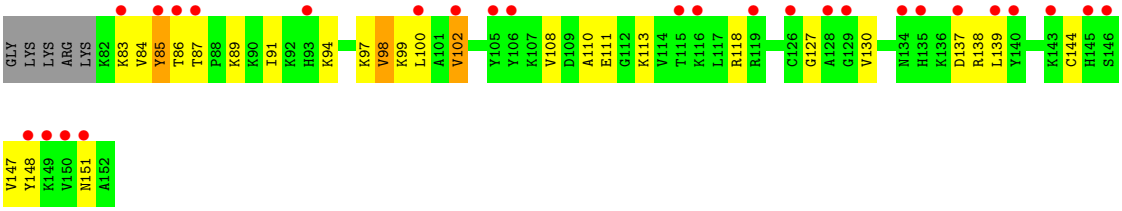
• Molecule 32: 40S ribosomal protein S30-A

Chain e0:



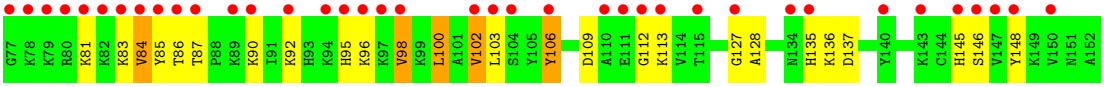
• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:



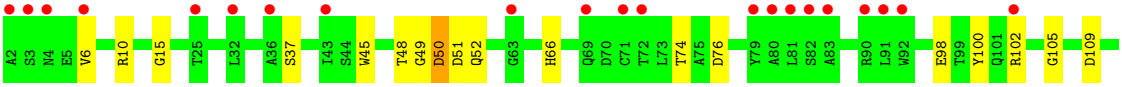
• Molecule 33: Ubiquitin-40S ribosomal protein S31

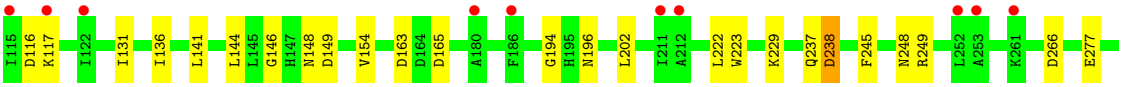
Chain e1:

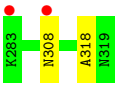


• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:

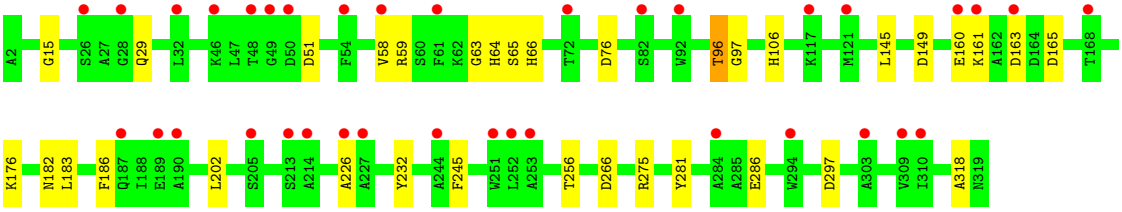






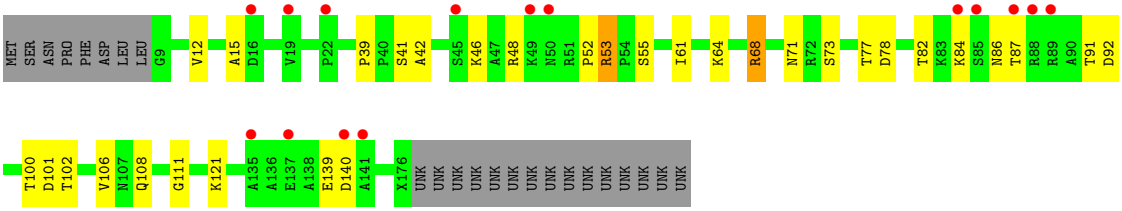
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:



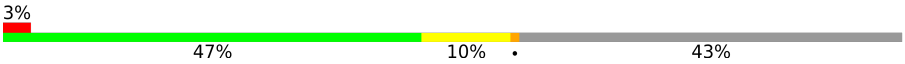
• Molecule 35: Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1

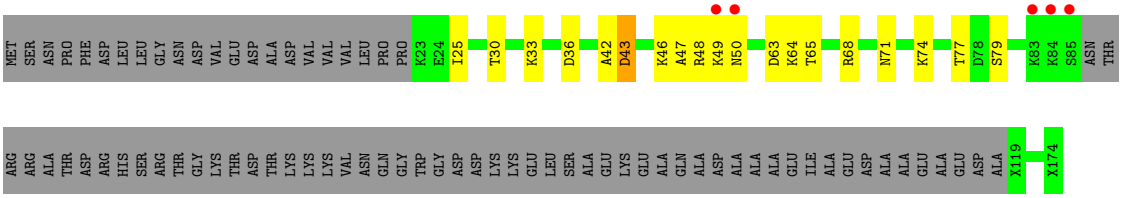
Chain SM:



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

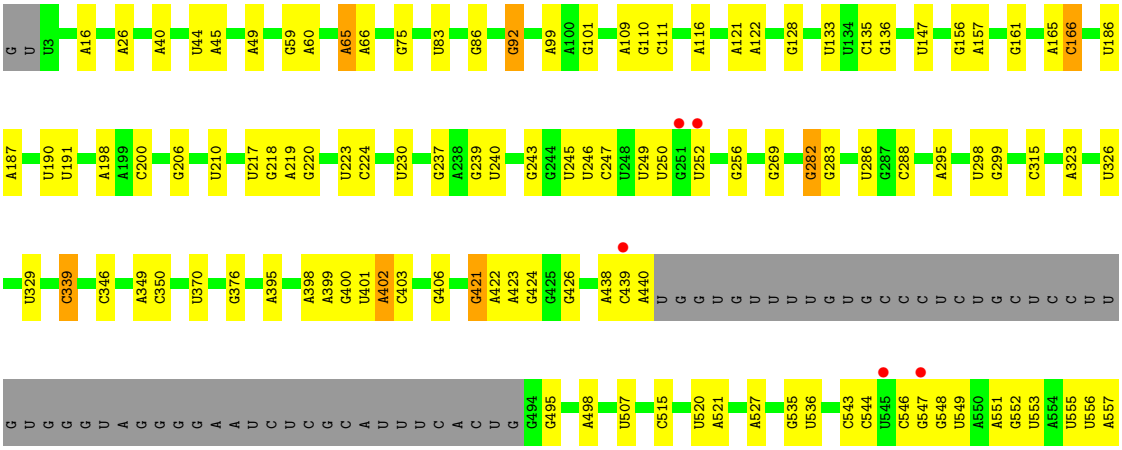
Chain sM:

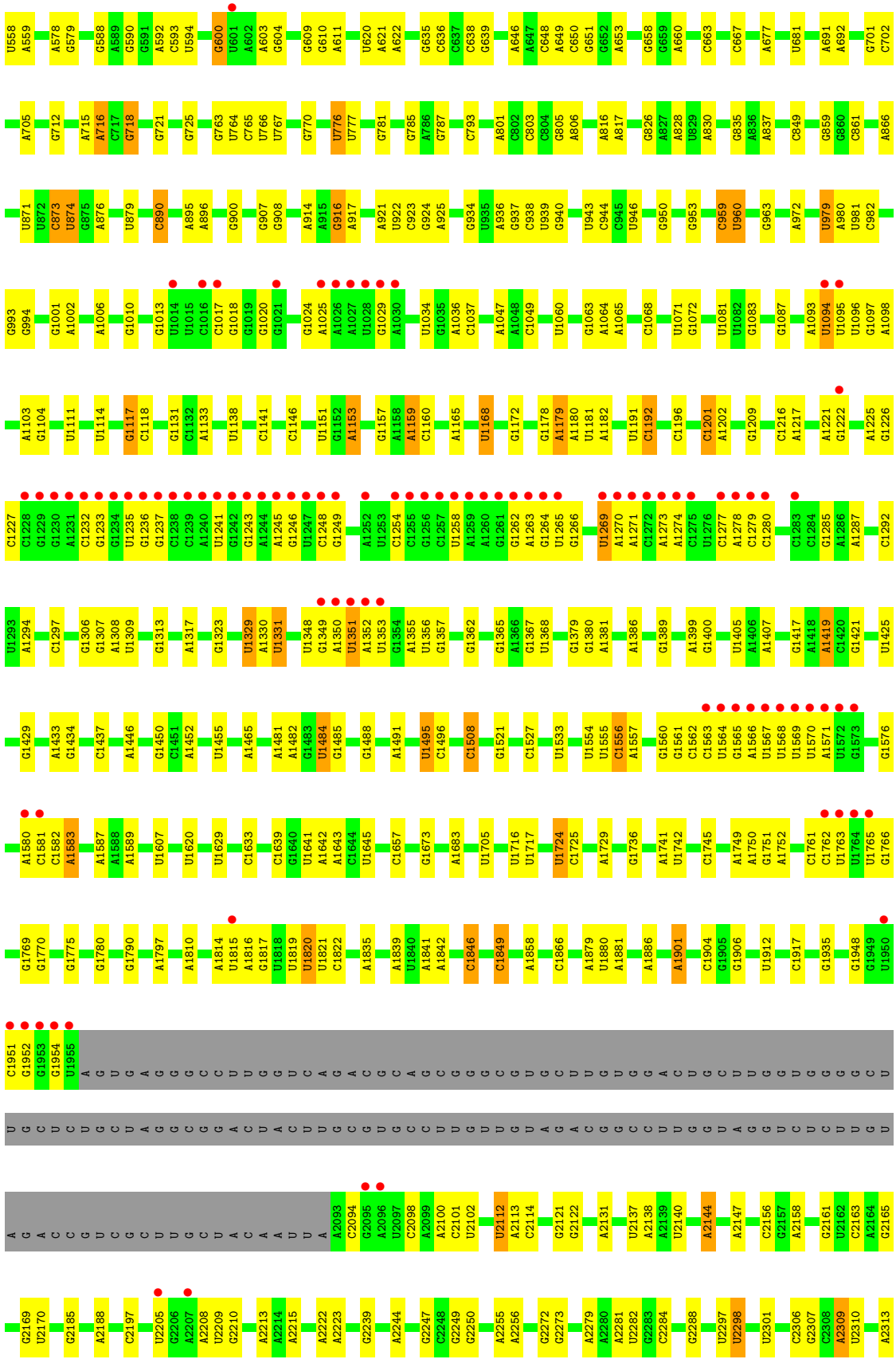




• Molecule 36: 25S ribosomal RNA

Chain 1:

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A705 G712 A715 A716 C717 G718 G721 G725 G763 U764 C765 U766 U767 G770 U776 U777 G781 G785 A786 G787 C793 A801 C802 C803 C804 G805 A806 A816 A817 G826 A827 A828 U829 A830 G835 A836 A837 C849 G859 G860 C861 A866
U871 U872 C873 U874 G875 A876 U879 C890 A895 A896 G900 G907 G908 A914 A915 G916 A917 A921 U922 C923 G924 A925 G934 U935 A936 G937 C938 U939 G940 U943 C944 C945 U946 G950 G953 C959 U960 G963 A972 U979 A980 U981 C982
G993 G994 G1001 A1002 A1006 G1010 G1013 U1014 U1015 C1016 C1017 G1018 G1019 G1020 G1021 G1024 A1025 A1026 A1027 U1028 G1029 A1030 U1034 G1035 A1036 C1037 A1047 A1048 C1049 U1060 G1063 A1064 A1065 C1068 U1071 G1072 U1081 U1082 G1083 G1087 A1093 U1094 U1095 U1096 G1097 A1098
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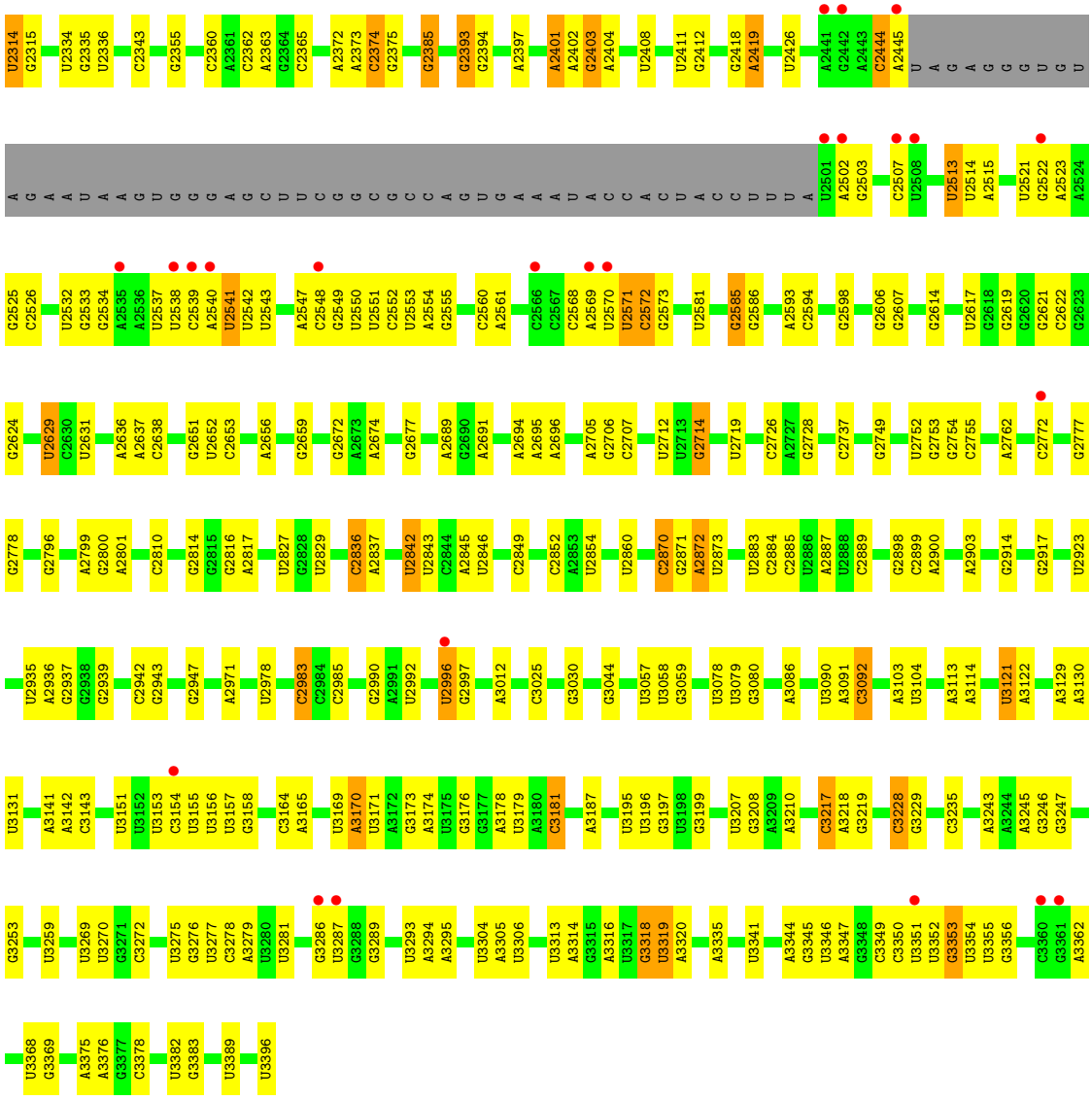
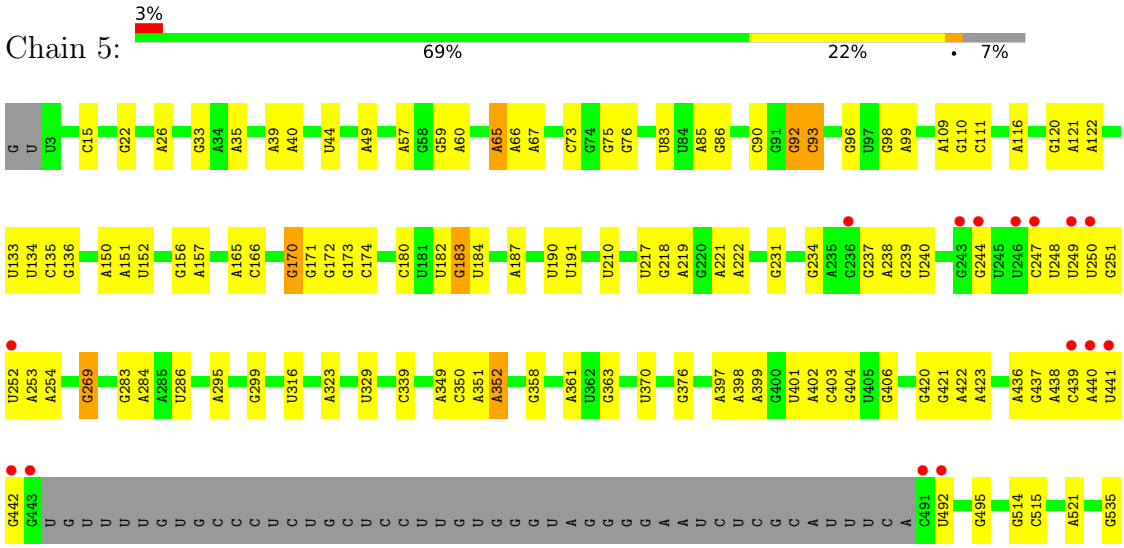
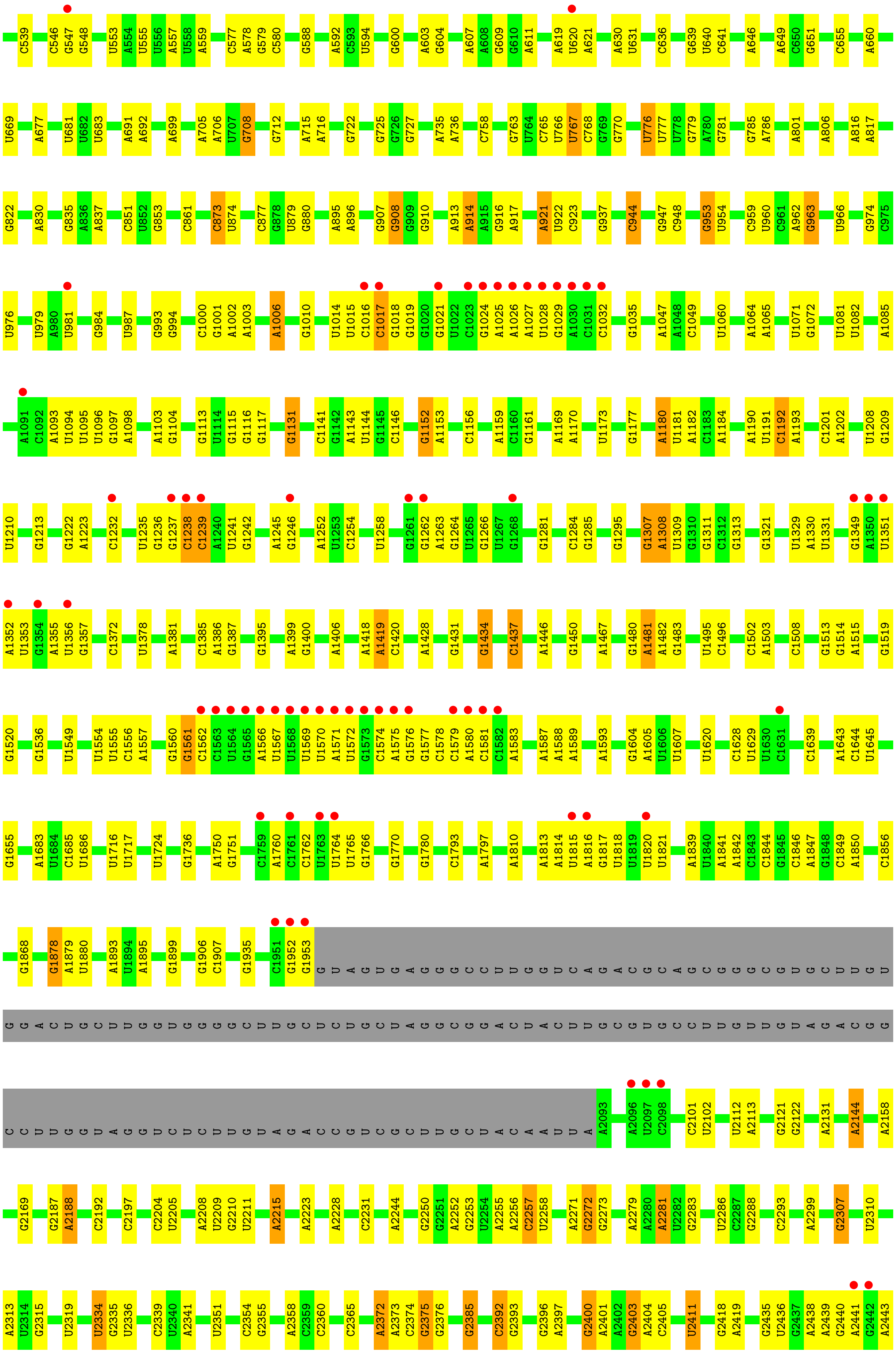
G1769 G1770 G1775 G1780 G1790 A1797 A1810 A1814 U1815 A1816 G1817 U1818 U1819 U1820 U1821 C1822 A1835 A1839 U1840 A1841 A1842 C1846 C1849 A1858 C1866 A1879 U1880 A1881 A1886 A1901 C1904 G1905 G1906 U1912 C1917 G1935 G1948 G1949 U1950
C1951 G1952 G1953 G1954 U1955 A G U G A G G C C U G U A C U U G C C U G C C G U A C U G C A A U C U G G C A C C U U G G G C A C U U G G A C U U G G U A G G G U C U G G G G C U
U G C U C U G C C U A G G C G G C U A C U G A A U U C U U G G C C G C U U G U A G C U G G U G G G C U C U G U U G G A C U U G G U G G G C U
A G A C C G U C G C U U G C C U A C A A U U A A2093 G C C G C A C U U G G C C U U G G G C A C U U G G C C U U G G G C C U
G2094 G2095 A2096 U2097 C2098 A2099 A2100 C2101 U2102 U2112 A2113 C2114 G2121 G2122 A2131 U2137 A2138 A2139 U2140 A2144 A2147 C2156 G2157 A2158 G2161 U2162 C2163 A2164 G2165
G2169 U2170 G2185 A2188 C2197 U2205 G2206 A2207 A2208 U2209 G2210 A2213 A2214 A2215 A2222 A2223 G2239 A2244 G2247 C2248 G2249 G2250 A2255 A2256 G2272 G2273 A2279 A2280 A2281 U2282 G2283 C2284 G2288 U2297 U2298 U2301 C2306 G2307 C2308 A2309 U2310 A2313



• Molecule 36: 25S ribosomal RNA

Chain 5:

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U669 A677 U681 U682 U683 A691 A692 A699 A705 A706 U707 G708 G712 A715 A716 G722 G725 G726 G727 A735 A736 C758 G763 U764 C765 U766 U767 C768 G769 G770 U776 U777 U778 G779 A780 G781 G785 A786 A801 A806 A816 A817
G822 A830 G835 A836 A837 C851 U852 G853 C861 C873 U874 C877 G878 U879 G880 A895 A896 G907 G908 G909 G910 A913 A914 A915 G916 A917 A921 U922 C923 G937 C944 G947 C948 G953 U954 C959 U960 C961 A962 G963 U966 G974 C975
U976 U979 A980 U981 G984 U987 G993 G994 C1000 G1001 A1002 A1003 A1006 G1010 U1014 U1015 C1016 C1017 G1018 G1019 G1020 G1021 U1022 C1023 G1024 A1025 A1026 A1027 U1028 G1029 A1030 C1031 C1032 G1035 A1047 A1048 C1049 U1060 A1064 A1065 U1071 G1072 U1081 U1082 A1085
A1091 C1092 A1093 U1094 U1095 U1096 G1097 A1098 A1103 G1104 G1113 U1114 G1115 G1116 G1117 G1131 C1141 G1142 A1143 U1144 G1145 C1146 G1152 A1153 C1156 A1159 C1160 G1161 A1169 A1170 U1173 G1177 A1180 U1181 A1182 C1183 A1184 A1190 U1191 C1192 A1193 C1201 A1202 U1208 G1209
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G G A C U G C U U G G U G G G C U U G C U C U G C U A G G C G G A C U A C U U G C G U G C C U U U G U U G U A G A C G G
C C U U G G U A G G U C U C U U G G U A G A C C G U C G C U U G C U A C A A U U A A2093 A2096 U2097 C2098 C2101 U2102 U2112 A2113 G2121 G2122 A2131 A2144 A2158
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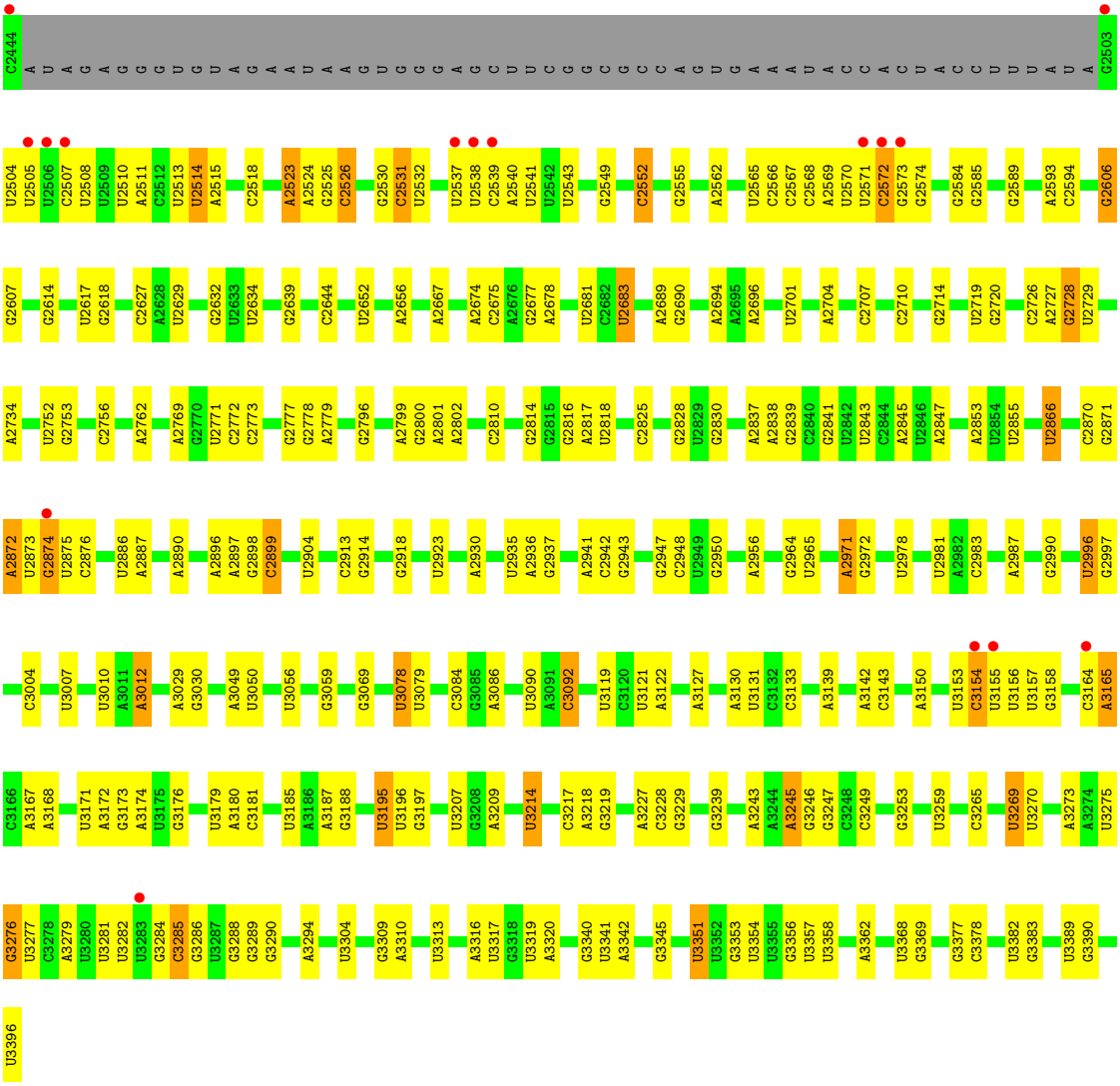
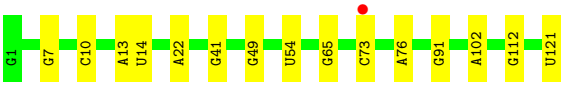
A2313 U2314 G2315 U2319 U2334 G2335 U2336 C2339 U2340 A2341 U2351 C2354 G2355 A2358 C2359 C2360 C2365 A2372 A2373 C2374 G2375 G2376 G2385 C2392 G2393 G2396 A2397 G2400 A2401 A2402 G2403 A2404 C2405 U2411 G2418 A2419 G2435 U2436 G2437 A2438 A2439 G2440 A2441 G2442 A2443



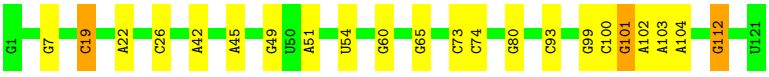
- Molecule 37: 5S ribosomal RNA

Chain 3:



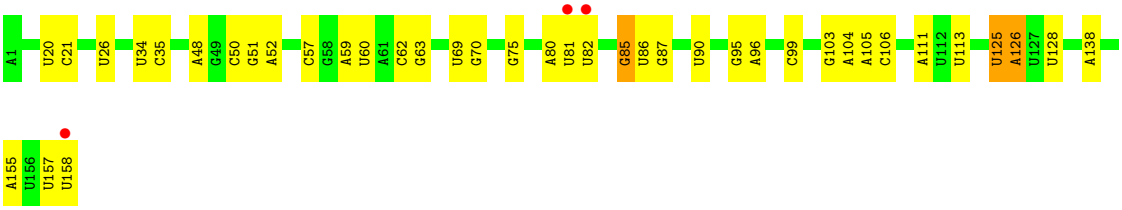
- Molecule 37: 5S ribosomal RNA

Chain 7:



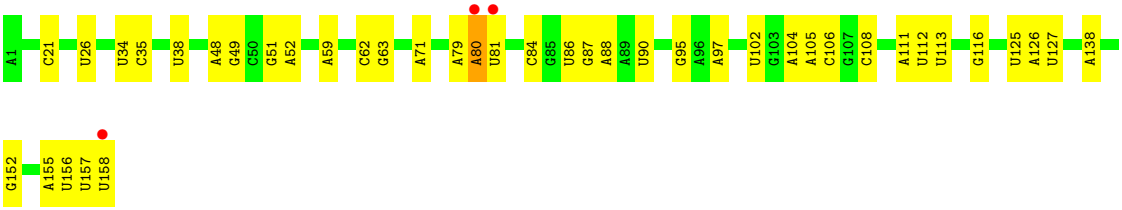
- Molecule 38: 5.8S ribosomal RNA

Chain 4:



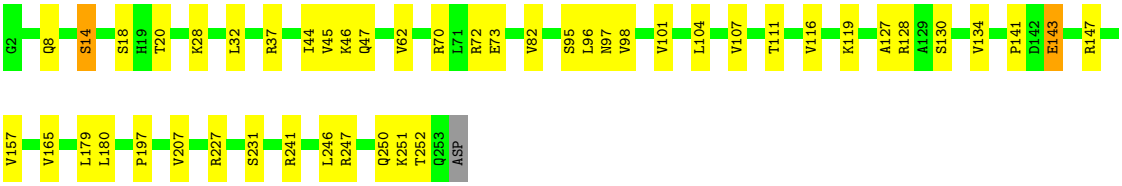
- Molecule 38: 5.8S ribosomal RNA

Chain 8:



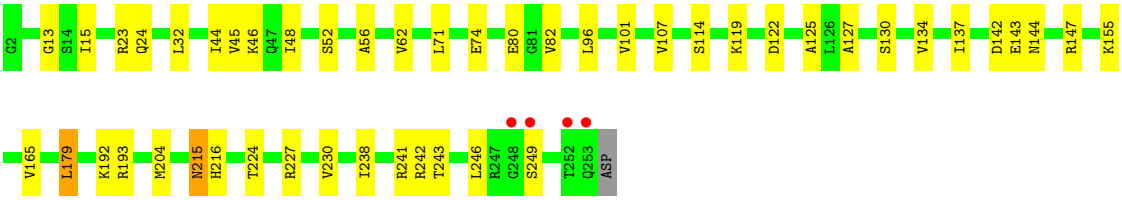
- Molecule 39: 60S ribosomal protein L2-A

Chain L2:



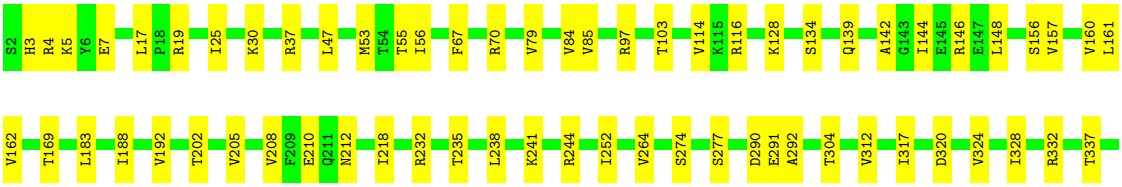
- Molecule 39: 60S ribosomal protein L2-A

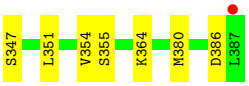
Chain l2:



- Molecule 40: 60S ribosomal protein L3

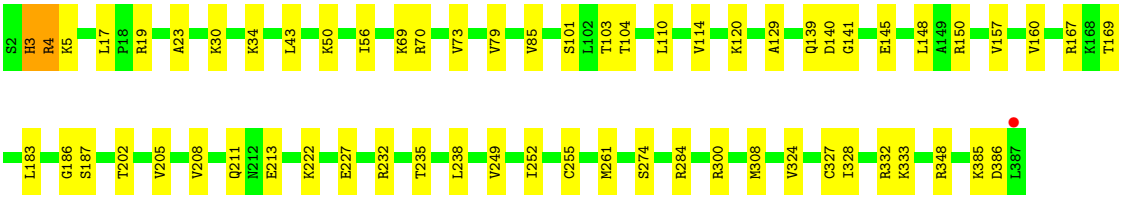
Chain L3:





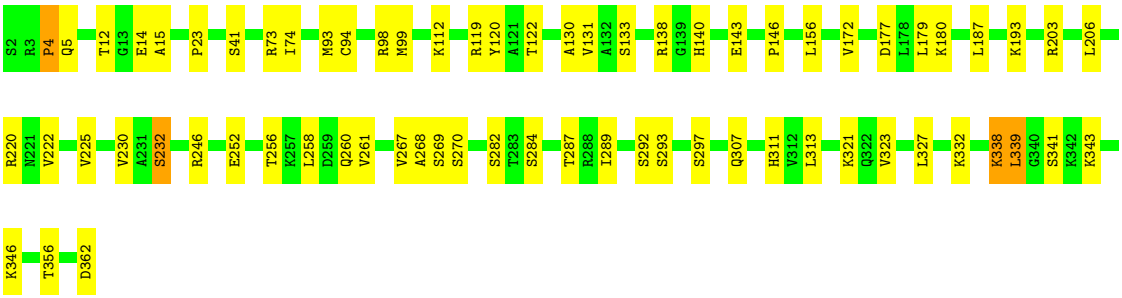
• Molecule 40: 60S ribosomal protein L3

Chain l3:



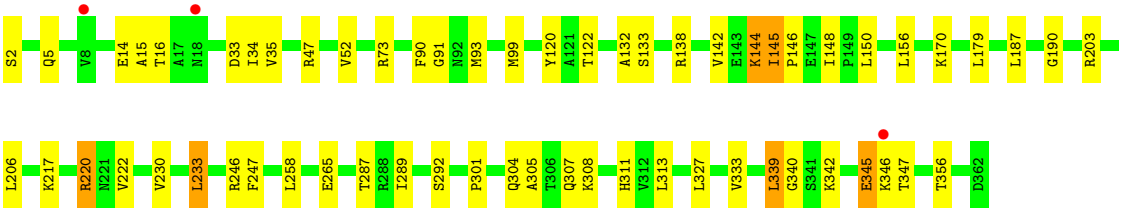
• Molecule 41: 60S ribosomal protein L4-A

Chain L4:



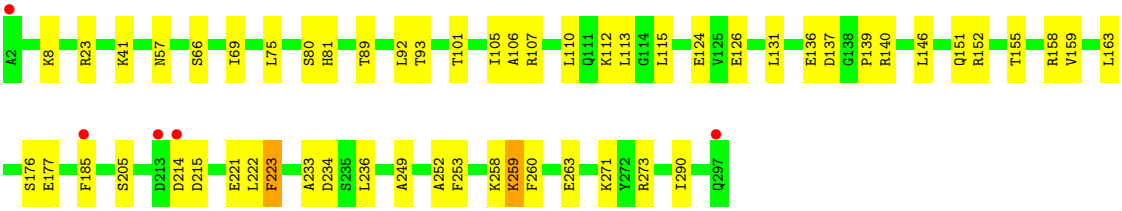
• Molecule 41: 60S ribosomal protein L4-A

Chain l4:



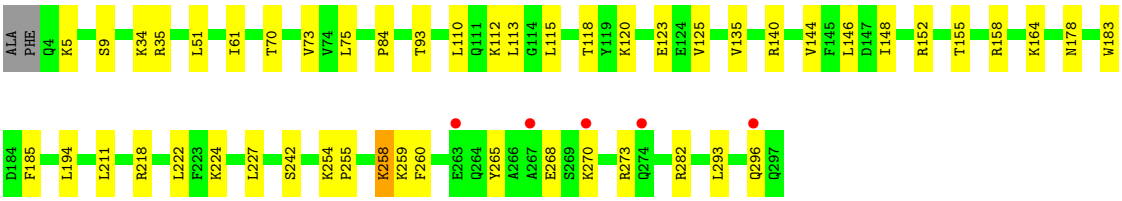
• Molecule 42: 60S ribosomal protein L5

Chain L5:



• Molecule 42: 60S ribosomal protein L5

Chain l5:



- Molecule 43: 60S ribosomal protein L6-A

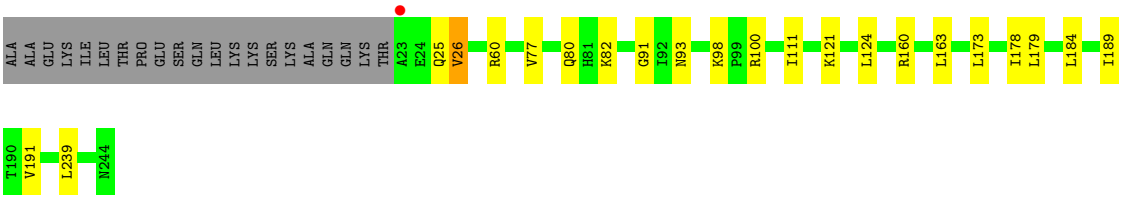
Chain L6:

- Molecule 43: 60S ribosomal protein L6-A

Chain l6:

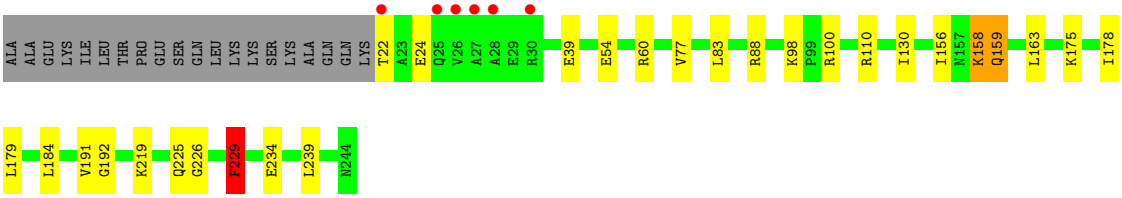
- Molecule 44: 60S ribosomal protein L7-A

Chain L7:



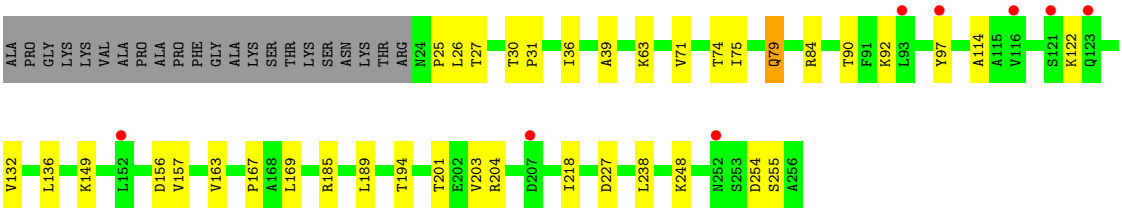
- Molecule 44: 60S ribosomal protein L7-A

Chain l7:



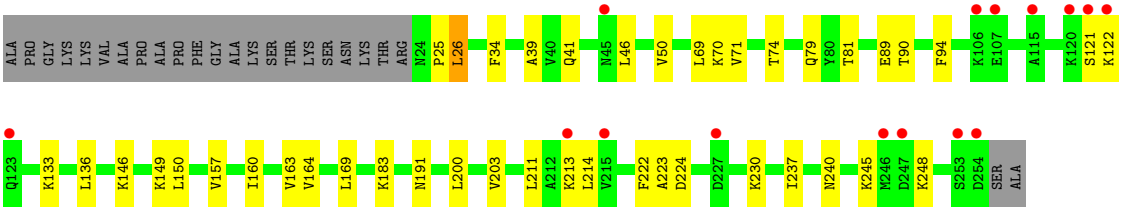
- Molecule 45: 60S ribosomal protein L8-A

Chain L8:



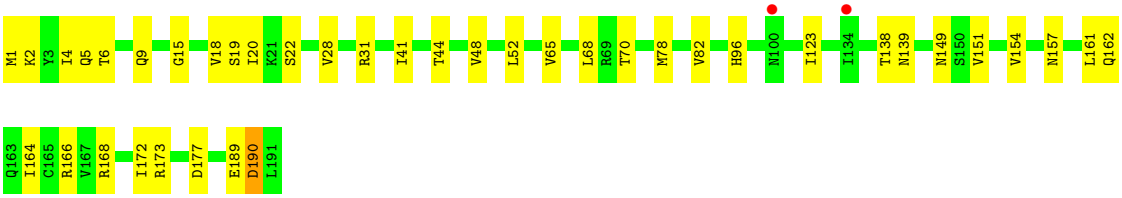
- Molecule 45: 60S ribosomal protein L8-A

Chain l8:



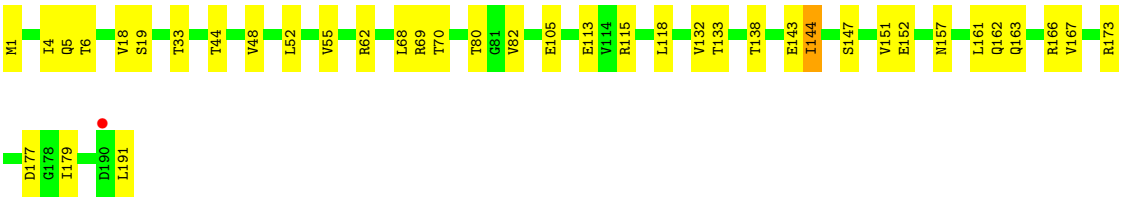
- Molecule 46: 60S ribosomal protein L9-A

Chain L9:



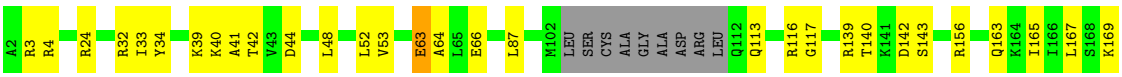
- Molecule 46: 60S ribosomal protein L9-A

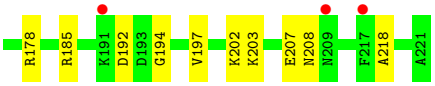
Chain l9:



- Molecule 47: 60S ribosomal protein L10

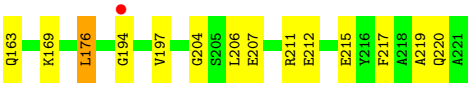
Chain M0:





• Molecule 47: 60S ribosomal protein L10

Chain m0:

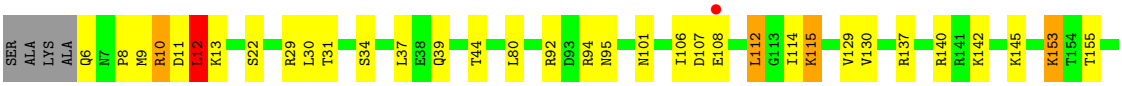


• Molecule 48: 60S ribosomal protein L11-A

Chain M1:

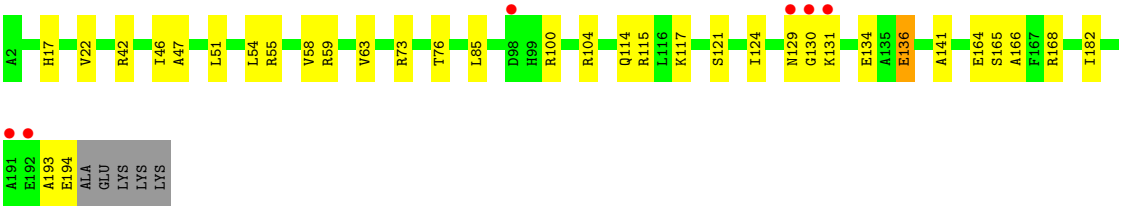
• Molecule 48: 60S ribosomal protein L11-A

Chain m1:



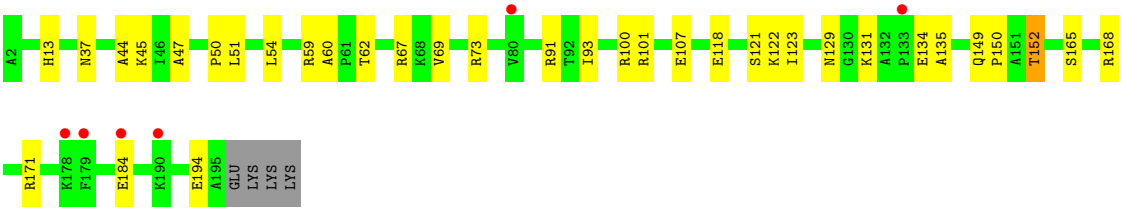
• Molecule 49: 60S ribosomal protein L13-A

Chain M3:



• Molecule 49: 60S ribosomal protein L13-A

Chain m3:

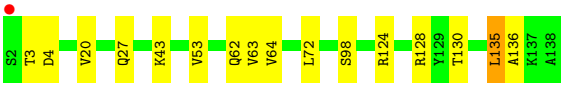


• Molecule 50: 60S ribosomal protein L14-A

Chain M4:

• Molecule 50: 60S ribosomal protein L14-A

Chain m4:



• Molecule 51: 60S ribosomal protein L15-A

Chain M5:

• Molecule 51: 60S ribosomal protein L15-A

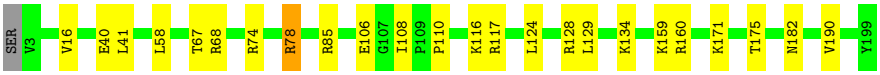
Chain m5:

• Molecule 52: 60S ribosomal protein L16-A

Chain M6:

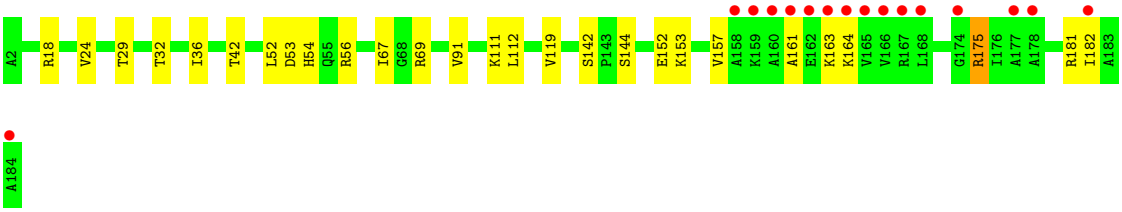
• Molecule 52: 60S ribosomal protein L16-A

Chain m6:



• Molecule 53: 60S ribosomal protein L17-A

Chain M7:

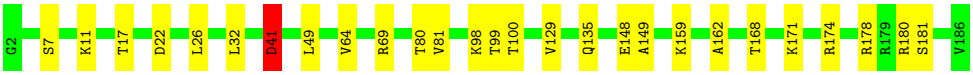


• Molecule 53: 60S ribosomal protein L17-A

Chain m7:

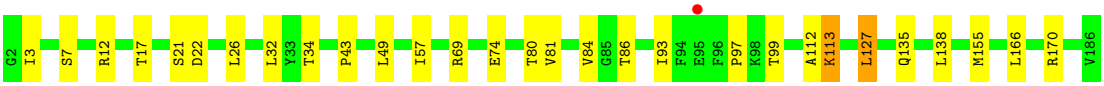
• Molecule 54: 60S ribosomal protein L18-A

Chain M8:



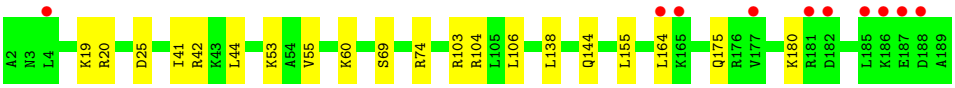
• Molecule 54: 60S ribosomal protein L18-A

Chain m8:



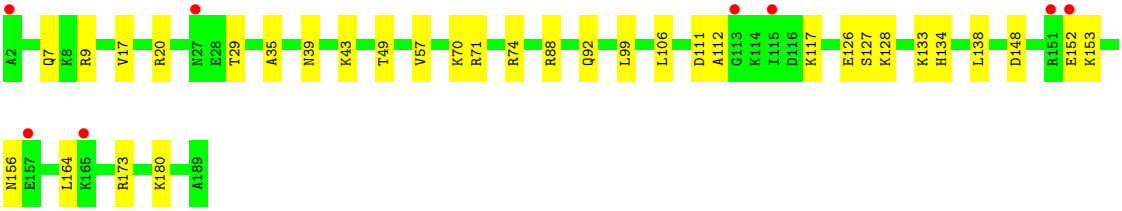
• Molecule 55: 60S ribosomal protein L19-A

Chain M9:



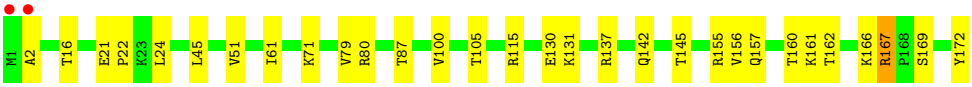
• Molecule 55: 60S ribosomal protein L19-A

Chain m9:



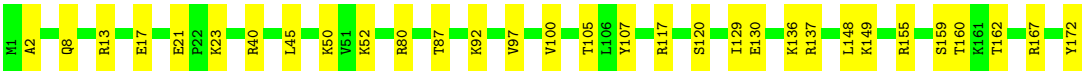
• Molecule 56: 60S ribosomal protein L20-A

Chain N0:



• Molecule 56: 60S ribosomal protein L20-A

Chain n0:

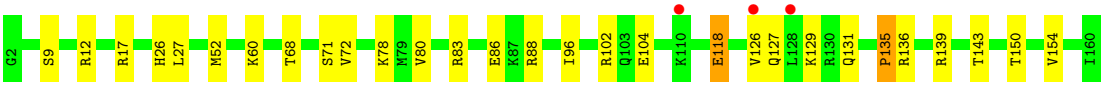


• Molecule 57: 60S ribosomal protein L21-A

Chain N1:

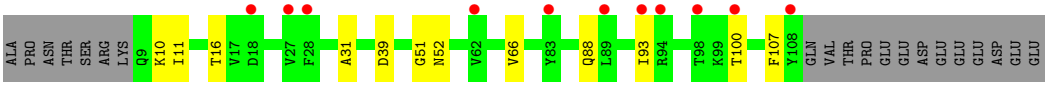
• Molecule 57: 60S ribosomal protein L21-A

Chain n1:



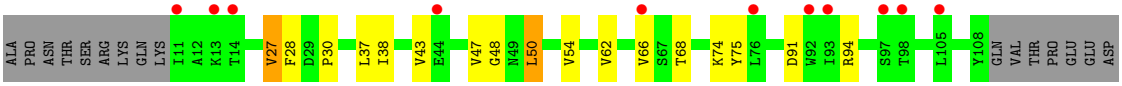
• Molecule 58: 60S ribosomal protein L22-A

Chain N2:



• Molecule 58: 60S ribosomal protein L22-A

Chain n2:



GLU GLU GLU ASP GLU GLU

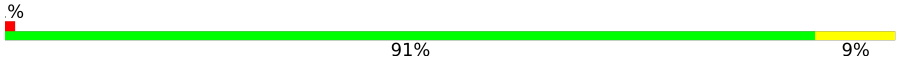
• Molecule 59: 60S ribosomal protein L23-A

Chain N3:

S2 G3 N4 G5 I13 S14 R45 L46 N47 R48 K63 K64 L69 K72 V73 K83 V91 I102 K106 T115 L125 S131 N132 S133 V137

• Molecule 59: 60S ribosomal protein L23-A

Chain n3:



S2 I13 K40 G41 R45 R48 K72 V73 M74 V91 I102 S112 T115 K120 V137

• Molecule 60: 60S ribosomal protein L24-A

Chain N4:

M1 E4 I5 R17 G18 T19 D25 L39 R47 R48 I49 T64 E65 E66 V67 A68 K69 K70 R71 S72 R73 K74 T75 V76 K77 A78 P81 G84 A85 S86 L87 D88 L89 I90 S95 L96 K97 P98 GLU VAL ARG LYS ALA ASN ARG GLU GLU LYS LEU LYS ALA

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

• Molecule 60: 60S ribosomal protein L24-A

Chain n4:

M1 E4 T19 D25 S26 L39 R47 L54 K57 I63 T64 E65 E66 V67 A68 K69 K70 R71 S72 R73 K74 T75 V76 K77 T83 L89 L96 V100 E107 A125 E126 K127 A128 K129 S130 A131 G132 T133 Q134 S135 SER LYS PHE SER LYS GLN

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

• Molecule 61: 60S ribosomal protein L25

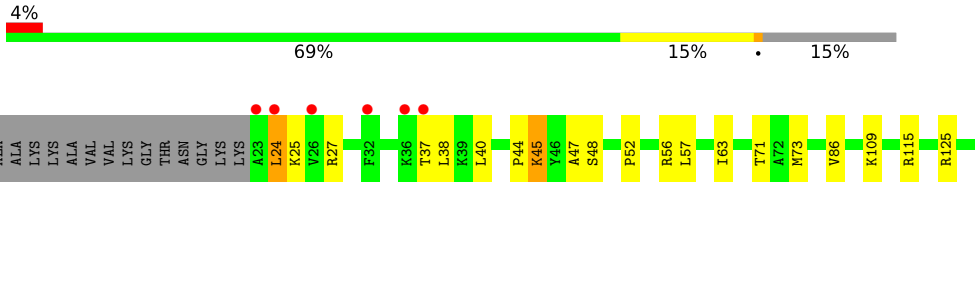
Chain N5:

ALA PRO SER ALA LYS ALA THR ALA ALA LYS LYS ALA VAL VAL LYS GLY THR ASN GLY LYS K22 R27 T37 L38 K39 L40 P44 K45 S48 S59 I63 T71 A72 M73 K74 K75 D78 K92 E104 L108 T112 R115 R125 D134 I135

A136 N137 R138 I139 I142

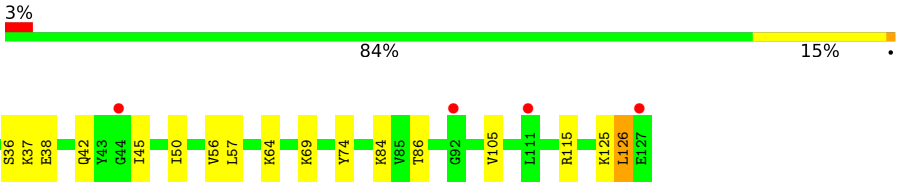
• Molecule 61: 60S ribosomal protein L25

Chain n5:



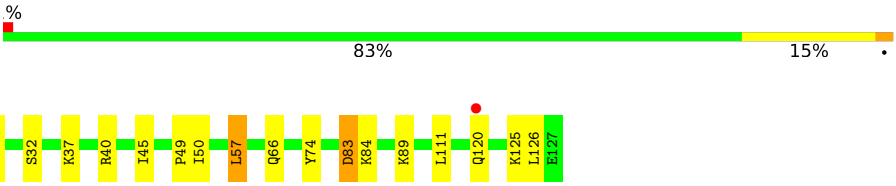
- Molecule 62: 60S ribosomal protein L26-A

Chain N6:



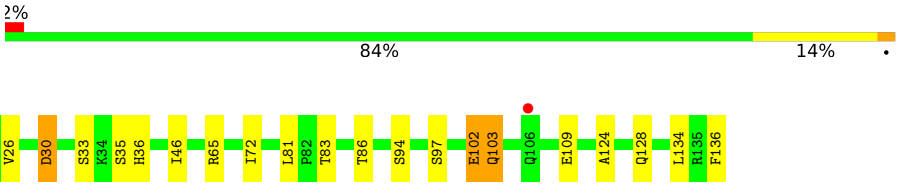
- Molecule 62: 60S ribosomal protein L26-A

Chain n6:



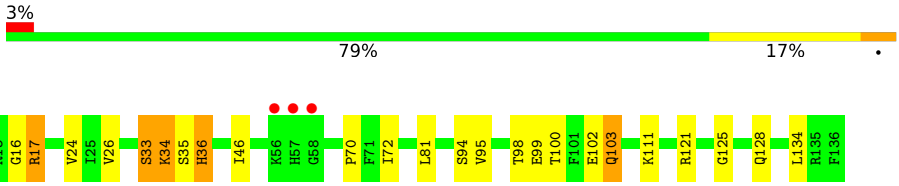
- Molecule 63: 60S ribosomal protein L27-A

Chain N7:



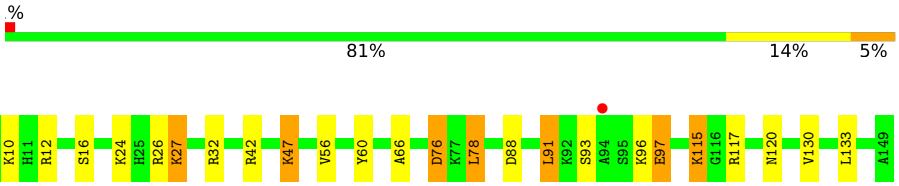
- Molecule 63: 60S ribosomal protein L27-A

Chain n7:



- Molecule 64: 60S ribosomal protein L28

Chain N8:

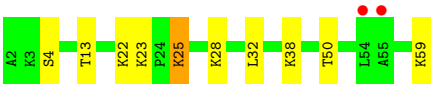


- Molecule 64: 60S ribosomal protein L28

Chain n8:

• Molecule 65: 60S ribosomal protein L29

Chain N9:

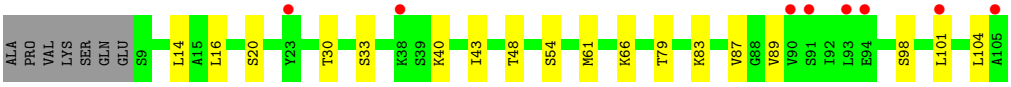


• Molecule 65: 60S ribosomal protein L29

Chain n9:

• Molecule 66: 60S ribosomal protein L30

Chain O0:

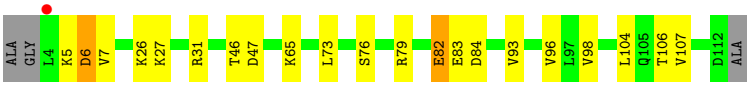


• Molecule 66: 60S ribosomal protein L30

Chain o0:

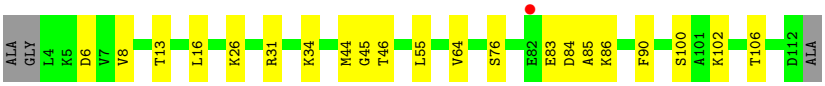
• Molecule 67: 60S ribosomal protein L31-A

Chain O1:



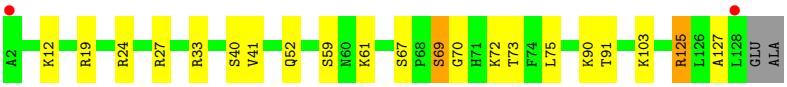
• Molecule 67: 60S ribosomal protein L31-A

Chain o1:



• Molecule 68: 60S ribosomal protein L32

Chain O2: 2% 82% 15%

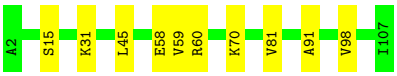


• Molecule 68: 60S ribosomal protein L32

Chain o2: % 81% 16%

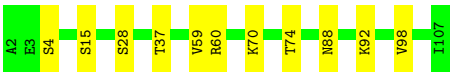
• Molecule 69: 60S ribosomal protein L33-A

Chain O3: 91% 9%



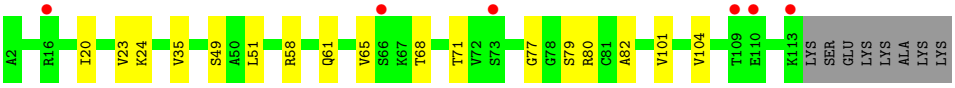
• Molecule 69: 60S ribosomal protein L33-A

Chain o3: 90% 10%



• Molecule 70: 60S ribosomal protein L34-A

Chain O4: 5% 79% 14% 7%

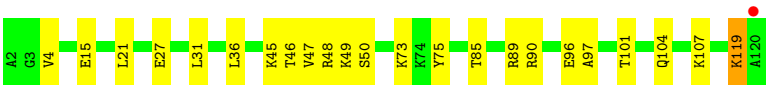


• Molecule 70: 60S ribosomal protein L34-A

Chain o4: 2% 78% 15% 7%

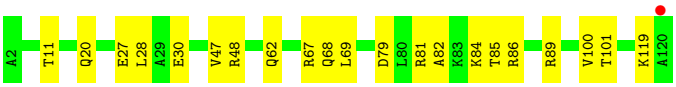
• Molecule 71: 60S ribosomal protein L35-A

Chain O5: % 81% 18%



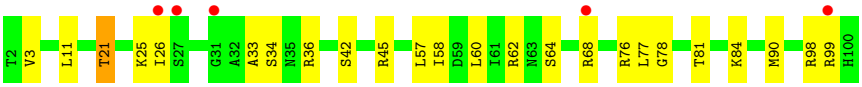
• Molecule 71: 60S ribosomal protein L35-A

Chain o5:



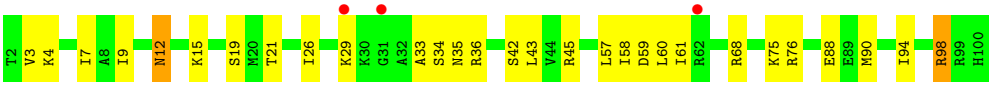
• Molecule 72: 60S ribosomal protein L36-A

Chain O6:



• Molecule 72: 60S ribosomal protein L36-A

Chain o6:

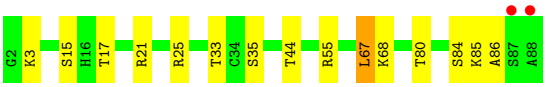


• Molecule 73: 60S ribosomal protein L37-A

Chain O7:

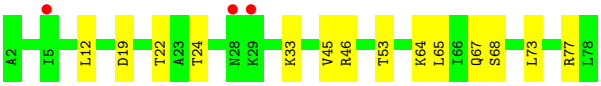
• Molecule 73: 60S ribosomal protein L37-A

Chain o7:



• Molecule 74: 60S ribosomal protein L38

Chain O8:

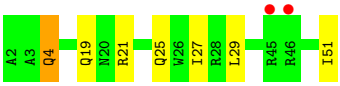


• Molecule 74: 60S ribosomal protein L38

Chain o8:

• Molecule 75: 60S ribosomal protein L39

Chain O9:



• Molecule 75: 60S ribosomal protein L39

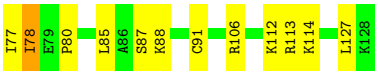
Chain o9:

• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:

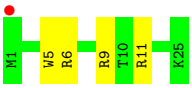
• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:



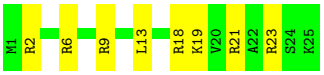
• Molecule 77: 60S ribosomal protein L41-A

Chain Q1:



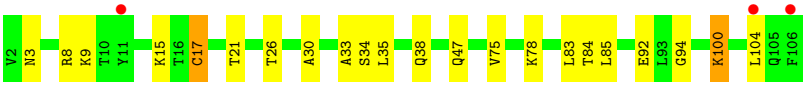
• Molecule 77: 60S ribosomal protein L41-A

Chain q1:



• Molecule 78: 60S ribosomal protein L42-A

Chain Q2:

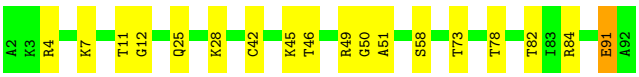


• Molecule 78: 60S ribosomal protein L42-A

Chain q2:

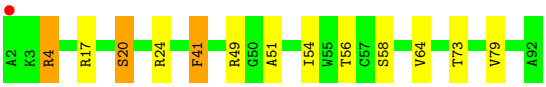
• Molecule 79: 60S ribosomal protein L43-A

Chain Q3:



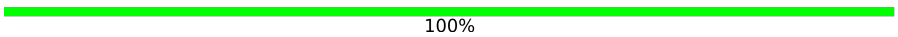
• Molecule 79: 60S ribosomal protein L43-A

Chain q3:



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

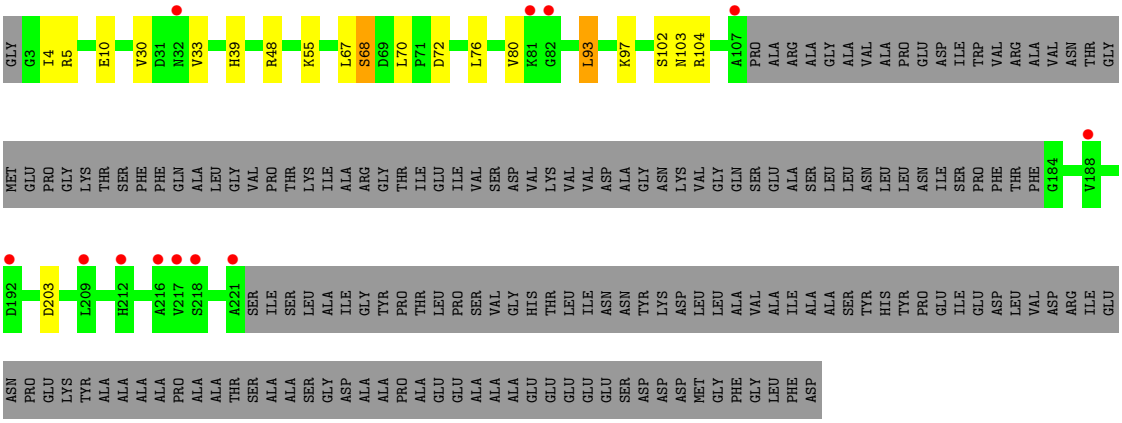
Chain m2:



There are no outlier residues recorded for this chain.

• Molecule 81: 60S acidic ribosomal protein P0

Chain p0:



• Molecule 82: 60S ribosomal protein P1 alpha

Chain p1: 100%

There are no outlier residues recorded for this chain.

- Molecule 83: 60S ribosomal protein P2 beta

Chain p2: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	436.11Å 287.31Å 303.99Å 90.00° 98.86° 90.00°	Depositor
Resolution (Å)	49.96 – 3.10 49.96 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.96-3.10) 89.6 (49.96-3.10)	Depositor EDS
R_{merge}	0.39	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.84 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.234 , 0.291 0.243 , 0.288	Depositor DCC
R_{free} test set	26664 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	63.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 51.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	410912	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	2	0.50	0/42468	1.01	74/66173 (0.1%)
1	6	0.60	0/42790	1.06	102/66673 (0.2%)
2	S0	0.35	0/1617	0.56	0/2215
2	s0	0.34	0/1653	0.55	0/2261
3	S1	0.32	0/1735	0.59	0/2335
3	s1	0.36	0/1748	0.58	0/2352
4	S2	0.37	0/1665	0.57	0/2263
4	s2	0.42	0/1665	0.62	0/2263
5	S3	0.37	0/1759	0.55	0/2368
5	s3	0.33	0/1759	0.52	0/2368
6	S4	0.36	0/2109	0.59	0/2839
6	s4	0.39	0/2109	0.61	0/2839
7	S5	0.33	0/1629	0.55	0/2202
7	s5	0.33	0/1629	0.55	0/2202
8	S6	0.38	0/1823	0.55	0/2439
8	s6	0.39	0/1779	0.56	0/2379
9	S7	0.34	0/1506	0.57	0/2028
9	s7	0.34	0/1517	0.58	0/2044
10	S8	0.38	0/1514	0.59	1/2021 (0.0%)
10	s8	0.43	0/1514	0.58	0/2021
11	S9	0.36	0/1519	0.56	0/2035
11	s9	0.39	0/1519	0.57	0/2035
12	C0	0.34	0/730	0.52	0/985
12	c0	0.29	0/718	0.53	1/968 (0.1%)
13	C1	0.43	0/1195	0.57	0/1612
13	c1	0.44	0/1195	0.60	0/1612
14	C2	0.34	0/898	0.55	0/1220
14	c2	0.25	0/898	0.50	0/1220
15	C3	0.36	0/1215	0.57	1/1638 (0.1%)
15	c3	0.38	0/1215	0.58	0/1638
16	C4	0.30	0/901	0.56	0/1217
16	c4	0.39	0/960	0.62	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	C5	0.34	0/998	0.57	0/1341
17	c5	0.38	0/1060	0.59	0/1426
18	C6	0.36	0/1125	0.62	3/1510 (0.2%)
18	c6	0.35	0/1131	0.57	0/1518
19	C7	0.37	0/935	0.60	0/1254
19	c7	0.31	0/953	0.53	0/1275
20	C8	0.36	0/1211	0.55	0/1628
20	c8	0.36	0/1211	0.58	0/1628
21	C9	0.33	0/1130	0.52	0/1517
21	c9	0.35	0/1130	0.55	0/1517
22	D0	0.36	0/865	0.57	0/1169
22	d0	0.36	0/892	0.58	0/1205
23	D1	0.36	0/693	0.54	0/935
23	d1	0.35	0/693	0.50	0/935
24	D2	0.37	0/1038	0.63	3/1395 (0.2%)
24	d2	0.44	0/1038	0.62	1/1395 (0.1%)
25	D3	0.44	0/1139	0.64	0/1518
25	d3	0.49	0/1139	0.66	1/1518 (0.1%)
26	D4	0.37	0/1087	0.55	0/1449
26	d4	0.40	0/1087	0.61	0/1449
27	D5	0.33	0/571	0.60	0/768
27	d5	0.33	0/566	0.54	0/761
28	D6	0.36	0/782	0.57	0/1047
28	d6	0.47	0/782	0.58	0/1047
29	D7	0.35	0/620	0.58	0/838
29	d7	0.36	0/620	0.56	0/838
30	D8	0.32	0/499	0.53	0/670
30	d8	0.34	0/499	0.54	0/670
31	D9	0.36	0/452	0.58	1/600 (0.2%)
31	d9	0.36	0/453	0.53	0/602
32	E0	0.37	0/483	0.54	0/643
32	e0	0.39	0/499	0.62	0/665
33	E1	0.35	0/577	0.61	0/770
33	e1	0.34	0/619	0.65	0/822
34	SR	0.31	0/2490	0.52	0/3389
34	sR	0.29	0/2498	0.49	0/3398
35	SM	0.38	0/984	0.56	0/1323
35	sM	0.40	0/480	0.60	0/642
36	1	0.78	3/75394 (0.0%)	1.21	317/117545 (0.3%)
36	5	0.82	7/75418 (0.0%)	1.21	316/117583 (0.3%)
37	3	0.65	0/2883	1.03	1/4491 (0.0%)
37	7	0.79	0/2883	1.20	8/4491 (0.2%)
38	4	0.73	0/3746	1.15	8/5832 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	8	0.68	0/3746	1.12	4/5832 (0.1%)
39	L2	0.50	0/1948	0.66	0/2617
39	l2	0.48	0/1952	0.69	2/2622 (0.1%)
40	L3	0.52	0/3136	0.64	0/4213
40	l3	0.59	1/3142 (0.0%)	0.68	1/4224 (0.0%)
41	L4	0.55	1/2800 (0.0%)	0.72	1/3790 (0.0%)
41	l4	0.53	0/2801	0.69	2/3792 (0.1%)
42	L5	0.43	0/2425	0.61	0/3271
42	l5	0.53	0/2408	0.65	0/3248
43	L6	0.53	0/1260	0.64	0/1694
43	l6	0.49	0/1269	0.62	0/1705
44	L7	0.53	0/1821	0.66	0/2451
44	l7	0.58	0/1828	0.70	1/2461 (0.0%)
45	L8	0.42	0/1836	0.60	0/2481
45	l8	0.40	0/1795	0.56	0/2429
46	L9	0.47	0/1539	0.59	0/2073
46	l9	0.54	0/1539	0.64	0/2073
47	M0	0.54	0/1741	0.66	0/2335
47	m0	0.55	0/1769	0.68	0/2372
48	M1	0.39	0/1374	0.59	0/1842
48	m1	0.47	0/1374	0.68	2/1842 (0.1%)
49	M3	0.51	0/1568	0.67	1/2106 (0.0%)
49	m3	0.47	0/1573	0.66	0/2113
50	M4	0.51	0/1068	0.64	0/1438
50	m4	0.53	0/1074	0.66	0/1446
51	M5	0.50	0/1757	0.64	0/2354
51	m5	0.47	0/1757	0.63	0/2354
52	M6	0.55	0/1585	0.69	1/2128 (0.0%)
52	m6	0.68	1/1585 (0.1%)	0.74	2/2128 (0.1%)
53	M7	0.53	0/1443	0.67	0/1944
53	m7	0.59	0/1250	0.69	0/1683
54	M8	0.51	0/1465	0.68	1/1965 (0.1%)
54	m8	0.53	0/1465	0.72	1/1965 (0.1%)
55	M9	0.38	0/1538	0.56	0/2050
55	m9	0.43	0/1538	0.57	0/2050
56	N0	0.55	0/1481	0.65	0/1990
56	n0	0.58	0/1481	0.70	0/1990
57	N1	0.56	0/1300	0.67	0/1743
57	n1	0.60	0/1300	0.62	0/1743
58	N2	0.36	0/812	0.54	0/1099
58	n2	0.39	0/794	0.60	0/1076
59	N3	0.53	0/1018	0.64	0/1369
59	n3	0.60	0/1018	0.74	0/1369

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
60	N4	0.42	0/712	0.57	0/958
60	n4	0.47	0/1103	0.60	0/1458
61	N5	0.44	0/979	0.64	1/1321 (0.1%)
61	n5	0.46	0/974	0.64	0/1314
62	N6	0.51	0/1004	0.69	0/1341
62	n6	0.45	0/1004	0.65	1/1341 (0.1%)
63	N7	0.40	0/1118	0.58	0/1497
63	n7	0.36	0/1118	0.53	0/1497
64	N8	0.54	0/1204	0.71	0/1612
64	n8	0.55	0/1204	0.71	0/1612
65	N9	0.48	0/473	0.68	1/629 (0.2%)
65	n9	0.54	0/473	0.82	1/629 (0.2%)
66	O0	0.38	0/751	0.51	0/1008
66	o0	0.40	0/775	0.58	1/1040 (0.1%)
67	O1	0.43	0/890	0.58	0/1196
67	o1	0.52	0/904	0.63	0/1213
68	O2	0.53	0/1041	0.67	0/1394
68	o2	0.57	0/1041	0.66	0/1394
69	O3	0.59	0/868	0.63	0/1168
69	o3	0.60	0/868	0.69	0/1168
70	O4	0.43	0/890	0.61	1/1189 (0.1%)
70	o4	0.43	0/891	0.63	0/1191
71	O5	0.49	0/978	0.64	0/1301
71	o5	0.42	0/978	0.54	0/1301
72	O6	0.46	0/778	0.62	0/1034
72	o6	0.43	0/778	0.58	0/1034
73	O7	0.57	0/696	0.70	1/923 (0.1%)
73	o7	0.49	0/696	0.66	0/923
74	O8	0.39	0/618	0.57	0/826
74	o8	0.34	0/618	0.50	0/826
75	O9	0.55	0/443	0.72	0/588
75	o9	0.47	0/443	0.66	0/588
76	Q0	0.52	0/423	0.69	0/562
76	q0	0.64	0/423	0.74	0/562
77	Q1	0.43	0/234	0.60	0/300
77	q1	0.49	0/234	0.71	0/300
78	Q2	0.65	1/860 (0.1%)	0.72	0/1136
78	q2	0.58	1/860 (0.1%)	0.69	1/1136 (0.1%)
79	Q3	0.52	0/701	0.66	0/934
79	q3	0.52	0/701	0.66	0/934
81	p0	0.34	0/1092	0.52	0/1474
All	All	0.62	15/430516 (0.0%)	0.98	865/632094 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	s5	0	1
9	S7	0	1
17	c5	0	1
19	C7	0	1
26	d4	0	1
27	D5	0	1
28	D6	0	1
44	l7	0	2
52	M6	0	1
56	N0	0	2
59	n3	0	1
64	n8	0	1
79	q3	0	1
All	All	0	15

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	11.25	2.01	1.82
36	5	1152	G	N9-C4	-9.21	1.30	1.38
78	q2	17	CYS	CB-SG	8.36	1.96	1.82
36	5	1152	G	N3-C4	-6.38	1.30	1.35
36	5	2941	A	N9-C4	-6.19	1.34	1.37

The worst 5 of 865 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1152	G	N3-C4-N9	-17.27	115.64	126.00
36	5	1152	G	N3-C4-C5	16.41	136.81	128.60
36	5	1152	G	C2-N3-C4	-11.50	106.15	111.90
36	1	2617	U	N3-C2-O2	-10.99	114.51	122.20
36	5	1307	G	P-O3'-C3'	10.06	131.77	119.70

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	C7	85	VAL	Peptide

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Mol	Chain	Res	Type	Group
27	D5	94	LYS	Peptide
28	D6	10	ARG	Peptide
52	M6	110	PRO	Peptide
9	S7	131	PHE	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	157 (77%)	31 (15%)	16 (8%)	1	5
2	s0	204/251 (81%)	150 (74%)	39 (19%)	15 (7%)	1	6
3	S1	212/254 (84%)	155 (73%)	31 (15%)	26 (12%)	0	1
3	s1	214/254 (84%)	170 (79%)	28 (13%)	16 (8%)	1	6
4	S2	215/253 (85%)	180 (84%)	21 (10%)	14 (6%)	1	8
4	s2	215/253 (85%)	173 (80%)	32 (15%)	10 (5%)	2	14
5	S3	221/239 (92%)	187 (85%)	26 (12%)	8 (4%)	3	20
5	s3	221/239 (92%)	179 (81%)	29 (13%)	13 (6%)	1	10
6	S4	258/260 (99%)	205 (80%)	38 (15%)	15 (6%)	1	10
6	s4	258/260 (99%)	215 (83%)	23 (9%)	20 (8%)	1	5
7	S5	204/224 (91%)	155 (76%)	32 (16%)	17 (8%)	1	5
7	s5	204/224 (91%)	154 (76%)	37 (18%)	13 (6%)	1	8
8	S6	224/236 (95%)	187 (84%)	26 (12%)	11 (5%)	2	14
8	s6	216/236 (92%)	189 (88%)	18 (8%)	9 (4%)	3	16
9	S7	182/189 (96%)	133 (73%)	32 (18%)	17 (9%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	s7	184/189 (97%)	152 (83%)	22 (12%)	10 (5%)	2	12
10	S8	184/200 (92%)	158 (86%)	18 (10%)	8 (4%)	2	16
10	s8	184/200 (92%)	150 (82%)	29 (16%)	5 (3%)	5	25
11	S9	183/196 (93%)	142 (78%)	35 (19%)	6 (3%)	4	21
11	s9	183/196 (93%)	145 (79%)	32 (18%)	6 (3%)	4	21
12	C0	83/96 (86%)	71 (86%)	9 (11%)	3 (4%)	3	20
12	c0	82/96 (85%)	61 (74%)	11 (13%)	10 (12%)	0	1
13	C1	145/155 (94%)	121 (83%)	16 (11%)	8 (6%)	2	11
13	c1	144/155 (93%)	118 (82%)	21 (15%)	5 (4%)	3	20
14	C2	122/142 (86%)	72 (59%)	31 (25%)	19 (16%)	0	0
14	c2	122/142 (86%)	72 (59%)	33 (27%)	17 (14%)	0	1
15	C3	148/150 (99%)	130 (88%)	12 (8%)	6 (4%)	3	16
15	c3	148/150 (99%)	119 (80%)	21 (14%)	8 (5%)	2	12
16	C4	125/136 (92%)	99 (79%)	14 (11%)	12 (10%)	0	3
16	c4	126/136 (93%)	99 (79%)	17 (14%)	10 (8%)	1	5
17	C5	122/141 (86%)	89 (73%)	25 (20%)	8 (7%)	1	7
17	c5	133/141 (94%)	98 (74%)	17 (13%)	18 (14%)	0	1
18	C6	139/142 (98%)	111 (80%)	21 (15%)	7 (5%)	2	13
18	c6	140/142 (99%)	122 (87%)	10 (7%)	8 (6%)	1	10
19	C7	116/136 (85%)	83 (72%)	26 (22%)	7 (6%)	1	9
19	c7	113/136 (83%)	89 (79%)	16 (14%)	8 (7%)	1	6
20	C8	143/145 (99%)	116 (81%)	14 (10%)	13 (9%)	1	4
20	c8	143/145 (99%)	117 (82%)	15 (10%)	11 (8%)	1	5
21	C9	141/143 (99%)	114 (81%)	20 (14%)	7 (5%)	2	13
21	c9	141/143 (99%)	119 (84%)	17 (12%)	5 (4%)	3	20
22	D0	105/120 (88%)	89 (85%)	10 (10%)	6 (6%)	1	10
22	d0	108/120 (90%)	81 (75%)	20 (18%)	7 (6%)	1	8
23	D1	85/87 (98%)	60 (71%)	15 (18%)	10 (12%)	0	1
23	d1	85/87 (98%)	69 (81%)	13 (15%)	3 (4%)	3	20
24	D2	127/129 (98%)	108 (85%)	17 (13%)	2 (2%)	9	37
24	d2	127/129 (98%)	113 (89%)	12 (9%)	2 (2%)	9	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	D3	142/144 (99%)	110 (78%)	19 (13%)	13 (9%)	1	4
25	d3	142/144 (99%)	127 (89%)	12 (8%)	3 (2%)	7	30
26	D4	132/134 (98%)	101 (76%)	19 (14%)	12 (9%)	1	4
26	d4	132/134 (98%)	102 (77%)	20 (15%)	10 (8%)	1	5
27	D5	68/107 (64%)	48 (71%)	15 (22%)	5 (7%)	1	6
27	d5	67/107 (63%)	54 (81%)	9 (13%)	4 (6%)	1	9
28	D6	95/97 (98%)	59 (62%)	23 (24%)	13 (14%)	0	1
28	d6	95/97 (98%)	71 (75%)	17 (18%)	7 (7%)	1	6
29	D7	79/81 (98%)	60 (76%)	16 (20%)	3 (4%)	3	19
29	d7	79/81 (98%)	65 (82%)	10 (13%)	4 (5%)	2	13
30	D8	61/66 (92%)	47 (77%)	10 (16%)	4 (7%)	1	7
30	d8	61/66 (92%)	48 (79%)	8 (13%)	5 (8%)	1	5
31	D9	51/55 (93%)	35 (69%)	12 (24%)	4 (8%)	1	5
31	d9	51/55 (93%)	43 (84%)	4 (8%)	4 (8%)	1	5
32	E0	58/62 (94%)	43 (74%)	12 (21%)	3 (5%)	2	12
32	e0	60/62 (97%)	46 (77%)	8 (13%)	6 (10%)	0	3
33	E1	69/76 (91%)	40 (58%)	13 (19%)	16 (23%)	0	0
33	e1	74/76 (97%)	34 (46%)	21 (28%)	19 (26%)	0	0
34	SR	316/318 (99%)	264 (84%)	38 (12%)	14 (4%)	2	15
34	sR	316/318 (99%)	266 (84%)	38 (12%)	12 (4%)	3	19
35	SM	131/182 (72%)	99 (76%)	18 (14%)	14 (11%)	0	2
35	sM	61/182 (34%)	39 (64%)	13 (21%)	9 (15%)	0	0
39	L2	250/253 (99%)	218 (87%)	24 (10%)	8 (3%)	4	22
39	l2	250/253 (99%)	213 (85%)	23 (9%)	14 (6%)	2	11
40	L3	384/386 (100%)	329 (86%)	48 (12%)	7 (2%)	8	34
40	l3	384/386 (100%)	346 (90%)	28 (7%)	10 (3%)	5	26
41	L4	359/361 (99%)	301 (84%)	38 (11%)	20 (6%)	2	11
41	l4	359/361 (99%)	289 (80%)	49 (14%)	21 (6%)	1	10
42	L5	294/296 (99%)	232 (79%)	41 (14%)	21 (7%)	1	6
42	l5	292/296 (99%)	249 (85%)	33 (11%)	10 (3%)	3	21
43	L6	152/175 (87%)	135 (89%)	15 (10%)	2 (1%)	12	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	l6	153/175 (87%)	130 (85%)	17 (11%)	6 (4%)	3	18
44	L7	220/243 (90%)	194 (88%)	20 (9%)	6 (3%)	5	25
44	l7	221/243 (91%)	199 (90%)	17 (8%)	5 (2%)	6	28
45	L8	231/255 (91%)	182 (79%)	34 (15%)	15 (6%)	1	8
45	l8	229/255 (90%)	178 (78%)	38 (17%)	13 (6%)	1	10
46	L9	189/191 (99%)	162 (86%)	23 (12%)	4 (2%)	7	30
46	l9	189/191 (99%)	170 (90%)	17 (9%)	2 (1%)	14	46
47	M0	207/220 (94%)	169 (82%)	28 (14%)	10 (5%)	2	14
47	m0	209/220 (95%)	168 (80%)	32 (15%)	9 (4%)	2	16
48	M1	167/173 (96%)	126 (75%)	24 (14%)	17 (10%)	0	3
48	m1	167/173 (96%)	142 (85%)	13 (8%)	12 (7%)	1	6
49	M3	191/198 (96%)	152 (80%)	26 (14%)	13 (7%)	1	7
49	m3	192/198 (97%)	157 (82%)	19 (10%)	16 (8%)	1	5
50	M4	134/137 (98%)	113 (84%)	14 (10%)	7 (5%)	2	12
50	m4	135/137 (98%)	116 (86%)	17 (13%)	2 (2%)	10	39
51	M5	201/203 (99%)	185 (92%)	10 (5%)	6 (3%)	4	23
51	m5	201/203 (99%)	179 (89%)	14 (7%)	8 (4%)	3	17
52	M6	195/198 (98%)	173 (89%)	17 (9%)	5 (3%)	5	26
52	m6	195/198 (98%)	183 (94%)	11 (6%)	1 (0%)	29	64
53	M7	181/183 (99%)	154 (85%)	20 (11%)	7 (4%)	3	18
53	m7	153/183 (84%)	134 (88%)	16 (10%)	3 (2%)	7	31
54	M8	183/185 (99%)	161 (88%)	17 (9%)	5 (3%)	5	25
54	m8	183/185 (99%)	149 (81%)	25 (14%)	9 (5%)	2	14
55	M9	186/188 (99%)	165 (89%)	20 (11%)	1 (0%)	29	64
55	m9	186/188 (99%)	165 (89%)	19 (10%)	2 (1%)	14	46
56	N0	170/172 (99%)	156 (92%)	10 (6%)	4 (2%)	6	27
56	n0	170/172 (99%)	154 (91%)	14 (8%)	2 (1%)	13	44
57	N1	157/159 (99%)	137 (87%)	17 (11%)	3 (2%)	8	33
57	n1	157/159 (99%)	141 (90%)	13 (8%)	3 (2%)	8	33
58	N2	98/120 (82%)	77 (79%)	18 (18%)	3 (3%)	4	23
58	n2	96/120 (80%)	80 (83%)	11 (12%)	5 (5%)	2	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	N3	134/136 (98%)	119 (89%)	12 (9%)	3 (2%)	6	29
59	n3	134/136 (98%)	123 (92%)	11 (8%)	0	100	100
60	N4	96/155 (62%)	68 (71%)	22 (23%)	6 (6%)	1	8
60	n4	133/155 (86%)	103 (77%)	23 (17%)	7 (5%)	2	12
61	N5	119/141 (84%)	99 (83%)	17 (14%)	3 (2%)	5	27
61	n5	118/141 (84%)	93 (79%)	16 (14%)	9 (8%)	1	5
62	N6	124/126 (98%)	106 (86%)	15 (12%)	3 (2%)	6	27
62	n6	124/126 (98%)	106 (86%)	13 (10%)	5 (4%)	3	17
63	N7	133/135 (98%)	109 (82%)	17 (13%)	7 (5%)	2	12
63	n7	133/135 (98%)	109 (82%)	13 (10%)	11 (8%)	1	5
64	N8	146/148 (99%)	121 (83%)	15 (10%)	10 (7%)	1	7
64	n8	146/148 (99%)	122 (84%)	17 (12%)	7 (5%)	2	14
65	N9	56/58 (97%)	47 (84%)	8 (14%)	1 (2%)	8	34
65	n9	56/58 (97%)	44 (79%)	6 (11%)	6 (11%)	0	2
66	O0	95/104 (91%)	84 (88%)	11 (12%)	0	100	100
66	o0	98/104 (94%)	84 (86%)	10 (10%)	4 (4%)	3	16
67	O1	107/112 (96%)	95 (89%)	7 (6%)	5 (5%)	2	14
67	o1	107/112 (96%)	92 (86%)	10 (9%)	5 (5%)	2	14
68	O2	125/129 (97%)	104 (83%)	14 (11%)	7 (6%)	2	11
68	o2	125/129 (97%)	105 (84%)	16 (13%)	4 (3%)	4	22
69	O3	104/106 (98%)	95 (91%)	8 (8%)	1 (1%)	15	49
69	o3	104/106 (98%)	94 (90%)	9 (9%)	1 (1%)	15	49
70	O4	110/120 (92%)	92 (84%)	16 (14%)	2 (2%)	8	34
70	o4	110/120 (92%)	96 (87%)	8 (7%)	6 (6%)	2	11
71	O5	117/119 (98%)	100 (86%)	12 (10%)	5 (4%)	2	16
71	o5	117/119 (98%)	100 (86%)	14 (12%)	3 (3%)	5	26
72	O6	97/99 (98%)	77 (79%)	12 (12%)	8 (8%)	1	5
72	o6	97/99 (98%)	82 (84%)	10 (10%)	5 (5%)	2	12
73	O7	85/87 (98%)	72 (85%)	13 (15%)	0	100	100
73	o7	85/87 (98%)	68 (80%)	12 (14%)	5 (6%)	1	10
74	O8	75/77 (97%)	64 (85%)	9 (12%)	2 (3%)	5	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
74	o8	75/77 (97%)	59 (79%)	13 (17%)	3 (4%)	3 17
75	O9	48/50 (96%)	41 (85%)	6 (12%)	1 (2%)	7 30
75	o9	48/50 (96%)	41 (85%)	6 (12%)	1 (2%)	7 30
76	Q0	50/52 (96%)	39 (78%)	9 (18%)	2 (4%)	3 17
76	q0	50/52 (96%)	48 (96%)	1 (2%)	1 (2%)	7 31
77	Q1	23/25 (92%)	20 (87%)	3 (13%)	0	100 100
77	q1	23/25 (92%)	23 (100%)	0	0	100 100
78	Q2	103/105 (98%)	82 (80%)	14 (14%)	7 (7%)	1 7
78	q2	103/105 (98%)	95 (92%)	6 (6%)	2 (2%)	8 33
79	Q3	89/91 (98%)	67 (75%)	15 (17%)	7 (8%)	1 5
79	q3	89/91 (98%)	78 (88%)	7 (8%)	4 (4%)	2 15
81	p0	139/311 (45%)	117 (84%)	16 (12%)	6 (4%)	2 16
All	All	22243/23945 (93%)	18323 (82%)	2769 (12%)	1151 (5%)	2 12

5 of 1151 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	158	VAL
2	S0	187	ALA
2	S0	191	ARG
2	S0	194	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	S0	164/209 (78%)	139 (85%)	25 (15%)	3 12
2	s0	173/209 (83%)	145 (84%)	28 (16%)	2 10
3	S1	191/223 (86%)	166 (87%)	25 (13%)	4 17
3	s1	192/223 (86%)	161 (84%)	31 (16%)	2 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	S2	176/204 (86%)	148 (84%)	28 (16%)	2	11
4	s2	176/204 (86%)	137 (78%)	39 (22%)	1	4
5	S3	182/194 (94%)	149 (82%)	33 (18%)	1	7
5	s3	182/194 (94%)	160 (88%)	22 (12%)	5	20
6	S4	221/221 (100%)	186 (84%)	35 (16%)	2	11
6	s4	221/221 (100%)	182 (82%)	39 (18%)	2	8
7	S5	173/190 (91%)	141 (82%)	32 (18%)	1	7
7	s5	173/190 (91%)	147 (85%)	26 (15%)	3	12
8	S6	188/201 (94%)	152 (81%)	36 (19%)	1	6
8	s6	187/201 (93%)	156 (83%)	31 (17%)	2	9
9	S7	165/169 (98%)	136 (82%)	29 (18%)	2	8
9	s7	166/169 (98%)	141 (85%)	25 (15%)	3	12
10	S8	150/161 (93%)	129 (86%)	21 (14%)	3	15
10	s8	150/161 (93%)	131 (87%)	19 (13%)	4	18
11	S9	158/165 (96%)	128 (81%)	30 (19%)	1	6
11	s9	158/165 (96%)	138 (87%)	20 (13%)	4	18
12	C0	77/78 (99%)	64 (83%)	13 (17%)	2	9
12	c0	73/78 (94%)	64 (88%)	9 (12%)	4	19
13	C1	129/129 (100%)	114 (88%)	15 (12%)	5	22
13	c1	129/129 (100%)	106 (82%)	23 (18%)	2	8
14	C2	88/118 (75%)	71 (81%)	17 (19%)	1	6
14	c2	88/118 (75%)	71 (81%)	17 (19%)	1	6
15	C3	127/127 (100%)	104 (82%)	23 (18%)	1	7
15	c3	127/127 (100%)	103 (81%)	24 (19%)	1	6
16	C4	81/104 (78%)	64 (79%)	17 (21%)	1	5
16	c4	97/104 (93%)	78 (80%)	19 (20%)	1	6
17	C5	101/117 (86%)	87 (86%)	14 (14%)	3	15
17	c5	103/117 (88%)	90 (87%)	13 (13%)	4	18
18	C6	117/118 (99%)	98 (84%)	19 (16%)	2	10
18	c6	118/118 (100%)	101 (86%)	17 (14%)	3	14
19	C7	94/124 (76%)	75 (80%)	19 (20%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	c7	106/124 (86%)	91 (86%)	15 (14%)	3	14
20	C8	128/128 (100%)	102 (80%)	26 (20%)	1	5
20	c8	128/128 (100%)	102 (80%)	26 (20%)	1	5
21	C9	115/115 (100%)	93 (81%)	22 (19%)	1	6
21	c9	115/115 (100%)	98 (85%)	17 (15%)	3	13
22	D0	100/113 (88%)	83 (83%)	17 (17%)	2	9
22	d0	103/113 (91%)	79 (77%)	24 (23%)	1	3
23	D1	74/74 (100%)	62 (84%)	12 (16%)	2	10
23	d1	74/74 (100%)	64 (86%)	10 (14%)	4	16
24	D2	110/110 (100%)	91 (83%)	19 (17%)	2	9
24	d2	110/110 (100%)	95 (86%)	15 (14%)	3	16
25	D3	119/119 (100%)	103 (87%)	16 (13%)	4	16
25	d3	119/119 (100%)	103 (87%)	16 (13%)	4	16
26	D4	112/112 (100%)	96 (86%)	16 (14%)	3	14
26	d4	112/112 (100%)	96 (86%)	16 (14%)	3	14
27	D5	61/88 (69%)	45 (74%)	16 (26%)	0	1
27	d5	61/88 (69%)	56 (92%)	5 (8%)	11	38
28	D6	83/83 (100%)	63 (76%)	20 (24%)	0	2
28	d6	83/83 (100%)	73 (88%)	10 (12%)	5	20
29	D7	70/70 (100%)	58 (83%)	12 (17%)	2	9
29	d7	70/70 (100%)	61 (87%)	9 (13%)	4	18
30	D8	56/59 (95%)	45 (80%)	11 (20%)	1	6
30	d8	56/59 (95%)	47 (84%)	9 (16%)	2	10
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2	9
31	d9	47/48 (98%)	42 (89%)	5 (11%)	6	26
32	E0	51/53 (96%)	45 (88%)	6 (12%)	5	21
32	e0	53/53 (100%)	41 (77%)	12 (23%)	1	3
33	E1	62/66 (94%)	48 (77%)	14 (23%)	1	3
33	e1	66/66 (100%)	54 (82%)	12 (18%)	1	7
34	SR	259/261 (99%)	226 (87%)	33 (13%)	4	18
34	sR	261/261 (100%)	238 (91%)	23 (9%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	SM	97/115 (84%)	77 (79%)	20 (21%)	1	5
35	sM	54/115 (47%)	43 (80%)	11 (20%)	1	5
39	L2	193/195 (99%)	152 (79%)	41 (21%)	1	5
39	l2	194/195 (100%)	160 (82%)	34 (18%)	2	8
40	L3	320/322 (99%)	256 (80%)	64 (20%)	1	5
40	l3	322/322 (100%)	270 (84%)	52 (16%)	2	10
41	L4	288/288 (100%)	237 (82%)	51 (18%)	2	8
41	l4	288/288 (100%)	244 (85%)	44 (15%)	2	12
42	L5	244/244 (100%)	207 (85%)	37 (15%)	3	12
42	l5	243/244 (100%)	202 (83%)	41 (17%)	2	9
43	L6	134/152 (88%)	115 (86%)	19 (14%)	3	14
43	l6	135/152 (89%)	112 (83%)	23 (17%)	2	9
44	L7	186/204 (91%)	169 (91%)	17 (9%)	9	33
44	l7	187/204 (92%)	163 (87%)	24 (13%)	4	18
45	L8	187/207 (90%)	163 (87%)	24 (13%)	4	18
45	l8	177/207 (86%)	146 (82%)	31 (18%)	2	8
46	L9	171/171 (100%)	134 (78%)	37 (22%)	1	4
46	l9	171/171 (100%)	133 (78%)	38 (22%)	1	4
47	M0	177/186 (95%)	146 (82%)	31 (18%)	2	8
47	m0	182/186 (98%)	151 (83%)	31 (17%)	2	9
48	M1	147/149 (99%)	117 (80%)	30 (20%)	1	5
48	m1	147/149 (99%)	119 (81%)	28 (19%)	1	6
49	M3	154/158 (98%)	133 (86%)	21 (14%)	3	16
49	m3	154/158 (98%)	134 (87%)	20 (13%)	4	18
50	M4	107/108 (99%)	91 (85%)	16 (15%)	3	12
50	m4	108/108 (100%)	93 (86%)	15 (14%)	3	15
51	M5	175/175 (100%)	144 (82%)	31 (18%)	2	8
51	m5	175/175 (100%)	154 (88%)	21 (12%)	5	20
52	M6	160/161 (99%)	138 (86%)	22 (14%)	3	16
52	m6	160/161 (99%)	138 (86%)	22 (14%)	3	16
53	M7	140/145 (97%)	119 (85%)	21 (15%)	3	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	m7	125/145 (86%)	110 (88%)	15 (12%)	5	20
54	M8	150/150 (100%)	127 (85%)	23 (15%)	2	12
54	m8	150/150 (100%)	129 (86%)	21 (14%)	3	15
55	M9	153/153 (100%)	134 (88%)	19 (12%)	4	19
55	m9	153/153 (100%)	122 (80%)	31 (20%)	1	5
56	N0	156/156 (100%)	131 (84%)	25 (16%)	2	11
56	n0	156/156 (100%)	127 (81%)	29 (19%)	1	7
57	N1	136/136 (100%)	110 (81%)	26 (19%)	1	6
57	n1	136/136 (100%)	108 (79%)	28 (21%)	1	5
58	N2	87/106 (82%)	78 (90%)	9 (10%)	7	27
58	n2	85/106 (80%)	71 (84%)	14 (16%)	2	10
59	N3	104/104 (100%)	88 (85%)	16 (15%)	2	11
59	n3	104/104 (100%)	93 (89%)	11 (11%)	6	26
60	N4	57/129 (44%)	51 (90%)	6 (10%)	7	26
60	n4	114/129 (88%)	99 (87%)	15 (13%)	4	17
61	N5	104/117 (89%)	81 (78%)	23 (22%)	1	4
61	n5	104/117 (89%)	88 (85%)	16 (15%)	2	11
62	N6	109/109 (100%)	91 (84%)	18 (16%)	2	10
62	n6	109/109 (100%)	92 (84%)	17 (16%)	2	11
63	N7	115/115 (100%)	97 (84%)	18 (16%)	2	11
63	n7	115/115 (100%)	93 (81%)	22 (19%)	1	6
64	N8	118/118 (100%)	93 (79%)	25 (21%)	1	5
64	n8	118/118 (100%)	96 (81%)	22 (19%)	1	7
65	N9	46/46 (100%)	37 (80%)	9 (20%)	1	6
65	n9	46/46 (100%)	38 (83%)	8 (17%)	2	9
66	O0	81/87 (93%)	63 (78%)	18 (22%)	1	4
66	o0	84/87 (97%)	67 (80%)	17 (20%)	1	5
67	O1	92/96 (96%)	74 (80%)	18 (20%)	1	6
67	o1	96/96 (100%)	80 (83%)	16 (17%)	2	9
68	O2	109/110 (99%)	93 (85%)	16 (15%)	3	13
68	o2	109/110 (99%)	88 (81%)	21 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	O3	90/90 (100%)	81 (90%)	9 (10%)	7	28
69	o3	90/90 (100%)	80 (89%)	10 (11%)	6	24
70	O4	95/102 (93%)	81 (85%)	14 (15%)	3	13
70	o4	95/102 (93%)	81 (85%)	14 (15%)	3	13
71	O5	104/104 (100%)	85 (82%)	19 (18%)	1	7
71	o5	104/104 (100%)	86 (83%)	18 (17%)	2	9
72	O6	81/81 (100%)	64 (79%)	17 (21%)	1	5
72	o6	81/81 (100%)	55 (68%)	26 (32%)	0	0
73	O7	70/70 (100%)	56 (80%)	14 (20%)	1	5
73	o7	70/70 (100%)	59 (84%)	11 (16%)	2	11
74	O8	68/68 (100%)	56 (82%)	12 (18%)	2	8
74	o8	68/68 (100%)	59 (87%)	9 (13%)	4	17
75	O9	45/45 (100%)	38 (84%)	7 (16%)	2	11
75	o9	45/45 (100%)	41 (91%)	4 (9%)	9	34
76	Q0	47/47 (100%)	40 (85%)	7 (15%)	3	13
76	q0	47/47 (100%)	35 (74%)	12 (26%)	0	1
77	Q1	23/23 (100%)	19 (83%)	4 (17%)	2	9
77	q1	23/23 (100%)	15 (65%)	8 (35%)	0	0
78	Q2	90/90 (100%)	74 (82%)	16 (18%)	2	8
78	q2	90/90 (100%)	76 (84%)	14 (16%)	2	11
79	Q3	71/71 (100%)	59 (83%)	12 (17%)	2	9
79	q3	71/71 (100%)	60 (84%)	11 (16%)	2	11
81	p0	105/253 (42%)	89 (85%)	16 (15%)	3	12
All	All	18777/19961 (94%)	15699 (84%)	3078 (16%)	2	10

5 of 3078 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	c1	21	ASN
41	l4	99	MET
15	c3	115	LEU
13	c1	5	LEU
25	d3	107	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
21	c9	25	GLN
52	m6	72	HIS
22	d0	16	GLN
39	l2	194	ASN
55	m9	36	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1777/1800 (98%)	461 (25%)	48 (2%)
1	6	1792/1800 (99%)	448 (25%)	45 (2%)
36	1	3145/3396 (92%)	658 (20%)	62 (1%)
36	5	3146/3396 (92%)	650 (20%)	68 (2%)
37	3	120/121 (99%)	13 (10%)	2 (1%)
37	7	120/121 (99%)	19 (15%)	1 (0%)
38	4	157/158 (99%)	37 (23%)	3 (1%)
38	8	157/158 (99%)	38 (24%)	1 (0%)
All	All	10414/10950 (95%)	2324 (22%)	230 (2%)

5 of 2324 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	25	C
1	2	26	A
1	2	27	U

5 of 230 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	6	25	C
36	5	3207	U
1	6	1207	C
36	5	3154	C
36	5	2204	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2030 ligands modelled in this entry, 995 are monoatomic - leaving 1035 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	1	3795	-	0,6,6	-	-	-		
85	OHX	8	224	-	0,6,6	-	-	-		
85	OHX	6	2068	-	0,6,6	-	-	-		
85	OHX	5	3915	-	0,6,6	-	-	-		
85	OHX	1	4015	-	0,6,6	-	-	-		
85	OHX	1	3994	-	0,6,6	-	-	-		
85	OHX	5	3957	-	0,6,6	-	-	-		
85	OHX	1	3850	-	0,6,6	-	-	-		
85	OHX	1	4005	-	0,6,6	-	-	-		
85	OHX	6	2098	-	0,6,6	-	-	-		
85	OHX	5	3964	-	0,6,6	-	-	-		
85	OHX	1	3929	-	0,6,6	-	-	-		
85	OHX	6	2058	-	0,6,6	-	-	-		
85	OHX	1	3999	-	0,6,6	-	-	-		
85	OHX	5	3991	-	0,6,6	-	-	-		
85	OHX	1	3933	-	0,6,6	-	-	-		
85	OHX	2	2034	-	0,6,6	-	-	-		
85	OHX	2	1994	-	0,6,6	-	-	-		
85	OHX	5	4044	-	0,6,6	-	-	-		
85	OHX	1	3836	-	0,6,6	-	-	-		
85	OHX	2	2048	-	0,6,6	-	-	-		
85	OHX	6	2136	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	1	3927	-	0,6,6	-	-	-		
85	OHX	2	2031	-	0,6,6	-	-	-		
85	OHX	1	3808	-	0,6,6	-	-	-		
85	OHX	1	3888	-	0,6,6	-	-	-		
85	OHX	6	2099	-	0,6,6	-	-	-		
85	OHX	5	3822	-	0,6,6	-	-	-		
85	OHX	2	2094	-	0,6,6	-	-	-		
85	OHX	6	2095	-	0,6,6	-	-	-		
85	OHX	5	3841	-	0,6,6	-	-	-		
85	OHX	5	3891	-	0,6,6	-	-	-		
85	OHX	2	2006	-	0,6,6	-	-	-		
85	OHX	1	3797	-	0,6,6	-	-	-		
85	OHX	1	3759	-	0,6,6	-	-	-		
85	OHX	2	2005	-	0,6,6	-	-	-		
85	OHX	5	3850	-	0,6,6	-	-	-		
85	OHX	5	3885	-	0,6,6	-	-	-		
85	OHX	5	3970	-	0,6,6	-	-	-		
85	OHX	l5	302	-	0,6,6	-	-	-		
85	OHX	5	3835	-	0,6,6	-	-	-		
85	OHX	5	3895	-	0,6,6	-	-	-		
85	OHX	1	3855	-	0,6,6	-	-	-		
85	OHX	1	3902	-	0,6,6	-	-	-		
85	OHX	5	3932	-	0,6,6	-	-	-		
85	OHX	5	3981	-	0,6,6	-	-	-		
85	OHX	C8	201	-	0,6,6	-	-	-		
85	OHX	1	3818	-	0,6,6	-	-	-		
85	OHX	2	2046	-	0,6,6	-	-	-		
85	OHX	2	1985	-	0,6,6	-	-	-		
85	OHX	1	3832	-	0,6,6	-	-	-		
85	OHX	1	3971	-	0,6,6	-	-	-		
85	OHX	1	3758	-	0,6,6	-	-	-		
85	OHX	5	3761	-	0,6,6	-	-	-		
85	OHX	m7	204	-	0,6,6	-	-	-		
85	OHX	6	2148	-	0,6,6	-	-	-		
85	OHX	5	4061	-	0,6,6	-	-	-		
85	OHX	5	3872	-	0,6,6	-	-	-		
85	OHX	7	213	-	0,6,6	-	-	-		
85	OHX	6	2062	-	0,6,6	-	-	-		
85	OHX	2	2084	-	0,6,6	-	-	-		
85	OHX	6	2022	-	0,6,6	-	-	-		
85	OHX	5	4015	-	0,6,6	-	-	-		
85	OHX	1	3750	-	0,6,6	-	-	-		
85	OHX	1	4031	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	8	217	-	0,6,6	-	-	-		
85	OHX	6	2080	-	0,6,6	-	-	-		
85	OHX	6	2084	-	0,6,6	-	-	-		
85	OHX	2	2077	-	0,6,6	-	-	-		
85	OHX	1	3742	-	0,6,6	-	-	-		
85	OHX	1	3809	-	0,6,6	-	-	-		
85	OHX	6	2050	-	0,6,6	-	-	-		
85	OHX	6	2138	-	0,6,6	-	-	-		
85	OHX	6	2065	-	0,6,6	-	-	-		
85	OHX	2	2022	-	0,6,6	-	-	-		
85	OHX	2	2051	-	0,6,6	-	-	-		
85	OHX	s4	301	-	0,6,6	-	-	-		
85	OHX	5	3751	-	0,6,6	-	-	-		
85	OHX	5	3839	-	0,6,6	-	-	-		
85	OHX	1	3769	-	0,6,6	-	-	-		
85	OHX	5	3972	-	0,6,6	-	-	-		
85	OHX	q2	502	-	0,6,6	-	-	-		
85	OHX	sR	401	-	0,6,6	-	-	-		
85	OHX	1	3923	-	0,6,6	-	-	-		
85	OHX	1	4002	-	0,6,6	-	-	-		
85	OHX	5	3833	-	0,6,6	-	-	-		
85	OHX	2	2020	-	0,6,6	-	-	-		
85	OHX	5	3893	-	0,6,6	-	-	-		
85	OHX	5	3746	-	0,6,6	-	-	-		
85	OHX	7	216	-	0,6,6	-	-	-		
85	OHX	5	3883	-	0,6,6	-	-	-		
85	OHX	5	4052	-	0,6,6	-	-	-		
85	OHX	6	2028	-	0,6,6	-	-	-		
85	OHX	1	3877	-	0,6,6	-	-	-		
85	OHX	1	3978	-	0,6,6	-	-	-		
85	OHX	1	3918	-	0,6,6	-	-	-		
85	OHX	5	4003	-	0,6,6	-	-	-		
85	OHX	5	3861	-	0,6,6	-	-	-		
85	OHX	6	2072	-	0,6,6	-	-	-		
85	OHX	1	3752	-	0,6,6	-	-	-		
85	OHX	1	3827	-	0,6,6	-	-	-		
85	OHX	3	212	-	0,6,6	-	-	-		
85	OHX	5	3809	-	0,6,6	-	-	-		
85	OHX	8	215	-	0,6,6	-	-	-		
85	OHX	1	4036	-	0,6,6	-	-	-		
85	OHX	o3	202	-	0,6,6	-	-	-		
85	OHX	5	3921	-	0,6,6	-	-	-		
85	OHX	1	3948	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	d4	201	-	0,6,6	-	-	-		
85	OHX	8	219	-	0,6,6	-	-	-		
85	OHX	5	4060	-	0,6,6	-	-	-		
85	OHX	5	3843	-	0,6,6	-	-	-		
85	OHX	O3	202	-	0,6,6	-	-	-		
85	OHX	6	2036	-	0,6,6	-	-	-		
85	OHX	1	3866	-	0,6,6	-	-	-		
85	OHX	5	4029	-	0,6,6	-	-	-		
85	OHX	1	4008	-	0,6,6	-	-	-		
85	OHX	5	3886	-	0,6,6	-	-	-		
85	OHX	2	2021	-	0,6,6	-	-	-		
85	OHX	1	3908	-	0,6,6	-	-	-		
85	OHX	5	3904	-	0,6,6	-	-	-		
85	OHX	8	220	-	0,6,6	-	-	-		
85	OHX	1	3892	-	0,6,6	-	-	-		
85	OHX	5	4011	-	0,6,6	-	-	-		
85	OHX	1	3938	-	0,6,6	-	-	-		
85	OHX	5	3936	-	0,6,6	-	-	-		
85	OHX	1	3779	-	0,6,6	-	-	-		
85	OHX	5	4037	-	0,6,6	-	-	-		
85	OHX	5	3801	-	0,6,6	-	-	-		
85	OHX	1	4028	-	0,6,6	-	-	-		
85	OHX	2	2070	-	0,6,6	-	-	-		
85	OHX	2	2044	-	0,6,6	-	-	-		
85	OHX	6	2087	-	0,6,6	-	-	-		
85	OHX	5	4035	-	0,6,6	-	-	-		
85	OHX	1	3756	-	0,6,6	-	-	-		
85	OHX	4	216	-	0,6,6	-	-	-		
85	OHX	1	3822	-	0,6,6	-	-	-		
85	OHX	5	3958	-	0,6,6	-	-	-		
85	OHX	1	3760	-	0,6,6	-	-	-		
85	OHX	5	3999	-	0,6,6	-	-	-		
85	OHX	5	3826	-	0,6,6	-	-	-		
85	OHX	5	3776	-	0,6,6	-	-	-		
85	OHX	5	4057	-	0,6,6	-	-	-		
85	OHX	1	4017	-	0,6,6	-	-	-		
85	OHX	2	2037	-	0,6,6	-	-	-		
85	OHX	1	3767	-	0,6,6	-	-	-		
85	OHX	1	3868	-	0,6,6	-	-	-		
85	OHX	1	3959	-	0,6,6	-	-	-		
85	OHX	5	3772	-	0,6,6	-	-	-		
85	OHX	5	4043	-	0,6,6	-	-	-		
85	OHX	2	2004	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	2	2012	-	0,6,6	-	-	-		
85	OHX	5	4008	-	0,6,6	-	-	-		
85	OHX	1	3859	-	0,6,6	-	-	-		
85	OHX	1	3928	-	0,6,6	-	-	-		
85	OHX	6	2053	-	0,6,6	-	-	-		
85	OHX	1	3911	-	0,6,6	-	-	-		
85	OHX	5	3844	-	0,6,6	-	-	-		
85	OHX	5	3775	-	0,6,6	-	-	-		
85	OHX	L4	401	-	0,6,6	-	-	-		
85	OHX	5	4039	-	0,6,6	-	-	-		
85	OHX	1	3845	-	0,6,6	-	-	-		
85	OHX	1	3776	-	0,6,6	-	-	-		
85	OHX	5	3778	-	0,6,6	-	-	-		
85	OHX	5	3988	-	0,6,6	-	-	-		
85	OHX	1	4022	-	0,6,6	-	-	-		
85	OHX	1	3968	-	0,6,6	-	-	-		
85	OHX	6	2019	-	0,6,6	-	-	-		
85	OHX	5	3881	-	0,6,6	-	-	-		
85	OHX	5	3830	-	0,6,6	-	-	-		
85	OHX	2	2049	-	0,6,6	-	-	-		
85	OHX	5	3817	-	0,6,6	-	-	-		
85	OHX	1	3785	-	0,6,6	-	-	-		
85	OHX	6	2140	-	0,6,6	-	-	-		
85	OHX	1	3986	-	0,6,6	-	-	-		
85	OHX	5	3848	-	0,6,6	-	-	-		
85	OHX	5	3832	-	0,6,6	-	-	-		
85	OHX	5	3758	-	0,6,6	-	-	-		
85	OHX	5	3851	-	0,6,6	-	-	-		
85	OHX	1	3988	-	0,6,6	-	-	-		
85	OHX	5	3790	-	0,6,6	-	-	-		
85	OHX	5	4042	-	0,6,6	-	-	-		
85	OHX	5	3940	-	0,6,6	-	-	-		
85	OHX	2	2098	-	0,6,6	-	-	-		
85	OHX	1	3805	-	0,6,6	-	-	-		
85	OHX	5	3820	-	0,6,6	-	-	-		
85	OHX	2	2015	-	0,6,6	-	-	-		
85	OHX	2	2058	-	0,6,6	-	-	-		
85	OHX	1	3946	-	0,6,6	-	-	-		
85	OHX	5	3879	-	0,6,6	-	-	-		
85	OHX	1	3789	-	0,6,6	-	-	-		
85	OHX	5	4050	-	0,6,6	-	-	-		
85	OHX	1	3858	-	0,6,6	-	-	-		
85	OHX	m0	302	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	1	3874	-	0,6,6	-	-	-		
85	OHX	8	212	-	0,6,6	-	-	-		
85	OHX	5	3742	-	0,6,6	-	-	-		
85	OHX	1	3903	-	0,6,6	-	-	-		
85	OHX	1	3990	-	0,6,6	-	-	-		
85	OHX	1	3787	-	0,6,6	-	-	-		
85	OHX	1	3955	-	0,6,6	-	-	-		
85	OHX	5	3871	-	0,6,6	-	-	-		
85	OHX	1	4010	-	0,6,6	-	-	-		
85	OHX	5	4048	-	0,6,6	-	-	-		
85	OHX	5	3961	-	0,6,6	-	-	-		
85	OHX	6	2041	-	0,6,6	-	-	-		
85	OHX	1	3952	-	0,6,6	-	-	-		
85	OHX	1	3817	-	0,6,6	-	-	-		
85	OHX	2	2116	-	0,6,6	-	-	-		
85	OHX	1	3914	-	0,6,6	-	-	-		
85	OHX	1	3953	-	0,6,6	-	-	-		
85	OHX	6	2014	-	0,6,6	-	-	-		
85	OHX	8	211	-	0,6,6	-	-	-		
85	OHX	5	3877	-	0,6,6	-	-	-		
85	OHX	2	2075	-	0,6,6	-	-	-		
85	OHX	1	3848	-	0,6,6	-	-	-		
85	OHX	6	2118	-	0,6,6	-	-	-		
85	OHX	1	3989	-	0,6,6	-	-	-		
85	OHX	1	3921	-	0,6,6	-	-	-		
85	OHX	1	3950	-	0,6,6	-	-	-		
85	OHX	1	3824	-	0,6,6	-	-	-		
85	OHX	1	3917	-	0,6,6	-	-	-		
85	OHX	2	2073	-	0,6,6	-	-	-		
85	OHX	6	2147	-	0,6,6	-	-	-		
85	OHX	1	3747	-	0,6,6	-	-	-		
85	OHX	5	3774	-	0,6,6	-	-	-		
85	OHX	2	2000	-	0,6,6	-	-	-		
85	OHX	5	3955	-	0,6,6	-	-	-		
85	OHX	5	3971	-	0,6,6	-	-	-		
85	OHX	1	3873	-	0,6,6	-	-	-		
85	OHX	5	3944	-	0,6,6	-	-	-		
85	OHX	5	3764	-	0,6,6	-	-	-		
85	OHX	5	3831	-	0,6,6	-	-	-		
85	OHX	2	2079	-	0,6,6	-	-	-		
85	OHX	1	3847	-	0,6,6	-	-	-		
85	OHX	6	2158	-	0,6,6	-	-	-		
85	OHX	5	3866	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	6	2128	-	0,6,6	-	-	-		
85	OHX	1	4011	-	0,6,6	-	-	-		
85	OHX	6	2031	-	0,6,6	-	-	-		
85	OHX	5	4018	-	0,6,6	-	-	-		
85	OHX	2	2101	-	0,6,6	-	-	-		
85	OHX	6	2035	-	0,6,6	-	-	-		
85	OHX	8	225	-	0,6,6	-	-	-		
85	OHX	1	3788	-	0,6,6	-	-	-		
85	OHX	D9	103	-	0,6,6	-	-	-		
85	OHX	2	2024	-	0,6,6	-	-	-		
85	OHX	5	3779	-	0,6,6	-	-	-		
85	OHX	5	3993	-	0,6,6	-	-	-		
85	OHX	7	212	-	0,6,6	-	-	-		
85	OHX	1	3867	-	0,6,6	-	-	-		
85	OHX	6	2078	-	0,6,6	-	-	-		
85	OHX	2	1988	-	0,6,6	-	-	-		
85	OHX	5	3874	-	0,6,6	-	-	-		
85	OHX	1	3761	-	0,6,6	-	-	-		
85	OHX	2	2074	-	0,6,6	-	-	-		
85	OHX	N8	203	-	0,6,6	-	-	-		
85	OHX	5	3782	-	0,6,6	-	-	-		
85	OHX	5	4066	-	0,6,6	-	-	-		
85	OHX	2	2019	-	0,6,6	-	-	-		
85	OHX	1	3798	-	0,6,6	-	-	-		
85	OHX	2	2010	-	0,6,6	-	-	-		
85	OHX	1	3974	-	0,6,6	-	-	-		
85	OHX	2	1998	-	0,6,6	-	-	-		
85	OHX	1	3957	-	0,6,6	-	-	-		
85	OHX	2	2066	-	0,6,6	-	-	-		
85	OHX	1	4020	-	0,6,6	-	-	-		
85	OHX	1	3942	-	0,6,6	-	-	-		
85	OHX	3	215	-	0,6,6	-	-	-		
85	OHX	6	2038	-	0,6,6	-	-	-		
85	OHX	5	3899	-	0,6,6	-	-	-		
85	OHX	5	4063	-	0,6,6	-	-	-		
85	OHX	1	3913	-	0,6,6	-	-	-		
85	OHX	1	3813	-	0,6,6	-	-	-		
85	OHX	1	3768	-	0,6,6	-	-	-		
85	OHX	3	217	-	0,6,6	-	-	-		
85	OHX	4	221	-	0,6,6	-	-	-		
85	OHX	1	3782	-	0,6,6	-	-	-		
85	OHX	6	2045	-	0,6,6	-	-	-		
85	OHX	1	3922	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	5	3875	-	0,6,6	-	-	-		
85	OHX	1	3733	-	0,6,6	-	-	-		
85	OHX	1	3735	-	0,6,6	-	-	-		
85	OHX	6	2051	-	0,6,6	-	-	-		
85	OHX	5	3898	-	0,6,6	-	-	-		
85	OHX	5	4022	-	0,6,6	-	-	-		
85	OHX	5	4068	-	0,6,6	-	-	-		
85	OHX	6	2132	-	0,6,6	-	-	-		
85	OHX	1	3820	-	0,6,6	-	-	-		
85	OHX	2	2030	-	0,6,6	-	-	-		
85	OHX	6	2049	-	0,6,6	-	-	-		
85	OHX	8	221	-	0,6,6	-	-	-		
85	OHX	2	2026	-	0,6,6	-	-	-		
85	OHX	1	3889	-	0,6,6	-	-	-		
85	OHX	5	3974	-	0,6,6	-	-	-		
85	OHX	2	1989	-	0,6,6	-	-	-		
85	OHX	2	2016	-	0,6,6	-	-	-		
85	OHX	5	3986	-	0,6,6	-	-	-		
85	OHX	6	2009	-	0,6,6	-	-	-		
85	OHX	2	2111	-	0,6,6	-	-	-		
85	OHX	1	3734	-	0,6,6	-	-	-		
85	OHX	6	2039	-	0,6,6	-	-	-		
85	OHX	M9	201	-	0,6,6	-	-	-		
85	OHX	1	3800	-	0,6,6	-	-	-		
85	OHX	1	3894	-	0,6,6	-	-	-		
85	OHX	c5	201	-	0,6,6	-	-	-		
85	OHX	1	3794	-	0,6,6	-	-	-		
85	OHX	2	2008	-	0,6,6	-	-	-		
85	OHX	5	3813	-	0,6,6	-	-	-		
85	OHX	6	2104	-	0,6,6	-	-	-		
85	OHX	N1	201	-	0,6,6	-	-	-		
85	OHX	2	2039	-	0,6,6	-	-	-		
85	OHX	5	3949	-	0,6,6	-	-	-		
85	OHX	5	3989	-	0,6,6	-	-	-		
85	OHX	5	3829	-	0,6,6	-	-	-		
85	OHX	5	4046	-	0,6,6	-	-	-		
85	OHX	5	3792	-	0,6,6	-	-	-		
85	OHX	4	223	-	0,6,6	-	-	-		
85	OHX	6	2024	-	0,6,6	-	-	-		
85	OHX	2	2118	-	0,6,6	-	-	-		
85	OHX	1	3885	-	0,6,6	-	-	-		
85	OHX	2	2071	-	0,6,6	-	-	-		
85	OHX	6	2075	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	1	3925	-	0,6,6	-	-	-		
85	OHX	5	3783	-	0,6,6	-	-	-		
85	OHX	S6	301	-	0,6,6	-	-	-		
85	OHX	5	3980	-	0,6,6	-	-	-		
85	OHX	6	2021	-	0,6,6	-	-	-		
85	OHX	2	2103	-	0,6,6	-	-	-		
85	OHX	2	2105	-	0,6,6	-	-	-		
85	OHX	5	3794	-	0,6,6	-	-	-		
85	OHX	6	2037	-	0,6,6	-	-	-		
85	OHX	5	3786	-	0,6,6	-	-	-		
85	OHX	5	3873	-	0,6,6	-	-	-		
85	OHX	5	3750	-	0,6,6	-	-	-		
85	OHX	L3	402	-	0,6,6	-	-	-		
85	OHX	6	2012	-	0,6,6	-	-	-		
85	OHX	1	3771	-	0,6,6	-	-	-		
85	OHX	5	3807	-	0,6,6	-	-	-		
85	OHX	5	3894	-	0,6,6	-	-	-		
85	OHX	1	3898	-	0,6,6	-	-	-		
85	OHX	6	2124	-	0,6,6	-	-	-		
85	OHX	1	3745	-	0,6,6	-	-	-		
85	OHX	5	3796	-	0,6,6	-	-	-		
85	OHX	1	3932	-	0,6,6	-	-	-		
85	OHX	6	2046	-	0,6,6	-	-	-		
85	OHX	1	3980	-	0,6,6	-	-	-		
85	OHX	8	214	-	0,6,6	-	-	-		
85	OHX	1	4026	-	0,6,6	-	-	-		
85	OHX	2	2088	-	0,6,6	-	-	-		
85	OHX	1	3821	-	0,6,6	-	-	-		
85	OHX	6	2073	-	0,6,6	-	-	-		
85	OHX	1	3982	-	0,6,6	-	-	-		
85	OHX	8	213	-	0,6,6	-	-	-		
85	OHX	5	4058	-	0,6,6	-	-	-		
85	OHX	6	2063	-	0,6,6	-	-	-		
85	OHX	1	3977	-	0,6,6	-	-	-		
85	OHX	1	3944	-	0,6,6	-	-	-		
85	OHX	2	2113	-	0,6,6	-	-	-		
85	OHX	1	4027	-	0,6,6	-	-	-		
85	OHX	5	3929	-	0,6,6	-	-	-		
85	OHX	5	3853	-	0,6,6	-	-	-		
85	OHX	1	3886	-	0,6,6	-	-	-		
85	OHX	1	3764	-	0,6,6	-	-	-		
85	OHX	5	3757	-	0,6,6	-	-	-		
85	OHX	1	3746	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	1	3791	-	0,6,6	-	-	-		
85	OHX	1	3831	-	0,6,6	-	-	-		
85	OHX	6	2102	-	0,6,6	-	-	-		
85	OHX	5	3744	-	0,6,6	-	-	-		
85	OHX	5	3997	-	0,6,6	-	-	-		
85	OHX	2	2080	-	0,6,6	-	-	-		
85	OHX	2	2007	-	0,6,6	-	-	-		
85	OHX	5	3827	-	0,6,6	-	-	-		
85	OHX	5	4038	-	0,6,6	-	-	-		
85	OHX	5	3996	-	0,6,6	-	-	-		
85	OHX	5	3965	-	0,6,6	-	-	-		
85	OHX	2	1991	-	0,6,6	-	-	-		
85	OHX	6	2015	-	0,6,6	-	-	-		
85	OHX	1	3833	-	0,6,6	-	-	-		
85	OHX	n9	102	-	0,6,6	-	-	-		
85	OHX	1	3899	-	0,6,6	-	-	-		
85	OHX	6	2130	-	0,6,6	-	-	-		
85	OHX	1	3853	-	0,6,6	-	-	-		
85	OHX	1	3972	-	0,6,6	-	-	-		
85	OHX	1	3983	-	0,6,6	-	-	-		
85	OHX	5	3834	-	0,6,6	-	-	-		
85	OHX	1	3905	-	0,6,6	-	-	-		
85	OHX	5	3909	-	0,6,6	-	-	-		
85	OHX	5	3884	-	0,6,6	-	-	-		
85	OHX	1	3900	-	0,6,6	-	-	-		
85	OHX	6	2123	-	0,6,6	-	-	-		
85	OHX	2	2001	-	0,6,6	-	-	-		
85	OHX	6	2040	-	0,6,6	-	-	-		
85	OHX	5	3912	-	0,6,6	-	-	-		
85	OHX	6	2142	-	0,6,6	-	-	-		
85	OHX	1	3854	-	0,6,6	-	-	-		
85	OHX	1	3926	-	0,6,6	-	-	-		
85	OHX	6	2105	-	0,6,6	-	-	-		
85	OHX	2	2029	-	0,6,6	-	-	-		
85	OHX	1	4003	-	0,6,6	-	-	-		
85	OHX	6	2108	-	0,6,6	-	-	-		
85	OHX	5	3987	-	0,6,6	-	-	-		
85	OHX	1	3741	-	0,6,6	-	-	-		
85	OHX	5	3959	-	0,6,6	-	-	-		
85	OHX	2	1993	-	0,6,6	-	-	-		
85	OHX	1	3775	-	0,6,6	-	-	-		
85	OHX	1	3901	-	0,6,6	-	-	-		
85	OHX	2	1999	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	6	2079	-	0,6,6	-	-	-		
85	OHX	1	3792	-	0,6,6	-	-	-		
85	OHX	6	2096	-	0,6,6	-	-	-		
85	OHX	6	2122	-	0,6,6	-	-	-		
85	OHX	1	4021	-	0,6,6	-	-	-		
85	OHX	5	3878	-	0,6,6	-	-	-		
85	OHX	5	4055	-	0,6,6	-	-	-		
85	OHX	6	2017	-	0,6,6	-	-	-		
85	OHX	1	3728	-	0,6,6	-	-	-		
85	OHX	1	3816	-	0,6,6	-	-	-		
85	OHX	6	2013	-	0,6,6	-	-	-		
85	OHX	5	3754	-	0,6,6	-	-	-		
85	OHX	6	2026	-	0,6,6	-	-	-		
85	OHX	1	3949	-	0,6,6	-	-	-		
85	OHX	5	3860	-	0,6,6	-	-	-		
85	OHX	1	3839	-	0,6,6	-	-	-		
85	OHX	5	3890	-	0,6,6	-	-	-		
85	OHX	1	3995	-	0,6,6	-	-	-		
85	OHX	1	3840	-	0,6,6	-	-	-		
85	OHX	5	4000	-	0,6,6	-	-	-		
85	OHX	3	210	-	0,6,6	-	-	-		
85	OHX	2	2011	-	0,6,6	-	-	-		
85	OHX	3	211	-	0,6,6	-	-	-		
85	OHX	5	3975	-	0,6,6	-	-	-		
85	OHX	2	2038	-	0,6,6	-	-	-		
85	OHX	1	3784	-	0,6,6	-	-	-		
85	OHX	6	2081	-	0,6,6	-	-	-		
85	OHX	2	2082	-	0,6,6	-	-	-		
85	OHX	5	3759	-	0,6,6	-	-	-		
85	OHX	5	3865	-	0,6,6	-	-	-		
85	OHX	1	3807	-	0,6,6	-	-	-		
85	OHX	1	3811	-	0,6,6	-	-	-		
85	OHX	1	3835	-	0,6,6	-	-	-		
85	OHX	1	3943	-	0,6,6	-	-	-		
85	OHX	4	218	-	0,6,6	-	-	-		
85	OHX	2	2081	-	0,6,6	-	-	-		
85	OHX	1	3778	-	0,6,6	-	-	-		
85	OHX	5	3979	-	0,6,6	-	-	-		
85	OHX	1	3984	-	0,6,6	-	-	-		
85	OHX	1	4038	-	0,6,6	-	-	-		
85	OHX	1	3801	-	0,6,6	-	-	-		
85	OHX	6	2088	-	0,6,6	-	-	-		
85	OHX	1	3732	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	6	2094	-	0,6,6	-	-	-		
85	OHX	5	3941	-	0,6,6	-	-	-		
85	OHX	5	3905	-	0,6,6	-	-	-		
85	OHX	6	2056	-	0,6,6	-	-	-		
85	OHX	5	3859	-	0,6,6	-	-	-		
85	OHX	5	4027	-	0,6,6	-	-	-		
85	OHX	1	3865	-	0,6,6	-	-	-		
85	OHX	1	4001	-	0,6,6	-	-	-		
85	OHX	2	2018	-	0,6,6	-	-	-		
85	OHX	5	3760	-	0,6,6	-	-	-		
85	OHX	2	2092	-	0,6,6	-	-	-		
85	OHX	1	3834	-	0,6,6	-	-	-		
85	OHX	l3	406	-	0,6,6	-	-	-		
85	OHX	5	3984	-	0,6,6	-	-	-		
85	OHX	4	222	-	0,6,6	-	-	-		
85	OHX	7	215	-	0,6,6	-	-	-		
85	OHX	5	4030	-	0,6,6	-	-	-		
85	OHX	5	4024	-	0,6,6	-	-	-		
85	OHX	5	3948	-	0,6,6	-	-	-		
85	OHX	1	3904	-	0,6,6	-	-	-		
85	OHX	6	2042	-	0,6,6	-	-	-		
85	OHX	5	3919	-	0,6,6	-	-	-		
85	OHX	1	4016	-	0,6,6	-	-	-		
85	OHX	7	217	-	0,6,6	-	-	-		
85	OHX	6	2144	-	0,6,6	-	-	-		
85	OHX	6	2010	-	0,6,6	-	-	-		
85	OHX	5	4070	-	0,6,6	-	-	-		
85	OHX	5	3810	-	0,6,6	-	-	-		
85	OHX	5	3876	-	0,6,6	-	-	-		
85	OHX	6	2070	-	0,6,6	-	-	-		
85	OHX	6	2113	-	0,6,6	-	-	-		
85	OHX	2	1987	-	0,6,6	-	-	-		
85	OHX	6	2052	-	0,6,6	-	-	-		
85	OHX	5	3855	-	0,6,6	-	-	-		
85	OHX	5	3916	-	0,6,6	-	-	-		
85	OHX	1	3856	-	0,6,6	-	-	-		
85	OHX	5	3745	-	0,6,6	-	-	-		
85	OHX	5	3803	-	0,6,6	-	-	-		
85	OHX	1	3802	-	0,6,6	-	-	-		
85	OHX	1	3979	-	0,6,6	-	-	-		
85	OHX	1	3786	-	0,6,6	-	-	-		
85	OHX	6	2134	-	0,6,6	-	-	-		
85	OHX	5	3748	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	6	2150	-	0,6,6	-	-	-		
85	OHX	2	2002	-	0,6,6	-	-	-		
85	OHX	5	3977	-	0,6,6	-	-	-		
85	OHX	6	2125	-	0,6,6	-	-	-		
85	OHX	5	3766	-	0,6,6	-	-	-		
85	OHX	6	2057	-	0,6,6	-	-	-		
85	OHX	1	3992	-	0,6,6	-	-	-		
85	OHX	5	3816	-	0,6,6	-	-	-		
85	OHX	5	3856	-	0,6,6	-	-	-		
85	OHX	5	3902	-	0,6,6	-	-	-		
85	OHX	1	3830	-	0,6,6	-	-	-		
85	OHX	1	3966	-	0,6,6	-	-	-		
85	OHX	5	4051	-	0,6,6	-	-	-		
85	OHX	n3	202	-	0,6,6	-	-	-		
85	OHX	6	2155	-	0,6,6	-	-	-		
85	OHX	5	3780	-	0,6,6	-	-	-		
85	OHX	6	2157	-	0,6,6	-	-	-		
85	OHX	7	220	-	0,6,6	-	-	-		
85	OHX	5	3968	-	0,6,6	-	-	-		
85	OHX	5	3901	-	0,6,6	-	-	-		
85	OHX	1	3748	-	0,6,6	-	-	-		
85	OHX	6	2114	-	0,6,6	-	-	-		
85	OHX	5	4006	-	0,6,6	-	-	-		
85	OHX	5	3952	-	0,6,6	-	-	-		
85	OHX	5	3927	-	0,6,6	-	-	-		
85	OHX	6	2091	-	0,6,6	-	-	-		
85	OHX	1	4029	-	0,6,6	-	-	-		
85	OHX	2	2100	-	0,6,6	-	-	-		
85	OHX	4	219	-	0,6,6	-	-	-		
85	OHX	5	3943	-	0,6,6	-	-	-		
85	OHX	5	3947	-	0,6,6	-	-	-		
85	OHX	5	3918	-	0,6,6	-	-	-		
85	OHX	1	3825	-	0,6,6	-	-	-		
85	OHX	1	3852	-	0,6,6	-	-	-		
85	OHX	5	3951	-	0,6,6	-	-	-		
85	OHX	2	2068	-	0,6,6	-	-	-		
85	OHX	5	4023	-	0,6,6	-	-	-		
85	OHX	8	223	-	0,6,6	-	-	-		
85	OHX	2	2072	-	0,6,6	-	-	-		
85	OHX	5	3900	-	0,6,6	-	-	-		
85	OHX	1	3963	-	0,6,6	-	-	-		
85	OHX	6	2115	-	0,6,6	-	-	-		
85	OHX	5	3934	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	1	3814	-	0,6,6	-	-	-		
85	OHX	5	3917	-	0,6,6	-	-	-		
85	OHX	6	2145	-	0,6,6	-	-	-		
85	OHX	2	1984	-	0,6,6	-	-	-		
85	OHX	2	2040	-	0,6,6	-	-	-		
85	OHX	1	3793	-	0,6,6	-	-	-		
85	OHX	1	4035	-	0,6,6	-	-	-		
85	OHX	5	3762	-	0,6,6	-	-	-		
85	OHX	8	216	-	0,6,6	-	-	-		
85	OHX	2	2099	-	0,6,6	-	-	-		
85	OHX	6	2133	-	0,6,6	-	-	-		
85	OHX	1	3951	-	0,6,6	-	-	-		
85	OHX	5	3892	-	0,6,6	-	-	-		
85	OHX	m5	304	-	0,6,6	-	-	-		
85	OHX	5	3837	-	0,6,6	-	-	-		
85	OHX	6	2061	-	0,6,6	-	-	-		
85	OHX	1	3893	-	0,6,6	-	-	-		
85	OHX	1	3919	-	0,6,6	-	-	-		
85	OHX	4	231	-	0,6,6	-	-	-		
85	OHX	2	2055	-	0,6,6	-	-	-		
85	OHX	6	2011	-	0,6,6	-	-	-		
85	OHX	2	2061	-	0,6,6	-	-	-		
85	OHX	1	3910	-	0,6,6	-	-	-		
85	OHX	5	3806	-	0,6,6	-	-	-		
85	OHX	5	4045	-	0,6,6	-	-	-		
85	OHX	2	2009	-	0,6,6	-	-	-		
85	OHX	5	4049	-	0,6,6	-	-	-		
85	OHX	6	2126	-	0,6,6	-	-	-		
85	OHX	l5	301	-	0,6,6	-	-	-		
85	OHX	6	2110	-	0,6,6	-	-	-		
85	OHX	1	4030	-	0,6,6	-	-	-		
85	OHX	2	2097	-	0,6,6	-	-	-		
85	OHX	5	3985	-	0,6,6	-	-	-		
85	OHX	1	3837	-	0,6,6	-	-	-		
85	OHX	2	2104	-	0,6,6	-	-	-		
85	OHX	5	3787	-	0,6,6	-	-	-		
85	OHX	5	3768	-	0,6,6	-	-	-		
85	OHX	1	4032	-	0,6,6	-	-	-		
85	OHX	6	2117	-	0,6,6	-	-	-		
85	OHX	5	3870	-	0,6,6	-	-	-		
85	OHX	6	2034	-	0,6,6	-	-	-		
85	OHX	1	3812	-	0,6,6	-	-	-		
85	OHX	4	215	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	4	229	-	0,6,6	-	-	-		
85	OHX	5	3953	-	0,6,6	-	-	-		
85	OHX	1	3878	-	0,6,6	-	-	-		
85	OHX	5	3924	-	0,6,6	-	-	-		
85	OHX	6	2156	-	0,6,6	-	-	-		
85	OHX	2	2062	-	0,6,6	-	-	-		
85	OHX	1	3881	-	0,6,6	-	-	-		
85	OHX	3	219	-	0,6,6	-	-	-		
85	OHX	5	3795	-	0,6,6	-	-	-		
85	OHX	5	4054	-	0,6,6	-	-	-		
85	OHX	6	2033	-	0,6,6	-	-	-		
85	OHX	2	1992	-	0,6,6	-	-	-		
85	OHX	6	2074	-	0,6,6	-	-	-		
85	OHX	7	211	-	0,6,6	-	-	-		
85	OHX	1	3842	-	0,6,6	-	-	-		
85	OHX	2	2043	-	0,6,6	-	-	-		
85	OHX	2	2033	-	0,6,6	-	-	-		
85	OHX	5	3802	-	0,6,6	-	-	-		
85	OHX	6	2154	-	0,6,6	-	-	-		
85	OHX	6	2082	-	0,6,6	-	-	-		
85	OHX	8	218	-	0,6,6	-	-	-		
85	OHX	1	3774	-	0,6,6	-	-	-		
85	OHX	2	2064	-	0,6,6	-	-	-		
85	OHX	1	3936	-	0,6,6	-	-	-		
85	OHX	5	3973	-	0,6,6	-	-	-		
85	OHX	1	3909	-	0,6,6	-	-	-		
85	OHX	2	2108	-	0,6,6	-	-	-		
85	OHX	5	3950	-	0,6,6	-	-	-		
85	OHX	5	3946	-	0,6,6	-	-	-		
85	OHX	5	3747	-	0,6,6	-	-	-		
85	OHX	2	2023	-	0,6,6	-	-	-		
85	OHX	1	3766	-	0,6,6	-	-	-		
85	OHX	6	2048	-	0,6,6	-	-	-		
85	OHX	5	3939	-	0,6,6	-	-	-		
85	OHX	5	3994	-	0,6,6	-	-	-		
85	OHX	5	3828	-	0,6,6	-	-	-		
85	OHX	5	3770	-	0,6,6	-	-	-		
85	OHX	1	3826	-	0,6,6	-	-	-		
85	OHX	1	3947	-	0,6,6	-	-	-		
85	OHX	1	4019	-	0,6,6	-	-	-		
85	OHX	5	3926	-	0,6,6	-	-	-		
85	OHX	5	4064	-	0,6,6	-	-	-		
85	OHX	8	222	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	o9	101	-	0,6,6	-	-	-		
85	OHX	5	4062	-	0,6,6	-	-	-		
85	OHX	2	2093	-	0,6,6	-	-	-		
85	OHX	2	2095	-	0,6,6	-	-	-		
85	OHX	1	3920	-	0,6,6	-	-	-		
85	OHX	1	3828	-	0,6,6	-	-	-		
85	OHX	2	2013	-	0,6,6	-	-	-		
85	OHX	6	2020	-	0,6,6	-	-	-		
85	OHX	6	2151	-	0,6,6	-	-	-		
85	OHX	5	3935	-	0,6,6	-	-	-		
85	OHX	5	3818	-	0,6,6	-	-	-		
85	OHX	1	4018	-	0,6,6	-	-	-		
85	OHX	5	3976	-	0,6,6	-	-	-		
85	OHX	1	3790	-	0,6,6	-	-	-		
85	OHX	1	3960	-	0,6,6	-	-	-		
85	OHX	1	3849	-	0,6,6	-	-	-		
85	OHX	2	2102	-	0,6,6	-	-	-		
85	OHX	6	2116	-	0,6,6	-	-	-		
85	OHX	5	4019	-	0,6,6	-	-	-		
85	OHX	5	4021	-	0,6,6	-	-	-		
85	OHX	6	2018	-	0,6,6	-	-	-		
85	OHX	5	3938	-	0,6,6	-	-	-		
85	OHX	1	4009	-	0,6,6	-	-	-		
85	OHX	1	3879	-	0,6,6	-	-	-		
85	OHX	2	2017	-	0,6,6	-	-	-		
85	OHX	5	3920	-	0,6,6	-	-	-		
85	OHX	1	3841	-	0,6,6	-	-	-		
85	OHX	2	2014	-	0,6,6	-	-	-		
85	OHX	1	3803	-	0,6,6	-	-	-		
85	OHX	1	3757	-	0,6,6	-	-	-		
85	OHX	1	3985	-	0,6,6	-	-	-		
85	OHX	1	3970	-	0,6,6	-	-	-		
85	OHX	M7	205	-	0,6,6	-	-	-		
85	OHX	6	2120	-	0,6,6	-	-	-		
85	OHX	5	3907	-	0,6,6	-	-	-		
85	OHX	5	4002	-	0,6,6	-	-	-		
85	OHX	1	3975	-	0,6,6	-	-	-		
85	OHX	1	3864	-	0,6,6	-	-	-		
85	OHX	2	2025	-	0,6,6	-	-	-		
85	OHX	1	3906	-	0,6,6	-	-	-		
85	OHX	5	3847	-	0,6,6	-	-	-		
85	OHX	C3	201	-	0,6,6	-	-	-		
85	OHX	6	2109	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	6	2137	-	0,6,6	-	-	-		
85	OHX	5	3815	-	0,6,6	-	-	-		
85	OHX	n3	203	-	0,6,6	-	-	-		
85	OHX	5	3880	-	0,6,6	-	-	-		
85	OHX	5	4053	-	0,6,6	-	-	-		
85	OHX	c3	201	-	0,6,6	-	-	-		
85	OHX	6	2083	-	0,6,6	-	-	-		
85	OHX	1	3896	-	0,6,6	-	-	-		
85	OHX	1	3806	-	0,6,6	-	-	-		
85	OHX	6	2146	-	0,6,6	-	-	-		
85	OHX	5	4036	-	0,6,6	-	-	-		
85	OHX	1	3895	-	0,6,6	-	-	-		
85	OHX	1	4034	-	0,6,6	-	-	-		
85	OHX	2	2087	-	0,6,6	-	-	-		
85	OHX	6	2032	-	0,6,6	-	-	-		
85	OHX	Q2	503	-	0,6,6	-	-	-		
85	OHX	2	1990	-	0,6,6	-	-	-		
85	OHX	1	3915	-	0,6,6	-	-	-		
85	OHX	1	3973	-	0,6,6	-	-	-		
85	OHX	6	2093	-	0,6,6	-	-	-		
85	OHX	C5	201	-	0,6,6	-	-	-		
85	OHX	1	3872	-	0,6,6	-	-	-		
85	OHX	5	3781	-	0,6,6	-	-	-		
85	OHX	4	225	-	0,6,6	-	-	-		
85	OHX	2	2041	-	0,6,6	-	-	-		
85	OHX	2	2050	-	0,6,6	-	-	-		
85	OHX	5	3842	-	0,6,6	-	-	-		
85	OHX	5	4016	-	0,6,6	-	-	-		
85	OHX	5	3882	-	0,6,6	-	-	-		
85	OHX	1	3937	-	0,6,6	-	-	-		
85	OHX	5	4034	-	0,6,6	-	-	-		
85	OHX	5	3913	-	0,6,6	-	-	-		
85	OHX	O7	104	-	0,6,6	-	-	-		
85	OHX	1	3727	-	0,6,6	-	-	-		
85	OHX	M6	202	-	0,6,6	-	-	-		
85	OHX	2	2035	-	0,6,6	-	-	-		
85	OHX	1	3880	-	0,6,6	-	-	-		
85	OHX	1	3941	-	0,6,6	-	-	-		
85	OHX	5	3908	-	0,6,6	-	-	-		
85	OHX	5	4025	-	0,6,6	-	-	-		
85	OHX	1	3876	-	0,6,6	-	-	-		
85	OHX	2	2056	-	0,6,6	-	-	-		
85	OHX	1	3869	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	1	3804	-	0,6,6	-	-	-		
85	OHX	4	226	-	0,6,6	-	-	-		
85	OHX	1	3916	-	0,6,6	-	-	-		
85	OHX	1	3998	-	0,6,6	-	-	-		
85	OHX	3	214	-	0,6,6	-	-	-		
85	OHX	5	3791	-	0,6,6	-	-	-		
85	OHX	5	3911	-	0,6,6	-	-	-		
85	OHX	5	3960	-	0,6,6	-	-	-		
85	OHX	1	3823	-	0,6,6	-	-	-		
85	OHX	2	2117	-	0,6,6	-	-	-		
85	OHX	6	2025	-	0,6,6	-	-	-		
85	OHX	1	3736	-	0,6,6	-	-	-		
85	OHX	2	2065	-	0,6,6	-	-	-		
85	OHX	1	3954	-	0,6,6	-	-	-		
85	OHX	5	3755	-	0,6,6	-	-	-		
85	OHX	5	3771	-	0,6,6	-	-	-		
85	OHX	6	2139	-	0,6,6	-	-	-		
85	OHX	6	2023	-	0,6,6	-	-	-		
85	OHX	5	3862	-	0,6,6	-	-	-		
85	OHX	6	2112	-	0,6,6	-	-	-		
85	OHX	6	2055	-	0,6,6	-	-	-		
85	OHX	5	3967	-	0,6,6	-	-	-		
85	OHX	1	3754	-	0,6,6	-	-	-		
85	OHX	1	3965	-	0,6,6	-	-	-		
85	OHX	N9	101	-	0,6,6	-	-	-		
85	OHX	5	3765	-	0,6,6	-	-	-		
85	OHX	5	3749	-	0,6,6	-	-	-		
85	OHX	1	4006	-	0,6,6	-	-	-		
85	OHX	5	3769	-	0,6,6	-	-	-		
85	OHX	6	2097	-	0,6,6	-	-	-		
85	OHX	1	3912	-	0,6,6	-	-	-		
85	OHX	5	3773	-	0,6,6	-	-	-		
85	OHX	5	3982	-	0,6,6	-	-	-		
85	OHX	1	3863	-	0,6,6	-	-	-		
85	OHX	1	3755	-	0,6,6	-	-	-		
85	OHX	5	4009	-	0,6,6	-	-	-		
85	OHX	1	3964	-	0,6,6	-	-	-		
85	OHX	1	3935	-	0,6,6	-	-	-		
85	OHX	5	3937	-	0,6,6	-	-	-		
85	OHX	6	2090	-	0,6,6	-	-	-		
85	OHX	5	3797	-	0,6,6	-	-	-		
85	OHX	5	3963	-	0,6,6	-	-	-		
85	OHX	5	3852	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	5	3903	-	0,6,6	-	-	-		
85	OHX	1	3773	-	0,6,6	-	-	-		
85	OHX	5	3814	-	0,6,6	-	-	-		
87	ANM	1	3401	-	20,20,20	2.93	9 (45%)	22,27,27	2.80	10 (45%)
85	OHX	6	2029	-	0,6,6	-	-	-		
85	OHX	1	3924	-	0,6,6	-	-	-		
85	OHX	5	3888	-	0,6,6	-	-	-		
85	OHX	2	1983	-	0,6,6	-	-	-		
85	OHX	1	3796	-	0,6,6	-	-	-		
85	OHX	1	3956	-	0,6,6	-	-	-		
85	OHX	6	2016	-	0,6,6	-	-	-		
85	OHX	1	3762	-	0,6,6	-	-	-		
85	OHX	6	2047	-	0,6,6	-	-	-		
85	OHX	5	3887	-	0,6,6	-	-	-		
85	OHX	6	2101	-	0,6,6	-	-	-		
85	OHX	1	3751	-	0,6,6	-	-	-		
85	OHX	2	2085	-	0,6,6	-	-	-		
85	OHX	2	2047	-	0,6,6	-	-	-		
85	OHX	1	3860	-	0,6,6	-	-	-		
85	OHX	1	3969	-	0,6,6	-	-	-		
85	OHX	2	2078	-	0,6,6	-	-	-		
85	OHX	5	4032	-	0,6,6	-	-	-		
85	OHX	1	3744	-	0,6,6	-	-	-		
85	OHX	2	2053	-	0,6,6	-	-	-		
85	OHX	5	4026	-	0,6,6	-	-	-		
85	OHX	6	2127	-	0,6,6	-	-	-		
85	OHX	6	2119	-	0,6,6	-	-	-		
85	OHX	2	1996	-	0,6,6	-	-	-		
85	OHX	3	213	-	0,6,6	-	-	-		
85	OHX	3	218	-	0,6,6	-	-	-		
85	OHX	5	3767	-	0,6,6	-	-	-		
85	OHX	5	3868	-	0,6,6	-	-	-		
85	OHX	5	3978	-	0,6,6	-	-	-		
85	OHX	2	2067	-	0,6,6	-	-	-		
85	OHX	1	3997	-	0,6,6	-	-	-		
85	OHX	1	4014	-	0,6,6	-	-	-		
85	OHX	5	3954	-	0,6,6	-	-	-		
85	OHX	5	4033	-	0,6,6	-	-	-		
85	OHX	1	3883	-	0,6,6	-	-	-		
85	OHX	2	2110	-	0,6,6	-	-	-		
85	OHX	2	2086	-	0,6,6	-	-	-		
85	OHX	5	3756	-	0,6,6	-	-	-		
85	OHX	6	2066	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	1	4025	-	0,6,6	-	-	-		
85	OHX	5	3869	-	0,6,6	-	-	-		
85	OHX	l3	408	-	0,6,6	-	-	-		
85	OHX	2	2032	-	0,6,6	-	-	-		
85	OHX	2	2109	-	0,6,6	-	-	-		
85	OHX	O7	105	-	0,6,6	-	-	-		
85	OHX	5	3825	-	0,6,6	-	-	-		
85	OHX	5	3896	-	0,6,6	-	-	-		
85	OHX	2	2083	-	0,6,6	-	-	-		
85	OHX	1	3780	-	0,6,6	-	-	-		
85	OHX	1	4033	-	0,6,6	-	-	-		
85	OHX	5	3840	-	0,6,6	-	-	-		
85	OHX	m5	305	-	0,6,6	-	-	-		
85	OHX	5	3752	-	0,6,6	-	-	-		
85	OHX	1	3743	-	0,6,6	-	-	-		
85	OHX	4	224	-	0,6,6	-	-	-		
85	OHX	2	2003	-	0,6,6	-	-	-		
85	OHX	1	3875	-	0,6,6	-	-	-		
85	OHX	1	3967	-	0,6,6	-	-	-		
85	OHX	2	2063	-	0,6,6	-	-	-		
85	OHX	1	3940	-	0,6,6	-	-	-		
85	OHX	6	2071	-	0,6,6	-	-	-		
85	OHX	5	3863	-	0,6,6	-	-	-		
85	OHX	2	2089	-	0,6,6	-	-	-		
85	OHX	2	2054	-	0,6,6	-	-	-		
85	OHX	1	3738	-	0,6,6	-	-	-		
85	OHX	1	3843	-	0,6,6	-	-	-		
85	OHX	6	2152	-	0,6,6	-	-	-		
85	OHX	5	3811	-	0,6,6	-	-	-		
85	OHX	m0	301	-	0,6,6	-	-	-		
85	OHX	1	4037	-	0,6,6	-	-	-		
85	OHX	s8	302	-	0,6,6	-	-	-		
85	OHX	5	3942	-	0,6,6	-	-	-		
85	OHX	5	4069	-	0,6,6	-	-	-		
85	OHX	5	4067	-	0,6,6	-	-	-		
85	OHX	m1	202	-	0,6,6	-	-	-		
85	OHX	1	3749	-	0,6,6	-	-	-		
85	OHX	6	2143	-	0,6,6	-	-	-		
85	OHX	7	214	-	0,6,6	-	-	-		
85	OHX	5	3753	-	0,6,6	-	-	-		
85	OHX	6	2103	-	0,6,6	-	-	-		
85	OHX	5	4020	-	0,6,6	-	-	-		
85	OHX	5	3956	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	5	4031	-	0,6,6	-	-	-		
85	OHX	1	3961	-	0,6,6	-	-	-		
85	OHX	1	3897	-	0,6,6	-	-	-		
85	OHX	1	3810	-	0,6,6	-	-	-		
85	OHX	M5	302	-	0,6,6	-	-	-		
85	OHX	5	3784	-	0,6,6	-	-	-		
85	OHX	5	4065	-	0,6,6	-	-	-		
85	OHX	1	3976	-	0,6,6	-	-	-		
85	OHX	2	2107	-	0,6,6	-	-	-		
85	OHX	1	3857	-	0,6,6	-	-	-		
85	OHX	5	3923	-	0,6,6	-	-	-		
85	OHX	1	3882	-	0,6,6	-	-	-		
85	OHX	1	3772	-	0,6,6	-	-	-		
85	OHX	2	2069	-	0,6,6	-	-	-		
85	OHX	1	3770	-	0,6,6	-	-	-		
85	OHX	1	3887	-	0,6,6	-	-	-		
85	OHX	5	3743	-	0,6,6	-	-	-		
85	OHX	5	3793	-	0,6,6	-	-	-		
85	OHX	1	3777	-	0,6,6	-	-	-		
85	OHX	1	3753	-	0,6,6	-	-	-		
85	OHX	1	3783	-	0,6,6	-	-	-		
85	OHX	5	3925	-	0,6,6	-	-	-		
85	OHX	5	3812	-	0,6,6	-	-	-		
85	OHX	6	2131	-	0,6,6	-	-	-		
85	OHX	1	4004	-	0,6,6	-	-	-		
85	OHX	5	3889	-	0,6,6	-	-	-		
85	OHX	1	3799	-	0,6,6	-	-	-		
85	OHX	1	3931	-	0,6,6	-	-	-		
85	OHX	6	2129	-	0,6,6	-	-	-		
85	OHX	5	3823	-	0,6,6	-	-	-		
85	OHX	2	2045	-	0,6,6	-	-	-		
85	OHX	1	3844	-	0,6,6	-	-	-		
85	OHX	1	4013	-	0,6,6	-	-	-		
85	OHX	6	2106	-	0,6,6	-	-	-		
85	OHX	7	221	-	0,6,6	-	-	-		
85	OHX	l4	401	-	0,6,6	-	-	-		
85	OHX	4	230	-	0,6,6	-	-	-		
85	OHX	1	3890	-	0,6,6	-	-	-		
85	OHX	2	2027	-	0,6,6	-	-	-		
85	OHX	1	3726	-	0,6,6	-	-	-		
85	OHX	1	3958	-	0,6,6	-	-	-		
85	OHX	c8	201	-	0,6,6	-	-	-		
85	OHX	1	3737	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	5	4059	-	0,6,6	-	-	-		
85	OHX	2	2106	-	0,6,6	-	-	-		
85	OHX	1	3819	-	0,6,6	-	-	-		
85	OHX	1	3729	-	0,6,6	-	-	-		
85	OHX	1	4007	-	0,6,6	-	-	-		
85	OHX	SR	401	-	0,6,6	-	-	-		
85	OHX	4	217	-	0,6,6	-	-	-		
85	OHX	5	3906	-	0,6,6	-	-	-		
85	OHX	2	2112	-	0,6,6	-	-	-		
85	OHX	s9	201	-	0,6,6	-	-	-		
85	OHX	5	3846	-	0,6,6	-	-	-		
85	OHX	5	3864	-	0,6,6	-	-	-		
85	OHX	5	3990	-	0,6,6	-	-	-		
85	OHX	5	3777	-	0,6,6	-	-	-		
85	OHX	1	3815	-	0,6,6	-	-	-		
85	OHX	2	2096	-	0,6,6	-	-	-		
85	OHX	6	2149	-	0,6,6	-	-	-		
85	OHX	6	2111	-	0,6,6	-	-	-		
85	OHX	1	3739	-	0,6,6	-	-	-		
85	OHX	5	3836	-	0,6,6	-	-	-		
85	OHX	1	3993	-	0,6,6	-	-	-		
85	OHX	6	2085	-	0,6,6	-	-	-		
85	OHX	1	3740	-	0,6,6	-	-	-		
85	OHX	5	3798	-	0,6,6	-	-	-		
85	OHX	2	2090	-	0,6,6	-	-	-		
85	OHX	1	3939	-	0,6,6	-	-	-		
85	OHX	5	3945	-	0,6,6	-	-	-		
85	OHX	5	3962	-	0,6,6	-	-	-		
85	OHX	6	2076	-	0,6,6	-	-	-		
85	OHX	l4	402	-	0,6,6	-	-	-		
85	OHX	5	3910	-	0,6,6	-	-	-		
85	OHX	6	2153	-	0,6,6	-	-	-		
85	OHX	5	4014	-	0,6,6	-	-	-		
85	OHX	1	3871	-	0,6,6	-	-	-		
85	OHX	1	4024	-	0,6,6	-	-	-		
85	OHX	5	3983	-	0,6,6	-	-	-		
85	OHX	5	3824	-	0,6,6	-	-	-		
85	OHX	2	2076	-	0,6,6	-	-	-		
85	OHX	6	2060	-	0,6,6	-	-	-		
85	OHX	1	3930	-	0,6,6	-	-	-		
85	OHX	6	2107	-	0,6,6	-	-	-		
85	OHX	2	2042	-	0,6,6	-	-	-		
85	OHX	5	3789	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	5	3992	-	0,6,6	-	-	-		
85	OHX	S8	301	-	0,6,6	-	-	-		
85	OHX	1	3884	-	0,6,6	-	-	-		
85	OHX	1	4012	-	0,6,6	-	-	-		
85	OHX	5	3763	-	0,6,6	-	-	-		
85	OHX	2	2060	-	0,6,6	-	-	-		
85	OHX	5	3858	-	0,6,6	-	-	-		
85	OHX	4	220	-	0,6,6	-	-	-		
85	OHX	1	3731	-	0,6,6	-	-	-		
85	OHX	5	3897	-	0,6,6	-	-	-		
85	OHX	2	2114	-	0,6,6	-	-	-		
85	OHX	5	3933	-	0,6,6	-	-	-		
85	OHX	3	216	-	0,6,6	-	-	-		
85	OHX	5	3805	-	0,6,6	-	-	-		
85	OHX	2	2052	-	0,6,6	-	-	-		
85	OHX	5	4005	-	0,6,6	-	-	-		
85	OHX	6	2064	-	0,6,6	-	-	-		
85	OHX	5	3969	-	0,6,6	-	-	-		
85	OHX	5	3800	-	0,6,6	-	-	-		
85	OHX	6	2044	-	0,6,6	-	-	-		
85	OHX	l3	407	-	0,6,6	-	-	-		
85	OHX	5	3804	-	0,6,6	-	-	-		
85	OHX	5	3857	-	0,6,6	-	-	-		
85	OHX	2	2036	-	0,6,6	-	-	-		
85	OHX	2	1995	-	0,6,6	-	-	-		
85	OHX	1	3962	-	0,6,6	-	-	-		
85	OHX	6	2077	-	0,6,6	-	-	-		
85	OHX	5	3998	-	0,6,6	-	-	-		
85	OHX	1	3934	-	0,6,6	-	-	-		
85	OHX	2	2119	-	0,6,6	-	-	-		
85	OHX	6	2141	-	0,6,6	-	-	-		
85	OHX	5	4041	-	0,6,6	-	-	-		
85	OHX	5	3838	-	0,6,6	-	-	-		
85	OHX	5	3966	-	0,6,6	-	-	-		
85	OHX	1	3907	-	0,6,6	-	-	-		
85	OHX	5	3867	-	0,6,6	-	-	-		
85	OHX	o7	502	-	0,6,6	-	-	-		
85	OHX	2	2028	-	0,6,6	-	-	-		
85	OHX	6	2121	-	0,6,6	-	-	-		
85	OHX	6	2089	-	0,6,6	-	-	-		
85	OHX	7	218	-	0,6,6	-	-	-		
85	OHX	6	2100	-	0,6,6	-	-	-		
85	OHX	O9	101	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	5	3819	-	0,6,6	-	-	-		
85	OHX	6	2067	-	0,6,6	-	-	-		
85	OHX	5	4007	36	0,6,6	-	-	-		
85	OHX	1	3829	-	0,6,6	-	-	-		
85	OHX	4	228	-	0,6,6	-	-	-		
85	OHX	6	2092	-	0,6,6	-	-	-		
85	OHX	1	3987	-	0,6,6	-	-	-		
85	OHX	1	3991	-	0,6,6	-	-	-		
85	OHX	1	3838	-	0,6,6	-	-	-		
85	OHX	5	3808	-	0,6,6	-	-	-		
85	OHX	5	4013	-	0,6,6	-	-	-		
85	OHX	1	3981	-	0,6,6	-	-	-		
85	OHX	1	3765	-	0,6,6	-	-	-		
85	OHX	5	4028	-	0,6,6	-	-	-		
85	OHX	6	2135	-	0,6,6	-	-	-		
85	OHX	2	1997	-	0,6,6	-	-	-		
85	OHX	6	2086	-	0,6,6	-	-	-		
85	OHX	5	4017	-	0,6,6	-	-	-		
85	OHX	5	3931	-	0,6,6	-	-	-		
85	OHX	6	2059	-	0,6,6	-	-	-		
85	OHX	1	4023	-	0,6,6	-	-	-		
85	OHX	1	3846	-	0,6,6	-	-	-		
85	OHX	5	3845	-	0,6,6	-	-	-		
85	OHX	5	3928	-	0,6,6	-	-	-		
85	OHX	6	2027	-	0,6,6	-	-	-		
85	OHX	5	4056	-	0,6,6	-	-	-		
85	OHX	2	2059	-	0,6,6	-	-	-		
85	OHX	1	3851	-	0,6,6	-	-	-		
85	OHX	5	3995	-	0,6,6	-	-	-		
85	OHX	2	2057	-	0,6,6	-	-	-		
85	OHX	l9	202	-	0,6,6	-	-	-		
85	OHX	5	3785	-	0,6,6	-	-	-		
85	OHX	5	3922	-	0,6,6	-	-	-		
85	OHX	2	1986	-	0,6,6	-	-	-		
85	OHX	6	2054	-	0,6,6	-	-	-		
85	OHX	5	3914	-	0,6,6	-	-	-		
85	OHX	5	4001	-	0,6,6	-	-	-		
85	OHX	6	2043	-	0,6,6	-	-	-		
85	OHX	2	2115	-	0,6,6	-	-	-		
85	OHX	1	3996	-	0,6,6	-	-	-		
85	OHX	2	2091	-	0,6,6	-	-	-		
85	OHX	1	3730	-	0,6,6	-	-	-		
85	OHX	M0	302	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	5	4040	-	0,6,6	-	-	-		
85	OHX	5	4047	-	0,6,6	-	-	-		
85	OHX	1	3781	-	0,6,6	-	-	-		
85	OHX	5	3788	-	0,6,6	-	-	-		
85	OHX	1	3945	-	0,6,6	-	-	-		
85	OHX	1	3891	-	0,6,6	-	-	-		
85	OHX	5	3930	-	0,6,6	-	-	-		
85	OHX	1	3861	-	0,6,6	-	-	-		
85	OHX	5	3854	-	0,6,6	-	-	-		
85	OHX	1	3870	-	0,6,6	-	-	-		
85	OHX	6	2069	-	0,6,6	-	-	-		
85	OHX	5	3821	-	0,6,6	-	-	-		
85	OHX	5	4004	-	0,6,6	-	-	-		
85	OHX	5	4010	-	0,6,6	-	-	-		
85	OHX	1	3763	-	0,6,6	-	-	-		
85	OHX	1	4000	-	0,6,6	-	-	-		
85	OHX	5	3799	-	0,6,6	-	-	-		
85	OHX	7	219	-	0,6,6	-	-	-		
85	OHX	4	227	-	0,6,6	-	-	-		
85	OHX	5	4012	-	0,6,6	-	-	-		
85	OHX	L3	403	-	0,6,6	-	-	-		
85	OHX	5	3849	-	0,6,6	-	-	-		
85	OHX	1	3862	-	0,6,6	-	-	-		
85	OHX	6	2030	-	0,6,6	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	ANM	1	3401	-	3/3/4/5	3/10/23/23	0/2/2/2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	1	3401	ANM	C4-C3	-6.47	1.43	1.53
87	1	3401	ANM	C3-C2	-6.41	1.40	1.53
87	1	3401	ANM	O2-C2	-4.67	1.37	1.44
87	1	3401	ANM	C16-N1	-4.41	1.38	1.48
87	1	3401	ANM	C15-C16	-3.10	1.47	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	1	3401	ANM	C15-C16-N1	-5.90	104.18	111.47
87	1	3401	ANM	C2-O2-C5	-5.34	109.46	117.72
87	1	3401	ANM	O2-C5-O3	-5.31	112.42	122.96
87	1	3401	ANM	C4-C3-C2	-4.14	97.94	103.29
87	1	3401	ANM	O4-C3-C4	-4.08	101.29	110.90

All (3) chirality outliers are listed below:

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

All (3) torsion outliers are listed below:

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

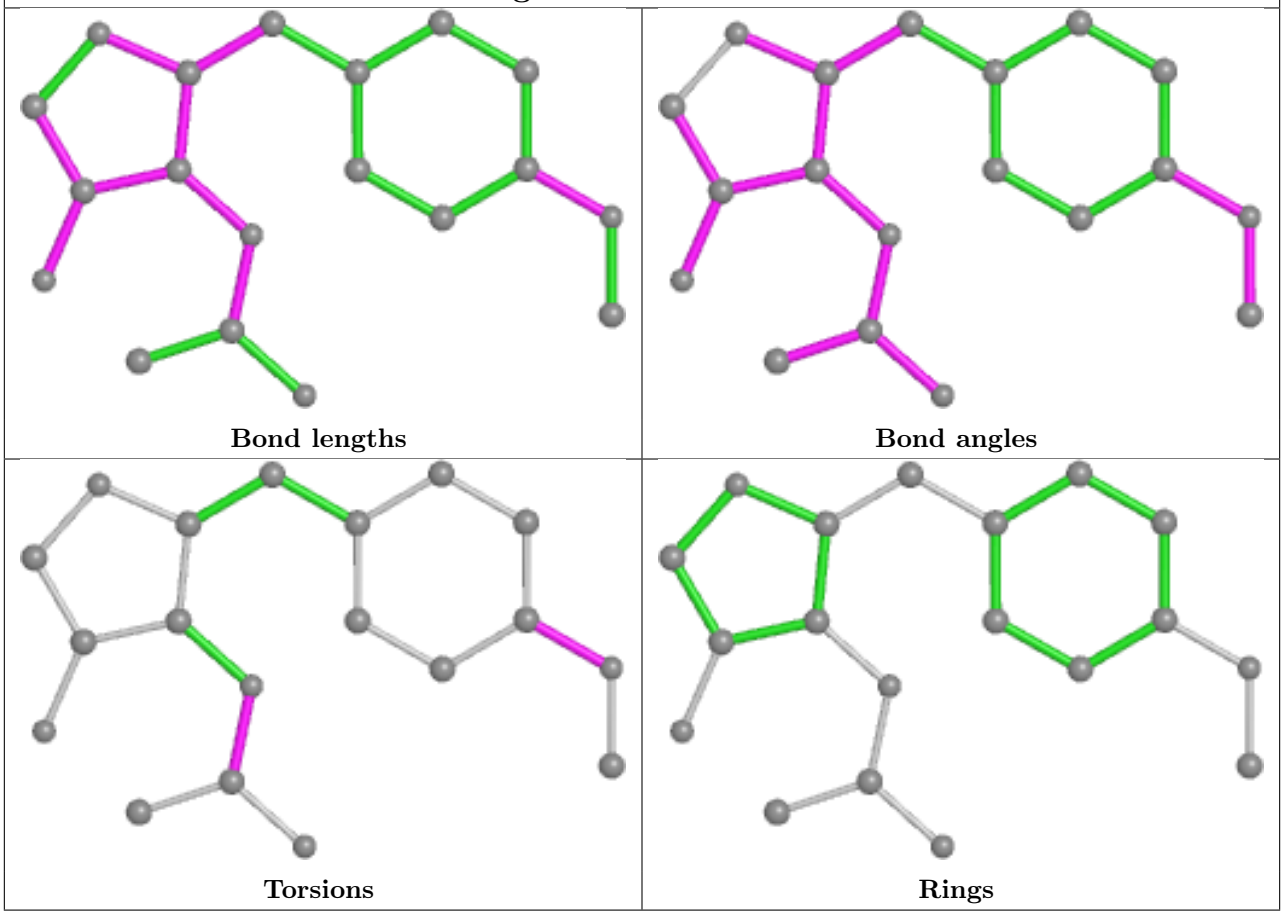
There are no ring outliers.

1 monomer is involved in 1 short contact:

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

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

Ligand ANM 1 3401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
80	m2	2
35	sM	1
35	SM	1
12	c0	1
1	2	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	139:UNK	C	155:UNK	N	37.86

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SM	141:ALA	C	151:UNK	N	26.40
1	c0	84:GLU	C	87:UNK	N	8.00
1	2	1716:C	O3'	1717:G	P	3.94
1	m2	23:UNK	C	28:UNK	N	3.86

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	C1	146/155 (94%)	0.17	6 (4%) 37 18	64, 72, 90, 101	0
13	c1	146/155 (94%)	0.26	9 (6%) 20 9	51, 66, 97, 152	0
14	C2	124/142 (87%)	1.60	46 (37%) 0 0	118, 124, 129, 132	0
14	c2	124/142 (87%)	2.93	76 (61%) 0 0	170, 185, 193, 202	0
15	C3	150/150 (100%)	0.06	6 (4%) 38 19	71, 85, 93, 97	0
15	c3	150/150 (100%)	-0.12	0 100 100	56, 72, 87, 92	0
16	C4	127/136 (93%)	1.07	25 (19%) 1 0	74, 116, 124, 126	0
16	c4	128/136 (94%)	0.21	2 (1%) 72 51	54, 81, 85, 88	0
17	C5	124/141 (87%)	0.08	3 (2%) 59 37	77, 88, 107, 114	0
17	c5	135/141 (95%)	0.32	10 (7%) 14 5	61, 91, 108, 115	0
18	C6	141/142 (99%)	0.41	6 (4%) 35 17	81, 99, 102, 103	0
18	c6	142/142 (100%)	0.67	18 (12%) 3 1	69, 89, 101, 104	0
19	C7	120/136 (88%)	0.51	11 (9%) 9 3	89, 99, 106, 107	0
19	c7	117/136 (86%)	0.82	17 (14%) 2 1	79, 95, 321, 380	0
20	C8	145/145 (100%)	0.78	18 (12%) 4 1	76, 94, 109, 114	0
20	c8	145/145 (100%)	0.46	8 (5%) 25 11	69, 87, 98, 103	0
21	C9	143/143 (100%)	0.47	7 (4%) 29 14	86, 97, 105, 110	0
21	c9	143/143 (100%)	0.17	0 100 100	71, 83, 93, 98	0
22	D0	107/120 (89%)	1.21	26 (24%) 0 0	76, 98, 107, 109	0
22	d0	110/120 (91%)	1.24	30 (27%) 0 0	73, 103, 118, 121	0
23	D1	87/87 (100%)	0.35	5 (5%) 23 11	84, 87, 97, 100	0
23	d1	87/87 (100%)	0.11	2 (2%) 60 39	70, 86, 139, 157	0
24	D2	129/129 (100%)	0.01	2 (1%) 72 51	73, 81, 87, 95	0
24	d2	129/129 (100%)	-0.03	0 100 100	56, 67, 74, 81	0
25	D3	144/144 (100%)	0.02	2 (1%) 75 56	63, 66, 72, 75	0
25	d3	144/144 (100%)	-0.26	0 100 100	47, 52, 60, 65	0
26	D4	134/134 (100%)	0.60	12 (8%) 9 3	74, 90, 97, 100	0
26	d4	134/134 (100%)	0.27	6 (4%) 33 16	58, 78, 88, 101	0
27	D5	70/107 (65%)	0.39	2 (2%) 51 28	103, 109, 114, 114	0
27	d5	69/107 (64%)	0.78	10 (14%) 2 1	86, 97, 101, 102	0
28	D6	97/97 (100%)	0.55	4 (4%) 37 18	76, 85, 121, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	d6	97/97 (100%)	0.08	1 (1%)	82	67	56, 66, 87, 91	0
29	D7	81/81 (100%)	0.51	7 (8%)	10	4	84, 95, 107, 108	0
29	d7	81/81 (100%)	0.54	7 (8%)	10	4	72, 86, 101, 103	0
30	D8	63/66 (95%)	1.38	17 (26%)	0	0	101, 108, 112, 115	0
30	d8	63/66 (95%)	1.49	18 (28%)	0	0	88, 96, 101, 106	0
31	D9	53/55 (96%)	0.40	1 (1%)	66	46	78, 82, 94, 95	0
31	d9	53/55 (96%)	0.58	4 (7%)	14	5	73, 85, 114, 122	0
32	E0	60/62 (96%)	0.67	6 (10%)	7	2	65, 90, 102, 104	0
32	e0	62/62 (100%)	0.75	9 (14%)	2	1	53, 78, 95, 99	0
33	E1	71/76 (93%)	1.58	27 (38%)	0	0	89, 115, 125, 126	0
33	e1	76/76 (100%)	2.55	38 (50%)	0	0	96, 155, 181, 183	0
34	SR	318/318 (100%)	0.63	33 (10%)	6	2	95, 103, 114, 120	0
34	sR	318/318 (100%)	0.71	36 (11%)	5	2	102, 116, 127, 175	0
35	SM	133/182 (73%)	0.61	15 (11%)	5	2	56, 80, 122, 131	0
35	sM	63/182 (34%)	0.50	5 (7%)	12	5	44, 87, 93, 95	0
36	1	3149/3396 (92%)	0.05	123 (3%)	39	20	31, 53, 104, 189	0
36	5	3150/3396 (92%)	0.01	97 (3%)	49	26	29, 51, 105, 149	0
37	3	121/121 (100%)	-0.07	1 (0%)	86	72	43, 66, 77, 80	0
37	7	121/121 (100%)	-0.24	0	100	100	34, 52, 64, 69	0
38	4	158/158 (100%)	-0.17	3 (1%)	66	46	35, 54, 84, 107	0
38	8	158/158 (100%)	-0.04	3 (1%)	66	46	40, 61, 93, 104	0
39	L2	252/253 (99%)	-0.16	0	100	100	39, 52, 65, 70	0
39	l2	252/253 (99%)	-0.17	4 (1%)	72	51	37, 55, 73, 146	0
40	L3	386/386 (100%)	-0.25	1 (0%)	94	88	38, 53, 64, 73	0
40	l3	386/386 (100%)	-0.33	1 (0%)	94	88	30, 43, 58, 82	0
41	L4	361/361 (100%)	-0.37	0	100	100	33, 44, 56, 62	0
41	l4	361/361 (100%)	-0.25	3 (0%)	86	72	36, 51, 66, 72	0
42	L5	296/296 (100%)	0.13	5 (1%)	70	49	52, 69, 81, 90	0
42	l5	294/296 (99%)	-0.09	5 (1%)	70	49	37, 55, 77, 101	0
43	L6	156/175 (89%)	-0.29	0	100	100	42, 49, 58, 71	0
43	l6	157/175 (89%)	-0.24	2 (1%)	77	59	42, 54, 65, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	L7	222/243 (91%)	-0.44	1 (0%) 91 81	36, 42, 58, 72	0
44	l7	223/243 (91%)	-0.30	6 (2%) 54 31	33, 41, 69, 86	0
45	L8	233/255 (91%)	0.09	8 (3%) 45 24	58, 71, 89, 96	0
45	l8	231/255 (90%)	0.41	15 (6%) 18 8	65, 80, 101, 106	0
46	L9	191/191 (100%)	0.04	2 (1%) 82 67	51, 59, 67, 72	0
46	l9	191/191 (100%)	-0.30	1 (0%) 91 81	39, 47, 59, 67	0
47	M0	211/220 (95%)	-0.25	3 (1%) 75 56	39, 50, 74, 80	0
47	m0	213/220 (96%)	-0.16	4 (1%) 66 46	33, 46, 75, 167	0
48	M1	169/173 (97%)	0.30	7 (4%) 37 18	61, 74, 82, 86	0
48	m1	169/173 (97%)	-0.09	2 (1%) 79 61	44, 57, 67, 76	0
49	M3	193/198 (97%)	-0.14	6 (3%) 49 26	35, 52, 76, 98	0
49	m3	194/198 (97%)	0.08	6 (3%) 49 26	35, 63, 86, 93	0
50	M4	136/137 (99%)	-0.25	2 (1%) 73 54	46, 52, 62, 64	0
50	m4	137/137 (100%)	-0.40	1 (0%) 87 75	41, 46, 61, 67	0
51	M5	203/203 (100%)	-0.17	0 100 100	36, 49, 59, 60	0
51	m5	203/203 (100%)	-0.08	0 100 100	40, 56, 66, 69	0
52	M6	197/198 (99%)	-0.40	1 (0%) 91 81	37, 43, 57, 58	0
52	m6	197/198 (99%)	-0.46	0 100 100	30, 35, 55, 58	0
53	M7	183/183 (100%)	0.10	16 (8%) 10 4	39, 47, 73, 82	0
53	m7	155/183 (84%)	-0.29	0 100 100	36, 43, 53, 61	0
54	M8	185/185 (100%)	-0.42	0 100 100	37, 47, 59, 68	0
54	m8	185/185 (100%)	-0.26	1 (0%) 91 81	36, 52, 60, 66	0
55	M9	188/188 (100%)	0.30	10 (5%) 26 12	58, 67, 117, 123	0
55	m9	188/188 (100%)	0.23	8 (4%) 35 17	53, 60, 108, 121	0
56	N0	172/172 (100%)	-0.29	2 (1%) 79 61	43, 49, 57, 63	0
56	n0	172/172 (100%)	-0.37	0 100 100	35, 41, 49, 52	0
57	N1	159/159 (100%)	-0.20	3 (1%) 66 46	39, 49, 71, 75	0
57	n1	159/159 (100%)	-0.22	3 (1%) 66 46	34, 41, 66, 71	0
58	N2	100/120 (83%)	0.89	11 (11%) 5 2	81, 89, 92, 92	0
58	n2	98/120 (81%)	0.61	11 (11%) 5 2	70, 79, 83, 86	0
59	N3	136/136 (100%)	0.01	4 (2%) 51 28	43, 50, 55, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
59	n3	136/136 (100%)	-0.30	1 (0%) 87 75	30, 39, 48, 51	0
60	N4	98/155 (63%)	0.94	21 (21%) 0 0	49, 63, 112, 120	0
60	n4	135/155 (87%)	0.64	19 (14%) 2 1	38, 87, 303, 442	0
61	N5	121/141 (85%)	-0.04	1 (0%) 86 72	51, 60, 72, 88	0
61	n5	120/141 (85%)	0.14	6 (5%) 28 13	50, 65, 80, 86	0
62	N6	126/126 (100%)	0.20	4 (3%) 47 25	40, 53, 61, 64	0
62	n6	126/126 (100%)	0.03	1 (0%) 86 72	46, 60, 71, 75	0
63	N7	135/135 (100%)	0.26	3 (2%) 62 41	71, 79, 92, 98	0
63	n7	135/135 (100%)	0.19	4 (2%) 50 27	75, 86, 100, 107	0
64	N8	148/148 (100%)	-0.26	1 (0%) 87 75	30, 48, 62, 72	0
64	n8	148/148 (100%)	-0.25	0 100 100	31, 54, 63, 65	0
65	N9	58/58 (100%)	0.12	2 (3%) 45 24	35, 53, 81, 89	0
65	n9	58/58 (100%)	-0.13	0 100 100	32, 49, 69, 73	0
66	O0	97/104 (93%)	0.27	8 (8%) 11 4	67, 73, 84, 87	0
66	o0	100/104 (96%)	0.30	5 (5%) 28 13	66, 76, 86, 92	0
67	O1	109/112 (97%)	0.08	1 (0%) 84 69	52, 62, 76, 82	0
67	o1	109/112 (97%)	0.09	1 (0%) 84 69	44, 56, 81, 163	0
68	O2	127/129 (98%)	-0.18	2 (1%) 72 51	32, 44, 49, 53	0
68	o2	127/129 (98%)	-0.31	1 (0%) 86 72	31, 50, 57, 61	0
69	O3	106/106 (100%)	-0.32	0 100 100	37, 42, 56, 60	0
69	o3	106/106 (100%)	-0.33	0 100 100	34, 43, 59, 65	0
70	O4	112/120 (93%)	0.36	6 (5%) 25 12	52, 67, 82, 87	0
70	o4	112/120 (93%)	0.22	3 (2%) 54 31	51, 66, 88, 91	0
71	O5	119/119 (100%)	-0.03	1 (0%) 86 72	49, 60, 66, 70	0
71	o5	119/119 (100%)	-0.07	1 (0%) 86 72	57, 68, 76, 81	0
72	O6	99/99 (100%)	0.12	5 (5%) 28 13	51, 60, 77, 83	0
72	o6	99/99 (100%)	0.16	3 (3%) 50 27	59, 67, 77, 85	0
73	O7	87/87 (100%)	-0.09	1 (1%) 80 64	37, 43, 60, 73	0
73	o7	87/87 (100%)	0.04	2 (2%) 60 39	37, 46, 74, 90	0
74	O8	77/77 (100%)	0.22	3 (3%) 39 20	75, 80, 87, 87	0
74	o8	77/77 (100%)	0.62	6 (7%) 13 5	81, 89, 108, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
75	O9	50/50 (100%)	-0.26	2 (4%) 38 19	45, 49, 51, 52	0
75	o9	50/50 (100%)	-0.27	0 100 100	45, 50, 57, 66	0
76	Q0	52/52 (100%)	-0.01	0 100 100	48, 52, 61, 65	0
76	q0	52/52 (100%)	-0.27	0 100 100	36, 39, 47, 51	0
77	Q1	25/25 (100%)	0.52	1 (4%) 38 19	62, 63, 67, 68	0
77	q1	25/25 (100%)	-0.11	0 100 100	49, 51, 53, 55	0
78	Q2	105/105 (100%)	0.45	3 (2%) 51 28	39, 51, 63, 74	0
78	q2	105/105 (100%)	0.33	4 (3%) 40 20	38, 49, 59, 71	0
79	Q3	91/91 (100%)	-0.11	0 100 100	46, 53, 63, 69	0
79	q3	91/91 (100%)	-0.25	1 (1%) 80 64	43, 51, 65, 71	0
80	m2	0/150	-	-	-	-
81	p0	143/311 (45%)	0.41	12 (8%) 11 4	83, 101, 174, 180	0
82	p1	0/47	-	-	-	-
83	p2	0/46	-	-	-	-
All	All	32994/35138 (93%)	0.17	1617 (4%) 29 14	29, 66, 117, 442	0

The worst 5 of 1617 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	c2	20	ALA	27.1
47	m0	111	LEU	12.8
16	C4	15	GLY	12.0
1	2	1702	A	10.4
60	n4	68	ALA	10.3

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
84	MG	6	1984	1/1	0.26	0.48	70,70,70,70	0
84	MG	1	3678	1/1	0.36	0.24	65,65,65,65	0
84	MG	M3	201	1/1	0.44	0.22	86,86,86,86	0
84	MG	5	3457	1/1	0.47	0.43	100,100,100,100	0
84	MG	2	1941	1/1	0.50	0.78	93,93,93,93	0
84	MG	2	1962	1/1	0.50	0.78	110,110,110,110	0
84	MG	5	3617	1/1	0.53	0.56	46,46,46,46	0
84	MG	l6	201	1/1	0.56	0.45	56,56,56,56	0
84	MG	5	3647	1/1	0.57	0.37	41,41,41,41	0
84	MG	5	3643	1/1	0.58	0.40	55,55,55,55	0
84	MG	SM	201	1/1	0.59	0.51	56,56,56,56	0
84	MG	1	3583	1/1	0.60	0.21	61,61,61,61	0
84	MG	6	1977	1/1	0.60	0.38	79,79,79,79	0
87	ANM	1	3401	19/19	0.61	0.52	62,62,62,62	19
84	MG	1	4043	1/1	0.62	0.72	33,33,33,33	0
84	MG	1	3494	1/1	0.62	0.38	52,52,52,52	0
84	MG	5	3613	1/1	0.63	0.34	58,58,58,58	0
84	MG	6	1971	1/1	0.64	0.60	90,90,90,90	0
84	MG	6	1996	1/1	0.64	0.36	54,54,54,54	0
84	MG	1	3714	1/1	0.64	0.22	45,45,45,45	0
84	MG	1	3722	1/1	0.65	0.37	60,60,60,60	0
84	MG	5	3460	1/1	0.65	0.29	44,44,44,44	0
84	MG	5	3462	1/1	0.65	0.29	58,58,58,58	0
84	MG	1	3570	1/1	0.66	0.69	67,67,67,67	0
84	MG	2	1904	1/1	0.66	0.67	77,77,77,77	0
84	MG	6	1961	1/1	0.66	0.43	61,61,61,61	0
84	MG	1	3599	1/1	0.66	0.49	59,59,59,59	0
84	MG	O7	103	1/1	0.67	0.61	64,64,64,64	0
84	MG	1	3624	1/1	0.68	0.23	44,44,44,44	0
84	MG	2	1970	1/1	0.68	0.56	76,76,76,76	0
84	MG	2	1912	1/1	0.68	0.55	74,74,74,74	0
84	MG	2	1969	1/1	0.69	0.71	66,66,66,66	0
84	MG	1	3496	1/1	0.69	0.48	39,39,39,39	0
84	MG	5	3715	1/1	0.69	0.29	39,39,39,39	0
84	MG	5	3426	1/1	0.69	0.30	36,36,36,36	0
84	MG	1	3673	1/1	0.69	0.51	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	5	3458	1/1	0.70	0.27	107,107,107,107	0
86	ZN	e1	501	1/1	0.70	0.07	160,160,160,160	0
84	MG	1	3667	1/1	0.70	0.66	62,62,62,62	0
84	MG	5	3409	1/1	0.71	0.26	58,58,58,58	0
84	MG	2	1972	1/1	0.71	0.50	71,71,71,71	0
84	MG	6	1969	1/1	0.71	0.48	65,65,65,65	0
84	MG	5	3709	1/1	0.71	0.41	61,61,61,61	0
84	MG	2	1909	1/1	0.71	0.58	81,81,81,81	0
84	MG	4	202	1/1	0.71	0.54	57,57,57,57	0
84	MG	1	3414	1/1	0.71	0.45	63,63,63,63	0
84	MG	1	3663	1/1	0.71	0.30	36,36,36,36	0
84	MG	2	1948	1/1	0.72	0.38	94,94,94,94	0
84	MG	5	3641	1/1	0.72	0.72	79,79,79,79	0
84	MG	3	201	1/1	0.72	0.24	71,71,71,71	0
84	MG	1	3487	1/1	0.72	0.62	49,49,49,49	0
84	MG	5	3693	1/1	0.72	0.40	80,80,80,80	0
84	MG	5	3404	1/1	0.73	0.24	33,33,33,33	0
84	MG	4	213	1/1	0.73	0.38	41,41,41,41	0
84	MG	1	3668	1/1	0.73	0.18	66,66,66,66	0
84	MG	l3	402	1/1	0.73	0.24	32,32,32,32	0
84	MG	6	1993	1/1	0.73	0.36	95,95,95,95	0
84	MG	m7	201	1/1	0.73	0.31	37,37,37,37	0
84	MG	1	3715	1/1	0.73	0.78	48,48,48,48	0
84	MG	6	1998	1/1	0.73	0.23	58,58,58,58	0
84	MG	2	1956	1/1	0.74	0.45	64,64,64,64	0
84	MG	6	1965	1/1	0.74	0.47	56,56,56,56	0
84	MG	2	1938	1/1	0.74	0.36	75,75,75,75	0
84	MG	1	3712	1/1	0.74	0.28	41,41,41,41	0
84	MG	6	2002	1/1	0.74	0.65	99,99,99,99	0
84	MG	5	3655	1/1	0.74	0.60	64,64,64,64	0
84	MG	1	3630	1/1	0.74	0.57	56,56,56,56	0
84	MG	6	2008	1/1	0.75	0.44	47,47,47,47	0
84	MG	1	3655	1/1	0.75	0.29	41,41,41,41	0
84	MG	2	1978	1/1	0.75	0.74	104,104,104,104	0
84	MG	5	3476	1/1	0.75	0.58	51,51,51,51	0
84	MG	1	3435	1/1	0.75	0.46	41,41,41,41	0
84	MG	1	3709	1/1	0.75	0.83	59,59,59,59	0
84	MG	1	3508	1/1	0.76	0.39	43,43,43,43	0
84	MG	5	3697	1/1	0.76	0.29	50,50,50,50	0
84	MG	2	1979	1/1	0.76	0.40	72,72,72,72	0
84	MG	1	3639	1/1	0.76	0.43	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	8	207	1/1	0.76	0.45	51,51,51,51	0
84	MG	1	3408	1/1	0.77	0.33	50,50,50,50	0
84	MG	5	3731	1/1	0.77	0.57	37,37,37,37	0
84	MG	5	3738	1/1	0.77	0.38	45,45,45,45	0
84	MG	2	1923	1/1	0.77	0.51	56,56,56,56	0
84	MG	2	1915	1/1	0.77	0.59	76,76,76,76	0
84	MG	6	1917	1/1	0.77	1.38	75,75,75,75	0
84	MG	5	3438	1/1	0.77	0.36	45,45,45,45	0
84	MG	5	3614	1/1	0.77	0.25	55,55,55,55	0
84	MG	6	1938	1/1	0.77	0.50	99,99,99,99	0
84	MG	5	3635	1/1	0.78	0.18	66,66,66,66	0
84	MG	1	3707	1/1	0.78	0.35	53,53,53,53	0
84	MG	5	3722	1/1	0.78	0.31	55,55,55,55	0
84	MG	5	3463	1/1	0.78	0.37	41,41,41,41	0
84	MG	5	3732	1/1	0.78	0.30	52,52,52,52	0
84	MG	5	3645	1/1	0.78	0.31	33,33,33,33	0
84	MG	2	1949	1/1	0.78	0.40	96,96,96,96	0
84	MG	2	1913	1/1	0.78	0.32	63,63,63,63	0
84	MG	5	3678	1/1	0.78	0.31	58,58,58,58	0
84	MG	5	3688	1/1	0.78	0.40	33,33,33,33	0
84	MG	1	3701	1/1	0.78	0.27	40,40,40,40	0
84	MG	6	1908	1/1	0.78	0.20	51,51,51,51	0
84	MG	5	3667	1/1	0.79	0.30	38,38,38,38	0
84	MG	1	3666	1/1	0.79	0.24	45,45,45,45	0
84	MG	2	1975	1/1	0.79	0.35	76,76,76,76	0
84	MG	O4	202	1/1	0.79	0.37	67,67,67,67	0
84	MG	1	3568	1/1	0.79	0.52	40,40,40,40	0
84	MG	1	3638	1/1	0.79	0.19	46,46,46,46	0
84	MG	6	1911	1/1	0.79	0.30	52,52,52,52	0
84	MG	6	2001	1/1	0.79	0.42	73,73,73,73	0
84	MG	2	1946	1/1	0.79	0.63	93,93,93,93	0
84	MG	6	1930	1/1	0.79	0.56	59,59,59,59	0
84	MG	5	3632	1/1	0.79	0.43	42,42,42,42	0
84	MG	1	3694	1/1	0.79	0.47	41,41,41,41	0
84	MG	2	1911	1/1	0.79	0.82	69,69,69,69	0
84	MG	1	3430	1/1	0.79	0.30	36,36,36,36	0
84	MG	4	208	1/1	0.79	0.27	54,54,54,54	0
84	MG	5	3450	1/1	0.79	0.25	58,58,58,58	0
84	MG	5	3453	1/1	0.79	0.23	42,42,42,42	0
84	MG	6	1903	1/1	0.80	0.50	45,45,45,45	0
84	MG	6	1946	1/1	0.80	0.56	49,49,49,49	0
84	MG	1	3442	1/1	0.80	0.15	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	5	3407	1/1	0.80	0.25	33,33,33,33	0
84	MG	5	3636	1/1	0.80	0.45	44,44,44,44	0
84	MG	6	1994	1/1	0.80	0.25	49,49,49,49	0
84	MG	1	3437	1/1	0.80	0.20	45,45,45,45	0
84	MG	5	3467	1/1	0.80	0.62	65,65,65,65	0
84	MG	1	3685	1/1	0.80	0.29	39,39,39,39	0
84	MG	5	3542	1/1	0.80	0.53	36,36,36,36	0
84	MG	5	3585	1/1	0.80	0.30	39,39,39,39	0
84	MG	l9	201	1/1	0.80	0.22	45,45,45,45	0
84	MG	5	3598	1/1	0.80	0.17	42,42,42,42	0
84	MG	5	3685	1/1	0.80	0.28	36,36,36,36	0
84	MG	4	210	1/1	0.80	0.38	58,58,58,58	0
84	MG	2	1947	1/1	0.81	1.03	93,93,93,93	0
84	MG	6	1995	1/1	0.81	0.71	52,52,52,52	0
84	MG	5	3723	1/1	0.81	0.42	38,38,38,38	0
84	MG	5	3574	1/1	0.81	0.42	53,53,53,53	0
84	MG	1	3417	1/1	0.81	0.47	58,58,58,58	0
84	MG	Q2	502	1/1	0.81	0.14	55,55,55,55	0
84	MG	7	202	1/1	0.81	0.30	32,32,32,32	0
84	MG	5	3600	1/1	0.81	0.28	34,34,34,34	0
84	MG	l2	302	1/1	0.81	0.37	42,42,42,42	0
84	MG	1	3456	1/1	0.81	0.18	32,32,32,32	0
84	MG	1	3688	1/1	0.81	0.22	47,47,47,47	0
84	MG	1	3406	1/1	0.81	0.73	130,130,130,130	0
84	MG	2	1981	1/1	0.81	0.42	76,76,76,76	0
84	MG	n6	201	1/1	0.81	0.39	65,65,65,65	0
84	MG	6	1928	1/1	0.81	0.51	51,51,51,51	0
84	MG	1	4039	1/1	0.81	0.42	46,46,46,46	0
84	MG	5	3461	1/1	0.82	0.19	40,40,40,40	0
84	MG	5	3728	1/1	0.82	0.32	50,50,50,50	0
84	MG	5	3608	1/1	0.82	0.41	89,89,89,89	0
84	MG	5	3664	1/1	0.82	0.19	53,53,53,53	0
84	MG	2	1971	1/1	0.82	0.33	77,77,77,77	0
84	MG	1	3697	1/1	0.82	0.51	41,41,41,41	0
84	MG	2	1961	1/1	0.82	0.22	75,75,75,75	0
84	MG	1	3536	1/1	0.82	0.42	56,56,56,56	0
84	MG	5	3456	1/1	0.82	0.40	54,54,54,54	0
84	MG	1	3657	1/1	0.82	0.33	50,50,50,50	0
84	MG	5	3701	1/1	0.82	0.45	47,47,47,47	0
84	MG	5	3704	1/1	0.82	0.44	54,54,54,54	0
84	MG	1	3690	1/1	0.82	0.31	48,48,48,48	0
84	MG	5	3595	1/1	0.82	0.13	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	6	1926	1/1	0.82	0.56	46,46,46,46	0
84	MG	5	3640	1/1	0.83	0.27	51,51,51,51	0
84	MG	1	3720	1/1	0.83	0.18	56,56,56,56	0
84	MG	1	3611	1/1	0.83	0.26	39,39,39,39	0
84	MG	5	3727	1/1	0.83	0.23	62,62,62,62	0
84	MG	6	2006	1/1	0.83	0.56	61,61,61,61	0
84	MG	1	3457	1/1	0.83	0.46	42,42,42,42	0
84	MG	1	3629	1/1	0.83	0.46	74,74,74,74	0
84	MG	1	3710	1/1	0.83	0.32	40,40,40,40	0
84	MG	5	3604	1/1	0.83	0.42	36,36,36,36	0
84	MG	5	3674	1/1	0.83	0.30	49,49,49,49	0
84	MG	5	3605	1/1	0.83	0.21	37,37,37,37	0
84	MG	1	3692	1/1	0.83	0.35	45,45,45,45	0
84	MG	l3	405	1/1	0.83	0.69	34,34,34,34	0
84	MG	6	1956	1/1	0.83	0.64	60,60,60,60	0
84	MG	l8	301	1/1	0.83	0.65	83,83,83,83	0
84	MG	1	3424	1/1	0.83	0.45	45,45,45,45	0
84	MG	5	3470	1/1	0.83	0.37	32,32,32,32	0
84	MG	5	3471	1/1	0.83	0.34	68,68,68,68	0
84	MG	1	3637	1/1	0.83	0.42	42,42,42,42	0
84	MG	5	3485	1/1	0.83	0.34	37,37,37,37	0
84	MG	1	3527	1/1	0.84	0.23	64,64,64,64	0
84	MG	1	3618	1/1	0.84	0.29	62,62,62,62	0
84	MG	5	3642	1/1	0.84	0.32	37,37,37,37	0
84	MG	2	1937	1/1	0.84	0.39	79,79,79,79	0
84	MG	5	3644	1/1	0.84	0.32	72,72,72,72	0
84	MG	1	3560	1/1	0.84	0.34	40,40,40,40	0
84	MG	6	1970	1/1	0.84	0.47	98,98,98,98	0
84	MG	5	3651	1/1	0.84	0.37	46,46,46,46	0
84	MG	6	1922	1/1	0.84	0.54	48,48,48,48	0
84	MG	2	1921	1/1	0.84	0.69	81,81,81,81	0
84	MG	1	3696	1/1	0.84	0.32	55,55,55,55	0
84	MG	6	1990	1/1	0.84	0.18	61,61,61,61	0
84	MG	5	3675	1/1	0.84	0.18	59,59,59,59	0
84	MG	5	3413	1/1	0.84	0.33	41,41,41,41	0
84	MG	5	3681	1/1	0.84	0.49	40,40,40,40	0
84	MG	l7	301	1/1	0.84	0.18	37,37,37,37	0
84	MG	D9	102	1/1	0.84	0.45	86,86,86,86	0
84	MG	1	3479	1/1	0.84	0.61	64,64,64,64	0
84	MG	m5	303	1/1	0.84	0.51	46,46,46,46	0
84	MG	5	3624	1/1	0.84	0.21	41,41,41,41	0
84	MG	1	3516	1/1	0.84	0.65	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	n6	202	1/1	0.84	0.39	52,52,52,52	0
84	MG	5	3532	1/1	0.84	0.68	50,50,50,50	0
84	MG	5	3541	1/1	0.84	0.39	50,50,50,50	0
84	MG	5	3710	1/1	0.85	0.21	44,44,44,44	0
84	MG	2	1924	1/1	0.85	0.85	86,86,86,86	0
84	MG	6	1916	1/1	0.85	0.46	46,46,46,46	0
84	MG	5	3411	1/1	0.85	0.34	34,34,34,34	0
84	MG	4	204	1/1	0.85	0.57	51,51,51,51	0
84	MG	5	3421	1/1	0.85	0.34	50,50,50,50	0
84	MG	5	3555	1/1	0.85	0.33	44,44,44,44	0
84	MG	1	3405	1/1	0.85	0.71	63,63,63,63	0
84	MG	1	3468	1/1	0.85	0.14	59,59,59,59	0
84	MG	5	3588	1/1	0.85	0.33	57,57,57,57	0
84	MG	8	206	1/1	0.85	0.58	52,52,52,52	0
84	MG	5	3444	1/1	0.85	0.22	32,32,32,32	0
84	MG	1	3472	1/1	0.85	0.36	52,52,52,52	0
84	MG	1	3693	1/1	0.85	0.27	58,58,58,58	0
84	MG	M7	201	1/1	0.85	0.48	60,60,60,60	0
84	MG	6	1942	1/1	0.85	0.98	79,79,79,79	0
84	MG	1	3477	1/1	0.85	0.27	54,54,54,54	0
84	MG	1	3421	1/1	0.85	0.35	41,41,41,41	0
84	MG	5	3687	1/1	0.85	0.46	31,31,31,31	0
84	MG	6	1959	1/1	0.85	0.66	86,86,86,86	0
84	MG	1	3439	1/1	0.85	0.26	60,60,60,60	0
84	MG	1	3569	1/1	0.85	0.46	53,53,53,53	0
84	MG	d6	102	1/1	0.85	0.49	56,56,56,56	0
86	ZN	D7	101	1/1	0.85	0.35	115,115,115,115	0
84	MG	5	3403	1/1	0.85	0.16	45,45,45,45	0
84	MG	1	3411	1/1	0.85	0.44	51,51,51,51	0
84	MG	1	3619	1/1	0.86	0.29	35,35,35,35	0
84	MG	5	3619	1/1	0.86	0.19	37,37,37,37	0
84	MG	5	3621	1/1	0.86	0.34	40,40,40,40	0
84	MG	2	1976	1/1	0.86	0.72	68,68,68,68	0
84	MG	5	3625	1/1	0.86	0.15	44,44,44,44	0
84	MG	5	3516	1/1	0.86	0.40	31,31,31,31	0
84	MG	5	3531	1/1	0.86	0.46	56,56,56,56	0
84	MG	1	3517	1/1	0.86	0.45	51,51,51,51	0
84	MG	5	3540	1/1	0.86	0.54	28,28,28,28	0
84	MG	1	3458	1/1	0.86	0.32	59,59,59,59	0
84	MG	1	3598	1/1	0.86	0.29	39,39,39,39	0
84	MG	5	3544	1/1	0.86	0.46	32,32,32,32	0
84	MG	2	1940	1/1	0.86	0.71	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	5	3559	1/1	0.86	0.35	40,40,40,40	0
84	MG	5	4078	1/1	0.86	0.57	40,40,40,40	0
84	MG	6	1962	1/1	0.86	0.17	84,84,84,84	0
84	MG	6	2003	1/1	0.86	1.02	63,63,63,63	0
84	MG	1	3684	1/1	0.86	0.82	51,51,51,51	0
84	MG	5	3657	1/1	0.86	0.21	57,57,57,57	0
84	MG	1	3610	1/1	0.86	0.61	42,42,42,42	0
84	MG	5	3666	1/1	0.86	0.21	37,37,37,37	0
84	MG	1	3640	1/1	0.86	0.35	74,74,74,74	0
84	MG	2	1974	1/1	0.86	0.22	93,93,93,93	0
84	MG	4	214	1/1	0.86	0.41	53,53,53,53	0
84	MG	5	3676	1/1	0.86	0.17	63,63,63,63	0
84	MG	5	3406	1/1	0.86	0.13	47,47,47,47	0
84	MG	5	3680	1/1	0.86	0.22	53,53,53,53	0
84	MG	6	1982	1/1	0.86	0.22	46,46,46,46	0
84	MG	5	3684	1/1	0.86	0.19	77,77,77,77	0
84	MG	L3	401	1/1	0.86	0.86	53,53,53,53	0
84	MG	2	1933	1/1	0.86	0.48	74,74,74,74	0
84	MG	5	3616	1/1	0.86	0.37	40,40,40,40	0
84	MG	5	3503	1/1	0.87	0.28	40,40,40,40	0
84	MG	2	1964	1/1	0.87	0.33	83,83,83,83	0
84	MG	5	3526	1/1	0.87	0.37	38,38,38,38	0
84	MG	5	3638	1/1	0.87	0.24	37,37,37,37	0
84	MG	5	3711	1/1	0.87	0.10	32,32,32,32	0
84	MG	1	3626	1/1	0.87	0.27	44,44,44,44	0
84	MG	2	1936	1/1	0.87	0.67	73,73,73,73	0
84	MG	5	3408	1/1	0.87	0.39	42,42,42,42	0
84	MG	O7	102	1/1	0.87	0.47	51,51,51,51	0
84	MG	1	3681	1/1	0.87	0.16	45,45,45,45	0
84	MG	1	3589	1/1	0.87	0.14	64,64,64,64	0
84	MG	5	3419	1/1	0.87	0.14	41,41,41,41	0
84	MG	5	3736	1/1	0.87	0.31	48,48,48,48	0
84	MG	6	1902	1/1	0.87	0.38	57,57,57,57	0
84	MG	1	3631	1/1	0.87	0.56	49,49,49,49	0
84	MG	1	3590	1/1	0.87	0.40	60,60,60,60	0
84	MG	7	206	1/1	0.87	0.45	42,42,42,42	0
84	MG	1	3448	1/1	0.87	0.40	64,64,64,64	0
84	MG	1	3548	1/1	0.87	0.27	31,31,31,31	0
84	MG	1	3608	1/1	0.87	0.48	87,87,87,87	0
84	MG	6	1919	1/1	0.87	0.66	67,67,67,67	0
84	MG	1	3649	1/1	0.87	0.26	43,43,43,43	0
84	MG	6	1924	1/1	0.87	0.70	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	1	3552	1/1	0.87	0.67	44,44,44,44	0
84	MG	1	3471	1/1	0.87	0.24	58,58,58,58	0
84	MG	4	212	1/1	0.87	0.20	54,54,54,54	0
84	MG	1	3616	1/1	0.87	0.47	81,81,81,81	0
84	MG	1	3449	1/1	0.87	0.99	64,64,64,64	0
84	MG	5	3686	1/1	0.87	0.25	44,44,44,44	0
84	MG	2	1932	1/1	0.87	0.58	68,68,68,68	0
85	OHX	1	4012	7/7	0.87	0.38	116,116,116,116	0
84	MG	6	1947	1/1	0.87	0.53	53,53,53,53	0
84	MG	6	1951	1/1	0.87	0.49	77,77,77,77	0
84	MG	6	1955	1/1	0.87	1.13	67,67,67,67	0
84	MG	1	3429	1/1	0.88	0.53	51,51,51,51	0
84	MG	1	3510	1/1	0.88	0.36	31,31,31,31	0
84	MG	1	3650	1/1	0.88	0.56	81,81,81,81	0
84	MG	1	3724	1/1	0.88	0.46	49,49,49,49	0
84	MG	1	3689	1/1	0.88	0.32	57,57,57,57	0
84	MG	1	3652	1/1	0.88	0.25	57,57,57,57	0
84	MG	1	3620	1/1	0.88	0.42	54,54,54,54	0
84	MG	3	202	1/1	0.88	0.68	67,67,67,67	0
84	MG	6	1976	1/1	0.88	0.19	91,91,91,91	0
84	MG	3	203	1/1	0.88	0.29	44,44,44,44	0
84	MG	1	3656	1/1	0.88	0.44	46,46,46,46	0
84	MG	2	1965	1/1	0.88	0.72	60,60,60,60	0
84	MG	1	3431	1/1	0.88	0.17	51,51,51,51	0
84	MG	1	3601	1/1	0.88	0.32	65,65,65,65	0
84	MG	6	1927	1/1	0.88	0.40	50,50,50,50	0
84	MG	1	3526	1/1	0.88	0.21	52,52,52,52	0
84	MG	5	3601	1/1	0.88	0.42	38,38,38,38	0
84	MG	S4	301	1/1	0.88	0.32	79,79,79,79	0
84	MG	6	1932	1/1	0.88	0.76	62,62,62,62	0
84	MG	6	1937	1/1	0.88	0.78	72,72,72,72	0
84	MG	5	3610	1/1	0.88	0.29	37,37,37,37	0
84	MG	1	3708	1/1	0.88	0.28	60,60,60,60	0
84	MG	1	3582	1/1	0.88	0.28	45,45,45,45	0
84	MG	m5	301	1/1	0.88	0.26	48,48,48,48	0
84	MG	1	3615	1/1	0.88	0.33	31,31,31,31	0
84	MG	1	3679	1/1	0.88	0.24	34,34,34,34	0
84	MG	n0	202	1/1	0.88	0.16	40,40,40,40	0
84	MG	c1	201	1/1	0.88	0.44	53,53,53,53	0
84	MG	M7	204	1/1	0.88	0.23	40,40,40,40	0
84	MG	n9	101	1/1	0.88	0.38	33,33,33,33	0
84	MG	5	3482	1/1	0.88	0.12	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	5	3402	1/1	0.88	0.66	61,61,61,61	0
84	MG	5	3501	1/1	0.88	0.53	27,27,27,27	0
84	MG	2	1954	1/1	0.88	0.49	90,90,90,90	0
84	MG	1	3704	1/1	0.89	0.36	34,34,34,34	0
84	MG	5	3671	1/1	0.89	0.28	35,35,35,35	0
84	MG	2	1943	1/1	0.89	0.75	71,71,71,71	0
84	MG	1	3441	1/1	0.89	0.32	31,31,31,31	0
84	MG	1	3664	1/1	0.89	0.33	36,36,36,36	0
84	MG	N3	201	1/1	0.89	0.35	40,40,40,40	0
84	MG	2	1955	1/1	0.89	0.33	68,68,68,68	0
84	MG	5	3566	1/1	0.89	0.56	46,46,46,46	0
84	MG	5	3571	1/1	0.89	0.78	53,53,53,53	0
84	MG	2	1902	1/1	0.89	0.41	55,55,55,55	0
84	MG	5	3581	1/1	0.89	0.57	35,35,35,35	0
84	MG	5	3583	1/1	0.89	0.12	42,42,42,42	0
84	MG	6	1963	1/1	0.89	0.32	76,76,76,76	0
84	MG	5	3587	1/1	0.89	0.32	39,39,39,39	0
84	MG	2	1939	1/1	0.89	0.43	74,74,74,74	0
84	MG	6	1966	1/1	0.89	0.40	53,53,53,53	0
84	MG	1	3450	1/1	0.89	0.37	33,33,33,33	0
84	MG	5	3705	1/1	0.89	0.14	36,36,36,36	0
84	MG	5	3707	1/1	0.89	0.16	43,43,43,43	0
84	MG	2	1919	1/1	0.89	0.70	73,73,73,73	0
84	MG	5	3428	1/1	0.89	0.52	39,39,39,39	0
84	MG	1	3721	1/1	0.89	0.56	42,42,42,42	0
84	MG	5	3712	1/1	0.89	0.24	44,44,44,44	0
84	MG	5	3442	1/1	0.89	0.32	36,36,36,36	0
84	MG	6	1975	1/1	0.89	0.32	79,79,79,79	0
84	MG	5	3445	1/1	0.89	0.60	49,49,49,49	0
84	MG	1	3587	1/1	0.89	0.20	42,42,42,42	0
84	MG	6	1910	1/1	0.89	0.40	74,74,74,74	0
84	MG	5	3615	1/1	0.89	0.56	56,56,56,56	0
84	MG	1	3723	1/1	0.89	0.30	37,37,37,37	0
84	MG	2	1982	1/1	0.89	0.27	65,65,65,65	0
84	MG	1	3634	1/1	0.89	0.38	39,39,39,39	0
84	MG	2	1905	1/1	0.89	0.77	63,63,63,63	0
84	MG	5	3622	1/1	0.89	0.17	55,55,55,55	0
84	MG	1	3461	1/1	0.89	0.35	36,36,36,36	0
84	MG	1	3462	1/1	0.89	0.31	38,38,38,38	0
84	MG	1	3600	1/1	0.89	0.34	52,52,52,52	0
84	MG	l2	301	1/1	0.89	0.60	48,48,48,48	0
84	MG	1	3643	1/1	0.89	0.52	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	1	3466	1/1	0.89	0.74	57,57,57,57	0
84	MG	1	3528	1/1	0.89	0.36	34,34,34,34	0
84	MG	1	3416	1/1	0.89	0.41	48,48,48,48	0
84	MG	5	3478	1/1	0.89	0.21	45,45,45,45	0
84	MG	6	2005	1/1	0.89	0.51	61,61,61,61	0
84	MG	4	211	1/1	0.89	0.23	42,42,42,42	0
84	MG	5	3487	1/1	0.89	0.42	32,32,32,32	0
84	MG	6	2007	1/1	0.89	0.29	61,61,61,61	0
84	MG	5	3646	1/1	0.89	0.18	35,35,35,35	0
84	MG	1	3538	1/1	0.89	0.42	42,42,42,42	0
84	MG	5	3507	1/1	0.89	0.43	44,44,44,44	0
84	MG	s8	301	1/1	0.89	0.32	47,47,47,47	0
84	MG	1	3700	1/1	0.89	0.46	36,36,36,36	0
85	OHX	2	2115	7/7	0.89	0.41	115,115,115,115	0
84	MG	5	3659	1/1	0.89	0.29	41,41,41,41	0
85	OHX	5	3938	7/7	0.89	0.22	115,115,115,115	0
85	OHX	5	4043	7/7	0.89	0.43	96,96,96,96	0
85	OHX	5	4068	7/7	0.89	0.27	96,96,96,96	0
84	MG	5	3662	1/1	0.89	0.26	34,34,34,34	0
84	MG	1	3438	1/1	0.89	0.32	32,32,32,32	0
84	MG	sM	201	1/1	0.89	0.32	44,44,44,44	0
84	MG	1	3460	1/1	0.90	0.28	52,52,52,52	0
84	MG	4	207	1/1	0.90	0.25	49,49,49,49	0
84	MG	5	3477	1/1	0.90	0.21	42,42,42,42	0
84	MG	5	3696	1/1	0.90	0.21	31,31,31,31	0
84	MG	2	1963	1/1	0.90	0.58	78,78,78,78	0
84	MG	5	3698	1/1	0.90	0.35	73,73,73,73	0
84	MG	5	3480	1/1	0.90	0.21	36,36,36,36	0
84	MG	1	3484	1/1	0.90	0.40	52,52,52,52	0
84	MG	1	3641	1/1	0.90	0.29	51,51,51,51	0
84	MG	1	3642	1/1	0.90	0.23	48,48,48,48	0
84	MG	5	3498	1/1	0.90	0.55	41,41,41,41	0
84	MG	5	3499	1/1	0.90	0.31	36,36,36,36	0
84	MG	1	3713	1/1	0.90	0.19	45,45,45,45	0
84	MG	6	1979	1/1	0.90	0.30	52,52,52,52	0
84	MG	6	1981	1/1	0.90	0.38	57,57,57,57	0
84	MG	5	3631	1/1	0.90	0.24	41,41,41,41	0
84	MG	5	3509	1/1	0.90	0.36	47,47,47,47	0
84	MG	5	3511	1/1	0.90	0.34	62,62,62,62	0
84	MG	5	3515	1/1	0.90	0.45	52,52,52,52	0
84	MG	5	3637	1/1	0.90	0.32	49,49,49,49	0
84	MG	2	1901	1/1	0.90	1.24	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	1	3452	1/1	0.90	0.43	38,38,38,38	0
84	MG	5	3737	1/1	0.90	0.08	52,52,52,52	0
84	MG	6	1987	1/1	0.90	0.14	55,55,55,55	0
84	MG	5	3739	1/1	0.90	0.30	88,88,88,88	0
84	MG	5	4076	1/1	0.90	0.50	52,52,52,52	0
84	MG	6	1988	1/1	0.90	0.27	73,73,73,73	0
84	MG	5	3538	1/1	0.90	0.52	41,41,41,41	0
84	MG	1	3467	1/1	0.90	0.23	47,47,47,47	0
84	MG	8	204	1/1	0.90	0.21	56,56,56,56	0
84	MG	8	205	1/1	0.90	0.25	48,48,48,48	0
84	MG	6	1934	1/1	0.90	0.29	67,67,67,67	0
84	MG	1	3539	1/1	0.90	0.52	44,44,44,44	0
84	MG	1	3420	1/1	0.90	0.10	38,38,38,38	0
84	MG	5	3650	1/1	0.90	0.11	46,46,46,46	0
84	MG	5	3550	1/1	0.90	0.55	31,31,31,31	0
84	MG	5	3652	1/1	0.90	0.17	44,44,44,44	0
84	MG	1	3549	1/1	0.90	0.38	53,53,53,53	0
84	MG	5	3446	1/1	0.90	0.33	45,45,45,45	0
84	MG	5	3447	1/1	0.90	0.57	34,34,34,34	0
84	MG	5	3660	1/1	0.90	0.34	41,41,41,41	0
84	MG	5	3448	1/1	0.90	0.32	28,28,28,28	0
84	MG	6	1945	1/1	0.90	0.41	66,66,66,66	0
84	MG	5	3578	1/1	0.90	0.82	40,40,40,40	0
84	MG	m7	203	1/1	0.90	0.41	40,40,40,40	0
84	MG	1	3404	1/1	0.90	0.23	42,42,42,42	0
84	MG	5	3668	1/1	0.90	0.46	71,71,71,71	0
84	MG	1	3658	1/1	0.90	0.33	52,52,52,52	0
84	MG	1	4040	1/1	0.90	0.35	39,39,39,39	0
84	MG	o3	201	1/1	0.90	0.29	49,49,49,49	0
84	MG	q1	101	1/1	0.90	0.57	47,47,47,47	0
84	MG	1	3659	1/1	0.90	0.45	47,47,47,47	0
85	OHX	1	3931	7/7	0.90	0.27	111,111,111,111	0
84	MG	1	3554	1/1	0.90	0.39	32,32,32,32	0
85	OHX	6	2158	7/7	0.90	0.35	140,140,140,140	0
84	MG	2	1910	1/1	0.90	0.43	64,64,64,64	0
84	MG	5	3597	1/1	0.90	0.27	29,29,29,29	0
84	MG	1	3605	1/1	0.90	0.19	46,46,46,46	0
84	MG	1	3561	1/1	0.90	0.43	43,43,43,43	0
84	MG	4	203	1/1	0.90	0.48	68,68,68,68	0
84	MG	6	1915	1/1	0.90	0.27	72,72,72,72	0
84	MG	2	1960	1/1	0.91	1.10	72,72,72,72	0
84	MG	5	3639	1/1	0.91	0.17	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	5	3714	1/1	0.91	0.24	34,34,34,34	0
84	MG	6	1929	1/1	0.91	0.30	67,67,67,67	0
84	MG	2	1952	1/1	0.91	0.98	77,77,77,77	0
84	MG	1	3407	1/1	0.91	0.45	45,45,45,45	0
84	MG	1	3623	1/1	0.91	0.19	51,51,51,51	0
84	MG	L6	201	1/1	0.91	0.14	48,48,48,48	0
84	MG	5	3729	1/1	0.91	0.22	52,52,52,52	0
84	MG	1	3427	1/1	0.91	0.41	48,48,48,48	0
84	MG	2	1953	1/1	0.91	0.94	84,84,84,84	0
84	MG	6	2000	1/1	0.91	0.28	86,86,86,86	0
84	MG	1	3584	1/1	0.91	0.88	54,54,54,54	0
84	MG	1	3585	1/1	0.91	0.70	59,59,59,59	0
84	MG	1	3531	1/1	0.91	0.72	45,45,45,45	0
84	MG	5	3741	1/1	0.91	0.31	54,54,54,54	0
84	MG	5	4073	1/1	0.91	0.78	31,31,31,31	0
84	MG	5	3653	1/1	0.91	0.17	67,67,67,67	0
84	MG	1	3491	1/1	0.91	0.55	41,41,41,41	0
84	MG	2	1942	1/1	0.91	0.20	69,69,69,69	0
84	MG	7	204	1/1	0.91	0.49	40,40,40,40	0
84	MG	1	3595	1/1	0.91	0.28	50,50,50,50	0
84	MG	6	1957	1/1	0.91	0.46	63,63,63,63	0
84	MG	6	2160	1/1	0.91	0.31	84,84,84,84	0
84	MG	5	3593	1/1	0.91	0.36	54,54,54,54	0
84	MG	5	3594	1/1	0.91	0.25	40,40,40,40	0
84	MG	6	1901	1/1	0.91	0.37	50,50,50,50	0
84	MG	1	3597	1/1	0.91	0.28	46,46,46,46	0
84	MG	5	3669	1/1	0.91	0.39	39,39,39,39	0
84	MG	l3	403	1/1	0.91	0.38	38,38,38,38	0
84	MG	2	1918	1/1	0.91	0.77	64,64,64,64	0
84	MG	5	3672	1/1	0.91	0.34	40,40,40,40	0
84	MG	1	3542	1/1	0.91	0.33	46,46,46,46	0
84	MG	1	3543	1/1	0.91	0.36	34,34,34,34	0
84	MG	1	3503	1/1	0.91	0.57	33,33,33,33	0
84	MG	5	3677	1/1	0.91	0.39	41,41,41,41	0
84	MG	6	1912	1/1	0.91	0.32	79,79,79,79	0
84	MG	6	1913	1/1	0.91	0.53	51,51,51,51	0
84	MG	1	3645	1/1	0.91	0.21	69,69,69,69	0
84	MG	1	3506	1/1	0.91	0.53	42,42,42,42	0
84	MG	5	3500	1/1	0.91	0.38	47,47,47,47	0
84	MG	2	1935	1/1	0.91	0.35	68,68,68,68	0
84	MG	1	3651	1/1	0.91	0.20	36,36,36,36	0
84	MG	2	1957	1/1	0.91	0.57	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	q0	202	1/1	0.91	0.28	44,44,44,44	0
84	MG	5	3690	1/1	0.91	0.43	30,30,30,30	0
85	OHX	2	2108	7/7	0.91	0.25	145,145,145,145	0
84	MG	5	3418	1/1	0.91	0.31	41,41,41,41	0
85	OHX	2	2118	7/7	0.91	0.30	132,132,132,132	0
85	OHX	1	3921	7/7	0.91	0.32	110,110,110,110	0
84	MG	6	1980	1/1	0.91	0.28	68,68,68,68	0
84	MG	1	3556	1/1	0.91	0.52	30,30,30,30	0
85	OHX	6	2131	7/7	0.91	0.34	121,121,121,121	0
84	MG	5	3425	1/1	0.91	0.19	31,31,31,31	0
84	MG	5	3520	1/1	0.91	0.44	40,40,40,40	0
84	MG	1	3512	1/1	0.91	0.35	55,55,55,55	0
85	OHX	5	4050	7/7	0.91	0.25	158,158,158,158	0
84	MG	5	3529	1/1	0.91	0.67	58,58,58,58	0
84	MG	1	3514	1/1	0.91	0.36	33,33,33,33	0
86	ZN	d6	101	1/1	0.91	0.09	60,60,60,60	0
84	MG	6	1985	1/1	0.91	0.29	65,65,65,65	0
84	MG	5	3536	1/1	0.91	0.58	46,46,46,46	0
84	MG	5	3412	1/1	0.92	0.46	39,39,39,39	0
84	MG	1	3547	1/1	0.92	0.49	33,33,33,33	0
84	MG	1	3665	1/1	0.92	0.29	67,67,67,67	0
84	MG	6	1958	1/1	0.92	0.68	47,47,47,47	0
84	MG	5	4071	1/1	0.92	0.23	43,43,43,43	0
84	MG	5	4072	1/1	0.92	0.29	33,33,33,33	0
84	MG	1	3447	1/1	0.92	0.48	37,37,37,37	0
84	MG	5	3496	1/1	0.92	0.43	56,56,56,56	0
84	MG	5	4077	1/1	0.92	0.87	38,38,38,38	0
84	MG	5	3423	1/1	0.92	0.56	45,45,45,45	0
84	MG	5	3603	1/1	0.92	0.35	47,47,47,47	0
84	MG	2	1951	1/1	0.92	0.47	58,58,58,58	0
84	MG	6	1999	1/1	0.92	0.28	49,49,49,49	0
84	MG	5	3427	1/1	0.92	0.11	47,47,47,47	0
84	MG	M6	201	1/1	0.92	0.16	45,45,45,45	0
84	MG	5	3429	1/1	0.92	0.15	78,78,78,78	0
84	MG	5	3431	1/1	0.92	0.18	37,37,37,37	0
84	MG	8	209	1/1	0.92	0.45	68,68,68,68	0
84	MG	5	3434	1/1	0.92	0.30	32,32,32,32	0
84	MG	5	3437	1/1	0.92	0.20	35,35,35,35	0
84	MG	l2	303	1/1	0.92	1.08	46,46,46,46	0
84	MG	6	1923	1/1	0.92	0.69	68,68,68,68	0
84	MG	5	3440	1/1	0.92	0.15	40,40,40,40	0
84	MG	6	1964	1/1	0.92	0.33	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	1	3489	1/1	0.92	0.52	49,49,49,49	0
84	MG	1	3672	1/1	0.92	0.28	42,42,42,42	0
84	MG	6	1967	1/1	0.92	0.20	51,51,51,51	0
84	MG	5	3689	1/1	0.92	0.23	30,30,30,30	0
84	MG	1	4044	1/1	0.92	0.30	51,51,51,51	0
84	MG	O2	201	1/1	0.92	0.24	35,35,35,35	0
84	MG	m6	201	1/1	0.92	0.28	37,37,37,37	0
84	MG	5	3633	1/1	0.92	0.86	36,36,36,36	0
84	MG	5	3634	1/1	0.92	0.16	31,31,31,31	0
84	MG	6	2159	1/1	0.92	0.59	58,58,58,58	0
84	MG	5	3451	1/1	0.92	0.35	33,33,33,33	0
84	MG	5	3703	1/1	0.92	0.41	36,36,36,36	0
84	MG	n8	201	1/1	0.92	0.34	50,50,50,50	0
84	MG	2	1966	1/1	0.92	0.35	67,67,67,67	0
84	MG	o1	201	1/1	0.92	0.61	49,49,49,49	0
84	MG	1	3705	1/1	0.92	0.82	52,52,52,52	0
84	MG	1	3676	1/1	0.92	0.25	48,48,48,48	0
84	MG	5	3551	1/1	0.92	0.34	35,35,35,35	0
84	MG	5	3553	1/1	0.92	0.42	38,38,38,38	0
85	OHX	2	2111	7/7	0.92	0.43	112,112,112,112	0
85	OHX	2	2114	7/7	0.92	0.20	170,170,170,170	0
84	MG	1	3443	1/1	0.92	0.45	43,43,43,43	0
84	MG	1	3459	1/1	0.92	0.44	46,46,46,46	0
84	MG	5	3563	1/1	0.92	0.37	38,38,38,38	0
84	MG	1	3541	1/1	0.92	0.45	55,55,55,55	0
84	MG	5	3716	1/1	0.92	0.40	29,29,29,29	0
84	MG	5	3721	1/1	0.92	0.58	35,35,35,35	0
85	OHX	6	2146	7/7	0.92	0.36	108,108,108,108	0
85	OHX	6	2157	7/7	0.92	0.47	115,115,115,115	0
84	MG	1	3592	1/1	0.92	0.21	61,61,61,61	0
85	OHX	5	3860	7/7	0.92	0.16	122,122,122,122	0
84	MG	1	3593	1/1	0.92	0.18	39,39,39,39	0
85	OHX	5	3969	7/7	0.92	0.25	138,138,138,138	0
85	OHX	5	4020	7/7	0.92	0.41	101,101,101,101	0
84	MG	1	3617	1/1	0.92	0.48	43,43,43,43	0
84	MG	1	3497	1/1	0.92	0.56	33,33,33,33	0
85	OHX	5	4061	7/7	0.92	0.39	121,121,121,121	0
84	MG	1	3662	1/1	0.92	0.24	45,45,45,45	0
84	MG	5	3730	1/1	0.92	0.37	43,43,43,43	0
84	MG	5	3473	1/1	0.92	0.41	44,44,44,44	0
86	ZN	d7	101	1/1	0.92	0.17	106,106,106,106	0
84	MG	6	1954	1/1	0.92	0.67	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	ZN	q2	501	1/1	0.92	0.21	64,64,64,64	0
84	MG	1	3482	1/1	0.92	0.15	53,53,53,53	0
84	MG	8	202	1/1	0.93	0.40	64,64,64,64	0
84	MG	1	3469	1/1	0.93	0.52	51,51,51,51	0
84	MG	2	1973	1/1	0.93	0.45	64,64,64,64	0
84	MG	5	3623	1/1	0.93	0.49	57,57,57,57	0
84	MG	2	1967	1/1	0.93	0.26	83,83,83,83	0
84	MG	6	1986	1/1	0.93	0.20	57,57,57,57	0
84	MG	8	210	1/1	0.93	0.23	57,57,57,57	0
84	MG	5	3549	1/1	0.93	0.41	48,48,48,48	0
84	MG	1	3501	1/1	0.93	0.53	43,43,43,43	0
84	MG	1	3532	1/1	0.93	0.19	57,57,57,57	0
84	MG	l3	401	1/1	0.93	0.51	29,29,29,29	0
84	MG	5	3414	1/1	0.93	0.17	31,31,31,31	0
84	MG	1	3564	1/1	0.93	0.62	40,40,40,40	0
84	MG	1	3444	1/1	0.93	0.27	51,51,51,51	0
84	MG	2	1907	1/1	0.93	0.51	64,64,64,64	0
84	MG	2	1903	1/1	0.93	0.69	55,55,55,55	0
84	MG	6	1909	1/1	0.93	0.40	98,98,98,98	0
84	MG	1	3602	1/1	0.93	0.52	41,41,41,41	0
84	MG	4	205	1/1	0.93	0.49	39,39,39,39	0
84	MG	1	3604	1/1	0.93	0.17	47,47,47,47	0
84	MG	1	3575	1/1	0.93	0.45	40,40,40,40	0
84	MG	5	3708	1/1	0.93	0.26	44,44,44,44	0
84	MG	1	3670	1/1	0.93	0.39	52,52,52,52	0
84	MG	1	3577	1/1	0.93	0.24	46,46,46,46	0
84	MG	1	3423	1/1	0.93	0.23	36,36,36,36	0
84	MG	5	3589	1/1	0.93	0.41	37,37,37,37	0
84	MG	5	3648	1/1	0.93	0.19	61,61,61,61	0
84	MG	n8	202	1/1	0.93	0.23	37,37,37,37	0
84	MG	2	1928	1/1	0.93	0.39	71,71,71,71	0
84	MG	6	1921	1/1	0.93	0.48	56,56,56,56	0
84	MG	5	3717	1/1	0.93	0.18	39,39,39,39	0
84	MG	5	3718	1/1	0.93	0.20	40,40,40,40	0
84	MG	1	3612	1/1	0.93	0.29	40,40,40,40	0
85	OHX	2	2034	7/7	0.93	0.26	113,113,113,113	0
85	OHX	2	2052	7/7	0.93	0.23	117,117,117,117	0
85	OHX	2	2100	7/7	0.93	0.20	116,116,116,116	0
85	OHX	2	2107	7/7	0.93	0.33	126,126,126,126	0
84	MG	5	3596	1/1	0.93	0.43	40,40,40,40	0
84	MG	5	3654	1/1	0.93	0.25	42,42,42,42	0
84	MG	1	3614	1/1	0.93	0.14	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	1	3719	1/1	0.93	0.71	45,45,45,45	0
84	MG	L7	301	1/1	0.93	0.36	42,42,42,42	0
84	MG	6	1973	1/1	0.93	0.21	78,78,78,78	0
84	MG	5	3518	1/1	0.93	0.38	41,41,41,41	0
84	MG	5	3663	1/1	0.93	0.25	62,62,62,62	0
85	OHX	6	2068	7/7	0.93	0.22	90,90,90,90	0
85	OHX	6	2127	7/7	0.93	0.25	138,138,138,138	0
84	MG	5	3735	1/1	0.93	0.22	65,65,65,65	0
85	OHX	6	2135	7/7	0.93	0.39	92,92,92,92	0
85	OHX	6	2144	7/7	0.93	0.35	102,102,102,102	0
84	MG	1	3648	1/1	0.93	0.22	37,37,37,37	0
85	OHX	6	2155	7/7	0.93	0.42	116,116,116,116	0
84	MG	5	3522	1/1	0.93	0.27	43,43,43,43	0
84	MG	5	3607	1/1	0.93	0.18	38,38,38,38	0
84	MG	1	3488	1/1	0.93	0.34	33,33,33,33	0
85	OHX	5	3870	7/7	0.93	0.28	76,76,76,76	0
85	OHX	5	3932	7/7	0.93	0.26	75,75,75,75	0
84	MG	5	3740	1/1	0.93	0.15	41,41,41,41	0
84	MG	5	3609	1/1	0.93	0.42	55,55,55,55	0
85	OHX	5	4005	7/7	0.93	0.27	104,104,104,104	0
84	MG	sM	202	1/1	0.93	0.11	43,43,43,43	0
85	OHX	5	4029	7/7	0.93	0.31	128,128,128,128	0
84	MG	1	3426	1/1	0.93	0.47	50,50,50,50	0
84	MG	5	3673	1/1	0.93	0.51	34,34,34,34	0
84	MG	2	1922	1/1	0.93	0.97	74,74,74,74	0
84	MG	5	3534	1/1	0.93	0.37	36,36,36,36	0
85	OHX	7	220	7/7	0.93	0.31	110,110,110,110	0
84	MG	5	3535	1/1	0.93	0.35	49,49,49,49	0
84	MG	1	3518	1/1	0.93	0.43	52,52,52,52	0
84	MG	N8	202	1/1	0.93	0.14	35,35,35,35	0
84	MG	5	3679	1/1	0.93	0.41	42,42,42,42	0
84	MG	7	209	1/1	0.93	0.34	51,51,51,51	0
84	MG	7	210	1/1	0.93	0.12	53,53,53,53	0
84	MG	1	3660	1/1	0.94	0.09	47,47,47,47	0
84	MG	O3	201	1/1	0.94	0.21	42,42,42,42	0
84	MG	5	3415	1/1	0.94	0.59	29,29,29,29	0
84	MG	5	4075	1/1	0.94	0.46	33,33,33,33	0
84	MG	5	3416	1/1	0.94	0.28	38,38,38,38	0
84	MG	5	3530	1/1	0.94	0.31	41,41,41,41	0
84	MG	5	3417	1/1	0.94	0.20	84,84,84,84	0
84	MG	1	3661	1/1	0.94	0.47	55,55,55,55	0
84	MG	5	3533	1/1	0.94	0.91	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	5	3649	1/1	0.94	0.23	35,35,35,35	0
84	MG	7	207	1/1	0.94	0.14	36,36,36,36	0
84	MG	1	3502	1/1	0.94	0.43	39,39,39,39	0
84	MG	1	3445	1/1	0.94	0.33	40,40,40,40	0
84	MG	8	201	1/1	0.94	0.24	42,42,42,42	0
84	MG	1	3415	1/1	0.94	0.38	41,41,41,41	0
84	MG	1	3545	1/1	0.94	0.54	36,36,36,36	0
84	MG	2	1920	1/1	0.94	0.69	74,74,74,74	0
84	MG	6	1972	1/1	0.94	0.31	51,51,51,51	0
84	MG	2	1925	1/1	0.94	0.76	74,74,74,74	0
84	MG	6	1906	1/1	0.94	0.34	51,51,51,51	0
84	MG	1	3594	1/1	0.94	0.35	48,48,48,48	0
84	MG	1	3669	1/1	0.94	0.27	48,48,48,48	0
84	MG	6	1978	1/1	0.94	0.59	76,76,76,76	0
84	MG	1	3476	1/1	0.94	0.20	42,42,42,42	0
84	MG	5	3665	1/1	0.94	0.45	39,39,39,39	0
84	MG	5	3439	1/1	0.94	0.33	33,33,33,33	0
84	MG	1	3725	1/1	0.94	0.38	52,52,52,52	0
84	MG	5	3562	1/1	0.94	0.35	32,32,32,32	0
84	MG	1	3596	1/1	0.94	0.16	46,46,46,46	0
84	MG	5	3670	1/1	0.94	0.32	35,35,35,35	0
84	MG	5	3564	1/1	0.94	0.45	38,38,38,38	0
84	MG	1	3633	1/1	0.94	0.44	56,56,56,56	0
84	MG	m1	201	1/1	0.94	0.40	48,48,48,48	0
84	MG	1	3432	1/1	0.94	0.22	49,49,49,49	0
84	MG	1	3677	1/1	0.94	0.27	43,43,43,43	0
84	MG	1	3515	1/1	0.94	0.46	41,41,41,41	0
84	MG	6	1918	1/1	0.94	0.48	58,58,58,58	0
84	MG	5	3582	1/1	0.94	0.23	49,49,49,49	0
84	MG	1	3433	1/1	0.94	0.35	36,36,36,36	0
84	MG	5	3584	1/1	0.94	0.11	45,45,45,45	0
84	MG	1	3455	1/1	0.94	0.34	32,32,32,32	0
84	MG	3	204	1/1	0.94	0.60	40,40,40,40	0
84	MG	5	3455	1/1	0.94	0.32	50,50,50,50	0
84	MG	3	205	1/1	0.94	0.24	66,66,66,66	0
84	MG	3	207	1/1	0.94	0.16	44,44,44,44	0
84	MG	4	201	1/1	0.94	0.52	53,53,53,53	0
84	MG	5	3459	1/1	0.94	0.35	40,40,40,40	0
84	MG	1	3682	1/1	0.94	0.50	33,33,33,33	0
85	OHX	2	2027	7/7	0.94	0.20	128,128,128,128	0
84	MG	1	3434	1/1	0.94	0.36	52,52,52,52	0
84	MG	1	3520	1/1	0.94	0.32	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	2	2063	7/7	0.94	0.22	160,160,160,160	0
85	OHX	2	2067	7/7	0.94	0.36	106,106,106,106	0
85	OHX	2	2076	7/7	0.94	0.18	135,135,135,135	0
85	OHX	2	2089	7/7	0.94	0.42	113,113,113,113	0
85	OHX	2	2090	7/7	0.94	0.19	121,121,121,121	0
84	MG	5	3695	1/1	0.94	0.25	48,48,48,48	0
85	OHX	2	2102	7/7	0.94	0.32	114,114,114,114	0
85	OHX	2	2106	7/7	0.94	0.35	123,123,123,123	0
84	MG	1	3687	1/1	0.94	0.19	48,48,48,48	0
84	MG	5	3464	1/1	0.94	0.34	29,29,29,29	0
85	OHX	2	2109	7/7	0.94	0.33	112,112,112,112	0
85	OHX	2	2110	7/7	0.94	0.38	130,130,130,130	0
84	MG	1	3565	1/1	0.94	0.47	32,32,32,32	0
84	MG	5	3700	1/1	0.94	0.23	38,38,38,38	0
84	MG	1	3567	1/1	0.94	0.93	50,50,50,50	0
84	MG	6	1936	1/1	0.94	0.38	42,42,42,42	0
85	OHX	2	2119	7/7	0.94	0.47	144,144,144,144	0
85	OHX	S6	301	7/7	0.94	0.38	117,117,117,117	0
85	OHX	1	3864	7/7	0.94	0.20	79,79,79,79	0
85	OHX	1	3889	7/7	0.94	0.21	99,99,99,99	0
85	OHX	1	3918	7/7	0.94	0.29	121,121,121,121	0
84	MG	5	3472	1/1	0.94	0.47	50,50,50,50	0
84	MG	4	209	1/1	0.94	0.29	54,54,54,54	0
85	OHX	1	3945	7/7	0.94	0.19	162,162,162,162	0
85	OHX	1	3997	7/7	0.94	0.39	82,82,82,82	0
85	OHX	1	4002	7/7	0.94	0.27	112,112,112,112	0
85	OHX	1	4003	7/7	0.94	0.39	108,108,108,108	0
84	MG	1	3644	1/1	0.94	0.72	41,41,41,41	0
85	OHX	1	4029	7/7	0.94	0.42	89,89,89,89	0
85	OHX	1	4036	7/7	0.94	0.36	104,104,104,104	0
84	MG	6	1941	1/1	0.94	0.38	43,43,43,43	0
85	OHX	6	2088	7/7	0.94	0.46	81,81,81,81	0
85	OHX	6	2101	7/7	0.94	0.26	105,105,105,105	0
85	OHX	6	2123	7/7	0.94	0.33	102,102,102,102	0
84	MG	5	3611	1/1	0.94	0.22	40,40,40,40	0
85	OHX	6	2128	7/7	0.94	0.31	112,112,112,112	0
84	MG	5	3612	1/1	0.94	0.36	40,40,40,40	0
84	MG	1	3606	1/1	0.94	0.39	34,34,34,34	0
85	OHX	6	2137	7/7	0.94	0.27	127,127,127,127	0
85	OHX	6	2142	7/7	0.94	0.24	117,117,117,117	0
84	MG	6	1943	1/1	0.94	0.57	58,58,58,58	0
84	MG	1	3646	1/1	0.94	0.14	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	6	2150	7/7	0.94	0.39	100,100,100,100	0
84	MG	5	3483	1/1	0.94	0.47	41,41,41,41	0
84	MG	2	1950	1/1	0.94	0.33	72,72,72,72	0
84	MG	1	3609	1/1	0.94	0.32	41,41,41,41	0
84	MG	5	3492	1/1	0.94	0.56	41,41,41,41	0
84	MG	5	3495	1/1	0.94	0.17	35,35,35,35	0
85	OHX	5	3906	7/7	0.94	0.21	101,101,101,101	0
85	OHX	5	3909	7/7	0.94	0.18	88,88,88,88	0
84	MG	6	1949	1/1	0.94	0.68	76,76,76,76	0
84	MG	2	1934	1/1	0.94	0.32	72,72,72,72	0
85	OHX	5	3943	7/7	0.94	0.18	116,116,116,116	0
84	MG	5	3725	1/1	0.94	0.28	38,38,38,38	0
85	OHX	5	3976	7/7	0.94	0.25	107,107,107,107	0
85	OHX	5	3980	7/7	0.94	0.23	102,102,102,102	0
84	MG	5	3401	1/1	0.94	0.26	32,32,32,32	0
85	OHX	5	4008	7/7	0.94	0.26	144,144,144,144	0
84	MG	5	3628	1/1	0.94	0.27	49,49,49,49	0
85	OHX	5	4024	7/7	0.94	0.32	116,116,116,116	0
84	MG	5	3629	1/1	0.94	0.35	35,35,35,35	0
85	OHX	5	4033	7/7	0.94	0.37	105,105,105,105	0
85	OHX	5	4034	7/7	0.94	0.34	84,84,84,84	0
84	MG	6	1952	1/1	0.94	0.51	54,54,54,54	0
85	OHX	5	4044	7/7	0.94	0.24	116,116,116,116	0
84	MG	1	3699	1/1	0.94	0.45	55,55,55,55	0
85	OHX	5	4055	7/7	0.94	0.36	114,114,114,114	0
84	MG	5	3502	1/1	0.94	0.46	32,32,32,32	0
84	MG	5	3733	1/1	0.94	0.43	32,32,32,32	0
84	MG	2	1926	1/1	0.94	0.33	74,74,74,74	0
84	MG	2	1927	1/1	0.94	0.47	65,65,65,65	0
86	ZN	E1	501	1/1	0.94	0.05	115,115,115,115	0
84	MG	1	3613	1/1	0.94	0.13	45,45,45,45	0
84	MG	1	3425	1/1	0.94	0.20	49,49,49,49	0
84	MG	2	1906	1/1	0.94	0.45	63,63,63,63	0
84	MG	2	1929	1/1	0.94	0.64	67,67,67,67	0
84	MG	1	3428	1/1	0.94	0.44	48,48,48,48	0
85	OHX	2	2003	7/7	0.95	0.11	101,101,101,101	0
85	OHX	2	2012	7/7	0.95	0.14	107,107,107,107	0
85	OHX	2	2025	7/7	0.95	0.14	108,108,108,108	0
85	OHX	2	2026	7/7	0.95	0.19	118,118,118,118	0
84	MG	2	1908	1/1	0.95	0.39	78,78,78,78	0
84	MG	1	3588	1/1	0.95	0.41	42,42,42,42	0
85	OHX	2	2040	7/7	0.95	0.24	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	5	3713	1/1	0.95	0.34	33,33,33,33	0
84	MG	1	3490	1/1	0.95	0.26	42,42,42,42	0
84	MG	M0	301	1/1	0.95	0.37	43,43,43,43	0
85	OHX	2	2068	7/7	0.95	0.33	122,122,122,122	0
85	OHX	2	2075	7/7	0.95	0.35	115,115,115,115	0
84	MG	5	3548	1/1	0.95	0.30	29,29,29,29	0
85	OHX	2	2084	7/7	0.95	0.33	98,98,98,98	0
85	OHX	2	2085	7/7	0.95	0.29	114,114,114,114	0
84	MG	5	3465	1/1	0.95	0.17	41,41,41,41	0
84	MG	1	3470	1/1	0.95	0.28	37,37,37,37	0
85	OHX	2	2092	7/7	0.95	0.32	106,106,106,106	0
85	OHX	2	2093	7/7	0.95	0.31	103,103,103,103	0
85	OHX	2	2098	7/7	0.95	0.38	125,125,125,125	0
84	MG	5	3719	1/1	0.95	0.15	32,32,32,32	0
84	MG	M5	301	1/1	0.95	0.24	39,39,39,39	0
85	OHX	2	2105	7/7	0.95	0.31	114,114,114,114	0
84	MG	1	3493	1/1	0.95	0.49	30,30,30,30	0
84	MG	6	1933	1/1	0.95	0.41	84,84,84,84	0
84	MG	5	3558	1/1	0.95	0.47	37,37,37,37	0
84	MG	2	1916	1/1	0.95	0.41	59,59,59,59	0
84	MG	5	3475	1/1	0.95	0.66	32,32,32,32	0
84	MG	1	3524	1/1	0.95	0.26	43,43,43,43	0
84	MG	1	3559	1/1	0.95	0.47	48,48,48,48	0
84	MG	1	3418	1/1	0.95	0.22	66,66,66,66	0
84	MG	5	3570	1/1	0.95	0.29	31,31,31,31	0
84	MG	5	3479	1/1	0.95	0.27	35,35,35,35	0
84	MG	5	3734	1/1	0.95	0.14	60,60,60,60	0
85	OHX	1	3826	7/7	0.95	0.14	93,93,93,93	0
85	OHX	1	3858	7/7	0.95	0.11	128,128,128,128	0
84	MG	5	3572	1/1	0.95	0.55	28,28,28,28	0
85	OHX	1	3888	7/7	0.95	0.30	85,85,85,85	0
84	MG	1	4042	1/1	0.95	0.15	45,45,45,45	0
84	MG	5	3575	1/1	0.95	0.47	31,31,31,31	0
84	MG	1	3474	1/1	0.95	0.18	53,53,53,53	0
84	MG	5	3580	1/1	0.95	0.57	37,37,37,37	0
84	MG	1	3500	1/1	0.95	0.66	44,44,44,44	0
85	OHX	1	3949	7/7	0.95	0.30	101,101,101,101	0
85	OHX	1	3960	7/7	0.95	0.30	122,122,122,122	0
85	OHX	1	3966	7/7	0.95	0.34	175,175,175,175	0
85	OHX	1	3969	7/7	0.95	0.33	103,103,103,103	0
85	OHX	1	3974	7/7	0.95	0.30	127,127,127,127	0
85	OHX	1	3978	7/7	0.95	0.22	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	1	3983	7/7	0.95	0.33	78,78,78,78	0
85	OHX	1	3992	7/7	0.95	0.32	116,116,116,116	0
84	MG	5	3656	1/1	0.95	0.12	36,36,36,36	0
84	MG	5	3484	1/1	0.95	0.35	35,35,35,35	0
84	MG	5	3658	1/1	0.95	0.31	46,46,46,46	0
85	OHX	1	4007	7/7	0.95	0.37	101,101,101,101	0
84	MG	1	3627	1/1	0.95	0.23	45,45,45,45	0
85	OHX	1	4013	7/7	0.95	0.26	104,104,104,104	0
85	OHX	1	4017	7/7	0.95	0.41	68,68,68,68	0
85	OHX	1	4018	7/7	0.95	0.32	88,88,88,88	0
84	MG	1	3446	1/1	0.95	0.17	47,47,47,47	0
85	OHX	1	4030	7/7	0.95	0.41	98,98,98,98	0
85	OHX	1	4031	7/7	0.95	0.23	102,102,102,102	0
85	OHX	1	4035	7/7	0.95	0.23	105,105,105,105	0
84	MG	1	3436	1/1	0.95	0.38	38,38,38,38	0
85	OHX	3	219	7/7	0.95	0.37	95,95,95,95	0
85	OHX	4	225	7/7	0.95	0.16	113,113,113,113	0
85	OHX	4	228	7/7	0.95	0.36	85,85,85,85	0
85	OHX	L4	401	7/7	0.95	0.30	92,92,92,92	0
85	OHX	M9	201	7/7	0.95	0.35	124,124,124,124	0
85	OHX	O9	101	7/7	0.95	0.46	77,77,77,77	0
85	OHX	6	2027	7/7	0.95	0.15	78,78,78,78	0
85	OHX	6	2040	7/7	0.95	0.13	89,89,89,89	0
84	MG	5	3586	1/1	0.95	0.42	34,34,34,34	0
85	OHX	6	2077	7/7	0.95	0.21	100,100,100,100	0
85	OHX	6	2080	7/7	0.95	0.29	109,109,109,109	0
85	OHX	6	2081	7/7	0.95	0.19	110,110,110,110	0
84	MG	5	3493	1/1	0.95	0.64	34,34,34,34	0
85	OHX	6	2095	7/7	0.95	0.41	119,119,119,119	0
85	OHX	6	2098	7/7	0.95	0.34	99,99,99,99	0
84	MG	5	3494	1/1	0.95	0.49	30,30,30,30	0
85	OHX	6	2109	7/7	0.95	0.26	84,84,84,84	0
85	OHX	6	2110	7/7	0.95	0.27	103,103,103,103	0
85	OHX	6	2116	7/7	0.95	0.18	111,111,111,111	0
84	MG	1	3533	1/1	0.95	0.43	39,39,39,39	0
84	MG	7	205	1/1	0.95	0.52	35,35,35,35	0
84	MG	5	3590	1/1	0.95	0.29	34,34,34,34	0
84	MG	5	3592	1/1	0.95	0.19	42,42,42,42	0
85	OHX	6	2132	7/7	0.95	0.30	112,112,112,112	0
85	OHX	6	2133	7/7	0.95	0.25	85,85,85,85	0
84	MG	6	1950	1/1	0.95	0.67	72,72,72,72	0
84	MG	1	3698	1/1	0.95	0.26	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	1	3402	1/1	0.95	0.61	46,46,46,46	0
85	OHX	6	2143	7/7	0.95	0.34	97,97,97,97	0
84	MG	6	1904	1/1	0.95	0.62	76,76,76,76	0
85	OHX	6	2145	7/7	0.95	0.35	106,106,106,106	0
84	MG	8	203	1/1	0.95	0.43	43,43,43,43	0
84	MG	1	3603	1/1	0.95	0.39	38,38,38,38	0
85	OHX	6	2154	7/7	0.95	0.38	100,100,100,100	0
84	MG	1	3403	1/1	0.95	0.65	51,51,51,51	0
84	MG	1	3572	1/1	0.95	0.52	33,33,33,33	0
84	MG	5	3505	1/1	0.95	0.51	36,36,36,36	0
85	OHX	c3	201	7/7	0.95	0.24	113,113,113,113	0
85	OHX	5	3849	7/7	0.95	0.15	90,90,90,90	0
84	MG	5	3602	1/1	0.95	0.50	49,49,49,49	0
85	OHX	5	3864	7/7	0.95	0.17	78,78,78,78	0
84	MG	5	3441	1/1	0.95	0.35	65,65,65,65	0
85	OHX	5	3886	7/7	0.95	0.21	82,82,82,82	0
85	OHX	5	3897	7/7	0.95	0.32	81,81,81,81	0
84	MG	5	3508	1/1	0.95	0.39	34,34,34,34	0
84	MG	1	3422	1/1	0.95	0.35	55,55,55,55	0
84	MG	5	3606	1/1	0.95	0.29	41,41,41,41	0
84	MG	5	3682	1/1	0.95	0.41	35,35,35,35	0
85	OHX	5	3940	7/7	0.95	0.23	99,99,99,99	0
84	MG	5	3443	1/1	0.95	0.20	38,38,38,38	0
85	OHX	5	3961	7/7	0.95	0.27	102,102,102,102	0
84	MG	5	3513	1/1	0.95	0.41	32,32,32,32	0
84	MG	5	3514	1/1	0.95	0.64	30,30,30,30	0
85	OHX	5	3978	7/7	0.95	0.27	92,92,92,92	0
84	MG	1	3706	1/1	0.95	0.65	32,32,32,32	0
85	OHX	5	3983	7/7	0.95	0.30	83,83,83,83	0
85	OHX	5	3988	7/7	0.95	0.28	116,116,116,116	0
85	OHX	5	3989	7/7	0.95	0.36	81,81,81,81	0
85	OHX	5	3990	7/7	0.95	0.40	76,76,76,76	0
85	OHX	5	3996	7/7	0.95	0.35	92,92,92,92	0
85	OHX	5	3997	7/7	0.95	0.37	87,87,87,87	0
85	OHX	5	4001	7/7	0.95	0.27	130,130,130,130	0
84	MG	1	3607	1/1	0.95	0.23	42,42,42,42	0
84	MG	5	3517	1/1	0.95	0.31	53,53,53,53	0
85	OHX	5	4018	7/7	0.95	0.35	105,105,105,105	0
85	OHX	5	4019	7/7	0.95	0.33	109,109,109,109	0
84	MG	1	3485	1/1	0.95	0.33	37,37,37,37	0
84	MG	1	3671	1/1	0.95	0.17	45,45,45,45	0
84	MG	5	3694	1/1	0.95	0.27	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	5	4031	7/7	0.95	0.27	106,106,106,106	0
84	MG	1	3511	1/1	0.95	0.50	39,39,39,39	0
84	MG	2	1968	1/1	0.95	0.44	85,85,85,85	0
84	MG	5	3527	1/1	0.95	0.33	69,69,69,69	0
84	MG	1	3674	1/1	0.95	0.50	37,37,37,37	0
85	OHX	5	4047	7/7	0.95	0.29	101,101,101,101	0
84	MG	n0	201	1/1	0.95	0.23	43,43,43,43	0
85	OHX	5	4053	7/7	0.95	0.29	105,105,105,105	0
84	MG	5	3452	1/1	0.95	0.34	43,43,43,43	0
85	OHX	5	4056	7/7	0.95	0.33	104,104,104,104	0
85	OHX	5	4058	7/7	0.95	0.35	115,115,115,115	0
84	MG	1	3544	1/1	0.95	0.57	35,35,35,35	0
85	OHX	5	4062	7/7	0.95	0.42	84,84,84,84	0
85	OHX	5	4067	7/7	0.95	0.22	93,93,93,93	0
84	MG	5	3702	1/1	0.95	0.13	35,35,35,35	0
84	MG	6	1968	1/1	0.95	0.35	55,55,55,55	0
85	OHX	l5	302	7/7	0.95	0.24	107,107,107,107	0
85	OHX	m0	301	7/7	0.95	0.13	109,109,109,109	0
86	ZN	D6	500	1/1	0.95	0.07	81,81,81,81	0
84	MG	6	1920	1/1	0.95	0.49	42,42,42,42	0
84	MG	2	1959	1/1	0.95	0.34	67,67,67,67	0
86	ZN	Q0	500	1/1	0.95	0.10	48,48,48,48	0
84	MG	5	3626	1/1	0.95	0.33	33,33,33,33	0
84	MG	L2	301	1/1	0.95	0.39	39,39,39,39	0
84	MG	L2	302	1/1	0.95	0.29	41,41,41,41	0
84	MG	5	3405	1/1	0.95	0.27	43,43,43,43	0
85	OHX	2	2000	7/7	0.95	0.13	89,89,89,89	0
85	OHX	1	3898	7/7	0.96	0.28	85,85,85,85	0
85	OHX	1	3905	7/7	0.96	0.20	79,79,79,79	0
85	OHX	1	3909	7/7	0.96	0.23	83,83,83,83	0
85	OHX	1	3914	7/7	0.96	0.16	111,111,111,111	0
85	OHX	1	3916	7/7	0.96	0.30	87,87,87,87	0
85	OHX	1	3917	7/7	0.96	0.13	133,133,133,133	0
84	MG	1	3478	1/1	0.96	0.15	40,40,40,40	0
85	OHX	1	3919	7/7	0.96	0.24	99,99,99,99	0
85	OHX	1	3920	7/7	0.96	0.17	121,121,121,121	0
84	MG	1	3504	1/1	0.96	0.36	40,40,40,40	0
85	OHX	1	3923	7/7	0.96	0.35	91,91,91,91	0
85	OHX	1	3929	7/7	0.96	0.34	83,83,83,83	0
85	OHX	1	3930	7/7	0.96	0.23	100,100,100,100	0
84	MG	4	206	1/1	0.96	0.27	35,35,35,35	0
85	OHX	1	3932	7/7	0.96	0.36	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	1	3935	7/7	0.96	0.31	88,88,88,88	0
85	OHX	1	3941	7/7	0.96	0.36	107,107,107,107	0
85	OHX	1	3943	7/7	0.96	0.31	112,112,112,112	0
84	MG	5	3521	1/1	0.96	0.41	39,39,39,39	0
85	OHX	1	3946	7/7	0.96	0.32	99,99,99,99	0
84	MG	1	3521	1/1	0.96	0.58	31,31,31,31	0
85	OHX	1	3950	7/7	0.96	0.26	121,121,121,121	0
85	OHX	1	3955	7/7	0.96	0.33	108,108,108,108	0
84	MG	1	3523	1/1	0.96	0.41	41,41,41,41	0
85	OHX	1	3964	7/7	0.96	0.28	89,89,89,89	0
84	MG	2	1958	1/1	0.96	0.49	96,96,96,96	0
84	MG	1	3525	1/1	0.96	0.39	46,46,46,46	0
84	MG	1	3711	1/1	0.96	0.23	46,46,46,46	0
85	OHX	1	3976	7/7	0.96	0.31	91,91,91,91	0
84	MG	1	3647	1/1	0.96	0.20	49,49,49,49	0
85	OHX	1	3981	7/7	0.96	0.24	95,95,95,95	0
84	MG	1	3546	1/1	0.96	0.24	36,36,36,36	0
85	OHX	1	3987	7/7	0.96	0.32	79,79,79,79	0
84	MG	1	3573	1/1	0.96	0.69	33,33,33,33	0
85	OHX	1	3993	7/7	0.96	0.37	87,87,87,87	0
84	MG	5	3692	1/1	0.96	0.44	68,68,68,68	0
85	OHX	1	4000	7/7	0.96	0.31	109,109,109,109	0
84	MG	5	3618	1/1	0.96	0.61	40,40,40,40	0
84	MG	l3	404	1/1	0.96	0.26	39,39,39,39	0
85	OHX	1	4006	7/7	0.96	0.43	102,102,102,102	0
84	MG	1	3621	1/1	0.96	0.16	36,36,36,36	0
84	MG	5	3620	1/1	0.96	0.35	35,35,35,35	0
84	MG	1	3622	1/1	0.96	0.23	35,35,35,35	0
85	OHX	1	4014	7/7	0.96	0.38	110,110,110,110	0
85	OHX	1	4015	7/7	0.96	0.36	91,91,91,91	0
85	OHX	1	4016	7/7	0.96	0.38	109,109,109,109	0
84	MG	1	3574	1/1	0.96	0.41	33,33,33,33	0
84	MG	5	3537	1/1	0.96	0.42	36,36,36,36	0
85	OHX	1	4023	7/7	0.96	0.33	109,109,109,109	0
85	OHX	1	4024	7/7	0.96	0.28	155,155,155,155	0
85	OHX	1	4028	7/7	0.96	0.31	115,115,115,115	0
84	MG	1	3653	1/1	0.96	0.17	40,40,40,40	0
84	MG	1	3654	1/1	0.96	0.16	45,45,45,45	0
84	MG	m5	302	1/1	0.96	0.17	53,53,53,53	0
85	OHX	1	4032	7/7	0.96	0.43	88,88,88,88	0
85	OHX	1	4034	7/7	0.96	0.36	104,104,104,104	0
84	MG	5	3466	1/1	0.96	0.23	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	5	3627	1/1	0.96	0.39	34,34,34,34	0
85	OHX	1	4037	7/7	0.96	0.45	98,98,98,98	0
85	OHX	1	4038	7/7	0.96	0.45	100,100,100,100	0
85	OHX	3	216	7/7	0.96	0.28	108,108,108,108	0
85	OHX	3	218	7/7	0.96	0.37	125,125,125,125	0
84	MG	1	3465	1/1	0.96	0.21	42,42,42,42	0
85	OHX	4	223	7/7	0.96	0.24	97,97,97,97	0
84	MG	m7	202	1/1	0.96	0.36	36,36,36,36	0
84	MG	5	3543	1/1	0.96	0.49	37,37,37,37	0
85	OHX	4	229	7/7	0.96	0.39	113,113,113,113	0
85	OHX	4	230	7/7	0.96	0.40	108,108,108,108	0
85	OHX	4	231	7/7	0.96	0.29	103,103,103,103	0
84	MG	5	3469	1/1	0.96	0.22	58,58,58,58	0
85	OHX	M0	302	7/7	0.96	0.18	86,86,86,86	0
84	MG	5	3410	1/1	0.96	0.62	42,42,42,42	0
85	OHX	N8	203	7/7	0.96	0.24	129,129,129,129	0
84	MG	1	3412	1/1	0.96	0.25	42,42,42,42	0
84	MG	1	3580	1/1	0.96	0.22	42,42,42,42	0
84	MG	1	3581	1/1	0.96	0.31	45,45,45,45	0
85	OHX	6	2054	7/7	0.96	0.22	84,84,84,84	0
85	OHX	6	2062	7/7	0.96	0.12	126,126,126,126	0
84	MG	5	3474	1/1	0.96	0.14	54,54,54,54	0
84	MG	1	3691	1/1	0.96	0.16	54,54,54,54	0
84	MG	M7	202	1/1	0.96	0.36	41,41,41,41	0
84	MG	M7	203	1/1	0.96	0.31	38,38,38,38	0
85	OHX	6	2084	7/7	0.96	0.19	117,117,117,117	0
84	MG	2	1914	1/1	0.96	0.56	73,73,73,73	0
85	OHX	6	2089	7/7	0.96	0.32	85,85,85,85	0
85	OHX	6	2091	7/7	0.96	0.18	110,110,110,110	0
85	OHX	6	2093	7/7	0.96	0.21	117,117,117,117	0
84	MG	1	3530	1/1	0.96	0.66	41,41,41,41	0
85	OHX	2	1991	7/7	0.96	0.12	97,97,97,97	0
84	MG	N8	201	1/1	0.96	0.21	37,37,37,37	0
85	OHX	6	2103	7/7	0.96	0.21	131,131,131,131	0
85	OHX	6	2105	7/7	0.96	0.32	115,115,115,115	0
85	OHX	6	2108	7/7	0.96	0.25	102,102,102,102	0
84	MG	5	3420	1/1	0.96	0.54	60,60,60,60	0
85	OHX	2	2008	7/7	0.96	0.14	105,105,105,105	0
85	OHX	6	2112	7/7	0.96	0.27	115,115,115,115	0
85	OHX	6	2115	7/7	0.96	0.18	106,106,106,106	0
84	MG	5	3720	1/1	0.96	0.19	32,32,32,32	0
85	OHX	6	2118	7/7	0.96	0.27	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	6	2121	7/7	0.96	0.33	108,108,108,108	0
85	OHX	2	2015	7/7	0.96	0.15	106,106,106,106	0
84	MG	1	3632	1/1	0.96	0.53	50,50,50,50	0
84	MG	5	3422	1/1	0.96	0.34	37,37,37,37	0
84	MG	6	1940	1/1	0.96	0.24	43,43,43,43	0
84	MG	5	3724	1/1	0.96	0.14	42,42,42,42	0
84	MG	5	3486	1/1	0.96	0.36	48,48,48,48	0
84	MG	5	3726	1/1	0.96	0.13	33,33,33,33	0
85	OHX	6	2136	7/7	0.96	0.37	108,108,108,108	0
85	OHX	2	2057	7/7	0.96	0.16	126,126,126,126	0
85	OHX	6	2141	7/7	0.96	0.35	109,109,109,109	0
85	OHX	2	2058	7/7	0.96	0.11	89,89,89,89	0
85	OHX	2	2059	7/7	0.96	0.23	119,119,119,119	0
85	OHX	2	2060	7/7	0.96	0.25	122,122,122,122	0
84	MG	5	3424	1/1	0.96	0.37	32,32,32,32	0
84	MG	5	3576	1/1	0.96	0.41	34,34,34,34	0
85	OHX	6	2148	7/7	0.96	0.51	114,114,114,114	0
85	OHX	6	2149	7/7	0.96	0.31	132,132,132,132	0
84	MG	5	3488	1/1	0.96	0.32	53,53,53,53	0
85	OHX	6	2151	7/7	0.96	0.33	127,127,127,127	0
85	OHX	6	2152	7/7	0.96	0.29	107,107,107,107	0
85	OHX	6	2153	7/7	0.96	0.36	109,109,109,109	0
85	OHX	2	2070	7/7	0.96	0.24	95,95,95,95	0
85	OHX	2	2073	7/7	0.96	0.20	120,120,120,120	0
84	MG	5	3489	1/1	0.96	0.28	34,34,34,34	0
84	MG	5	3491	1/1	0.96	0.50	42,42,42,42	0
85	OHX	s4	301	7/7	0.96	0.26	110,110,110,110	0
85	OHX	s8	302	7/7	0.96	0.38	132,132,132,132	0
85	OHX	s9	201	7/7	0.96	0.43	96,96,96,96	0
85	OHX	2	2077	7/7	0.96	0.33	110,110,110,110	0
85	OHX	c5	201	7/7	0.96	0.22	128,128,128,128	0
85	OHX	sR	401	7/7	0.96	0.24	132,132,132,132	0
85	OHX	5	3802	7/7	0.96	0.12	70,70,70,70	0
85	OHX	5	3819	7/7	0.96	0.12	78,78,78,78	0
85	OHX	5	3843	7/7	0.96	0.14	91,91,91,91	0
85	OHX	2	2082	7/7	0.96	0.24	114,114,114,114	0
84	MG	1	3486	1/1	0.96	0.45	36,36,36,36	0
84	MG	1	3498	1/1	0.96	0.46	32,32,32,32	0
85	OHX	2	2086	7/7	0.96	0.35	104,104,104,104	0
85	OHX	5	3871	7/7	0.96	0.21	77,77,77,77	0
85	OHX	5	3878	7/7	0.96	0.15	80,80,80,80	0
85	OHX	5	3884	7/7	0.96	0.10	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	6	1992	1/1	0.96	0.66	60,60,60,60	0
85	OHX	5	3895	7/7	0.96	0.30	76,76,76,76	0
84	MG	O4	201	1/1	0.96	0.52	51,51,51,51	0
85	OHX	2	2091	7/7	0.96	0.20	122,122,122,122	0
84	MG	1	3635	1/1	0.96	0.28	41,41,41,41	0
85	OHX	5	3914	7/7	0.96	0.24	93,93,93,93	0
85	OHX	5	3919	7/7	0.96	0.28	97,97,97,97	0
84	MG	1	3475	1/1	0.96	0.45	40,40,40,40	0
85	OHX	5	3937	7/7	0.96	0.29	112,112,112,112	0
85	OHX	2	2094	7/7	0.96	0.26	108,108,108,108	0
85	OHX	2	2096	7/7	0.96	0.30	122,122,122,122	0
85	OHX	2	2097	7/7	0.96	0.25	110,110,110,110	0
85	OHX	5	3945	7/7	0.96	0.17	119,119,119,119	0
85	OHX	5	3955	7/7	0.96	0.23	104,104,104,104	0
85	OHX	5	3959	7/7	0.96	0.34	118,118,118,118	0
84	MG	5	3432	1/1	0.96	0.21	31,31,31,31	0
85	OHX	5	3963	7/7	0.96	0.23	108,108,108,108	0
85	OHX	5	3966	7/7	0.96	0.33	108,108,108,108	0
85	OHX	5	3967	7/7	0.96	0.14	116,116,116,116	0
85	OHX	5	3968	7/7	0.96	0.22	86,86,86,86	0
85	OHX	2	2099	7/7	0.96	0.25	128,128,128,128	0
85	OHX	5	3972	7/7	0.96	0.33	87,87,87,87	0
85	OHX	5	3973	7/7	0.96	0.27	96,96,96,96	0
84	MG	2	1945	1/1	0.96	0.21	63,63,63,63	0
85	OHX	2	2101	7/7	0.96	0.31	129,129,129,129	0
84	MG	5	3661	1/1	0.96	0.23	33,33,33,33	0
85	OHX	5	3982	7/7	0.96	0.30	80,80,80,80	0
85	OHX	2	2103	7/7	0.96	0.27	132,132,132,132	0
85	OHX	5	3984	7/7	0.96	0.31	86,86,86,86	0
85	OHX	5	3986	7/7	0.96	0.35	105,105,105,105	0
85	OHX	2	2104	7/7	0.96	0.37	96,96,96,96	0
84	MG	5	3435	1/1	0.96	0.21	34,34,34,34	0
84	MG	5	3591	1/1	0.96	0.27	33,33,33,33	0
85	OHX	5	3995	7/7	0.96	0.33	80,80,80,80	0
84	MG	6	1997	1/1	0.96	0.20	63,63,63,63	0
84	MG	6	1948	1/1	0.96	0.48	47,47,47,47	0
85	OHX	5	4000	7/7	0.96	0.24	106,106,106,106	0
84	MG	1	3409	1/1	0.96	0.39	40,40,40,40	0
84	MG	5	3506	1/1	0.96	0.63	47,47,47,47	0
85	OHX	5	4007	7/7	0.96	0.32	63,63,63,63	0
84	MG	3	208	1/1	0.96	0.40	65,65,65,65	0
85	OHX	5	4009	7/7	0.96	0.27	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	5	4014	7/7	0.96	0.28	96,96,96,96	0
85	OHX	5	4016	7/7	0.96	0.39	90,90,90,90	0
85	OHX	5	4017	7/7	0.96	0.27	128,128,128,128	0
85	OHX	2	2112	7/7	0.96	0.34	116,116,116,116	0
85	OHX	2	2113	7/7	0.96	0.34	110,110,110,110	0
84	MG	3	209	1/1	0.96	0.17	74,74,74,74	0
85	OHX	5	4023	7/7	0.96	0.32	89,89,89,89	0
84	MG	7	201	1/1	0.96	0.68	49,49,49,49	0
85	OHX	2	2117	7/7	0.96	0.47	128,128,128,128	0
84	MG	1	3702	1/1	0.96	0.44	36,36,36,36	0
85	OHX	5	4032	7/7	0.96	0.33	86,86,86,86	0
84	MG	5	3599	1/1	0.96	0.25	43,43,43,43	0
84	MG	6	1953	1/1	0.96	0.63	43,43,43,43	0
85	OHX	5	4042	7/7	0.96	0.34	100,100,100,100	0
85	OHX	C3	201	7/7	0.96	0.18	115,115,115,115	0
85	OHX	D9	103	7/7	0.96	0.38	108,108,108,108	0
85	OHX	1	3770	7/7	0.96	0.18	74,74,74,74	0
85	OHX	1	3788	7/7	0.96	0.13	86,86,86,86	0
85	OHX	5	4051	7/7	0.96	0.36	100,100,100,100	0
85	OHX	1	3799	7/7	0.96	0.11	88,88,88,88	0
85	OHX	5	4054	7/7	0.96	0.33	87,87,87,87	0
85	OHX	1	3800	7/7	0.96	0.11	88,88,88,88	0
85	OHX	1	3810	7/7	0.96	0.10	99,99,99,99	0
85	OHX	1	3813	7/7	0.96	0.21	77,77,77,77	0
85	OHX	5	4059	7/7	0.96	0.37	74,74,74,74	0
85	OHX	1	3823	7/7	0.96	0.17	73,73,73,73	0
84	MG	5	3512	1/1	0.96	0.14	31,31,31,31	0
85	OHX	5	4063	7/7	0.96	0.28	121,121,121,121	0
85	OHX	5	4064	7/7	0.96	0.37	90,90,90,90	0
85	OHX	1	3828	7/7	0.96	0.10	104,104,104,104	0
85	OHX	1	3835	7/7	0.96	0.18	85,85,85,85	0
85	OHX	5	4070	7/7	0.96	0.29	135,135,135,135	0
85	OHX	1	3855	7/7	0.96	0.35	86,86,86,86	0
85	OHX	7	221	7/7	0.96	0.32	110,110,110,110	0
85	OHX	8	221	7/7	0.96	0.33	92,92,92,92	0
85	OHX	8	223	7/7	0.96	0.33	95,95,95,95	0
85	OHX	l3	408	7/7	0.96	0.35	111,111,111,111	0
85	OHX	1	3856	7/7	0.96	0.15	107,107,107,107	0
84	MG	6	2004	1/1	0.96	0.24	70,70,70,70	0
85	OHX	m0	302	7/7	0.96	0.25	88,88,88,88	0
85	OHX	m1	202	7/7	0.96	0.29	107,107,107,107	0
84	MG	1	3703	1/1	0.96	0.26	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	1	3869	7/7	0.96	0.21	91,91,91,91	0
85	OHX	1	3873	7/7	0.96	0.18	112,112,112,112	0
85	OHX	1	3877	7/7	0.96	0.12	126,126,126,126	0
85	OHX	1	3879	7/7	0.96	0.24	101,101,101,101	0
85	OHX	1	3884	7/7	0.96	0.23	109,109,109,109	0
86	ZN	d9	101	1/1	0.96	0.13	86,86,86,86	0
84	MG	1	3563	1/1	0.96	0.83	54,54,54,54	0
84	MG	6	1907	1/1	0.96	0.42	75,75,75,75	0
85	OHX	1	3897	7/7	0.96	0.16	109,109,109,109	0
85	OHX	1	3837	7/7	0.97	0.19	71,71,71,71	0
85	OHX	1	3840	7/7	0.97	0.15	82,82,82,82	0
84	MG	5	3525	1/1	0.97	0.53	36,36,36,36	0
85	OHX	6	2087	7/7	0.97	0.34	109,109,109,109	0
85	OHX	2	2028	7/7	0.97	0.22	94,94,94,94	0
85	OHX	2	2032	7/7	0.97	0.15	121,121,121,121	0
85	OHX	1	3862	7/7	0.97	0.21	74,74,74,74	0
84	MG	5	3699	1/1	0.97	0.19	42,42,42,42	0
85	OHX	6	2094	7/7	0.97	0.23	96,96,96,96	0
85	OHX	1	3865	7/7	0.97	0.21	93,93,93,93	0
85	OHX	2	2035	7/7	0.97	0.17	95,95,95,95	0
85	OHX	6	2100	7/7	0.97	0.20	96,96,96,96	0
85	OHX	2	2036	7/7	0.97	0.14	103,103,103,103	0
85	OHX	2	2039	7/7	0.97	0.19	133,133,133,133	0
84	MG	1	3507	1/1	0.97	0.41	34,34,34,34	0
85	OHX	6	2106	7/7	0.97	0.30	96,96,96,96	0
85	OHX	6	2107	7/7	0.97	0.26	99,99,99,99	0
85	OHX	1	3881	7/7	0.97	0.29	87,87,87,87	0
85	OHX	2	2045	7/7	0.97	0.23	90,90,90,90	0
85	OHX	1	3887	7/7	0.97	0.14	99,99,99,99	0
85	OHX	2	2047	7/7	0.97	0.22	101,101,101,101	0
85	OHX	6	2113	7/7	0.97	0.35	86,86,86,86	0
85	OHX	2	2049	7/7	0.97	0.23	100,100,100,100	0
85	OHX	1	3890	7/7	0.97	0.23	102,102,102,102	0
85	OHX	6	2117	7/7	0.97	0.25	86,86,86,86	0
85	OHX	1	3892	7/7	0.97	0.25	95,95,95,95	0
85	OHX	6	2119	7/7	0.97	0.24	106,106,106,106	0
85	OHX	6	2120	7/7	0.97	0.24	85,85,85,85	0
84	MG	5	3430	1/1	0.97	0.19	33,33,33,33	0
85	OHX	2	2053	7/7	0.97	0.09	130,130,130,130	0
85	OHX	6	2124	7/7	0.97	0.27	89,89,89,89	0
85	OHX	6	2126	7/7	0.97	0.30	96,96,96,96	0
85	OHX	1	3899	7/7	0.97	0.32	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	1	3903	7/7	0.97	0.24	77,77,77,77	0
85	OHX	6	2129	7/7	0.97	0.25	152,152,152,152	0
85	OHX	6	2130	7/7	0.97	0.42	88,88,88,88	0
85	OHX	2	2054	7/7	0.97	0.20	122,122,122,122	0
85	OHX	1	3906	7/7	0.97	0.30	85,85,85,85	0
85	OHX	2	2055	7/7	0.97	0.31	111,111,111,111	0
85	OHX	1	3910	7/7	0.97	0.24	84,84,84,84	0
85	OHX	1	3912	7/7	0.97	0.25	110,110,110,110	0
84	MG	1	3473	1/1	0.97	0.28	45,45,45,45	0
85	OHX	6	2139	7/7	0.97	0.44	84,84,84,84	0
85	OHX	6	2140	7/7	0.97	0.30	101,101,101,101	0
85	OHX	1	3915	7/7	0.97	0.28	69,69,69,69	0
84	MG	1	3571	1/1	0.97	0.43	35,35,35,35	0
84	MG	5	3433	1/1	0.97	0.34	42,42,42,42	0
84	MG	3	206	1/1	0.97	0.79	59,59,59,59	0
85	OHX	2	2062	7/7	0.97	0.32	106,106,106,106	0
84	MG	1	3509	1/1	0.97	0.32	33,33,33,33	0
85	OHX	6	2147	7/7	0.97	0.37	100,100,100,100	0
84	MG	5	3436	1/1	0.97	0.23	30,30,30,30	0
84	MG	5	3481	1/1	0.97	0.44	35,35,35,35	0
85	OHX	1	3928	7/7	0.97	0.24	95,95,95,95	0
84	MG	1	3675	1/1	0.97	0.31	41,41,41,41	0
85	OHX	2	2071	7/7	0.97	0.28	127,127,127,127	0
84	MG	1	3495	1/1	0.97	0.46	41,41,41,41	0
84	MG	3	220	1/1	0.97	0.42	46,46,46,46	0
85	OHX	1	3933	7/7	0.97	0.17	92,92,92,92	0
85	OHX	6	2156	7/7	0.97	0.37	115,115,115,115	0
85	OHX	1	3934	7/7	0.97	0.33	94,94,94,94	0
84	MG	6	1974	1/1	0.97	0.14	50,50,50,50	0
85	OHX	1	3936	7/7	0.97	0.23	98,98,98,98	0
85	OHX	1	3937	7/7	0.97	0.43	88,88,88,88	0
85	OHX	1	3940	7/7	0.97	0.40	88,88,88,88	0
84	MG	1	3440	1/1	0.97	0.27	48,48,48,48	0
85	OHX	1	3942	7/7	0.97	0.30	88,88,88,88	0
85	OHX	d4	201	7/7	0.97	0.28	115,115,115,115	0
85	OHX	2	2078	7/7	0.97	0.28	105,105,105,105	0
85	OHX	5	3786	7/7	0.97	0.11	75,75,75,75	0
85	OHX	5	3795	7/7	0.97	0.12	104,104,104,104	0
85	OHX	2	2080	7/7	0.97	0.31	112,112,112,112	0
85	OHX	5	3810	7/7	0.97	0.11	87,87,87,87	0
85	OHX	5	3818	7/7	0.97	0.11	90,90,90,90	0
84	MG	2	1930	1/1	0.97	0.52	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	5	3824	7/7	0.97	0.13	82,82,82,82	0
85	OHX	5	3839	7/7	0.97	0.14	84,84,84,84	0
85	OHX	1	3947	7/7	0.97	0.23	85,85,85,85	0
84	MG	1	3529	1/1	0.97	0.48	50,50,50,50	0
85	OHX	5	3850	7/7	0.97	0.12	107,107,107,107	0
85	OHX	5	3852	7/7	0.97	0.18	71,71,71,71	0
84	MG	1	3680	1/1	0.97	0.13	40,40,40,40	0
85	OHX	1	3953	7/7	0.97	0.26	108,108,108,108	0
85	OHX	5	3869	7/7	0.97	0.15	79,79,79,79	0
84	MG	5	3545	1/1	0.97	0.68	30,30,30,30	0
84	MG	5	3490	1/1	0.97	0.60	39,39,39,39	0
85	OHX	5	3873	7/7	0.97	0.20	68,68,68,68	0
85	OHX	5	3874	7/7	0.97	0.16	87,87,87,87	0
85	OHX	1	3962	7/7	0.97	0.20	101,101,101,101	0
85	OHX	5	3879	7/7	0.97	0.16	103,103,103,103	0
85	OHX	5	3880	7/7	0.97	0.22	91,91,91,91	0
84	MG	1	3578	1/1	0.97	0.27	35,35,35,35	0
84	MG	1	3551	1/1	0.97	0.57	37,37,37,37	0
85	OHX	5	3889	7/7	0.97	0.25	72,72,72,72	0
85	OHX	5	3892	7/7	0.97	0.23	80,80,80,80	0
85	OHX	1	3967	7/7	0.97	0.35	94,94,94,94	0
85	OHX	5	3896	7/7	0.97	0.21	77,77,77,77	0
84	MG	6	1944	1/1	0.97	0.60	69,69,69,69	0
85	OHX	5	3901	7/7	0.97	0.19	110,110,110,110	0
85	OHX	5	3903	7/7	0.97	0.11	110,110,110,110	0
85	OHX	5	3904	7/7	0.97	0.20	76,76,76,76	0
85	OHX	5	3905	7/7	0.97	0.26	93,93,93,93	0
85	OHX	1	3970	7/7	0.97	0.31	94,94,94,94	0
85	OHX	1	3971	7/7	0.97	0.41	98,98,98,98	0
85	OHX	5	3911	7/7	0.97	0.27	80,80,80,80	0
85	OHX	5	3913	7/7	0.97	0.21	88,88,88,88	0
85	OHX	1	3972	7/7	0.97	0.31	77,77,77,77	0
85	OHX	1	3973	7/7	0.97	0.40	105,105,105,105	0
85	OHX	5	3922	7/7	0.97	0.16	97,97,97,97	0
85	OHX	5	3926	7/7	0.97	0.18	104,104,104,104	0
85	OHX	5	3930	7/7	0.97	0.37	75,75,75,75	0
84	MG	1	3683	1/1	0.97	0.36	34,34,34,34	0
85	OHX	5	3935	7/7	0.97	0.20	92,92,92,92	0
84	MG	5	3449	1/1	0.97	0.23	34,34,34,34	0
85	OHX	1	3977	7/7	0.97	0.29	98,98,98,98	0
85	OHX	2	2095	7/7	0.97	0.36	96,96,96,96	0
85	OHX	5	3941	7/7	0.97	0.28	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	1	3979	7/7	0.97	0.36	94,94,94,94	0
85	OHX	5	3944	7/7	0.97	0.36	74,74,74,74	0
84	MG	2	1931	1/1	0.97	0.54	65,65,65,65	0
85	OHX	5	3946	7/7	0.97	0.23	100,100,100,100	0
85	OHX	5	3947	7/7	0.97	0.36	79,79,79,79	0
85	OHX	5	3950	7/7	0.97	0.40	101,101,101,101	0
85	OHX	5	3951	7/7	0.97	0.27	92,92,92,92	0
85	OHX	5	3954	7/7	0.97	0.25	82,82,82,82	0
85	OHX	1	3982	7/7	0.97	0.32	107,107,107,107	0
85	OHX	5	3956	7/7	0.97	0.35	76,76,76,76	0
85	OHX	5	3957	7/7	0.97	0.28	84,84,84,84	0
85	OHX	5	3958	7/7	0.97	0.29	98,98,98,98	0
84	MG	1	3413	1/1	0.97	0.46	43,43,43,43	0
85	OHX	5	3960	7/7	0.97	0.32	105,105,105,105	0
85	OHX	1	3984	7/7	0.97	0.26	102,102,102,102	0
85	OHX	1	3985	7/7	0.97	0.41	97,97,97,97	0
85	OHX	1	3986	7/7	0.97	0.19	112,112,112,112	0
84	MG	1	3717	1/1	0.97	0.16	60,60,60,60	0
85	OHX	1	3988	7/7	0.97	0.32	104,104,104,104	0
85	OHX	1	3989	7/7	0.97	0.42	104,104,104,104	0
85	OHX	5	3970	7/7	0.97	0.37	90,90,90,90	0
85	OHX	1	3990	7/7	0.97	0.38	99,99,99,99	0
85	OHX	1	3991	7/7	0.97	0.28	119,119,119,119	0
85	OHX	5	3975	7/7	0.97	0.39	85,85,85,85	0
84	MG	1	3718	1/1	0.97	0.24	78,78,78,78	0
85	OHX	5	3977	7/7	0.97	0.42	70,70,70,70	0
84	MG	5	3454	1/1	0.97	0.40	37,37,37,37	0
85	OHX	1	3994	7/7	0.97	0.32	92,92,92,92	0
85	OHX	1	3995	7/7	0.97	0.12	86,86,86,86	0
85	OHX	1	3996	7/7	0.97	0.31	97,97,97,97	0
84	MG	1	3419	1/1	0.97	0.53	44,44,44,44	0
85	OHX	1	3998	7/7	0.97	0.42	102,102,102,102	0
85	OHX	5	3987	7/7	0.97	0.45	81,81,81,81	0
84	MG	6	1989	1/1	0.97	0.20	74,74,74,74	0
84	MG	2	1980	1/1	0.97	0.12	58,58,58,58	0
84	MG	1	3534	1/1	0.97	0.72	36,36,36,36	0
85	OHX	5	3992	7/7	0.97	0.39	97,97,97,97	0
85	OHX	5	3993	7/7	0.97	0.32	101,101,101,101	0
84	MG	5	3573	1/1	0.97	0.32	37,37,37,37	0
84	MG	n3	201	1/1	0.97	0.55	28,28,28,28	0
85	OHX	1	4008	7/7	0.97	0.19	82,82,82,82	0
85	OHX	5	3998	7/7	0.97	0.44	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	1	4010	7/7	0.97	0.45	104,104,104,104	0
84	MG	1	3636	1/1	0.97	0.27	46,46,46,46	0
85	OHX	5	4002	7/7	0.97	0.33	102,102,102,102	0
85	OHX	5	4003	7/7	0.97	0.25	86,86,86,86	0
85	OHX	5	4004	7/7	0.97	0.29	119,119,119,119	0
84	MG	1	3586	1/1	0.97	0.56	68,68,68,68	0
84	MG	1	3480	1/1	0.97	0.36	36,36,36,36	0
84	MG	5	3630	1/1	0.97	0.15	31,31,31,31	0
84	MG	1	3537	1/1	0.97	0.34	33,33,33,33	0
85	OHX	5	4010	7/7	0.97	0.38	75,75,75,75	0
84	MG	1	3519	1/1	0.97	0.77	38,38,38,38	0
84	MG	1	3695	1/1	0.97	0.28	40,40,40,40	0
85	OHX	1	4019	7/7	0.97	0.36	85,85,85,85	0
85	OHX	1	4020	7/7	0.97	0.39	118,118,118,118	0
85	OHX	1	4021	7/7	0.97	0.31	128,128,128,128	0
84	MG	o4	201	1/1	0.97	0.35	52,52,52,52	0
85	OHX	5	4021	7/7	0.97	0.38	82,82,82,82	0
84	MG	1	4041	1/1	0.97	0.30	41,41,41,41	0
85	OHX	1	4027	7/7	0.97	0.37	103,103,103,103	0
85	OHX	5	4026	7/7	0.97	0.37	105,105,105,105	0
85	OHX	5	4027	7/7	0.97	0.28	92,92,92,92	0
85	OHX	5	4028	7/7	0.97	0.32	86,86,86,86	0
85	OHX	2	2116	7/7	0.97	0.42	109,109,109,109	0
85	OHX	5	4030	7/7	0.97	0.40	89,89,89,89	0
84	MG	6	1960	1/1	0.97	0.26	45,45,45,45	0
84	MG	1	3492	1/1	0.97	0.35	39,39,39,39	0
85	OHX	2	1993	7/7	0.97	0.14	99,99,99,99	0
85	OHX	2	1997	7/7	0.97	0.11	115,115,115,115	0
85	OHX	5	4037	7/7	0.97	0.28	89,89,89,89	0
85	OHX	5	4038	7/7	0.97	0.30	91,91,91,91	0
85	OHX	5	4039	7/7	0.97	0.40	105,105,105,105	0
85	OHX	5	4040	7/7	0.97	0.41	102,102,102,102	0
85	OHX	5	4041	7/7	0.97	0.44	96,96,96,96	0
85	OHX	1	4033	7/7	0.97	0.27	100,100,100,100	0
85	OHX	S8	301	7/7	0.97	0.26	124,124,124,124	0
84	MG	5	3468	1/1	0.97	0.49	51,51,51,51	0
85	OHX	5	4045	7/7	0.97	0.37	99,99,99,99	0
85	OHX	5	4046	7/7	0.97	0.35	75,75,75,75	0
85	OHX	C5	201	7/7	0.97	0.21	127,127,127,127	0
85	OHX	5	4048	7/7	0.97	0.28	104,104,104,104	0
84	MG	1	3591	1/1	0.97	0.15	44,44,44,44	0
85	OHX	SR	401	7/7	0.97	0.13	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	5	4052	7/7	0.97	0.38	94,94,94,94	0
85	OHX	3	215	7/7	0.97	0.18	98,98,98,98	0
85	OHX	1	3765	7/7	0.97	0.11	79,79,79,79	0
85	OHX	2	2005	7/7	0.97	0.13	94,94,94,94	0
85	OHX	1	3778	7/7	0.97	0.12	84,84,84,84	0
85	OHX	5	4057	7/7	0.97	0.34	96,96,96,96	0
85	OHX	4	221	7/7	0.97	0.32	88,88,88,88	0
85	OHX	1	3780	7/7	0.97	0.09	100,100,100,100	0
84	MG	5	3519	1/1	0.97	0.54	34,34,34,34	0
85	OHX	4	227	7/7	0.97	0.39	85,85,85,85	0
85	OHX	1	3795	7/7	0.97	0.13	83,83,83,83	0
84	MG	1	3566	1/1	0.97	0.37	37,37,37,37	0
85	OHX	5	4065	7/7	0.97	0.13	92,92,92,92	0
85	OHX	2	2014	7/7	0.97	0.20	89,89,89,89	0
85	OHX	1	3806	7/7	0.97	0.10	92,92,92,92	0
85	OHX	5	4069	7/7	0.97	0.11	129,129,129,129	0
85	OHX	1	3807	7/7	0.97	0.12	76,76,76,76	0
85	OHX	7	213	7/7	0.97	0.13	79,79,79,79	0
85	OHX	7	218	7/7	0.97	0.30	92,92,92,92	0
85	OHX	7	219	7/7	0.97	0.24	80,80,80,80	0
85	OHX	1	3809	7/7	0.97	0.09	107,107,107,107	0
84	MG	2	1977	1/1	0.97	0.27	75,75,75,75	0
85	OHX	8	212	7/7	0.97	0.10	91,91,91,91	0
85	OHX	8	215	7/7	0.97	0.15	94,94,94,94	0
85	OHX	8	217	7/7	0.97	0.20	101,101,101,101	0
85	OHX	8	218	7/7	0.97	0.29	79,79,79,79	0
85	OHX	8	219	7/7	0.97	0.29	90,90,90,90	0
85	OHX	1	3812	7/7	0.97	0.12	88,88,88,88	0
85	OHX	8	222	7/7	0.97	0.27	114,114,114,114	0
85	OHX	2	2017	7/7	0.97	0.15	89,89,89,89	0
85	OHX	8	224	7/7	0.97	0.45	94,94,94,94	0
85	OHX	l3	407	7/7	0.97	0.28	78,78,78,78	0
85	OHX	1	3820	7/7	0.97	0.14	87,87,87,87	0
85	OHX	l4	401	7/7	0.97	0.26	96,96,96,96	0
85	OHX	l4	402	7/7	0.97	0.52	99,99,99,99	0
85	OHX	l5	301	7/7	0.97	0.17	106,106,106,106	0
85	OHX	6	2036	7/7	0.97	0.10	110,110,110,110	0
85	OHX	l9	202	7/7	0.97	0.23	92,92,92,92	0
85	OHX	6	2037	7/7	0.97	0.09	112,112,112,112	0
85	OHX	1	3822	7/7	0.97	0.11	95,95,95,95	0
85	OHX	6	2048	7/7	0.97	0.08	117,117,117,117	0
85	OHX	m7	204	7/7	0.97	0.40	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	o9	101	7/7	0.97	0.28	87,87,87,87	0
85	OHX	2	2018	7/7	0.97	0.12	106,106,106,106	0
85	OHX	6	2057	7/7	0.97	0.12	108,108,108,108	0
85	OHX	6	2058	7/7	0.97	0.17	99,99,99,99	0
85	OHX	2	2021	7/7	0.97	0.17	99,99,99,99	0
86	ZN	Q2	501	1/1	0.97	0.16	64,64,64,64	0
85	OHX	6	2066	7/7	0.97	0.17	83,83,83,83	0
84	MG	1	3522	1/1	0.97	0.34	32,32,32,32	0
85	OHX	6	2069	7/7	0.97	0.23	86,86,86,86	0
85	OHX	6	2074	7/7	0.97	0.14	106,106,106,106	0
84	MG	5	3524	1/1	0.97	0.66	34,34,34,34	0
85	OHX	6	2079	7/7	0.97	0.23	110,110,110,110	0
85	OHX	2	1990	7/7	0.98	0.09	95,95,95,95	0
85	OHX	6	2122	7/7	0.98	0.37	92,92,92,92	0
84	MG	1	3499	1/1	0.98	0.47	39,39,39,39	0
84	MG	5	3579	1/1	0.98	0.55	32,32,32,32	0
85	OHX	6	2125	7/7	0.98	0.27	87,87,87,87	0
85	OHX	1	3922	7/7	0.98	0.43	92,92,92,92	0
85	OHX	2	1995	7/7	0.98	0.09	91,91,91,91	0
85	OHX	1	3924	7/7	0.98	0.26	76,76,76,76	0
85	OHX	1	3925	7/7	0.98	0.10	116,116,116,116	0
85	OHX	1	3926	7/7	0.98	0.31	81,81,81,81	0
85	OHX	1	3927	7/7	0.98	0.29	92,92,92,92	0
84	MG	1	3540	1/1	0.98	0.45	35,35,35,35	0
85	OHX	2	1998	7/7	0.98	0.10	89,89,89,89	0
85	OHX	6	2134	7/7	0.98	0.29	112,112,112,112	0
85	OHX	2	1999	7/7	0.98	0.10	84,84,84,84	0
84	MG	7	208	1/1	0.98	0.58	43,43,43,43	0
85	OHX	2	2002	7/7	0.98	0.08	84,84,84,84	0
85	OHX	6	2138	7/7	0.98	0.27	77,77,77,77	0
84	MG	5	3504	1/1	0.98	0.45	37,37,37,37	0
84	MG	6	1939	1/1	0.98	0.31	56,56,56,56	0
85	OHX	2	2007	7/7	0.98	0.14	94,94,94,94	0
84	MG	1	3410	1/1	0.98	0.45	35,35,35,35	0
85	OHX	2	2009	7/7	0.98	0.15	95,95,95,95	0
85	OHX	1	3939	7/7	0.98	0.32	94,94,94,94	0
84	MG	1	3555	1/1	0.98	0.16	35,35,35,35	0
85	OHX	2	2013	7/7	0.98	0.21	105,105,105,105	0
84	MG	5	3539	1/1	0.98	0.42	29,29,29,29	0
84	MG	6	1991	1/1	0.98	0.15	50,50,50,50	0
85	OHX	1	3944	7/7	0.98	0.18	100,100,100,100	0
85	OHX	2	2016	7/7	0.98	0.20	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	2	1944	1/1	0.98	0.57	91,91,91,91	0
84	MG	5	3510	1/1	0.98	0.56	36,36,36,36	0
85	OHX	2	2020	7/7	0.98	0.09	103,103,103,103	0
84	MG	1	3557	1/1	0.98	0.70	37,37,37,37	0
85	OHX	1	3952	7/7	0.98	0.23	111,111,111,111	0
85	OHX	2	2022	7/7	0.98	0.12	107,107,107,107	0
85	OHX	1	3954	7/7	0.98	0.37	96,96,96,96	0
85	OHX	2	2023	7/7	0.98	0.22	90,90,90,90	0
85	OHX	1	3956	7/7	0.98	0.36	100,100,100,100	0
85	OHX	1	3959	7/7	0.98	0.28	84,84,84,84	0
85	OHX	2	2024	7/7	0.98	0.20	89,89,89,89	0
85	OHX	1	3961	7/7	0.98	0.23	104,104,104,104	0
84	MG	8	208	1/1	0.98	0.10	63,63,63,63	0
85	OHX	c8	201	7/7	0.98	0.15	117,117,117,117	0
85	OHX	1	3963	7/7	0.98	0.26	88,88,88,88	0
84	MG	1	3558	1/1	0.98	0.32	45,45,45,45	0
85	OHX	5	3770	7/7	0.98	0.13	63,63,63,63	0
85	OHX	5	3773	7/7	0.98	0.11	64,64,64,64	0
85	OHX	5	3775	7/7	0.98	0.11	60,60,60,60	0
85	OHX	5	3784	7/7	0.98	0.12	70,70,70,70	0
85	OHX	1	3965	7/7	0.98	0.20	109,109,109,109	0
85	OHX	5	3787	7/7	0.98	0.10	63,63,63,63	0
85	OHX	5	3788	7/7	0.98	0.08	78,78,78,78	0
84	MG	1	3716	1/1	0.98	0.10	33,33,33,33	0
85	OHX	5	3796	7/7	0.98	0.09	89,89,89,89	0
85	OHX	5	3799	7/7	0.98	0.16	82,82,82,82	0
85	OHX	5	3800	7/7	0.98	0.09	78,78,78,78	0
84	MG	5	3546	1/1	0.98	0.67	39,39,39,39	0
85	OHX	5	3803	7/7	0.98	0.10	63,63,63,63	0
85	OHX	5	3804	7/7	0.98	0.11	63,63,63,63	0
85	OHX	5	3806	7/7	0.98	0.08	74,74,74,74	0
85	OHX	5	3807	7/7	0.98	0.10	74,74,74,74	0
85	OHX	5	3809	7/7	0.98	0.13	88,88,88,88	0
85	OHX	1	3968	7/7	0.98	0.28	86,86,86,86	0
85	OHX	5	3816	7/7	0.98	0.13	66,66,66,66	0
85	OHX	5	3817	7/7	0.98	0.12	67,67,67,67	0
85	OHX	2	2029	7/7	0.98	0.12	108,108,108,108	0
85	OHX	2	2030	7/7	0.98	0.20	103,103,103,103	0
85	OHX	5	3820	7/7	0.98	0.12	81,81,81,81	0
85	OHX	5	3821	7/7	0.98	0.10	74,74,74,74	0
85	OHX	5	3823	7/7	0.98	0.13	76,76,76,76	0
84	MG	1	3463	1/1	0.98	0.47	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	5	3827	7/7	0.98	0.20	76,76,76,76	0
85	OHX	5	3831	7/7	0.98	0.11	77,77,77,77	0
85	OHX	5	3834	7/7	0.98	0.14	79,79,79,79	0
85	OHX	5	3836	7/7	0.98	0.15	81,81,81,81	0
85	OHX	5	3837	7/7	0.98	0.26	72,72,72,72	0
85	OHX	C8	201	7/7	0.98	0.08	97,97,97,97	0
85	OHX	5	3840	7/7	0.98	0.20	73,73,73,73	0
85	OHX	2	2033	7/7	0.98	0.27	94,94,94,94	0
85	OHX	5	3845	7/7	0.98	0.11	87,87,87,87	0
85	OHX	5	3846	7/7	0.98	0.22	58,58,58,58	0
84	MG	1	3625	1/1	0.98	0.40	63,63,63,63	0
85	OHX	1	3975	7/7	0.98	0.34	85,85,85,85	0
85	OHX	1	3751	7/7	0.98	0.13	67,67,67,67	0
85	OHX	5	3853	7/7	0.98	0.10	83,83,83,83	0
85	OHX	5	3854	7/7	0.98	0.21	80,80,80,80	0
85	OHX	5	3855	7/7	0.98	0.23	83,83,83,83	0
85	OHX	5	3856	7/7	0.98	0.07	120,120,120,120	0
85	OHX	5	3857	7/7	0.98	0.20	71,71,71,71	0
85	OHX	5	3859	7/7	0.98	0.17	81,81,81,81	0
85	OHX	1	3755	7/7	0.98	0.12	67,67,67,67	0
85	OHX	1	3756	7/7	0.98	0.12	68,68,68,68	0
85	OHX	5	3866	7/7	0.98	0.19	87,87,87,87	0
85	OHX	5	3867	7/7	0.98	0.21	85,85,85,85	0
85	OHX	1	3757	7/7	0.98	0.11	70,70,70,70	0
85	OHX	1	3980	7/7	0.98	0.37	83,83,83,83	0
85	OHX	1	3764	7/7	0.98	0.15	64,64,64,64	0
85	OHX	5	3872	7/7	0.98	0.18	65,65,65,65	0
84	MG	1	3451	1/1	0.98	0.37	47,47,47,47	0
84	MG	1	3513	1/1	0.98	0.95	38,38,38,38	0
85	OHX	5	3875	7/7	0.98	0.10	112,112,112,112	0
85	OHX	5	3876	7/7	0.98	0.29	76,76,76,76	0
85	OHX	5	3877	7/7	0.98	0.19	80,80,80,80	0
85	OHX	1	3771	7/7	0.98	0.09	76,76,76,76	0
85	OHX	1	3773	7/7	0.98	0.08	73,73,73,73	0
85	OHX	1	3776	7/7	0.98	0.13	69,69,69,69	0
85	OHX	5	3883	7/7	0.98	0.19	91,91,91,91	0
85	OHX	1	3777	7/7	0.98	0.07	84,84,84,84	0
85	OHX	5	3885	7/7	0.98	0.26	92,92,92,92	0
85	OHX	2	2037	7/7	0.98	0.22	106,106,106,106	0
85	OHX	5	3887	7/7	0.98	0.23	72,72,72,72	0
84	MG	5	3552	1/1	0.98	0.57	36,36,36,36	0
85	OHX	5	3890	7/7	0.98	0.20	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	5	3891	7/7	0.98	0.22	84,84,84,84	0
85	OHX	1	3781	7/7	0.98	0.12	78,78,78,78	0
85	OHX	5	3893	7/7	0.98	0.15	111,111,111,111	0
85	OHX	5	3894	7/7	0.98	0.40	80,80,80,80	0
85	OHX	1	3783	7/7	0.98	0.11	70,70,70,70	0
85	OHX	1	3784	7/7	0.98	0.10	77,77,77,77	0
84	MG	6	1925	1/1	0.98	0.38	72,72,72,72	0
85	OHX	5	3899	7/7	0.98	0.25	80,80,80,80	0
85	OHX	5	3900	7/7	0.98	0.24	103,103,103,103	0
85	OHX	1	3789	7/7	0.98	0.10	88,88,88,88	0
85	OHX	5	3902	7/7	0.98	0.27	87,87,87,87	0
85	OHX	1	3791	7/7	0.98	0.11	73,73,73,73	0
85	OHX	1	3792	7/7	0.98	0.11	80,80,80,80	0
85	OHX	2	2041	7/7	0.98	0.10	119,119,119,119	0
85	OHX	1	3797	7/7	0.98	0.10	76,76,76,76	0
85	OHX	5	3907	7/7	0.98	0.17	116,116,116,116	0
85	OHX	5	3908	7/7	0.98	0.23	84,84,84,84	0
85	OHX	1	3999	7/7	0.98	0.25	82,82,82,82	0
85	OHX	5	3910	7/7	0.98	0.12	95,95,95,95	0
85	OHX	2	2042	7/7	0.98	0.15	110,110,110,110	0
85	OHX	5	3912	7/7	0.98	0.30	108,108,108,108	0
85	OHX	1	4001	7/7	0.98	0.25	108,108,108,108	0
85	OHX	2	2044	7/7	0.98	0.22	113,113,113,113	0
85	OHX	5	3915	7/7	0.98	0.25	91,91,91,91	0
85	OHX	5	3916	7/7	0.98	0.32	85,85,85,85	0
85	OHX	5	3917	7/7	0.98	0.23	86,86,86,86	0
85	OHX	5	3918	7/7	0.98	0.33	84,84,84,84	0
85	OHX	1	3804	7/7	0.98	0.10	88,88,88,88	0
85	OHX	1	4004	7/7	0.98	0.35	85,85,85,85	0
85	OHX	5	3923	7/7	0.98	0.20	85,85,85,85	0
85	OHX	5	3924	7/7	0.98	0.28	77,77,77,77	0
85	OHX	5	3925	7/7	0.98	0.22	81,81,81,81	0
85	OHX	1	3805	7/7	0.98	0.10	72,72,72,72	0
85	OHX	5	3927	7/7	0.98	0.23	87,87,87,87	0
85	OHX	5	3928	7/7	0.98	0.22	91,91,91,91	0
84	MG	5	3683	1/1	0.98	0.11	46,46,46,46	0
85	OHX	5	3931	7/7	0.98	0.18	68,68,68,68	0
85	OHX	2	2046	7/7	0.98	0.16	105,105,105,105	0
85	OHX	5	3933	7/7	0.98	0.30	77,77,77,77	0
85	OHX	5	3934	7/7	0.98	0.26	91,91,91,91	0
84	MG	5	3554	1/1	0.98	0.42	29,29,29,29	0
85	OHX	5	3936	7/7	0.98	0.23	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	1	4011	7/7	0.98	0.32	100,100,100,100	0
85	OHX	2	2048	7/7	0.98	0.24	87,87,87,87	0
85	OHX	5	3939	7/7	0.98	0.26	83,83,83,83	0
84	MG	1	3628	1/1	0.98	0.72	50,50,50,50	0
85	OHX	2	2050	7/7	0.98	0.36	102,102,102,102	0
85	OHX	5	3942	7/7	0.98	0.25	98,98,98,98	0
85	OHX	1	3814	7/7	0.98	0.14	71,71,71,71	0
85	OHX	1	3816	7/7	0.98	0.12	84,84,84,84	0
85	OHX	1	3817	7/7	0.98	0.16	75,75,75,75	0
85	OHX	1	3819	7/7	0.98	0.09	90,90,90,90	0
85	OHX	2	2051	7/7	0.98	0.32	93,93,93,93	0
85	OHX	5	3948	7/7	0.98	0.31	92,92,92,92	0
84	MG	5	3556	1/1	0.98	0.41	36,36,36,36	0
84	MG	5	3557	1/1	0.98	0.68	42,42,42,42	0
85	OHX	5	3952	7/7	0.98	0.33	77,77,77,77	0
85	OHX	1	4022	7/7	0.98	0.41	77,77,77,77	0
84	MG	1	3579	1/1	0.98	0.42	40,40,40,40	0
85	OHX	1	3827	7/7	0.98	0.20	72,72,72,72	0
85	OHX	1	4025	7/7	0.98	0.44	101,101,101,101	0
85	OHX	1	4026	7/7	0.98	0.39	90,90,90,90	0
84	MG	6	1905	1/1	0.98	0.83	61,61,61,61	0
85	OHX	1	3829	7/7	0.98	0.15	82,82,82,82	0
85	OHX	1	3831	7/7	0.98	0.18	86,86,86,86	0
85	OHX	5	3962	7/7	0.98	0.23	111,111,111,111	0
85	OHX	1	3833	7/7	0.98	0.20	78,78,78,78	0
85	OHX	5	3964	7/7	0.98	0.34	106,106,106,106	0
85	OHX	1	3834	7/7	0.98	0.09	99,99,99,99	0
85	OHX	2	2056	7/7	0.98	0.09	127,127,127,127	0
85	OHX	1	3836	7/7	0.98	0.21	83,83,83,83	0
84	MG	5	3561	1/1	0.98	0.93	48,48,48,48	0
84	MG	5	3691	1/1	0.98	0.12	43,43,43,43	0
85	OHX	5	3971	7/7	0.98	0.23	94,94,94,94	0
85	OHX	1	3842	7/7	0.98	0.14	96,96,96,96	0
85	OHX	1	3843	7/7	0.98	0.23	79,79,79,79	0
85	OHX	5	3974	7/7	0.98	0.36	89,89,89,89	0
85	OHX	1	3844	7/7	0.98	0.19	71,71,71,71	0
85	OHX	3	210	7/7	0.98	0.09	77,77,77,77	0
85	OHX	3	212	7/7	0.98	0.11	81,81,81,81	0
85	OHX	3	213	7/7	0.98	0.18	97,97,97,97	0
85	OHX	5	3979	7/7	0.98	0.28	85,85,85,85	0
85	OHX	3	214	7/7	0.98	0.18	95,95,95,95	0
85	OHX	5	3981	7/7	0.98	0.28	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	1	3845	7/7	0.98	0.25	77,77,77,77	0
85	OHX	1	3846	7/7	0.98	0.19	97,97,97,97	0
85	OHX	3	217	7/7	0.98	0.31	85,85,85,85	0
85	OHX	5	3985	7/7	0.98	0.39	97,97,97,97	0
85	OHX	1	3847	7/7	0.98	0.21	91,91,91,91	0
85	OHX	1	3849	7/7	0.98	0.20	80,80,80,80	0
85	OHX	4	218	7/7	0.98	0.18	77,77,77,77	0
85	OHX	4	219	7/7	0.98	0.10	93,93,93,93	0
85	OHX	4	220	7/7	0.98	0.17	96,96,96,96	0
85	OHX	5	3991	7/7	0.98	0.23	87,87,87,87	0
85	OHX	1	3852	7/7	0.98	0.14	110,110,110,110	0
85	OHX	4	222	7/7	0.98	0.26	83,83,83,83	0
85	OHX	5	3994	7/7	0.98	0.30	97,97,97,97	0
85	OHX	1	3853	7/7	0.98	0.14	93,93,93,93	0
85	OHX	4	224	7/7	0.98	0.27	82,82,82,82	0
84	MG	2	1917	1/1	0.98	0.52	62,62,62,62	0
85	OHX	4	226	7/7	0.98	0.22	106,106,106,106	0
84	MG	5	3523	1/1	0.98	0.33	27,27,27,27	0
85	OHX	1	3857	7/7	0.98	0.21	79,79,79,79	0
85	OHX	2	2061	7/7	0.98	0.25	115,115,115,115	0
85	OHX	1	3859	7/7	0.98	0.16	119,119,119,119	0
85	OHX	1	3860	7/7	0.98	0.27	82,82,82,82	0
85	OHX	L3	403	7/7	0.98	0.22	86,86,86,86	0
85	OHX	5	4006	7/7	0.98	0.37	89,89,89,89	0
84	MG	1	3505	1/1	0.98	0.29	38,38,38,38	0
85	OHX	1	3863	7/7	0.98	0.16	95,95,95,95	0
85	OHX	M5	302	7/7	0.98	0.22	88,88,88,88	0
85	OHX	M7	205	7/7	0.98	0.30	101,101,101,101	0
85	OHX	5	4012	7/7	0.98	0.27	89,89,89,89	0
85	OHX	5	4013	7/7	0.98	0.41	96,96,96,96	0
84	MG	5	3565	1/1	0.98	0.54	49,49,49,49	0
85	OHX	5	4015	7/7	0.98	0.29	98,98,98,98	0
85	OHX	2	2064	7/7	0.98	0.20	92,92,92,92	0
85	OHX	O3	202	7/7	0.98	0.33	85,85,85,85	0
85	OHX	O7	104	7/7	0.98	0.09	77,77,77,77	0
85	OHX	O7	105	7/7	0.98	0.19	76,76,76,76	0
85	OHX	1	3866	7/7	0.98	0.26	91,91,91,91	0
85	OHX	6	2017	7/7	0.98	0.09	85,85,85,85	0
85	OHX	5	4022	7/7	0.98	0.38	94,94,94,94	0
85	OHX	1	3867	7/7	0.98	0.20	75,75,75,75	0
85	OHX	6	2028	7/7	0.98	0.09	89,89,89,89	0
85	OHX	5	4025	7/7	0.98	0.37	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	6	2029	7/7	0.98	0.08	110,110,110,110	0
85	OHX	6	2032	7/7	0.98	0.09	87,87,87,87	0
85	OHX	6	2033	7/7	0.98	0.13	74,74,74,74	0
85	OHX	1	3868	7/7	0.98	0.23	83,83,83,83	0
85	OHX	2	2065	7/7	0.98	0.21	104,104,104,104	0
85	OHX	6	2039	7/7	0.98	0.11	83,83,83,83	0
85	OHX	1	3870	7/7	0.98	0.22	97,97,97,97	0
85	OHX	6	2041	7/7	0.98	0.12	74,74,74,74	0
85	OHX	6	2042	7/7	0.98	0.13	100,100,100,100	0
85	OHX	5	4035	7/7	0.98	0.18	63,63,63,63	0
85	OHX	5	4036	7/7	0.98	0.22	82,82,82,82	0
85	OHX	6	2043	7/7	0.98	0.19	77,77,77,77	0
85	OHX	6	2046	7/7	0.98	0.10	95,95,95,95	0
85	OHX	6	2047	7/7	0.98	0.12	91,91,91,91	0
85	OHX	1	3872	7/7	0.98	0.18	98,98,98,98	0
85	OHX	6	2049	7/7	0.98	0.14	85,85,85,85	0
85	OHX	6	2051	7/7	0.98	0.12	93,93,93,93	0
85	OHX	6	2053	7/7	0.98	0.15	84,84,84,84	0
85	OHX	2	2066	7/7	0.98	0.20	93,93,93,93	0
85	OHX	6	2055	7/7	0.98	0.10	95,95,95,95	0
85	OHX	6	2056	7/7	0.98	0.13	82,82,82,82	0
85	OHX	1	3875	7/7	0.98	0.21	100,100,100,100	0
84	MG	1	3686	1/1	0.98	0.11	37,37,37,37	0
85	OHX	5	4049	7/7	0.98	0.33	85,85,85,85	0
85	OHX	6	2059	7/7	0.98	0.10	106,106,106,106	0
85	OHX	6	2060	7/7	0.98	0.12	138,138,138,138	0
85	OHX	6	2061	7/7	0.98	0.18	98,98,98,98	0
84	MG	5	3568	1/1	0.98	0.56	35,35,35,35	0
85	OHX	6	2063	7/7	0.98	0.11	134,134,134,134	0
85	OHX	6	2064	7/7	0.98	0.07	141,141,141,141	0
85	OHX	6	2065	7/7	0.98	0.11	94,94,94,94	0
85	OHX	1	3880	7/7	0.98	0.23	89,89,89,89	0
85	OHX	6	2067	7/7	0.98	0.16	98,98,98,98	0
84	MG	5	3569	1/1	0.98	0.63	29,29,29,29	0
85	OHX	5	4060	7/7	0.98	0.30	125,125,125,125	0
85	OHX	1	3882	7/7	0.98	0.19	90,90,90,90	0
85	OHX	6	2070	7/7	0.98	0.28	98,98,98,98	0
85	OHX	6	2071	7/7	0.98	0.17	79,79,79,79	0
85	OHX	6	2072	7/7	0.98	0.23	92,92,92,92	0
84	MG	1	3453	1/1	0.98	0.39	33,33,33,33	0
85	OHX	6	2075	7/7	0.98	0.24	96,96,96,96	0
85	OHX	1	3886	7/7	0.98	0.22	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	2	2072	7/7	0.98	0.29	106,106,106,106	0
84	MG	5	4074	1/1	0.98	0.41	32,32,32,32	0
85	OHX	7	211	7/7	0.98	0.09	74,74,74,74	0
85	OHX	7	212	7/7	0.98	0.14	70,70,70,70	0
85	OHX	2	2074	7/7	0.98	0.24	101,101,101,101	0
85	OHX	7	214	7/7	0.98	0.15	71,71,71,71	0
85	OHX	7	217	7/7	0.98	0.15	95,95,95,95	0
85	OHX	6	2083	7/7	0.98	0.19	116,116,116,116	0
84	MG	5	3497	1/1	0.98	0.56	30,30,30,30	0
85	OHX	6	2085	7/7	0.98	0.24	78,78,78,78	0
85	OHX	6	2086	7/7	0.98	0.32	103,103,103,103	0
85	OHX	1	3891	7/7	0.98	0.22	81,81,81,81	0
85	OHX	8	213	7/7	0.98	0.18	83,83,83,83	0
85	OHX	8	214	7/7	0.98	0.13	102,102,102,102	0
84	MG	5	3528	1/1	0.98	0.26	36,36,36,36	0
85	OHX	8	216	7/7	0.98	0.31	86,86,86,86	0
85	OHX	1	3894	7/7	0.98	0.14	114,114,114,114	0
85	OHX	6	2090	7/7	0.98	0.23	115,115,115,115	0
85	OHX	1	3895	7/7	0.98	0.22	70,70,70,70	0
85	OHX	8	220	7/7	0.98	0.17	120,120,120,120	0
85	OHX	6	2092	7/7	0.98	0.17	96,96,96,96	0
85	OHX	1	3896	7/7	0.98	0.22	88,88,88,88	0
84	MG	1	3454	1/1	0.98	0.39	34,34,34,34	0
84	MG	6	1983	1/1	0.98	0.19	73,73,73,73	0
85	OHX	8	225	7/7	0.98	0.37	101,101,101,101	0
85	OHX	6	2096	7/7	0.98	0.21	100,100,100,100	0
85	OHX	6	2097	7/7	0.98	0.19	103,103,103,103	0
85	OHX	2	2079	7/7	0.98	0.23	115,115,115,115	0
85	OHX	1	3900	7/7	0.98	0.25	83,83,83,83	0
85	OHX	1	3901	7/7	0.98	0.19	106,106,106,106	0
85	OHX	6	2102	7/7	0.98	0.27	104,104,104,104	0
85	OHX	1	3902	7/7	0.98	0.26	88,88,88,88	0
85	OHX	6	2104	7/7	0.98	0.30	103,103,103,103	0
84	MG	6	1935	1/1	0.98	0.47	44,44,44,44	0
85	OHX	2	2081	7/7	0.98	0.28	109,109,109,109	0
85	OHX	m5	304	7/7	0.98	0.11	74,74,74,74	0
85	OHX	m5	305	7/7	0.98	0.18	94,94,94,94	0
84	MG	1	3550	1/1	0.98	0.26	40,40,40,40	0
85	OHX	n3	203	7/7	0.98	0.21	76,76,76,76	0
85	OHX	o7	502	7/7	0.98	0.13	79,79,79,79	0
85	OHX	1	3907	7/7	0.98	0.21	96,96,96,96	0
85	OHX	q2	502	7/7	0.98	0.16	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	2	2083	7/7	0.98	0.30	115,115,115,115	0
84	MG	7	203	1/1	0.98	0.38	58,58,58,58	0
86	ZN	D9	101	1/1	0.98	0.12	79,79,79,79	0
85	OHX	1	3911	7/7	0.98	0.23	103,103,103,103	0
84	MG	5	3706	1/1	0.98	0.23	37,37,37,37	0
85	OHX	6	2114	7/7	0.98	0.26	114,114,114,114	0
86	ZN	Q3	501	1/1	0.98	0.06	58,58,58,58	0
85	OHX	1	3913	7/7	0.98	0.27	70,70,70,70	0
85	OHX	2	1985	7/7	0.98	0.16	84,84,84,84	0
85	OHX	2	2087	7/7	0.98	0.26	119,119,119,119	0
85	OHX	2	2088	7/7	0.98	0.19	94,94,94,94	0
86	ZN	q0	201	1/1	0.98	0.10	36,36,36,36	0
85	OHX	2	1988	7/7	0.98	0.17	90,90,90,90	0
85	OHX	2	1989	7/7	0.98	0.08	92,92,92,92	0
85	OHX	1	3736	7/7	0.99	0.11	63,63,63,63	0
85	OHX	1	3821	7/7	0.99	0.15	77,77,77,77	0
85	OHX	6	2099	7/7	0.99	0.30	95,95,95,95	0
85	OHX	1	3738	7/7	0.99	0.08	56,56,56,56	0
85	OHX	1	3739	7/7	0.99	0.07	62,62,62,62	0
85	OHX	1	3824	7/7	0.99	0.09	56,56,56,56	0
85	OHX	1	3825	7/7	0.99	0.15	83,83,83,83	0
85	OHX	1	3740	7/7	0.99	0.13	60,60,60,60	0
85	OHX	1	3741	7/7	0.99	0.09	55,55,55,55	0
85	OHX	1	3742	7/7	0.99	0.11	65,65,65,65	0
85	OHX	1	3743	7/7	0.99	0.12	60,60,60,60	0
85	OHX	1	3830	7/7	0.99	0.11	86,86,86,86	0
85	OHX	1	3746	7/7	0.99	0.10	65,65,65,65	0
85	OHX	1	3832	7/7	0.99	0.19	75,75,75,75	0
85	OHX	6	2111	7/7	0.99	0.21	84,84,84,84	0
85	OHX	1	3747	7/7	0.99	0.14	64,64,64,64	0
85	OHX	1	3748	7/7	0.99	0.10	72,72,72,72	0
85	OHX	3	211	7/7	0.99	0.20	85,85,85,85	0
85	OHX	1	3749	7/7	0.99	0.11	67,67,67,67	0
85	OHX	1	3750	7/7	0.99	0.12	76,76,76,76	0
85	OHX	2	2038	7/7	0.99	0.24	93,93,93,93	0
85	OHX	5	3920	7/7	0.99	0.12	73,73,73,73	0
85	OHX	5	3921	7/7	0.99	0.24	95,95,95,95	0
85	OHX	1	3838	7/7	0.99	0.25	68,68,68,68	0
85	OHX	1	3938	7/7	0.99	0.24	92,92,92,92	0
85	OHX	1	3839	7/7	0.99	0.18	80,80,80,80	0
85	OHX	1	3753	7/7	0.99	0.09	67,67,67,67	0
85	OHX	1	3841	7/7	0.99	0.17	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	4	215	7/7	0.99	0.10	54,54,54,54	0
85	OHX	4	216	7/7	0.99	0.09	58,58,58,58	0
85	OHX	5	3929	7/7	0.99	0.18	76,76,76,76	0
85	OHX	4	217	7/7	0.99	0.08	68,68,68,68	0
85	OHX	2	2011	7/7	0.99	0.16	98,98,98,98	0
85	OHX	2	2069	7/7	0.99	0.15	112,112,112,112	0
85	OHX	2	1987	7/7	0.99	0.10	74,74,74,74	0
85	OHX	1	3758	7/7	0.99	0.05	67,67,67,67	0
85	OHX	1	3759	7/7	0.99	0.11	79,79,79,79	0
85	OHX	1	3760	7/7	0.99	0.09	68,68,68,68	0
85	OHX	1	3948	7/7	0.99	0.18	70,70,70,70	0
85	OHX	1	3848	7/7	0.99	0.15	90,90,90,90	0
85	OHX	1	3762	7/7	0.99	0.07	66,66,66,66	0
85	OHX	1	3951	7/7	0.99	0.29	81,81,81,81	0
85	OHX	1	3850	7/7	0.99	0.24	83,83,83,83	0
85	OHX	1	3851	7/7	0.99	0.23	82,82,82,82	0
85	OHX	1	3763	7/7	0.99	0.09	68,68,68,68	0
84	MG	1	3535	1/1	0.99	0.37	43,43,43,43	0
85	OHX	L3	402	7/7	0.99	0.27	86,86,86,86	0
85	OHX	1	3854	7/7	0.99	0.17	74,74,74,74	0
85	OHX	1	3957	7/7	0.99	0.32	111,111,111,111	0
85	OHX	1	3958	7/7	0.99	0.34	84,84,84,84	0
85	OHX	5	3949	7/7	0.99	0.18	63,63,63,63	0
84	MG	1	3562	1/1	0.99	0.56	48,48,48,48	0
85	OHX	M6	202	7/7	0.99	0.18	80,80,80,80	0
85	OHX	1	3766	7/7	0.99	0.08	76,76,76,76	0
85	OHX	5	3953	7/7	0.99	0.20	81,81,81,81	0
85	OHX	1	3767	7/7	0.99	0.12	69,69,69,69	0
85	OHX	N1	201	7/7	0.99	0.08	59,59,59,59	0
85	OHX	1	3768	7/7	0.99	0.06	83,83,83,83	0
85	OHX	N9	101	7/7	0.99	0.11	56,56,56,56	0
85	OHX	1	3769	7/7	0.99	0.07	63,63,63,63	0
85	OHX	2	2043	7/7	0.99	0.19	89,89,89,89	0
85	OHX	1	3861	7/7	0.99	0.14	67,67,67,67	0
84	MG	5	3560	1/1	0.99	0.47	35,35,35,35	0
85	OHX	Q2	503	7/7	0.99	0.20	59,59,59,59	0
85	OHX	6	2010	7/7	0.99	0.18	73,73,73,73	0
85	OHX	6	2011	7/7	0.99	0.09	61,61,61,61	0
85	OHX	5	3965	7/7	0.99	0.29	88,88,88,88	0
85	OHX	6	2012	7/7	0.99	0.10	67,67,67,67	0
85	OHX	6	2013	7/7	0.99	0.12	70,70,70,70	0
85	OHX	6	2015	7/7	0.99	0.11	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	6	2016	7/7	0.99	0.14	71,71,71,71	0
85	OHX	1	3772	7/7	0.99	0.06	74,74,74,74	0
85	OHX	6	2018	7/7	0.99	0.10	60,60,60,60	0
85	OHX	6	2019	7/7	0.99	0.13	77,77,77,77	0
85	OHX	6	2020	7/7	0.99	0.09	69,69,69,69	0
85	OHX	6	2021	7/7	0.99	0.09	74,74,74,74	0
85	OHX	5	3742	7/7	0.99	0.18	46,46,46,46	0
85	OHX	5	3746	7/7	0.99	0.16	54,54,54,54	0
85	OHX	5	3747	7/7	0.99	0.12	53,53,53,53	0
85	OHX	5	3748	7/7	0.99	0.10	55,55,55,55	0
85	OHX	5	3749	7/7	0.99	0.13	52,52,52,52	0
85	OHX	5	3750	7/7	0.99	0.11	54,54,54,54	0
85	OHX	5	3751	7/7	0.99	0.12	52,52,52,52	0
85	OHX	5	3753	7/7	0.99	0.16	68,68,68,68	0
85	OHX	5	3754	7/7	0.99	0.09	50,50,50,50	0
85	OHX	5	3755	7/7	0.99	0.09	50,50,50,50	0
85	OHX	5	3758	7/7	0.99	0.11	55,55,55,55	0
85	OHX	5	3759	7/7	0.99	0.08	62,62,62,62	0
85	OHX	5	3760	7/7	0.99	0.09	56,56,56,56	0
85	OHX	5	3761	7/7	0.99	0.08	55,55,55,55	0
85	OHX	5	3762	7/7	0.99	0.10	63,63,63,63	0
85	OHX	5	3764	7/7	0.99	0.06	57,57,57,57	0
85	OHX	5	3765	7/7	0.99	0.10	59,59,59,59	0
85	OHX	5	3767	7/7	0.99	0.11	63,63,63,63	0
85	OHX	5	3768	7/7	0.99	0.06	58,58,58,58	0
85	OHX	6	2022	7/7	0.99	0.09	87,87,87,87	0
85	OHX	5	3771	7/7	0.99	0.04	66,66,66,66	0
85	OHX	5	3772	7/7	0.99	0.05	61,61,61,61	0
85	OHX	6	2023	7/7	0.99	0.06	71,71,71,71	0
85	OHX	6	2024	7/7	0.99	0.07	71,71,71,71	0
85	OHX	5	3999	7/7	0.99	0.28	76,76,76,76	0
85	OHX	5	3776	7/7	0.99	0.10	86,86,86,86	0
85	OHX	5	3777	7/7	0.99	0.07	59,59,59,59	0
85	OHX	5	3778	7/7	0.99	0.06	64,64,64,64	0
85	OHX	5	3779	7/7	0.99	0.06	65,65,65,65	0
85	OHX	5	3780	7/7	0.99	0.05	59,59,59,59	0
85	OHX	5	3781	7/7	0.99	0.09	65,65,65,65	0
85	OHX	5	3782	7/7	0.99	0.10	76,76,76,76	0
85	OHX	5	3783	7/7	0.99	0.06	77,77,77,77	0
85	OHX	6	2025	7/7	0.99	0.09	73,73,73,73	0
85	OHX	5	3785	7/7	0.99	0.07	68,68,68,68	0
85	OHX	6	2026	7/7	0.99	0.07	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	5	4011	7/7	0.99	0.20	63,63,63,63	0
84	MG	6	1914	1/1	0.99	0.46	41,41,41,41	0
85	OHX	1	3774	7/7	0.99	0.06	74,74,74,74	0
85	OHX	5	3789	7/7	0.99	0.06	59,59,59,59	0
85	OHX	5	3790	7/7	0.99	0.08	58,58,58,58	0
85	OHX	5	3791	7/7	0.99	0.07	73,73,73,73	0
85	OHX	5	3792	7/7	0.99	0.06	81,81,81,81	0
85	OHX	5	3793	7/7	0.99	0.07	87,87,87,87	0
85	OHX	5	3794	7/7	0.99	0.08	69,69,69,69	0
85	OHX	1	3775	7/7	0.99	0.10	83,83,83,83	0
85	OHX	6	2030	7/7	0.99	0.19	74,74,74,74	0
85	OHX	5	3797	7/7	0.99	0.13	57,57,57,57	0
85	OHX	5	3798	7/7	0.99	0.08	80,80,80,80	0
85	OHX	6	2031	7/7	0.99	0.13	76,76,76,76	0
85	OHX	2	1992	7/7	0.99	0.10	89,89,89,89	0
85	OHX	5	3801	7/7	0.99	0.09	69,69,69,69	0
84	MG	6	1931	1/1	0.99	0.29	48,48,48,48	0
85	OHX	6	2034	7/7	0.99	0.07	91,91,91,91	0
85	OHX	6	2035	7/7	0.99	0.19	71,71,71,71	0
85	OHX	5	3805	7/7	0.99	0.09	73,73,73,73	0
85	OHX	2	2019	7/7	0.99	0.18	87,87,87,87	0
85	OHX	1	3779	7/7	0.99	0.08	71,71,71,71	0
85	OHX	5	3808	7/7	0.99	0.09	67,67,67,67	0
85	OHX	6	2038	7/7	0.99	0.11	71,71,71,71	0
85	OHX	1	3871	7/7	0.99	0.22	100,100,100,100	0
85	OHX	5	3811	7/7	0.99	0.11	73,73,73,73	0
85	OHX	5	3812	7/7	0.99	0.08	74,74,74,74	0
85	OHX	5	3813	7/7	0.99	0.09	81,81,81,81	0
85	OHX	5	3814	7/7	0.99	0.07	84,84,84,84	0
85	OHX	5	3815	7/7	0.99	0.11	68,68,68,68	0
85	OHX	2	1994	7/7	0.99	0.11	99,99,99,99	0
84	MG	1	3481	1/1	0.99	0.21	45,45,45,45	0
85	OHX	1	3874	7/7	0.99	0.20	91,91,91,91	0
85	OHX	1	3782	7/7	0.99	0.07	77,77,77,77	0
85	OHX	6	2044	7/7	0.99	0.11	81,81,81,81	0
85	OHX	6	2045	7/7	0.99	0.10	87,87,87,87	0
85	OHX	5	3822	7/7	0.99	0.17	64,64,64,64	0
85	OHX	1	3876	7/7	0.99	0.23	86,86,86,86	0
85	OHX	2	1996	7/7	0.99	0.10	83,83,83,83	0
85	OHX	5	3825	7/7	0.99	0.12	68,68,68,68	0
85	OHX	5	3826	7/7	0.99	0.10	62,62,62,62	0
85	OHX	1	3878	7/7	0.99	0.21	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	5	3828	7/7	0.99	0.19	73,73,73,73	0
85	OHX	5	3829	7/7	0.99	0.12	68,68,68,68	0
85	OHX	5	3830	7/7	0.99	0.14	64,64,64,64	0
84	MG	1	3576	1/1	0.99	0.57	28,28,28,28	0
85	OHX	5	3832	7/7	0.99	0.12	103,103,103,103	0
85	OHX	5	3833	7/7	0.99	0.07	61,61,61,61	0
85	OHX	6	2050	7/7	0.99	0.12	92,92,92,92	0
85	OHX	5	3835	7/7	0.99	0.13	73,73,73,73	0
85	OHX	1	3786	7/7	0.99	0.08	101,101,101,101	0
85	OHX	6	2052	7/7	0.99	0.09	110,110,110,110	0
85	OHX	5	3838	7/7	0.99	0.15	101,101,101,101	0
85	OHX	1	3787	7/7	0.99	0.07	73,73,73,73	0
84	MG	5	3577	1/1	0.99	0.50	45,45,45,45	0
85	OHX	5	4066	7/7	0.99	0.43	114,114,114,114	0
85	OHX	5	3841	7/7	0.99	0.08	97,97,97,97	0
85	OHX	5	3842	7/7	0.99	0.10	91,91,91,91	0
85	OHX	1	3883	7/7	0.99	0.19	106,106,106,106	0
85	OHX	5	3844	7/7	0.99	0.12	70,70,70,70	0
84	MG	1	3553	1/1	0.99	0.51	30,30,30,30	0
85	OHX	1	3885	7/7	0.99	0.22	78,78,78,78	0
85	OHX	5	3847	7/7	0.99	0.12	67,67,67,67	0
85	OHX	5	3848	7/7	0.99	0.20	80,80,80,80	0
85	OHX	7	215	7/7	0.99	0.09	82,82,82,82	0
85	OHX	7	216	7/7	0.99	0.13	87,87,87,87	0
85	OHX	1	3790	7/7	0.99	0.11	72,72,72,72	0
84	MG	1	3464	1/1	0.99	0.28	36,36,36,36	0
85	OHX	5	3851	7/7	0.99	0.08	52,52,52,52	0
85	OHX	2	2001	7/7	0.99	0.09	83,83,83,83	0
85	OHX	1	3793	7/7	0.99	0.06	89,89,89,89	0
85	OHX	8	211	7/7	0.99	0.08	55,55,55,55	0
85	OHX	1	3794	7/7	0.99	0.06	62,62,62,62	0
84	MG	5	3567	1/1	0.99	0.49	30,30,30,30	0
85	OHX	1	3796	7/7	0.99	0.07	79,79,79,79	0
85	OHX	1	3893	7/7	0.99	0.28	81,81,81,81	0
85	OHX	5	3858	7/7	0.99	0.21	82,82,82,82	0
84	MG	1	3483	1/1	0.99	0.31	45,45,45,45	0
85	OHX	1	3798	7/7	0.99	0.08	75,75,75,75	0
85	OHX	5	3861	7/7	0.99	0.06	103,103,103,103	0
85	OHX	5	3862	7/7	0.99	0.25	77,77,77,77	0
85	OHX	5	3863	7/7	0.99	0.22	86,86,86,86	0
85	OHX	2	2004	7/7	0.99	0.09	86,86,86,86	0
85	OHX	5	3865	7/7	0.99	0.11	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	2	2031	7/7	0.99	0.18	95,95,95,95	0
85	OHX	1	3801	7/7	0.99	0.11	81,81,81,81	0
85	OHX	l3	406	7/7	0.99	0.14	79,79,79,79	0
85	OHX	5	3868	7/7	0.99	0.07	96,96,96,96	0
85	OHX	1	3802	7/7	0.99	0.13	75,75,75,75	0
85	OHX	1	3803	7/7	0.99	0.20	74,74,74,74	0
85	OHX	6	2073	7/7	0.99	0.28	86,86,86,86	0
85	OHX	1	4005	7/7	0.99	0.25	95,95,95,95	0
85	OHX	2	1983	7/7	0.99	0.11	75,75,75,75	0
85	OHX	6	2076	7/7	0.99	0.23	81,81,81,81	0
85	OHX	2	2006	7/7	0.99	0.12	113,113,113,113	0
85	OHX	6	2078	7/7	0.99	0.24	98,98,98,98	0
85	OHX	2	1984	7/7	0.99	0.11	78,78,78,78	0
85	OHX	1	4009	7/7	0.99	0.20	83,83,83,83	0
85	OHX	1	3904	7/7	0.99	0.16	82,82,82,82	0
85	OHX	6	2082	7/7	0.99	0.21	91,91,91,91	0
85	OHX	n3	202	7/7	0.99	0.08	72,72,72,72	0
85	OHX	5	3881	7/7	0.99	0.11	106,106,106,106	0
85	OHX	n9	102	7/7	0.99	0.14	59,59,59,59	0
85	OHX	o3	202	7/7	0.99	0.19	82,82,82,82	0
85	OHX	5	3882	7/7	0.99	0.26	67,67,67,67	0
84	MG	5	3547	1/1	0.99	0.53	33,33,33,33	0
85	OHX	1	3808	7/7	0.99	0.10	93,93,93,93	0
85	OHX	2	1986	7/7	0.99	0.10	81,81,81,81	0
85	OHX	1	3908	7/7	0.99	0.18	103,103,103,103	0
85	OHX	2	2010	7/7	0.99	0.17	88,88,88,88	0
85	OHX	5	3888	7/7	0.99	0.26	91,91,91,91	0
86	ZN	O7	101	1/1	0.99	0.07	42,42,42,42	0
85	OHX	1	3811	7/7	0.99	0.09	78,78,78,78	0
85	OHX	1	3730	7/7	0.99	0.18	55,55,55,55	0
85	OHX	1	3731	7/7	0.99	0.11	50,50,50,50	0
85	OHX	1	3732	7/7	0.99	0.13	57,57,57,57	0
85	OHX	1	3815	7/7	0.99	0.14	71,71,71,71	0
85	OHX	1	3733	7/7	0.99	0.10	47,47,47,47	0
85	OHX	1	3734	7/7	0.99	0.09	56,56,56,56	0
86	ZN	o7	501	1/1	0.99	0.07	45,45,45,45	0
85	OHX	1	3818	7/7	0.99	0.16	58,58,58,58	0
85	OHX	1	3735	7/7	0.99	0.11	54,54,54,54	0
86	ZN	q3	501	1/1	0.99	0.10	57,57,57,57	0
85	OHX	5	3898	7/7	0.99	0.17	80,80,80,80	0
85	OHX	1	3727	7/7	1.00	0.10	52,52,52,52	0
85	OHX	1	3728	7/7	1.00	0.10	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	5	3769	7/7	1.00	0.06	52,52,52,52	0
85	OHX	6	2014	7/7	1.00	0.09	62,62,62,62	0
85	OHX	1	3737	7/7	1.00	0.06	56,56,56,56	0
85	OHX	1	3729	7/7	1.00	0.14	53,53,53,53	0
85	OHX	1	3744	7/7	1.00	0.04	54,54,54,54	0
85	OHX	5	3774	7/7	1.00	0.11	53,53,53,53	0
85	OHX	5	3752	7/7	1.00	0.09	40,40,40,40	0
85	OHX	1	3761	7/7	1.00	0.06	60,60,60,60	0
85	OHX	1	3752	7/7	1.00	0.09	59,59,59,59	0
85	OHX	1	3745	7/7	1.00	0.09	66,66,66,66	0
85	OHX	5	3756	7/7	1.00	0.08	60,60,60,60	0
85	OHX	5	3757	7/7	1.00	0.10	58,58,58,58	0
85	OHX	1	3754	7/7	1.00	0.05	63,63,63,63	0
85	OHX	6	2009	7/7	1.00	0.12	57,57,57,57	0
85	OHX	1	3785	7/7	1.00	0.06	66,66,66,66	0
85	OHX	1	3726	7/7	1.00	0.13	43,43,43,43	0
85	OHX	5	3743	7/7	1.00	0.14	43,43,43,43	0
85	OHX	5	3763	7/7	1.00	0.09	61,61,61,61	0
85	OHX	5	3744	7/7	1.00	0.12	40,40,40,40	0
85	OHX	5	3745	7/7	1.00	0.10	43,43,43,43	0
85	OHX	5	3766	7/7	1.00	0.07	63,63,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.