wwPDB X-ray Structure Validation Summary Report (i)

Nov 29, 2022 – 09:03 pm GMT

PDB ID	:	5TGM
Title	:	Crystal structure of the S.cerevisiae 80S ribosome in complex with the A-site bound aminoacyl-tRNA analog ACCA-Pro
Authors	:	Melnikov, S.; Mailliot, J.; Yusupov, M.
Deposited on	:	2016-09-28
Resolution	:	3.50 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:

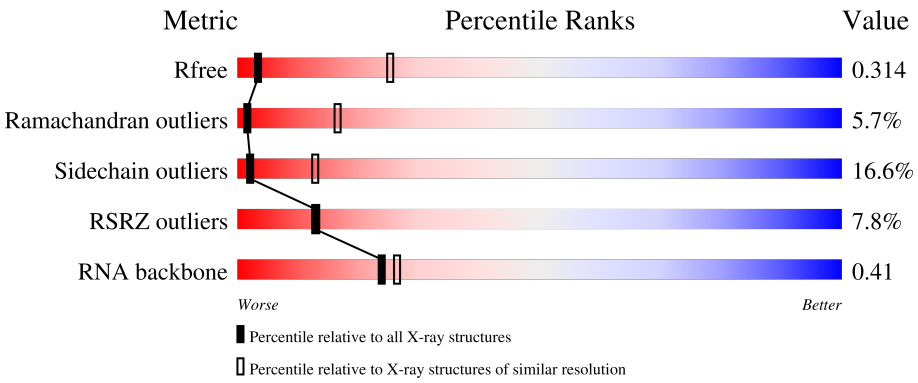
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.50 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	1659 (3.60-3.40)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1812	8%, 17%, 61%, 20%, •
2	S0	206	30%, 83%, 16%
2	s0	206	9%, 78%, 20%, •
3	S1	216	8%, 74%, 24%, • •
3	s1	216	6%, 74%, 23%, •

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Mol	Chain	Length	Quality of chain
4	S2	217	31% 85% 13%
4	s2	217	15% 76% 22%
5	S3	223	30% 85% 14%
5	s3	223	36% 82% 17%
6	S4	260	12% 79% 19%
6	s4	260	3% 80% 20%
7	S5	206	28% 84% 14%
7	s5	206	20% 84% 15%
8	S6	226	19% 79% 19%
8	s6	226	18% 76% 18%
9	S7	186	8% 83% 15%
9	s7	186	4% 81% 17%
10	S8	199	18% 79% 13% 6%
10	s8	199	10% 79% 15% 6%
11	S9	185	19% 84% 14%
11	s9	185	2% 82% 17%
12	C0	105	9% 74% 16% 9%
12	c0	105	24% 72% 14% 5% 9%
13	C1	156	27% 85% 15%
13	c1	156	6% 78% 16% 6%
14	C2	143	30% 67% 18% 13%
14	c2	143	24% 67% 19% 13%
15	C3	150	6% 79% 19%
15	c3	150	% 83% 14%
16	C4	128	9% 82% 14%

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Mol	Chain	Length	Quality of chain
16	c4	128	13% 83% 16%
17	C5	142	6% 72% 14% 13%
17	c5	142	7% 74% 20% 5%
18	C6	142	48% 78% 19%
18	c6	142	30% 84% 16%
19	C7	125	33% 77% 17%
19	c7	125	14% 72% 21% 6%
20	C8	145	6% 84% 12%
20	c8	145	7% 79% 20%
21	C9	143	22% 81% 19%
21	c9	143	8% 89% 10%
22	D0	110	24% 79% 18%
22	d0	110	46% 77% 19%
23	D1	87	18% 76% 24%
23	d1	87	6% 83% 16%
24	D2	129	22% 81% 19%
24	d2	129	85% 15%
25	D3	144	5% 83% 17%
25	d3	144	2% 82% 17%
26	D4	134	2% 81% 17%
26	d4	134	4% 78% 18%
27	D5	70	10% 67% 30%
27	d5	70	7% 80% 19%
28	D6	97	43% 70% 23% 7%
28	d6	97	53% 72% 28%

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Mol	Chain	Length	Quality of chain
29	D7	81	16% 95% 5%
29	d7	81	5% 78% 22%
30	D8	63	51% 79% 19%
30	d8	63	63% 75% 24%
31	D9	53	4% 75% 25%
31	d9	53	25% 70% 30%
32	E0	62	15% 73% 23%
32	e0	62	10% 82% 15%
33	E1	76	11% 58% 32% 7%
33	e1	76	20% 59% 36% 5%
34	SR	318	26% 89% 10%
35	SM	299	9% 43% 9% 47%
36	1	3149	2% 74% 23%
37	3	121	3% 82% 15%
37	7	121	% 80% 18%
38	4	158	% 71% 28%
38	8	158	% 5% 71% 24%
39	L2	252	3% 79% 19%
39	l2	252	2% 76% 21%
40	L3	386	% 73% 24%
40	l3	386	% 75% 22%
41	L4	361	75% 20% 6%
41	l4	361	75% 20% 5%
42	L5	296	12% 78% 20%
42	l5	296	% 74% 22%

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Mol	Chain	Length	Quality of chain
43	L6	175	75% 13% 11%
43	l6	175	2% 73% 15% 10%
44	L7	223	74% 22%
44	l7	223	75% 22%
45	L8	233	2% 83% 16%
46	L9	191	7% 69% 28%
46	l9	191	2% 74% 24%
47	M0	220	70% 24%
47	m0	220	4% 70% 20% 5%
48	M1	169	11% 76% 18%
48	m1	169	77% 22%
49	M3	194	% 72% 24%
49	m3	194	3% 74% 25%
50	M4	137	2% 74% 23%
50	m4	137	% 74% 25%
51	M5	203	74% 23%
51	m5	203	78% 20%
52	M6	197	% 75% 23%
52	m6	197	74% 23%
53	M7	183	5% 75% 23%
53	m7	183	58% 24% 15%
54	M8	185	76% 23%
54	m8	185	72% 26%
55	M9	188	4% 86% 13%
55	m9	188	% 80% 19%

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Mol	Chain	Length	Quality of chain
56	N0	172	12% 78% 20%
56	n0	172	.% 75% 23%
57	N1	159	4% 75% 21%
57	n1	159	5% 74% 25%
58	N2	100	5% 79% 20%
58	n2	100	4% 79% 18%
59	N3	136	2% 77% 22%
59	n3	136	76% 21%
60	N4	98	31% 88% 12%
61	N5	121	2% 80% 18%
61	n5	121	.% 67% 30%
62	N6	126	.% 70% 26%
62	n6	126	71% 25%
63	N7	135	5% 79% 20%
63	n7	135	5% 76% 21%
64	N8	148	78% 18%
64	n8	148	.% 73% 25%
65	N9	58	81% 17%
65	n9	58	5% 76% 19% 5%
66	O0	100	3% 79% 18%
66	o0	100	5% 82% 16%
67	O1	109	3% 79% 17%
67	o1	109	2% 72% 24%
68	O2	127	70% 27%
68	o2	127	66% 31%

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Mol	Chain	Length	Quality of chain
69	O3	106	69% 26%
69	o3	106	72% 25%
70	O4	112	4% 81% 18%
70	o4	112	4% 81% 18%
71	O5	119	% 81% 16%
71	o5	119	% 74% 22%
72	O6	99	2% 71% 27%
72	o6	99	76% 22%
73	O7	87	% 76% 22%
73	o7	87	3% 76% 21%
74	O8	77	% 71% 26%
74	o8	77	4% 79% 19%
75	O9	50	72% 26%
75	o9	50	72% 28%
76	Q0	52	2% 67% 31%
76	q0	52	71% 29%
77	Q1	25	76% 24%
77	q1	25	64% 32%
78	Q2	105	10% 67% 31%
78	q2	105	9% 73% 23%
79	Q3	91	5% 70% 29%
79	q3	91	3% 74% 25%
80	6	1800	7% 13% 65% 21%
81	sR	318	30% 90% 10%
82	sM	273	5% 32% 5% 62%

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Mol	Chain	Length	Quality of chain
83	5	3150	2% 73% 24%
84	l8	256	4% 71% 18% 10%
85	m2	165	18% 73% 15% 9%
86	n4	135	24% 79% 19%
87	p0	312	10% 39% 6% 54%
88	p1	128	13% 32% 63%
88	p2	128	15% 30% 5% 64%
89	P	4	50% 50%
89	p	4	50% 50%

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
91	MG	1	3732	-	-	-	X
91	MG	1	3735	-	-	-	X
91	MG	1	3743	-	-	-	X
91	MG	1	3764	-	-	-	X
91	MG	1	3773	-	-	-	X
91	MG	1	3782	-	-	-	X
91	MG	1	3785	-	-	-	X
91	MG	1	3817	-	-	-	X
91	MG	1	3831	-	-	-	X
91	MG	1	3847	-	-	-	X
91	MG	1	3854	-	-	-	X
91	MG	1	3873	-	-	-	X
91	MG	1	3914	-	-	-	X
91	MG	1	3932	-	-	-	X
91	MG	1	3944	-	-	-	X
91	MG	1	3946	-	-	-	X
91	MG	1	3963	-	-	-	X
91	MG	1	3964	-	-	-	X
91	MG	1	3976	-	-	-	X
91	MG	1	3984	-	-	-	X
91	MG	1	3989	-	-	-	X
91	MG	1	4000	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	MG	1	4008	-	-	-	X
91	MG	1	4012	-	-	-	X
91	MG	1	4024	-	-	-	X
91	MG	1	4031	-	-	-	X
91	MG	1	4042	-	-	-	X
91	MG	1	4052	-	-	-	X
91	MG	1	4053	-	-	-	X
91	MG	1	4063	-	-	-	X
91	MG	1	4077	-	-	-	X
91	MG	1	4079	-	-	-	X
91	MG	1	4093	-	-	-	X
91	MG	2	2061	-	-	-	X
91	MG	2	2068	-	-	-	X
91	MG	2	2070	-	-	-	X
91	MG	2	2076	-	-	-	X
91	MG	2	2078	-	-	-	X
91	MG	2	2084	-	-	-	X
91	MG	2	2089	-	-	-	X
91	MG	2	2092	-	-	-	X
91	MG	2	2094	-	-	-	X
91	MG	2	2101	-	-	-	X
91	MG	2	2110	-	-	-	X
91	MG	2	2112	-	-	-	X
91	MG	2	2114	-	-	-	X
91	MG	2	2117	-	-	-	X
91	MG	2	2118	-	-	-	X
91	MG	2	2132	-	-	-	X
91	MG	2	2138	-	-	-	X
91	MG	2	2141	-	-	-	X
91	MG	5	3754	-	-	-	X
91	MG	5	3763	-	-	-	X
91	MG	5	3789	-	-	-	X
91	MG	5	3792	-	-	-	X
91	MG	5	3809	-	-	-	X
91	MG	5	3831	-	-	-	X
91	MG	5	3838	-	-	-	X
91	MG	5	3860	-	-	-	X
91	MG	5	3874	-	-	-	X
91	MG	5	3895	-	-	-	X
91	MG	5	3943	-	-	-	X
91	MG	5	3948	-	-	-	X
91	MG	5	3969	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	MG	5	3985	-	-	-	X
91	MG	5	3988	-	-	-	X
91	MG	5	4007	-	-	-	X
91	MG	5	4019	-	-	-	X
91	MG	5	4021	-	-	-	X
91	MG	5	4037	-	-	-	X
91	MG	5	4048	-	-	-	X
91	MG	5	4062	-	-	-	X
91	MG	5	4065	-	-	-	X
91	MG	5	4084	-	-	-	X
91	MG	5	4086	-	-	-	X
91	MG	5	4097	-	-	-	X
91	MG	5	4102	-	-	-	X
91	MG	5	4107	-	-	-	X
91	MG	5	4112	-	-	-	X
91	MG	5	4122	-	-	-	X
91	MG	5	4126	-	-	-	X
91	MG	5	4132	-	-	-	X
91	MG	5	4153	-	-	-	X
91	MG	5	4168	-	-	-	X
91	MG	5	4171	-	-	-	X
91	MG	6	2062	-	-	-	X
91	MG	6	2064	-	-	-	X
91	MG	6	2067	-	-	-	X
91	MG	6	2073	-	-	-	X
91	MG	6	2080	-	-	-	X
91	MG	6	2091	-	-	-	X
91	MG	6	2093	-	-	-	X
91	MG	6	2098	-	-	-	X
91	MG	6	2102	-	-	-	X
91	MG	6	2105	-	-	-	X
91	MG	6	2106	-	-	-	X
91	MG	6	2108	-	-	-	X
91	MG	6	2111	-	-	-	X
91	MG	6	2114	-	-	-	X
91	MG	6	2120	-	-	-	X
91	MG	6	2125	-	-	-	X
91	MG	6	2129	-	-	-	X
91	MG	6	2130	-	-	-	X
91	MG	6	2133	-	-	-	X
91	MG	6	2136	-	-	-	X
91	MG	6	2137	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	MG	6	2141	-	-	-	X
91	MG	6	2147	-	-	-	X
91	MG	6	2152	-	-	-	X
91	MG	6	2156	-	-	-	X
91	MG	6	2166	-	-	-	X
91	MG	6	2167	-	-	-	X
91	MG	6	2180	-	-	-	X
91	MG	6	2183	-	-	-	X
91	MG	7	212	-	-	-	X
91	MG	7	225	-	-	-	X
91	MG	C1	201	-	-	-	X
91	MG	C9	201	-	-	-	X
91	MG	L4	404	-	-	-	X
91	MG	M7	202	-	-	-	X
91	MG	O7	105	-	-	-	X
91	MG	S4	301	-	-	-	X
91	MG	c6	201	-	-	-	X
91	MG	d3	201	-	-	-	X
91	MG	d7	102	-	-	-	X
91	MG	l6	201	-	-	-	X
91	MG	n6	201	-	-	-	X
91	MG	o2	201	-	-	-	X
91	MG	o9	101	-	-	-	X
91	MG	s6	301	-	-	-	X
93	PHE	5	3401	-	-	-	X

2 Entry composition (i)

There are 96 unique types of molecules in this entry. The entry contains 411566 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

- 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	1583	1017	281	283	2	0	0	0

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

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S1	56	SER	ASN	conflict	UNP P23248
S1	84	ILE	VAL	conflict	UNP P23248
S1	174	LYS	ARG	conflict	UNP P23248
S1	178	GLY	ASN	conflict	UNP P23248
s1	56	SER	ASN	conflict	UNP P23248
s1	84	ILE	VAL	conflict	UNP P23248
s1	174	LYS	ARG	conflict	UNP P23248
s1	178	GLY	ASN	conflict	UNP P23248

- 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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	s7	186	1491	957	267	267	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
			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.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	C1	155	1213	774	230	206	3	0	0	0
			Total	C	N	O	S			
13	c1	146	1168	747	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
15	c3	150	1192	759	224	207	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	C4	127	891	545	182	163	1	0	0	0
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
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
18	c6	142	1111	711	204	196	0	0	0

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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
31	d9	53	442	274	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
32	e0	62	491	309	101	80	1	0	0	0

- Molecule 33 is a protein called 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
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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SR	161	ALA	LYS	conflict	UNP P38011

- Molecule 35 is a protein called Suppressor protein STM1,Ribosome-bound protein Stm1,Suppressor protein STM1,Ribosome-bound protein Stm1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
35	SM	159	1104	654	221	229	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SM	134	LEU	ASP	conflict	UNP P39015

- 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

- 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	1912	1190	388	333	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	3075	1950	584	533	8	0	0	0
40	l3	386	3075	1950	584	533	8	0	0	0

- 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	2748	1729	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

- 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
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
47	m0	213	1722	1094	325	297	6	0	0	0

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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

- 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
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	883	559	167	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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
70	o4	112	880	545	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
			Total	C	N	O	S			
71	o5	119	965	612	185	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
			Total	C	N	O	S			
72	o6	99	770	481	156	131	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
			Total	C	N	O	S			
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	608	388	114	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 60S ribosomal protein L40-A.

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
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 RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
80	6	1795	38260	17105	6763	12596	1796	0	1	0

- Molecule 81 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
81	sR	318	2442	1544	418	472	8	0	0	0

- Molecule 82 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
82	sM	104	680	403	140	137	0	0	0

- Molecule 83 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
83	5	3150	67376	30095	12145	21987	3149	0	0	0

- Molecule 84 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
84	l8	231	1763	1130	316	314	3	0	0	0

- Molecule 85 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
85	m2	150	737	437	150	150	0	0	0

- Molecule 86 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
86	n4	135	1038	651	206	180	1	0	0	0

- Molecule 87 is a protein called 60S acidic ribosomal protein P0.

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

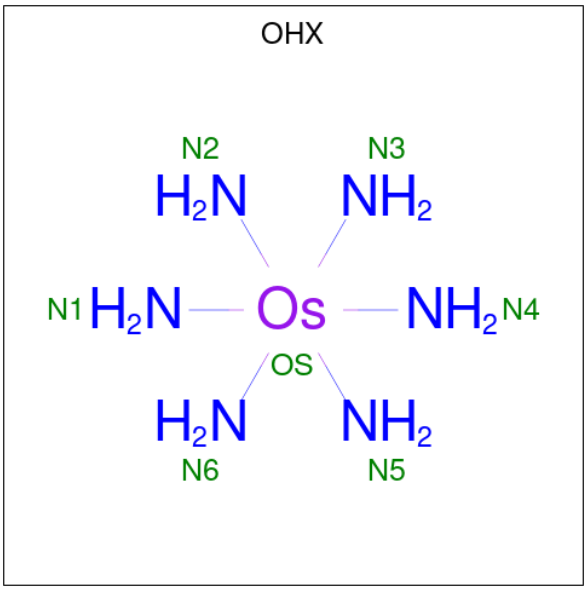
- Molecule 88 is a protein called 60S ribosomal protein L40-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
88	p1	47	232	138	47	47	0	0	0
88	p2	46	228	136	46	46	0	0	0

- Molecule 89 is a RNA chain called Peptidyl-tRNA analog ACCA-Leu-Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
89	P	2	37	18	6	12	1	0	0	0
89	p	2	40	18	6	14	2	0	0	0

- Molecule 90 is osmium (III) hexammine (three-letter code: OHX) (formula: $H_{12}N_6Os$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
90	2	1	7	6	1	0	0
			Total	N	Os		
90	2	1	7	6	1	0	0
			Total	N	Os		
90	2	1	7	6	1	0	0
			Total	N	Os		
90	2	1	7	6	1	0	0
			Total	N	Os		
90	2	1	7	6	1	0	0
			Total	N	Os		
90	2	1	7	6	1	0	0
			Total	N	Os		
90	2	1	7	6	1	0	0
			Total	N	Os		
90	2	1	7	6	1	0	0
			Total	N	Os		
90	2	1	7	6	1	0	0
			Total	N	Os		
90	2	1	7	6	1	0	0
			Total	N	Os		
90	2	1	7	6	1	0	0
			Total	N	Os		
90	2	1	7	6	1	0	0
			Total	N	Os		
90	2	1	7	6	1	0	0
			Total	N	Os		
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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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			Total	N	Os		
90	S9	1	7	6	1	0	0
			Total	N	Os		
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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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90	1	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		
90	1	1	7	6	1	0	0
			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
90	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
90	1	1	7	6	1	0	0
90	1	1	7	6	1	0	0
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90	1	1	7	6	1	0	0
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90	1	1	7	6	1	0	0
90	1	1	7	6	1	0	0
90	1	1	7	6	1	0	0
90	1	1	7	6	1	0	0
90	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
90	1	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		
90	1	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
90	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
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90	1	1	7	6	1	0	0
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
90	1	1	7	6	1	0	0
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90	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
90	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
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90	1	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
90	1	1	7	6	1	0	0
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90	1	1	7	6	1	0	0
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90	1	1	7	6	1	0	0
			Total	N	Os		
90	1	1	7	6	1	0	0
			Total	N	Os		
90	1	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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90	3	1	7	6	1	0	0
			Total	N	Os		
90	3	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		
90	4	1	7	6	1	0	0
			Total	N	Os		
90	4	1	7	6	1	0	0
			Total	N	Os		
90	4	1	7	6	1	0	0
			Total	N	Os		
90	4	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
90	4	1	7	6	1	0	0
			Total	N	Os		
90	4	1	7	6	1	0	0
			Total	N	Os		
90	4	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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90	4	1	7	6	1	0	0
			Total	N	Os		
90	4	1	7	6	1	0	0
			Total	N	Os		
90	4	1	7	6	1	0	0
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			Total	N	Os		
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			Total	N	Os		
90	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		
90	L3	1	7	6	1	0	0
			Total	N	Os		
90	L3	1	7	6	1	0	0
			Total	N	Os		
90	L4	1	7	6	1	0	0
			Total	N	Os		
90	L6	1	7	6	1	0	0
			Total	N	Os		
90	L6	1	7	6	1	0	0
			Total	N	Os		
90	M0	1	7	6	1	0	0
			Total	N	Os		
90	M5	1	7	6	1	0	0
			Total	N	Os		
90	M5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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90	M6	1	7	6	1	0	0
90	M7	1	7	6	1	0	0
90	M8	1	7	6	1	0	0
90	M9	1	7	6	1	0	0
90	N9	1	7	6	1	0	0
90	O3	1	7	6	1	0	0
90	O4	1	7	6	1	0	0
90	O7	1	7	6	1	0	0
90	O9	1	7	6	1	0	0
90	Q2	1	7	6	1	0	0
90	6	1	7	6	1	0	0
90	6	1	7	6	1	0	0
90	6	1	7	6	1	0	0
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90	6	1	7	6	1	0	0
90	6	1	7	6	1	0	0
90	6	1	7	6	1	0	0
90	6	1	7	6	1	0	0
90	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
90	6	1	7	6	1	0	0
			Total	N	Os		
90	6	1	7	6	1	0	0
			Total	N	Os		
90	6	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
90	6	1	7	6	1	0	0
			Total	N	Os		
90	6	1	7	6	1	0	0
			Total	N	Os		
90	6	1	7	6	1	0	0
			Total	N	Os		
90	6	1	7	6	1	0	0
			Total	N	Os		
90	6	1	7	6	1	0	0
			Total	N	Os		
90	6	1	7	6	1	0	0
			Total	N	Os		
90	6	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
90	6	1	7	6	1	0	0
			Total	N	Os		
90	6	1	7	6	1	0	0
			Total	N	Os		
90	6	1	7	6	1	0	0
			Total	N	Os		
90	6	1	7	6	1	0	0
			Total	N	Os		
90	6	1	7	6	1	0	0
			Total	N	Os		
90	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
90	6	1	7	6	1	0	0
			Total	N	Os		
90	6	1	7	6	1	0	0
			Total	N	Os		
90	6	1	7	6	1	0	0
			Total	N	Os		
90	6	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		
90	6	1	7	6	1	0	0
			Total	N	Os		
90	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
90	6	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
90	6	1	7	6	1	0	0
			Total	N	Os		
90	6	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		
90	6	1	7	6	1	0	0
			Total	N	Os		
90	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		
90	6	1	7	6	1	0	0
			Total	N	Os		
90	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
90	6	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		
90	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
90	6	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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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		
90	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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90	s8	1	7	6	1	0	0
90	s9	1	7	6	1	0	0
90	c3	1	7	6	1	0	0
90	c5	1	7	6	1	0	0
90	c8	1	7	6	1	0	0
90	d4	1	7	6	1	0	0
90	sR	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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			Total	N	Os		
90	5	1	7	6	1	0	0
			Total	N	Os		
90	5	1	7	6	1	0	0
			Total	N	Os		
90	5	1	7	6	1	0	0
			Total	N	Os		
90	5	1	7	6	1	0	0
			Total	N	Os		
90	5	1	7	6	1	0	0
			Total	N	Os		
90	5	1	7	6	1	0	0
			Total	N	Os		
90	5	1	7	6	1	0	0
			Total	N	Os		
90	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
90	5	1	Total N Os 7 6 1	0	0
90	5	1	Total N Os 7 6 1	0	0
90	5	1	Total N Os 7 6 1	0	0
90	5	1	Total N Os 7 6 1	0	0
90	5	1	Total N Os 7 6 1	0	0
90	5	1	Total N Os 7 6 1	0	0
90	5	1	Total N Os 7 6 1	0	0
90	5	1	Total N Os 7 6 1	0	0
90	5	1	Total N Os 7 6 1	0	0
90	5	1	Total N Os 7 6 1	0	0
90	5	1	Total N Os 7 6 1	0	0
90	5	1	Total N Os 7 6 1	0	0
90	5	1	Total N Os 7 6 1	0	0
90	5	1	Total N Os 7 6 1	0	0
90	5	1	Total N Os 7 6 1	0	0
90	5	1	Total N Os 7 6 1	0	0
90	5	1	Total N Os 7 6 1	0	0
90	5	1	Total N Os 7 6 1	0	0
90	5	1	Total N Os 7 6 1	0	0
90	5	1	Total N Os 7 6 1	0	0
90	7	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
90	7	1	7	6	1	0	0
			Total	N	Os		
90	7	1	7	6	1	0	0
			Total	N	Os		
90	7	1	7	6	1	0	0
			Total	N	Os		
90	7	1	7	6	1	0	0
			Total	N	Os		
90	7	1	7	6	1	0	0
			Total	N	Os		
90	7	1	7	6	1	0	0
			Total	N	Os		
90	7	1	7	6	1	0	0
			Total	N	Os		
90	7	1	7	6	1	0	0
			Total	N	Os		
90	7	1	7	6	1	0	0
			Total	N	Os		
90	7	1	7	6	1	0	0
			Total	N	Os		
90	8	1	7	6	1	0	0
			Total	N	Os		
90	8	1	7	6	1	0	0
			Total	N	Os		
90	8	1	7	6	1	0	0
			Total	N	Os		
90	8	1	7	6	1	0	0
			Total	N	Os		
90	8	1	7	6	1	0	0
			Total	N	Os		
90	8	1	7	6	1	0	0
			Total	N	Os		
90	8	1	7	6	1	0	0
			Total	N	Os		
90	8	1	7	6	1	0	0
			Total	N	Os		
90	8	1	7	6	1	0	0
			Total	N	Os		
90	8	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
90	8	1	7	6	1	0	0
			Total	N	Os		
90	8	1	7	6	1	0	0
			Total	N	Os		
90	8	1	7	6	1	0	0
			Total	N	Os		
90	8	1	7	6	1	0	0
			Total	N	Os		
90	8	1	7	6	1	0	0
			Total	N	Os		
90	l3	1	7	6	1	0	0
			Total	N	Os		
90	l3	1	7	6	1	0	0
			Total	N	Os		
90	l5	1	7	6	1	0	0
			Total	N	Os		
90	l5	1	7	6	1	0	0
			Total	N	Os		
90	l9	1	7	6	1	0	0
			Total	N	Os		
90	m0	1	7	6	1	0	0
			Total	N	Os		
90	m0	1	7	6	1	0	0
			Total	N	Os		
90	m0	1	7	6	1	0	0
			Total	N	Os		
90	m5	1	7	6	1	0	0
			Total	N	Os		
90	m5	1	7	6	1	0	0
			Total	N	Os		
90	m6	1	7	6	1	0	0
			Total	N	Os		
90	m8	1	7	6	1	0	0
			Total	N	Os		
90	m9	1	7	6	1	0	0
			Total	N	Os		
90	n9	1	7	6	1	0	0
			Total	N	Os		
90	o3	1	7	6	1	0	0
			Total	N	Os		
90	o7	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
90	o7	1	7	6	1	0	0
90	q2	1	7	6	1	0	0

- Molecule 91 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
91	2	90	90	90	0	0
91	S4	1	1	1	0	0
91	C1	1	1	1	0	0
91	C8	1	1	1	0	0
91	C9	1	1	1	0	0
91	D9	2	2	2	0	0
91	1	394	394	394	0	0
91	3	7	7	7	0	0
91	4	17	17	17	0	0
91	L2	2	2	2	0	0
91	L3	3	3	3	0	0
91	L4	5	5	5	0	0
91	L7	2	2	2	0	0
91	M0	1	1	1	0	0
91	M3	1	1	1	0	0
91	M5	1	1	1	0	0
91	M7	5	5	5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
91	N0	2	2	2	0	0
91	N3	3	3	3	0	0
91	N5	1	1	1	0	0
91	N6	2	2	2	0	0
91	N8	6	6	6	0	0
91	O4	1	1	1	0	0
91	O5	1	1	1	0	0
91	O7	4	4	4	0	0
91	Q2	1	1	1	0	0
91	6	126	126	126	0	0
91	s4	1	1	1	0	0
91	s6	1	1	1	0	0
91	c6	1	1	1	0	0
91	c8	2	2	2	0	0
91	c9	1	1	1	0	0
91	d3	1	1	1	0	0
91	d4	1	1	1	0	0
91	d6	1	1	1	0	0
91	d7	1	1	1	0	0
91	sM	2	2	2	0	0
91	5	427	427	427	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
91	7	15	15	15	0	0
91	8	14	14	14	0	0
91	l2	3	3	3	0	0
91	l3	4	4	4	0	0
91	l5	1	1	1	0	0
91	l6	1	1	1	0	0
91	l7	1	1	1	0	0
91	l9	1	1	1	0	0
91	m0	1	1	1	0	0
91	m4	1	1	1	0	0
91	m5	2	2	2	0	0
91	m6	4	4	4	0	0
91	m7	3	3	3	0	0
91	n0	2	2	2	0	0
91	n3	1	1	1	0	0
91	n6	2	2	2	0	0
91	n8	3	3	3	0	0
91	n9	2	2	2	0	0
91	o2	2	2	2	0	0
91	o3	2	2	2	0	0
91	o4	1	1	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
91	o9	1	Total Mg 1 1	0	0
91	q1	1	Total Mg 1 1	0	0
91	P	1	Total Mg 1 1	0	0
91	p	2	Total Mg 2 2	0	0

- Molecule 92 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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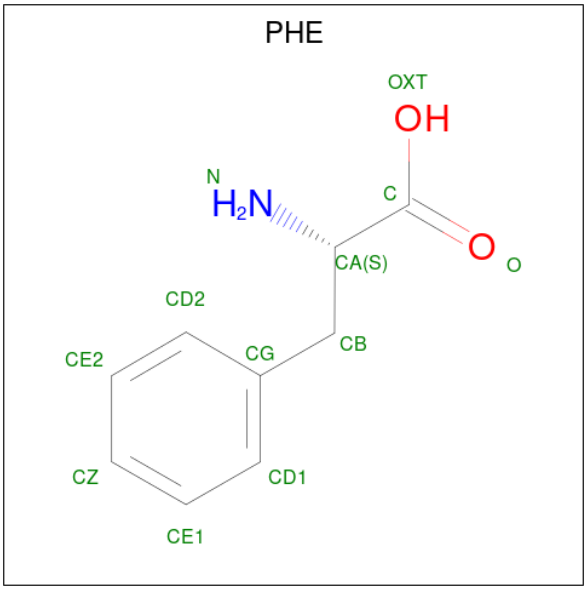
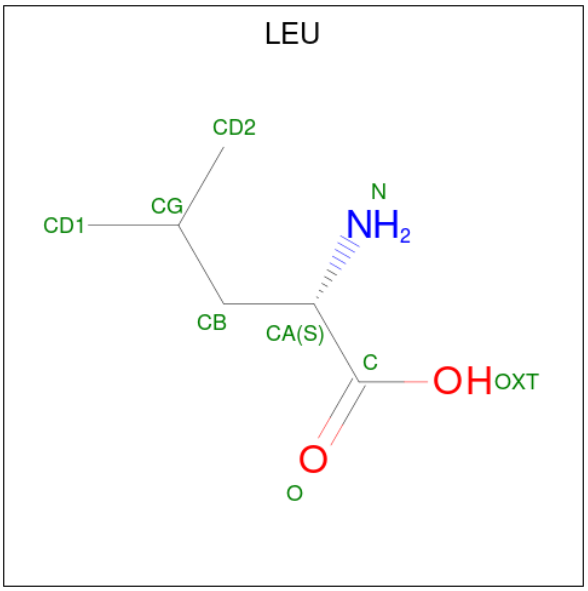
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
92	q3	1	1	1	0	0

- Molecule 93 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



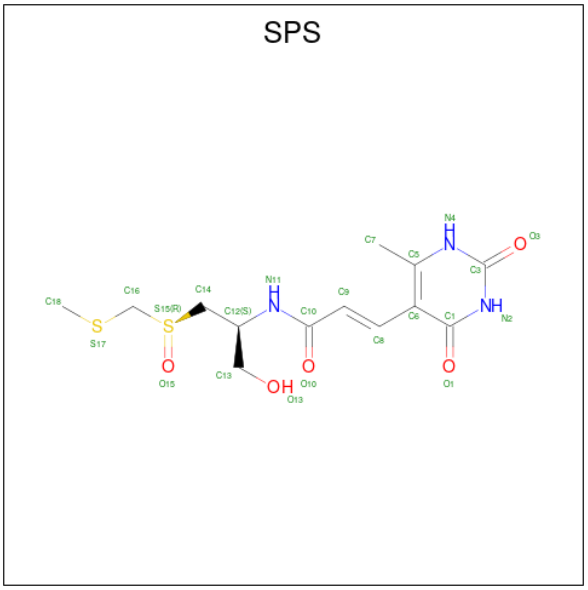
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
93	1	1	11	9	1	1	0	0
			Total	C	N	O		
93	5	1	11	9	1	1	0	0

- Molecule 94 is LEUCINE (three-letter code: LEU) (formula: $C_6H_{13}NO_2$).



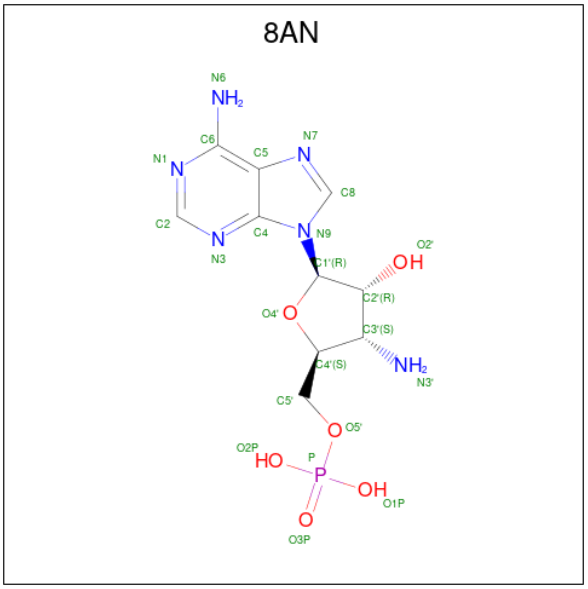
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
94	1	1	8	6	1	1	0	0
94	5	1	8	6	1	1	0	0

- Molecule 95 is SPARSOMYCIN (three-letter code: SPS) (formula: $C_{13}H_{19}N_3O_5S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
95	1	1	23	13	3	5	2	0	0
95	5	1	23	13	3	5	2	0	0

- Molecule 96 is 3'-amino-3'-deoxyadenosine 5'-(dihydrogen phosphate) (three-letter code: 8AN) (formula: $C_{10}H_{15}N_6O_6P$).



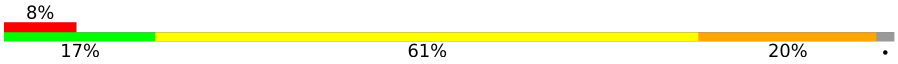
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
96	P	1	22	10	6	5	1	0	0
			Total	C	N	O	P		
96	p	1	22	10	6	5	1	0	0

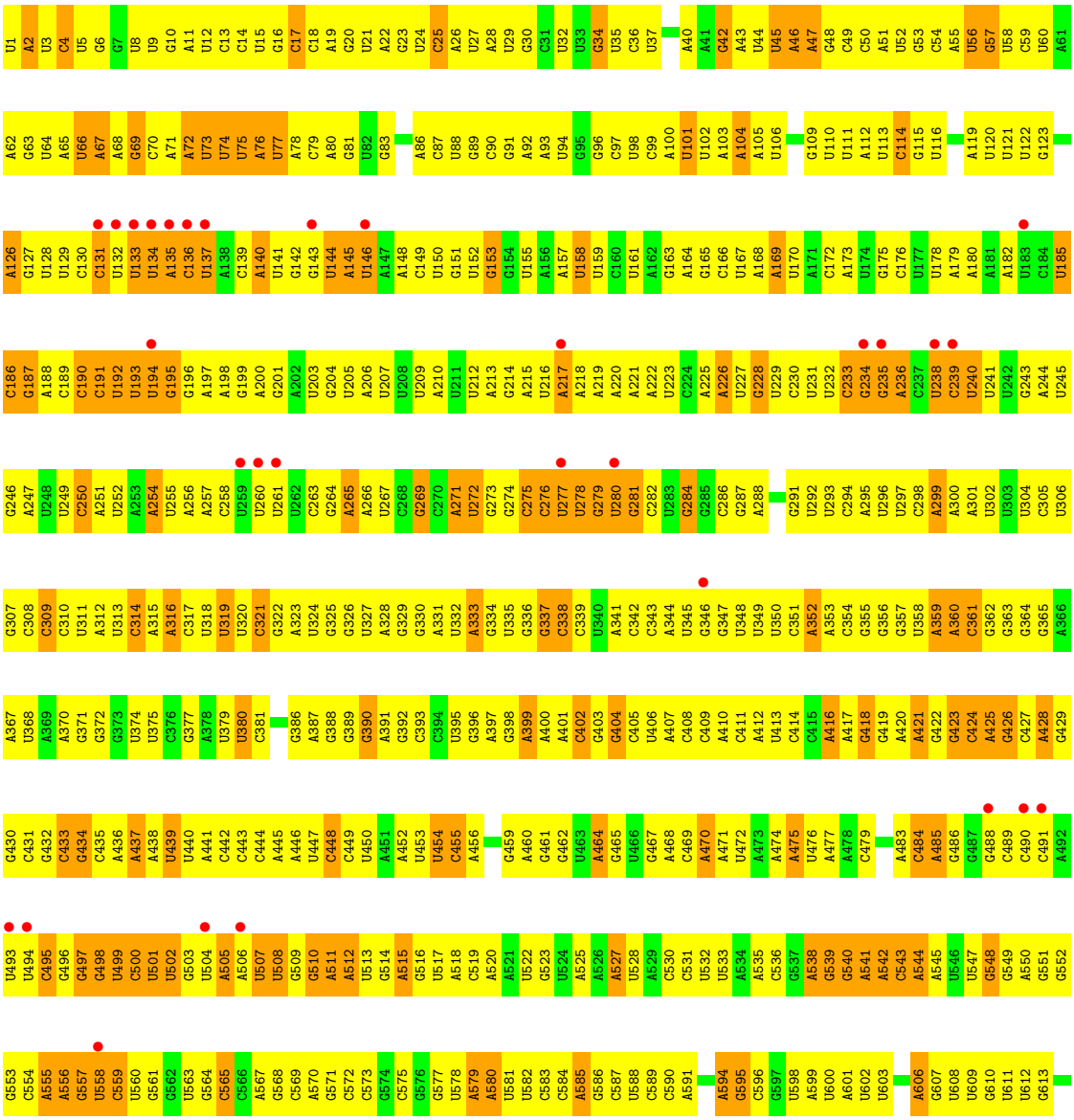
3 Residue-property plots (i)

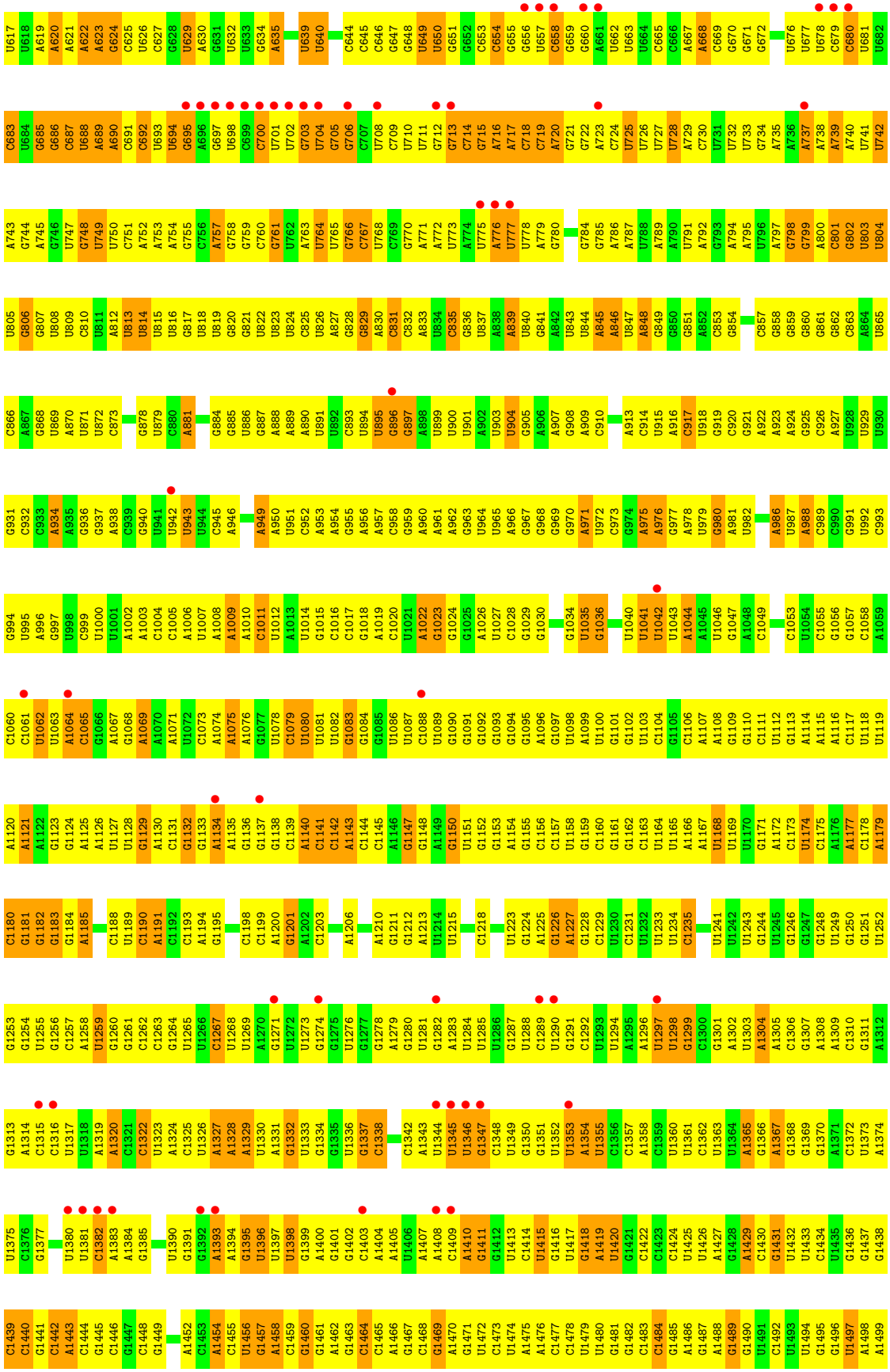
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

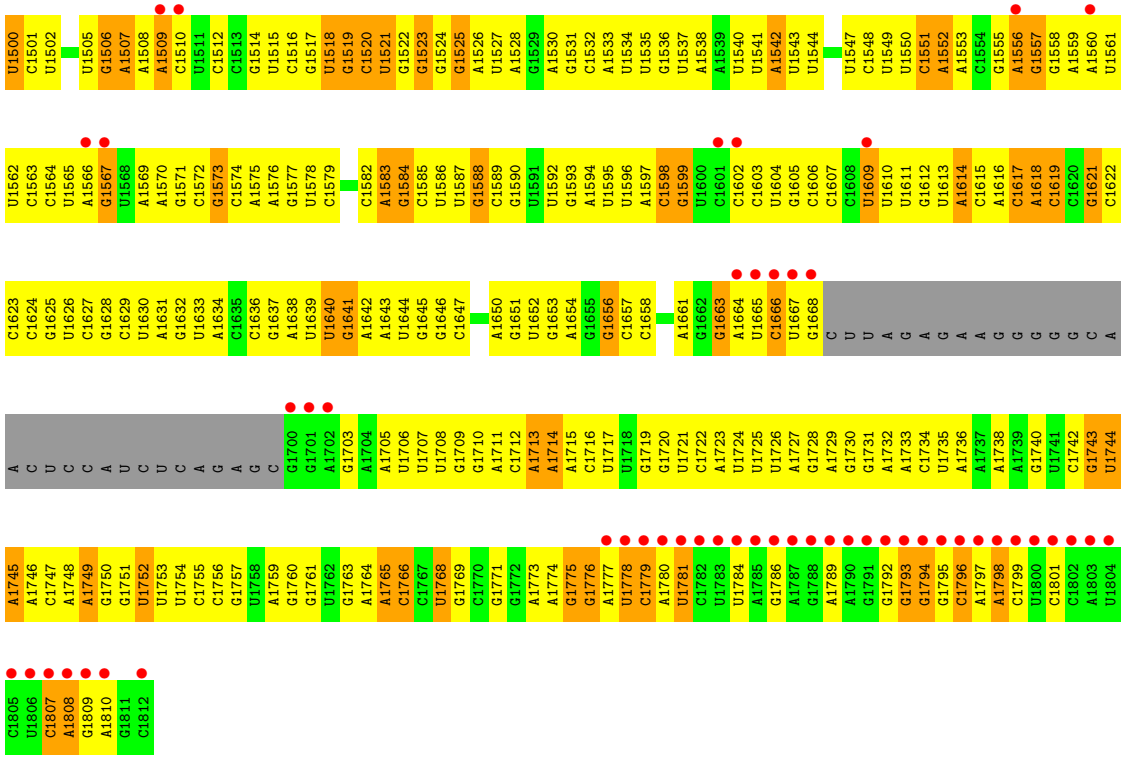
- Molecule 1: 18S ribosomal RNA

Chain 2:



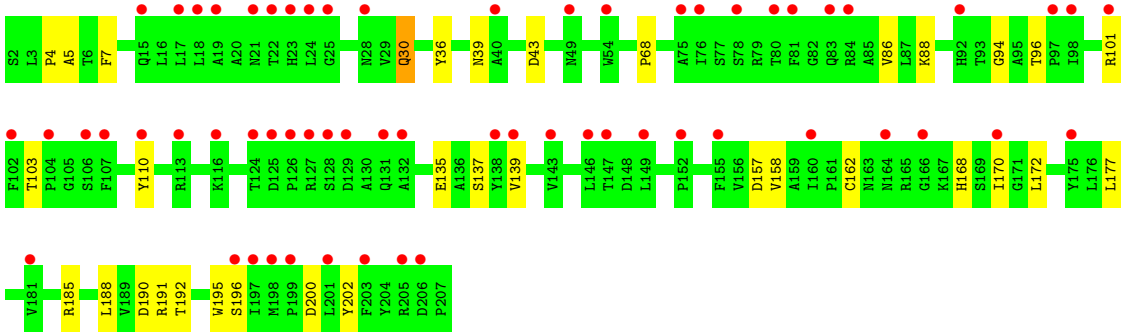



U617 U618 A619 A620 A621 A622 A623 G624 C625 U626 C627 G628 U629 A630 G631 U632 U633 G634 A635 U639 U640 C644 C645 C646 G647 G648 U649 U650 G651 G652 C653 C654 G655 G656 U657 C658 G659 G660 A661 U662 U663 U664 C665 C666 A667 A668 C669 G670 G671 G672 U676 U677 U678 C679 C680 U681 U682
C683 U684 G685 G686 C687 U688 A689 A690 C691 C692 U693 U694 G695 A696 G697 U698 C699 C700 U701 U702 G703 U704 G705 G706 C707 U708 C709 U710 U711 G712 G713 C714 G715 A716 A717 C718 C719 A720 G721 G722 A723 C724 U725 U726 U727 U728 A729 C730 U731 U732 U733 G734 A735 A736 A737 A738 A739 A740 U741 U742
A743 G744 A745 G746 U747 G748 U749 U750 C751 A752 A753 A754 G755 C756 A757 G758 G759 C760 G761 U762 A763 U764 U765 G766 C767 U768 C769 G770 A771 A772 U773 A774 U775 A776 U777 U778 A779 G780 G784 G785 A786 A787 U788 A789 A790 U791 A792 G793 A794 A795 U796 A797 G798 G799 A800 C801 G802 U803 U804
U805 G806 G807 U808 U809 C810 U811 A812 U813 U814 U815 U816 G817 U818 U819 G820 G821 U822 U823 U824 C825 U826 A827 G828 G829 A830 C831 C832 A833 U834 C835 G836 U837 A838 A839 U840 G841 A842 U843 U844 A845 A846 U847 A848 G849 G850 G851 A852 C853 G854 C857 G858 G859 G860 G861 G862 C863 A864 U865
C866 A867 G868 U869 A870 U871 U872 C873 G878 U879 C880 A881 G884 G885 U886 C887 A888 A889 A890 U891 U892 C893 U894 U895 G896 G897 A898 U899 U900 U901 A902 U903 U904 G905 A906 A907 G908 A909 C910 A913 C914 U915 A916 C917 U918 G919 C920 G921 A922 A923 A924 G925 C926 A927 U928 U929 U930
G931 C932 C933 A934 A935 G936 G937 A938 C939 G940 U941 U942 U943 U944 C945 A946 A949 A950 U951 C952 A953 A954 G955 A956 A957 C958 G959 A960 A961 A962 G963 U964 U965 A966 G967 G968 G969 G970 A971 U972 C973 G974 A975 A976 G977 A978 U979 G980 A981 U982 A986 U987 A988 C989 C990 G991 U992 C993
G994 U995 A996 G997 U998 C999 U1000 U1001 A1002 A1003 C1004 C1005 A1006 U1007 A1008 A1009 A1010 C1011 U1012 A1013 U1014 G1015 C1016 C1017 G1018 A1019 C1020 U1021 A1022 G1023 G1024 G1025 A1026 U1027 C1028 G1029 G1030 G1034 U1035 G1036 U1040 U1041 U1042 U1043 A1044 A1045 U1046 G1047 A1048 C1049 C1053 U1054 C1055 G1056 G1057 C1058 A1059
C1060 C1061 U1062 U1063 A1064 C1065 G1066 A1067 G1068 A1069 A1070 A1071 U1072 C1073 A1074 A1075 A1076 G1077 U1078 C1079 U1080 U1081 U1082 G1083 G1084 G1085 U1086 U1087 C1088 U1089 G1090 G1091 G1092 G1093 G1094 G1095 A1096 G1097 U1098 A1099 U1100 G1101 G1102 U1103 C1104 G1105 C1106 A1107 A1108 G1109 G1110 C1111 U1112 G1113 A1114 A1115 A1116 C1117 U1118 U1119
A1120 A1121 A1122 G1123 G1124 A1125 A1126 U1127 U1128 G1129 A1130 C1131 G1132 G1133 A1134 A1135 G1136 G1137 G1138 C1139 A1140 C1141 C1142 A1143 C1144 C1145 A1146 G1147 G1148 A1149 G1150 U1151 G1152 G1153 A1154 G1155 C1156 C1157 U1158 G1159 C1160 G1161 G1162 C1163 U1164 U1165 A1166 A1167 U1168 U1169 U1170 G1171 A1172 C1173 A1174 C1175 A1176 A1177 C1178 A1179
C1180 G1181 G1182 G1183 G1184 A1185 C1188 U1189 C1190 A1191 C1192 C1193 A1194 G1195 C1198 C1199 A1200 G1201 A1202 C1203 A1206 A1210 G1211 G1212 A1213 U1214 U1215 C1218 U1223 G1224 A1225 G1226 A1227 G1228 C1229 U1230 C1231 U1232 U1233 U1234 C1235 U1241 U1242 U1243 G1244 U1245 G1246 G1247 G1248 U1249 G1250 G1251 U1252
G1253 G1254 U1255 G1256 C1257 A1258 U1259 G1260 G1261 C1262 C1263 G1264 U1265 U1266 C1267 U1268 U1269 A1270 G1271 U1272 U1273 G1274 G1275 U1276 G1277 G1278 A1279 G1280 U1281 G1282 A1283 U1284 U1285 U1286 G1287 U1288 C1289 U1290 G1291 C1292 U1293 U1294 A1295 A1296 U1297 U1298 G1299 C1300 G1301 A1302 U1303 A1304 A1305 C1306 G1307 A1308 A1309 C1310 G1311 A1312
G1313 A1314 C1315 C1316 U1317 U1318 A1319 A1320 C1321 C1322 U1323 A1324 C1325 U1326 A1327 A1328 A1329 U1330 A1331 G1332 U1333 G1334 G1335 U1336 G1337 C1338 C1342 A1343 U1344 U1345 U1346 G1347 C1348 U1349 G1350 G1351 U1352 U1353 A1354 U1355 C1356 C1357 A1358 C1359 U1360 U1361 C1362 U1363 U1364 A1365 G1366 A1367 G1368 G1369 G1370 A1371 C1372 U1373 A1374
U1375 C1376 G1377 U1380 U1381 C1382 A1383 A1384 G1385 U1390 G1391 G1392 A1393 A1394 G1395 U1396 U1397 U1398 G1399 A1400 G1401 G1402 C1403 A1404 A1405 U1406 A1407 A1408 C1409 A1410 G1411 G1412 U1413 C1414 U1415 G1416 U1417 G1418 A1419 U1420 G1421 C1422 C1423 C1424 U1425 U1426 A1427 G1428 A1429 C1430 G1431 U1432 U1433 C1434 U1435 G1436 G1437 G1438
C1439 C1440 G1441 C1442 A1443 C1444 G1445 C1446 G1447 C1448 G1449 A1452 C1453 A1454 C1455 U1456 G1457 A1458 C1459 G1460 G1461 A1462 G1463 C1464 C1465 A1466 G1467 C1468 G1469 A1470 G1471 U1472 C1473 U1474 A1475 A1476 C1477 C1478 U1479 U1480 G1481 G1482 C1483 C1484 G1485 A1486 G1487 A1488 G1489 G1490 U1491 C1492 U1493 U1494 G1495 G1496 U1497 A1498 A1499



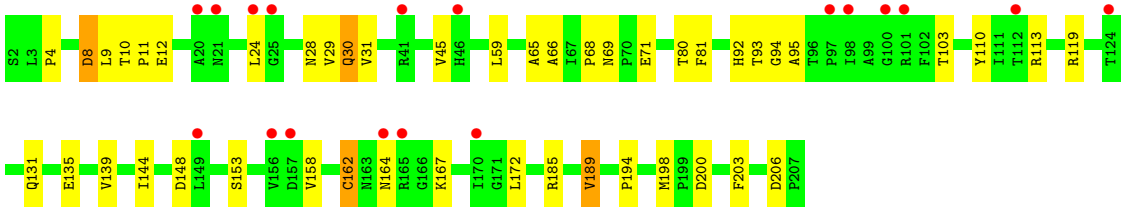
- Molecule 2: 40S ribosomal protein S0-A

Chain S0:



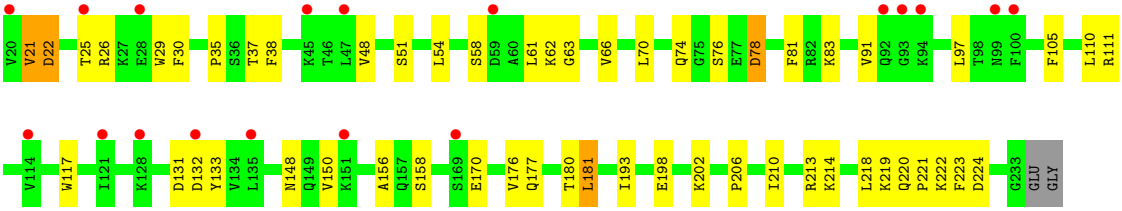
- Molecule 2: 40S ribosomal protein S0-A

Chain s0:



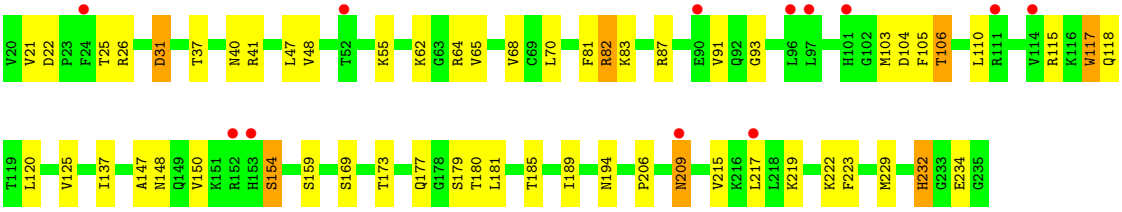
- Molecule 3: 40S ribosomal protein S1-B

Chain S1: 8% 74% 24%



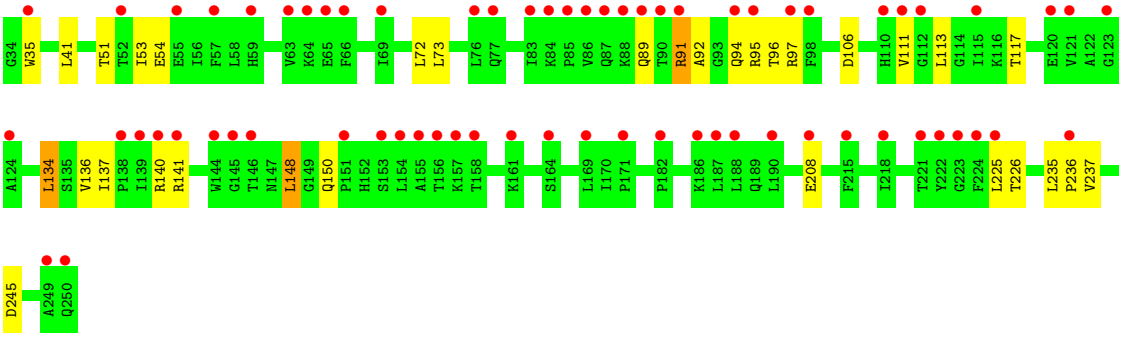
- Molecule 3: 40S ribosomal protein S1-B

Chain s1: 6% 74% 23%



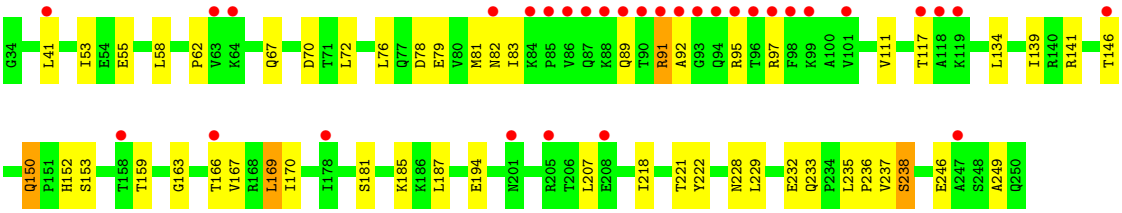
- Molecule 4: 40S ribosomal protein S2

Chain S2: 31% 85% 13%



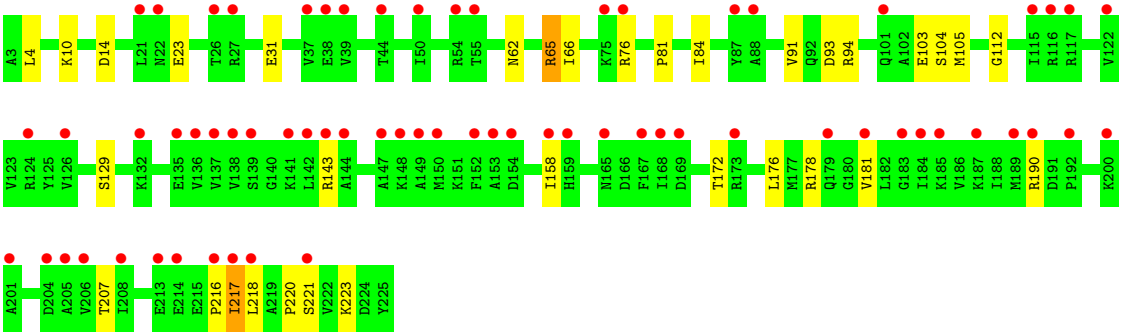
- Molecule 4: 40S ribosomal protein S2

Chain s2: 15% 76% 22%



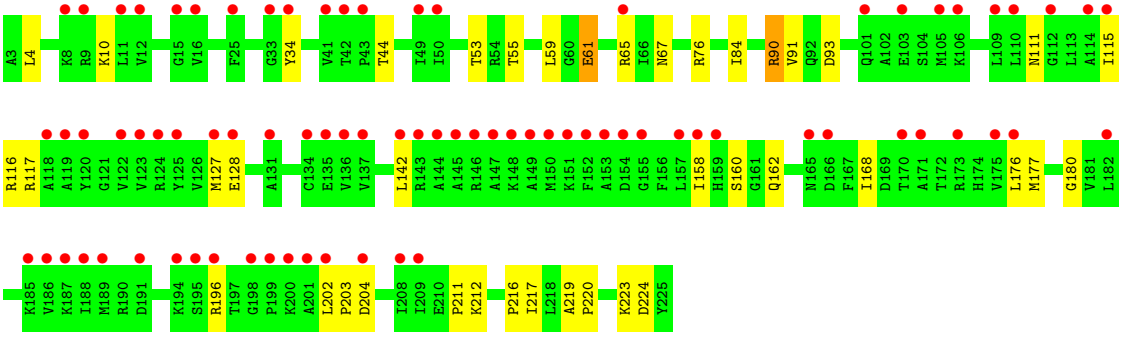
- Molecule 5: 40S ribosomal protein S3

Chain S3: 30% 85% 14%



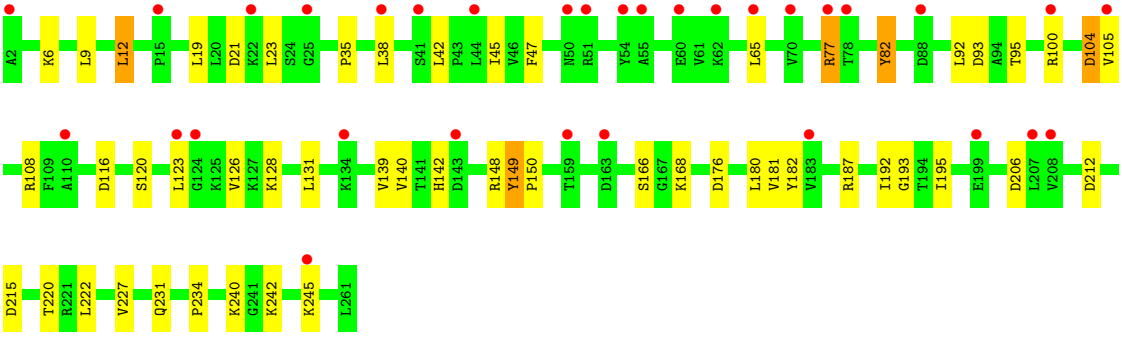
- Molecule 5: 40S ribosomal protein S3

Chain s3:



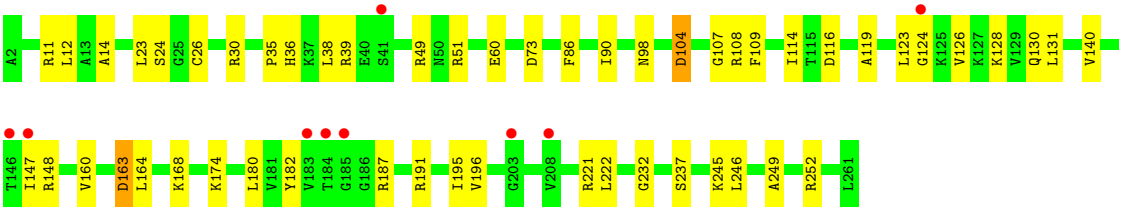
- Molecule 6: 40S ribosomal protein S4-A

Chain S4:



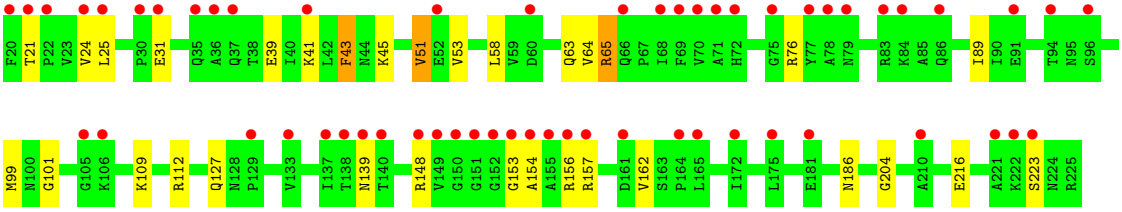
- Molecule 6: 40S ribosomal protein S4-A

Chain s4:



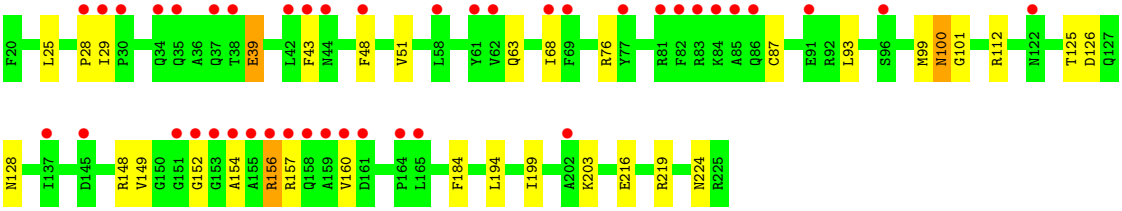
- Molecule 7: 40S ribosomal protein S5

Chain S5:



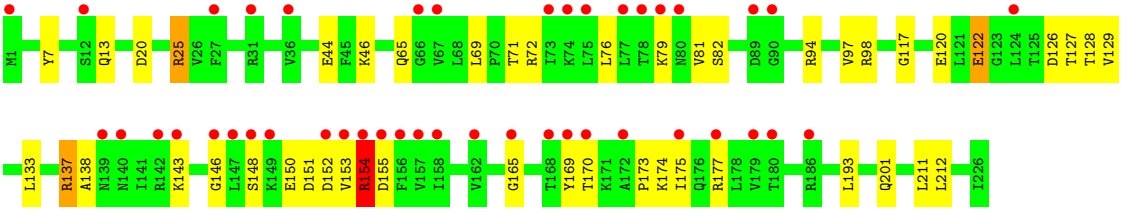
- Molecule 7: 40S ribosomal protein S5

Chain s5:



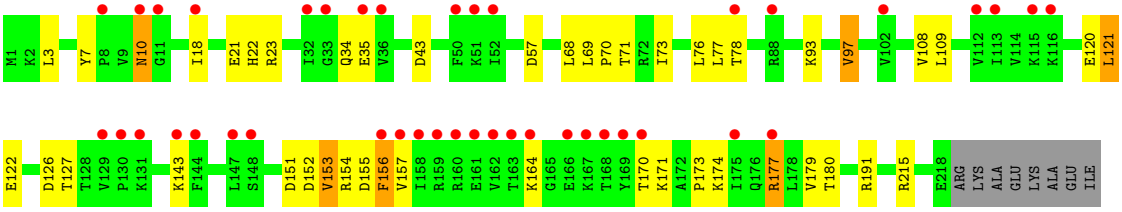
- Molecule 8: 40S ribosomal protein S6-A

Chain S6:



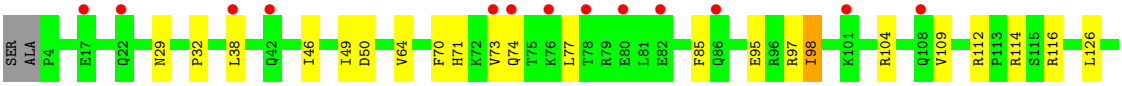
- Molecule 8: 40S ribosomal protein S6-A

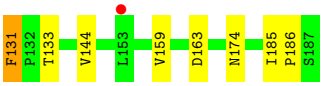
Chain s6:



- Molecule 9: 40S ribosomal protein S7-A

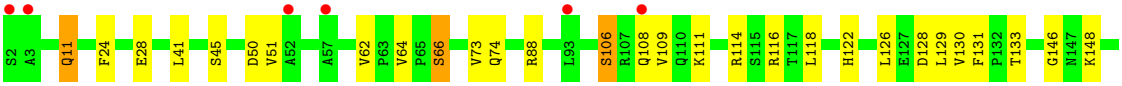
Chain S7:

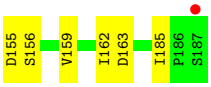




• Molecule 9: 40S ribosomal protein S7-A

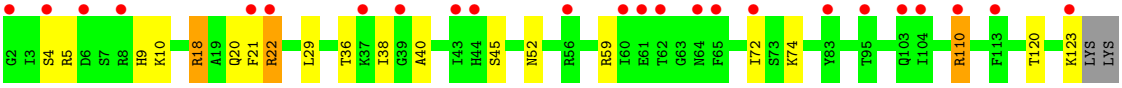
Chain s7:

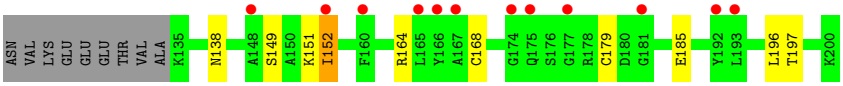




• Molecule 10: 40S ribosomal protein S8-A

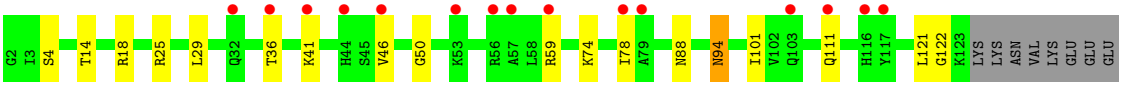
Chain S8:

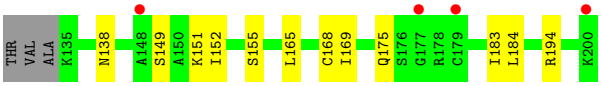




• Molecule 10: 40S ribosomal protein S8-A

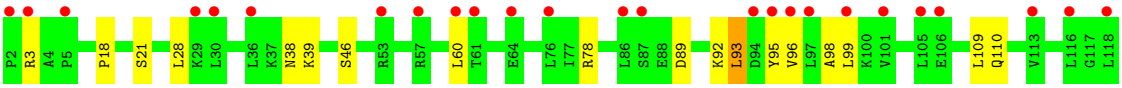
Chain s8:

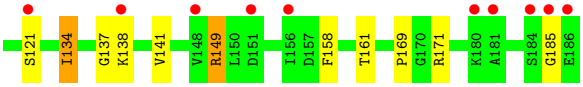




• Molecule 11: 40S ribosomal protein S9-A

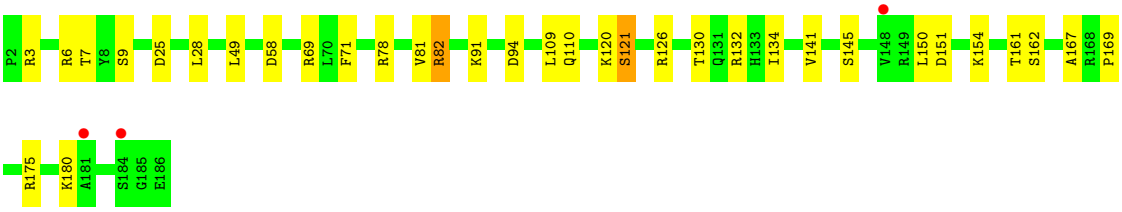
Chain S9:





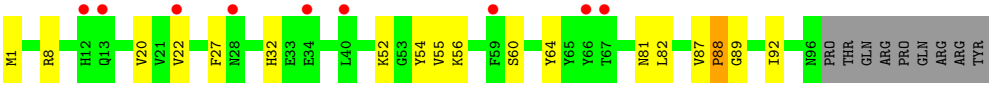
• Molecule 11: 40S ribosomal protein S9-A

Chain s9:



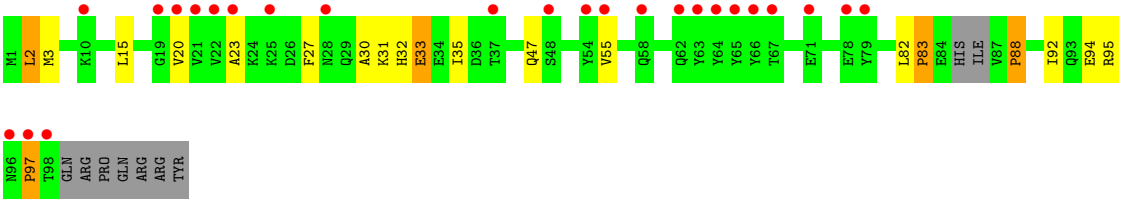
• Molecule 12: 40S ribosomal protein S10-A

Chain C0:



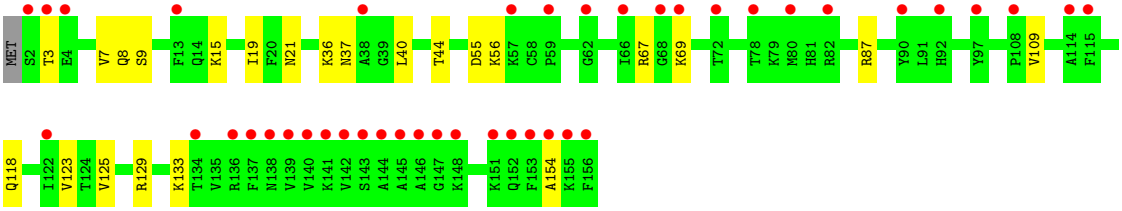
• Molecule 12: 40S ribosomal protein S10-A

Chain c0:



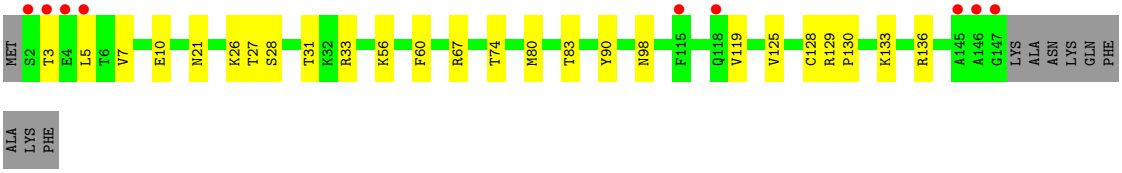
• Molecule 13: 40S ribosomal protein S11-A

Chain C1:



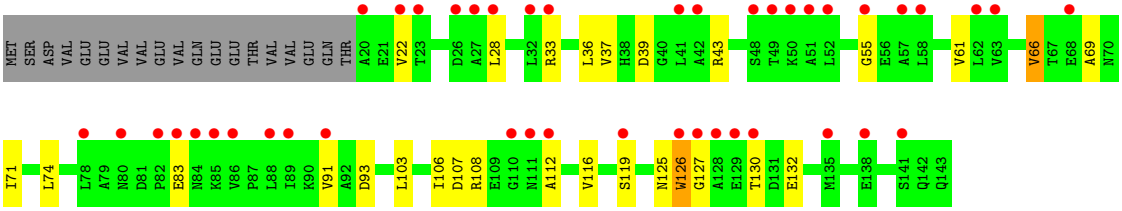
• Molecule 13: 40S ribosomal protein S11-A

Chain c1:



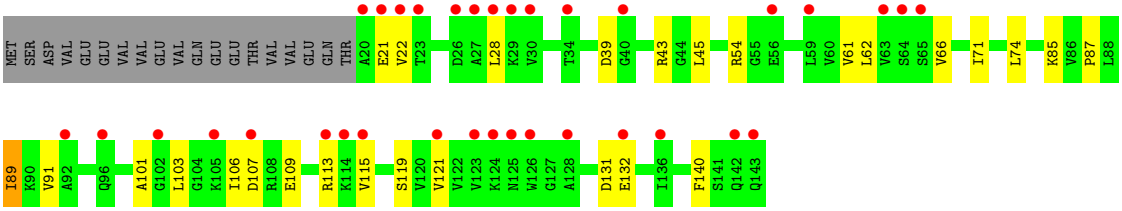
• Molecule 14: 40S ribosomal protein S12

Chain C2:



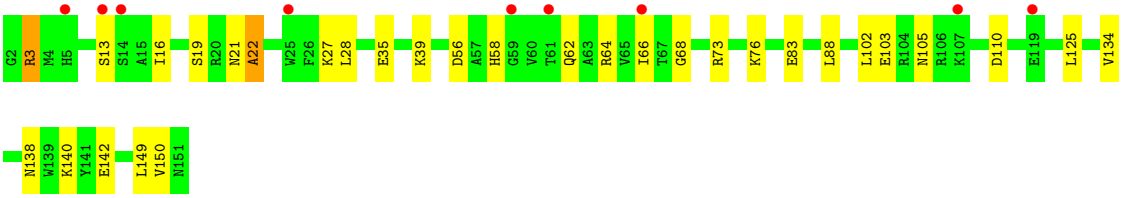
- Molecule 14: 40S ribosomal protein S12

Chain c2:



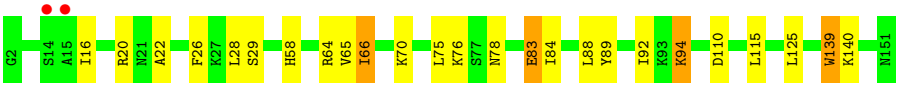
- Molecule 15: 40S ribosomal protein S13

Chain C3:



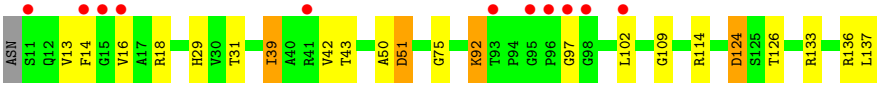
- Molecule 15: 40S ribosomal protein S13

Chain c3:



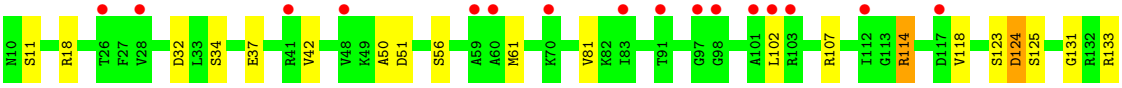
- Molecule 16: 40S ribosomal protein S14-B

Chain C4:



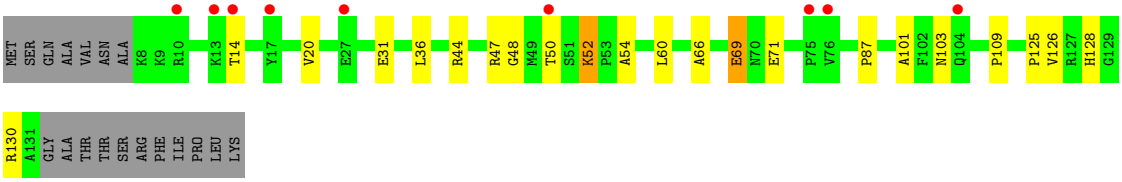
- Molecule 16: 40S ribosomal protein S14-B

Chain c4:



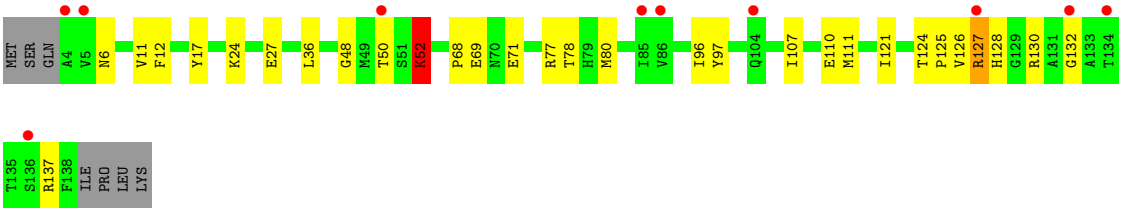
• Molecule 17: 40S ribosomal protein S15

Chain C5:



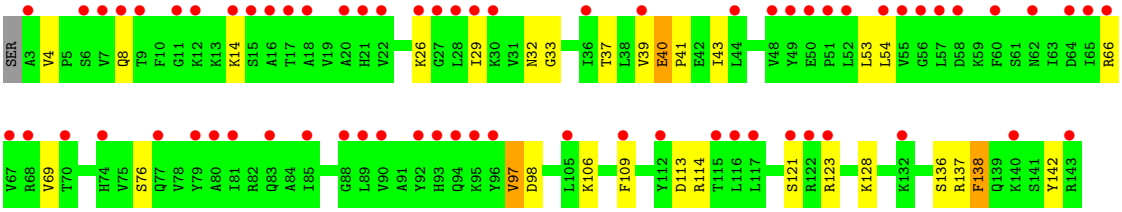
• Molecule 17: 40S ribosomal protein S15

Chain c5:



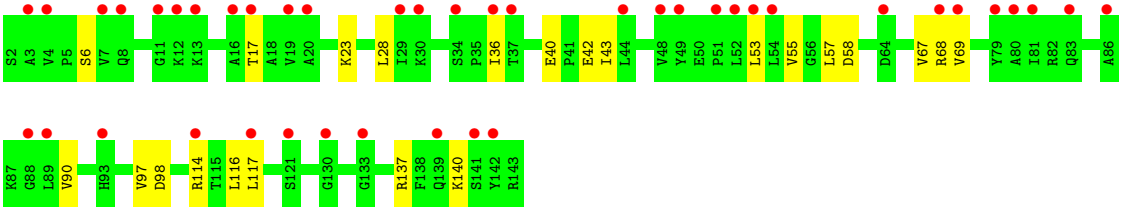
• Molecule 18: 40S ribosomal protein S16-A

Chain C6:



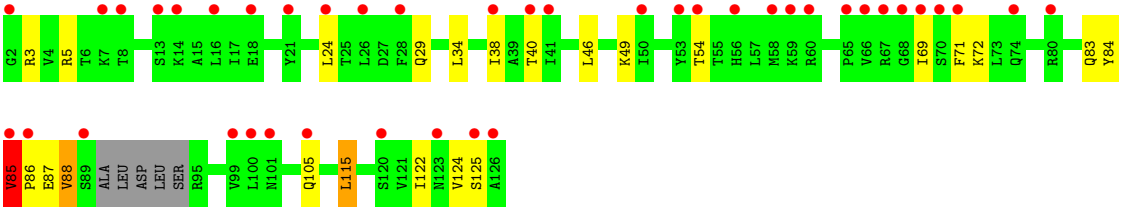
• Molecule 18: 40S ribosomal protein S16-A

Chain c6:



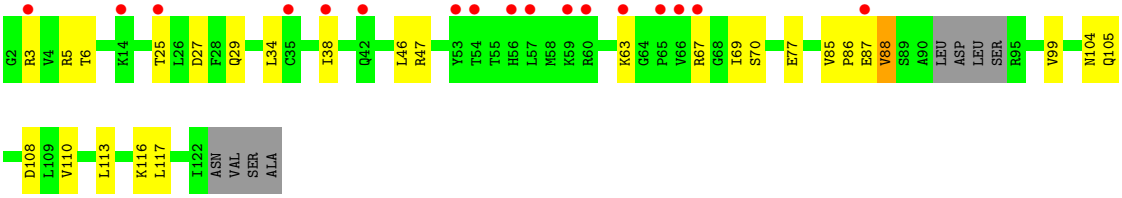
• Molecule 19: 40S ribosomal protein S17-B

Chain C7:



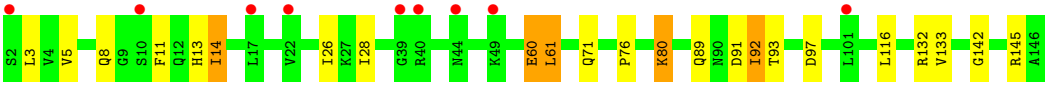
• Molecule 19: 40S ribosomal protein S17-B

Chain c7:



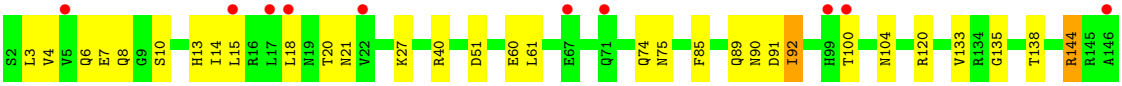
• Molecule 20: 40S ribosomal protein S18-A

Chain C8:



• Molecule 20: 40S ribosomal protein S18-A

Chain c8:

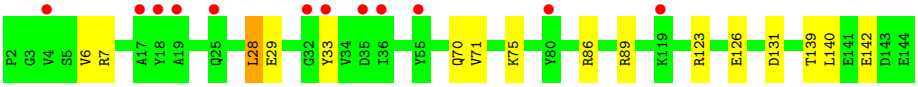


• Molecule 21: 40S ribosomal protein S19-A

Chain C9:

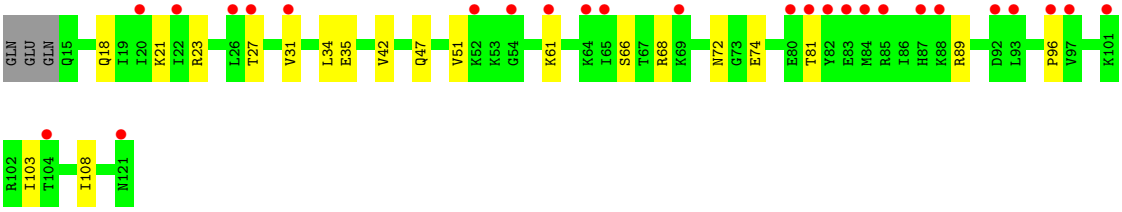
• Molecule 21: 40S ribosomal protein S19-A

Chain c9:



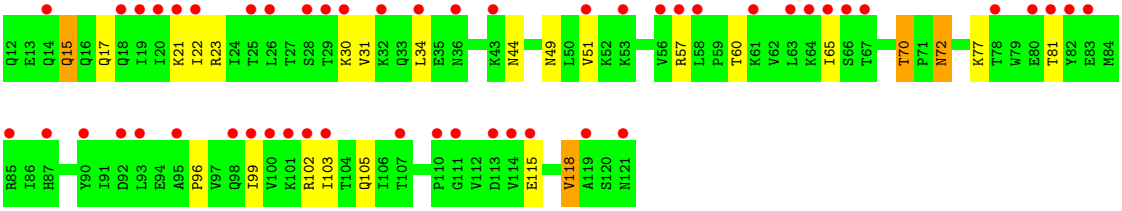
• Molecule 22: 40S ribosomal protein S20

Chain D0:



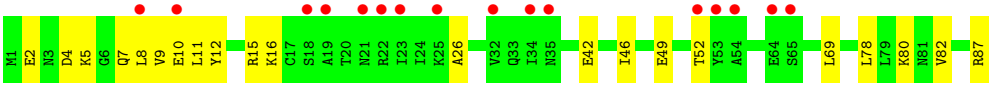
• Molecule 22: 40S ribosomal protein S20

Chain d0:



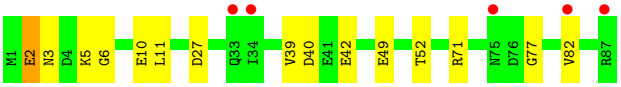
• Molecule 23: 40S ribosomal protein S21-A

Chain D1:



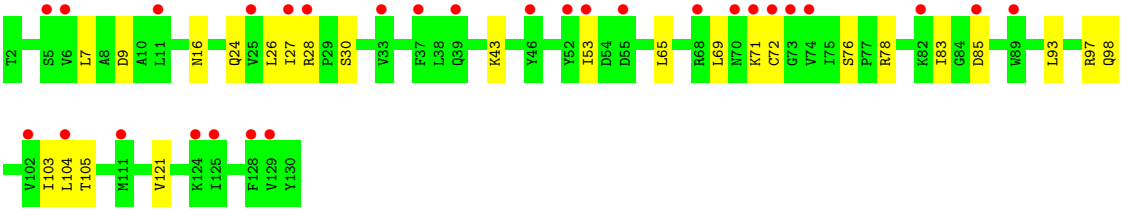
• Molecule 23: 40S ribosomal protein S21-A

Chain d1:



• Molecule 24: 40S ribosomal protein S22-A

Chain D2:

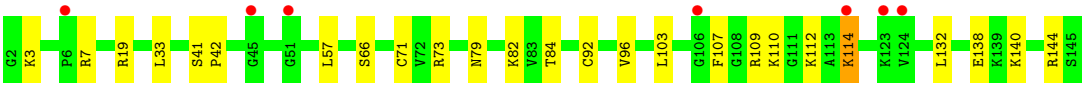


• Molecule 24: 40S ribosomal protein S22-A

Chain d2:

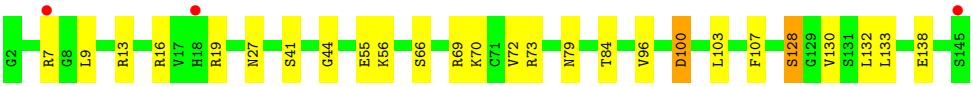
• Molecule 25: 40S ribosomal protein S23-A

Chain D3:



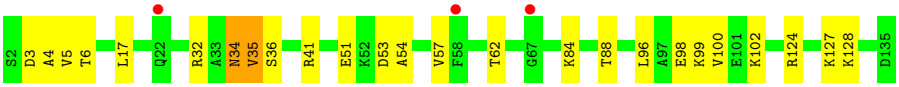
• Molecule 25: 40S ribosomal protein S23-A

Chain d3:



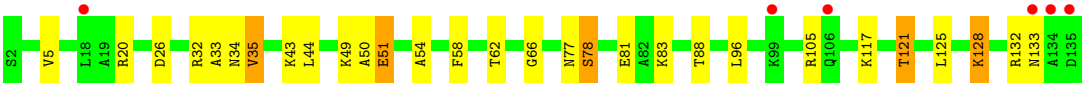
• Molecule 26: 40S ribosomal protein S24-A

Chain D4:



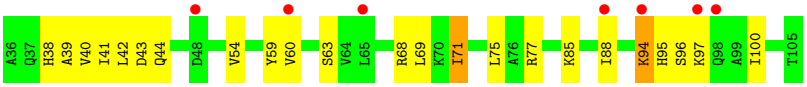
• Molecule 26: 40S ribosomal protein S24-A

Chain d4:



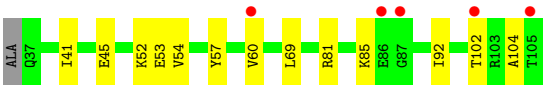
• Molecule 27: 40S ribosomal protein S25-A

Chain D5:



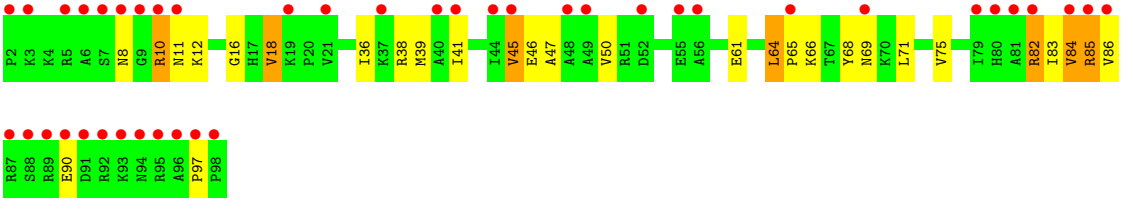
• Molecule 27: 40S ribosomal protein S25-A

Chain d5:



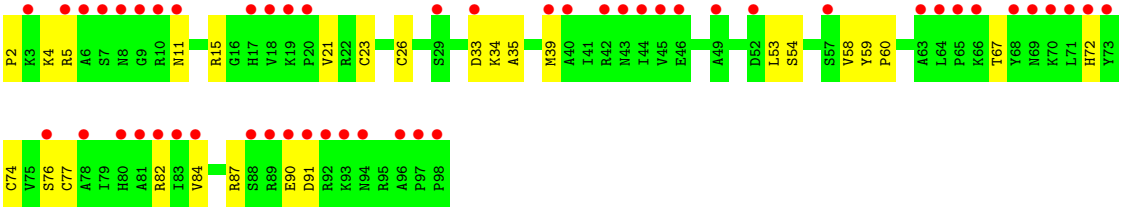
• Molecule 28: 40S ribosomal protein S26-B

Chain D6:



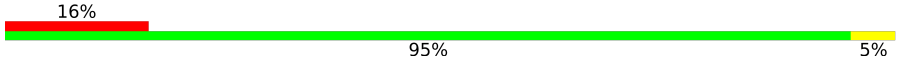
• Molecule 28: 40S ribosomal protein S26-B

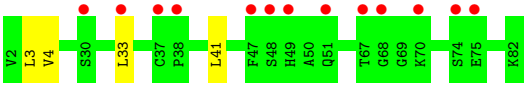
Chain d6:



• Molecule 29: 40S ribosomal protein S27-A

Chain D7:



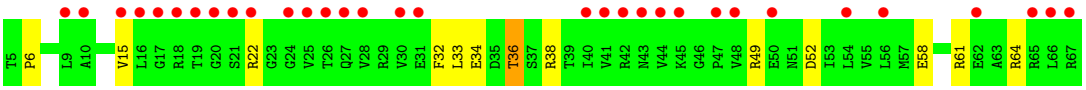


• Molecule 29: 40S ribosomal protein S27-A

Chain d7:

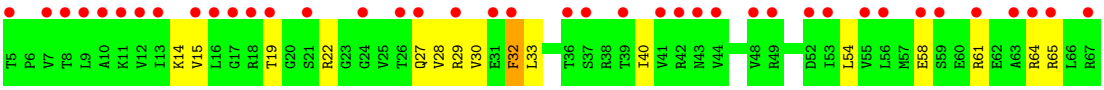
• Molecule 30: 40S ribosomal protein S28-A

Chain D8:



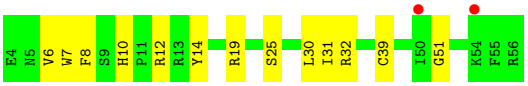
• Molecule 30: 40S ribosomal protein S28-A

Chain d8:



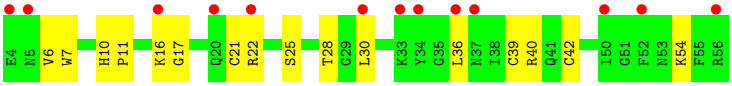
• Molecule 31: 40S ribosomal protein S29-A

Chain D9:



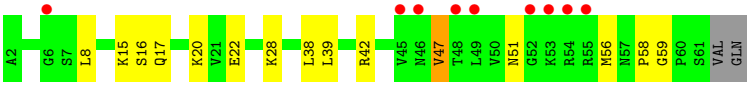
• Molecule 31: 40S ribosomal protein S29-A

Chain d9:



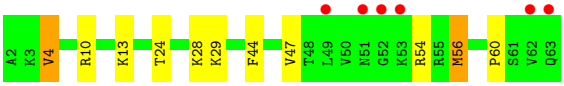
• Molecule 32: 40S ribosomal protein S30-A

Chain E0:



• Molecule 32: 40S ribosomal protein S30-A

Chain e0:

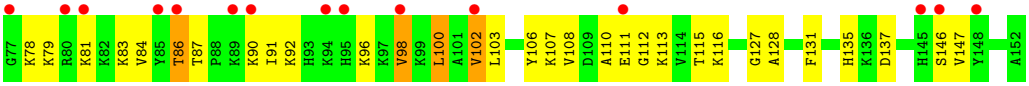


• Molecule 33: 40S ribosomal protein S31

Chain E1:

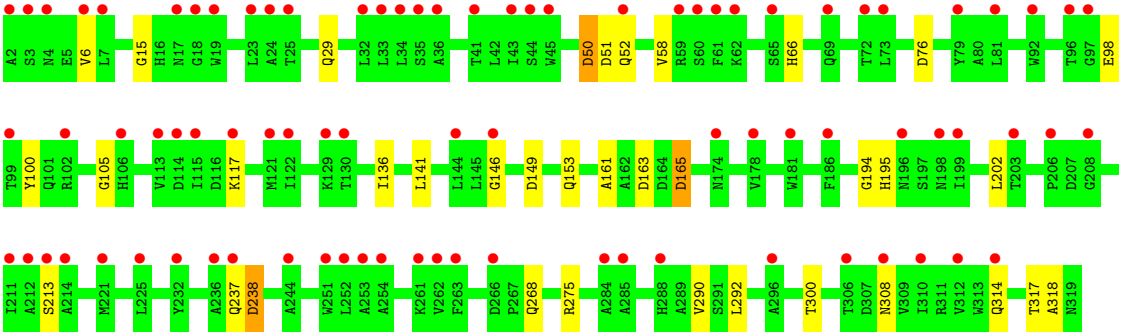
• Molecule 33: 40S ribosomal protein S31

Chain e1:



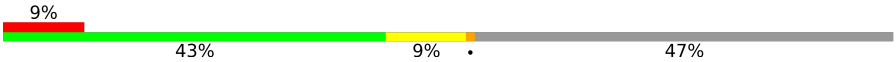
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

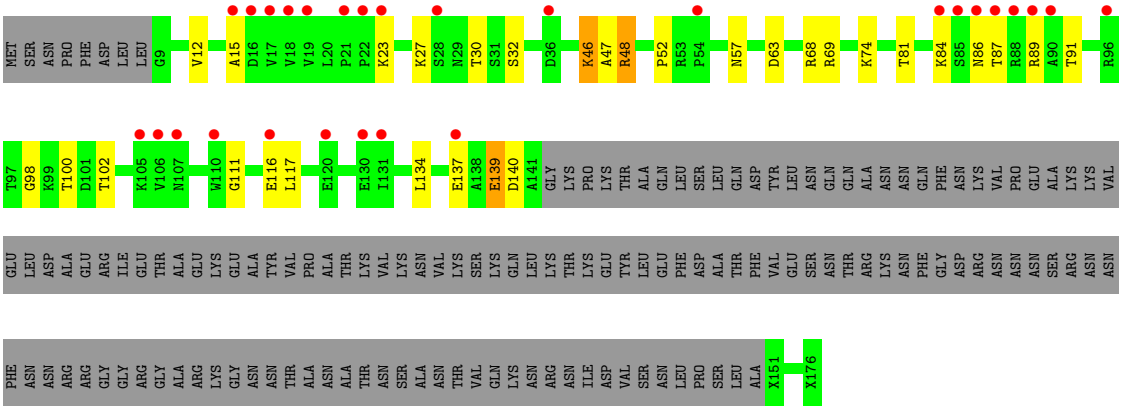
Chain SR:



• Molecule 35: Suppressor protein STM1,Ribosome-bound protein Stm1,Suppressor protein STM1,Ribosome-bound protein Stm1

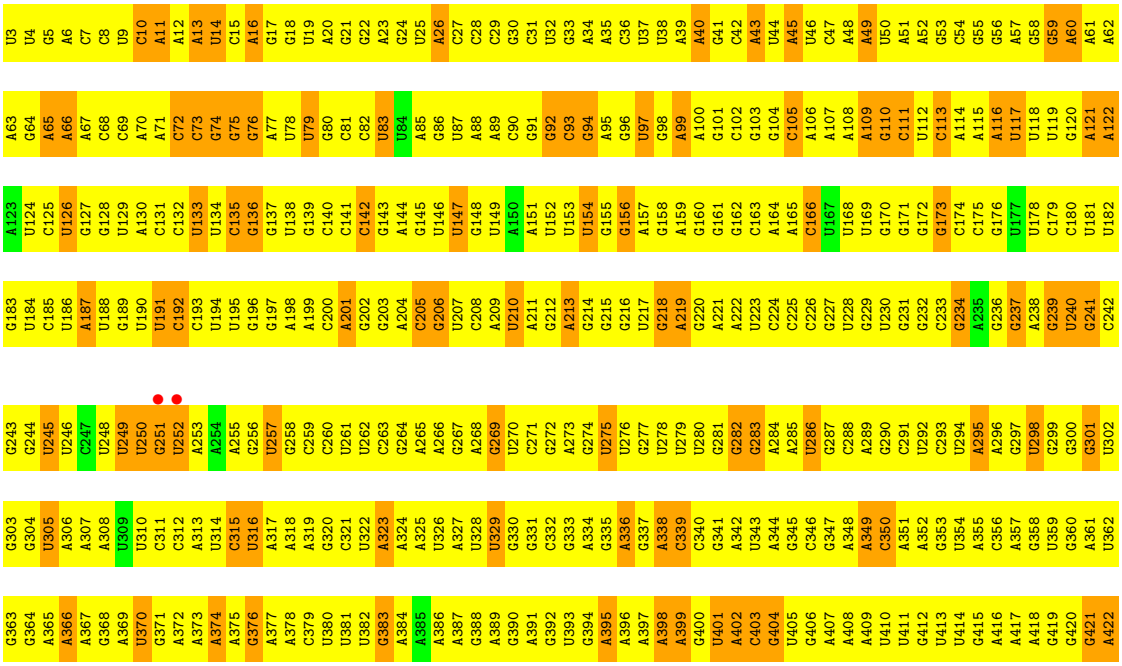
Chain SM:

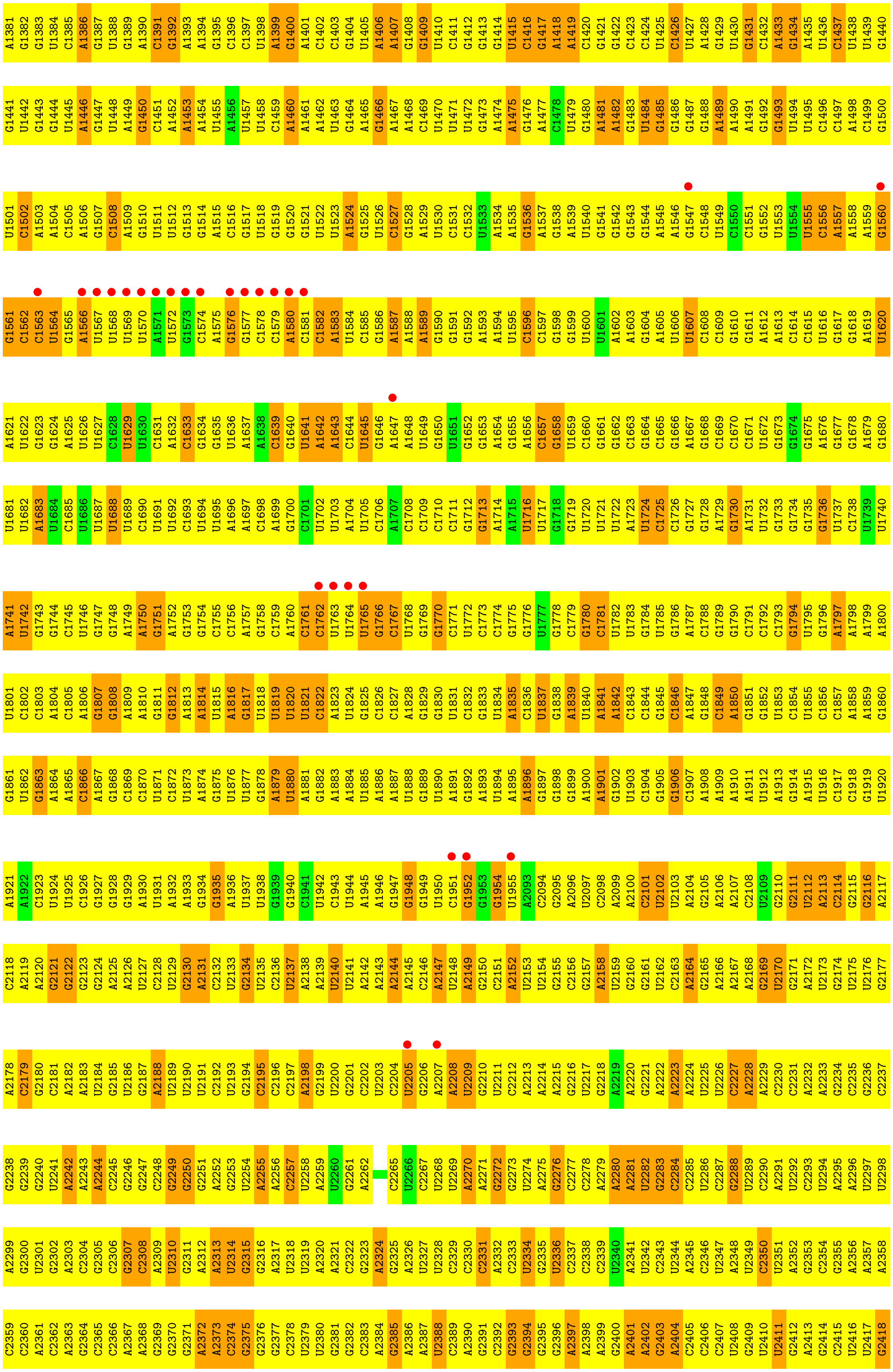




• Molecule 36: 25S ribosomal RNA

Chain 1:

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U3255 G3256 C3257 U3258 U3259 G3260 C3261 U3262 G3263 G3264 C3265 G3266 A3267 A3268 U3269 U3270 G3271 C3272 A3273 A3274 U3275 G3276 U3277 C3278 A3279 U3280 U3281 U3282 U3283 G3284 C3285 U3286 U3287 G3288 G3289 G3290 G3291 U3292 G3293 A3294 A3295 A3296 U3297 C3298 A3299 U3300 U3301 A3302 U3303 U3304 A3305 U3306 A3307 C3308 G3309 A3310 C3311 U3312 U3313 A3314
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A3375 A3376 G3377 C3378 C3379 U3380 U3381 U3382 G3383 U3384 U3385 G3386 U3387 C3388 U3389 G3390 A3391 U3392 U3393 U3394 G3395 U3396

- Molecule 37: 5S ribosomal RNA

Chain 3:

G1 G2 U3 U4 G5 C6 G7 G8 C9 C10 A11 U12 A13 U14 C15 U16 A17 C18 C19 A20 G21 A22 A23 A24 G25 C26 A27 C28 C29 G30 U31 U32 U33 C34 C35 C36 G37 U38 C39 C40 G41 A42 U43 C44 A45 A46 C47 U48 G49 U50 A51 G52 U53 U54 A55 A56 G57 C58 U59 G60

G61 U62 A63 A64 G65 A66 G67 C68 C69 U70 G71 A72 C73 C74 G75 A76 G77 U78 A79 G80 U81 G82 U83 A84 G85 U86 G87 G88 G89 U90 G91 A92 C93 C94 A95 U96 A97 U98 G99 C100 G101 A102 A103 A104 C105 U106 C107 A108 G109 G110 U111 G112 C113 U114 G115 C116 A117 A118 U119 C120

U121

- Molecule 37: 5S ribosomal RNA

Chain 7:

G1 G2 U3 U4 G5 C6 G7 G8 C9 C10 A11 U12 A13 U14 C15 U16 A17 C18 C19 A20 G21 A22 A23 A24 G25 C26 A27 C28 C29 G30 U31 U32 U33 C34 C35 C36 G37 U38 C39 C40 G41 A42 U43 C44 A45 A46 C47 U48 G49 U50 A51 G52 U53 U54 A55 A56 G57 C58 U59 G60

G61 U62 A63 A64 G65 A66 G67 C68 C69 U70 G71 A72 C73 C74 G75 A76 G77 U78 A79 G80 U81 G82 U83 A84 G85 U86 G87 G88 G89 U90 G91 A92 C93 C94 A95 U96 A97 C98 G99 C100 G101 A102 A103 A104 C105 U106 C107 A108 G109 G110 U111 G112 C113 U114 G115 C116 A117 A118 U119 C120

U121

- Molecule 38: 5.8S ribosomal RNA

Chain 4:

A1 A2 A3 C4 U5 U6 U7 C8 A9 A10 C11 A12 A13 C14 G15 G16 A17 U18 C19 U20 C21 U22 U23 G24 G25 U26 U27 C28 U29 C30 G31 C32 A33 U34 C35 G36 A37 U38 G39 A40 A41 G42 A43 A44 C45 G46 C47 A48 G49 C50 G51 A52 A53 A54 U55 G56 C57 G58 A59 U60

A61 C62 G63 U64 A65 A66 U67 G68 U69 G70 A71 A72 U73 U74 G75 C76 A77 G78 A79 A80 U81 U82 C83 C84 G85 U86 G87 A88 A89 U90 C91 A92 U93 C94 G95 A96 A97 U98 C99 U100 U101 U102 G103 A104 A105 C106 G107 C108 A109 C110 A111 U112 U113 G114 C115 G116 C117 C118 C119 C120

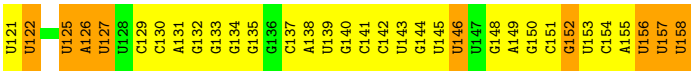
U121 U122 G123 G124 U125 A126 U127 U128 C129 C130 A131 G132 G133 G134 G135 G136 C137 A138 U139 G140 C141 C142 U143 G144 U145 U146 U147 G148 A149 G150 C151 G152 U153 C154 A155 U156 U157 U158

- Molecule 38: 5.8S ribosomal RNA

Chain 8:

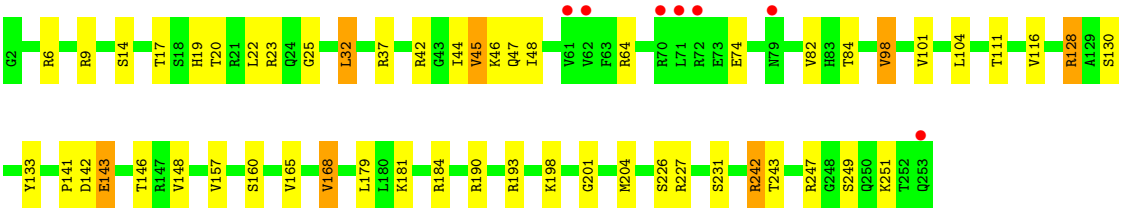
A1 A2 A3 C4 U5 U6 U7 C8 A9 A10 C11 A12 A13 C14 G15 G16 A17 U18 C19 U20 C21 U22 U23 G24 G25 U26 U27 C28 U29 C30 G31 C32 A33 U34 C35 G36 A37 U38 G39 A40 A41 G42 A43 A44 C45 G46 C47 A48 G49 C50 G51 A52 A53 A54 U55 G56 C57 G58 A59 U60

A61 C62 G63 U64 A65 A66 U67 G68 U69 G70 A71 A72 U73 U74 G75 C76 A77 G78 A79 A80 U81 U82 C83 C84 G85 U86 G87 A88 A89 U90 C91 A92 U93 C94 G95 A96 A97 U98 C99 U100 U101 U102 G103 A104 A105 C106 G107 C108 A109 C110 A111 U112 U113 G114 C115 G116 C117 C118 C119 C120



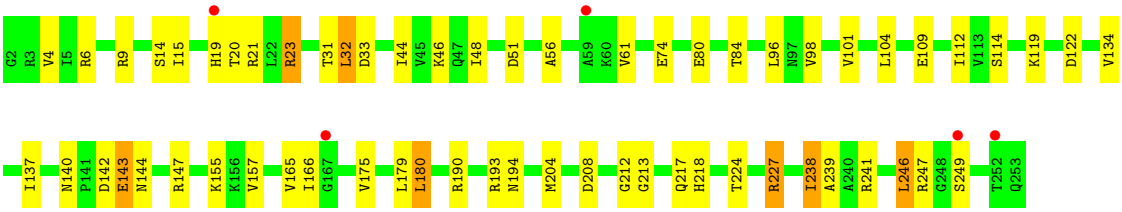
• Molecule 39: 60S ribosomal protein L2-A

Chain L2:



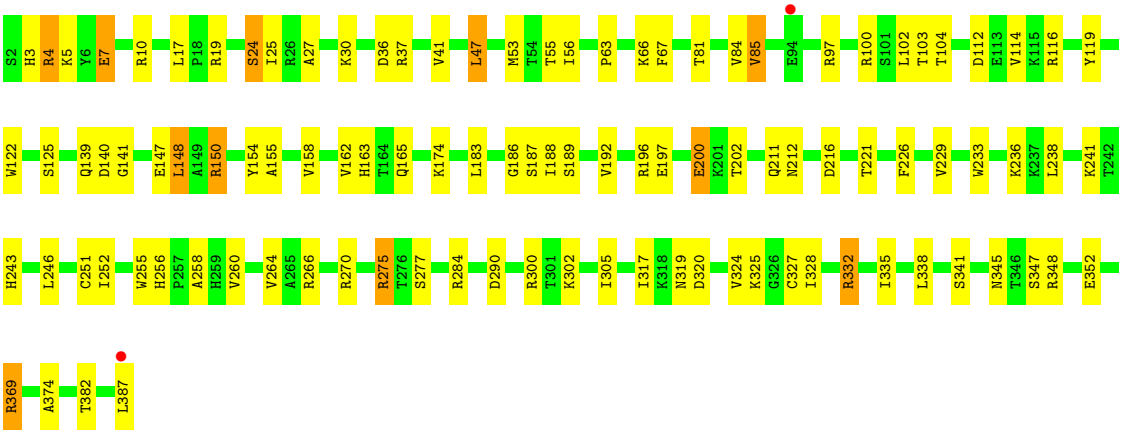
• Molecule 39: 60S ribosomal protein L2-A

Chain l2:



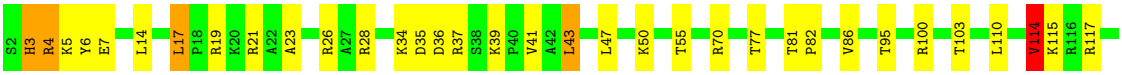
• Molecule 40: 60S ribosomal protein L3

Chain L3:



• Molecule 40: 60S ribosomal protein L3

Chain l3:



K120 K127 K128 A129 F130 A138 Q139 D140 G141 A142 R146 E147 L148 K153 Y154 A155 L161 R167 K168 G186 S187 D193 R196 E197 T202 V205 V208 N212 E213 M214 F226 V229 R232 W233 G234 T235 L238 R244 G245 L246 R247 K248

V249 W262 R275 I282 Y283 R284 K287 R300 T301 K302 K303 T304 Y314 N319 I322 M323 V324 K325 I328 R332 L338 R339 K340 S347 R348 L356 K367 G368 L383 K384 K385 D386 L387

- Molecule 41: 60S ribosomal protein L4-A

Chain L4: 75% 20% 6%

S2 R3 P4 Q5 V6 T7 L11 E14 A15 T16 L22 D33 R47 V52 S53 E54 Q59 S64 V71 I74 G79 T82 F90 M93 C94 R95 R98 M99 T105 W106 R107 K118 R119 Y120 A130 V131 R138 G139 H140 R141

I145 P146 E147 I148 P149 L150 L156 K170 A174 L179 K180 V181 L182 K183 S184 K185 R188 K193 Y194 R197 R202 R203 L206 V207 V216 L219 R220 N221 V222 T227 V230 L233 L238 R246 F247 V248 D259 Q260 V261 E265 T266 V267

A268 S269 S270 K271 V272 G273 S284 T287 R288 I289 S292 S293 R300 Q304 R309 T310 H311 V312 L313 L318 L324 L325 R326 L327 L339 T349 K350 D362

- Molecule 41: 60S ribosomal protein L4-A

Chain l4: 75% 20% 5%

S2 R3 L11 T12 G13 E14 A15 A24 V25 N43 R47 Y50 S53 E54 K55 T60 S61 A62 V71 A72 R73 F90 G91 N92 M93 C94 R98 T105 W106 V113 E117 Y120 A121 T122 I126 V135 L136 A137 R138 V142 E143 K144 I145

P146 E147 I148 P149 L150 V151 V152 L156 E157 S158 K163 E164 S176 D177 L178 L179 K186 L187 K193 Y194 R195 N196 R197 R202 R203 L206 R220 N221 V222 P223 L233 L244 G245 R246 F247 E252 L258 D259 Q260 V261 E265 V272 G273 Y274 T275 L276

S282 T283 S284 R288 I289 S292 I295 I299 R300 P301 A302 A305 T306 Q307 H311 V312 L313 N316 L327 V333 K342 E345 K346 T347 T356 D362

- Molecule 42: 60S ribosomal protein L5

Chain L5: 12% 78% 20%

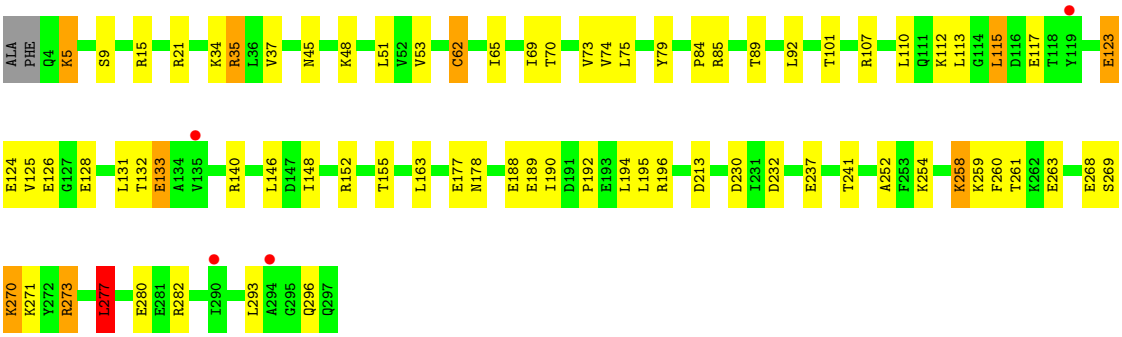
A2 A7 S10 R22 R23 G26 R35 K41 F55 T56 N57 I65 S66 S67 T68 I69 P84 H90 G91 L92 T93 N94 W95 Y99 I105 R108 T109 L110 L113 E117 V122 E123 E124 V125 E126 G127 E130 L131 T132 E133 D137

R140 V144 F145 L146 D147 I148 Q151 T155 V159 F160 G161 A162 L163 S167 D168 H175 S176 E177 F180 W183 D184 F185 E186 T187 E188 E189 I190 D191 P192 E193 L194 L195 Y198 I199 F200 H203 V204 S205 D213 D214 D215 E216 E217 R218 E221 L222 A233

D234 S235 L236 E237 D238 R248 A252 F253 K258 K259 E263 R273 R285 L293 A294 G295 Q296 Q297

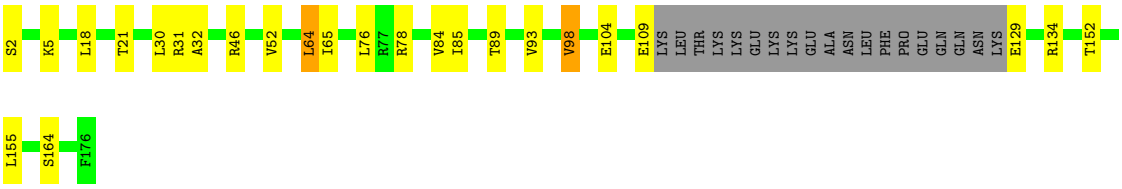
- Molecule 42: 60S ribosomal protein L5

Chain l5:



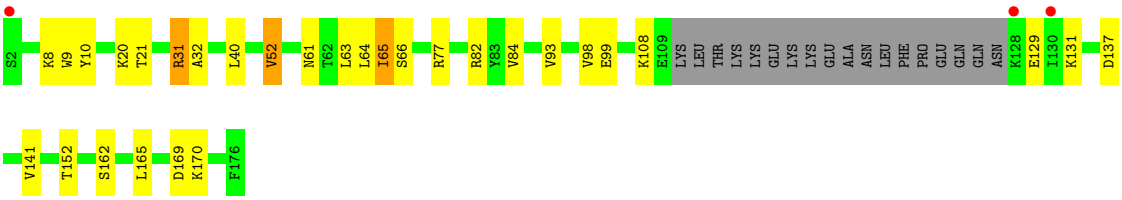
- Molecule 43: 60S ribosomal protein L6-A

Chain L6:



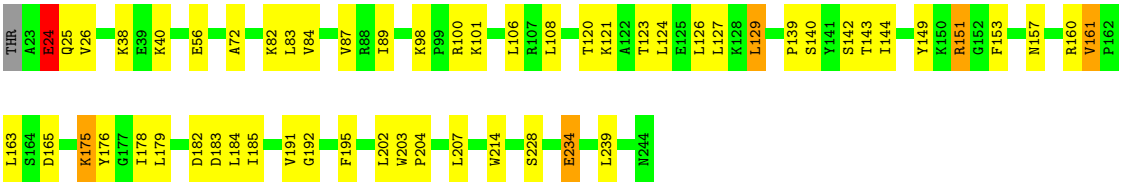
- Molecule 43: 60S ribosomal protein L6-A

Chain l6:



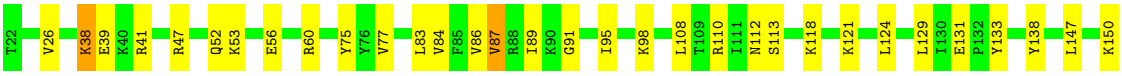
- Molecule 44: 60S ribosomal protein L7-A

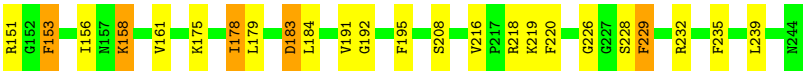
Chain L7:



- Molecule 44: 60S ribosomal protein L7-A

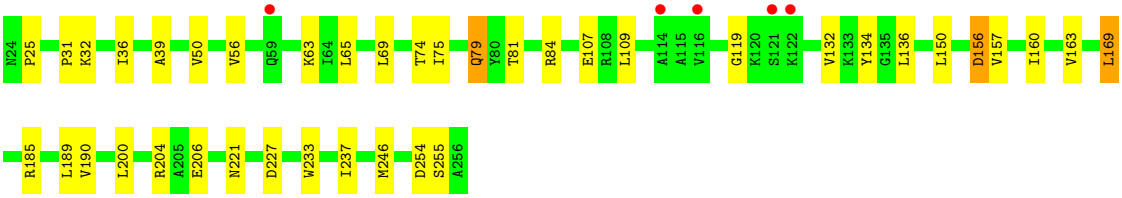
Chain l7:





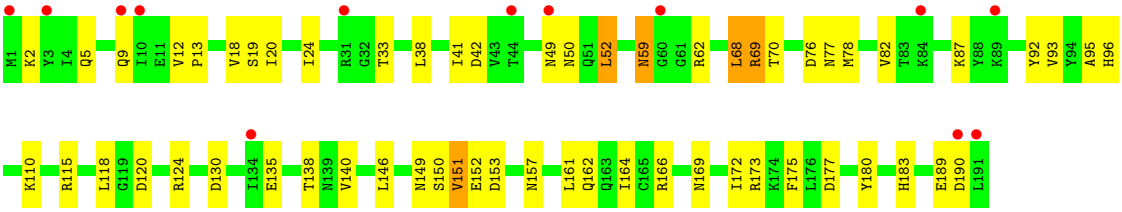
• Molecule 45: 60S ribosomal protein L8-A

Chain L8:



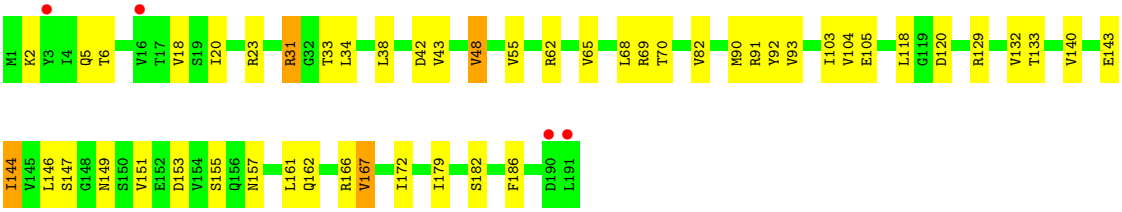
• Molecule 46: 60S ribosomal protein L9-A

Chain L9:



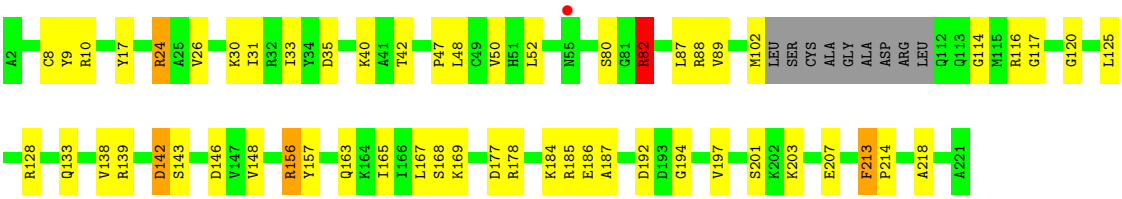
• Molecule 46: 60S ribosomal protein L9-A

Chain l9:



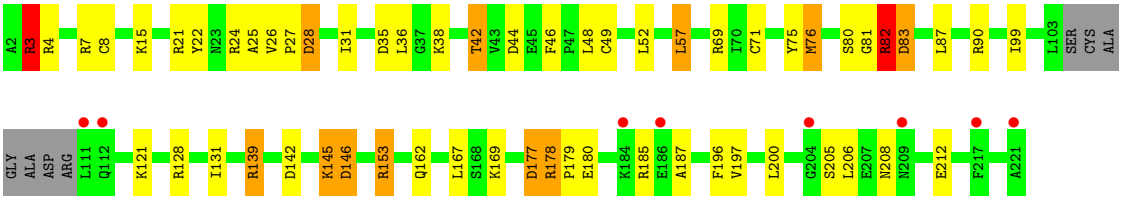
• Molecule 47: 60S ribosomal protein L10

Chain M0:



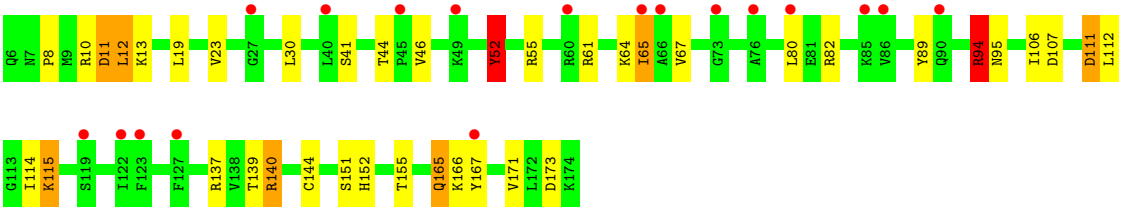
• Molecule 47: 60S ribosomal protein L10

Chain m0:



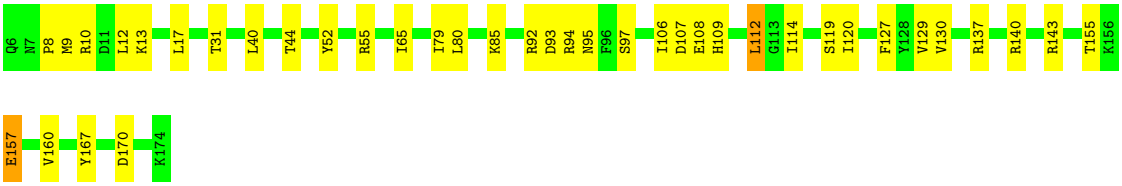
• Molecule 48: 60S ribosomal protein L11-B

Chain M1:



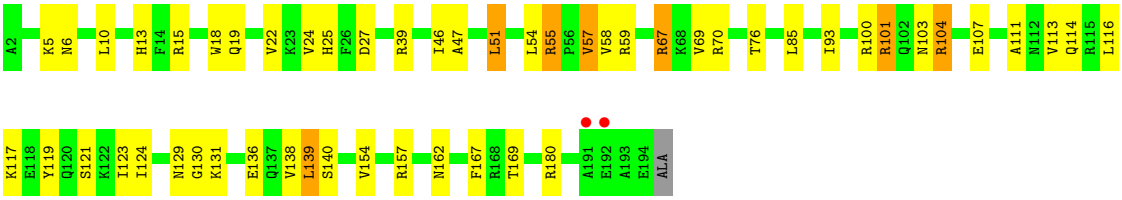
• Molecule 48: 60S ribosomal protein L11-B

Chain m1:



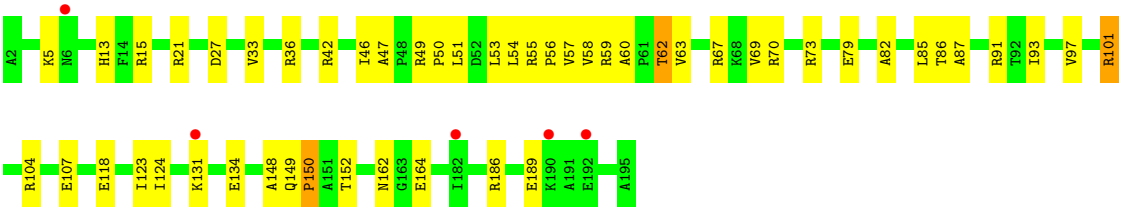
• Molecule 49: 60S ribosomal protein L13-A

Chain M3:



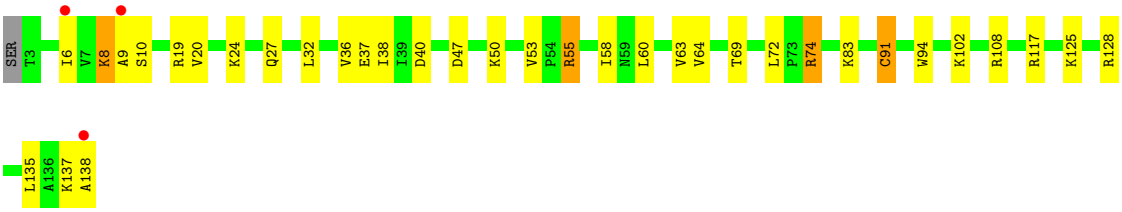
• Molecule 49: 60S ribosomal protein L13-A

Chain m3:



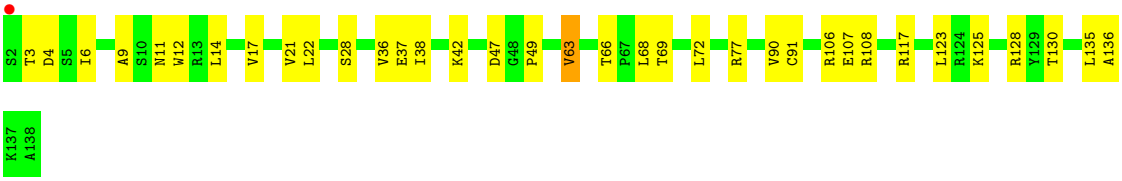
• Molecule 50: 60S ribosomal protein L14-A

Chain M4:



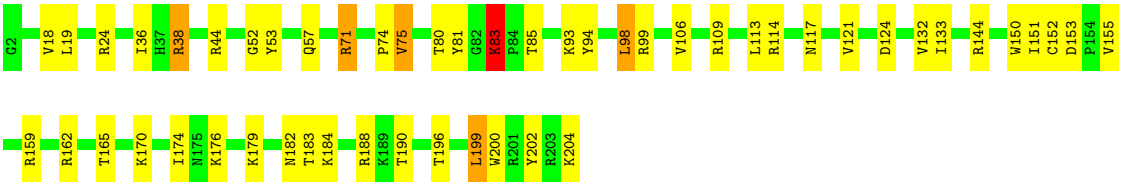
- Molecule 50: 60S ribosomal protein L14-A

Chain m4:



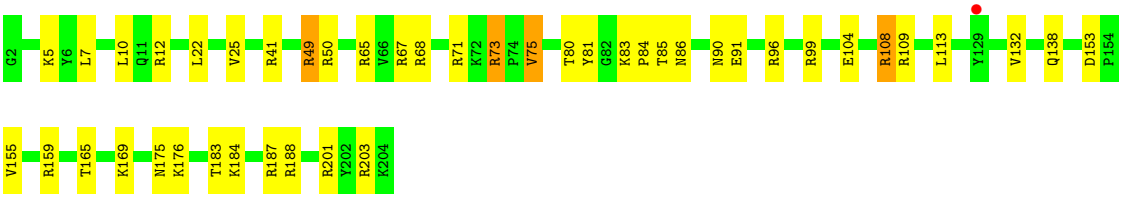
- Molecule 51: 60S ribosomal protein L15-A

Chain M5:



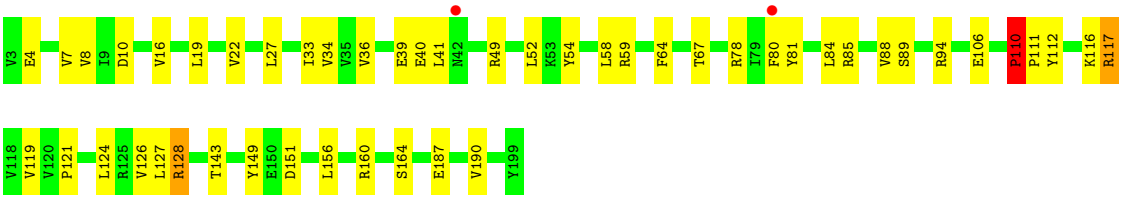
- Molecule 51: 60S ribosomal protein L15-A

Chain m5:



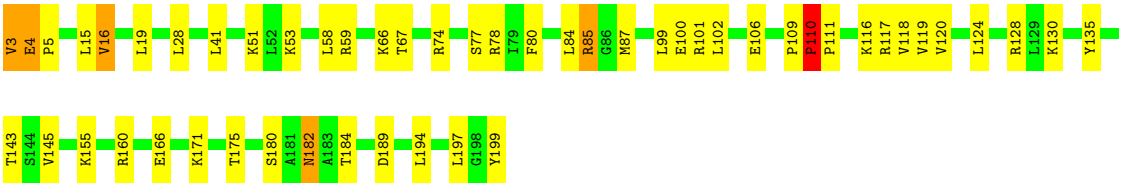
- Molecule 52: 60S ribosomal protein L16-A

Chain M6:



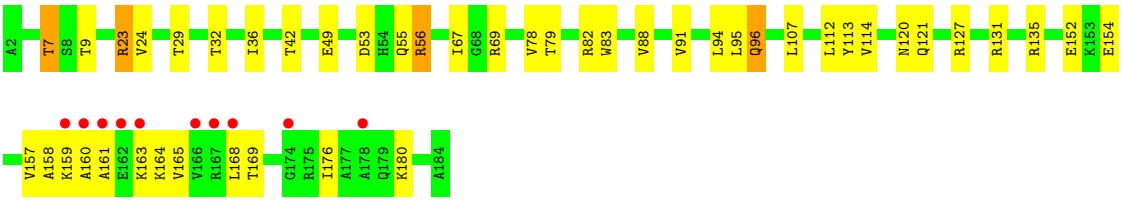
- Molecule 52: 60S ribosomal protein L16-A

Chain m6:



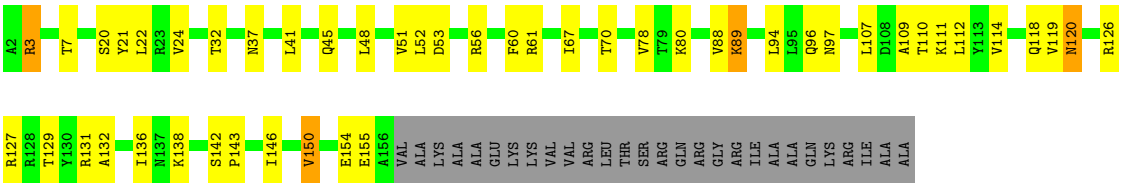
- Molecule 53: 60S ribosomal protein L17-A

Chain M7:



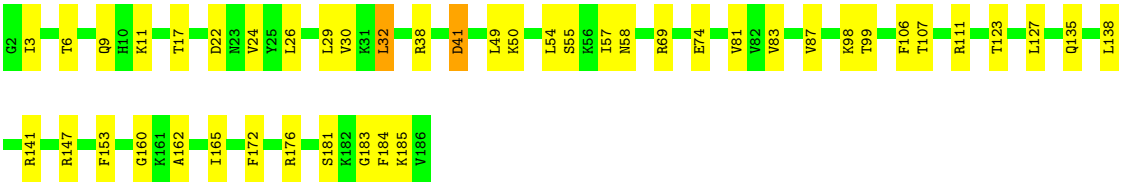
- Molecule 53: 60S ribosomal protein L17-A

Chain m7:



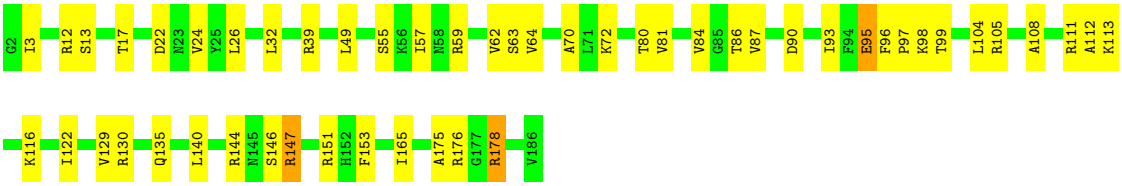
- Molecule 54: 60S ribosomal protein L18-A

Chain M8:



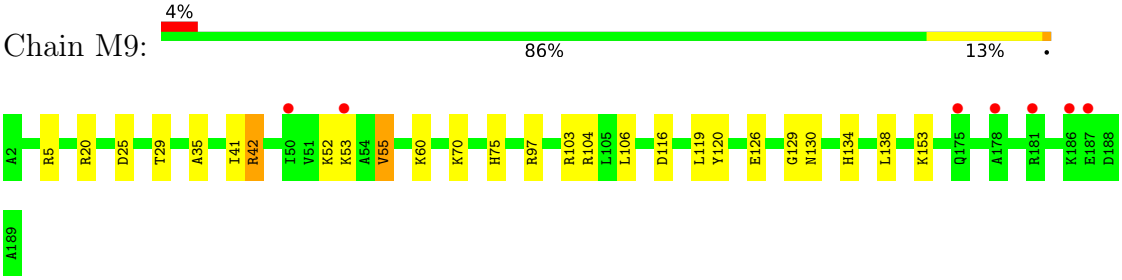
- Molecule 54: 60S ribosomal protein L18-A

Chain m8:



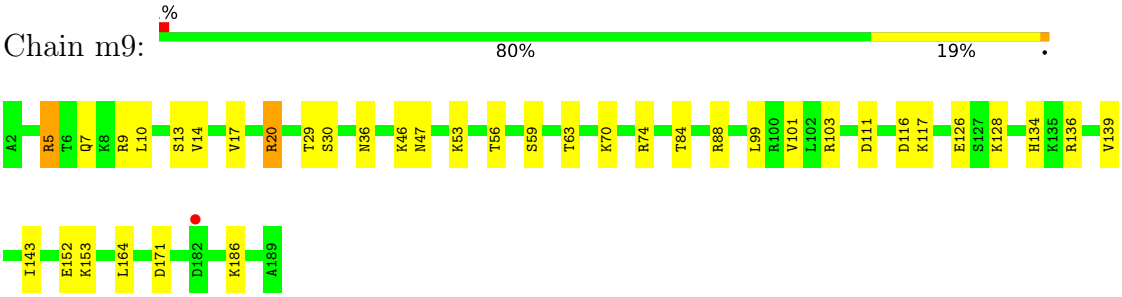
• Molecule 55: 60S ribosomal protein L19-A

Chain M9:



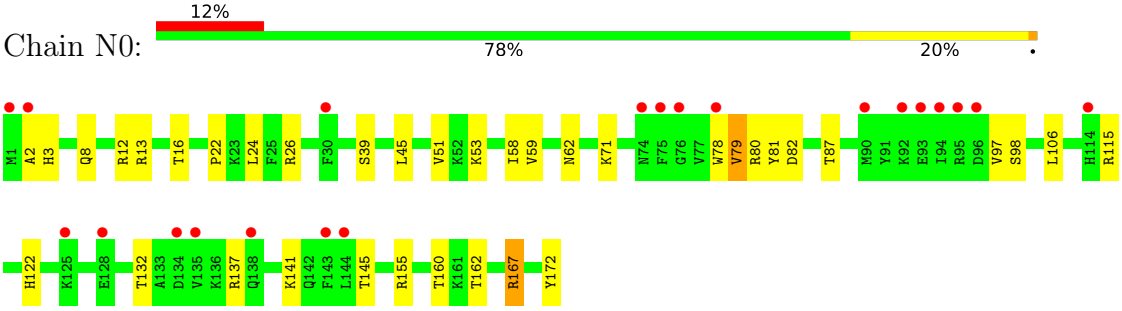
• Molecule 55: 60S ribosomal protein L19-A

Chain m9:



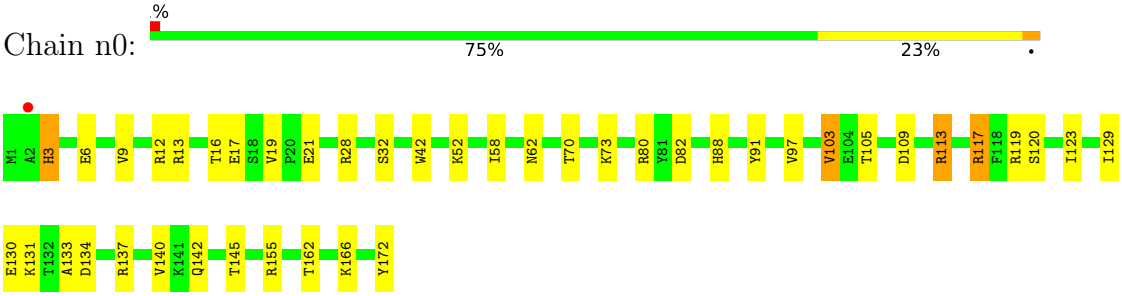
• Molecule 56: 60S ribosomal protein L20-A

Chain N0:



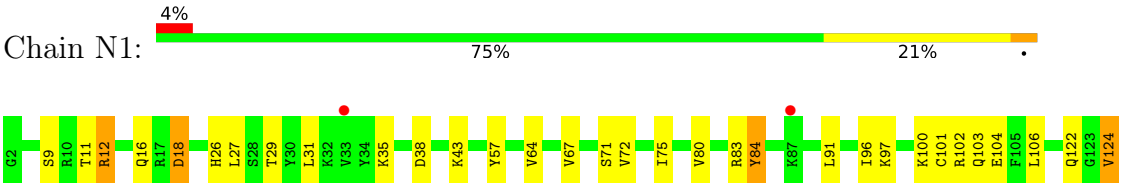
• Molecule 56: 60S ribosomal protein L20-A

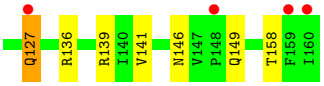
Chain n0:



• Molecule 57: 60S ribosomal protein L21-A

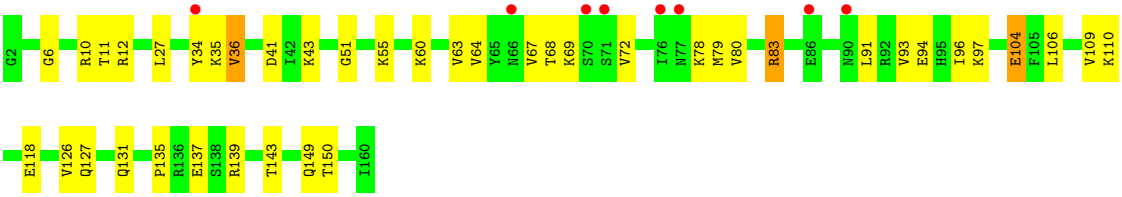
Chain N1:





• Molecule 57: 60S ribosomal protein L21-A

Chain n1:



• Molecule 58: 60S ribosomal protein L22-A

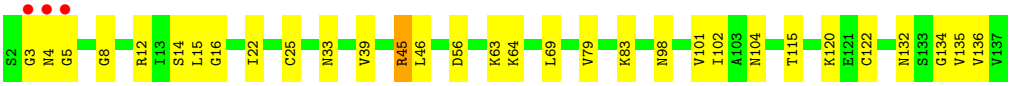
Chain N2:

• Molecule 58: 60S ribosomal protein L22-A

Chain n2:

• Molecule 59: 60S ribosomal protein L23-A

Chain N3:

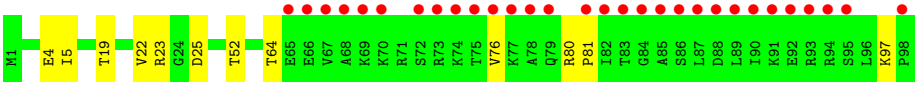


• Molecule 59: 60S ribosomal protein L23-A

Chain n3:

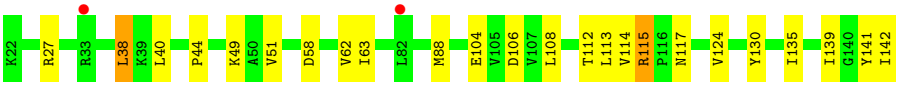
• Molecule 60: 60S ribosomal protein L24-A

Chain N4:



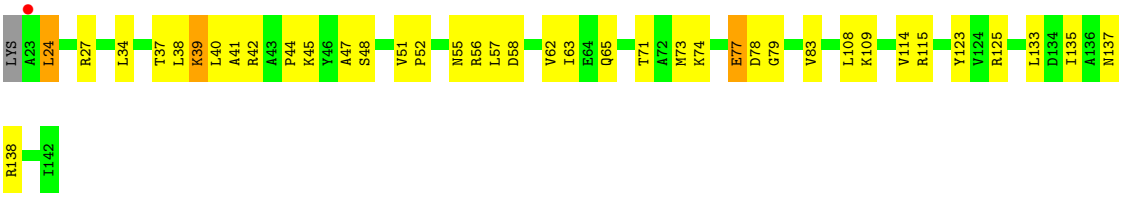
• Molecule 61: 60S ribosomal protein L25

Chain N5:



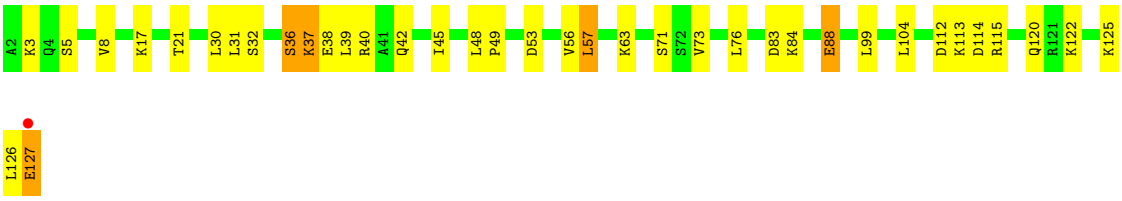
• Molecule 61: 60S ribosomal protein L25

Chain n5:



• Molecule 62: 60S ribosomal protein L26-A

Chain N6:

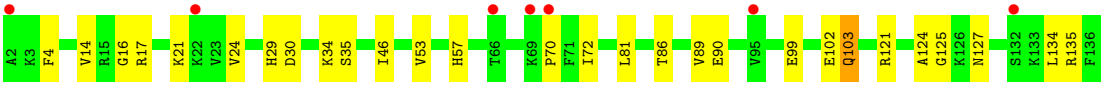


• Molecule 62: 60S ribosomal protein L26-A

Chain n6:

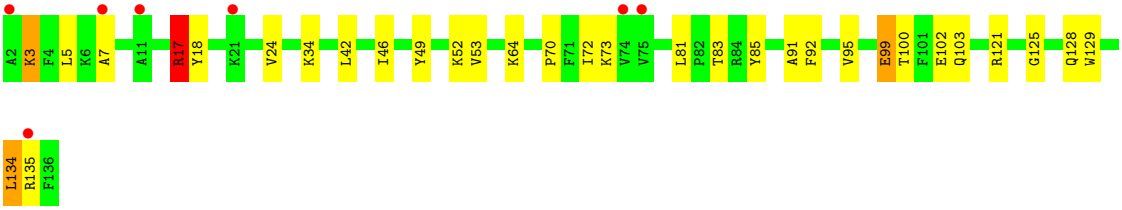
• Molecule 63: 60S ribosomal protein L27-A

Chain N7:



• Molecule 63: 60S ribosomal protein L27-A

Chain n7:

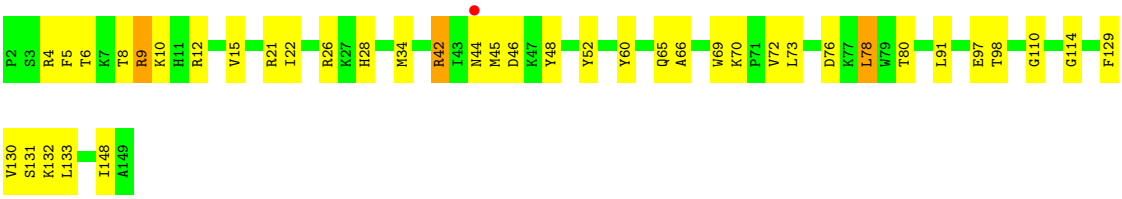


• Molecule 64: 60S ribosomal protein L28

Chain N8:

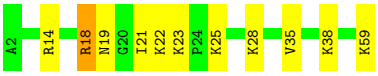
• Molecule 64: 60S ribosomal protein L28

Chain n8:



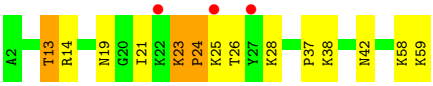
• Molecule 65: 60S ribosomal protein L29

Chain N9:



• Molecule 65: 60S ribosomal protein L29

Chain n9:

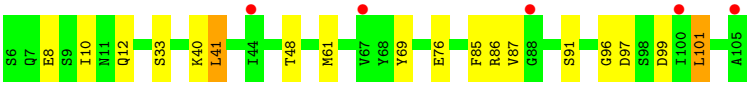


• Molecule 66: 60S ribosomal protein L30

Chain O0:

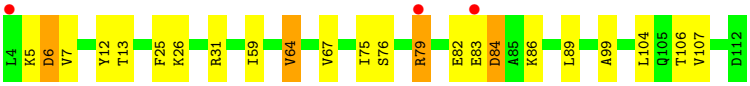
• Molecule 66: 60S ribosomal protein L30

Chain o0:



• Molecule 67: 60S ribosomal protein L31-A

Chain O1:

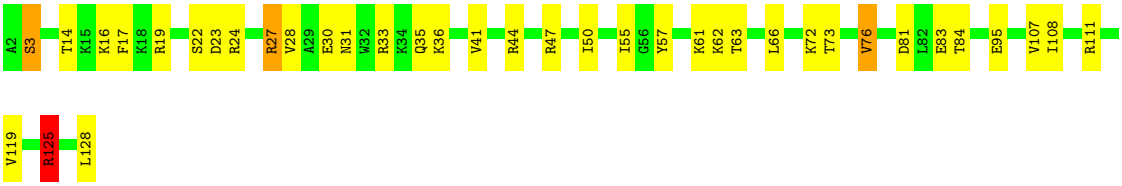


• Molecule 67: 60S ribosomal protein L31-A

Chain o1:

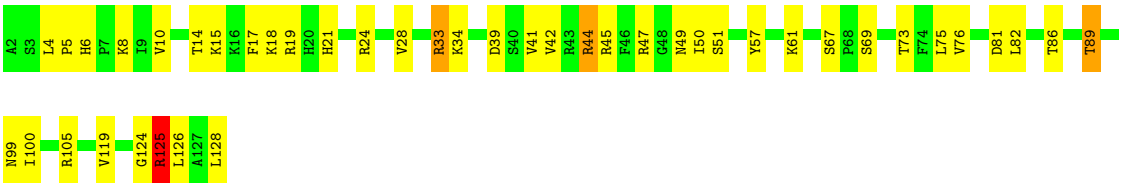
• Molecule 68: 60S ribosomal protein L32

Chain O2:



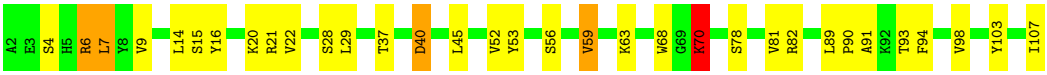
• Molecule 68: 60S ribosomal protein L32

Chain o2:



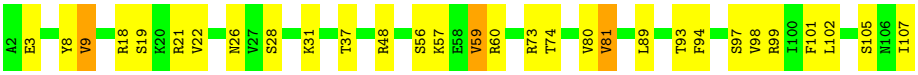
• Molecule 69: 60S ribosomal protein L33-A

Chain O3:



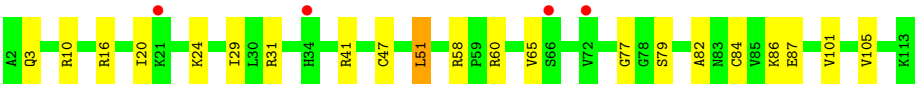
• Molecule 69: 60S ribosomal protein L33-A

Chain o3:



• Molecule 70: 60S ribosomal protein L34-A

Chain O4:



• Molecule 70: 60S ribosomal protein L34-A

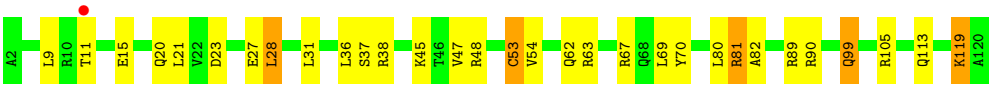
Chain o4:

• Molecule 71: 60S ribosomal protein L35-A

Chain O5:

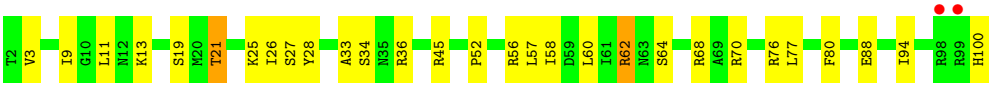
• Molecule 71: 60S ribosomal protein L35-A

Chain o5:



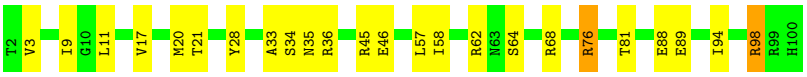
• Molecule 72: 60S ribosomal protein L36-A

Chain O6:



• Molecule 72: 60S ribosomal protein L36-A

Chain o6:

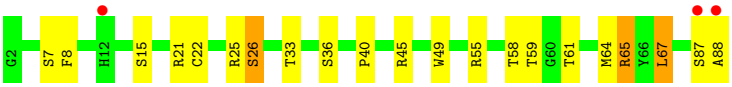


• Molecule 73: 60S ribosomal protein L37-A

Chain O7:

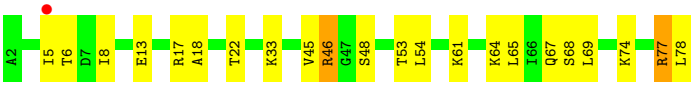
• Molecule 73: 60S ribosomal protein L37-A

Chain o7:



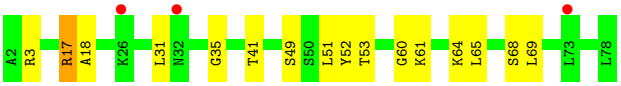
• Molecule 74: 60S ribosomal protein L38

Chain O8:



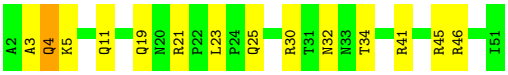
• Molecule 74: 60S ribosomal protein L38

Chain o8:



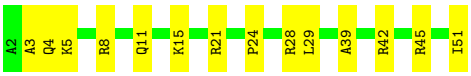
• Molecule 75: 60S ribosomal protein L39

Chain O9:



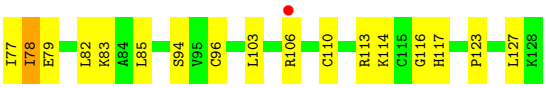
• Molecule 75: 60S ribosomal protein L39

Chain o9:



• Molecule 76: 60S ribosomal protein L40-A

Chain Q0:



• Molecule 76: 60S ribosomal protein L40-A

Chain q0: 71% 29%

I77 I78 E79 L85 K88 Y89 S94 V95 C96 L103 R106 C110 R111 K112 R113 K114 C115 L127 K128

• Molecule 77: 60S ribosomal protein L41-A

Chain Q1: 76% 24%

M1 R9 T10 R11 R17 R21 A22 R23 S24 K25

• Molecule 77: 60S ribosomal protein L41-A

Chain q1: 64% 32%

M1 R2 R6 T10 L13 R18 K19 V20 R21 A22 R23 S24 K25

• Molecule 78: 60S ribosomal protein L42-A

Chain Q2: 10% 67% 31%

V2 N3 T7 R8 K9 K15 T16 C17 H20 T21 Q22 T26 A30 S34 L35 Q38 R41 R42 Y43 Q47 S48 P56 V57 F58 H59 K60 K61 T65 R71 L72 K78 T79 L83 T84 L85 K86 R87 E92 L93 G94 G95 E96 Q99 K100

G101 Q102 A103 L104 Q105 F106

• Molecule 78: 60S ribosomal protein L42-A

Chain q2: 9% 73% 23%

V2 R8 G14 K15 T16 C17 K24 A33 R45 T54 K55 K60 K61 T64 L70 R71 L72 C77 K78 T79 T84 C88 F91 E92 L93 E96 K97 K98 Q99 K100 L104 Q105 F106

• Molecule 79: 60S ribosomal protein L43-A

Chain Q3: 5% 70% 29%

A2 T5 V8 T11 G12 K13 V16 R17 Y18 G19 S20 R23 R24 K28 L29 R36 Y37 S40 F41 C42 G43 K44 K45 T46 V47 K48 R49 W55 T56 C57 T70 V71 S72 T73 S81 R84 R85 E91 A92

• Molecule 79: 60S ribosomal protein L43-A

Chain q3: 3% 74% 25%

A2 K3 R4 V8 T11 V16 R17 Y18 R23 V26 A35 F41 T46 A51 A52 G53 I54 W55 T56 C57 S58 C59 C60 A65 G66 Y69 T73 V79 R80 S81 M89 A92

• Molecule 80: 18S ribosomal RNA

Chain 6: 7% 13% 65% 21%

U1 A2 U3 C4 G7 U8 U9 G10 A11 U12 C13 C14 U15 G16 C17 C18 A19 G20 U21 A22 G23 U24 C25 A26 U27 A28 U29 G30 C31 U32 U33 G34 U35 C36 U37 C38 A39 A40 A41 G42 A43 U44 U45 A46 A47 G48 C49 C50 A51 U52 G53 C54 A55 U56 G57 U58 C59 U60 A61

A62 G63 U64 A65 U66 A67 A68 G69 C70 A71 A72 U73 U74 U75 A76 U77 A78 C79 A80 G81 U82 G83 A84 A85 A86 C87 U88 G89 C90 G91 A92 A93 U94 G95 G96 C97 U98 C99 A100 U101 U102 A103 A104 A105 U106 C107 A108 G109 U110 U111 A112 U113 C114 G115 U116 U117 U118 A119 U120 U121

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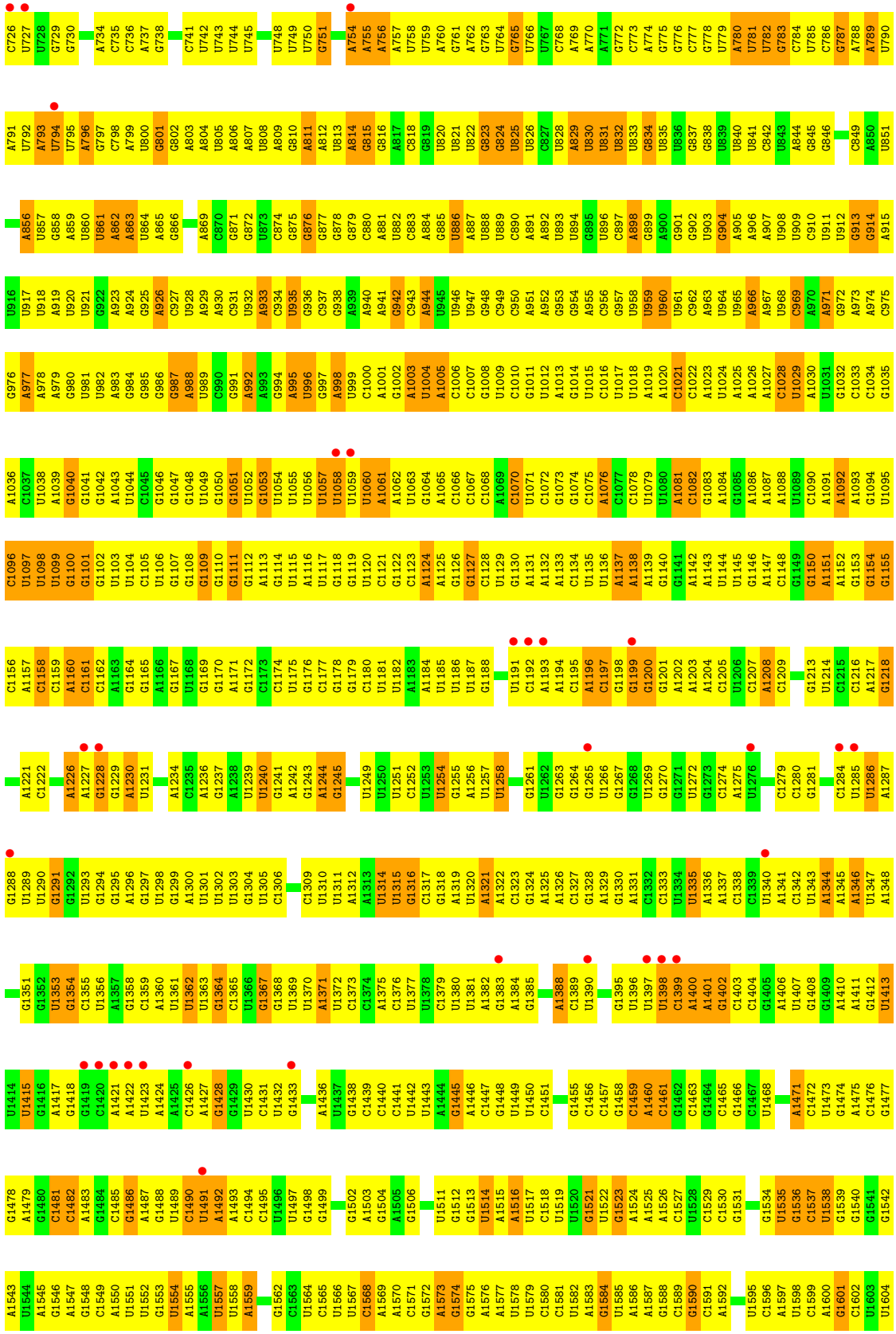
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A791 U792 A793 U794 U795 A796 G797 C798 A799 U800 G801 G802 A803 A804 U805 A806 A807 U808 A809 G810 A811 A812 U813 A814 G815 G816 A817 C818 G819 U820 U821 U822 G823 G824 U825 U826 C827 U828 A829 U830 U831 U832 U833 G834 U835 U836 G837 G838 U839 U840 U841 C842 U843 A844 G845 G846 C849 A850 U851
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G1288 U1289 U1290 G1291 G1292 U1293 G1294 G1295 A1296 G1297 U1298 G1299 A1300 U1301 U1302 U1303 G1304 U1305 C1306 C1309 U1310 U1311 A1312 A1313 U1314 U1315 G1316 C1317 G1318 A1319 U1320 A1321 A1322 C1323 G1324 A1325 A1326 C1327 G1328 A1329 G1330 A1331 C1332 C1333 U1334 U1335 A1336 A1337 C1338 C1339 U1340 A1341 C1342 U1343 A1344 A1345 A1346 U1347 A1348
G1351 G1352 U1353 G1354 C1355 U1356 A1357 G1358 C1359 A1360 U1361 U1362 U1363 G1364 C1365 U1366 G1367 G1368 U1369 U1370 A1371 U1372 C1373 C1374 A1375 C1376 U1377 U1378 C1379 U1380 U1381 A1382 G1383 A1384 G1385 A1388 C1389 U1390 G1395 U1396 U1397 U1398 C1399 A1400 A1401 G1402 C1403 C1404 G1405 A1406 U1407 G1408 G1409 A1410 A1411 U1412 U1413
U1414 U1415 G1416 A1417 G1418 G1419 C1420 A1421 A1422 U1423 A1424 A1425 C1426 A1427 G1428 G1429 U1430 C1431 U1432 G1433 A1436 U1437 G1438 C1439 A1440 C1441 U1442 A1443 A1444 G1445 A1446 C1447 G1448 U1449 U1450 C1451 G1455 C1456 C1457 G1458 C1459 A1460 C1461 G1462 C1463 G1464 C1465 C1466 C1467 U1468 A1471 C1472 U1473 G1474 A1475 C1476 G1477
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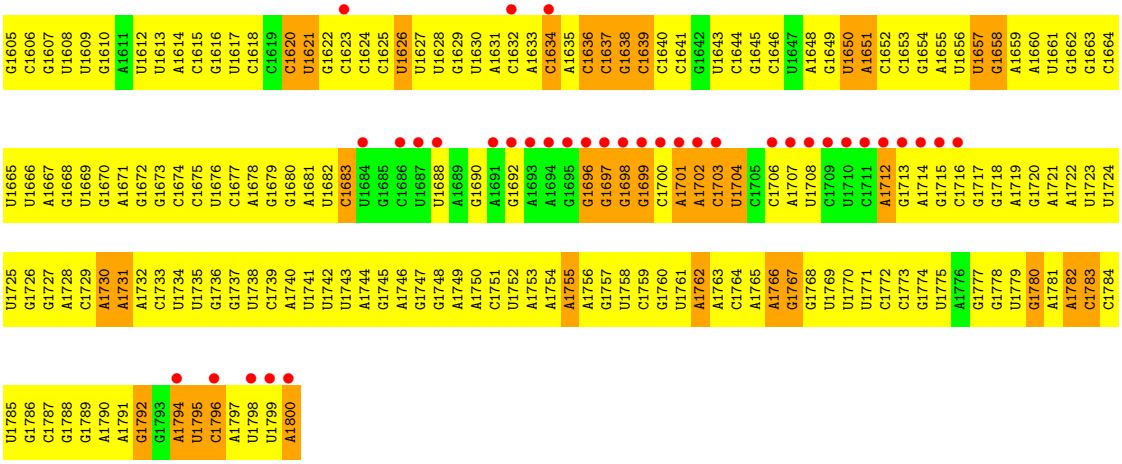
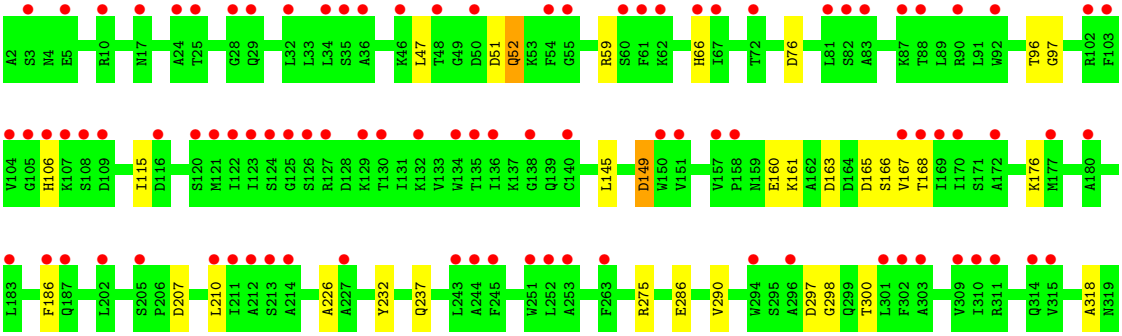


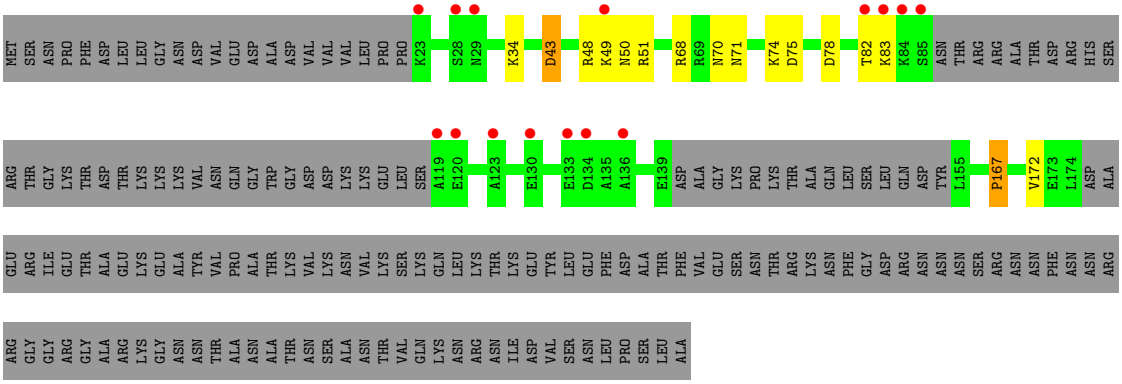
- Molecule 81: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:



- Molecule 82: Suppressor protein STM1

Chain sM:



- Molecule 83: 25S ribosomal RNA

Chain 5:

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C1192 A1193 G1194 A1195 C1196 A1197 C1198 C1199 A1200 C1201 A1202 A1203 A1204 A1205 G1206 G1207 U1208 G1209 U1210 U1211 A1212 G1213 U1214 U1215 C1216 A1217 U1218 C1219 U1220 A1221 G1222 A1223 C1224 A1225 G1226 C1227 C1228 G1229 G1230 A1231 C1232 U1235 G1236 G1237 C1238 C1239 A1240 U1241 G1242 G1243 A1244 A1245 G1246 U1247 C1248 G1249 G1250 A1251 A1252

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C1314 U1315 C1316 A1317 A1318 G1319 C1320 G1321 U1322 G1323 U1324 U1325 A1326 C1327 C1328 U1329 A1330 U1331 A1332 C1333 U1334 C1335 U1336 A1337 C1338 C1339 G1340 U1341 C1342 A1343 G1344 G1345 G1346 U1347 U1348 G1349 A1350 U1351 A1352 U1353 G1354 A1355 U1356 G1357 C1358 C1359 C1360 U1361 G1362 A1363 C1364 G1365 A1366 G1367 A1368 A1369 G1370 G1371 C1372 A1373

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U1795 G1796 A1797 A1798 A1799 A1800 U1801 C1802 C1803 A1804 C1805 A1806 G1807 G1808 A1809 A1810 G1811 G1812 A1813 A1814 U1815 A1816 A1817 U1818 U1819 U1820 U1821 C1822 A1823 U1824 G1825 C1826 C1827 A1828 G1829 G1830 U1831 C1832 G1833 U1834 A1835 C1836 U1837 G1838 A1839 U1840 A1841 A1842 C1843 C1844 G1845 C1846 A1847 G1848 C1849 A1850 G1851 G1852 U1853 G1854

U1855 C1856 C1857 A1858 A1859 G1860 G1861 U1862 G1863 A1864 A1865 C1866 A1867 G1868 C1869 C1870 U1871 C1872 U1873 A1874 G1875 U1876 U1877 G1878 A1879 U1880 A1881 G1882 A1883 A1884 U1885 A1886 A1887 U1888 G1889 U1890 A1891 G1892 A1893 U1894 A1895 A1896 G1897 G1898 G1899 A1900 A1901 G1902 U1903 C1904 G1905 G1906 C1907 A1908 A1909 A1910 A1911 U1912 A1913 C1914

A1915 U1916 C1917 C1918 G1919 U1920 A1921 A1922 C1923 U1924 U1925 C1926 G1927 G1928 G1929 A1930 U1931 A1932 A1933 G1934 G1935 A1936 U1937 U1938 G1939 G1940 C1941 U1942 C1943 U1944 A1945 A1946 G1947 G1948 G1949 U1950 C1951 U1952 G1953 A2093 C2094 G2095 A2096 U2097 C2098 A2099 A2100 C2101 U2102 U2103 A2104 G2105 A2106 A2107 C2108 U2109 G2110 G2111 U2112 A2113

C2114 G2115 G2116 A2117 C2118 A2119 A2120 G2121 G2122 G2123 G2124 A2125 A2126 U2127 C2128 U2129 G2130 A2131 C2132 U2133 G2134 U2135 C2136 U2137 A2138 A2139 U2140 U2141 A2142 A2143 A2144 A2145 C2146 A2147 U2148 A2149 G2150 C2151 A2152 U2153 U2154 G2155 C2156 G2157 A2158 U2159 G2160 G2161 U2162 C2163 A2164 G2165 A2166 A2167 A2168 G2169 U2170 G2171 A2172 U2173

C3194 U3195 U3196 G3197 U3198 G3199 G3200 C3201 G3202 U3203 C3204 G3205 C3206 U3207 G3208 A3209 A3210 C3211 C3212 A3213 U3214 A3215 G3216 G3217 A3218 G3219 G3220 C3221 U3222 A3223 G3224 C3225 A3226 A3227 C3228 G3229 G3230 U3231 G3232 C3233 A3234 C3235 U3236 U3237 G3238 G3239 C3240 G3241 G3242 A3243 A3244 A3245 G3246 G3247 C3248 C3249 U3250 U3251 G3252 G3253

G3254 U3255 G3256 C3257 U3258 U3259 G3260 C3261 U3262 G3263 G3264 C3265 G3266 A3267 A3268 U3269 U3270 G3271 C3272 A3273 A3274 U3275 G3276 U3277 C3278 A3279 U3280 U3281 U3282 U3283 G3284 C3285 G3286 U3287 G3288 G3289 G3290 G3291 A3292 U3293 A3294 A3295 A3296 U3297 C3298 A3299 C3300 U3301 U3302 G3303 U3304 A3305 U3306 A3307 C3308 G3309 A3310 C3311 U3312 U3313

A3314 G3315 A3316 U3317 G3318 U3319 A3320 C3321 A3322 A3323 C3324 G3325 G3326 G3327 G3328 U3329 A3330 U3331 U3332 U3333 U3334 A3335 A3336 G3337 C3338 A3339 G3340 U3341 A3342 G3343 A3344 G3345 U3346 A3347 G3348 C3349 C3350 U3351 U3352 G3353 U3354 U3355 G3356 U3357 U3358 A3359 C3360 G3361 A3362 U3363 C3364 U3365 G3366 C3367 U3368 G3369 A3370 G3371 A3372 U3373

U3374 A3375 A3376 G3377 C3378 C3379 U3380 U3381 U3382 G3383 U3384 U3385 G3386 U3387 C3388 U3389 G3390 A3391 U3392 U3393 U3394 G3395 U3396

- Molecule 84: 60S ribosomal protein L8-A

Chain l8: 4% 71% 18% 10%

MET ALA PRO GLY LYS LYS VAL ALA PRO ALA PRO PHE GLY ALA LYS SER THR LYS SER ASN LYS THR ARG N24 P25 L26 S29 K32 A39 V40 Q41 P42 K43 Y49 R57 R68 I69 K70 T74 Q77 F78 Q79 Y80 T81 E89 T90 N95 L109

K120 S121 K122 Q123 D124 A125 S126 K133 L136 K149 I153 V157 I160 E161 L169 K172 V180 K183 G187 L200 V203 E208 L211 A212 K213 L214 A223 D224 V229 K230 I237 L238 G239 N240 K241 K245 M246 D247 K248 N252

S253 D254 SER ALA

- Molecule 85: 60S ribosomal protein L12-A

Chain m2: 18% 73% 15% • 9%

MET PRO PRO LYS PHE ASP PRO ASN E9 V10 K11 Y12 L13 Y14 V18 G19 G20 E21 V22 G23 ALA SER ALA ALA L28 A29 P30 K31 I32 G33 P34 L37 S38 P39 E52 PHE K54 G55 I56 K57 V58 T59 V60 K63 I64 Q65 N66 R67 Q68 A69 A70 A71 S72 V73 V74 P75

S76 A77 S78 K86 E87 P88 P89 N97 V98 K99 N103 I104 R117 F121 G122 R123 T124 L125 A126 S127 V139 V143 D144 N147 P148 N156 E161 I162 P163 GLU ASN

- Molecule 86: 60S ribosomal protein L24-A

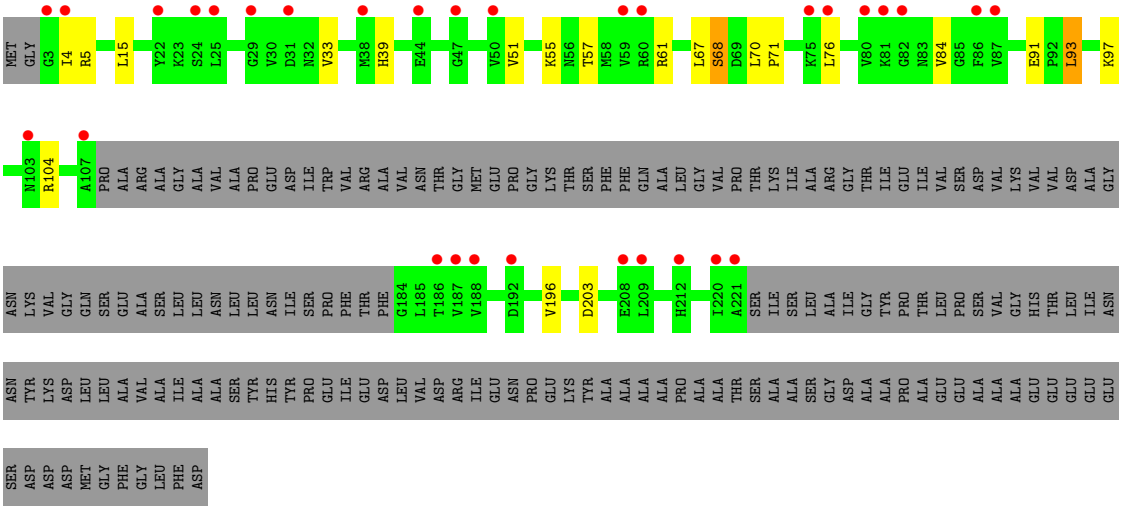
Chain n4: 24% 79% 19% •

M1 I5 D6 S7 R17 G18 R23 G24 D25 S26 L39 F40 K41 R48 T52 V53 L54 F55 R56 K57 H58 I63 T64 E65 E66 V67 A68 K69 K70 R71 S72 T75 V76 Q79 R80 P81 I82 T83 G84 A85 S86 L87 D88 L89 I90 K91 E92 R93 R94 S95 L96

E99 V100 R101 N104 R105 E106 E107 K127 A128 A131 G132 T133 Q134 S135

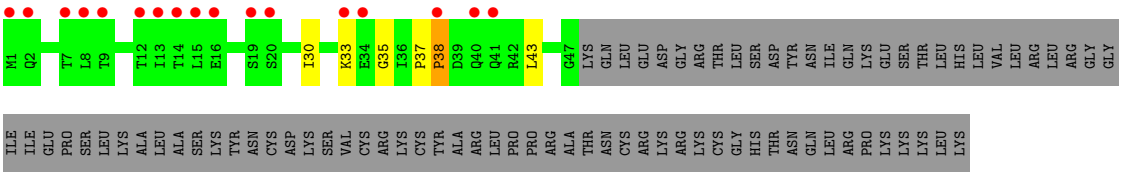
- Molecule 87: 60S acidic ribosomal protein P0

Chain p0:



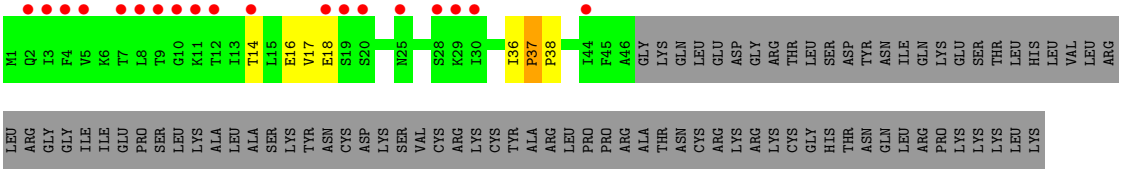
- Molecule 88: 60S ribosomal protein L40-A

Chain p1:



- Molecule 88: 60S ribosomal protein L40-A

Chain p2:



- Molecule 89: Peptidyl-tRNA analog ACCA-Leu-Phe

Chain P:

- Molecule 89: Peptidyl-tRNA analog ACCA-Leu-Phe

Chain p:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	434.73Å 286.77Å 303.15Å 90.00° 98.87° 90.00°	Depositor
Resolution (Å)	148.72 – 3.50 149.76 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (148.72-3.50) 99.7 (149.76-3.50)	Depositor EDS
R_{merge}	0.61	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.261 , 0.312 0.263 , 0.314	Depositor DCC
R_{free} test set	18373 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	83.6	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	411566	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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, OHX, SPS, MG, 8AN

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	1.53	426/42467 (1.0%)	2.41	4031/66169 (6.1%)
2	S0	0.67	0/1617	0.76	0/2215
2	s0	0.78	0/1623	0.86	1/2222 (0.0%)
3	S1	0.59	0/1735	0.75	1/2335 (0.0%)
3	s1	0.82	2/1748 (0.1%)	0.95	5/2352 (0.2%)
4	S2	0.73	0/1665	0.81	0/2263
4	s2	0.86	2/1665 (0.1%)	0.96	4/2263 (0.2%)
5	S3	0.68	0/1759	0.78	0/2368
5	s3	0.70	0/1759	0.79	0/2368
6	S4	0.85	2/2109 (0.1%)	0.91	2/2839 (0.1%)
6	s4	0.84	1/2109 (0.0%)	0.98	1/2839 (0.0%)
7	S5	0.66	0/1629	0.76	0/2202
7	s5	0.65	1/1629 (0.1%)	0.76	1/2202 (0.0%)
8	S6	0.84	3/1823 (0.2%)	0.92	5/2439 (0.2%)
8	s6	0.93	1/1779 (0.1%)	1.01	6/2379 (0.3%)
9	S7	0.73	2/1506 (0.1%)	0.79	0/2028
9	s7	0.78	0/1516	0.85	2/2043 (0.1%)
10	S8	0.79	1/1514 (0.1%)	0.90	2/2021 (0.1%)
10	s8	0.94	2/1514 (0.1%)	1.00	5/2021 (0.2%)
11	S9	0.75	2/1519 (0.1%)	0.88	1/2035 (0.0%)
11	s9	0.84	1/1519 (0.1%)	0.97	4/2035 (0.2%)
12	C0	0.60	0/789	0.74	1/1067 (0.1%)
12	c0	0.58	0/776	0.72	3/1047 (0.3%)
13	C1	0.85	1/1239 (0.1%)	0.84	0/1673
13	c1	0.95	1/1194 (0.1%)	0.96	1/1610 (0.1%)
14	C2	0.59	0/898	0.71	0/1220
14	c2	0.48	0/898	0.63	0/1220
15	C3	0.75	0/1215	0.86	1/1638 (0.1%)
15	c3	0.86	1/1215 (0.1%)	0.93	0/1638
16	C4	0.59	0/901	0.75	0/1217
16	c4	0.85	0/960	0.97	0/1290
17	C5	0.85	2/998 (0.2%)	0.85	0/1341

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	c5	0.75	0/1060	0.86	1/1426 (0.1%)
18	C6	0.65	0/1125	0.80	2/1510 (0.1%)
18	c6	0.69	0/1131	0.74	0/1518
19	C7	0.66	0/935	0.76	0/1254
19	c7	0.69	0/914	0.83	1/1224 (0.1%)
20	C8	0.70	0/1211	0.82	0/1628
20	c8	0.76	1/1211 (0.1%)	0.87	0/1628
21	C9	0.66	0/1130	0.75	0/1517
21	c9	0.70	0/1130	0.79	1/1517 (0.1%)
22	D0	0.64	0/865	0.80	1/1169 (0.1%)
22	d0	0.72	0/892	0.75	0/1205
23	D1	0.72	0/693	0.83	0/935
23	d1	0.87	0/693	0.96	1/935 (0.1%)
24	D2	0.81	0/1038	0.90	2/1395 (0.1%)
24	d2	0.90	2/1038 (0.2%)	0.95	2/1395 (0.1%)
25	D3	0.85	1/1139 (0.1%)	0.90	1/1518 (0.1%)
25	d3	1.05	1/1139 (0.1%)	1.07	4/1518 (0.3%)
26	D4	0.79	0/1087	0.85	0/1449
26	d4	0.93	0/1087	1.04	5/1449 (0.3%)
27	D5	0.66	0/571	0.78	0/768
27	d5	0.78	1/566 (0.2%)	0.76	0/761
28	D6	0.68	0/782	0.78	1/1047 (0.1%)
28	d6	0.84	2/782 (0.3%)	0.99	1/1047 (0.1%)
29	D7	0.76	0/620	0.80	0/838
29	d7	0.82	2/620 (0.3%)	0.89	0/838
30	D8	0.69	0/499	0.82	1/670 (0.1%)
30	d8	0.69	0/499	0.91	0/670
31	D9	0.76	1/452 (0.2%)	0.80	0/600
31	d9	0.78	1/452 (0.2%)	0.80	0/600
32	E0	0.74	0/483	0.78	0/643
32	e0	0.94	1/499 (0.2%)	0.94	1/665 (0.2%)
33	E1	0.72	0/577	0.80	0/770
33	e1	0.66	0/619	0.77	0/822
34	SR	0.57	0/2490	0.71	0/3389
35	SM	0.76	1/984 (0.1%)	0.86	1/1323 (0.1%)
36	1	2.49	4418/75394 (5.9%)	3.49	15681/117545 (13.3%)
37	3	2.00	80/2883 (2.8%)	3.26	543/4491 (12.1%)
37	7	2.57	171/2883 (5.9%)	3.80	680/4491 (15.1%)
38	4	2.46	206/3746 (5.5%)	3.78	898/5832 (15.4%)
38	8	2.34	182/3746 (4.9%)	3.37	707/5832 (12.1%)
39	L2	1.18	7/1948 (0.4%)	1.22	16/2617 (0.6%)
39	l2	1.09	6/1946 (0.3%)	1.23	16/2614 (0.6%)
40	L3	1.18	16/3146 (0.5%)	1.19	19/4228 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
40	l3	1.33	19/3146 (0.6%)	1.32	33/4228 (0.8%)
41	L4	1.29	18/2800 (0.6%)	1.30	28/3790 (0.7%)
41	l4	1.26	14/2800 (0.5%)	1.22	18/3790 (0.5%)
42	L5	1.02	5/2425 (0.2%)	1.04	10/3271 (0.3%)
42	l5	1.23	14/2408 (0.6%)	1.22	17/3248 (0.5%)
43	L6	1.21	2/1260 (0.2%)	1.15	3/1694 (0.2%)
43	l6	1.16	4/1269 (0.3%)	1.26	12/1705 (0.7%)
44	L7	1.32	12/1821 (0.7%)	1.23	14/2451 (0.6%)
44	l7	1.44	19/1828 (1.0%)	1.23	15/2461 (0.6%)
45	L8	0.98	2/1836 (0.1%)	0.99	3/2481 (0.1%)
46	L9	1.10	6/1539 (0.4%)	1.11	10/2073 (0.5%)
46	l9	1.19	4/1539 (0.3%)	1.21	13/2073 (0.6%)
47	M0	1.15	9/1741 (0.5%)	1.18	14/2335 (0.6%)
47	m0	1.24	5/1758 (0.3%)	1.37	21/2358 (0.9%)
48	M1	0.93	3/1374 (0.2%)	0.97	2/1842 (0.1%)
48	m1	1.05	4/1374 (0.3%)	1.17	10/1842 (0.5%)
49	M3	1.20	10/1568 (0.6%)	1.23	13/2106 (0.6%)
49	m3	1.05	3/1573 (0.2%)	1.20	13/2113 (0.6%)
50	M4	1.11	5/1068 (0.5%)	1.15	6/1438 (0.4%)
50	m4	1.21	7/1074 (0.7%)	1.27	10/1446 (0.7%)
51	M5	1.19	7/1757 (0.4%)	1.28	19/2354 (0.8%)
51	m5	1.10	5/1757 (0.3%)	1.16	10/2354 (0.4%)
52	M6	1.40	18/1585 (1.1%)	1.37	22/2128 (1.0%)
52	m6	1.50	13/1585 (0.8%)	1.35	22/2128 (1.0%)
53	M7	1.29	4/1443 (0.3%)	1.14	10/1944 (0.5%)
53	m7	1.47	17/1250 (1.4%)	1.29	13/1683 (0.8%)
54	M8	1.26	11/1465 (0.8%)	1.22	11/1965 (0.6%)
54	m8	1.23	10/1465 (0.7%)	1.30	11/1965 (0.6%)
55	M9	0.93	0/1538	0.98	2/2050 (0.1%)
55	m9	0.96	2/1538 (0.1%)	1.05	8/2050 (0.4%)
56	N0	1.20	4/1481 (0.3%)	1.15	6/1990 (0.3%)
56	n0	1.35	11/1481 (0.7%)	1.23	9/1990 (0.5%)
57	N1	1.16	3/1300 (0.2%)	1.13	5/1743 (0.3%)
57	n1	1.32	10/1300 (0.8%)	1.20	10/1743 (0.6%)
58	N2	0.95	0/812	0.90	1/1099 (0.1%)
58	n2	0.94	0/794	1.00	2/1076 (0.2%)
59	N3	1.16	5/1018 (0.5%)	1.21	8/1369 (0.6%)
59	n3	1.39	11/1018 (1.1%)	1.34	13/1369 (0.9%)
60	N4	0.94	1/712 (0.1%)	0.97	3/958 (0.3%)
61	N5	1.14	3/979 (0.3%)	1.16	7/1321 (0.5%)
61	n5	1.11	4/974 (0.4%)	1.19	4/1314 (0.3%)
62	N6	1.17	7/1004 (0.7%)	1.33	12/1341 (0.9%)
62	n6	1.17	5/1004 (0.5%)	1.34	15/1341 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
63	N7	0.91	0/1118	0.91	1/1497 (0.1%)
63	n7	0.96	2/1118 (0.2%)	0.95	3/1497 (0.2%)
64	N8	1.22	4/1204 (0.3%)	1.24	11/1612 (0.7%)
64	n8	1.25	10/1204 (0.8%)	1.26	10/1612 (0.6%)
65	N9	1.08	1/473 (0.2%)	1.14	2/629 (0.3%)
65	n9	1.17	2/473 (0.4%)	1.16	2/629 (0.3%)
66	O0	0.81	0/751	0.91	0/1008
66	o0	0.94	1/775 (0.1%)	0.99	2/1040 (0.2%)
67	O1	1.07	3/890 (0.3%)	1.07	4/1196 (0.3%)
67	o1	1.23	5/897 (0.6%)	1.22	5/1205 (0.4%)
68	O2	1.40	13/1041 (1.2%)	1.34	14/1394 (1.0%)
68	o2	1.24	6/1041 (0.6%)	1.33	11/1394 (0.8%)
69	O3	1.50	10/868 (1.2%)	1.22	7/1168 (0.6%)
69	o3	1.54	13/868 (1.5%)	1.32	7/1168 (0.6%)
70	O4	1.01	1/890 (0.1%)	1.14	7/1189 (0.6%)
70	o4	1.03	2/890 (0.2%)	1.11	6/1189 (0.5%)
71	O5	1.18	5/978 (0.5%)	1.26	11/1301 (0.8%)
71	o5	0.96	2/974 (0.2%)	1.13	6/1297 (0.5%)
72	O6	0.99	0/778	1.15	3/1034 (0.3%)
72	o6	1.03	2/777 (0.3%)	1.16	3/1033 (0.3%)
73	O7	1.30	2/696 (0.3%)	1.29	7/923 (0.8%)
73	o7	1.25	4/696 (0.6%)	1.16	3/923 (0.3%)
74	O8	0.96	2/618 (0.3%)	1.08	3/826 (0.4%)
74	o8	0.83	0/614	1.01	3/822 (0.4%)
75	O9	1.09	1/443 (0.2%)	1.31	7/588 (1.2%)
75	o9	1.02	0/443	1.26	6/588 (1.0%)
76	Q0	1.15	3/423 (0.7%)	1.21	4/562 (0.7%)
76	q0	1.33	6/423 (1.4%)	1.22	3/562 (0.5%)
77	Q1	0.79	0/234	1.15	3/300 (1.0%)
77	q1	0.96	0/234	1.40	2/300 (0.7%)
78	Q2	1.22	3/860 (0.3%)	1.23	7/1136 (0.6%)
78	q2	1.32	4/860 (0.5%)	1.33	9/1136 (0.8%)
79	Q3	1.26	9/701 (1.3%)	1.31	7/934 (0.7%)
79	q3	1.22	6/701 (0.9%)	1.10	3/934 (0.3%)
80	6	1.94	1088/42790 (2.5%)	2.88	5446/66673 (8.2%)
81	sR	0.61	0/2495	0.72	0/3395
82	sM	0.78	1/683 (0.1%)	0.84	1/923 (0.1%)
83	5	2.61	4902/75414 (6.5%)	3.71	16861/117575 (14.3%)
84	l8	0.92	1/1795 (0.1%)	0.94	3/2429 (0.1%)
85	m2	0.57	0/734	0.90	8/1015 (0.8%)
86	n4	1.08	0/1052	1.10	7/1398 (0.5%)
87	p0	0.79	0/1092	0.82	2/1474 (0.1%)
88	p1	0.38	0/231	0.72	2/320 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
88	p2	0.39	0/227	0.73	2/315 (0.6%)
89	P	2.37	2/40 (5.0%)	4.21	9/60 (15.0%)
89	p	13.84	3/43 (7.0%)	5.74	11/64 (17.2%)
All	All	1.87	11986/432003 (2.8%)	2.67	45685/634177 (7.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	S4	0	2
9	s7	0	1
11	S9	0	1
12	c0	0	1
17	c5	0	1
19	C7	0	1
22	d0	0	1
25	d3	0	1
27	D5	0	1
33	E1	0	2
39	L2	0	1
40	L3	0	1
40	l3	0	1
41	L4	0	2
41	l4	0	1
42	l5	0	2
44	L7	0	1
44	l7	0	2
47	M0	0	1
49	m3	0	1
52	M6	0	1
52	m6	0	1
53	M7	0	2
56	n0	0	2
57	N1	0	1
64	n8	0	1
65	N9	0	1
65	n9	0	1
68	o2	0	1
75	o9	0	1
80	6	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
83	5	0	1
All	All	0	39

The worst 5 of 11986 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	p	74	C	P-O5'	89.50	2.49	1.59
37	7	63	A	C6-N6	27.75	1.56	1.33
80	6	1498	G	C8-N7	24.00	1.45	1.30
83	5	748	U	C4-O4	23.12	1.42	1.23
80	6	54	C	C4-N4	22.95	1.54	1.33

The worst 5 of 45685 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	5	2707	C	N3-C4-C5	-50.63	101.65	121.90
80	6	54	C	N3-C4-C5	-49.41	102.13	121.90
80	6	1070	C	N3-C4-C5	-42.39	104.94	121.90
80	6	818	C	N3-C4-C5	-42.29	104.98	121.90
80	6	1498	G	C5-N7-C8	-42.11	83.24	104.30

There are no chirality outliers.

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	C7	85	VAL	Peptide
27	D5	94	LYS	Peptide
6	S4	148	ARG	Peptide
6	S4	193	GLY	Peptide
11	S9	38	ASN	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	204/206 (99%)	151 (74%)	38 (19%)	15 (7%)	1 11
2	s0	204/206 (99%)	151 (74%)	34 (17%)	19 (9%)	0 8
3	S1	212/216 (98%)	154 (73%)	34 (16%)	24 (11%)	0 6
3	s1	214/216 (99%)	166 (78%)	32 (15%)	16 (8%)	1 11
4	S2	215/217 (99%)	182 (85%)	24 (11%)	9 (4%)	3 23
4	s2	215/217 (99%)	172 (80%)	34 (16%)	9 (4%)	3 23
5	S3	221/223 (99%)	186 (84%)	24 (11%)	11 (5%)	2 19
5	s3	221/223 (99%)	176 (80%)	30 (14%)	15 (7%)	1 13
6	S4	258/260 (99%)	197 (76%)	45 (17%)	16 (6%)	1 15
6	s4	258/260 (99%)	197 (76%)	42 (16%)	19 (7%)	1 11
7	S5	204/206 (99%)	169 (83%)	20 (10%)	15 (7%)	1 11
7	s5	204/206 (99%)	159 (78%)	35 (17%)	10 (5%)	2 19
8	S6	224/226 (99%)	186 (83%)	23 (10%)	15 (7%)	1 13
8	s6	216/226 (96%)	182 (84%)	22 (10%)	12 (6%)	2 17
9	S7	182/186 (98%)	134 (74%)	36 (20%)	12 (7%)	1 13
9	s7	184/186 (99%)	143 (78%)	28 (15%)	13 (7%)	1 12
10	S8	184/199 (92%)	150 (82%)	25 (14%)	9 (5%)	2 19
10	s8	184/199 (92%)	156 (85%)	23 (12%)	5 (3%)	5 33
11	S9	183/185 (99%)	143 (78%)	33 (18%)	7 (4%)	3 25
11	s9	183/185 (99%)	149 (81%)	26 (14%)	8 (4%)	2 21
12	C0	94/105 (90%)	72 (77%)	15 (16%)	7 (7%)	1 11
12	c0	92/105 (88%)	68 (74%)	10 (11%)	14 (15%)	0 3
13	C1	153/156 (98%)	117 (76%)	31 (20%)	5 (3%)	4 28
13	c1	144/156 (92%)	115 (80%)	25 (17%)	4 (3%)	5 32
14	C2	122/143 (85%)	77 (63%)	28 (23%)	17 (14%)	0 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	c2	122/143 (85%)	78 (64%)	31 (25%)	13 (11%)	0	6
15	C3	148/150 (99%)	125 (84%)	17 (12%)	6 (4%)	3	23
15	c3	148/150 (99%)	122 (82%)	18 (12%)	8 (5%)	2	17
16	C4	125/128 (98%)	90 (72%)	23 (18%)	12 (10%)	0	8
16	c4	126/128 (98%)	101 (80%)	15 (12%)	10 (8%)	1	10
17	C5	122/142 (86%)	90 (74%)	21 (17%)	11 (9%)	1	8
17	c5	133/142 (94%)	92 (69%)	26 (20%)	15 (11%)	0	6
18	C6	139/142 (98%)	115 (83%)	13 (9%)	11 (8%)	1	10
18	c6	140/142 (99%)	121 (86%)	15 (11%)	4 (3%)	4	31
19	C7	116/125 (93%)	90 (78%)	16 (14%)	10 (9%)	1	9
19	c7	113/125 (90%)	87 (77%)	19 (17%)	7 (6%)	1	15
20	C8	143/145 (99%)	113 (79%)	22 (15%)	8 (6%)	2	17
20	c8	143/145 (99%)	113 (79%)	19 (13%)	11 (8%)	1	10
21	C9	141/143 (99%)	121 (86%)	10 (7%)	10 (7%)	1	12
21	c9	141/143 (99%)	124 (88%)	13 (9%)	4 (3%)	5	32
22	D0	105/110 (96%)	89 (85%)	13 (12%)	3 (3%)	4	31
22	d0	108/110 (98%)	86 (80%)	15 (14%)	7 (6%)	1	14
23	D1	85/87 (98%)	62 (73%)	11 (13%)	12 (14%)	0	3
23	d1	85/87 (98%)	64 (75%)	13 (15%)	8 (9%)	0	8
24	D2	127/129 (98%)	109 (86%)	14 (11%)	4 (3%)	4	30
24	d2	127/129 (98%)	105 (83%)	19 (15%)	3 (2%)	6	35
25	D3	142/144 (99%)	109 (77%)	26 (18%)	7 (5%)	2	19
25	d3	142/144 (99%)	116 (82%)	23 (16%)	3 (2%)	7	38
26	D4	132/134 (98%)	103 (78%)	20 (15%)	9 (7%)	1	13
26	d4	132/134 (98%)	109 (83%)	14 (11%)	9 (7%)	1	13
27	D5	68/70 (97%)	46 (68%)	13 (19%)	9 (13%)	0	4
27	d5	67/70 (96%)	53 (79%)	10 (15%)	4 (6%)	1	15
28	D6	95/97 (98%)	53 (56%)	26 (27%)	16 (17%)	0	2
28	d6	95/97 (98%)	75 (79%)	13 (14%)	7 (7%)	1	11
29	D7	79/81 (98%)	59 (75%)	20 (25%)	0	100	100
29	d7	79/81 (98%)	58 (73%)	18 (23%)	3 (4%)	3	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	D8	61/63 (97%)	49 (80%)	9 (15%)	3 (5%)	2	19
30	d8	61/63 (97%)	45 (74%)	14 (23%)	2 (3%)	4	28
31	D9	51/53 (96%)	40 (78%)	9 (18%)	2 (4%)	3	25
31	d9	51/53 (96%)	42 (82%)	2 (4%)	7 (14%)	0	4
32	E0	58/62 (94%)	46 (79%)	8 (14%)	4 (7%)	1	12
32	e0	60/62 (97%)	46 (77%)	11 (18%)	3 (5%)	2	19
33	E1	69/76 (91%)	38 (55%)	22 (32%)	9 (13%)	0	4
33	e1	74/76 (97%)	36 (49%)	19 (26%)	19 (26%)	0	0
34	SR	316/318 (99%)	262 (83%)	41 (13%)	13 (4%)	3	23
35	SM	131/299 (44%)	101 (77%)	17 (13%)	13 (10%)	0	7
39	L2	250/252 (99%)	218 (87%)	25 (10%)	7 (3%)	5	32
39	l2	250/252 (99%)	200 (80%)	32 (13%)	18 (7%)	1	11
40	L3	384/386 (100%)	323 (84%)	44 (12%)	17 (4%)	2	21
40	l3	384/386 (100%)	329 (86%)	36 (9%)	19 (5%)	2	19
41	L4	359/361 (99%)	288 (80%)	44 (12%)	27 (8%)	1	11
41	l4	359/361 (99%)	284 (79%)	48 (13%)	27 (8%)	1	11
42	L5	294/296 (99%)	232 (79%)	43 (15%)	19 (6%)	1	14
42	l5	292/296 (99%)	236 (81%)	41 (14%)	15 (5%)	2	19
43	L6	152/175 (87%)	130 (86%)	19 (12%)	3 (2%)	7	39
43	l6	153/175 (87%)	128 (84%)	22 (14%)	3 (2%)	7	39
44	L7	220/223 (99%)	184 (84%)	27 (12%)	9 (4%)	3	23
44	l7	221/223 (99%)	185 (84%)	30 (14%)	6 (3%)	5	33
45	L8	231/233 (99%)	180 (78%)	34 (15%)	17 (7%)	1	11
46	L9	189/191 (99%)	155 (82%)	22 (12%)	12 (6%)	1	14
46	l9	189/191 (99%)	161 (85%)	24 (13%)	4 (2%)	7	38
47	M0	207/220 (94%)	157 (76%)	39 (19%)	11 (5%)	2	17
47	m0	209/220 (95%)	162 (78%)	33 (16%)	14 (7%)	1	13
48	M1	167/169 (99%)	125 (75%)	22 (13%)	20 (12%)	0	5
48	m1	167/169 (99%)	132 (79%)	27 (16%)	8 (5%)	2	20
49	M3	191/194 (98%)	150 (78%)	31 (16%)	10 (5%)	2	18
49	m3	192/194 (99%)	150 (78%)	29 (15%)	13 (7%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	M4	134/137 (98%)	112 (84%)	15 (11%)	7 (5%)	2	18
50	m4	135/137 (98%)	107 (79%)	24 (18%)	4 (3%)	4	30
51	M5	201/203 (99%)	162 (81%)	33 (16%)	6 (3%)	4	30
51	m5	201/203 (99%)	164 (82%)	30 (15%)	7 (4%)	3	27
52	M6	195/197 (99%)	173 (89%)	19 (10%)	3 (2%)	10	45
52	m6	195/197 (99%)	176 (90%)	13 (7%)	6 (3%)	4	30
53	M7	181/183 (99%)	141 (78%)	29 (16%)	11 (6%)	1	15
53	m7	153/183 (84%)	128 (84%)	20 (13%)	5 (3%)	4	28
54	M8	183/185 (99%)	155 (85%)	22 (12%)	6 (3%)	4	28
54	m8	183/185 (99%)	152 (83%)	21 (12%)	10 (6%)	2	17
55	M9	186/188 (99%)	161 (87%)	19 (10%)	6 (3%)	4	29
55	m9	186/188 (99%)	163 (88%)	23 (12%)	0	100	100
56	N0	170/172 (99%)	139 (82%)	27 (16%)	4 (2%)	6	35
56	n0	170/172 (99%)	149 (88%)	20 (12%)	1 (1%)	25	64
57	N1	157/159 (99%)	129 (82%)	22 (14%)	6 (4%)	3	25
57	n1	157/159 (99%)	138 (88%)	15 (10%)	4 (2%)	5	34
58	N2	98/100 (98%)	72 (74%)	19 (19%)	7 (7%)	1	12
58	n2	96/100 (96%)	70 (73%)	23 (24%)	3 (3%)	4	30
59	N3	134/136 (98%)	108 (81%)	21 (16%)	5 (4%)	3	26
59	n3	134/136 (98%)	113 (84%)	19 (14%)	2 (2%)	10	45
60	N4	96/98 (98%)	75 (78%)	16 (17%)	5 (5%)	2	18
61	N5	119/121 (98%)	99 (83%)	17 (14%)	3 (2%)	5	34
61	n5	118/121 (98%)	90 (76%)	16 (14%)	12 (10%)	0	7
62	N6	124/126 (98%)	109 (88%)	12 (10%)	3 (2%)	6	35
62	n6	124/126 (98%)	104 (84%)	15 (12%)	5 (4%)	3	24
63	N7	133/135 (98%)	106 (80%)	17 (13%)	10 (8%)	1	11
63	n7	133/135 (98%)	93 (70%)	26 (20%)	14 (10%)	0	7
64	N8	146/148 (99%)	112 (77%)	28 (19%)	6 (4%)	3	23
64	n8	146/148 (99%)	118 (81%)	17 (12%)	11 (8%)	1	11
65	N9	56/58 (97%)	47 (84%)	8 (14%)	1 (2%)	8	41
65	n9	56/58 (97%)	39 (70%)	11 (20%)	6 (11%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	O0	95/100 (95%)	87 (92%)	7 (7%)	1 (1%)	14	52
66	o0	98/100 (98%)	83 (85%)	11 (11%)	4 (4%)	3	23
67	O1	107/109 (98%)	90 (84%)	10 (9%)	7 (6%)	1	14
67	o1	107/109 (98%)	84 (78%)	16 (15%)	7 (6%)	1	14
68	O2	125/127 (98%)	112 (90%)	11 (9%)	2 (2%)	9	43
68	o2	125/127 (98%)	100 (80%)	18 (14%)	7 (6%)	2	17
69	O3	104/106 (98%)	90 (86%)	8 (8%)	6 (6%)	1	16
69	o3	104/106 (98%)	92 (88%)	10 (10%)	2 (2%)	8	40
70	O4	110/112 (98%)	91 (83%)	17 (16%)	2 (2%)	8	41
70	o4	110/112 (98%)	92 (84%)	15 (14%)	3 (3%)	5	33
71	O5	117/119 (98%)	105 (90%)	9 (8%)	3 (3%)	5	33
71	o5	117/119 (98%)	93 (80%)	17 (14%)	7 (6%)	1	15
72	O6	97/99 (98%)	76 (78%)	11 (11%)	10 (10%)	0	7
72	o6	97/99 (98%)	84 (87%)	7 (7%)	6 (6%)	1	15
73	O7	85/87 (98%)	72 (85%)	10 (12%)	3 (4%)	3	27
73	o7	85/87 (98%)	66 (78%)	17 (20%)	2 (2%)	6	35
74	O8	75/77 (97%)	61 (81%)	11 (15%)	3 (4%)	3	24
74	o8	75/77 (97%)	59 (79%)	11 (15%)	5 (7%)	1	13
75	O9	48/50 (96%)	39 (81%)	8 (17%)	1 (2%)	7	38
75	o9	48/50 (96%)	43 (90%)	2 (4%)	3 (6%)	1	14
76	Q0	50/52 (96%)	41 (82%)	4 (8%)	5 (10%)	0	7
76	q0	50/52 (96%)	46 (92%)	3 (6%)	1 (2%)	7	39
77	Q1	23/25 (92%)	19 (83%)	4 (17%)	0	100	100
77	q1	23/25 (92%)	19 (83%)	4 (17%)	0	100	100
78	Q2	103/105 (98%)	76 (74%)	20 (19%)	7 (7%)	1	13
78	q2	103/105 (98%)	89 (86%)	9 (9%)	5 (5%)	2	19
79	Q3	89/91 (98%)	71 (80%)	16 (18%)	2 (2%)	6	37
79	q3	89/91 (98%)	70 (79%)	15 (17%)	4 (4%)	2	21
81	sR	316/318 (99%)	252 (80%)	51 (16%)	13 (4%)	3	23
82	sM	98/273 (36%)	72 (74%)	20 (20%)	6 (6%)	1	15
84	l8	229/256 (90%)	182 (80%)	29 (13%)	18 (8%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
85	m2	144/165 (87%)	79 (55%)	37 (26%)	28 (19%)	0 2
86	n4	133/135 (98%)	109 (82%)	12 (9%)	12 (9%)	1 8
87	p0	139/312 (45%)	115 (83%)	19 (14%)	5 (4%)	3 26
88	p1	45/128 (35%)	33 (73%)	7 (16%)	5 (11%)	0 6
88	p2	44/128 (34%)	35 (80%)	3 (7%)	6 (14%)	0 4
All	All	22542/23829 (95%)	18075 (80%)	3183 (14%)	1284 (6%)	1 16

5 of 1284 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	39	ASN
2	S0	158	VAL
2	S0	191	ARG
2	S0	195	TRP

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	164/173 (95%)	144 (88%)	20 (12%)	5 23
2	s0	165/173 (95%)	135 (82%)	30 (18%)	1 9
3	S1	191/192 (100%)	157 (82%)	34 (18%)	2 10
3	s1	192/192 (100%)	151 (79%)	41 (21%)	1 5
4	S2	176/176 (100%)	150 (85%)	26 (15%)	3 17
4	s2	176/176 (100%)	135 (77%)	41 (23%)	1 4
5	S3	182/182 (100%)	158 (87%)	24 (13%)	4 21
5	s3	182/182 (100%)	154 (85%)	28 (15%)	2 16
6	S4	221/221 (100%)	184 (83%)	37 (17%)	2 12
6	s4	221/221 (100%)	187 (85%)	34 (15%)	2 16
7	S5	173/173 (100%)	153 (88%)	20 (12%)	5 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	s5	173/173 (100%)	149 (86%)	24 (14%)	3	20
8	S6	188/193 (97%)	157 (84%)	31 (16%)	2	13
8	s6	187/193 (97%)	154 (82%)	33 (18%)	2	10
9	S7	165/166 (99%)	147 (89%)	18 (11%)	6	29
9	s7	165/166 (99%)	143 (87%)	22 (13%)	4	21
10	S8	150/160 (94%)	128 (85%)	22 (15%)	3	18
10	s8	150/160 (94%)	131 (87%)	19 (13%)	4	22
11	S9	158/158 (100%)	137 (87%)	21 (13%)	4	21
11	s9	158/158 (100%)	134 (85%)	24 (15%)	3	17
12	C0	77/98 (79%)	66 (86%)	11 (14%)	3	19
12	c0	73/98 (74%)	66 (90%)	7 (10%)	8	34
13	C1	129/137 (94%)	112 (87%)	17 (13%)	4	21
13	c1	129/137 (94%)	110 (85%)	19 (15%)	3	18
14	C2	88/119 (74%)	75 (85%)	13 (15%)	3	17
14	c2	88/119 (74%)	72 (82%)	16 (18%)	1	9
15	C3	127/127 (100%)	101 (80%)	26 (20%)	1	6
15	c3	127/127 (100%)	107 (84%)	20 (16%)	2	15
16	C4	81/97 (84%)	67 (83%)	14 (17%)	2	11
16	c4	97/97 (100%)	83 (86%)	14 (14%)	3	18
17	C5	101/118 (86%)	90 (89%)	11 (11%)	6	29
17	c5	103/118 (87%)	87 (84%)	16 (16%)	2	16
18	C6	117/118 (99%)	96 (82%)	21 (18%)	2	9
18	c6	118/118 (100%)	99 (84%)	19 (16%)	2	14
19	C7	94/113 (83%)	77 (82%)	17 (18%)	1	9
19	c7	92/113 (81%)	72 (78%)	20 (22%)	1	5
20	C8	128/128 (100%)	108 (84%)	20 (16%)	2	16
20	c8	128/128 (100%)	107 (84%)	21 (16%)	2	13
21	C9	115/115 (100%)	98 (85%)	17 (15%)	3	17
21	c9	115/115 (100%)	103 (90%)	12 (10%)	7	31
22	D0	100/103 (97%)	84 (84%)	16 (16%)	2	14
22	d0	103/103 (100%)	82 (80%)	21 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	D1	74/74 (100%)	65 (88%)	9 (12%)	5	23
23	d1	74/74 (100%)	67 (90%)	7 (10%)	8	34
24	D2	110/110 (100%)	91 (83%)	19 (17%)	2	11
24	d2	110/110 (100%)	98 (89%)	12 (11%)	6	29
25	D3	119/119 (100%)	102 (86%)	17 (14%)	3	19
25	d3	119/119 (100%)	98 (82%)	21 (18%)	2	10
26	D4	112/112 (100%)	94 (84%)	18 (16%)	2	14
26	d4	112/112 (100%)	92 (82%)	20 (18%)	2	9
27	D5	61/61 (100%)	46 (75%)	15 (25%)	0	4
27	d5	61/61 (100%)	53 (87%)	8 (13%)	4	21
28	D6	83/83 (100%)	64 (77%)	19 (23%)	1	4
28	d6	83/83 (100%)	66 (80%)	17 (20%)	1	6
29	D7	70/70 (100%)	66 (94%)	4 (6%)	20	53
29	d7	70/70 (100%)	57 (81%)	13 (19%)	1	8
30	D8	56/56 (100%)	46 (82%)	10 (18%)	2	9
30	d8	56/56 (100%)	41 (73%)	15 (27%)	0	3
31	D9	47/47 (100%)	37 (79%)	10 (21%)	1	5
31	d9	47/47 (100%)	39 (83%)	8 (17%)	2	12
32	E0	51/53 (96%)	39 (76%)	12 (24%)	1	4
32	e0	53/53 (100%)	45 (85%)	8 (15%)	3	17
33	E1	62/66 (94%)	43 (69%)	19 (31%)	0	2
33	e1	66/66 (100%)	50 (76%)	16 (24%)	0	4
34	SR	259/260 (100%)	233 (90%)	26 (10%)	7	32
35	SM	97/228 (42%)	78 (80%)	19 (20%)	1	7
39	L2	193/194 (100%)	162 (84%)	31 (16%)	2	14
39	l2	192/194 (99%)	159 (83%)	33 (17%)	2	11
40	L3	320/322 (99%)	252 (79%)	68 (21%)	1	5
40	l3	319/322 (99%)	268 (84%)	51 (16%)	2	14
41	L4	288/288 (100%)	239 (83%)	49 (17%)	2	12
41	l4	288/288 (100%)	231 (80%)	57 (20%)	1	7
42	L5	244/244 (100%)	205 (84%)	39 (16%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	l5	243/244 (100%)	201 (83%)	42 (17%)	2	11
43	L6	134/152 (88%)	114 (85%)	20 (15%)	3	17
43	l6	135/152 (89%)	119 (88%)	16 (12%)	5	25
44	L7	186/187 (100%)	156 (84%)	30 (16%)	2	14
44	l7	187/187 (100%)	155 (83%)	32 (17%)	2	12
45	L8	187/191 (98%)	166 (89%)	21 (11%)	6	27
46	L9	171/171 (100%)	134 (78%)	37 (22%)	1	5
46	l9	171/171 (100%)	134 (78%)	37 (22%)	1	5
47	M0	177/186 (95%)	147 (83%)	30 (17%)	2	12
47	m0	179/186 (96%)	139 (78%)	40 (22%)	1	4
48	M1	147/147 (100%)	120 (82%)	27 (18%)	1	8
48	m1	147/147 (100%)	126 (86%)	21 (14%)	3	19
49	M3	154/154 (100%)	125 (81%)	29 (19%)	1	8
49	m3	154/154 (100%)	127 (82%)	27 (18%)	2	10
50	M4	107/108 (99%)	86 (80%)	21 (20%)	1	7
50	m4	108/108 (100%)	91 (84%)	17 (16%)	2	15
51	M5	175/175 (100%)	145 (83%)	30 (17%)	2	12
51	m5	175/175 (100%)	148 (85%)	27 (15%)	2	16
52	M6	160/160 (100%)	141 (88%)	19 (12%)	5	25
52	m6	160/160 (100%)	135 (84%)	25 (16%)	2	16
53	M7	140/145 (97%)	114 (81%)	26 (19%)	1	8
53	m7	125/145 (86%)	99 (79%)	26 (21%)	1	6
54	M8	150/150 (100%)	126 (84%)	24 (16%)	2	14
54	m8	150/150 (100%)	122 (81%)	28 (19%)	1	8
55	M9	153/153 (100%)	133 (87%)	20 (13%)	4	21
55	m9	153/153 (100%)	121 (79%)	32 (21%)	1	6
56	N0	156/156 (100%)	129 (83%)	27 (17%)	2	11
56	n0	156/156 (100%)	130 (83%)	26 (17%)	2	12
57	N1	136/136 (100%)	106 (78%)	30 (22%)	1	5
57	n1	136/136 (100%)	112 (82%)	24 (18%)	2	10
58	N2	87/87 (100%)	73 (84%)	14 (16%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	n2	85/87 (98%)	70 (82%)	15 (18%)	2	10
59	N3	104/104 (100%)	89 (86%)	15 (14%)	3	18
59	n3	104/104 (100%)	93 (89%)	11 (11%)	6	30
60	N4	57/86 (66%)	53 (93%)	4 (7%)	15	46
61	N5	104/105 (99%)	89 (86%)	15 (14%)	3	18
61	n5	104/105 (99%)	80 (77%)	24 (23%)	1	4
62	N6	109/109 (100%)	85 (78%)	24 (22%)	1	5
62	n6	109/109 (100%)	88 (81%)	21 (19%)	1	7
63	N7	115/115 (100%)	97 (84%)	18 (16%)	2	15
63	n7	115/115 (100%)	96 (84%)	19 (16%)	2	13
64	N8	118/118 (100%)	99 (84%)	19 (16%)	2	14
64	n8	118/118 (100%)	101 (86%)	17 (14%)	3	18
65	N9	46/46 (100%)	39 (85%)	7 (15%)	3	17
65	n9	46/46 (100%)	39 (85%)	7 (15%)	3	17
66	O0	81/84 (96%)	64 (79%)	17 (21%)	1	5
66	o0	84/84 (100%)	71 (84%)	13 (16%)	2	16
67	O1	92/96 (96%)	79 (86%)	13 (14%)	3	19
67	o1	94/96 (98%)	74 (79%)	20 (21%)	1	5
68	O2	109/109 (100%)	88 (81%)	21 (19%)	1	7
68	o2	109/109 (100%)	83 (76%)	26 (24%)	0	4
69	O3	90/90 (100%)	72 (80%)	18 (20%)	1	7
69	o3	90/90 (100%)	74 (82%)	16 (18%)	2	10
70	O4	95/95 (100%)	82 (86%)	13 (14%)	3	20
70	o4	95/95 (100%)	83 (87%)	12 (13%)	4	22
71	O5	104/104 (100%)	93 (89%)	11 (11%)	6	30
71	o5	103/104 (99%)	82 (80%)	21 (20%)	1	6
72	O6	81/81 (100%)	63 (78%)	18 (22%)	1	5
72	o6	80/81 (99%)	64 (80%)	16 (20%)	1	7
73	O7	70/70 (100%)	58 (83%)	12 (17%)	2	12
73	o7	70/70 (100%)	54 (77%)	16 (23%)	1	4
74	O8	68/68 (100%)	52 (76%)	16 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	o8	67/68 (98%)	58 (87%)	9 (13%)	4	21
75	O9	45/45 (100%)	37 (82%)	8 (18%)	2	10
75	o9	45/45 (100%)	40 (89%)	5 (11%)	6	28
76	Q0	47/47 (100%)	40 (85%)	7 (15%)	3	17
76	q0	47/47 (100%)	40 (85%)	7 (15%)	3	17
77	Q1	23/23 (100%)	19 (83%)	4 (17%)	2	11
77	q1	23/23 (100%)	14 (61%)	9 (39%)	0	1
78	Q2	90/90 (100%)	65 (72%)	25 (28%)	0	3
78	q2	90/90 (100%)	71 (79%)	19 (21%)	1	5
79	Q3	71/71 (100%)	59 (83%)	12 (17%)	2	12
79	q3	71/71 (100%)	58 (82%)	13 (18%)	1	8
81	sR	260/261 (100%)	238 (92%)	22 (8%)	10	39
82	sM	54/228 (24%)	44 (82%)	10 (18%)	1	8
84	l8	177/208 (85%)	147 (83%)	30 (17%)	2	12
86	n4	100/114 (88%)	87 (87%)	13 (13%)	4	21
87	p0	105/254 (41%)	89 (85%)	16 (15%)	3	17
All	All	18726/19636 (95%)	15610 (83%)	3116 (17%)	2	13

5 of 3116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	c2	85	LYS
41	l4	179	LEU
17	c5	121	ILE
14	c2	71	ILE
28	d6	67	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
14	c2	125	ASN
42	l5	57	ASN
19	c7	105	GLN
30	d8	27	GLN
47	m0	55	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1776/1812 (98%)	474 (26%)	47 (2%)
36	1	3145/3149 (99%)	753 (23%)	72 (2%)
37	3	120/121 (99%)	16 (13%)	3 (2%)
37	7	120/121 (99%)	21 (17%)	2 (1%)
38	4	157/158 (99%)	46 (29%)	3 (1%)
38	8	157/158 (99%)	39 (24%)	2 (1%)
80	6	1792/1800 (99%)	461 (25%)	54 (3%)
83	5	3145/3150 (99%)	767 (24%)	85 (2%)
89	P	1/4 (25%)	0	0
89	p	1/4 (25%)	0	0
All	All	10414/10477 (99%)	2577 (24%)	268 (2%)

5 of 2577 RNA backbone outliers are listed below:

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

5 of 268 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
83	5	2281	A
83	5	2539	C
83	5	3317	U
36	1	2541	U
36	1	2418	G

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 2310 ligands modelled in this entry, 1207 are monoatomic - leaving 1103 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	$\#\|Z\| > 2$
90	OHX	1	3697	36	0,6,6	-	-	-		
90	OHX	6	1916	-	0,6,6	-	-	-		
90	OHX	6	1940	80	0,6,6	-	-	-		
90	OHX	1	3667	-	0,6,6	-	-	-		
90	OHX	1	3604	-	0,6,6	-	-	-		
90	OHX	5	3541	-	0,6,6	-	-	-		
90	OHX	1	3609	-	0,6,6	-	-	-		
90	OHX	5	3455	-	0,6,6	-	-	-		
90	OHX	6	2019	80	0,6,6	-	-	-		
90	OHX	5	3746	83	0,6,6	-	-	-		
90	OHX	1	3625	-	0,6,6	-	-	-		
90	OHX	6	1910	-	0,6,6	-	-	-		
90	OHX	1	3430	-	0,6,6	-	-	-		
90	OHX	4	218	-	0,6,6	-	-	-		
90	OHX	2	1958	-	0,6,6	-	-	-		
90	OHX	6	1938	-	0,6,6	-	-	-		
90	OHX	2	1921	-	0,6,6	-	-	-		
90	OHX	d4	201	-	0,6,6	-	-	-		
90	OHX	5	3480	83	0,6,6	-	-	-		
90	OHX	5	3438	-	0,6,6	-	-	-		
90	OHX	5	3507	-	0,6,6	-	-	-		
90	OHX	1	3407	-	0,6,6	-	-	-		
90	OHX	5	3456	83	0,6,6	-	-	-		
90	OHX	m0	303	-	0,6,6	-	-	-		
90	OHX	1	3700	-	0,6,6	-	-	-		
90	OHX	6	1947	-	0,6,6	-	-	-		
90	OHX	1	3680	-	0,6,6	-	-	-		
90	OHX	5	3666	83	0,6,6	-	-	-		
90	OHX	5	3613	-	0,6,6	-	-	-		
90	OHX	1	3427	36	0,6,6	-	-	-		
90	OHX	6	1946	-	0,6,6	-	-	-		
90	OHX	1	3685	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	1	3628	-	0,6,6	-	-	-		
90	OHX	6	1951	80	0,6,6	-	-	-		
90	OHX	5	3700	83	0,6,6	-	-	-		
90	OHX	5	3408	83	0,6,6	-	-	-		
90	OHX	5	3624	-	0,6,6	-	-	-		
90	OHX	5	3727	-	0,6,6	-	-	-		
90	OHX	6	1959	-	0,6,6	-	-	-		
90	OHX	2	2039	1	0,6,6	-	-	-		
90	OHX	1	3513	-	0,6,6	-	-	-		
90	OHX	6	1939	80	0,6,6	-	-	-		
90	OHX	1	3500	-	0,6,6	-	-	-		
90	OHX	1	3723	-	0,6,6	-	-	-		
90	OHX	6	1943	-	0,6,6	-	-	-		
90	OHX	5	3447	83	0,6,6	-	-	-		
90	OHX	1	3428	-	0,6,6	-	-	-		
90	OHX	1	3439	-	0,6,6	-	-	-		
90	OHX	1	3725	-	0,6,6	-	-	-		
90	OHX	7	210	-	0,6,6	-	-	-		
90	OHX	6	2055	80	0,6,6	-	-	-		
90	OHX	1	3692	-	0,6,6	-	-	-		
90	OHX	1	3519	-	0,6,6	-	-	-		
90	OHX	5	3718	83	0,6,6	-	-	-		
90	OHX	8	206	-	0,6,6	-	-	-		
90	OHX	6	1983	-	0,6,6	-	-	-		
90	OHX	6	2051	80	0,6,6	-	-	-		
90	OHX	2	1965	-	0,6,6	-	-	-		
90	OHX	s4	302	-	0,6,6	-	-	-		
90	OHX	6	2038	-	0,6,6	-	-	-		
90	OHX	2	1962	-	0,6,6	-	-	-		
90	OHX	5	3439	-	0,6,6	-	-	-		
90	OHX	1	3706	-	0,6,6	-	-	-		
90	OHX	6	1965	-	0,6,6	-	-	-		
90	OHX	5	3477	83	0,6,6	-	-	-		
90	OHX	6	2033	80	0,6,6	-	-	-		
90	OHX	1	3708	-	0,6,6	-	-	-		
90	OHX	5	3569	-	0,6,6	-	-	-		
90	OHX	1	3414	-	0,6,6	-	-	-		
90	OHX	1	3412	-	0,6,6	-	-	-		
90	OHX	2	1909	-	0,6,6	-	-	-		
90	OHX	2	1932	-	0,6,6	-	-	-		
90	OHX	1	3543	-	0,6,6	-	-	-		
90	OHX	1	3556	-	0,6,6	-	-	-		
90	OHX	1	3612	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	1	3626	-	0,6,6	-	-	-		
90	OHX	l3	401	-	0,6,6	-	-	-		
90	OHX	1	3434	-	0,6,6	-	-	-		
90	OHX	2	1989	-	0,6,6	-	-	-		
90	OHX	1	3466	-	0,6,6	-	-	-		
90	OHX	1	3438	-	0,6,6	-	-	-		
90	OHX	1	3572	36	0,6,6	-	-	-		
90	OHX	5	3520	-	0,6,6	-	-	-		
90	OHX	l5	301	-	0,6,6	-	-	-		
90	OHX	5	3664	-	0,6,6	-	-	-		
90	OHX	2	2034	-	0,6,6	-	-	-		
90	OHX	5	3490	83	0,6,6	-	-	-		
90	OHX	5	3547	-	0,6,6	-	-	-		
90	OHX	1	3518	-	0,6,6	-	-	-		
90	OHX	2	2002	-	0,6,6	-	-	-		
90	OHX	5	3423	83	0,6,6	-	-	-		
90	OHX	6	2002	80	0,6,6	-	-	-		
90	OHX	1	3727	36	0,6,6	-	-	-		
90	OHX	6	1907	80	0,6,6	-	-	-		
90	OHX	5	3528	-	0,6,6	-	-	-		
90	OHX	1	3570	-	0,6,6	-	-	-		
90	OHX	5	3518	-	0,6,6	-	-	-		
90	OHX	1	3429	-	0,6,6	-	-	-		
90	OHX	2	2017	-	0,6,6	-	-	-		
90	OHX	2	2013	-	0,6,6	-	-	-		
90	OHX	6	2052	80	0,6,6	-	-	-		
90	OHX	5	3443	37	0,6,6	-	-	-		
90	OHX	5	3469	83	0,6,6	-	-	-		
90	OHX	2	2023	-	0,6,6	-	-	-		
90	OHX	1	3649	-	0,6,6	-	-	-		
90	OHX	5	3493	83	0,6,6	-	-	-		
90	OHX	1	3527	-	0,6,6	-	-	-		
90	OHX	2	2037	1	0,6,6	-	-	-		
90	OHX	5	3610	-	0,6,6	-	-	-		
90	OHX	5	3464	83	0,6,6	-	-	-		
90	OHX	1	3465	-	0,6,6	-	-	-		
90	OHX	1	3599	-	0,6,6	-	-	-		
90	OHX	5	3656	-	0,6,6	-	-	-		
90	OHX	2	2043	1	0,6,6	-	-	-		
90	OHX	2	1994	-	0,6,6	-	-	-		
90	OHX	1	3425	-	0,6,6	-	-	-		
90	OHX	1	3584	-	0,6,6	-	-	-		
90	OHX	1	3569	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	1	3639	-	0,6,6	-	-	-		
90	OHX	6	2012	-	0,6,6	-	-	-		
90	OHX	5	3515	-	0,6,6	-	-	-		
90	OHX	2	1931	-	0,6,6	-	-	-		
90	OHX	4	214	-	0,6,6	-	-	-		
90	OHX	2	1919	-	0,6,6	-	-	-		
90	OHX	5	3692	-	0,6,6	-	-	-		
90	OHX	1	3480	-	0,6,6	-	-	-		
90	OHX	5	3695	-	0,6,6	-	-	-		
90	OHX	1	3525	-	0,6,6	-	-	-		
90	OHX	2	1969	1	0,6,6	-	-	-		
90	OHX	5	3460	83	0,6,6	-	-	-		
90	OHX	5	3599	83	0,6,6	-	-	-		
90	OHX	2	2019	-	0,6,6	-	-	-		
90	OHX	6	1912	-	0,6,6	-	-	-		
90	OHX	5	3601	-	0,6,6	-	-	-		
90	OHX	2	1912	-	0,6,6	-	-	-		
90	OHX	5	3726	83	0,6,6	-	-	-		
90	OHX	6	1972	80	0,6,6	-	-	-		
90	OHX	L3	402	-	0,6,6	-	-	-		
90	OHX	5	3662	-	0,6,6	-	-	-		
90	OHX	5	3644	-	0,6,6	-	-	-		
90	OHX	1	3537	-	0,6,6	-	-	-		
90	OHX	1	3613	-	0,6,6	-	-	-		
90	OHX	4	216	-	0,6,6	-	-	-		
90	OHX	8	211	38	0,6,6	-	-	-		
90	OHX	5	3421	-	0,6,6	-	-	-		
90	OHX	2	1956	-	0,6,6	-	-	-		
90	OHX	6	1902	80	0,6,6	-	-	-		
90	OHX	4	215	-	0,6,6	-	-	-		
90	OHX	2	1947	-	0,6,6	-	-	-		
90	OHX	6	1997	-	0,6,6	-	-	-		
90	OHX	6	2001	-	0,6,6	-	-	-		
90	OHX	5	3719	-	0,6,6	-	-	-		
90	OHX	l3	402	-	0,6,6	-	-	-		
90	OHX	2	1960	-	0,6,6	-	-	-		
90	OHX	6	1905	-	0,6,6	-	-	-		
90	OHX	6	1988	-	0,6,6	-	-	-		
90	OHX	1	3528	-	0,6,6	-	-	-		
90	OHX	5	3707	-	0,6,6	-	-	-		
90	OHX	1	3554	-	0,6,6	-	-	-		
90	OHX	5	3632	-	0,6,6	-	-	-		
90	OHX	1	3588	36	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	5	3556	83	0,6,6	-	-	-		
90	OHX	5	3561	83	0,6,6	-	-	-		
90	OHX	1	3539	-	0,6,6	-	-	-		
90	OHX	5	3590	83	0,6,6	-	-	-		
90	OHX	2	1934	-	0,6,6	-	-	-		
90	OHX	5	3653	83	0,6,6	-	-	-		
90	OHX	1	3718	-	0,6,6	-	-	-		
90	OHX	2	1941	-	0,6,6	-	-	-		
90	OHX	6	1967	80	0,6,6	-	-	-		
90	OHX	1	3521	-	0,6,6	-	-	-		
90	OHX	6	1975	-	0,6,6	-	-	-		
90	OHX	2	2046	-	0,6,6	-	-	-		
90	OHX	5	3529	83	0,6,6	-	-	-		
90	OHX	8	218	38	0,6,6	-	-	-		
90	OHX	4	222	-	0,6,6	-	-	-		
90	OHX	1	3610	-	0,6,6	-	-	-		
90	OHX	5	3747	83	0,6,6	-	-	-		
90	OHX	2	1970	-	0,6,6	-	-	-		
90	OHX	1	3564	36	0,6,6	-	-	-		
90	OHX	5	3524	83	0,6,6	-	-	-		
90	OHX	2	1986	1	0,6,6	-	-	-		
90	OHX	5	3521	83	0,6,6	-	-	-		
90	OHX	6	2034	-	0,6,6	-	-	-		
90	OHX	5	3688	-	0,6,6	-	-	-		
90	OHX	6	1990	-	0,6,6	-	-	-		
90	OHX	1	3468	-	0,6,6	-	-	-		
90	OHX	6	1977	80	0,6,6	-	-	-		
90	OHX	5	3736	83	0,6,6	-	-	-		
90	OHX	7	202	37	0,6,6	-	-	-		
90	OHX	1	3650	-	0,6,6	-	-	-		
90	OHX	1	3619	-	0,6,6	-	-	-		
90	OHX	1	3695	36	0,6,6	-	-	-		
90	OHX	2	1937	-	0,6,6	-	-	-		
90	OHX	1	3460	-	0,6,6	-	-	-		
90	OHX	1	3710	36	0,6,6	-	-	-		
90	OHX	5	3415	-	0,6,6	-	-	-		
90	OHX	1	3474	-	0,6,6	-	-	-		
90	OHX	2	2007	-	0,6,6	-	-	-		
90	OHX	5	3495	83	0,6,6	-	-	-		
90	OHX	5	3548	83	0,6,6	-	-	-		
90	OHX	5	3595	83	0,6,6	-	-	-		
90	OHX	1	3726	-	0,6,6	-	-	-		
90	OHX	1	3453	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	1	3559	-	0,6,6	-	-	-		
90	OHX	5	3526	-	0,6,6	-	-	-		
90	OHX	6	2041	-	0,6,6	-	-	-		
90	OHX	1	3627	36	0,6,6	-	-	-		
90	OHX	5	3562	-	0,6,6	-	-	-		
90	OHX	6	1901	-	0,6,6	-	-	-		
90	OHX	5	3643	83	0,6,6	-	-	-		
93	PHE	1	3401	-	10,11,12	1.23	1 (10%)	10,13,15	0.62	0
90	OHX	1	3421	-	0,6,6	-	-	-		
90	OHX	1	3423	-	0,6,6	-	-	-		
90	OHX	2	1991	-	0,6,6	-	-	-		
90	OHX	5	3603	-	0,6,6	-	-	-		
90	OHX	5	3712	83	0,6,6	-	-	-		
90	OHX	2	2040	-	0,6,6	-	-	-		
90	OHX	5	3721	83	0,6,6	-	-	-		
90	OHX	5	3697	-	0,6,6	-	-	-		
90	OHX	1	3551	-	0,6,6	-	-	-		
90	OHX	5	3730	-	0,6,6	-	-	-		
90	OHX	1	3568	-	0,6,6	-	-	-		
90	OHX	5	3406	-	0,6,6	-	-	-		
90	OHX	2	1926	-	0,6,6	-	-	-		
90	OHX	2	2009	1	0,6,6	-	-	-		
90	OHX	C3	201	-	0,6,6	-	-	-		
90	OHX	1	3566	36	0,6,6	-	-	-		
90	OHX	6	1999	80	0,6,6	-	-	-		
90	OHX	1	3591	-	0,6,6	-	-	-		
90	OHX	4	221	-	0,6,6	-	-	-		
90	OHX	1	3632	-	0,6,6	-	-	-		
90	OHX	1	3535	-	0,6,6	-	-	-		
90	OHX	5	3446	-	0,6,6	-	-	-		
90	OHX	2	1936	1	0,6,6	-	-	-		
90	OHX	1	3561	-	0,6,6	-	-	-		
90	OHX	6	2026	80	0,6,6	-	-	-		
90	OHX	1	3469	-	0,6,6	-	-	-		
90	OHX	6	1955	80	0,6,6	-	-	-		
90	OHX	5	3452	-	0,6,6	-	-	-		
90	OHX	2	2047	1	0,6,6	-	-	-		
90	OHX	4	206	-	0,6,6	-	-	-		
90	OHX	1	3715	36	0,6,6	-	-	-		
90	OHX	5	3591	-	0,6,6	-	-	-		
90	OHX	5	3404	-	0,6,6	-	-	-		
90	OHX	2	1930	-	0,6,6	-	-	-		
90	OHX	1	3660	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	5	3473	83	0,6,6	-	-	-		
90	OHX	5	3701	-	0,6,6	-	-	-		
90	OHX	5	3472	83	0,6,6	-	-	-		
90	OHX	1	3515	-	0,6,6	-	-	-		
90	OHX	1	3664	-	0,6,6	-	-	-		
90	OHX	5	3533	83	0,6,6	-	-	-		
90	OHX	5	3717	83	0,6,6	-	-	-		
90	OHX	1	3637	36	0,6,6	-	-	-		
90	OHX	6	1924	80	0,6,6	-	-	-		
90	OHX	1	3455	-	0,6,6	-	-	-		
90	OHX	1	3563	-	0,6,6	-	-	-		
90	OHX	2	2020	-	0,6,6	-	-	-		
90	OHX	2	1993	-	0,6,6	-	-	-		
90	OHX	5	3503	-	0,6,6	-	-	-		
90	OHX	5	3508	-	0,6,6	-	-	-		
90	OHX	2	1959	-	0,6,6	-	-	-		
90	OHX	5	3538	-	0,6,6	-	-	-		
90	OHX	1	3699	-	0,6,6	-	-	-		
90	OHX	1	3585	-	0,6,6	-	-	-		
90	OHX	5	3576	-	0,6,6	-	-	-		
90	OHX	5	3670	83	0,6,6	-	-	-		
90	OHX	1	3526	-	0,6,6	-	-	-		
90	OHX	7	207	37	0,6,6	-	-	-		
90	OHX	6	2010	80	0,6,6	-	-	-		
90	OHX	2	2045	-	0,6,6	-	-	-		
90	OHX	1	3562	-	0,6,6	-	-	-		
90	OHX	C8	202	36	0,6,6	-	-	-		
90	OHX	1	3676	-	0,6,6	-	-	-		
90	OHX	5	3575	-	0,6,6	-	-	-		
90	OHX	1	3656	-	0,6,6	-	-	-		
90	OHX	5	3741	-	0,6,6	-	-	-		
90	OHX	5	3748	-	0,6,6	-	-	-		
90	OHX	1	3499	-	0,6,6	-	-	-		
90	OHX	1	3514	-	0,6,6	-	-	-		
90	OHX	1	3520	-	0,6,6	-	-	-		
90	OHX	5	3424	-	0,6,6	-	-	-		
90	OHX	5	3494	-	0,6,6	-	-	-		
90	OHX	5	3708	-	0,6,6	-	-	-		
90	OHX	8	215	-	0,6,6	-	-	-		
90	OHX	1	3730	36	0,6,6	-	-	-		
90	OHX	5	3621	-	0,6,6	-	-	-		
90	OHX	1	3686	-	0,6,6	-	-	-		
90	OHX	2	2032	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	2	2049	-	0,6,6	-	-	-		
90	OHX	6	1979	-	0,6,6	-	-	-		
90	OHX	2	2030	1	0,6,6	-	-	-		
90	OHX	1	3431	-	0,6,6	-	-	-		
90	OHX	1	3696	-	0,6,6	-	-	-		
90	OHX	6	2025	80	0,6,6	-	-	-		
90	OHX	8	210	-	0,6,6	-	-	-		
90	OHX	2	1946	-	0,6,6	-	-	-		
90	OHX	1	3611	-	0,6,6	-	-	-		
90	OHX	2	2001	-	0,6,6	-	-	-		
90	OHX	1	3452	-	0,6,6	-	-	-		
90	OHX	6	1929	80	0,6,6	-	-	-		
90	OHX	5	3637	83	0,6,6	-	-	-		
90	OHX	1	3608	-	0,6,6	-	-	-		
90	OHX	L3	403	-	0,6,6	-	-	-		
90	OHX	5	3710	-	0,6,6	-	-	-		
90	OHX	5	3636	-	0,6,6	-	-	-		
90	OHX	6	1987	80	0,6,6	-	-	-		
90	OHX	1	3669	-	0,6,6	-	-	-		
90	OHX	2	1952	1	0,6,6	-	-	-		
90	OHX	6	1922	80	0,6,6	-	-	-		
90	OHX	c8	202	-	0,6,6	-	-	-		
90	OHX	7	206	37	0,6,6	-	-	-		
90	OHX	2	1997	-	0,6,6	-	-	-		
90	OHX	5	3572	83	0,6,6	-	-	-		
90	OHX	1	3495	-	0,6,6	-	-	-		
90	OHX	1	3409	-	0,6,6	-	-	-		
90	OHX	5	3694	-	0,6,6	-	-	-		
90	OHX	2	2038	-	0,6,6	-	-	-		
90	OHX	5	3696	83	0,6,6	-	-	-		
90	OHX	1	3486	-	0,6,6	-	-	-		
90	OHX	1	3422	-	0,6,6	-	-	-		
90	OHX	1	3670	-	0,6,6	-	-	-		
90	OHX	5	3691	-	0,6,6	-	-	-		
90	OHX	1	3688	36	0,6,6	-	-	-		
90	OHX	5	3617	-	0,6,6	-	-	-		
90	OHX	1	3643	-	0,6,6	-	-	-		
90	OHX	5	3535	83	0,6,6	-	-	-		
90	OHX	6	1914	80	0,6,6	-	-	-		
90	OHX	6	2008	-	0,6,6	-	-	-		
90	OHX	1	3507	-	0,6,6	-	-	-		
90	OHX	m5	301	-	0,6,6	-	-	-		
90	OHX	4	220	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	6	1986	-	0,6,6	-	-	-		
90	OHX	6	2000	80	0,6,6	-	-	-		
90	OHX	5	3420	-	0,6,6	-	-	-		
90	OHX	5	3578	83	0,6,6	-	-	-		
90	OHX	5	3552	83	0,6,6	-	-	-		
90	OHX	1	3646	-	0,6,6	-	-	-		
90	OHX	1	3540	-	0,6,6	-	-	-		
90	OHX	1	3684	-	0,6,6	-	-	-		
90	OHX	L4	402	-	0,6,6	-	-	-		
90	OHX	2	2016	-	0,6,6	-	-	-		
90	OHX	6	2004	-	0,6,6	-	-	-		
90	OHX	2	1917	-	0,6,6	-	-	-		
90	OHX	5	3678	83	0,6,6	-	-	-		
90	OHX	5	3560	-	0,6,6	-	-	-		
90	OHX	C5	201	-	0,6,6	-	-	-		
90	OHX	2	2050	1	0,6,6	-	-	-		
90	OHX	2	2004	-	0,6,6	-	-	-		
90	OHX	6	2018	80	0,6,6	-	-	-		
90	OHX	5	3646	-	0,6,6	-	-	-		
90	OHX	8	214	38	0,6,6	-	-	-		
90	OHX	5	3684	83	0,6,6	-	-	-		
90	OHX	2	1911	-	0,6,6	-	-	-		
90	OHX	1	3598	-	0,6,6	-	-	-		
90	OHX	1	3689	-	0,6,6	-	-	-		
90	OHX	1	3693	-	0,6,6	-	-	-		
90	OHX	6	2015	-	0,6,6	-	-	-		
90	OHX	5	3600	83	0,6,6	-	-	-		
90	OHX	5	3582	-	0,6,6	-	-	-		
90	OHX	5	3677	83	0,6,6	-	-	-		
90	OHX	1	3472	-	0,6,6	-	-	-		
90	OHX	2	1905	-	0,6,6	-	-	-		
90	OHX	1	3493	36	0,6,6	-	-	-		
90	OHX	6	1995	-	0,6,6	-	-	-		
90	OHX	7	204	-	0,6,6	-	-	-		
90	OHX	5	3486	-	0,6,6	-	-	-		
90	OHX	5	3713	83	0,6,6	-	-	-		
90	OHX	5	3553	83	0,6,6	-	-	-		
90	OHX	5	3459	83	0,6,6	-	-	-		
90	OHX	8	212	38	0,6,6	-	-	-		
90	OHX	6	1957	80	0,6,6	-	-	-		
90	OHX	1	3687	-	0,6,6	-	-	-		
90	OHX	1	3672	-	0,6,6	-	-	-		
90	OHX	1	3404	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	5	3604	83	0,6,6	-	-	-		
90	OHX	4	204	-	0,6,6	-	-	-		
90	OHX	1	3679	-	0,6,6	-	-	-		
90	OHX	2	1929	-	0,6,6	-	-	-		
90	OHX	1	3545	-	0,6,6	-	-	-		
90	OHX	1	3576	36	0,6,6	-	-	-		
90	OHX	2	1927	-	0,6,6	-	-	-		
90	OHX	6	1970	80	0,6,6	-	-	-		
90	OHX	8	209	38	0,6,6	-	-	-		
90	OHX	6	1925	-	0,6,6	-	-	-		
90	OHX	4	211	-	0,6,6	-	-	-		
90	OHX	6	1996	80	0,6,6	-	-	-		
90	OHX	1	3661	-	0,6,6	-	-	-		
90	OHX	1	3575	-	0,6,6	-	-	-		
90	OHX	c5	201	-	0,6,6	-	-	-		
90	OHX	5	3672	-	0,6,6	-	-	-		
90	OHX	6	2005	-	0,6,6	-	-	-		
90	OHX	1	3481	-	0,6,6	-	-	-		
90	OHX	5	3577	83	0,6,6	-	-	-		
90	OHX	O9	101	-	0,6,6	-	-	-		
90	OHX	5	3436	83	0,6,6	-	-	-		
90	OHX	3	210	-	0,6,6	-	-	-		
90	OHX	5	3679	-	0,6,6	-	-	-		
90	OHX	5	3705	-	0,6,6	-	-	-		
90	OHX	1	3482	-	0,6,6	-	-	-		
90	OHX	6	1923	80	0,6,6	-	-	-		
90	OHX	1	3714	-	0,6,6	-	-	-		
90	OHX	2	1924	-	0,6,6	-	-	-		
90	OHX	2	1943	-	0,6,6	-	-	-		
90	OHX	1	3504	-	0,6,6	-	-	-		
90	OHX	1	3614	-	0,6,6	-	-	-		
90	OHX	1	3483	-	0,6,6	-	-	-		
90	OHX	5	3481	-	0,6,6	-	-	-		
90	OHX	5	3628	-	0,6,6	-	-	-		
90	OHX	M0	301	-	0,6,6	-	-	-		
90	OHX	5	3647	-	0,6,6	-	-	-		
90	OHX	5	3709	-	0,6,6	-	-	-		
90	OHX	2	1979	-	0,6,6	-	-	-		
90	OHX	o3	201	-	0,6,6	-	-	-		
90	OHX	5	3745	-	0,6,6	-	-	-		
90	OHX	1	3635	-	0,6,6	-	-	-		
90	OHX	2	1961	-	0,6,6	-	-	-		
90	OHX	6	1908	80	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	2	1977	-	0,6,6	-	-	-		
90	OHX	5	3449	-	0,6,6	-	-	-		
90	OHX	M5	302	-	0,6,6	-	-	-		
90	OHX	5	3437	83	0,6,6	-	-	-		
90	OHX	2	2025	-	0,6,6	-	-	-		
90	OHX	1	3600	-	0,6,6	-	-	-		
90	OHX	2	1953	-	0,6,6	-	-	-		
90	OHX	1	3665	-	0,6,6	-	-	-		
90	OHX	4	213	-	0,6,6	-	-	-		
90	OHX	1	3677	-	0,6,6	-	-	-		
90	OHX	1	3582	36	0,6,6	-	-	-		
90	OHX	5	3655	-	0,6,6	-	-	-		
90	OHX	5	3422	83	0,6,6	-	-	-		
90	OHX	6	1953	80	0,6,6	-	-	-		
90	OHX	4	208	38	0,6,6	-	-	-		
90	OHX	5	3720	83	0,6,6	-	-	-		
90	OHX	1	3641	-	0,6,6	-	-	-		
90	OHX	6	2059	-	0,6,6	-	-	-		
90	OHX	5	3465	-	0,6,6	-	-	-		
90	OHX	S8	301	-	0,6,6	-	-	-		
95	SPS	5	4176	91	20,23,23	3.41	10 (50%)	18,30,30	4.56	11 (61%)
90	OHX	2	2048	-	0,6,6	-	-	-		
90	OHX	1	3707	-	0,6,6	-	-	-		
90	OHX	6	1915	80	0,6,6	-	-	-		
90	OHX	5	3417	-	0,6,6	-	-	-		
90	OHX	5	3630	-	0,6,6	-	-	-		
90	OHX	5	3665	83	0,6,6	-	-	-		
90	OHX	5	3609	-	0,6,6	-	-	-		
90	OHX	2	1918	-	0,6,6	-	-	-		
90	OHX	2	2044	-	0,6,6	-	-	-		
90	OHX	1	3587	-	0,6,6	-	-	-		
90	OHX	5	3627	-	0,6,6	-	-	-		
90	OHX	5	3693	-	0,6,6	-	-	-		
90	OHX	6	2017	80	0,6,6	-	-	-		
90	OHX	1	3494	36	0,6,6	-	-	-		
90	OHX	2	2015	-	0,6,6	-	-	-		
90	OHX	6	1963	-	0,6,6	-	-	-		
90	OHX	5	3484	83	0,6,6	-	-	-		
90	OHX	6	2040	80	0,6,6	-	-	-		
90	OHX	1	3573	36	0,6,6	-	-	-		
90	OHX	6	2037	80	0,6,6	-	-	-		
90	OHX	s1	301	-	0,6,6	-	-	-		
90	OHX	2	1950	1	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	3	207	-	0,6,6	-	-	-		
90	OHX	1	3705	-	0,6,6	-	-	-		
90	OHX	1	3577	-	0,6,6	-	-	-		
90	OHX	5	3434	-	0,6,6	-	-	-		
90	OHX	1	3436	-	0,6,6	-	-	-		
90	OHX	5	3479	-	0,6,6	-	-	-		
90	OHX	6	1926	80	0,6,6	-	-	-		
90	OHX	5	3623	-	0,6,6	-	-	-		
90	OHX	1	3491	-	0,6,6	-	-	-		
90	OHX	5	3566	-	0,6,6	-	-	-		
90	OHX	5	3593	-	0,6,6	-	-	-		
90	OHX	1	3633	-	0,6,6	-	-	-		
90	OHX	1	3532	-	0,6,6	-	-	-		
90	OHX	5	3635	83	0,6,6	-	-	-		
90	OHX	5	3542	83	0,6,6	-	-	-		
90	OHX	5	3652	-	0,6,6	-	-	-		
90	OHX	2	1928	-	0,6,6	-	-	-		
90	OHX	5	3557	-	0,6,6	-	-	-		
90	OHX	1	3605	-	0,6,6	-	-	-		
90	OHX	5	3669	83	0,6,6	-	-	-		
90	OHX	1	3509	36	0,6,6	-	-	-		
90	OHX	1	3560	-	0,6,6	-	-	-		
90	OHX	4	210	-	0,6,6	-	-	-		
90	OHX	1	3524	-	0,6,6	-	-	-		
90	OHX	2	1976	-	0,6,6	-	-	-		
90	OHX	1	3506	-	0,6,6	-	-	-		
90	OHX	2	1904	1	0,6,6	-	-	-		
90	OHX	1	3490	-	0,6,6	-	-	-		
90	OHX	1	3550	-	0,6,6	-	-	-		
90	OHX	1	3712	36	0,6,6	-	-	-		
90	OHX	6	1913	80	0,6,6	-	-	-		
90	OHX	5	3427	-	0,6,6	-	-	-		
90	OHX	1	3713	-	0,6,6	-	-	-		
90	OHX	5	3461	83	0,6,6	-	-	-		
90	OHX	1	3449	36	0,6,6	-	-	-		
90	OHX	5	3492	-	0,6,6	-	-	-		
90	OHX	5	3605	-	0,6,6	-	-	-		
90	OHX	l9	201	-	0,6,6	-	-	-		
90	OHX	6	2058	-	0,6,6	-	-	-		
90	OHX	1	3606	-	0,6,6	-	-	-		
90	OHX	1	3549	-	0,6,6	-	-	-		
90	OHX	5	3661	-	0,6,6	-	-	-		
90	OHX	2	1933	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	2	1942	-	0,6,6	-	-	-		
90	OHX	2	2000	-	0,6,6	-	-	-		
90	OHX	1	3410	-	0,6,6	-	-	-		
90	OHX	2	2029	-	0,6,6	-	-	-		
90	OHX	5	3555	-	0,6,6	-	-	-		
90	OHX	5	3668	83	0,6,6	-	-	-		
90	OHX	5	3458	83	0,6,6	-	-	-		
90	OHX	5	3425	-	0,6,6	-	-	-		
90	OHX	8	207	-	0,6,6	-	-	-		
90	OHX	1	3616	36	0,6,6	-	-	-		
90	OHX	1	3654	-	0,6,6	-	-	-		
90	OHX	6	1921	80	0,6,6	-	-	-		
90	OHX	6	2016	80	0,6,6	-	-	-		
90	OHX	2	1987	1	0,6,6	-	-	-		
90	OHX	2	1975	-	0,6,6	-	-	-		
90	OHX	1	3484	-	0,6,6	-	-	-		
90	OHX	5	3483	-	0,6,6	-	-	-		
90	OHX	6	1980	-	0,6,6	-	-	-		
90	OHX	5	3525	83	0,6,6	-	-	-		
90	OHX	7	203	37	0,6,6	-	-	-		
90	OHX	1	3479	-	0,6,6	-	-	-		
90	OHX	6	2032	-	0,6,6	-	-	-		
90	OHX	5	3478	-	0,6,6	-	-	-		
90	OHX	6	2036	80	0,6,6	-	-	-		
90	OHX	m0	304	-	0,6,6	-	-	-		
90	OHX	8	208	38	0,6,6	-	-	-		
90	OHX	1	3574	-	0,6,6	-	-	-		
90	OHX	1	3644	-	0,6,6	-	-	-		
90	OHX	1	3702	-	0,6,6	-	-	-		
90	OHX	7	205	37	0,6,6	-	-	-		
90	OHX	5	3517	-	0,6,6	-	-	-		
90	OHX	L6	201	-	0,6,6	-	-	-		
90	OHX	5	3596	83	0,6,6	-	-	-		
90	OHX	o7	502	-	0,6,6	-	-	-		
90	OHX	2	1990	-	0,6,6	-	-	-		
90	OHX	1	3579	-	0,6,6	-	-	-		
90	OHX	5	3419	83	0,6,6	-	-	-		
90	OHX	3	201	-	0,6,6	-	-	-		
90	OHX	1	3721	-	0,6,6	-	-	-		
90	OHX	1	3698	36	0,6,6	-	-	-		
90	OHX	5	3413	-	0,6,6	-	-	-		
90	OHX	5	3650	-	0,6,6	-	-	-		
90	OHX	2	1948	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	2	1996	-	0,6,6	-	-	-		
90	OHX	2	1983	-	0,6,6	-	-	-		
90	OHX	1	3655	-	0,6,6	-	-	-		
90	OHX	M9	201	-	0,6,6	-	-	-		
90	OHX	5	3416	83	0,6,6	-	-	-		
90	OHX	5	3554	-	0,6,6	-	-	-		
90	OHX	2	2005	-	0,6,6	-	-	-		
90	OHX	M5	301	-	0,6,6	-	-	-		
90	OHX	5	3725	-	0,6,6	-	-	-		
90	OHX	6	1966	80	0,6,6	-	-	-		
90	OHX	5	3606	83	0,6,6	-	-	-		
90	OHX	5	3550	83	0,6,6	-	-	-		
90	OHX	5	3731	-	0,6,6	-	-	-		
90	OHX	1	3634	-	0,6,6	-	-	-		
90	OHX	1	3503	-	0,6,6	-	-	-		
90	OHX	2	1908	-	0,6,6	-	-	-		
90	OHX	2	2014	-	0,6,6	-	-	-		
90	OHX	1	3592	-	0,6,6	-	-	-		
90	OHX	5	3724	83	0,6,6	-	-	-		
90	OHX	m6	202	-	0,6,6	-	-	-		
90	OHX	1	3440	-	0,6,6	-	-	-		
90	OHX	5	3615	83	0,6,6	-	-	-		
90	OHX	1	3593	-	0,6,6	-	-	-		
90	OHX	5	3442	-	0,6,6	-	-	-		
90	OHX	6	1937	-	0,6,6	-	-	-		
90	OHX	6	2031	80	0,6,6	-	-	-		
90	OHX	5	3418	-	0,6,6	-	-	-		
90	OHX	2	1914	-	0,6,6	-	-	-		
90	OHX	1	3512	36	0,6,6	-	-	-		
90	OHX	2	1992	-	0,6,6	-	-	-		
90	OHX	5	3581	-	0,6,6	-	-	-		
90	OHX	6	1932	80	0,6,6	-	-	-		
90	OHX	6	1998	80	0,6,6	-	-	-		
90	OHX	5	3592	83	0,6,6	-	-	-		
90	OHX	5	3690	-	0,6,6	-	-	-		
90	OHX	2	1910	-	0,6,6	-	-	-		
90	OHX	5	3642	83	0,6,6	-	-	-		
90	OHX	2	1922	-	0,6,6	-	-	-		
90	OHX	2	1938	-	0,6,6	-	-	-		
90	OHX	5	3667	-	0,6,6	-	-	-		
90	OHX	1	3406	-	0,6,6	-	-	-		
90	OHX	6	1989	80	0,6,6	-	-	-		
90	OHX	M8	201	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	1	3454	-	0,6,6	-	-	-		
90	OHX	2	1999	-	0,6,6	-	-	-		
90	OHX	5	3409	-	0,6,6	-	-	-		
90	OHX	5	3598	83	0,6,6	-	-	-		
90	OHX	n9	101	-	0,6,6	-	-	-		
90	OHX	1	3478	-	0,6,6	-	-	-		
90	OHX	5	3702	-	0,6,6	-	-	-		
90	OHX	2	1968	-	0,6,6	-	-	-		
90	OHX	1	3557	-	0,6,6	-	-	-		
90	OHX	6	2024	-	0,6,6	-	-	-		
90	OHX	5	3441	83	0,6,6	-	-	-		
90	OHX	5	3454	-	0,6,6	-	-	-		
93	PHE	5	3401	-	10,11,12	1.23	1 (10%)	10,13,15	0.62	0
90	OHX	1	3595	-	0,6,6	-	-	-		
90	OHX	1	3447	-	0,6,6	-	-	-		
90	OHX	5	3629	83	0,6,6	-	-	-		
90	OHX	6	1911	-	0,6,6	-	-	-		
90	OHX	1	3419	36	0,6,6	-	-	-		
90	OHX	1	3542	-	0,6,6	-	-	-		
90	OHX	L6	202	-	0,6,6	-	-	-		
90	OHX	6	1944	80	0,6,6	-	-	-		
90	OHX	1	3533	-	0,6,6	-	-	-		
90	OHX	5	3564	83	0,6,6	-	-	-		
90	OHX	2	2022	-	0,6,6	-	-	-		
90	OHX	6	1945	80	0,6,6	-	-	-		
90	OHX	6	2057	80	0,6,6	-	-	-		
90	OHX	1	3464	-	0,6,6	-	-	-		
90	OHX	6	2039	80	0,6,6	-	-	-		
90	OHX	5	3735	-	0,6,6	-	-	-		
90	OHX	6	2013	80	0,6,6	-	-	-		
90	OHX	5	3597	83	0,6,6	-	-	-		
90	OHX	8	204	38	0,6,6	-	-	-		
90	OHX	1	3640	-	0,6,6	-	-	-		
90	OHX	1	3555	-	0,6,6	-	-	-		
90	OHX	2	1984	-	0,6,6	-	-	-		
90	OHX	5	3451	-	0,6,6	-	-	-		
90	OHX	4	212	-	0,6,6	-	-	-		
90	OHX	5	3634	-	0,6,6	-	-	-		
90	OHX	5	3514	83	0,6,6	-	-	-		
90	OHX	1	3668	-	0,6,6	-	-	-		
90	OHX	1	3442	-	0,6,6	-	-	-		
90	OHX	6	1994	-	0,6,6	-	-	-		
90	OHX	1	3458	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	5	3611	-	0,6,6	-	-	-		
90	OHX	1	3662	-	0,6,6	-	-	-		
90	OHX	1	3435	-	0,6,6	-	-	-		
90	OHX	5	3732	-	0,6,6	-	-	-		
90	OHX	5	3579	-	0,6,6	-	-	-		
90	OHX	5	3563	83	0,6,6	-	-	-		
90	OHX	5	3559	-	0,6,6	-	-	-		
90	OHX	5	3626	83	0,6,6	-	-	-		
90	OHX	5	3660	83	0,6,6	-	-	-		
90	OHX	5	3722	83	0,6,6	-	-	-		
90	OHX	2	1963	1	0,6,6	-	-	-		
90	OHX	5	3586	83	0,6,6	-	-	-		
90	OHX	5	3739	-	0,6,6	-	-	-		
90	OHX	5	3516	83	0,6,6	-	-	-		
90	OHX	2	1971	-	0,6,6	-	-	-		
90	OHX	1	3596	-	0,6,6	-	-	-		
90	OHX	6	1920	80	0,6,6	-	-	-		
90	OHX	5	3466	-	0,6,6	-	-	-		
90	OHX	2	2011	1	0,6,6	-	-	-		
90	OHX	6	1960	80	0,6,6	-	-	-		
90	OHX	3	206	-	0,6,6	-	-	-		
90	OHX	1	3629	36	0,6,6	-	-	-		
90	OHX	1	3489	-	0,6,6	-	-	-		
90	OHX	1	3624	-	0,6,6	-	-	-		
90	OHX	O3	201	-	0,6,6	-	-	-		
90	OHX	5	3453	83	0,6,6	-	-	-		
90	OHX	5	3523	-	0,6,6	-	-	-		
90	OHX	1	3416	-	0,6,6	-	-	-		
90	OHX	5	3699	-	0,6,6	-	-	-		
90	OHX	1	3420	-	0,6,6	-	-	-		
90	OHX	5	3641	-	0,6,6	-	-	-		
90	OHX	1	3511	-	0,6,6	-	-	-		
90	OHX	6	1934	-	0,6,6	-	-	-		
90	OHX	6	1969	-	0,6,6	-	-	-		
90	OHX	5	3414	-	0,6,6	-	-	-		
90	OHX	5	3489	-	0,6,6	-	-	-		
90	OHX	6	1941	80	0,6,6	-	-	-		
90	OHX	1	3510	-	0,6,6	-	-	-		
90	OHX	1	3418	-	0,6,6	-	-	-		
90	OHX	1	3437	-	0,6,6	-	-	-		
90	OHX	1	3678	36	0,6,6	-	-	-		
90	OHX	1	3443	-	0,6,6	-	-	-		
90	OHX	s9	201	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	1	3492	-	0,6,6	-	-	-		
90	OHX	5	3570	-	0,6,6	-	-	-		
90	OHX	5	3633	-	0,6,6	-	-	-		
90	OHX	1	3461	-	0,6,6	-	-	-		
90	OHX	2	2028	-	0,6,6	-	-	-		
90	OHX	1	3711	-	0,6,6	-	-	-		
90	OHX	7	208	-	0,6,6	-	-	-		
90	OHX	1	3456	-	0,6,6	-	-	-		
90	OHX	5	3671	83	0,6,6	-	-	-		
90	OHX	4	219	-	0,6,6	-	-	-		
90	OHX	8	216	38	0,6,6	-	-	-		
90	OHX	4	217	38	0,6,6	-	-	-		
90	OHX	2	1972	1	0,6,6	-	-	-		
90	OHX	5	3574	-	0,6,6	-	-	-		
90	OHX	1	3642	-	0,6,6	-	-	-		
90	OHX	5	3711	-	0,6,6	-	-	-		
90	OHX	6	2046	-	0,6,6	-	-	-		
90	OHX	5	3491	-	0,6,6	-	-	-		
90	OHX	6	1948	80	0,6,6	-	-	-		
90	OHX	5	3651	-	0,6,6	-	-	-		
90	OHX	6	1928	80	0,6,6	-	-	-		
90	OHX	5	3658	83	0,6,6	-	-	-		
90	OHX	6	1931	80	0,6,6	-	-	-		
90	OHX	5	3703	-	0,6,6	-	-	-		
90	OHX	1	3666	-	0,6,6	-	-	-		
90	OHX	sR	401	-	0,6,6	-	-	-		
90	OHX	1	3594	-	0,6,6	-	-	-		
90	OHX	1	3441	-	0,6,6	-	-	-		
90	OHX	5	3431	83	0,6,6	-	-	-		
90	OHX	O7	104	-	0,6,6	-	-	-		
90	OHX	1	3487	-	0,6,6	-	-	-		
90	OHX	5	3435	-	0,6,6	-	-	-		
90	OHX	1	3547	-	0,6,6	-	-	-		
90	OHX	5	3522	-	0,6,6	-	-	-		
90	OHX	3	204	-	0,6,6	-	-	-		
90	OHX	2	1978	-	0,6,6	-	-	-		
90	OHX	5	3432	-	0,6,6	-	-	-		
90	OHX	5	3551	83	0,6,6	-	-	-		
90	OHX	4	209	-	0,6,6	-	-	-		
90	OHX	6	1956	-	0,6,6	-	-	-		
90	OHX	1	3523	-	0,6,6	-	-	-		
90	OHX	6	2009	-	0,6,6	-	-	-		
90	OHX	5	3733	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	6	2044	-	0,6,6	-	-	-		
90	OHX	5	3681	83	0,6,6	-	-	-		
90	OHX	1	3709	-	0,6,6	-	-	-		
90	OHX	6	1933	-	0,6,6	-	-	-		
90	OHX	6	1936	-	0,6,6	-	-	-		
90	OHX	M6	201	-	0,6,6	-	-	-		
90	OHX	5	3571	-	0,6,6	-	-	-		
90	OHX	2	1944	-	0,6,6	-	-	-		
90	OHX	6	1964	80	0,6,6	-	-	-		
90	OHX	6	2035	-	0,6,6	-	-	-		
90	OHX	2	1967	-	0,6,6	-	-	-		
90	OHX	5	3488	83	0,6,6	-	-	-		
90	OHX	5	3544	83	0,6,6	-	-	-		
90	OHX	6	1973	80	0,6,6	-	-	-		
90	OHX	5	3654	-	0,6,6	-	-	-		
90	OHX	2	2042	-	0,6,6	-	-	-		
90	OHX	5	3602	-	0,6,6	-	-	-		
90	OHX	5	3567	-	0,6,6	-	-	-		
90	OHX	1	3673	-	0,6,6	-	-	-		
90	OHX	6	2053	80	0,6,6	-	-	-		
90	OHX	1	3694	-	0,6,6	-	-	-		
90	OHX	1	3704	-	0,6,6	-	-	-		
90	OHX	5	3614	-	0,6,6	-	-	-		
90	OHX	5	3476	-	0,6,6	-	-	-		
90	OHX	5	3648	-	0,6,6	-	-	-		
90	OHX	2	2031	-	0,6,6	-	-	-		
90	OHX	6	2047	-	0,6,6	-	-	-		
90	OHX	5	3510	83	0,6,6	-	-	-		
90	OHX	5	3673	83	0,6,6	-	-	-		
90	OHX	5	3687	-	0,6,6	-	-	-		
90	OHX	5	3608	-	0,6,6	-	-	-		
90	OHX	2	1966	1	0,6,6	-	-	-		
90	OHX	6	1993	80	0,6,6	-	-	-		
90	OHX	5	3407	-	0,6,6	-	-	-		
90	OHX	1	3417	-	0,6,6	-	-	-		
90	OHX	1	3658	-	0,6,6	-	-	-		
90	OHX	1	3722	-	0,6,6	-	-	-		
90	OHX	1	3586	-	0,6,6	-	-	-		
90	OHX	2	1913	-	0,6,6	-	-	-		
90	OHX	Q2	502	-	0,6,6	-	-	-		
90	OHX	6	2045	-	0,6,6	-	-	-		
90	OHX	1	3675	-	0,6,6	-	-	-		
90	OHX	5	3594	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	5	3589	83	0,6,6	-	-	-		
90	OHX	6	1984	-	0,6,6	-	-	-		
90	OHX	1	3433	-	0,6,6	-	-	-		
90	OHX	2	1901	-	0,6,6	-	-	-		
90	OHX	1	3728	-	0,6,6	-	-	-		
90	OHX	5	3698	-	0,6,6	-	-	-		
90	OHX	5	3620	-	0,6,6	-	-	-		
90	OHX	1	3432	-	0,6,6	-	-	-		
90	OHX	2	1981	-	0,6,6	-	-	-		
90	OHX	8	217	38	0,6,6	-	-	-		
90	OHX	1	3529	36	0,6,6	-	-	-		
90	OHX	5	3622	83	0,6,6	-	-	-		
90	OHX	5	3474	83	0,6,6	-	-	-		
90	OHX	m0	302	-	0,6,6	-	-	-		
90	OHX	6	2030	80	0,6,6	-	-	-		
90	OHX	1	3475	-	0,6,6	-	-	-		
90	OHX	5	3659	-	0,6,6	-	-	-		
90	OHX	3	208	-	0,6,6	-	-	-		
90	OHX	2	2026	-	0,6,6	-	-	-		
94	LEU	1	3402	-	5,7,8	0.43	0	5,8,10	0.61	0
90	OHX	2	1955	-	0,6,6	-	-	-		
90	OHX	6	1992	-	0,6,6	-	-	-		
90	OHX	5	3663	-	0,6,6	-	-	-		
90	OHX	1	3607	-	0,6,6	-	-	-		
90	OHX	5	3631	83	0,6,6	-	-	-		
90	OHX	2	1985	-	0,6,6	-	-	-		
90	OHX	7	209	37	0,6,6	-	-	-		
90	OHX	2	1903	-	0,6,6	-	-	-		
90	OHX	1	3544	-	0,6,6	-	-	-		
90	OHX	1	3682	-	0,6,6	-	-	-		
90	OHX	5	3463	-	0,6,6	-	-	-		
90	OHX	5	3737	83	0,6,6	-	-	-		
90	OHX	5	3501	83	0,6,6	-	-	-		
90	OHX	1	3602	-	0,6,6	-	-	-		
90	OHX	1	3645	-	0,6,6	-	-	-		
90	OHX	2	2021	-	0,6,6	-	-	-		
90	OHX	5	3485	83	0,6,6	-	-	-		
90	OHX	1	3652	-	0,6,6	-	-	-		
90	OHX	1	3538	-	0,6,6	-	-	-		
90	OHX	5	3607	-	0,6,6	-	-	-		
90	OHX	1	3476	-	0,6,6	-	-	-		
90	OHX	1	3648	-	0,6,6	-	-	-		
90	OHX	1	3717	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	2	2035	1	0,6,6	-	-	-		
90	OHX	1	3617	-	0,6,6	-	-	-		
90	OHX	1	3601	-	0,6,6	-	-	-		
90	OHX	5	3682	83	0,6,6	-	-	-		
90	OHX	m5	302	-	0,6,6	-	-	-		
90	OHX	o7	503	-	0,6,6	-	-	-		
90	OHX	1	3690	-	0,6,6	-	-	-		
90	OHX	1	3651	-	0,6,6	-	-	-		
90	OHX	M7	201	-	0,6,6	-	-	-		
90	OHX	1	3457	-	0,6,6	-	-	-		
90	OHX	5	3645	-	0,6,6	-	-	-		
90	OHX	5	3704	83	0,6,6	-	-	-		
90	OHX	6	1968	80	0,6,6	-	-	-		
90	OHX	l5	302	-	0,6,6	-	-	-		
90	OHX	1	3450	-	0,6,6	-	-	-		
90	OHX	2	1916	-	0,6,6	-	-	-		
90	OHX	6	1971	80	0,6,6	-	-	-		
90	OHX	1	3405	-	0,6,6	-	-	-		
90	OHX	1	3597	-	0,6,6	-	-	-		
96	8AN	p	101	91,89	19,24,25	1.06	1 (5%)	13,35,38	1.71	4 (30%)
90	OHX	5	3573	-	0,6,6	-	-	-		
90	OHX	1	3583	-	0,6,6	-	-	-		
90	OHX	1	3589	-	0,6,6	-	-	-		
90	OHX	1	3590	-	0,6,6	-	-	-		
90	OHX	5	3433	-	0,6,6	-	-	-		
90	OHX	1	3470	-	0,6,6	-	-	-		
90	OHX	1	3647	-	0,6,6	-	-	-		
90	OHX	5	3588	83	0,6,6	-	-	-		
90	OHX	1	3719	-	0,6,6	-	-	-		
90	OHX	5	3405	83	0,6,6	-	-	-		
90	OHX	4	205	-	0,6,6	-	-	-		
90	OHX	6	2007	80	0,6,6	-	-	-		
90	OHX	1	3620	-	0,6,6	-	-	-		
90	OHX	1	3623	-	0,6,6	-	-	-		
90	OHX	6	1958	80	0,6,6	-	-	-		
90	OHX	1	3683	36	0,6,6	-	-	-		
90	OHX	5	3585	83	0,6,6	-	-	-		
90	OHX	2	1940	-	0,6,6	-	-	-		
90	OHX	m9	201	-	0,6,6	-	-	-		
90	OHX	5	3502	-	0,6,6	-	-	-		
90	OHX	5	3540	83	0,6,6	-	-	-		
90	OHX	1	3567	-	0,6,6	-	-	-		
90	OHX	1	3621	36	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	6	1917	80	0,6,6	-	-	-		
90	OHX	6	1974	80	0,6,6	-	-	-		
90	OHX	1	3565	-	0,6,6	-	-	-		
90	OHX	1	3408	-	0,6,6	-	-	-		
90	OHX	1	3636	-	0,6,6	-	-	-		
90	OHX	5	3509	83	0,6,6	-	-	-		
90	OHX	1	3473	-	0,6,6	-	-	-		
90	OHX	5	3729	83	0,6,6	-	-	-		
90	OHX	1	3659	-	0,6,6	-	-	-		
90	OHX	1	3571	-	0,6,6	-	-	-		
90	OHX	1	3531	-	0,6,6	-	-	-		
90	OHX	1	3581	-	0,6,6	-	-	-		
90	OHX	1	3703	-	0,6,6	-	-	-		
90	OHX	6	1978	-	0,6,6	-	-	-		
90	OHX	2	2027	-	0,6,6	-	-	-		
90	OHX	6	2011	-	0,6,6	-	-	-		
90	OHX	5	3428	83	0,6,6	-	-	-		
90	OHX	5	3742	-	0,6,6	-	-	-		
90	OHX	1	3701	36	0,6,6	-	-	-		
90	OHX	1	3663	-	0,6,6	-	-	-		
90	OHX	1	3502	-	0,6,6	-	-	-		
90	OHX	5	3740	-	0,6,6	-	-	-		
90	OHX	3	203	-	0,6,6	-	-	-		
90	OHX	2	1939	-	0,6,6	-	-	-		
90	OHX	2	1988	-	0,6,6	-	-	-		
90	OHX	2	1957	-	0,6,6	-	-	-		
90	OHX	1	3546	-	0,6,6	-	-	-		
90	OHX	5	3549	-	0,6,6	-	-	-		
90	OHX	6	1982	80	0,6,6	-	-	-		
90	OHX	6	2050	80	0,6,6	-	-	-		
90	OHX	2	1945	-	0,6,6	-	-	-		
90	OHX	6	1949	-	0,6,6	-	-	-		
90	OHX	5	3440	-	0,6,6	-	-	-		
90	OHX	5	3715	83	0,6,6	-	-	-		
90	OHX	5	3689	-	0,6,6	-	-	-		
90	OHX	2	2036	-	0,6,6	-	-	-		
90	OHX	q2	502	-	0,6,6	-	-	-		
90	OHX	5	3543	83	0,6,6	-	-	-		
90	OHX	5	3587	-	0,6,6	-	-	-		
90	OHX	s8	301	-	0,6,6	-	-	-		
90	OHX	1	3517	-	0,6,6	-	-	-		
90	OHX	6	1927	80	0,6,6	-	-	-		
90	OHX	5	3545	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	5	3558	-	0,6,6	-	-	-		
90	OHX	1	3477	-	0,6,6	-	-	-		
90	OHX	4	207	38	0,6,6	-	-	-		
90	OHX	5	3534	83	0,6,6	-	-	-		
90	OHX	6	2020	-	0,6,6	-	-	-		
90	OHX	2	1964	-	0,6,6	-	-	-		
90	OHX	5	3444	-	0,6,6	-	-	-		
90	OHX	5	3639	-	0,6,6	-	-	-		
90	OHX	5	3482	83	0,6,6	-	-	-		
90	OHX	D9	102	-	0,6,6	-	-	-		
90	OHX	1	3463	-	0,6,6	-	-	-		
90	OHX	5	3531	83	0,6,6	-	-	-		
90	OHX	5	3580	-	0,6,6	-	-	-		
90	OHX	2	1998	-	0,6,6	-	-	-		
90	OHX	5	3457	-	0,6,6	-	-	-		
90	OHX	2	2051	-	0,6,6	-	-	-		
90	OHX	2	2008	-	0,6,6	-	-	-		
90	OHX	5	3583	-	0,6,6	-	-	-		
90	OHX	5	3744	-	0,6,6	-	-	-		
90	OHX	1	3622	-	0,6,6	-	-	-		
90	OHX	3	205	-	0,6,6	-	-	-		
90	OHX	3	202	-	0,6,6	-	-	-		
90	OHX	6	1906	-	0,6,6	-	-	-		
90	OHX	2	2003	-	0,6,6	-	-	-		
90	OHX	6	2056	80	0,6,6	-	-	-		
90	OHX	5	3539	83	0,6,6	-	-	-		
90	OHX	SR	401	-	0,6,6	-	-	-		
90	OHX	6	2006	80	0,6,6	-	-	-		
90	OHX	1	3536	-	0,6,6	-	-	-		
90	OHX	1	3446	-	0,6,6	-	-	-		
90	OHX	1	3720	-	0,6,6	-	-	-		
90	OHX	3	209	-	0,6,6	-	-	-		
90	OHX	6	1935	80	0,6,6	-	-	-		
90	OHX	5	3445	-	0,6,6	-	-	-		
90	OHX	5	3448	-	0,6,6	-	-	-		
90	OHX	1	3459	-	0,6,6	-	-	-		
90	OHX	5	3527	83	0,6,6	-	-	-		
90	OHX	5	3674	83	0,6,6	-	-	-		
90	OHX	1	3411	-	0,6,6	-	-	-		
90	OHX	c3	201	-	0,6,6	-	-	-		
90	OHX	1	3631	-	0,6,6	-	-	-		
90	OHX	6	1909	80	0,6,6	-	-	-		
90	OHX	5	3657	83	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	2	1915	-	0,6,6	-	-	-		
90	OHX	2	2018	-	0,6,6	-	-	-		
90	OHX	1	3630	-	0,6,6	-	-	-		
90	OHX	5	3450	83	0,6,6	-	-	-		
90	OHX	5	3584	83	0,6,6	-	-	-		
90	OHX	5	3734	-	0,6,6	-	-	-		
90	OHX	5	3467	-	0,6,6	-	-	-		
90	OHX	5	3743	-	0,6,6	-	-	-		
90	OHX	1	3501	-	0,6,6	-	-	-		
90	OHX	5	3714	83	0,6,6	-	-	-		
90	OHX	5	3411	-	0,6,6	-	-	-		
90	OHX	2	1995	-	0,6,6	-	-	-		
90	OHX	5	3565	83	0,6,6	-	-	-		
90	OHX	1	3653	-	0,6,6	-	-	-		
90	OHX	6	2048	80	0,6,6	-	-	-		
90	OHX	5	3738	83	0,6,6	-	-	-		
90	OHX	2	1902	-	0,6,6	-	-	-		
90	OHX	2	1951	-	0,6,6	-	-	-		
90	OHX	5	3619	-	0,6,6	-	-	-		
90	OHX	C7	201	-	0,6,6	-	-	-		
90	OHX	8	205	-	0,6,6	-	-	-		
94	LEU	5	3402	-	5,7,8	0.44	0	5,8,10	0.60	0
90	OHX	1	3451	-	0,6,6	-	-	-		
90	OHX	6	1918	80	0,6,6	-	-	-		
90	OHX	1	3471	-	0,6,6	-	-	-		
90	OHX	1	3508	-	0,6,6	-	-	-		
90	OHX	5	3683	83	0,6,6	-	-	-		
90	OHX	5	3716	-	0,6,6	-	-	-		
90	OHX	2	1907	-	0,6,6	-	-	-		
90	OHX	N9	101	-	0,6,6	-	-	-		
90	OHX	O4	201	-	0,6,6	-	-	-		
90	OHX	5	3616	-	0,6,6	-	-	-		
90	OHX	5	3471	83	0,6,6	-	-	-		
90	OHX	6	2027	-	0,6,6	-	-	-		
90	OHX	6	2023	80	0,6,6	-	-	-		
90	OHX	5	3498	83	0,6,6	-	-	-		
90	OHX	2	1925	-	0,6,6	-	-	-		
90	OHX	2	1973	-	0,6,6	-	-	-		
90	OHX	1	3534	-	0,6,6	-	-	-		
90	OHX	1	3691	-	0,6,6	-	-	-		
90	OHX	5	3426	-	0,6,6	-	-	-		
90	OHX	5	3537	-	0,6,6	-	-	-		
90	OHX	1	3444	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	5	3462	-	0,6,6	-	-	-		
90	OHX	6	1952	80	0,6,6	-	-	-		
90	OHX	5	3496	-	0,6,6	-	-	-		
90	OHX	6	2043	-	0,6,6	-	-	-		
90	OHX	1	3424	-	0,6,6	-	-	-		
90	OHX	1	3716	-	0,6,6	-	-	-		
90	OHX	1	3415	-	0,6,6	-	-	-		
90	OHX	5	3497	83	0,6,6	-	-	-		
90	OHX	2	1923	1	0,6,6	-	-	-		
95	SPS	1	4125	91	20,23,23	3.41	9 (45%)	18,30,30	5.63	12 (66%)
90	OHX	4	203	-	0,6,6	-	-	-		
90	OHX	5	3504	-	0,6,6	-	-	-		
90	OHX	6	1950	-	0,6,6	-	-	-		
90	OHX	6	1962	80	0,6,6	-	-	-		
90	OHX	5	3487	-	0,6,6	-	-	-		
90	OHX	5	3546	-	0,6,6	-	-	-		
90	OHX	1	3516	-	0,6,6	-	-	-		
90	OHX	1	3729	-	0,6,6	-	-	-		
90	OHX	6	2054	-	0,6,6	-	-	-		
90	OHX	m8	201	-	0,6,6	-	-	-		
90	OHX	1	3674	-	0,6,6	-	-	-		
90	OHX	1	3448	36	0,6,6	-	-	-		
90	OHX	6	1976	80	0,6,6	-	-	-		
90	OHX	6	2003	-	0,6,6	-	-	-		
90	OHX	2	1954	-	0,6,6	-	-	-		
90	OHX	5	3513	83	0,6,6	-	-	-		
90	OHX	5	3568	-	0,6,6	-	-	-		
90	OHX	6	2042	80	0,6,6	-	-	-		
90	OHX	5	3511	83	0,6,6	-	-	-		
90	OHX	5	3640	83	0,6,6	-	-	-		
96	8AN	P	101	91,89	19,24,25	1.06	1 (5%)	13,35,38	1.71	4 (30%)
90	OHX	2	1974	-	0,6,6	-	-	-		
90	OHX	5	3706	-	0,6,6	-	-	-		
90	OHX	1	3657	-	0,6,6	-	-	-		
90	OHX	5	3723	83	0,6,6	-	-	-		
90	OHX	2	1920	-	0,6,6	-	-	-		
90	OHX	2	2033	1	0,6,6	-	-	-		
90	OHX	1	3522	-	0,6,6	-	-	-		
90	OHX	1	3530	36	0,6,6	-	-	-		
90	OHX	1	3553	-	0,6,6	-	-	-		
90	OHX	1	3618	-	0,6,6	-	-	-		
90	OHX	6	2049	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	1	3505	-	0,6,6	-	-	-		
90	OHX	5	3499	83	0,6,6	-	-	-		
90	OHX	5	3728	83	0,6,6	-	-	-		
90	OHX	2	1906	-	0,6,6	-	-	-		
90	OHX	6	1961	-	0,6,6	-	-	-		
90	OHX	2	1949	-	0,6,6	-	-	-		
90	OHX	6	1942	80	0,6,6	-	-	-		
90	OHX	6	2014	80	0,6,6	-	-	-		
90	OHX	5	3536	-	0,6,6	-	-	-		
90	OHX	5	3612	-	0,6,6	-	-	-		
90	OHX	5	3519	-	0,6,6	-	-	-		
90	OHX	2	2010	-	0,6,6	-	-	-		
90	OHX	5	3638	83	0,6,6	-	-	-		
90	OHX	1	3578	-	0,6,6	-	-	-		
90	OHX	6	2029	80	0,6,6	-	-	-		
90	OHX	5	3530	-	0,6,6	-	-	-		
90	OHX	5	3618	-	0,6,6	-	-	-		
90	OHX	2	1980	-	0,6,6	-	-	-		
90	OHX	5	3512	-	0,6,6	-	-	-		
90	OHX	5	3505	-	0,6,6	-	-	-		
90	OHX	1	3403	-	0,6,6	-	-	-		
90	OHX	5	3468	-	0,6,6	-	-	-		
90	OHX	1	3671	-	0,6,6	-	-	-		
90	OHX	5	3625	83	0,6,6	-	-	-		
90	OHX	1	3558	-	0,6,6	-	-	-		
90	OHX	1	3485	-	0,6,6	-	-	-		
90	OHX	5	3475	83	0,6,6	-	-	-		
90	OHX	5	3675	-	0,6,6	-	-	-		
90	OHX	5	3676	-	0,6,6	-	-	-		
90	OHX	7	211	-	0,6,6	-	-	-		
90	OHX	2	2024	-	0,6,6	-	-	-		
90	OHX	5	3412	-	0,6,6	-	-	-		
90	OHX	1	3498	36	0,6,6	-	-	-		
90	OHX	6	2028	80	0,6,6	-	-	-		
90	OHX	1	3488	-	0,6,6	-	-	-		
90	OHX	5	3403	83	0,6,6	-	-	-		
90	OHX	1	3426	-	0,6,6	-	-	-		
90	OHX	4	223	-	0,6,6	-	-	-		
90	OHX	6	1981	80	0,6,6	-	-	-		
90	OHX	1	3462	-	0,6,6	-	-	-		
90	OHX	1	3496	-	0,6,6	-	-	-		
90	OHX	1	3580	-	0,6,6	-	-	-		
90	OHX	8	213	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	OHX	5	3680	-	0,6,6	-	-	-		
90	OHX	1	3497	-	0,6,6	-	-	-		
90	OHX	1	3413	-	0,6,6	-	-	-		
90	OHX	5	3686	-	0,6,6	-	-	-		
90	OHX	1	3552	-	0,6,6	-	-	-		
90	OHX	5	3410	-	0,6,6	-	-	-		
90	OHX	5	3429	83	0,6,6	-	-	-		
90	OHX	5	3685	-	0,6,6	-	-	-		
90	OHX	2	1982	-	0,6,6	-	-	-		
90	OHX	6	1930	80	0,6,6	-	-	-		
90	OHX	2	2041	-	0,6,6	-	-	-		
90	OHX	1	3445	-	0,6,6	-	-	-		
90	OHX	6	1985	-	0,6,6	-	-	-		
90	OHX	6	1903	-	0,6,6	-	-	-		
90	OHX	5	3532	83	0,6,6	-	-	-		
90	OHX	1	3603	-	0,6,6	-	-	-		
90	OHX	6	1919	80	0,6,6	-	-	-		
90	OHX	5	3500	-	0,6,6	-	-	-		
90	OHX	1	3724	-	0,6,6	-	-	-		
90	OHX	S9	201	-	0,6,6	-	-	-		
90	OHX	2	2012	1	0,6,6	-	-	-		
90	OHX	2	2006	-	0,6,6	-	-	-		
90	OHX	1	3548	-	0,6,6	-	-	-		
90	OHX	6	2021	-	0,6,6	-	-	-		
90	OHX	6	2022	-	0,6,6	-	-	-		
90	OHX	2	1935	-	0,6,6	-	-	-		
90	OHX	1	3467	-	0,6,6	-	-	-		
90	OHX	1	3615	-	0,6,6	-	-	-		
90	OHX	6	1991	80	0,6,6	-	-	-		
90	OHX	1	3681	-	0,6,6	-	-	-		
90	OHX	6	1954	-	0,6,6	-	-	-		
90	OHX	5	3470	-	0,6,6	-	-	-		
90	OHX	7	201	-	0,6,6	-	-	-		
90	OHX	1	3541	-	0,6,6	-	-	-		
90	OHX	6	1904	-	0,6,6	-	-	-		
90	OHX	5	3430	-	0,6,6	-	-	-		
90	OHX	5	3506	-	0,6,6	-	-	-		
90	OHX	1	3638	-	0,6,6	-	-	-		
90	OHX	5	3649	-	0,6,6	-	-	-		
90	OHX	8	203	-	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
96	8AN	p	101	91,89	-	1/3/25/26	0/3/3/3
95	SPS	1	4125	91	-	1/15/18/18	0/1/1/1
96	8AN	P	101	91,89	-	1/3/25/26	0/3/3/3
94	LEU	1	3402	-	-	4/5/6/8	-
95	SPS	5	4176	91	-	3/15/18/18	0/1/1/1
93	PHE	5	3401	-	-	3/5/6/8	0/1/1/1
93	PHE	1	3401	-	-	3/5/6/8	0/1/1/1
94	LEU	5	3402	-	-	4/5/6/8	-

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
95	1	4125	SPS	C9-C8	8.26	1.54	1.33
95	5	4176	SPS	C9-C8	7.69	1.53	1.33
95	5	4176	SPS	C9-C10	-7.39	1.32	1.48
95	1	4125	SPS	C9-C10	-5.96	1.35	1.48
95	1	4125	SPS	C10-N11	5.15	1.46	1.34

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
95	1	4125	SPS	C3-N2-C1	12.81	125.96	115.14
95	1	4125	SPS	O15-S15-C16	-11.93	92.28	106.47
95	5	4176	SPS	C3-N2-C1	9.98	123.57	115.14
95	1	4125	SPS	C6-C1-N2	-9.49	117.79	124.40
95	1	4125	SPS	O13-C13-C12	7.47	131.24	111.95

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

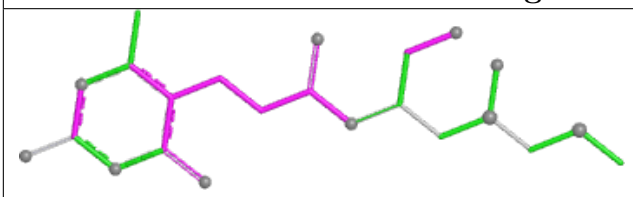
Mol	Chain	Res	Type	Atoms
93	1	3401	PHE	O-C-CA-CB
93	5	3401	PHE	O-C-CA-CB
94	1	3402	LEU	C-CA-CB-CG
94	5	3402	LEU	C-CA-CB-CG
95	1	4125	SPS	N11-C12-C14-S15

There are no ring outliers.

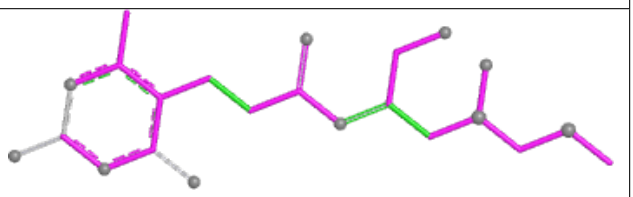
No monomer is involved in short contacts.

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.

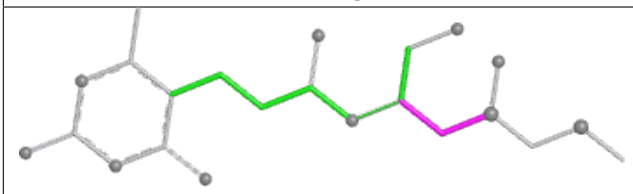
Ligand SPS 5 4176



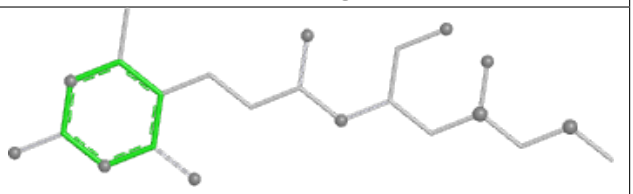
Bond lengths



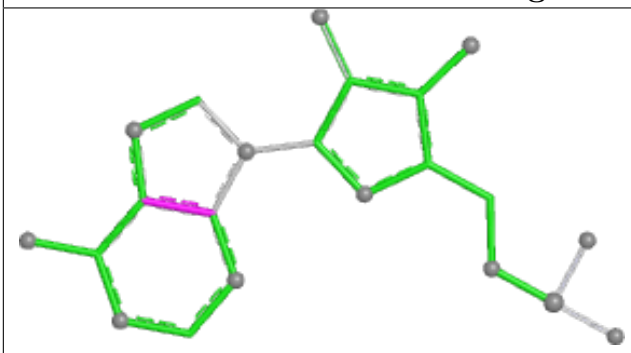
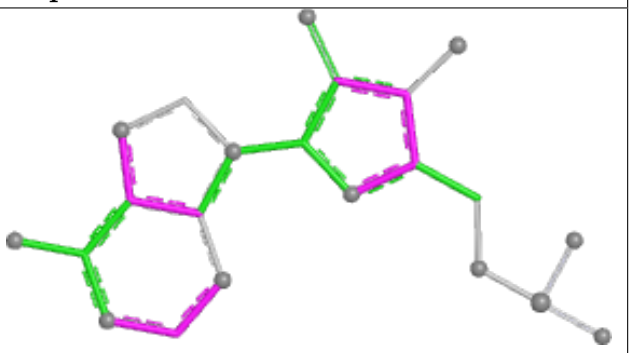
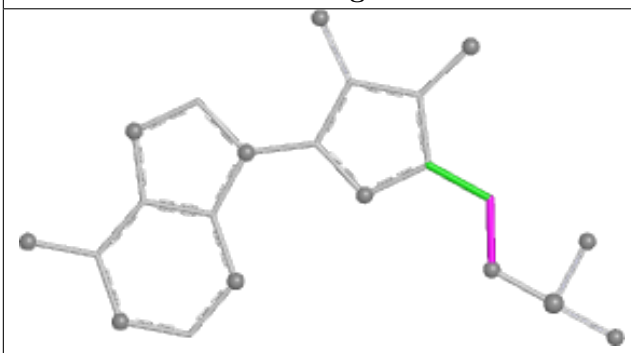
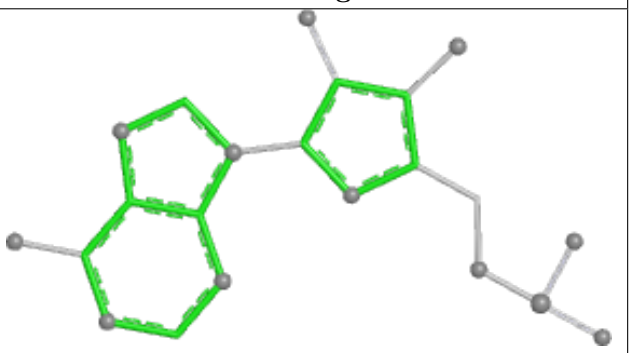
Bond angles

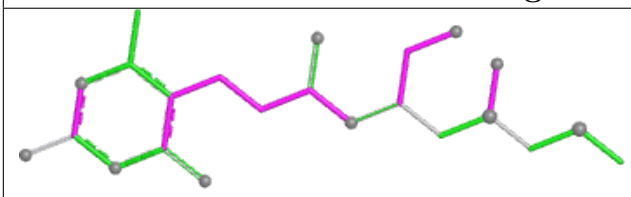
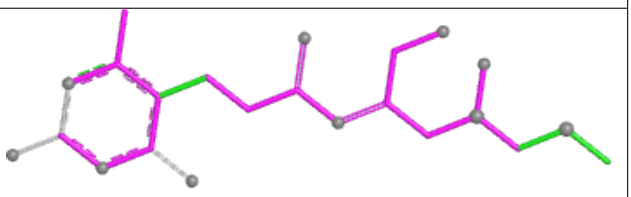
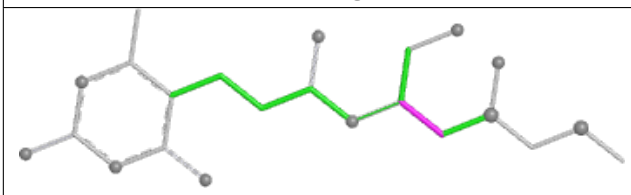
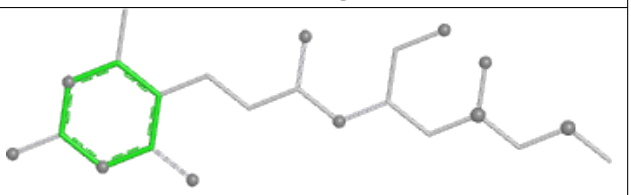


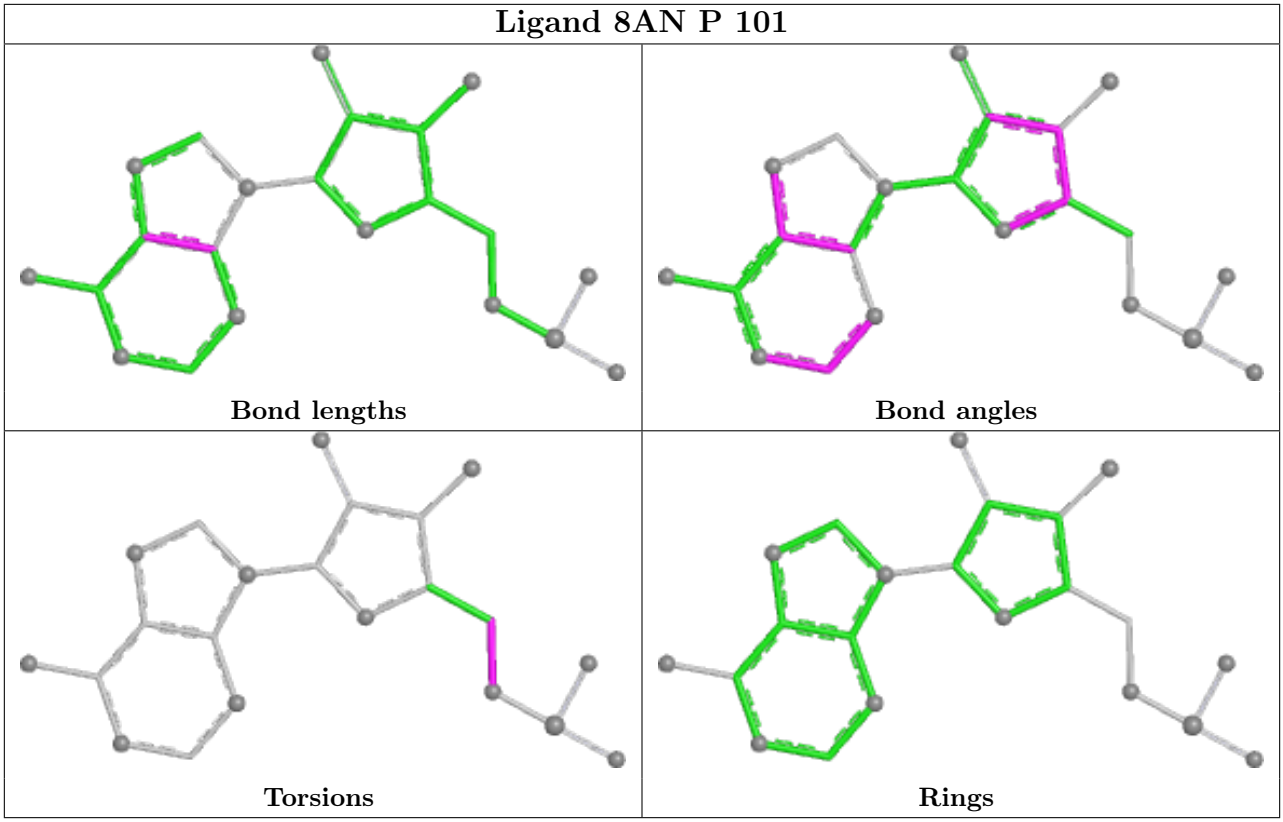
Torsions



Rings

Ligand 8AN p 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPS 1 4125	
 Bond lengths	 Bond angles
 Torsions	 Rings



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
36	1	3
83	5	3
1	2	2
41	l4	2
13	C1	1
57	n1	1
68	O2	1
40	l3	1
6	S4	1

The worst 5 of 15 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1781:U	O3'	1782:C	P	145.43
1	1	1955:U	O3'	2093:A	P	25.58
1	5	2444:C	O3'	2503:G	P	19.59
1	2	658:C	O3'	659:G	P	18.47
1	5	1953:G	O3'	2093:A	P	16.42

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	1781/1812 (98%)	0.61	139 (7%)	13	13	60, 89, 120, 149	0
2	S0	206/206 (100%)	1.45	61 (29%)	0	0	93, 99, 105, 107	0
2	s0	206/206 (100%)	0.62	18 (8%)	10	11	77, 83, 89, 90	0
3	S1	214/216 (99%)	0.58	18 (8%)	11	11	95, 106, 113, 113	0
3	s1	216/216 (100%)	0.64	12 (5%)	24	22	70, 75, 81, 84	0
4	S2	217/217 (100%)	1.42	67 (30%)	0	0	81, 88, 96, 99	0
4	s2	217/217 (100%)	0.95	32 (14%)	2	3	67, 73, 79, 81	0
5	S3	223/223 (100%)	1.50	67 (30%)	0	0	85, 96, 110, 115	0
5	s3	223/223 (100%)	1.65	80 (35%)	0	0	91, 102, 113, 114	0
6	S4	260/260 (100%)	0.93	32 (12%)	4	5	75, 88, 91, 93	0
6	s4	260/260 (100%)	0.49	9 (3%)	44	39	59, 73, 78, 80	0
7	S5	206/206 (100%)	1.39	57 (27%)	0	0	97, 105, 111, 113	0
7	s5	206/206 (100%)	0.91	42 (20%)	1	1	90, 95, 101, 103	0
8	S6	226/226 (100%)	0.92	43 (19%)	1	1	62, 76, 96, 101	0
8	s6	218/226 (96%)	1.04	41 (18%)	1	1	55, 63, 82, 86	0
9	S7	184/186 (98%)	0.50	14 (7%)	13	14	92, 102, 108, 109	0
9	s7	186/186 (100%)	0.08	7 (3%)	40	36	75, 90, 101, 104	0
10	S8	188/199 (94%)	1.15	36 (19%)	1	1	72, 78, 92, 95	0
10	s8	188/199 (94%)	0.77	19 (10%)	7	7	57, 68, 89, 95	0
11	S9	185/185 (100%)	1.09	35 (18%)	1	1	81, 89, 99, 103	0
11	s9	185/185 (100%)	0.13	3 (1%)	72	66	63, 74, 82, 84	0
12	C0	96/105 (91%)	0.58	9 (9%)	8	9	94, 101, 110, 115	0
12	c0	96/105 (91%)	1.26	25 (26%)	0	0	105, 116, 122, 123	0
13	C1	155/156 (99%)	1.54	42 (27%)	0	0	75, 79, 87, 90	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	c1	146/156 (93%)	0.53	9 (6%) 20 18	62, 67, 81, 92	0
14	C2	124/143 (86%)	1.54	43 (34%) 0 0	111, 116, 119, 122	0
14	c2	124/143 (86%)	1.60	34 (27%) 0 0	133, 142, 148, 154	0
15	C3	150/150 (100%)	0.41	9 (6%) 21 19	80, 88, 92, 94	0
15	c3	150/150 (100%)	0.01	2 (1%) 77 71	65, 75, 80, 82	0
16	C4	127/128 (99%)	0.36	11 (8%) 10 11	82, 105, 111, 112	0
16	c4	128/128 (100%)	0.93	17 (13%) 3 4	63, 74, 79, 80	0
17	C5	124/142 (87%)	0.52	9 (7%) 15 15	80, 90, 96, 101	0
17	c5	135/142 (95%)	0.35	10 (7%) 14 14	50, 91, 98, 100	0
18	C6	141/142 (99%)	2.22	68 (48%) 0 0	88, 105, 109, 110	0
18	c6	142/142 (100%)	1.47	42 (29%) 0 0	90, 98, 102, 104	0
19	C7	120/125 (96%)	1.53	41 (34%) 0 0	98, 104, 108, 109	0
19	c7	117/125 (93%)	0.83	17 (14%) 2 3	86, 94, 99, 100	0
20	C8	145/145 (100%)	0.60	9 (6%) 20 18	83, 95, 107, 110	0
20	c8	145/145 (100%)	0.41	10 (6%) 16 16	69, 86, 93, 97	0
21	C9	143/143 (100%)	1.26	31 (21%) 0 0	92, 101, 106, 108	0
21	c9	143/143 (100%)	0.47	12 (8%) 11 11	87, 92, 96, 98	0
22	D0	107/110 (97%)	1.14	26 (24%) 0 0	87, 100, 105, 106	0
22	d0	110/110 (100%)	2.07	51 (46%) 0 0	92, 104, 110, 111	0
23	D1	87/87 (100%)	0.93	16 (18%) 1 1	90, 94, 102, 106	0
23	d1	87/87 (100%)	0.65	5 (5%) 23 21	74, 78, 86, 89	0
24	D2	129/129 (100%)	1.27	29 (22%) 0 0	82, 88, 92, 98	0
24	d2	129/129 (100%)	0.26	0 100 100	67, 73, 75, 76	0
25	D3	144/144 (100%)	0.33	7 (4%) 29 26	71, 76, 79, 80	0
25	d3	144/144 (100%)	0.10	3 (2%) 63 58	57, 59, 64, 66	0
26	D4	134/134 (100%)	0.28	3 (2%) 62 56	76, 88, 92, 94	0
26	d4	134/134 (100%)	0.13	6 (4%) 33 29	60, 71, 74, 76	0
27	D5	70/70 (100%)	0.62	7 (10%) 7 8	104, 108, 111, 112	0
27	d5	69/70 (98%)	0.41	5 (7%) 15 15	93, 97, 100, 101	0
28	D6	97/97 (100%)	1.99	42 (43%) 0 0	84, 91, 112, 113	0
28	d6	97/97 (100%)	1.98	51 (52%) 0 0	65, 72, 81, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
29	D7	81/81 (100%)	1.08	13 (16%) 1 2	90, 94, 99, 100	0
29	d7	81/81 (100%)	0.64	4 (4%) 29 26	74, 80, 88, 89	0
30	D8	63/63 (100%)	2.18	32 (50%) 0 0	98, 107, 112, 113	0
30	d8	63/63 (100%)	2.42	40 (63%) 0 0	90, 95, 99, 100	0
31	D9	53/53 (100%)	0.46	2 (3%) 40 36	89, 91, 96, 97	0
31	d9	53/53 (100%)	1.26	13 (24%) 0 0	93, 97, 113, 120	0
32	E0	60/62 (96%)	0.93	9 (15%) 2 3	72, 87, 97, 101	0
32	e0	62/62 (100%)	0.30	6 (9%) 7 8	58, 72, 77, 80	0
33	E1	71/76 (93%)	0.57	8 (11%) 5 6	92, 108, 113, 113	0
33	e1	76/76 (100%)	0.91	15 (19%) 1 1	99, 127, 139, 140	0
34	SR	318/318 (100%)	1.37	84 (26%) 0 0	104, 111, 118, 122	0
35	SM	133/299 (44%)	1.23	28 (21%) 1 1	55, 83, 97, 98	0
36	1	3149/3149 (100%)	0.17	64 (2%) 65 60	31, 49, 82, 154	0
37	3	121/121 (100%)	-0.14	4 (3%) 46 41	41, 59, 64, 65	0
37	7	121/121 (100%)	-0.22	1 (0%) 86 81	36, 47, 51, 54	0
38	4	158/158 (100%)	0.01	1 (0%) 89 86	33, 45, 63, 84	0
38	8	158/158 (100%)	0.05	2 (1%) 77 71	36, 49, 68, 76	0
39	L2	252/252 (100%)	0.32	7 (2%) 53 47	40, 52, 61, 73	0
39	l2	252/252 (100%)	0.18	5 (1%) 65 60	39, 53, 62, 66	0
40	L3	386/386 (100%)	-0.20	2 (0%) 91 88	38, 50, 58, 62	0
40	l3	386/386 (100%)	-0.30	2 (0%) 91 88	32, 39, 47, 58	0
41	L4	361/361 (100%)	-0.28	0 100 100	31, 37, 47, 51	0
41	l4	361/361 (100%)	-0.22	1 (0%) 94 91	33, 41, 48, 58	0
42	L5	296/296 (100%)	0.61	36 (12%) 4 5	50, 60, 67, 69	0
42	l5	294/296 (99%)	0.02	4 (1%) 75 69	43, 49, 57, 66	0
43	L6	156/175 (89%)	-0.36	0 100 100	38, 46, 49, 55	0
43	l6	157/175 (89%)	-0.29	3 (1%) 66 61	40, 46, 49, 52	0
44	L7	222/223 (99%)	-0.09	0 100 100	36, 40, 48, 50	0
44	l7	223/223 (100%)	-0.28	0 100 100	34, 38, 48, 54	0
45	L8	233/233 (100%)	0.28	5 (2%) 63 58	54, 60, 74, 77	0
46	L9	191/191 (100%)	0.38	13 (6%) 17 16	48, 51, 53, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
46	l9	191/191 (100%)	0.22	4 (2%) 63 58	39, 44, 52, 63	0
47	M0	211/220 (95%)	-0.05	1 (0%) 91 88	39, 48, 61, 66	0
47	m0	213/220 (96%)	0.18	8 (3%) 40 36	36, 42, 57, 67	0
48	M1	169/169 (100%)	0.81	18 (10%) 6 6	57, 67, 73, 76	0
48	m1	169/169 (100%)	-0.27	0 100 100	44, 54, 59, 63	0
49	M3	193/194 (99%)	0.03	2 (1%) 82 77	33, 46, 59, 74	0
49	m3	194/194 (100%)	-0.05	5 (2%) 56 49	35, 50, 61, 70	0
50	M4	136/137 (99%)	-0.18	3 (2%) 62 56	45, 49, 54, 56	0
50	m4	137/137 (100%)	-0.34	1 (0%) 87 83	39, 43, 52, 60	0
51	M5	203/203 (100%)	0.14	0 100 100	35, 46, 54, 56	0
51	m5	203/203 (100%)	0.04	1 (0%) 91 88	38, 50, 57, 59	0
52	M6	197/197 (100%)	-0.08	2 (1%) 82 77	39, 42, 50, 52	0
52	m6	197/197 (100%)	-0.29	0 100 100	32, 36, 49, 50	0
53	M7	183/183 (100%)	0.10	10 (5%) 25 22	38, 43, 58, 62	0
53	m7	155/183 (84%)	-0.30	0 100 100	34, 37, 40, 43	0
54	M8	185/185 (100%)	0.08	0 100 100	36, 44, 54, 61	0
54	m8	185/185 (100%)	0.06	0 100 100	35, 44, 48, 50	0
55	M9	188/188 (100%)	0.20	7 (3%) 41 37	49, 61, 103, 111	0
55	m9	188/188 (100%)	-0.01	1 (0%) 91 88	43, 55, 98, 106	0
56	N0	172/172 (100%)	0.73	21 (12%) 4 5	42, 46, 51, 53	0
56	n0	172/172 (100%)	-0.10	1 (0%) 89 86	36, 39, 44, 48	0
57	N1	159/159 (100%)	0.47	6 (3%) 40 36	40, 47, 56, 57	0
57	n1	159/159 (100%)	0.44	8 (5%) 28 25	36, 42, 53, 55	0
58	N2	100/100 (100%)	0.34	5 (5%) 28 25	65, 69, 72, 73	0
58	n2	98/100 (98%)	0.14	4 (4%) 37 33	56, 59, 60, 61	0
59	N3	136/136 (100%)	0.07	3 (2%) 62 56	43, 49, 52, 54	0
59	n3	136/136 (100%)	0.05	0 100 100	33, 37, 41, 43	0
60	N4	98/98 (100%)	2.05	30 (30%) 0 0	49, 59, 89, 91	0
61	N5	121/121 (100%)	0.22	2 (1%) 70 64	43, 45, 62, 72	0
61	n5	120/121 (99%)	0.12	1 (0%) 86 81	44, 48, 65, 67	0
62	N6	126/126 (100%)	0.00	1 (0%) 86 81	35, 41, 44, 45	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
62	n6	126/126 (100%)	-0.14	0	100	100	38, 45, 49, 50	0
63	N7	135/135 (100%)	0.53	7 (5%)	27	24	62, 67, 76, 79	0
63	n7	135/135 (100%)	0.46	7 (5%)	27	24	65, 71, 78, 83	0
64	N8	148/148 (100%)	0.02	0	100	100	31, 43, 50, 57	0
64	n8	148/148 (100%)	0.04	1 (0%)	87	83	31, 45, 48, 50	0
65	N9	58/58 (100%)	0.28	0	100	100	36, 49, 66, 71	0
65	n9	58/58 (100%)	0.30	3 (5%)	27	24	34, 45, 52, 53	0
66	O0	97/100 (97%)	0.15	3 (3%)	49	43	60, 64, 70, 71	0
66	o0	100/100 (100%)	0.46	5 (5%)	28	25	61, 66, 73, 75	0
67	O1	109/109 (100%)	0.28	3 (2%)	53	47	51, 55, 59, 67	0
67	o1	109/109 (100%)	0.17	2 (1%)	68	62	41, 43, 47, 49	0
68	O2	127/127 (100%)	-0.20	0	100	100	32, 39, 41, 43	0
68	o2	127/127 (100%)	-0.19	0	100	100	31, 40, 43, 44	0
69	O3	106/106 (100%)	-0.19	0	100	100	37, 42, 50, 52	0
69	o3	106/106 (100%)	-0.10	0	100	100	34, 40, 50, 51	0
70	O4	112/112 (100%)	0.53	4 (3%)	42	38	47, 60, 70, 73	0
70	o4	112/112 (100%)	0.56	4 (3%)	42	38	46, 62, 70, 72	0
71	O5	119/119 (100%)	0.02	1 (0%)	86	81	42, 44, 56, 58	0
71	o5	119/119 (100%)	-0.16	1 (0%)	86	81	46, 48, 60, 64	0
72	O6	99/99 (100%)	-0.15	2 (2%)	65	60	44, 54, 62, 66	0
72	o6	99/99 (100%)	-0.28	0	100	100	48, 57, 62, 66	0
73	O7	87/87 (100%)	0.13	1 (1%)	80	75	35, 41, 46, 49	0
73	o7	87/87 (100%)	0.25	3 (3%)	45	40	37, 42, 51, 58	0
74	O8	77/77 (100%)	-0.41	1 (1%)	77	71	57, 60, 66, 66	0
74	o8	77/77 (100%)	0.55	3 (3%)	39	35	59, 63, 66, 68	0
75	O9	50/50 (100%)	0.09	0	100	100	40, 42, 44, 45	0
75	o9	50/50 (100%)	0.24	0	100	100	40, 44, 46, 49	0
76	Q0	52/52 (100%)	-0.03	1 (1%)	66	61	46, 49, 50, 52	0
76	q0	52/52 (100%)	-0.26	0	100	100	38, 39, 43, 45	0
77	Q1	25/25 (100%)	-0.10	0	100	100	60, 70, 78, 78	0
77	q1	25/25 (100%)	-0.32	0	100	100	49, 56, 59, 60	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
78	Q2	105/105 (100%)	0.75	11 (10%)	6	7	38, 49, 58, 66	0
78	q2	105/105 (100%)	0.76	9 (8%)	10	11	37, 44, 49, 57	0
79	Q3	91/91 (100%)	0.35	5 (5%)	25	22	49, 53, 57, 58	0
79	q3	91/91 (100%)	0.19	3 (3%)	46	41	45, 53, 60, 64	0
80	6	1795/1800 (99%)	0.47	132 (7%)	14	14	46, 75, 111, 134	0
81	sR	318/318 (100%)	1.45	94 (29%)	0	0	90, 107, 111, 114	0
82	sM	104/273 (38%)	0.67	15 (14%)	2	3	45, 89, 142, 143	0
83	5	3150/3150 (100%)	0.17	54 (1%)	70	64	31, 45, 82, 107	0
84	l8	231/256 (90%)	0.22	11 (4%)	30	27	58, 64, 78, 81	0
85	m2	150/165 (90%)	1.03	29 (19%)	1	1	65, 93, 100, 101	0
86	n4	135/135 (100%)	1.01	33 (24%)	0	0	37, 62, 81, 82	0
87	p0	143/312 (45%)	1.34	31 (21%)	0	0	78, 91, 138, 143	0
88	p1	47/128 (36%)	2.03	17 (36%)	0	0	114, 142, 154, 156	0
88	p2	46/128 (35%)	1.95	19 (41%)	0	0	168, 176, 181, 181	0
89	P	2/4 (50%)	-0.02	0	100	100	38, 38, 38, 40	0
89	p	2/4 (50%)	0.86	0	100	100	34, 34, 34, 38	0
All	All	33315/34306 (97%)	0.42	2597 (7%)	13	13	31, 60, 108, 181	0

The worst 5 of 2597 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	c2	20	ALA	14.0
60	N4	88	ASP	13.2
60	N4	75	THR	11.3
1	2	1805	C	11.3
1	2	1807	C	11.1

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
91	MG	6	2136	1/1	-0.06	0.46	75,75,75,75	0
91	MG	6	2166	1/1	0.14	0.52	114,114,114,114	0
91	MG	6	2152	1/1	0.19	1.16	62,62,62,62	0
91	MG	2	2117	1/1	0.20	0.59	94,94,94,94	0
91	MG	1	4043	1/1	0.22	0.35	52,52,52,52	0
91	MG	1	3847	1/1	0.22	1.15	36,36,36,36	0
91	MG	2	2094	1/1	0.23	0.73	81,81,81,81	0
91	MG	6	2073	1/1	0.31	0.47	91,91,91,91	0
91	MG	2	2059	1/1	0.32	0.33	86,86,86,86	0
91	MG	2	2139	1/1	0.38	0.34	93,93,93,93	0
91	MG	2	2108	1/1	0.42	0.40	92,92,92,92	0
91	MG	s6	301	1/1	0.45	1.02	67,67,67,67	0
91	MG	5	3807	1/1	0.45	0.24	88,88,88,88	0
91	MG	6	2086	1/1	0.46	0.28	75,75,75,75	0
91	MG	6	2111	1/1	0.46	0.48	69,69,69,69	0
91	MG	6	2133	1/1	0.46	0.45	94,94,94,94	0
91	MG	c8	203	1/1	0.46	0.39	84,84,84,84	0
91	MG	1	3938	1/1	0.46	0.32	54,54,54,54	0
91	MG	1	3764	1/1	0.47	0.80	42,42,42,42	0
91	MG	C1	201	1/1	0.48	0.67	76,76,76,76	0
91	MG	6	2182	1/1	0.49	0.32	66,66,66,66	0
91	MG	d7	102	1/1	0.49	0.44	74,74,74,74	0
91	MG	1	4063	1/1	0.49	0.52	43,43,43,43	0
91	MG	6	2114	1/1	0.52	0.51	89,89,89,89	0
91	MG	1	4031	1/1	0.53	0.61	34,34,34,34	0
91	MG	5	4084	1/1	0.53	0.48	34,34,34,34	0
91	MG	2	2141	1/1	0.55	0.62	79,79,79,79	0
91	MG	1	3782	1/1	0.56	0.54	41,41,41,41	0
91	MG	o9	101	1/1	0.56	0.60	41,41,41,41	0
91	MG	6	2147	1/1	0.57	0.52	66,66,66,66	0
91	MG	5	4147	1/1	0.57	0.36	41,41,41,41	0
91	MG	1	4117	1/1	0.57	0.34	43,43,43,43	0
91	MG	6	2140	1/1	0.58	0.12	71,71,71,71	0
91	MG	1	3964	1/1	0.59	0.63	51,51,51,51	0
91	MG	1	3914	1/1	0.60	0.95	50,50,50,50	0
91	MG	5	3948	1/1	0.60	0.42	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	1	3773	1/1	0.60	0.67	51,51,51,51	0
91	MG	6	2082	1/1	0.60	0.37	87,87,87,87	0
91	MG	n6	201	1/1	0.60	0.50	46,46,46,46	0
91	MG	6	2178	1/1	0.60	0.34	67,67,67,67	0
91	MG	5	4062	1/1	0.62	0.43	59,59,59,59	0
91	MG	4	236	1/1	0.62	0.25	43,43,43,43	0
91	MG	5	4122	1/1	0.62	0.47	37,37,37,37	0
91	MG	6	2180	1/1	0.62	0.92	98,98,98,98	0
91	MG	7	225	1/1	0.62	1.62	44,44,44,44	0
91	MG	6	2091	1/1	0.62	0.74	66,66,66,66	0
91	MG	6	2169	1/1	0.62	0.34	97,97,97,97	0
93	PHE	5	3401	11/12	0.62	0.53	31,31,41,41	0
91	MG	1	4053	1/1	0.63	0.43	34,34,34,34	0
91	MG	5	4175	1/1	0.63	0.28	39,39,39,39	0
91	MG	S4	301	1/1	0.63	0.63	83,83,83,83	0
91	MG	1	3743	1/1	0.64	0.46	52,52,52,52	0
91	MG	6	2125	1/1	0.64	0.98	57,57,57,57	0
91	MG	5	3988	1/1	0.64	0.79	35,35,35,35	0
91	MG	6	2092	1/1	0.64	0.20	88,88,88,88	0
91	MG	6	2093	1/1	0.64	0.41	90,90,90,90	0
92	ZN	D7	101	1/1	0.64	0.29	100,100,100,100	0
91	MG	1	3952	1/1	0.64	0.29	48,48,48,48	0
91	MG	5	3969	1/1	0.65	0.70	73,73,73,73	0
91	MG	M7	202	1/1	0.65	0.81	52,52,52,52	0
91	MG	1	4077	1/1	0.65	0.48	40,40,40,40	0
91	MG	5	3809	1/1	0.65	0.56	39,39,39,39	0
91	MG	5	3838	1/1	0.65	0.54	45,45,45,45	0
91	MG	6	2167	1/1	0.65	1.09	55,55,55,55	0
91	MG	5	4139	1/1	0.66	0.25	60,60,60,60	0
91	MG	1	4093	1/1	0.66	0.69	55,55,55,55	0
91	MG	1	3831	1/1	0.66	0.42	31,31,31,31	0
91	MG	6	2120	1/1	0.66	0.48	102,102,102,102	0
91	MG	5	3806	1/1	0.67	0.26	50,50,50,50	0
91	MG	1	3808	1/1	0.67	0.30	37,37,37,37	0
91	MG	2	2113	1/1	0.67	0.31	101,101,101,101	0
91	MG	1	3955	1/1	0.68	0.29	50,50,50,50	0
91	MG	6	2130	1/1	0.68	0.46	67,67,67,67	0
91	MG	2	2100	1/1	0.68	0.39	102,102,102,102	0
91	MG	5	4132	1/1	0.68	0.40	50,50,50,50	0
91	MG	d4	202	1/1	0.68	0.27	65,65,65,65	0
91	MG	5	4010	1/1	0.68	0.13	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	6	2076	1/1	0.69	0.36	70,70,70,70	0
91	MG	6	2129	1/1	0.69	0.64	61,61,61,61	0
91	MG	6	2080	1/1	0.69	0.68	63,63,63,63	0
91	MG	1	3946	1/1	0.69	0.59	98,98,98,98	0
91	MG	O7	105	1/1	0.69	0.55	42,42,42,42	0
91	MG	1	3735	1/1	0.69	0.49	125,125,125,125	0
91	MG	5	3971	1/1	0.69	0.22	84,84,84,84	0
91	MG	5	3763	1/1	0.70	0.47	34,34,34,34	0
91	MG	1	4042	1/1	0.70	0.51	43,43,43,43	0
91	MG	2	2075	1/1	0.70	0.24	96,96,96,96	0
91	MG	1	3984	1/1	0.70	0.88	42,42,42,42	0
91	MG	5	3831	1/1	0.70	0.60	44,44,44,44	0
91	MG	m6	204	1/1	0.70	0.38	34,34,34,34	0
91	MG	2	2076	1/1	0.70	0.53	86,86,86,86	0
91	MG	5	4097	1/1	0.70	0.70	52,52,52,52	0
91	MG	5	4107	1/1	0.70	0.81	42,42,42,42	0
91	MG	1	4075	1/1	0.70	0.30	59,59,59,59	0
91	MG	5	3754	1/1	0.71	0.60	45,45,45,45	0
91	MG	1	3944	1/1	0.71	0.59	45,45,45,45	0
91	MG	5	4086	1/1	0.71	0.41	41,41,41,41	0
91	MG	2	2098	1/1	0.71	0.22	87,87,87,87	0
91	MG	D9	103	1/1	0.71	0.33	92,92,92,92	0
91	MG	1	3817	1/1	0.71	0.42	51,51,51,51	0
91	MG	2	2092	1/1	0.71	0.41	80,80,80,80	0
91	MG	2	2101	1/1	0.71	0.47	79,79,79,79	0
91	MG	5	3891	1/1	0.71	0.34	43,43,43,43	0
91	MG	1	4000	1/1	0.71	0.41	61,61,61,61	0
91	MG	2	2106	1/1	0.71	0.24	96,96,96,96	0
91	MG	2	2084	1/1	0.71	0.66	88,88,88,88	0
91	MG	6	2145	1/1	0.71	0.14	89,89,89,89	0
91	MG	6	2098	1/1	0.71	0.86	99,99,99,99	0
91	MG	5	4019	1/1	0.71	0.55	50,50,50,50	0
91	MG	5	4055	1/1	0.71	0.23	48,48,48,48	0
91	MG	2	2118	1/1	0.72	0.42	92,92,92,92	0
91	MG	6	2153	1/1	0.72	0.36	86,86,86,86	0
91	MG	5	4034	1/1	0.72	0.23	89,89,89,89	0
91	MG	5	4039	1/1	0.72	0.37	43,43,43,43	0
91	MG	5	4168	1/1	0.72	0.62	41,41,41,41	0
91	MG	2	2110	1/1	0.72	0.49	76,76,76,76	0
91	MG	5	3946	1/1	0.73	0.33	61,61,61,61	0
91	MG	5	3813	1/1	0.73	0.34	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	2	2062	1/1	0.73	0.28	98,98,98,98	0
91	MG	5	4115	1/1	0.73	0.26	63,63,63,63	0
91	MG	5	4048	1/1	0.73	0.44	57,57,57,57	0
91	MG	2	2089	1/1	0.73	0.41	85,85,85,85	0
91	MG	1	4062	1/1	0.73	0.33	105,105,105,105	0
91	MG	5	3943	1/1	0.73	0.47	44,44,44,44	0
91	MG	6	2141	1/1	0.74	0.54	95,95,95,95	0
91	MG	d3	201	1/1	0.74	0.56	55,55,55,55	0
91	MG	5	4172	1/1	0.74	0.17	81,81,81,81	0
91	MG	1	4109	1/1	0.74	0.36	43,43,43,43	0
91	MG	5	4112	1/1	0.74	0.74	62,62,62,62	0
91	MG	L4	404	1/1	0.74	0.41	31,31,31,31	0
91	MG	sM	301	1/1	0.74	0.27	45,45,45,45	0
91	MG	o2	201	1/1	0.74	0.46	32,32,32,32	0
91	MG	5	4126	1/1	0.74	0.63	57,57,57,57	0
91	MG	6	2183	1/1	0.74	0.49	72,72,72,72	0
91	MG	6	2062	1/1	0.74	0.77	61,61,61,61	0
91	MG	5	4021	1/1	0.75	0.73	33,33,33,33	0
91	MG	6	2156	1/1	0.75	0.48	68,68,68,68	0
91	MG	6	2106	1/1	0.75	0.57	60,60,60,60	0
91	MG	1	3989	1/1	0.75	0.48	40,40,40,40	0
91	MG	5	3833	1/1	0.75	0.34	40,40,40,40	0
91	MG	5	3985	1/1	0.75	0.68	42,42,42,42	0
91	MG	1	3937	1/1	0.75	0.20	57,57,57,57	0
91	MG	1	4024	1/1	0.75	0.50	49,49,49,49	0
91	MG	1	3960	1/1	0.75	0.40	40,40,40,40	0
91	MG	5	4104	1/1	0.76	0.09	93,93,93,93	0
91	MG	1	3751	1/1	0.76	0.36	38,38,38,38	0
91	MG	6	2105	1/1	0.76	0.62	65,65,65,65	0
91	MG	2	2114	1/1	0.76	0.77	77,77,77,77	0
91	MG	2	2131	1/1	0.76	0.31	80,80,80,80	0
91	MG	2	2078	1/1	0.76	0.51	92,92,92,92	0
91	MG	5	3778	1/1	0.76	0.30	57,57,57,57	0
91	MG	1	3873	1/1	0.76	0.44	33,33,33,33	0
91	MG	1	3785	1/1	0.76	0.56	51,51,51,51	0
92	ZN	e1	501	1/1	0.76	0.07	130,130,130,130	0
91	MG	5	4154	1/1	0.76	0.34	50,50,50,50	0
91	MG	1	4008	1/1	0.77	0.49	34,34,34,34	0
91	MG	5	4037	1/1	0.77	0.43	39,39,39,39	0
91	MG	2	2132	1/1	0.77	0.45	76,76,76,76	0
91	MG	1	3963	1/1	0.77	1.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	6	2102	1/1	0.77	0.53	96,96,96,96	0
91	MG	5	3762	1/1	0.77	0.22	50,50,50,50	0
91	MG	5	4065	1/1	0.77	0.58	37,37,37,37	0
91	MG	6	2137	1/1	0.77	0.47	85,85,85,85	0
91	MG	1	4079	1/1	0.77	0.44	54,54,54,54	0
91	MG	5	4096	1/1	0.77	0.39	45,45,45,45	0
91	MG	1	3931	1/1	0.77	0.30	37,37,37,37	0
91	MG	1	3951	1/1	0.77	0.29	32,32,32,32	0
91	MG	1	4052	1/1	0.77	0.43	59,59,59,59	0
91	MG	1	3854	1/1	0.77	0.81	56,56,56,56	0
91	MG	5	3815	1/1	0.77	0.34	46,46,46,46	0
91	MG	2	2068	1/1	0.77	0.86	75,75,75,75	0
91	MG	5	3751	1/1	0.78	0.34	45,45,45,45	0
91	MG	1	3732	1/1	0.78	0.90	48,48,48,48	0
91	MG	2	2056	1/1	0.78	0.31	74,74,74,74	0
91	MG	2	2064	1/1	0.78	0.40	85,85,85,85	0
91	MG	6	2175	1/1	0.78	0.38	64,64,64,64	0
91	MG	1	4004	1/1	0.78	0.33	40,40,40,40	0
91	MG	N0	202	1/1	0.78	0.39	44,44,44,44	0
91	MG	2	2061	1/1	0.78	0.53	83,83,83,83	0
91	MG	1	3825	1/1	0.78	0.36	49,49,49,49	0
91	MG	6	2067	1/1	0.78	0.42	57,57,57,57	0
91	MG	5	3819	1/1	0.78	0.27	41,41,41,41	0
91	MG	c6	201	1/1	0.78	0.43	90,90,90,90	0
91	MG	C9	201	1/1	0.78	0.49	96,96,96,96	0
91	MG	2	2070	1/1	0.78	0.75	71,71,71,71	0
91	MG	l6	201	1/1	0.78	0.46	44,44,44,44	0
91	MG	l9	202	1/1	0.78	0.33	41,41,41,41	0
91	MG	m5	304	1/1	0.78	0.40	47,47,47,47	0
91	MG	5	3874	1/1	0.78	0.63	35,35,35,35	0
91	MG	5	4066	1/1	0.78	0.30	42,42,42,42	0
91	MG	1	4102	1/1	0.78	0.39	39,39,39,39	0
91	MG	5	3895	1/1	0.78	0.43	48,48,48,48	0
91	MG	1	3976	1/1	0.78	0.53	36,36,36,36	0
91	MG	6	2159	1/1	0.78	0.20	88,88,88,88	0
91	MG	5	4102	1/1	0.78	0.64	43,43,43,43	0
91	MG	5	4153	1/1	0.79	0.43	52,52,52,52	0
91	MG	5	3998	1/1	0.79	0.35	39,39,39,39	0
91	MG	5	4007	1/1	0.79	0.63	48,48,48,48	0
91	MG	5	4171	1/1	0.79	0.51	31,31,31,31	0
91	MG	5	4092	1/1	0.79	0.36	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	5	3860	1/1	0.79	0.56	32,32,32,32	0
91	MG	1	3932	1/1	0.79	0.49	37,37,37,37	0
91	MG	5	4020	1/1	0.79	0.30	65,65,65,65	0
91	MG	2	2112	1/1	0.79	0.63	83,83,83,83	0
91	MG	2	2072	1/1	0.79	0.33	83,83,83,83	0
91	MG	1	3953	1/1	0.79	0.31	55,55,55,55	0
91	MG	1	4096	1/1	0.79	0.27	49,49,49,49	0
91	MG	1	4012	1/1	0.79	0.46	50,50,50,50	0
91	MG	6	2064	1/1	0.79	0.48	68,68,68,68	0
91	MG	1	3826	1/1	0.79	0.39	33,33,33,33	0
91	MG	6	2154	1/1	0.79	0.33	94,94,94,94	0
91	MG	1	4025	1/1	0.79	0.40	49,49,49,49	0
94	LEU	5	3402	8/9	0.79	0.35	36,36,36,36	0
91	MG	6	2115	1/1	0.80	0.41	69,69,69,69	0
91	MG	4	232	1/1	0.80	0.29	72,72,72,72	0
91	MG	1	3979	1/1	0.80	0.38	48,48,48,48	0
91	MG	6	2071	1/1	0.80	0.64	63,63,63,63	0
91	MG	7	212	1/1	0.80	0.53	46,46,46,46	0
91	MG	5	3789	1/1	0.80	0.57	36,36,36,36	0
91	MG	l3	404	1/1	0.80	0.34	32,32,32,32	0
91	MG	l5	303	1/1	0.80	0.09	50,50,50,50	0
91	MG	5	3792	1/1	0.80	0.54	39,39,39,39	0
91	MG	5	3900	1/1	0.80	0.24	49,49,49,49	0
91	MG	5	3805	1/1	0.80	0.40	36,36,36,36	0
91	MG	1	3981	1/1	0.80	0.27	58,58,58,58	0
91	MG	1	3809	1/1	0.80	0.48	49,49,49,49	0
91	MG	5	4128	1/1	0.80	0.36	33,33,33,33	0
91	MG	2	2138	1/1	0.80	0.80	87,87,87,87	0
91	MG	1	3818	1/1	0.80	0.29	62,62,62,62	0
91	MG	6	2108	1/1	0.80	0.45	63,63,63,63	0
91	MG	6	2085	1/1	0.80	0.56	58,58,58,58	0
91	MG	4	227	1/1	0.80	0.49	47,47,47,47	0
91	MG	1	4098	1/1	0.81	0.57	58,58,58,58	0
91	MG	1	3912	1/1	0.81	0.51	43,43,43,43	0
91	MG	1	3756	1/1	0.81	0.44	43,43,43,43	0
91	MG	5	4059	1/1	0.81	0.67	33,33,33,33	0
91	MG	6	2079	1/1	0.81	0.48	72,72,72,72	0
91	MG	2	2125	1/1	0.81	0.54	78,78,78,78	0
91	MG	1	3868	1/1	0.81	0.38	41,41,41,41	0
91	MG	6	2128	1/1	0.81	0.40	88,88,88,88	0
91	MG	1	3869	1/1	0.81	0.45	49,49,49,49	0
91	MG	2	2095	1/1	0.81	0.41	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	6	2088	1/1	0.81	0.37	65,65,65,65	0
91	MG	1	4014	1/1	0.81	0.37	36,36,36,36	0
91	MG	1	4076	1/1	0.81	0.56	51,51,51,51	0
91	MG	5	4004	1/1	0.81	0.72	29,29,29,29	0
91	MG	1	3887	1/1	0.81	0.42	35,35,35,35	0
91	MG	1	3899	1/1	0.81	0.37	33,33,33,33	0
91	MG	5	4017	1/1	0.81	0.26	42,42,42,42	0
91	MG	1	4086	1/1	0.81	0.36	41,41,41,41	0
91	MG	1	4026	1/1	0.81	0.71	39,39,39,39	0
91	MG	1	3904	1/1	0.81	0.64	38,38,38,38	0
91	MG	6	2107	1/1	0.81	0.47	63,63,63,63	0
91	MG	5	3866	1/1	0.81	0.44	33,33,33,33	0
91	MG	6	2138	1/1	0.82	0.17	82,82,82,82	0
91	MG	6	2094	1/1	0.82	0.24	77,77,77,77	0
91	MG	1	3845	1/1	0.82	0.61	38,38,38,38	0
91	MG	6	2124	1/1	0.82	0.28	89,89,89,89	0
91	MG	5	3945	1/1	0.82	0.67	32,32,32,32	0
91	MG	7	223	1/1	0.82	0.27	36,36,36,36	0
91	MG	5	4031	1/1	0.82	0.53	54,54,54,54	0
91	MG	8	221	1/1	0.82	0.73	46,46,46,46	0
91	MG	8	224	1/1	0.82	0.27	53,53,53,53	0
91	MG	1	3803	1/1	0.82	0.49	46,46,46,46	0
91	MG	1	3776	1/1	0.82	0.53	47,47,47,47	0
91	MG	4	237	1/1	0.82	0.38	31,31,31,31	0
91	MG	5	4117	1/1	0.82	0.31	43,43,43,43	0
91	MG	5	3770	1/1	0.82	0.33	41,41,41,41	0
91	MG	C8	201	1/1	0.82	0.08	94,94,94,94	0
91	MG	5	4056	1/1	0.82	0.22	40,40,40,40	0
91	MG	5	3986	1/1	0.82	0.41	60,60,60,60	0
91	MG	2	2128	1/1	0.82	0.36	89,89,89,89	0
91	MG	1	4118	1/1	0.82	0.20	44,44,44,44	0
91	MG	5	3867	1/1	0.82	0.29	40,40,40,40	0
91	MG	N6	201	1/1	0.82	0.42	40,40,40,40	0
91	MG	5	4162	1/1	0.82	0.61	49,49,49,49	0
91	MG	1	3804	1/1	0.83	0.16	58,58,58,58	0
91	MG	4	224	1/1	0.83	0.50	48,48,48,48	0
91	MG	1	3999	1/1	0.83	0.49	43,43,43,43	0
91	MG	5	4000	1/1	0.83	0.44	40,40,40,40	0
91	MG	2	2135	1/1	0.83	0.59	68,68,68,68	0
91	MG	1	3783	1/1	0.83	0.73	39,39,39,39	0
91	MG	5	3752	1/1	0.83	0.30	32,32,32,32	0
91	MG	5	4082	1/1	0.83	0.58	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	5	3917	1/1	0.83	0.61	32,32,32,32	0
91	MG	5	4151	1/1	0.83	0.30	46,46,46,46	0
91	MG	2	2081	1/1	0.83	0.44	87,87,87,87	0
91	MG	6	2087	1/1	0.83	0.33	66,66,66,66	0
91	MG	5	4159	1/1	0.83	0.37	45,45,45,45	0
91	MG	6	2070	1/1	0.83	0.28	94,94,94,94	0
91	MG	6	2155	1/1	0.83	0.23	76,76,76,76	0
92	ZN	d7	101	1/1	0.83	0.24	89,89,89,89	0
91	MG	1	3793	1/1	0.83	0.46	39,39,39,39	0
91	MG	5	3856	1/1	0.83	0.49	42,42,42,42	0
91	MG	1	3759	1/1	0.83	0.63	45,45,45,45	0
91	MG	6	2078	1/1	0.84	0.25	58,58,58,58	0
91	MG	2	2086	1/1	0.84	0.33	71,71,71,71	0
91	MG	1	4060	1/1	0.84	0.30	37,37,37,37	0
91	MG	5	4131	1/1	0.84	0.49	35,35,35,35	0
91	MG	1	4061	1/1	0.84	0.35	32,32,32,32	0
91	MG	1	3954	1/1	0.84	0.22	57,57,57,57	0
91	MG	1	3747	1/1	0.84	0.96	49,49,49,49	0
91	MG	1	4006	1/1	0.84	0.52	61,61,61,61	0
91	MG	2	2057	1/1	0.84	0.46	73,73,73,73	0
91	MG	2	2103	1/1	0.84	0.55	74,74,74,74	0
91	MG	6	2139	1/1	0.84	0.60	57,57,57,57	0
91	MG	2	2104	1/1	0.84	0.54	97,97,97,97	0
91	MG	1	3967	1/1	0.84	0.51	51,51,51,51	0
91	MG	O4	202	1/1	0.84	0.19	61,61,61,61	0
91	MG	5	3885	1/1	0.84	0.32	34,34,34,34	0
91	MG	5	3890	1/1	0.84	0.34	40,40,40,40	0
91	MG	1	3880	1/1	0.84	0.69	41,41,41,41	0
91	MG	1	3802	1/1	0.84	0.39	36,36,36,36	0
91	MG	5	3898	1/1	0.84	0.54	39,39,39,39	0
91	MG	2	2124	1/1	0.84	0.20	87,87,87,87	0
91	MG	6	2066	1/1	0.84	0.13	89,89,89,89	0
91	MG	8	227	1/1	0.84	0.17	51,51,51,51	0
91	MG	8	229	1/1	0.84	0.30	40,40,40,40	0
91	MG	5	4075	1/1	0.84	0.41	49,49,49,49	0
91	MG	5	3922	1/1	0.84	0.44	36,36,36,36	0
91	MG	1	3982	1/1	0.84	0.58	48,48,48,48	0
91	MG	5	3777	1/1	0.84	0.32	48,48,48,48	0
91	MG	1	4105	1/1	0.84	0.31	54,54,54,54	0
91	MG	5	3788	1/1	0.84	0.73	34,34,34,34	0
91	MG	1	4106	1/1	0.84	0.30	39,39,39,39	0
91	MG	1	3903	1/1	0.84	0.44	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	o2	202	1/1	0.84	0.36	32,32,32,32	0
91	MG	5	3977	1/1	0.84	0.19	48,48,48,48	0
91	MG	5	3982	1/1	0.84	0.51	41,41,41,41	0
91	MG	5	3796	1/1	0.84	0.62	42,42,42,42	0
91	MG	5	4114	1/1	0.84	0.24	44,44,44,44	0
91	MG	6	2074	1/1	0.84	0.67	88,88,88,88	0
91	MG	1	3738	1/1	0.84	0.50	37,37,37,37	0
91	MG	5	3808	1/1	0.85	0.38	37,37,37,37	0
91	MG	1	4048	1/1	0.85	0.18	44,44,44,44	0
91	MG	5	3993	1/1	0.85	0.52	41,41,41,41	0
91	MG	5	4125	1/1	0.85	0.30	41,41,41,41	0
91	MG	1	3911	1/1	0.85	0.85	52,52,52,52	0
91	MG	6	2077	1/1	0.85	0.30	55,55,55,55	0
91	MG	1	4121	1/1	0.85	0.36	39,39,39,39	0
91	MG	6	2127	1/1	0.85	0.15	54,54,54,54	0
91	MG	1	3993	1/1	0.85	0.55	45,45,45,45	0
91	MG	5	4145	1/1	0.85	0.37	48,48,48,48	0
91	MG	1	4058	1/1	0.85	0.34	38,38,38,38	0
91	MG	5	3849	1/1	0.85	0.62	31,31,31,31	0
91	MG	1	3995	1/1	0.85	0.58	47,47,47,47	0
91	MG	c9	201	1/1	0.85	0.19	90,90,90,90	0
91	MG	5	4026	1/1	0.85	0.38	33,33,33,33	0
91	MG	6	2084	1/1	0.85	0.43	60,60,60,60	0
91	MG	5	4164	1/1	0.85	0.27	33,33,33,33	0
91	MG	1	3748	1/1	0.85	0.40	69,69,69,69	0
91	MG	2	2096	1/1	0.85	0.28	75,75,75,75	0
91	MG	1	3921	1/1	0.85	0.26	42,42,42,42	0
91	MG	5	4041	1/1	0.85	0.30	41,41,41,41	0
91	MG	M3	1000	1/1	0.85	0.37	64,64,64,64	0
91	MG	1	3736	1/1	0.85	0.43	47,47,47,47	0
91	MG	5	3894	1/1	0.85	0.80	33,33,33,33	0
91	MG	2	2054	1/1	0.85	0.41	81,81,81,81	0
90	OHX	2	2048	7/7	0.85	0.29	100,100,100,100	0
91	MG	8	225	1/1	0.85	0.47	62,62,62,62	0
91	MG	2	2111	1/1	0.85	0.43	78,78,78,78	0
91	MG	6	2097	1/1	0.85	0.18	92,92,92,92	0
91	MG	1	4017	1/1	0.85	0.32	61,61,61,61	0
91	MG	l3	405	1/1	0.85	0.42	38,38,38,38	0
91	MG	5	4081	1/1	0.85	0.36	32,32,32,32	0
91	MG	5	3937	1/1	0.85	0.38	43,43,43,43	0
91	MG	1	3940	1/1	0.85	0.26	51,51,51,51	0
91	MG	1	3942	1/1	0.85	0.28	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	m6	203	1/1	0.85	0.74	29,29,29,29	0
91	MG	1	3901	1/1	0.85	0.79	37,37,37,37	0
91	MG	5	4093	1/1	0.85	0.43	35,35,35,35	0
91	MG	1	3857	1/1	0.85	0.44	35,35,35,35	0
91	MG	6	2161	1/1	0.85	0.37	59,59,59,59	0
91	MG	5	3798	1/1	0.85	0.44	52,52,52,52	0
91	MG	1	4037	1/1	0.85	0.96	46,46,46,46	0
91	MG	5	4106	1/1	0.85	0.55	37,37,37,37	0
91	MG	5	3979	1/1	0.85	0.22	50,50,50,50	0
91	MG	1	3859	1/1	0.85	0.67	41,41,41,41	0
91	MG	1	3987	1/1	0.85	0.43	35,35,35,35	0
91	MG	2	2093	1/1	0.86	0.14	81,81,81,81	0
91	MG	1	3795	1/1	0.86	0.24	39,39,39,39	0
91	MG	5	3828	1/1	0.86	0.39	35,35,35,35	0
91	MG	2	2058	1/1	0.86	0.25	81,81,81,81	0
91	MG	5	3974	1/1	0.86	0.34	38,38,38,38	0
91	MG	5	4068	1/1	0.86	0.70	40,40,40,40	0
91	MG	N8	203	1/1	0.86	0.96	32,32,32,32	0
91	MG	5	3978	1/1	0.86	0.36	56,56,56,56	0
91	MG	1	3778	1/1	0.86	0.42	37,37,37,37	0
91	MG	5	3846	1/1	0.86	0.44	50,50,50,50	0
91	MG	7	219	1/1	0.86	0.38	45,45,45,45	0
91	MG	1	4113	1/1	0.86	0.37	39,39,39,39	0
91	MG	6	2163	1/1	0.86	0.46	66,66,66,66	0
91	MG	8	201	1/1	0.86	0.28	36,36,36,36	0
91	MG	1	3757	1/1	0.86	0.19	42,42,42,42	0
91	MG	6	2089	1/1	0.86	0.17	70,70,70,70	0
91	MG	1	4074	1/1	0.86	0.28	54,54,54,54	0
91	MG	1	4036	1/1	0.86	0.20	56,56,56,56	0
91	MG	1	3832	1/1	0.86	0.55	39,39,39,39	0
91	MG	8	230	1/1	0.86	0.49	56,56,56,56	0
91	MG	4	226	1/1	0.86	0.66	49,49,49,49	0
91	MG	6	2096	1/1	0.86	0.61	59,59,59,59	0
91	MG	5	4110	1/1	0.86	0.77	45,45,45,45	0
91	MG	5	3893	1/1	0.86	0.64	47,47,47,47	0
91	MG	1	4038	1/1	0.86	0.71	52,52,52,52	0
91	MG	5	3800	1/1	0.86	0.42	48,48,48,48	0
91	MG	5	3802	1/1	0.86	0.31	38,38,38,38	0
90	OHX	2	2044	7/7	0.86	0.52	88,88,88,88	0
91	MG	5	3908	1/1	0.86	0.63	44,44,44,44	0
91	MG	1	3749	1/1	0.86	0.55	55,55,55,55	0
91	MG	1	3852	1/1	0.86	0.64	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	5	3934	1/1	0.86	0.38	31,31,31,31	0
91	MG	1	3934	1/1	0.86	0.46	37,37,37,37	0
91	MG	5	4045	1/1	0.86	0.35	41,41,41,41	0
91	MG	5	4047	1/1	0.86	0.30	36,36,36,36	0
91	MG	M0	302	1/1	0.86	0.16	46,46,46,46	0
91	MG	1	3985	1/1	0.86	0.29	42,42,42,42	0
91	MG	5	4161	1/1	0.87	0.26	39,39,39,39	0
91	MG	5	3834	1/1	0.87	0.34	41,41,41,41	0
91	MG	5	4079	1/1	0.87	0.63	43,43,43,43	0
91	MG	5	3999	1/1	0.87	0.32	45,45,45,45	0
91	MG	5	3918	1/1	0.87	0.57	42,42,42,42	0
91	MG	1	3770	1/1	0.87	0.47	41,41,41,41	0
91	MG	5	4173	1/1	0.87	0.56	30,30,30,30	0
91	MG	1	4069	1/1	0.87	0.26	46,46,46,46	0
91	MG	5	4008	1/1	0.87	0.31	56,56,56,56	0
91	MG	5	3936	1/1	0.87	0.56	38,38,38,38	0
91	MG	7	221	1/1	0.87	0.46	47,47,47,47	0
91	MG	2	2073	1/1	0.87	0.30	93,93,93,93	0
91	MG	5	4018	1/1	0.87	0.29	38,38,38,38	0
91	MG	5	3939	1/1	0.87	0.53	38,38,38,38	0
91	MG	8	220	1/1	0.87	0.25	49,49,49,49	0
91	MG	5	3940	1/1	0.87	0.55	34,34,34,34	0
91	MG	6	2165	1/1	0.87	0.29	69,69,69,69	0
91	MG	6	2104	1/1	0.87	0.30	90,90,90,90	0
91	MG	5	4028	1/1	0.87	0.36	36,36,36,36	0
91	MG	5	4029	1/1	0.87	0.23	56,56,56,56	0
91	MG	6	2142	1/1	0.87	0.84	48,48,48,48	0
91	MG	5	4033	1/1	0.87	0.27	47,47,47,47	0
91	MG	1	3737	1/1	0.87	0.25	48,48,48,48	0
91	MG	5	4118	1/1	0.87	0.48	35,35,35,35	0
91	MG	5	3964	1/1	0.87	0.32	55,55,55,55	0
91	MG	6	2170	1/1	0.87	0.41	64,64,64,64	0
91	MG	m4	201	1/1	0.87	0.28	42,42,42,42	0
91	MG	m5	303	1/1	0.87	0.44	37,37,37,37	0
91	MG	6	2146	1/1	0.87	0.24	75,75,75,75	0
91	MG	1	3777	1/1	0.87	0.32	31,31,31,31	0
91	MG	M7	205	1/1	0.87	0.34	38,38,38,38	0
91	MG	m7	203	1/1	0.87	0.32	33,33,33,33	0
91	MG	5	3892	1/1	0.87	0.63	43,43,43,43	0
91	MG	n8	201	1/1	0.87	0.14	43,43,43,43	0
91	MG	5	4134	1/1	0.87	0.33	36,36,36,36	0
91	MG	1	4021	1/1	0.87	0.20	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	o3	203	1/1	0.87	0.67	36,36,36,36	0
91	MG	5	3775	1/1	0.87	0.34	32,32,32,32	0
91	MG	p	102	1/1	0.87	0.34	35,35,35,35	0
91	MG	p	103	1/1	0.87	0.78	40,40,40,40	0
91	MG	6	2109	1/1	0.87	0.82	90,90,90,90	0
91	MG	2	2119	1/1	0.87	0.13	87,87,87,87	0
91	MG	5	3784	1/1	0.87	0.46	37,37,37,37	0
91	MG	1	3876	1/1	0.87	0.74	43,43,43,43	0
91	MG	5	3995	1/1	0.87	0.22	34,34,34,34	0
91	MG	1	4028	1/1	0.88	0.19	43,43,43,43	0
91	MG	2	2060	1/1	0.88	0.76	74,74,74,74	0
91	MG	N8	206	1/1	0.88	0.31	37,37,37,37	0
91	MG	5	4036	1/1	0.88	0.31	41,41,41,41	0
91	MG	1	4087	1/1	0.88	0.81	34,34,34,34	0
91	MG	1	3742	1/1	0.88	0.50	41,41,41,41	0
90	OHX	6	1970	7/7	0.88	0.56	105,105,105,105	0
91	MG	6	2063	1/1	0.88	0.26	89,89,89,89	0
91	MG	2	2126	1/1	0.88	0.56	78,78,78,78	0
91	MG	1	4100	1/1	0.88	0.20	37,37,37,37	0
91	MG	5	4054	1/1	0.88	0.29	36,36,36,36	0
91	MG	1	3943	1/1	0.88	0.34	47,47,47,47	0
91	MG	6	2113	1/1	0.88	0.43	55,55,55,55	0
91	MG	6	2068	1/1	0.88	0.49	105,105,105,105	0
91	MG	6	2176	1/1	0.88	0.46	58,58,58,58	0
91	MG	5	3812	1/1	0.88	0.21	42,42,42,42	0
90	OHX	5	3647	7/7	0.88	0.38	64,64,64,64	0
91	MG	1	3824	1/1	0.88	0.68	38,38,38,38	0
91	MG	5	3970	1/1	0.88	0.45	32,32,32,32	0
91	MG	2	2130	1/1	0.88	0.23	85,85,85,85	0
91	MG	5	3825	1/1	0.88	0.65	35,35,35,35	0
90	OHX	8	217	7/7	0.88	0.46	55,55,55,55	0
91	MG	1	4115	1/1	0.88	0.47	63,63,63,63	0
91	MG	1	4055	1/1	0.88	0.98	32,32,32,32	0
91	MG	5	3981	1/1	0.88	0.39	35,35,35,35	0
91	MG	1	3784	1/1	0.88	0.34	57,57,57,57	0
91	MG	5	3983	1/1	0.88	0.18	41,41,41,41	0
91	MG	5	3837	1/1	0.88	0.54	34,34,34,34	0
91	MG	1	3754	1/1	0.88	0.26	35,35,35,35	0
91	MG	5	3843	1/1	0.88	0.35	34,34,34,34	0
91	MG	5	3992	1/1	0.88	0.65	40,40,40,40	0
91	MG	3	215	1/1	0.88	0.15	59,59,59,59	0
91	MG	1	3838	1/1	0.88	0.48	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	2	2115	1/1	0.88	0.66	84,84,84,84	0
91	MG	2	2088	1/1	0.88	0.45	77,77,77,77	0
91	MG	m6	205	1/1	0.88	0.49	36,36,36,36	0
91	MG	5	3863	1/1	0.88	0.58	38,38,38,38	0
91	MG	5	3750	1/1	0.88	0.74	60,60,60,60	0
91	MG	n6	202	1/1	0.88	0.33	42,42,42,42	0
91	MG	1	4064	1/1	0.88	1.02	54,54,54,54	0
91	MG	1	4067	1/1	0.88	0.45	39,39,39,39	0
91	MG	1	3849	1/1	0.88	0.52	39,39,39,39	0
91	MG	5	3888	1/1	0.88	0.40	48,48,48,48	0
91	MG	o4	201	1/1	0.88	0.11	63,63,63,63	0
91	MG	5	4127	1/1	0.88	0.55	36,36,36,36	0
91	MG	q1	101	1/1	0.88	0.38	58,58,58,58	0
91	MG	5	3758	1/1	0.88	0.57	43,43,43,43	0
91	MG	1	4072	1/1	0.88	0.63	37,37,37,37	0
91	MG	1	3797	1/1	0.88	0.29	51,51,51,51	0
90	OHX	2	1994	7/7	0.88	0.32	98,98,98,98	0
91	MG	1	3856	1/1	0.88	0.70	36,36,36,36	0
91	MG	2	2099	1/1	0.88	0.60	80,80,80,80	0
91	MG	1	4078	1/1	0.88	0.28	36,36,36,36	0
91	MG	5	4116	1/1	0.89	0.66	44,44,44,44	0
91	MG	5	3814	1/1	0.89	0.56	38,38,38,38	0
91	MG	2	2087	1/1	0.89	0.34	77,77,77,77	0
91	MG	6	2101	1/1	0.89	0.45	53,53,53,53	0
91	MG	5	3822	1/1	0.89	0.35	42,42,42,42	0
91	MG	5	3823	1/1	0.89	0.62	50,50,50,50	0
91	MG	2	2121	1/1	0.89	0.47	68,68,68,68	0
91	MG	5	3989	1/1	0.89	0.22	44,44,44,44	0
91	MG	5	3826	1/1	0.89	0.34	43,43,43,43	0
91	MG	1	4007	1/1	0.89	0.20	51,51,51,51	0
91	MG	5	4133	1/1	0.89	0.47	47,47,47,47	0
91	MG	M7	204	1/1	0.89	0.52	38,38,38,38	0
90	OHX	1	3682	7/7	0.89	0.38	87,87,87,87	0
91	MG	5	4140	1/1	0.89	0.73	39,39,39,39	0
91	MG	1	3958	1/1	0.89	0.32	36,36,36,36	0
91	MG	5	3836	1/1	0.89	0.27	37,37,37,37	0
91	MG	5	4149	1/1	0.89	0.45	34,34,34,34	0
91	MG	6	2181	1/1	0.89	0.17	77,77,77,77	0
91	MG	5	4006	1/1	0.89	0.30	33,33,33,33	0
91	MG	1	3916	1/1	0.89	0.63	35,35,35,35	0
91	MG	5	4156	1/1	0.89	0.32	39,39,39,39	0
91	MG	1	4015	1/1	0.89	0.96	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	N8	204	1/1	0.89	0.24	44,44,44,44	0
91	MG	5	4011	1/1	0.89	0.53	32,32,32,32	0
91	MG	1	3961	1/1	0.89	0.43	31,31,31,31	0
91	MG	5	3853	1/1	0.89	0.22	36,36,36,36	0
91	MG	1	4019	1/1	0.89	0.14	49,49,49,49	0
91	MG	1	4083	1/1	0.89	0.31	56,56,56,56	0
90	OHX	1	3721	7/7	0.89	0.51	62,62,62,62	0
91	MG	5	4022	1/1	0.89	0.34	37,37,37,37	0
91	MG	1	4022	1/1	0.89	0.27	34,34,34,34	0
91	MG	7	213	1/1	0.89	0.81	33,33,33,33	0
91	MG	5	4027	1/1	0.89	0.23	40,40,40,40	0
91	MG	d6	102	1/1	0.89	0.62	64,64,64,64	0
91	MG	1	3926	1/1	0.89	0.15	38,38,38,38	0
91	MG	1	3965	1/1	0.89	0.36	44,44,44,44	0
91	MG	1	3966	1/1	0.89	0.29	32,32,32,32	0
91	MG	1	3930	1/1	0.89	0.42	60,60,60,60	0
90	OHX	2	1976	7/7	0.89	0.45	110,110,110,110	0
91	MG	6	2132	1/1	0.89	0.51	59,59,59,59	0
91	MG	5	3757	1/1	0.89	0.46	42,42,42,42	0
91	MG	1	3977	1/1	0.89	0.32	65,65,65,65	0
91	MG	5	3759	1/1	0.89	0.22	32,32,32,32	0
91	MG	1	3978	1/1	0.89	0.70	43,43,43,43	0
91	MG	1	3827	1/1	0.89	0.89	50,50,50,50	0
91	MG	5	3906	1/1	0.89	0.61	33,33,33,33	0
91	MG	1	4110	1/1	0.89	0.64	41,41,41,41	0
91	MG	1	3870	1/1	0.89	0.48	52,52,52,52	0
91	MG	2	2127	1/1	0.89	0.74	77,77,77,77	0
91	MG	1	4046	1/1	0.89	0.59	43,43,43,43	0
91	MG	5	3780	1/1	0.89	0.29	35,35,35,35	0
91	MG	2	2055	1/1	0.89	0.79	75,75,75,75	0
91	MG	1	3835	1/1	0.89	0.74	32,32,32,32	0
91	MG	1	3779	1/1	0.89	0.53	37,37,37,37	0
91	MG	3	216	1/1	0.89	0.11	59,59,59,59	0
91	MG	m7	201	1/1	0.89	0.38	34,34,34,34	0
91	MG	m7	202	1/1	0.89	0.32	36,36,36,36	0
91	MG	6	2151	1/1	0.89	0.69	64,64,64,64	0
91	MG	n3	201	1/1	0.89	0.44	32,32,32,32	0
91	MG	1	3805	1/1	0.89	0.51	52,52,52,52	0
91	MG	5	3799	1/1	0.89	0.37	31,31,31,31	0
91	MG	5	3947	1/1	0.89	0.24	40,40,40,40	0
91	MG	5	4089	1/1	0.89	0.24	51,51,51,51	0
91	MG	4	225	1/1	0.89	0.53	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	o3	202	1/1	0.89	0.52	44,44,44,44	0
91	MG	5	3956	1/1	0.89	0.45	33,33,33,33	0
91	MG	5	3957	1/1	0.89	0.28	38,38,38,38	0
91	MG	5	3962	1/1	0.89	0.55	46,46,46,46	0
91	MG	2	2067	1/1	0.89	0.60	78,78,78,78	0
91	MG	1	3902	1/1	0.89	0.51	40,40,40,40	0
91	MG	4	228	1/1	0.89	0.61	40,40,40,40	0
91	MG	1	3996	1/1	0.89	0.50	40,40,40,40	0
91	MG	4	235	1/1	0.89	0.21	41,41,41,41	0
91	MG	1	3997	1/1	0.89	0.34	43,43,43,43	0
93	PHE	1	3401	11/12	0.89	0.29	34,34,44,44	0
91	MG	1	3740	1/1	0.89	0.29	48,48,48,48	0
91	MG	1	3810	1/1	0.89	0.27	40,40,40,40	0
91	MG	1	4023	1/1	0.90	0.45	60,60,60,60	0
91	MG	1	3962	1/1	0.90	0.70	54,54,54,54	0
90	OHX	2	2015	7/7	0.90	0.34	92,92,92,92	0
90	OHX	2	2024	7/7	0.90	0.27	103,103,103,103	0
90	OHX	1	3727	7/7	0.90	0.40	50,50,50,50	0
91	MG	2	2065	1/1	0.90	0.42	88,88,88,88	0
91	MG	1	4108	1/1	0.90	0.39	44,44,44,44	0
91	MG	1	3906	1/1	0.90	0.47	49,49,49,49	0
91	MG	5	4078	1/1	0.90	0.26	32,32,32,32	0
91	MG	1	3972	1/1	0.90	0.32	43,43,43,43	0
91	MG	2	2066	1/1	0.90	0.81	72,72,72,72	0
91	MG	1	4040	1/1	0.90	0.25	49,49,49,49	0
90	OHX	2	2030	7/7	0.90	0.43	95,95,95,95	0
91	MG	2	2133	1/1	0.90	0.31	85,85,85,85	0
90	OHX	6	2016	7/7	0.90	0.37	95,95,95,95	0
91	MG	5	3991	1/1	0.90	0.61	38,38,38,38	0
91	MG	5	3869	1/1	0.90	0.45	59,59,59,59	0
91	MG	1	4047	1/1	0.90	0.51	43,43,43,43	0
91	MG	5	3880	1/1	0.90	0.40	37,37,37,37	0
91	MG	5	3997	1/1	0.90	0.28	31,31,31,31	0
91	MG	2	2136	1/1	0.90	0.19	90,90,90,90	0
90	OHX	6	2037	7/7	0.90	0.45	77,77,77,77	0
90	OHX	6	2048	7/7	0.90	0.31	77,77,77,77	0
91	MG	2	2140	1/1	0.90	0.27	83,83,83,83	0
91	MG	2	2105	1/1	0.90	0.23	96,96,96,96	0
90	OHX	6	2055	7/7	0.90	0.30	118,118,118,118	0
91	MG	1	3936	1/1	0.90	0.34	40,40,40,40	0
91	MG	4	234	1/1	0.90	0.37	45,45,45,45	0
90	OHX	2	2039	7/7	0.90	0.23	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	5	4013	1/1	0.90	0.43	38,38,38,38	0
90	OHX	7	210	7/7	0.90	0.34	91,91,91,91	0
91	MG	2	2077	1/1	0.90	1.23	59,59,59,59	0
91	MG	L3	404	1/1	0.90	0.54	51,51,51,51	0
90	OHX	2	2011	7/7	0.90	0.38	104,104,104,104	0
91	MG	L7	301	1/1	0.90	0.49	39,39,39,39	0
91	MG	2	2053	1/1	0.90	0.83	70,70,70,70	0
91	MG	5	3924	1/1	0.90	0.55	36,36,36,36	0
91	MG	1	3863	1/1	0.90	0.31	30,30,30,30	0
91	MG	n8	202	1/1	0.90	0.23	34,34,34,34	0
91	MG	n8	203	1/1	0.90	0.96	34,34,34,34	0
91	MG	6	2103	1/1	0.90	0.59	62,62,62,62	0
91	MG	5	4136	1/1	0.90	0.35	38,38,38,38	0
91	MG	6	2171	1/1	0.90	0.94	68,68,68,68	0
90	OHX	2	2012	7/7	0.90	0.28	108,108,108,108	0
91	MG	1	3950	1/1	0.90	0.38	44,44,44,44	0
91	MG	5	4146	1/1	0.90	0.29	37,37,37,37	0
91	MG	2	2085	1/1	0.90	0.68	76,76,76,76	0
90	OHX	2	2049	7/7	0.90	0.41	108,108,108,108	0
90	OHX	2	2050	7/7	0.90	0.23	115,115,115,115	0
91	MG	N8	201	1/1	0.90	0.23	31,31,31,31	0
90	OHX	C5	201	7/7	0.90	0.28	105,105,105,105	0
90	OHX	SR	401	7/7	0.90	0.23	121,121,121,121	0
91	MG	1	3883	1/1	0.90	0.81	42,42,42,42	0
90	OHX	1	3593	7/7	0.90	0.37	66,66,66,66	0
90	OHX	1	3604	7/7	0.90	0.42	43,43,43,43	0
96	8AN	P	101	22/23	0.90	0.26	37,38,38,38	0
96	8AN	p	101	22/23	0.90	0.24	33,34,35,35	0
91	MG	5	3889	1/1	0.91	0.57	39,39,39,39	0
91	MG	5	4135	1/1	0.91	0.47	38,38,38,38	0
91	MG	4	233	1/1	0.91	0.23	44,44,44,44	0
91	MG	1	3860	1/1	0.91	0.72	44,44,44,44	0
91	MG	5	4015	1/1	0.91	0.72	66,66,66,66	0
91	MG	6	2143	1/1	0.91	0.51	75,75,75,75	0
91	MG	1	3969	1/1	0.91	0.67	42,42,42,42	0
90	OHX	5	3738	7/7	0.91	0.50	69,69,69,69	0
91	MG	1	3933	1/1	0.91	0.28	51,51,51,51	0
91	MG	5	3786	1/1	0.91	0.21	33,33,33,33	0
91	MG	6	2148	1/1	0.91	0.21	58,58,58,58	0
91	MG	5	4023	1/1	0.91	0.60	41,41,41,41	0
91	MG	5	4024	1/1	0.91	0.32	49,49,49,49	0
91	MG	2	2063	1/1	0.91	0.23	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	5	3791	1/1	0.91	0.21	42,42,42,42	0
91	MG	5	3909	1/1	0.91	0.60	31,31,31,31	0
91	MG	5	3913	1/1	0.91	0.65	30,30,30,30	0
91	MG	5	4166	1/1	0.91	1.03	44,44,44,44	0
91	MG	5	4030	1/1	0.91	0.43	33,33,33,33	0
91	MG	2	2116	1/1	0.91	0.13	85,85,85,85	0
91	MG	1	4027	1/1	0.91	0.17	41,41,41,41	0
91	MG	5	3919	1/1	0.91	0.54	34,34,34,34	0
90	OHX	2	1947	7/7	0.91	0.24	106,106,106,106	0
91	MG	5	3923	1/1	0.91	0.51	38,38,38,38	0
91	MG	1	3980	1/1	0.91	1.06	63,63,63,63	0
91	MG	5	4040	1/1	0.91	0.17	54,54,54,54	0
91	MG	1	3741	1/1	0.91	0.59	35,35,35,35	0
90	OHX	6	1931	7/7	0.91	0.21	86,86,86,86	0
91	MG	7	224	1/1	0.91	0.22	36,36,36,36	0
90	OHX	2	1974	7/7	0.91	0.26	112,112,112,112	0
91	MG	7	226	1/1	0.91	0.12	46,46,46,46	0
91	MG	N0	201	1/1	0.91	0.91	43,43,43,43	0
91	MG	5	4051	1/1	0.91	0.45	34,34,34,34	0
91	MG	6	2164	1/1	0.91	0.25	57,57,57,57	0
90	OHX	2	2042	7/7	0.91	0.23	126,126,126,126	0
91	MG	1	4101	1/1	0.91	1.01	43,43,43,43	0
91	MG	1	3886	1/1	0.91	0.68	38,38,38,38	0
91	MG	5	4060	1/1	0.91	0.19	48,48,48,48	0
91	MG	5	4061	1/1	0.91	0.62	39,39,39,39	0
91	MG	2	2123	1/1	0.91	0.45	96,96,96,96	0
91	MG	1	3947	1/1	0.91	0.55	43,43,43,43	0
91	MG	5	3954	1/1	0.91	0.12	48,48,48,48	0
91	MG	5	3955	1/1	0.91	0.71	35,35,35,35	0
91	MG	5	4071	1/1	0.91	0.34	35,35,35,35	0
90	OHX	6	2031	7/7	0.91	0.39	106,106,106,106	0
91	MG	1	3900	1/1	0.91	0.19	31,31,31,31	0
91	MG	5	3959	1/1	0.91	0.36	41,41,41,41	0
91	MG	1	4049	1/1	0.91	0.52	47,47,47,47	0
91	MG	1	3792	1/1	0.91	0.36	38,38,38,38	0
90	OHX	2	2051	7/7	0.91	0.39	105,105,105,105	0
91	MG	1	3839	1/1	0.91	0.54	42,42,42,42	0
91	MG	1	3842	1/1	0.91	0.59	38,38,38,38	0
91	MG	5	3829	1/1	0.91	0.35	41,41,41,41	0
91	MG	6	2117	1/1	0.91	0.47	55,55,55,55	0
91	MG	6	2118	1/1	0.91	0.41	96,96,96,96	0
90	OHX	6	2040	7/7	0.91	0.37	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	6	2121	1/1	0.91	0.36	62,62,62,62	0
91	MG	6	2123	1/1	0.91	0.07	93,93,93,93	0
91	MG	1	4124	1/1	0.91	0.99	49,49,49,49	0
91	MG	1	3796	1/1	0.91	0.38	35,35,35,35	0
90	OHX	6	2042	7/7	0.91	0.30	94,94,94,94	0
91	MG	5	4111	1/1	0.91	0.30	35,35,35,35	0
91	MG	6	2072	1/1	0.91	0.53	59,59,59,59	0
91	MG	4	201	1/1	0.91	0.31	32,32,32,32	0
90	OHX	1	3684	7/7	0.91	0.42	65,65,65,65	0
91	MG	1	3758	1/1	0.91	1.06	41,41,41,41	0
90	OHX	1	3701	7/7	0.91	0.31	38,38,38,38	0
91	MG	5	3865	1/1	0.91	0.53	44,44,44,44	0
91	MG	6	2135	1/1	0.91	0.43	64,64,64,64	0
91	MG	1	4068	1/1	0.91	0.25	43,43,43,43	0
91	MG	5	3868	1/1	0.91	0.53	32,32,32,32	0
90	OHX	2	2028	7/7	0.91	0.28	109,109,109,109	0
91	MG	4	231	1/1	0.91	0.37	46,46,46,46	0
91	MG	1	3767	1/1	0.91	0.47	46,46,46,46	0
95	SPS	1	4125	23/23	0.91	0.24	37,37,48,51	0
91	MG	6	2083	1/1	0.91	0.81	56,56,56,56	0
91	MG	5	3769	1/1	0.91	0.40	35,35,35,35	0
90	OHX	c3	201	7/7	0.92	0.28	89,89,89,89	0
91	MG	1	4103	1/1	0.92	0.39	39,39,39,39	0
90	OHX	c5	201	7/7	0.92	0.26	99,99,99,99	0
90	OHX	5	3619	7/7	0.92	0.29	73,73,73,73	0
91	MG	1	4013	1/1	0.92	0.41	37,37,37,37	0
90	OHX	2	2009	7/7	0.92	0.22	117,117,117,117	0
91	MG	1	3939	1/1	0.92	0.43	54,54,54,54	0
90	OHX	5	3709	7/7	0.92	0.40	57,57,57,57	0
90	OHX	1	3695	7/7	0.92	0.35	64,64,64,64	0
90	OHX	1	3697	7/7	0.92	0.31	58,58,58,58	0
91	MG	6	2174	1/1	0.92	0.26	60,60,60,60	0
91	MG	5	4137	1/1	0.92	0.45	38,38,38,38	0
91	MG	5	4003	1/1	0.92	0.28	36,36,36,36	0
90	OHX	2	2031	7/7	0.92	0.36	103,103,103,103	0
90	OHX	l3	402	7/7	0.92	0.51	67,67,67,67	0
91	MG	6	2177	1/1	0.92	0.12	94,94,94,94	0
91	MG	2	2052	1/1	0.92	0.91	69,69,69,69	0
91	MG	1	3948	1/1	0.92	0.50	48,48,48,48	0
91	MG	1	3774	1/1	0.92	0.37	44,44,44,44	0
91	MG	5	4152	1/1	0.92	0.38	40,40,40,40	0
90	OHX	1	3703	7/7	0.92	0.39	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	1	3707	7/7	0.92	0.28	114,114,114,114	0
91	MG	s4	301	1/1	0.92	0.32	63,63,63,63	0
90	OHX	2	2032	7/7	0.92	0.39	106,106,106,106	0
91	MG	1	4033	1/1	0.92	0.28	34,34,34,34	0
91	MG	5	3877	1/1	0.92	0.47	37,37,37,37	0
91	MG	5	4163	1/1	0.92	0.56	37,37,37,37	0
91	MG	5	3879	1/1	0.92	0.75	36,36,36,36	0
90	OHX	2	2033	7/7	0.92	0.22	123,123,123,123	0
91	MG	5	3881	1/1	0.92	0.97	35,35,35,35	0
91	MG	1	3864	1/1	0.92	0.73	49,49,49,49	0
91	MG	5	4025	1/1	0.92	0.37	39,39,39,39	0
91	MG	1	3956	1/1	0.92	0.21	56,56,56,56	0
91	MG	5	4174	1/1	0.92	0.15	43,43,43,43	0
91	MG	1	3957	1/1	0.92	0.27	39,39,39,39	0
91	MG	2	2097	1/1	0.92	0.19	118,118,118,118	0
90	OHX	S9	201	7/7	0.92	0.50	93,93,93,93	0
91	MG	7	215	1/1	0.92	0.49	36,36,36,36	0
90	OHX	2	2038	7/7	0.92	0.35	95,95,95,95	0
90	OHX	6	1973	7/7	0.92	0.25	68,68,68,68	0
91	MG	1	3874	1/1	0.92	0.51	44,44,44,44	0
91	MG	1	3789	1/1	0.92	0.50	33,33,33,33	0
91	MG	5	3753	1/1	0.92	0.34	43,43,43,43	0
91	MG	L4	403	1/1	0.92	0.54	50,50,50,50	0
91	MG	1	4050	1/1	0.92	0.99	53,53,53,53	0
91	MG	8	202	1/1	0.92	0.41	39,39,39,39	0
91	MG	8	219	1/1	0.92	0.36	37,37,37,37	0
91	MG	6	2116	1/1	0.92	0.34	63,63,63,63	0
90	OHX	2	1980	7/7	0.92	0.22	140,140,140,140	0
91	MG	5	3761	1/1	0.92	0.44	33,33,33,33	0
91	MG	5	3916	1/1	0.92	0.74	44,44,44,44	0
91	MG	1	3882	1/1	0.92	0.39	44,44,44,44	0
91	MG	2	2102	1/1	0.92	0.25	98,98,98,98	0
91	MG	5	4052	1/1	0.92	0.56	65,65,65,65	0
90	OHX	6	2019	7/7	0.92	0.38	75,75,75,75	0
90	OHX	2	2025	7/7	0.92	0.41	85,85,85,85	0
91	MG	1	3974	1/1	0.92	0.48	35,35,35,35	0
91	MG	1	3889	1/1	0.92	0.93	36,36,36,36	0
90	OHX	6	2036	7/7	0.92	0.39	73,73,73,73	0
91	MG	1	3798	1/1	0.92	0.25	34,34,34,34	0
90	OHX	1	3594	7/7	0.92	0.43	68,68,68,68	0
91	MG	5	3785	1/1	0.92	0.34	33,33,33,33	0
91	MG	1	3733	1/1	0.92	0.48	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	6	2038	7/7	0.92	0.25	105,105,105,105	0
91	MG	5	4069	1/1	0.92	0.49	33,33,33,33	0
91	MG	2	2109	1/1	0.92	0.30	80,80,80,80	0
91	MG	1	3807	1/1	0.92	0.32	48,48,48,48	0
91	MG	O5	201	1/1	0.92	0.55	42,42,42,42	0
91	MG	5	3795	1/1	0.92	0.30	37,37,37,37	0
91	MG	O7	102	1/1	0.92	0.20	42,42,42,42	0
90	OHX	2	1995	7/7	0.92	0.29	103,103,103,103	0
91	MG	Q2	503	1/1	0.92	0.24	48,48,48,48	0
91	MG	1	3986	1/1	0.92	0.39	43,43,43,43	0
90	OHX	1	3663	7/7	0.92	0.45	73,73,73,73	0
90	OHX	1	3666	7/7	0.92	0.36	81,81,81,81	0
90	OHX	2	2046	7/7	0.92	0.46	100,100,100,100	0
91	MG	5	3968	1/1	0.92	0.30	40,40,40,40	0
91	MG	6	2144	1/1	0.92	0.29	94,94,94,94	0
91	MG	5	4098	1/1	0.92	1.34	32,32,32,32	0
90	OHX	6	2056	7/7	0.92	0.20	99,99,99,99	0
90	OHX	6	2057	7/7	0.92	0.44	92,92,92,92	0
91	MG	5	3972	1/1	0.92	0.47	37,37,37,37	0
91	MG	5	3973	1/1	0.92	0.13	46,46,46,46	0
91	MG	5	4108	1/1	0.92	0.42	32,32,32,32	0
91	MG	1	3927	1/1	0.92	0.17	56,56,56,56	0
91	MG	1	3746	1/1	0.92	0.17	48,48,48,48	0
91	MG	2	2074	1/1	0.92	0.76	80,80,80,80	0
91	MG	1	4097	1/1	0.92	0.36	41,41,41,41	0
91	MG	1	4001	1/1	0.92	0.32	52,52,52,52	0
91	MG	6	2075	1/1	0.92	0.46	71,71,71,71	0
90	OHX	6	2059	7/7	0.92	0.31	103,103,103,103	0
90	OHX	s9	201	7/7	0.92	0.40	77,77,77,77	0
91	MG	1	3959	1/1	0.93	0.15	41,41,41,41	0
91	MG	1	3844	1/1	0.93	0.71	39,39,39,39	0
90	OHX	5	3723	7/7	0.93	0.34	36,36,36,36	0
91	MG	5	3914	1/1	0.93	0.55	48,48,48,48	0
90	OHX	6	1980	7/7	0.93	0.21	112,112,112,112	0
91	MG	6	2081	1/1	0.93	0.23	70,70,70,70	0
90	OHX	5	3746	7/7	0.93	0.26	61,61,61,61	0
90	OHX	6	1987	7/7	0.93	0.28	89,89,89,89	0
91	MG	5	3920	1/1	0.93	0.71	44,44,44,44	0
91	MG	1	3853	1/1	0.93	0.80	43,43,43,43	0
91	MG	1	4082	1/1	0.93	0.46	54,54,54,54	0
90	OHX	6	1988	7/7	0.93	0.36	82,82,82,82	0
91	MG	5	3929	1/1	0.93	0.76	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	5	4103	1/1	0.93	0.28	38,38,38,38	0
91	MG	1	4084	1/1	0.93	0.21	33,33,33,33	0
91	MG	1	3855	1/1	0.93	0.28	32,32,32,32	0
91	MG	1	3750	1/1	0.93	0.51	39,39,39,39	0
91	MG	1	4088	1/1	0.93	0.69	44,44,44,44	0
91	MG	1	4091	1/1	0.93	0.26	33,33,33,33	0
91	MG	5	3942	1/1	0.93	0.39	40,40,40,40	0
91	MG	5	3755	1/1	0.93	0.19	34,34,34,34	0
91	MG	5	3756	1/1	0.93	0.70	44,44,44,44	0
90	OHX	6	1998	7/7	0.93	0.27	65,65,65,65	0
90	OHX	6	2002	7/7	0.93	0.33	71,71,71,71	0
90	OHX	2	1945	7/7	0.93	0.18	90,90,90,90	0
91	MG	5	3951	1/1	0.93	0.34	39,39,39,39	0
90	OHX	6	2017	7/7	0.93	0.34	99,99,99,99	0
90	OHX	S8	301	7/7	0.93	0.33	96,96,96,96	0
91	MG	6	2099	1/1	0.93	0.23	65,65,65,65	0
91	MG	5	3766	1/1	0.93	0.38	46,46,46,46	0
91	MG	5	3768	1/1	0.93	0.22	51,51,51,51	0
91	MG	6	2100	1/1	0.93	0.84	45,45,45,45	0
90	OHX	6	2023	7/7	0.93	0.49	91,91,91,91	0
91	MG	5	3967	1/1	0.93	0.28	40,40,40,40	0
91	MG	5	3774	1/1	0.93	0.20	33,33,33,33	0
91	MG	1	3762	1/1	0.93	0.30	34,34,34,34	0
90	OHX	6	2025	7/7	0.93	0.40	70,70,70,70	0
91	MG	1	3872	1/1	0.93	0.51	41,41,41,41	0
90	OHX	6	2027	7/7	0.93	0.43	91,91,91,91	0
90	OHX	2	2013	7/7	0.93	0.28	104,104,104,104	0
90	OHX	1	3693	7/7	0.93	0.35	80,80,80,80	0
91	MG	1	3878	1/1	0.93	0.61	33,33,33,33	0
90	OHX	2	1996	7/7	0.93	0.24	103,103,103,103	0
90	OHX	2	2020	7/7	0.93	0.31	96,96,96,96	0
91	MG	5	3980	1/1	0.93	0.56	43,43,43,43	0
91	MG	6	2112	1/1	0.93	0.23	63,63,63,63	0
90	OHX	6	2039	7/7	0.93	0.25	94,94,94,94	0
91	MG	2	2122	1/1	0.93	0.32	74,74,74,74	0
90	OHX	1	3700	7/7	0.93	0.31	87,87,87,87	0
91	MG	1	3998	1/1	0.93	0.58	43,43,43,43	0
91	MG	5	4160	1/1	0.93	0.20	44,44,44,44	0
91	MG	1	3780	1/1	0.93	0.49	52,52,52,52	0
91	MG	1	3890	1/1	0.93	0.30	40,40,40,40	0
91	MG	1	3896	1/1	0.93	0.67	44,44,44,44	0
91	MG	1	3781	1/1	0.93	0.42	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	1	3501	7/7	0.93	0.18	66,66,66,66	0
91	MG	5	3994	1/1	0.93	0.48	31,31,31,31	0
90	OHX	6	2044	7/7	0.93	0.35	63,63,63,63	0
91	MG	5	3996	1/1	0.93	0.33	35,35,35,35	0
90	OHX	6	2047	7/7	0.93	0.40	87,87,87,87	0
90	OHX	1	3552	7/7	0.93	0.30	58,58,58,58	0
91	MG	5	3810	1/1	0.93	0.15	89,89,89,89	0
91	MG	1	3786	1/1	0.93	0.41	33,33,33,33	0
91	MG	5	4001	1/1	0.93	0.35	37,37,37,37	0
90	OHX	2	2047	7/7	0.93	0.47	105,105,105,105	0
91	MG	7	218	1/1	0.93	0.23	37,37,37,37	0
91	MG	1	3908	1/1	0.93	0.63	41,41,41,41	0
91	MG	7	220	1/1	0.93	0.21	48,48,48,48	0
91	MG	2	2129	1/1	0.93	0.15	80,80,80,80	0
90	OHX	1	3715	7/7	0.93	0.33	51,51,51,51	0
91	MG	1	3794	1/1	0.93	0.53	58,58,58,58	0
90	OHX	1	3720	7/7	0.93	0.36	61,61,61,61	0
91	MG	4	238	1/1	0.93	0.44	42,42,42,42	0
90	OHX	2	1986	7/7	0.93	0.35	107,107,107,107	0
91	MG	L3	405	1/1	0.93	0.14	41,41,41,41	0
90	OHX	2	2035	7/7	0.93	0.29	107,107,107,107	0
91	MG	2	2134	1/1	0.93	1.01	59,59,59,59	0
91	MG	1	3928	1/1	0.93	0.41	51,51,51,51	0
91	MG	1	3929	1/1	0.93	0.56	51,51,51,51	0
90	OHX	1	3612	7/7	0.93	0.31	87,87,87,87	0
91	MG	8	226	1/1	0.93	0.54	53,53,53,53	0
90	OHX	6	1939	7/7	0.93	0.16	102,102,102,102	0
91	MG	8	228	1/1	0.93	0.26	47,47,47,47	0
90	OHX	sR	401	7/7	0.93	0.25	116,116,116,116	0
91	MG	5	3842	1/1	0.93	0.60	38,38,38,38	0
91	MG	1	4035	1/1	0.93	0.67	37,37,37,37	0
90	OHX	5	3553	7/7	0.93	0.37	50,50,50,50	0
91	MG	l3	406	1/1	0.93	0.68	34,34,34,34	0
91	MG	5	3848	1/1	0.93	1.04	41,41,41,41	0
91	MG	6	2150	1/1	0.93	1.08	58,58,58,58	0
90	OHX	5	3601	7/7	0.93	0.26	84,84,84,84	0
91	MG	5	3854	1/1	0.93	0.54	53,53,53,53	0
90	OHX	6	1959	7/7	0.93	0.23	67,67,67,67	0
91	MG	1	4039	1/1	0.93	0.14	49,49,49,49	0
90	OHX	5	3645	7/7	0.93	0.41	56,56,56,56	0
91	MG	1	4041	1/1	0.93	0.51	53,53,53,53	0
90	OHX	1	3637	7/7	0.93	0.19	145,145,145,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	1	3814	1/1	0.93	0.38	50,50,50,50	0
91	MG	1	3816	1/1	0.93	0.28	34,34,34,34	0
91	MG	6	2162	1/1	0.93	0.34	55,55,55,55	0
90	OHX	5	3651	7/7	0.93	0.43	48,48,48,48	0
90	OHX	5	3658	7/7	0.93	0.38	58,58,58,58	0
90	OHX	5	3664	7/7	0.93	0.33	92,92,92,92	0
91	MG	5	4050	1/1	0.93	0.92	24,24,24,24	0
91	MG	6	2061	1/1	0.93	0.16	69,69,69,69	0
90	OHX	5	3668	7/7	0.93	0.36	60,60,60,60	0
91	MG	5	4053	1/1	0.93	0.32	43,43,43,43	0
90	OHX	5	3671	7/7	0.93	0.25	103,103,103,103	0
90	OHX	5	3685	7/7	0.93	0.35	73,73,73,73	0
91	MG	1	3949	1/1	0.93	0.46	36,36,36,36	0
91	MG	5	4058	1/1	0.93	0.30	47,47,47,47	0
90	OHX	5	3689	7/7	0.93	0.36	79,79,79,79	0
90	OHX	5	3699	7/7	0.93	0.38	63,63,63,63	0
91	MG	1	3833	1/1	0.93	0.47	39,39,39,39	0
91	MG	1	3834	1/1	0.93	0.45	35,35,35,35	0
90	OHX	5	3700	7/7	0.93	0.41	53,53,53,53	0
92	ZN	E1	501	1/1	0.93	0.06	109,109,109,109	0
91	MG	1	3836	1/1	0.93	0.66	34,34,34,34	0
90	OHX	2	1909	7/7	0.93	0.15	97,97,97,97	0
92	ZN	q2	501	1/1	0.93	0.09	47,47,47,47	0
90	OHX	5	3718	7/7	0.93	0.25	102,102,102,102	0
91	MG	5	4070	1/1	0.93	0.19	40,40,40,40	0
91	MG	5	3902	1/1	0.93	0.77	37,37,37,37	0
91	MG	5	4073	1/1	0.93	0.27	34,34,34,34	0
95	SPS	5	4176	23/23	0.93	0.24	33,34,45,47	0
90	OHX	5	3721	7/7	0.93	0.28	99,99,99,99	0
91	MG	5	4077	1/1	0.93	0.49	43,43,43,43	0
91	MG	N8	202	1/1	0.94	0.26	31,31,31,31	0
90	OHX	6	1953	7/7	0.94	0.15	109,109,109,109	0
91	MG	1	4029	1/1	0.94	0.60	44,44,44,44	0
91	MG	6	2172	1/1	0.94	0.60	64,64,64,64	0
91	MG	5	3905	1/1	0.94	0.85	38,38,38,38	0
91	MG	1	3910	1/1	0.94	0.48	38,38,38,38	0
90	OHX	5	3670	7/7	0.94	0.36	40,40,40,40	0
91	MG	5	4088	1/1	0.94	0.21	42,42,42,42	0
90	OHX	2	2017	7/7	0.94	0.31	88,88,88,88	0
91	MG	O7	101	1/1	0.94	0.23	40,40,40,40	0
91	MG	1	3913	1/1	0.94	0.61	49,49,49,49	0
90	OHX	5	3681	7/7	0.94	0.34	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	6	1960	7/7	0.94	0.19	77,77,77,77	0
90	OHX	5	3687	7/7	0.94	0.44	66,66,66,66	0
90	OHX	6	1968	7/7	0.94	0.38	74,74,74,74	0
91	MG	1	3788	1/1	0.94	0.87	39,39,39,39	0
91	MG	5	3921	1/1	0.94	0.61	31,31,31,31	0
90	OHX	5	3692	7/7	0.94	0.32	70,70,70,70	0
90	OHX	1	3601	7/7	0.94	0.40	62,62,62,62	0
90	OHX	2	1959	7/7	0.94	0.21	98,98,98,98	0
91	MG	5	3925	1/1	0.94	0.47	38,38,38,38	0
90	OHX	5	3703	7/7	0.94	0.22	57,57,57,57	0
90	OHX	2	2023	7/7	0.94	0.31	91,91,91,91	0
90	OHX	5	3715	7/7	0.94	0.41	59,59,59,59	0
90	OHX	1	3613	7/7	0.94	0.40	58,58,58,58	0
90	OHX	1	3625	7/7	0.94	0.38	70,70,70,70	0
90	OHX	5	3722	7/7	0.94	0.38	62,62,62,62	0
90	OHX	1	3630	7/7	0.94	0.31	59,59,59,59	0
91	MG	5	4119	1/1	0.94	0.16	41,41,41,41	0
90	OHX	5	3737	7/7	0.94	0.16	56,56,56,56	0
90	OHX	2	1970	7/7	0.94	0.38	98,98,98,98	0
90	OHX	6	2003	7/7	0.94	0.24	89,89,89,89	0
90	OHX	5	3748	7/7	0.94	0.34	87,87,87,87	0
90	OHX	6	2010	7/7	0.94	0.27	91,91,91,91	0
91	MG	5	4129	1/1	0.94	0.40	40,40,40,40	0
90	OHX	8	211	7/7	0.94	0.27	78,78,78,78	0
90	OHX	8	215	7/7	0.94	0.36	62,62,62,62	0
90	OHX	6	2015	7/7	0.94	0.38	79,79,79,79	0
90	OHX	1	3645	7/7	0.94	0.36	57,57,57,57	0
91	MG	5	3760	1/1	0.94	0.23	42,42,42,42	0
90	OHX	m9	201	7/7	0.94	0.46	89,89,89,89	0
91	MG	1	3820	1/1	0.94	0.24	49,49,49,49	0
91	MG	1	3822	1/1	0.94	0.47	44,44,44,44	0
90	OHX	2	1971	7/7	0.94	0.18	108,108,108,108	0
91	MG	5	4141	1/1	0.94	0.17	38,38,38,38	0
90	OHX	6	2018	7/7	0.94	0.21	114,114,114,114	0
90	OHX	2	2027	7/7	0.94	0.32	93,93,93,93	0
90	OHX	1	3667	7/7	0.94	0.38	92,92,92,92	0
91	MG	1	3830	1/1	0.94	0.36	38,38,38,38	0
90	OHX	6	2024	7/7	0.94	0.44	103,103,103,103	0
91	MG	6	2095	1/1	0.94	0.45	55,55,55,55	0
90	OHX	1	3674	7/7	0.94	0.35	61,61,61,61	0
90	OHX	1	3679	7/7	0.94	0.31	67,67,67,67	0
90	OHX	2	1915	7/7	0.94	0.15	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	5	4158	1/1	0.94	0.21	57,57,57,57	0
90	OHX	6	2032	7/7	0.94	0.28	92,92,92,92	0
90	OHX	2	1999	7/7	0.94	0.38	106,106,106,106	0
90	OHX	2	2003	7/7	0.94	0.27	100,100,100,100	0
91	MG	1	4094	1/1	0.94	0.48	37,37,37,37	0
90	OHX	2	1975	7/7	0.94	0.15	77,77,77,77	0
90	OHX	C3	201	7/7	0.94	0.23	96,96,96,96	0
91	MG	5	3793	1/1	0.94	0.28	62,62,62,62	0
91	MG	5	4167	1/1	0.94	0.54	33,33,33,33	0
90	OHX	2	1926	7/7	0.94	0.16	91,91,91,91	0
91	MG	5	4169	1/1	0.94	0.45	47,47,47,47	0
91	MG	1	4099	1/1	0.94	0.76	45,45,45,45	0
91	MG	5	3797	1/1	0.94	0.20	38,38,38,38	0
90	OHX	2	1978	7/7	0.94	0.28	103,103,103,103	0
91	MG	1	3846	1/1	0.94	0.30	33,33,33,33	0
91	MG	1	3973	1/1	0.94	0.41	47,47,47,47	0
91	MG	6	2110	1/1	0.94	0.21	91,91,91,91	0
91	MG	5	3804	1/1	0.94	0.52	39,39,39,39	0
91	MG	7	214	1/1	0.94	0.44	47,47,47,47	0
90	OHX	1	3488	7/7	0.94	0.23	47,47,47,47	0
90	OHX	1	3704	7/7	0.94	0.43	49,49,49,49	0
91	MG	1	3851	1/1	0.94	0.72	36,36,36,36	0
91	MG	1	3734	1/1	0.94	0.49	53,53,53,53	0
90	OHX	2	1950	7/7	0.94	0.31	101,101,101,101	0
91	MG	5	4002	1/1	0.94	0.33	43,43,43,43	0
91	MG	2	2071	1/1	0.94	0.55	79,79,79,79	0
90	OHX	6	2050	7/7	0.94	0.47	68,68,68,68	0
91	MG	1	4114	1/1	0.94	0.36	34,34,34,34	0
90	OHX	1	3709	7/7	0.94	0.52	47,47,47,47	0
91	MG	1	3739	1/1	0.94	0.45	33,33,33,33	0
91	MG	5	4009	1/1	0.94	0.76	43,43,43,43	0
91	MG	6	2122	1/1	0.94	0.17	74,74,74,74	0
90	OHX	1	3548	7/7	0.94	0.18	91,91,91,91	0
91	MG	8	222	1/1	0.94	0.37	43,43,43,43	0
90	OHX	1	3718	7/7	0.94	0.43	83,83,83,83	0
91	MG	1	4123	1/1	0.94	0.40	46,46,46,46	0
90	OHX	1	3719	7/7	0.94	0.38	65,65,65,65	0
91	MG	1	3988	1/1	0.94	0.70	59,59,59,59	0
90	OHX	2	1982	7/7	0.94	0.26	94,94,94,94	0
90	OHX	1	3559	7/7	0.94	0.36	54,54,54,54	0
91	MG	6	2131	1/1	0.94	0.49	60,60,60,60	0
91	MG	l2	302	1/1	0.94	0.34	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	1	3722	7/7	0.94	0.42	76,76,76,76	0
91	MG	2	2082	1/1	0.94	0.49	74,74,74,74	0
91	MG	2	2083	1/1	0.94	0.65	83,83,83,83	0
90	OHX	1	3724	7/7	0.94	0.35	75,75,75,75	0
91	MG	5	3839	1/1	0.94	0.25	35,35,35,35	0
90	OHX	5	3518	7/7	0.94	0.16	78,78,78,78	0
90	OHX	1	3726	7/7	0.94	0.42	69,69,69,69	0
90	OHX	5	3570	7/7	0.94	0.32	61,61,61,61	0
91	MG	5	3847	1/1	0.94	0.55	33,33,33,33	0
91	MG	1	4002	1/1	0.94	0.26	41,41,41,41	0
90	OHX	5	3577	7/7	0.94	0.35	50,50,50,50	0
91	MG	1	4005	1/1	0.94	0.39	45,45,45,45	0
91	MG	5	4035	1/1	0.94	0.36	40,40,40,40	0
90	OHX	5	3596	7/7	0.94	0.25	68,68,68,68	0
91	MG	2	2091	1/1	0.94	0.43	77,77,77,77	0
91	MG	n0	202	1/1	0.94	0.33	37,37,37,37	0
91	MG	5	3859	1/1	0.94	0.50	30,30,30,30	0
91	MG	1	3760	1/1	0.94	0.43	45,45,45,45	0
91	MG	L3	401	1/1	0.94	0.71	41,41,41,41	0
90	OHX	5	3600	7/7	0.94	0.27	44,44,44,44	0
90	OHX	1	3560	7/7	0.94	0.26	60,60,60,60	0
91	MG	6	2149	1/1	0.94	0.24	73,73,73,73	0
91	MG	n9	103	1/1	0.94	0.42	34,34,34,34	0
90	OHX	1	3730	7/7	0.94	0.17	94,94,94,94	0
91	MG	1	3892	1/1	0.94	0.28	32,32,32,32	0
91	MG	5	3871	1/1	0.94	0.24	33,33,33,33	0
91	MG	5	3873	1/1	0.94	0.41	51,51,51,51	0
91	MG	1	3893	1/1	0.94	0.57	46,46,46,46	0
91	MG	1	3769	1/1	0.94	0.53	36,36,36,36	0
91	MG	5	3878	1/1	0.94	0.89	37,37,37,37	0
91	MG	P	102	1/1	0.94	0.43	39,39,39,39	0
91	MG	1	4020	1/1	0.94	0.42	39,39,39,39	0
91	MG	M5	303	1/1	0.94	0.16	37,37,37,37	0
90	OHX	5	3622	7/7	0.94	0.26	59,59,59,59	0
91	MG	5	3882	1/1	0.94	0.33	30,30,30,30	0
90	OHX	5	3625	7/7	0.94	0.33	79,79,79,79	0
91	MG	5	3886	1/1	0.94	0.35	61,61,61,61	0
90	OHX	4	220	7/7	0.94	0.39	67,67,67,67	0
91	MG	5	4067	1/1	0.94	0.44	35,35,35,35	0
90	OHX	O7	104	7/7	0.94	0.23	52,52,52,52	0
94	LEU	1	3402	8/9	0.94	0.30	39,40,40,40	0
90	OHX	6	1927	7/7	0.94	0.12	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	N3	202	1/1	0.94	0.24	51,51,51,51	0
91	MG	N5	201	1/1	0.94	0.35	43,43,43,43	0
90	OHX	1	3588	7/7	0.94	0.26	45,45,45,45	0
90	OHX	2	2041	7/7	0.94	0.42	83,83,83,83	0
91	MG	5	4038	1/1	0.95	0.46	37,37,37,37	0
90	OHX	5	3729	7/7	0.95	0.29	74,74,74,74	0
90	OHX	5	3730	7/7	0.95	0.31	97,97,97,97	0
91	MG	5	3824	1/1	0.95	0.15	45,45,45,45	0
91	MG	5	4043	1/1	0.95	0.59	41,41,41,41	0
91	MG	5	4044	1/1	0.95	0.68	47,47,47,47	0
90	OHX	5	3734	7/7	0.95	0.39	70,70,70,70	0
90	OHX	1	3678	7/7	0.95	0.33	84,84,84,84	0
90	OHX	6	2013	7/7	0.95	0.32	72,72,72,72	0
90	OHX	5	3739	7/7	0.95	0.39	55,55,55,55	0
91	MG	1	3895	1/1	0.95	0.68	37,37,37,37	0
90	OHX	5	3741	7/7	0.95	0.39	56,56,56,56	0
91	MG	1	4057	1/1	0.95	0.79	38,38,38,38	0
91	MG	1	3898	1/1	0.95	0.46	34,34,34,34	0
90	OHX	5	3744	7/7	0.95	0.21	59,59,59,59	0
90	OHX	2	1998	7/7	0.95	0.39	95,95,95,95	0
91	MG	5	4057	1/1	0.95	0.41	35,35,35,35	0
90	OHX	C7	201	7/7	0.95	0.27	106,106,106,106	0
90	OHX	D9	102	7/7	0.95	0.39	98,98,98,98	0
90	OHX	7	211	7/7	0.95	0.35	69,69,69,69	0
90	OHX	1	3688	7/7	0.95	0.34	65,65,65,65	0
90	OHX	8	214	7/7	0.95	0.37	76,76,76,76	0
91	MG	5	4063	1/1	0.95	0.21	38,38,38,38	0
91	MG	1	3907	1/1	0.95	0.23	53,53,53,53	0
91	MG	1	4071	1/1	0.95	0.65	34,34,34,34	0
90	OHX	2	1973	7/7	0.95	0.15	112,112,112,112	0
91	MG	1	3745	1/1	0.95	0.24	40,40,40,40	0
90	OHX	8	216	7/7	0.95	0.38	59,59,59,59	0
91	MG	5	3857	1/1	0.95	0.47	32,32,32,32	0
91	MG	5	3858	1/1	0.95	0.41	39,39,39,39	0
90	OHX	1	3694	7/7	0.95	0.30	73,73,73,73	0
91	MG	5	4074	1/1	0.95	0.51	47,47,47,47	0
91	MG	6	2119	1/1	0.95	0.32	59,59,59,59	0
91	MG	5	3861	1/1	0.95	0.63	39,39,39,39	0
91	MG	5	3862	1/1	0.95	0.46	35,35,35,35	0
90	OHX	8	218	7/7	0.95	0.42	60,60,60,60	0
90	OHX	1	3464	7/7	0.95	0.14	66,66,66,66	0
90	OHX	l5	302	7/7	0.95	0.37	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	5	4083	1/1	0.95	0.55	35,35,35,35	0
91	MG	1	4081	1/1	0.95	0.31	38,38,38,38	0
91	MG	5	4085	1/1	0.95	0.59	49,49,49,49	0
91	MG	1	3920	1/1	0.95	0.94	34,34,34,34	0
90	OHX	m0	302	7/7	0.95	0.24	68,68,68,68	0
91	MG	1	3922	1/1	0.95	0.30	34,34,34,34	0
91	MG	1	3925	1/1	0.95	0.34	39,39,39,39	0
90	OHX	1	3481	7/7	0.95	0.17	66,66,66,66	0
91	MG	5	4095	1/1	0.95	0.62	34,34,34,34	0
91	MG	5	3876	1/1	0.95	0.18	45,45,45,45	0
91	MG	1	3755	1/1	0.95	0.47	54,54,54,54	0
90	OHX	6	2026	7/7	0.95	0.55	90,90,90,90	0
91	MG	5	4099	1/1	0.95	0.45	33,33,33,33	0
91	MG	5	4101	1/1	0.95	0.74	60,60,60,60	0
90	OHX	1	3699	7/7	0.95	0.48	80,80,80,80	0
90	OHX	2	1918	7/7	0.95	0.16	83,83,83,83	0
90	OHX	2	2004	7/7	0.95	0.38	96,96,96,96	0
90	OHX	6	2033	7/7	0.95	0.42	78,78,78,78	0
91	MG	5	3884	1/1	0.95	0.43	39,39,39,39	0
91	MG	1	3761	1/1	0.95	0.50	46,46,46,46	0
90	OHX	1	3535	7/7	0.95	0.20	50,50,50,50	0
90	OHX	1	3540	7/7	0.95	0.27	66,66,66,66	0
90	OHX	2	1946	7/7	0.95	0.17	99,99,99,99	0
90	OHX	2	2036	7/7	0.95	0.43	112,112,112,112	0
90	OHX	2	2037	7/7	0.95	0.29	98,98,98,98	0
91	MG	1	3772	1/1	0.95	0.17	57,57,57,57	0
91	MG	1	3941	1/1	0.95	0.54	42,42,42,42	0
90	OHX	2	1925	7/7	0.95	0.17	85,85,85,85	0
90	OHX	1	3587	7/7	0.95	0.19	81,81,81,81	0
91	MG	5	4121	1/1	0.95	0.30	33,33,33,33	0
91	MG	5	3896	1/1	0.95	0.64	44,44,44,44	0
91	MG	5	3897	1/1	0.95	0.38	37,37,37,37	0
90	OHX	6	2045	7/7	0.95	0.38	94,94,94,94	0
91	MG	5	3899	1/1	0.95	0.32	32,32,32,32	0
90	OHX	2	1948	7/7	0.95	0.21	80,80,80,80	0
90	OHX	1	3590	7/7	0.95	0.21	92,92,92,92	0
91	MG	5	3904	1/1	0.95	0.72	32,32,32,32	0
90	OHX	2	1903	7/7	0.95	0.14	95,95,95,95	0
90	OHX	6	2051	7/7	0.95	0.41	84,84,84,84	0
90	OHX	6	2052	7/7	0.95	0.16	65,65,65,65	0
91	MG	1	4120	1/1	0.95	0.28	38,38,38,38	0
90	OHX	2	2014	7/7	0.95	0.19	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	1	3725	7/7	0.95	0.45	87,87,87,87	0
90	OHX	2	2043	7/7	0.95	0.40	85,85,85,85	0
91	MG	6	2158	1/1	0.95	0.08	54,54,54,54	0
90	OHX	1	3603	7/7	0.95	0.36	62,62,62,62	0
91	MG	5	4143	1/1	0.95	0.44	32,32,32,32	0
91	MG	5	4144	1/1	0.95	0.17	33,33,33,33	0
90	OHX	s8	301	7/7	0.95	0.30	96,96,96,96	0
90	OHX	2	1958	7/7	0.95	0.22	109,109,109,109	0
90	OHX	3	209	7/7	0.95	0.30	84,84,84,84	0
90	OHX	3	210	7/7	0.95	0.44	85,85,85,85	0
91	MG	2	2080	1/1	0.95	0.33	82,82,82,82	0
90	OHX	4	219	7/7	0.95	0.37	69,69,69,69	0
90	OHX	5	3475	7/7	0.95	0.23	42,42,42,42	0
90	OHX	5	3497	7/7	0.95	0.20	62,62,62,62	0
91	MG	5	4155	1/1	0.95	0.25	72,72,72,72	0
91	MG	5	3931	1/1	0.95	0.41	31,31,31,31	0
90	OHX	2	2045	7/7	0.95	0.48	100,100,100,100	0
91	MG	5	3935	1/1	0.95	0.55	34,34,34,34	0
90	OHX	5	3531	7/7	0.95	0.18	84,84,84,84	0
90	OHX	5	3535	7/7	0.95	0.20	65,65,65,65	0
90	OHX	5	3542	7/7	0.95	0.23	53,53,53,53	0
90	OHX	4	221	7/7	0.95	0.33	65,65,65,65	0
90	OHX	4	223	7/7	0.95	0.35	61,61,61,61	0
91	MG	5	4165	1/1	0.95	0.27	32,32,32,32	0
90	OHX	O4	201	7/7	0.95	0.49	73,73,73,73	0
91	MG	L2	301	1/1	0.95	0.27	42,42,42,42	0
90	OHX	2	1985	7/7	0.95	0.34	98,98,98,98	0
90	OHX	5	3597	7/7	0.95	0.35	51,51,51,51	0
91	MG	5	4170	1/1	0.95	0.28	42,42,42,42	0
90	OHX	2	2018	7/7	0.95	0.40	84,84,84,84	0
90	OHX	2	1936	7/7	0.95	0.14	102,102,102,102	0
91	MG	5	3953	1/1	0.95	0.18	41,41,41,41	0
91	MG	6	2185	1/1	0.95	0.37	92,92,92,92	0
91	MG	1	3815	1/1	0.95	0.30	41,41,41,41	0
91	MG	L4	406	1/1	0.95	0.82	33,33,33,33	0
90	OHX	6	1937	7/7	0.95	0.16	81,81,81,81	0
91	MG	5	3958	1/1	0.95	0.19	39,39,39,39	0
90	OHX	1	3635	7/7	0.95	0.37	59,59,59,59	0
90	OHX	6	1949	7/7	0.95	0.22	81,81,81,81	0
91	MG	5	3963	1/1	0.95	0.13	36,36,36,36	0
90	OHX	5	3626	7/7	0.95	0.18	84,84,84,84	0
91	MG	5	3965	1/1	0.95	0.24	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	1	3821	1/1	0.95	0.33	40,40,40,40	0
91	MG	M7	203	1/1	0.95	0.27	38,38,38,38	0
90	OHX	5	3628	7/7	0.95	0.27	90,90,90,90	0
90	OHX	5	3631	7/7	0.95	0.36	51,51,51,51	0
90	OHX	5	3632	7/7	0.95	0.34	65,65,65,65	0
90	OHX	5	3633	7/7	0.95	0.53	70,70,70,70	0
91	MG	N3	201	1/1	0.95	0.57	41,41,41,41	0
90	OHX	5	3636	7/7	0.95	0.28	63,63,63,63	0
91	MG	1	3990	1/1	0.95	0.41	39,39,39,39	0
90	OHX	5	3638	7/7	0.95	0.33	56,56,56,56	0
90	OHX	5	3641	7/7	0.95	0.27	72,72,72,72	0
90	OHX	5	3643	7/7	0.95	0.30	48,48,48,48	0
90	OHX	2	1989	7/7	0.95	0.19	93,93,93,93	0
90	OHX	6	1957	7/7	0.95	0.22	72,72,72,72	0
90	OHX	6	1958	7/7	0.95	0.23	89,89,89,89	0
90	OHX	5	3657	7/7	0.95	0.32	50,50,50,50	0
90	OHX	1	3641	7/7	0.95	0.29	64,64,64,64	0
90	OHX	2	1993	7/7	0.95	0.29	96,96,96,96	0
91	MG	l3	403	1/1	0.95	0.74	31,31,31,31	0
91	MG	5	3764	1/1	0.95	0.24	34,34,34,34	0
91	MG	5	3990	1/1	0.95	0.15	50,50,50,50	0
91	MG	5	3765	1/1	0.95	0.56	31,31,31,31	0
91	MG	1	4003	1/1	0.95	0.28	39,39,39,39	0
90	OHX	5	3665	7/7	0.95	0.29	55,55,55,55	0
90	OHX	5	3666	7/7	0.95	0.28	51,51,51,51	0
90	OHX	1	3646	7/7	0.95	0.30	93,93,93,93	0
90	OHX	2	1960	7/7	0.95	0.24	100,100,100,100	0
90	OHX	2	2026	7/7	0.95	0.30	109,109,109,109	0
91	MG	2	2120	1/1	0.95	0.08	95,95,95,95	0
91	MG	1	3850	1/1	0.95	0.45	33,33,33,33	0
91	MG	5	3779	1/1	0.95	0.62	33,33,33,33	0
90	OHX	5	3678	7/7	0.95	0.41	55,55,55,55	0
91	MG	5	3781	1/1	0.95	0.17	37,37,37,37	0
90	OHX	6	1975	7/7	0.95	0.16	93,93,93,93	0
91	MG	6	2069	1/1	0.95	0.40	61,61,61,61	0
91	MG	5	4005	1/1	0.95	0.60	37,37,37,37	0
90	OHX	2	1939	7/7	0.95	0.16	92,92,92,92	0
90	OHX	1	3672	7/7	0.95	0.38	67,67,67,67	0
90	OHX	1	3673	7/7	0.95	0.44	73,73,73,73	0
90	OHX	6	1989	7/7	0.95	0.40	97,97,97,97	0
90	OHX	5	3695	7/7	0.95	0.25	92,92,92,92	0
91	MG	1	3858	1/1	0.95	0.64	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	6	1991	7/7	0.95	0.24	81,81,81,81	0
90	OHX	6	1993	7/7	0.95	0.22	99,99,99,99	0
91	MG	5	4016	1/1	0.95	0.32	31,31,31,31	0
90	OHX	6	1997	7/7	0.95	0.29	83,83,83,83	0
90	OHX	2	1943	7/7	0.95	0.34	101,101,101,101	0
91	MG	1	3867	1/1	0.95	0.41	44,44,44,44	0
90	OHX	5	3710	7/7	0.95	0.28	89,89,89,89	0
90	OHX	5	3713	7/7	0.95	0.22	39,39,39,39	0
90	OHX	6	1999	7/7	0.95	0.33	75,75,75,75	0
91	MG	1	4034	1/1	0.95	0.32	47,47,47,47	0
90	OHX	5	3716	7/7	0.95	0.29	84,84,84,84	0
90	OHX	6	2001	7/7	0.95	0.29	93,93,93,93	0
90	OHX	5	3719	7/7	0.95	0.34	67,67,67,67	0
90	OHX	1	3675	7/7	0.95	0.31	64,64,64,64	0
90	OHX	1	3677	7/7	0.95	0.38	54,54,54,54	0
91	MG	5	3811	1/1	0.95	0.43	44,44,44,44	0
90	OHX	6	2006	7/7	0.95	0.28	72,72,72,72	0
90	OHX	5	3724	7/7	0.95	0.44	55,55,55,55	0
90	OHX	5	3726	7/7	0.95	0.48	60,60,60,60	0
91	MG	1	3884	1/1	0.95	0.55	35,35,35,35	0
91	MG	5	3816	1/1	0.95	0.33	43,43,43,43	0
91	MG	1	4045	1/1	0.95	0.29	40,40,40,40	0
91	MG	5	3820	1/1	0.95	0.31	54,54,54,54	0
90	OHX	5	3728	7/7	0.96	0.37	49,49,49,49	0
91	MG	1	4032	1/1	0.96	0.29	47,47,47,47	0
90	OHX	1	3446	7/7	0.96	0.16	53,53,53,53	0
90	OHX	1	3602	7/7	0.96	0.27	74,74,74,74	0
90	OHX	5	3733	7/7	0.96	0.25	91,91,91,91	0
91	MG	1	3799	1/1	0.96	0.45	39,39,39,39	0
90	OHX	1	3705	7/7	0.96	0.32	74,74,74,74	0
90	OHX	2	1906	7/7	0.96	0.12	89,89,89,89	0
90	OHX	6	2020	7/7	0.96	0.34	94,94,94,94	0
90	OHX	6	2022	7/7	0.96	0.46	91,91,91,91	0
91	MG	1	3806	1/1	0.96	0.27	41,41,41,41	0
90	OHX	2	1938	7/7	0.96	0.24	79,79,79,79	0
90	OHX	5	3742	7/7	0.96	0.34	70,70,70,70	0
90	OHX	1	3713	7/7	0.96	0.38	72,72,72,72	0
91	MG	6	2157	1/1	0.96	0.24	57,57,57,57	0
90	OHX	1	3714	7/7	0.96	0.29	82,82,82,82	0
90	OHX	1	3607	7/7	0.96	0.25	63,63,63,63	0
90	OHX	1	3716	7/7	0.96	0.37	65,65,65,65	0
90	OHX	6	2028	7/7	0.96	0.30	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	8	208	7/7	0.96	0.19	57,57,57,57	0
90	OHX	6	2029	7/7	0.96	0.49	69,69,69,69	0
90	OHX	8	212	7/7	0.96	0.37	57,57,57,57	0
91	MG	1	4054	1/1	0.96	0.52	38,38,38,38	0
90	OHX	8	213	7/7	0.96	0.29	60,60,60,60	0
90	OHX	2	1972	7/7	0.96	0.27	105,105,105,105	0
90	OHX	1	3492	7/7	0.96	0.25	61,61,61,61	0
90	OHX	1	3614	7/7	0.96	0.31	77,77,77,77	0
90	OHX	6	2034	7/7	0.96	0.28	99,99,99,99	0
91	MG	6	2173	1/1	0.96	0.23	70,70,70,70	0
90	OHX	6	2035	7/7	0.96	0.45	84,84,84,84	0
90	OHX	1	3618	7/7	0.96	0.33	59,59,59,59	0
90	OHX	1	3620	7/7	0.96	0.28	70,70,70,70	0
91	MG	5	4014	1/1	0.96	0.40	42,42,42,42	0
91	MG	1	4065	1/1	0.96	0.54	44,44,44,44	0
91	MG	1	4066	1/1	0.96	0.75	38,38,38,38	0
90	OHX	1	3723	7/7	0.96	0.33	65,65,65,65	0
90	OHX	m8	201	7/7	0.96	0.35	60,60,60,60	0
90	OHX	1	3495	7/7	0.96	0.16	56,56,56,56	0
91	MG	1	4070	1/1	0.96	0.26	35,35,35,35	0
90	OHX	o7	503	7/7	0.96	0.15	59,59,59,59	0
90	OHX	1	3626	7/7	0.96	0.30	73,73,73,73	0
90	OHX	2	1997	7/7	0.96	0.26	96,96,96,96	0
90	OHX	6	2043	7/7	0.96	0.45	81,81,81,81	0
91	MG	1	3840	1/1	0.96	0.48	41,41,41,41	0
90	OHX	1	3633	7/7	0.96	0.28	66,66,66,66	0
90	OHX	1	3728	7/7	0.96	0.40	55,55,55,55	0
90	OHX	6	2046	7/7	0.96	0.34	93,93,93,93	0
90	OHX	1	3509	7/7	0.96	0.18	60,60,60,60	0
90	OHX	3	203	7/7	0.96	0.17	59,59,59,59	0
90	OHX	6	2049	7/7	0.96	0.44	81,81,81,81	0
91	MG	5	4032	1/1	0.96	0.73	34,34,34,34	0
91	MG	5	3749	1/1	0.96	0.27	36,36,36,36	0
90	OHX	3	208	7/7	0.96	0.22	81,81,81,81	0
90	OHX	1	3636	7/7	0.96	0.22	75,75,75,75	0
90	OHX	1	3527	7/7	0.96	0.34	52,52,52,52	0
90	OHX	6	2053	7/7	0.96	0.38	87,87,87,87	0
91	MG	1	4090	1/1	0.96	0.51	42,42,42,42	0
90	OHX	6	2054	7/7	0.96	0.29	89,89,89,89	0
91	MG	1	4092	1/1	0.96	0.65	33,33,33,33	0
90	OHX	4	218	7/7	0.96	0.30	57,57,57,57	0
90	OHX	1	3529	7/7	0.96	0.26	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	1	3643	7/7	0.96	0.30	48,48,48,48	0
91	MG	2	2069	1/1	0.96	0.44	79,79,79,79	0
90	OHX	6	2058	7/7	0.96	0.30	100,100,100,100	0
90	OHX	1	3533	7/7	0.96	0.24	55,55,55,55	0
91	MG	1	3862	1/1	0.96	0.34	36,36,36,36	0
90	OHX	s4	302	7/7	0.96	0.33	90,90,90,90	0
90	OHX	4	222	7/7	0.96	0.37	66,66,66,66	0
91	MG	1	3865	1/1	0.96	0.41	31,31,31,31	0
90	OHX	2	1984	7/7	0.96	0.29	83,83,83,83	0
90	OHX	L3	403	7/7	0.96	0.20	62,62,62,62	0
91	MG	1	4107	1/1	0.96	0.35	48,48,48,48	0
90	OHX	L4	402	7/7	0.96	0.33	54,54,54,54	0
90	OHX	c8	202	7/7	0.96	0.22	96,96,96,96	0
90	OHX	d4	201	7/7	0.96	0.44	84,84,84,84	0
91	MG	1	4111	1/1	0.96	0.28	45,45,45,45	0
90	OHX	M0	301	7/7	0.96	0.28	55,55,55,55	0
90	OHX	5	3462	7/7	0.96	0.15	48,48,48,48	0
91	MG	1	3875	1/1	0.96	0.72	45,45,45,45	0
91	MG	5	3782	1/1	0.96	0.36	42,42,42,42	0
91	MG	5	3783	1/1	0.96	0.37	33,33,33,33	0
90	OHX	5	3474	7/7	0.96	0.16	47,47,47,47	0
90	OHX	M7	201	7/7	0.96	0.39	62,62,62,62	0
91	MG	1	4119	1/1	0.96	0.31	58,58,58,58	0
91	MG	1	3879	1/1	0.96	0.44	41,41,41,41	0
90	OHX	5	3476	7/7	0.96	0.14	56,56,56,56	0
91	MG	1	3881	1/1	0.96	0.30	33,33,33,33	0
90	OHX	M8	201	7/7	0.96	0.38	65,65,65,65	0
91	MG	3	211	1/1	0.96	0.28	60,60,60,60	0
91	MG	3	212	1/1	0.96	0.55	59,59,59,59	0
90	OHX	5	3501	7/7	0.96	0.15	59,59,59,59	0
90	OHX	5	3503	7/7	0.96	0.16	61,61,61,61	0
91	MG	5	4080	1/1	0.96	0.93	40,40,40,40	0
91	MG	3	217	1/1	0.96	0.50	39,39,39,39	0
90	OHX	5	3508	7/7	0.96	0.23	63,63,63,63	0
91	MG	4	202	1/1	0.96	0.33	42,42,42,42	0
90	OHX	M9	201	7/7	0.96	0.38	74,74,74,74	0
91	MG	5	3803	1/1	0.96	0.37	34,34,34,34	0
91	MG	2	2090	1/1	0.96	0.18	83,83,83,83	0
91	MG	5	4087	1/1	0.96	0.15	41,41,41,41	0
90	OHX	5	3524	7/7	0.96	0.13	75,75,75,75	0
90	OHX	5	3526	7/7	0.96	0.28	47,47,47,47	0
90	OHX	5	3527	7/7	0.96	0.25	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	4	229	1/1	0.96	0.38	36,36,36,36	0
91	MG	1	3894	1/1	0.96	0.66	42,42,42,42	0
90	OHX	5	3529	7/7	0.96	0.26	42,42,42,42	0
90	OHX	5	3530	7/7	0.96	0.28	55,55,55,55	0
90	OHX	1	3652	7/7	0.96	0.31	57,57,57,57	0
90	OHX	5	3534	7/7	0.96	0.19	53,53,53,53	0
90	OHX	1	3654	7/7	0.96	0.36	55,55,55,55	0
90	OHX	5	3536	7/7	0.96	0.25	73,73,73,73	0
90	OHX	5	3540	7/7	0.96	0.11	93,93,93,93	0
91	MG	5	3817	1/1	0.96	0.30	43,43,43,43	0
91	MG	5	3818	1/1	0.96	0.50	31,31,31,31	0
90	OHX	5	3541	7/7	0.96	0.25	57,57,57,57	0
91	MG	L2	302	1/1	0.96	0.36	42,42,42,42	0
91	MG	5	3821	1/1	0.96	0.60	55,55,55,55	0
90	OHX	6	1920	7/7	0.96	0.13	95,95,95,95	0
90	OHX	5	3551	7/7	0.96	0.23	46,46,46,46	0
91	MG	5	4113	1/1	0.96	0.49	35,35,35,35	0
90	OHX	6	1923	7/7	0.96	0.13	81,81,81,81	0
90	OHX	5	3559	7/7	0.96	0.19	79,79,79,79	0
90	OHX	5	3562	7/7	0.96	0.21	70,70,70,70	0
91	MG	5	3827	1/1	0.96	0.62	31,31,31,31	0
91	MG	L4	405	1/1	0.96	0.22	33,33,33,33	0
90	OHX	5	3569	7/7	0.96	0.27	63,63,63,63	0
90	OHX	6	1925	7/7	0.96	0.14	76,76,76,76	0
91	MG	5	3832	1/1	0.96	0.79	41,41,41,41	0
91	MG	5	4124	1/1	0.96	0.45	40,40,40,40	0
90	OHX	1	3656	7/7	0.96	0.29	50,50,50,50	0
90	OHX	5	3584	7/7	0.96	0.34	58,58,58,58	0
90	OHX	5	3586	7/7	0.96	0.31	47,47,47,47	0
91	MG	1	3918	1/1	0.96	0.58	32,32,32,32	0
90	OHX	5	3588	7/7	0.96	0.28	46,46,46,46	0
90	OHX	5	3593	7/7	0.96	0.34	74,74,74,74	0
90	OHX	5	3594	7/7	0.96	0.20	76,76,76,76	0
90	OHX	1	3657	7/7	0.96	0.39	65,65,65,65	0
91	MG	5	3845	1/1	0.96	0.65	32,32,32,32	0
90	OHX	6	1932	7/7	0.96	0.15	59,59,59,59	0
90	OHX	5	3598	7/7	0.96	0.33	68,68,68,68	0
90	OHX	1	3660	7/7	0.96	0.24	77,77,77,77	0
91	MG	N3	203	1/1	0.96	0.22	46,46,46,46	0
90	OHX	1	3661	7/7	0.96	0.38	50,50,50,50	0
90	OHX	5	3604	7/7	0.96	0.29	46,46,46,46	0
91	MG	N6	202	1/1	0.96	0.25	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	5	3606	7/7	0.96	0.34	59,59,59,59	0
90	OHX	5	3611	7/7	0.96	0.25	49,49,49,49	0
90	OHX	5	3613	7/7	0.96	0.21	71,71,71,71	0
90	OHX	5	3615	7/7	0.96	0.25	54,54,54,54	0
91	MG	N8	205	1/1	0.96	0.28	35,35,35,35	0
91	MG	1	3935	1/1	0.96	0.47	40,40,40,40	0
90	OHX	5	3616	7/7	0.96	0.39	63,63,63,63	0
90	OHX	5	3617	7/7	0.96	0.36	74,74,74,74	0
90	OHX	5	3618	7/7	0.96	0.35	68,68,68,68	0
90	OHX	6	1941	7/7	0.96	0.24	96,96,96,96	0
90	OHX	6	1942	7/7	0.96	0.14	73,73,73,73	0
90	OHX	6	1948	7/7	0.96	0.24	82,82,82,82	0
91	MG	6	2060	1/1	0.96	0.29	63,63,63,63	0
90	OHX	1	3537	7/7	0.96	0.32	66,66,66,66	0
90	OHX	5	3627	7/7	0.96	0.19	60,60,60,60	0
90	OHX	6	1951	7/7	0.96	0.14	119,119,119,119	0
90	OHX	6	1952	7/7	0.96	0.18	80,80,80,80	0
91	MG	6	2065	1/1	0.96	0.38	61,61,61,61	0
90	OHX	1	3665	7/7	0.96	0.30	87,87,87,87	0
91	MG	2	2137	1/1	0.96	0.14	85,85,85,85	0
90	OHX	2	1930	7/7	0.96	0.13	95,95,95,95	0
90	OHX	5	3634	7/7	0.96	0.30	57,57,57,57	0
90	OHX	1	3541	7/7	0.96	0.24	60,60,60,60	0
90	OHX	1	3668	7/7	0.96	0.31	63,63,63,63	0
90	OHX	1	3670	7/7	0.96	0.34	65,65,65,65	0
91	MG	5	3887	1/1	0.96	0.20	36,36,36,36	0
90	OHX	6	1961	7/7	0.96	0.32	75,75,75,75	0
90	OHX	5	3644	7/7	0.96	0.35	53,53,53,53	0
90	OHX	6	1967	7/7	0.96	0.19	78,78,78,78	0
90	OHX	1	3542	7/7	0.96	0.25	69,69,69,69	0
91	MG	D9	104	1/1	0.96	0.31	89,89,89,89	0
91	MG	1	3731	1/1	0.96	0.21	47,47,47,47	0
90	OHX	5	3648	7/7	0.96	0.34	50,50,50,50	0
91	MG	7	216	1/1	0.96	0.71	34,34,34,34	0
91	MG	7	217	1/1	0.96	0.48	33,33,33,33	0
90	OHX	6	1969	7/7	0.96	0.24	99,99,99,99	0
90	OHX	5	3655	7/7	0.96	0.22	71,71,71,71	0
90	OHX	2	2034	7/7	0.96	0.30	87,87,87,87	0
90	OHX	1	3550	7/7	0.96	0.26	75,75,75,75	0
90	OHX	5	3659	7/7	0.96	0.34	70,70,70,70	0
90	OHX	5	3663	7/7	0.96	0.34	71,71,71,71	0
91	MG	5	3901	1/1	0.96	0.77	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	6	1974	7/7	0.96	0.27	106,106,106,106	0
91	MG	1	3968	1/1	0.96	0.31	42,42,42,42	0
90	OHX	1	3551	7/7	0.96	0.24	60,60,60,60	0
91	MG	1	3970	1/1	0.96	0.56	37,37,37,37	0
90	OHX	6	1977	7/7	0.96	0.23	97,97,97,97	0
90	OHX	2	2000	7/7	0.96	0.28	95,95,95,95	0
91	MG	5	3911	1/1	0.96	0.74	37,37,37,37	0
91	MG	5	3912	1/1	0.96	0.35	35,35,35,35	0
90	OHX	6	1981	7/7	0.96	0.21	87,87,87,87	0
91	MG	1	3744	1/1	0.96	0.44	41,41,41,41	0
90	OHX	6	1982	7/7	0.96	0.20	96,96,96,96	0
90	OHX	5	3672	7/7	0.96	0.28	76,76,76,76	0
90	OHX	5	3677	7/7	0.96	0.33	60,60,60,60	0
90	OHX	2	2001	7/7	0.96	0.26	99,99,99,99	0
91	MG	l2	301	1/1	0.96	0.68	42,42,42,42	0
90	OHX	5	3679	7/7	0.96	0.38	67,67,67,67	0
90	OHX	2	2021	7/7	0.96	0.33	110,110,110,110	0
91	MG	1	3983	1/1	0.96	0.49	37,37,37,37	0
90	OHX	1	3681	7/7	0.96	0.26	84,84,84,84	0
91	MG	1	3752	1/1	0.96	0.17	40,40,40,40	0
91	MG	1	3753	1/1	0.96	0.19	45,45,45,45	0
91	MG	5	3927	1/1	0.96	0.60	34,34,34,34	0
90	OHX	6	1990	7/7	0.96	0.23	79,79,79,79	0
91	MG	5	3930	1/1	0.96	0.60	37,37,37,37	0
90	OHX	1	3568	7/7	0.96	0.33	63,63,63,63	0
90	OHX	5	3690	7/7	0.96	0.38	49,49,49,49	0
91	MG	m6	201	1/1	0.96	0.86	35,35,35,35	0
90	OHX	1	3570	7/7	0.96	0.28	58,58,58,58	0
91	MG	1	3991	1/1	0.96	0.32	45,45,45,45	0
90	OHX	1	3686	7/7	0.96	0.30	67,67,67,67	0
90	OHX	5	3696	7/7	0.96	0.34	70,70,70,70	0
90	OHX	5	3697	7/7	0.96	0.44	59,59,59,59	0
90	OHX	5	3698	7/7	0.96	0.30	70,70,70,70	0
90	OHX	1	3578	7/7	0.96	0.36	59,59,59,59	0
91	MG	1	3763	1/1	0.96	0.09	50,50,50,50	0
90	OHX	1	3582	7/7	0.96	0.26	53,53,53,53	0
91	MG	1	3765	1/1	0.96	0.52	47,47,47,47	0
90	OHX	5	3702	7/7	0.96	0.26	52,52,52,52	0
91	MG	5	3949	1/1	0.96	0.51	33,33,33,33	0
91	MG	5	3950	1/1	0.96	0.40	34,34,34,34	0
91	MG	n9	102	1/1	0.96	0.93	29,29,29,29	0
90	OHX	2	2022	7/7	0.96	0.26	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	5	3705	7/7	0.96	0.42	54,54,54,54	0
90	OHX	5	3707	7/7	0.96	0.47	67,67,67,67	0
90	OHX	5	3708	7/7	0.96	0.37	68,68,68,68	0
90	OHX	2	1932	7/7	0.96	0.26	76,76,76,76	0
90	OHX	2	1961	7/7	0.96	0.27	103,103,103,103	0
90	OHX	5	3711	7/7	0.96	0.35	48,48,48,48	0
90	OHX	5	3712	7/7	0.96	0.29	53,53,53,53	0
91	MG	5	3960	1/1	0.96	0.56	39,39,39,39	0
91	MG	5	3961	1/1	0.96	0.43	43,43,43,43	0
90	OHX	6	2005	7/7	0.96	0.23	79,79,79,79	0
90	OHX	5	3714	7/7	0.96	0.29	95,95,95,95	0
90	OHX	1	3698	7/7	0.96	0.34	60,60,60,60	0
90	OHX	6	2007	7/7	0.96	0.41	82,82,82,82	0
90	OHX	5	3717	7/7	0.96	0.46	48,48,48,48	0
90	OHX	6	2008	7/7	0.96	0.26	100,100,100,100	0
90	OHX	6	2009	7/7	0.96	0.29	88,88,88,88	0
90	OHX	1	3591	7/7	0.96	0.29	65,65,65,65	0
90	OHX	6	2012	7/7	0.96	0.34	76,76,76,76	0
90	OHX	2	2007	7/7	0.96	0.41	88,88,88,88	0
91	MG	1	3790	1/1	0.96	0.46	32,32,32,32	0
90	OHX	6	2014	7/7	0.96	0.30	64,64,64,64	0
90	OHX	2	1964	7/7	0.96	0.18	97,97,97,97	0
90	OHX	5	3727	7/7	0.96	0.34	71,71,71,71	0
90	OHX	5	3661	7/7	0.97	0.41	51,51,51,51	0
90	OHX	2	1935	7/7	0.97	0.13	82,82,82,82	0
90	OHX	1	3680	7/7	0.97	0.29	76,76,76,76	0
90	OHX	1	3553	7/7	0.97	0.24	63,63,63,63	0
90	OHX	1	3555	7/7	0.97	0.24	81,81,81,81	0
90	OHX	5	3667	7/7	0.97	0.24	72,72,72,72	0
90	OHX	2	1923	7/7	0.97	0.13	84,84,84,84	0
90	OHX	5	3669	7/7	0.97	0.35	50,50,50,50	0
90	OHX	1	3685	7/7	0.97	0.24	65,65,65,65	0
90	OHX	6	2004	7/7	0.97	0.24	84,84,84,84	0
90	OHX	2	1951	7/7	0.97	0.15	82,82,82,82	0
90	OHX	5	3673	7/7	0.97	0.38	56,56,56,56	0
90	OHX	5	3674	7/7	0.97	0.27	43,43,43,43	0
90	OHX	5	3676	7/7	0.97	0.30	66,66,66,66	0
90	OHX	1	3561	7/7	0.97	0.25	64,64,64,64	0
91	MG	5	3975	1/1	0.97	0.28	35,35,35,35	0
91	MG	5	3976	1/1	0.97	0.68	40,40,40,40	0
91	MG	6	2134	1/1	0.97	0.31	57,57,57,57	0
90	OHX	1	3689	7/7	0.97	0.24	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	1	4009	1/1	0.97	0.21	37,37,37,37	0
91	MG	1	4010	1/1	0.97	0.17	47,47,47,47	0
91	MG	1	4011	1/1	0.97	0.16	50,50,50,50	0
90	OHX	1	3691	7/7	0.97	0.30	80,80,80,80	0
90	OHX	5	3680	7/7	0.97	0.38	45,45,45,45	0
91	MG	5	3984	1/1	0.97	0.12	49,49,49,49	0
90	OHX	1	3562	7/7	0.97	0.22	58,58,58,58	0
90	OHX	5	3682	7/7	0.97	0.30	83,83,83,83	0
91	MG	5	3987	1/1	0.97	0.18	38,38,38,38	0
90	OHX	5	3683	7/7	0.97	0.51	72,72,72,72	0
91	MG	1	4018	1/1	0.97	0.21	36,36,36,36	0
90	OHX	5	3684	7/7	0.97	0.26	73,73,73,73	0
90	OHX	1	3563	7/7	0.97	0.25	70,70,70,70	0
90	OHX	1	3565	7/7	0.97	0.26	57,57,57,57	0
90	OHX	1	3696	7/7	0.97	0.17	46,46,46,46	0
91	MG	1	3768	1/1	0.97	0.78	36,36,36,36	0
90	OHX	1	3567	7/7	0.97	0.23	45,45,45,45	0
90	OHX	2	1977	7/7	0.97	0.23	99,99,99,99	0
90	OHX	2	1952	7/7	0.97	0.26	104,104,104,104	0
90	OHX	1	3574	7/7	0.97	0.29	57,57,57,57	0
90	OHX	1	3575	7/7	0.97	0.32	47,47,47,47	0
91	MG	1	3775	1/1	0.97	0.12	44,44,44,44	0
91	MG	1	4030	1/1	0.97	0.29	40,40,40,40	0
90	OHX	1	3577	7/7	0.97	0.25	51,51,51,51	0
90	OHX	2	1979	7/7	0.97	0.29	82,82,82,82	0
90	OHX	6	2021	7/7	0.97	0.39	84,84,84,84	0
90	OHX	5	3701	7/7	0.97	0.18	50,50,50,50	0
90	OHX	1	3580	7/7	0.97	0.17	79,79,79,79	0
90	OHX	1	3581	7/7	0.97	0.22	53,53,53,53	0
90	OHX	5	3704	7/7	0.97	0.39	59,59,59,59	0
90	OHX	2	2016	7/7	0.97	0.30	84,84,84,84	0
90	OHX	1	3710	7/7	0.97	0.29	56,56,56,56	0
90	OHX	1	3712	7/7	0.97	0.44	58,58,58,58	0
91	MG	6	2168	1/1	0.97	0.22	57,57,57,57	0
90	OHX	1	3583	7/7	0.97	0.41	78,78,78,78	0
90	OHX	2	1953	7/7	0.97	0.26	83,83,83,83	0
90	OHX	2	1981	7/7	0.97	0.19	75,75,75,75	0
91	MG	1	4044	1/1	0.97	0.44	35,35,35,35	0
90	OHX	6	2030	7/7	0.97	0.30	74,74,74,74	0
91	MG	1	3791	1/1	0.97	0.38	35,35,35,35	0
90	OHX	1	3589	7/7	0.97	0.36	53,53,53,53	0
90	OHX	1	3717	7/7	0.97	0.36	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	2	2019	7/7	0.97	0.41	91,91,91,91	0
90	OHX	2	1954	7/7	0.97	0.12	89,89,89,89	0
91	MG	1	4051	1/1	0.97	0.42	33,33,33,33	0
90	OHX	2	1983	7/7	0.97	0.24	81,81,81,81	0
90	OHX	2	1955	7/7	0.97	0.24	96,96,96,96	0
90	OHX	1	3595	7/7	0.97	0.43	60,60,60,60	0
91	MG	6	2184	1/1	0.97	0.20	57,57,57,57	0
90	OHX	1	3596	7/7	0.97	0.32	56,56,56,56	0
91	MG	1	3800	1/1	0.97	0.38	32,32,32,32	0
90	OHX	1	3598	7/7	0.97	0.38	50,50,50,50	0
90	OHX	2	1956	7/7	0.97	0.24	92,92,92,92	0
90	OHX	2	1957	7/7	0.97	0.33	85,85,85,85	0
90	OHX	5	3725	7/7	0.97	0.32	90,90,90,90	0
90	OHX	1	3431	7/7	0.97	0.23	46,46,46,46	0
90	OHX	1	3440	7/7	0.97	0.21	44,44,44,44	0
90	OHX	1	3729	7/7	0.97	0.14	60,60,60,60	0
90	OHX	1	3441	7/7	0.97	0.12	55,55,55,55	0
90	OHX	1	3610	7/7	0.97	0.33	64,64,64,64	0
91	MG	1	3813	1/1	0.97	0.31	44,44,44,44	0
90	OHX	5	3731	7/7	0.97	0.36	65,65,65,65	0
91	MG	5	4042	1/1	0.97	0.17	35,35,35,35	0
90	OHX	5	3732	7/7	0.97	0.29	74,74,74,74	0
90	OHX	3	204	7/7	0.97	0.22	49,49,49,49	0
90	OHX	3	206	7/7	0.97	0.17	69,69,69,69	0
91	MG	5	4046	1/1	0.97	0.18	40,40,40,40	0
91	MG	1	4073	1/1	0.97	0.63	41,41,41,41	0
90	OHX	5	3735	7/7	0.97	0.41	81,81,81,81	0
90	OHX	3	207	7/7	0.97	0.17	68,68,68,68	0
90	OHX	1	3611	7/7	0.97	0.28	57,57,57,57	0
90	OHX	2	1988	7/7	0.97	0.30	87,87,87,87	0
91	MG	1	3823	1/1	0.97	0.30	37,37,37,37	0
90	OHX	5	3740	7/7	0.97	0.13	59,59,59,59	0
90	OHX	1	3453	7/7	0.97	0.13	59,59,59,59	0
90	OHX	4	209	7/7	0.97	0.16	55,55,55,55	0
90	OHX	5	3743	7/7	0.97	0.36	72,72,72,72	0
91	MG	1	3828	1/1	0.97	0.68	43,43,43,43	0
90	OHX	4	210	7/7	0.97	0.24	69,69,69,69	0
90	OHX	4	213	7/7	0.97	0.26	63,63,63,63	0
91	MG	5	3767	1/1	0.97	0.59	36,36,36,36	0
90	OHX	5	3747	7/7	0.97	0.15	92,92,92,92	0
91	MG	1	4089	1/1	0.97	0.55	31,31,31,31	0
91	MG	5	4064	1/1	0.97	1.04	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	4	215	7/7	0.97	0.24	72,72,72,72	0
91	MG	5	3771	1/1	0.97	0.33	38,38,38,38	0
91	MG	5	3772	1/1	0.97	0.80	46,46,46,46	0
91	MG	5	3773	1/1	0.97	0.33	33,33,33,33	0
90	OHX	7	202	7/7	0.97	0.14	52,52,52,52	0
90	OHX	7	203	7/7	0.97	0.13	48,48,48,48	0
90	OHX	7	207	7/7	0.97	0.18	59,59,59,59	0
91	MG	1	3837	1/1	0.97	0.58	39,39,39,39	0
91	MG	1	4095	1/1	0.97	0.10	52,52,52,52	0
90	OHX	7	208	7/7	0.97	0.27	61,61,61,61	0
91	MG	5	4076	1/1	0.97	0.29	61,61,61,61	0
90	OHX	4	217	7/7	0.97	0.38	48,48,48,48	0
90	OHX	2	1908	7/7	0.97	0.10	95,95,95,95	0
91	MG	1	3841	1/1	0.97	0.38	33,33,33,33	0
90	OHX	8	205	7/7	0.97	0.17	56,56,56,56	0
90	OHX	8	207	7/7	0.97	0.15	75,75,75,75	0
90	OHX	1	3616	7/7	0.97	0.11	131,131,131,131	0
91	MG	5	3787	1/1	0.97	0.36	32,32,32,32	0
90	OHX	8	209	7/7	0.97	0.34	56,56,56,56	0
91	MG	1	4104	1/1	0.97	0.48	54,54,54,54	0
90	OHX	8	210	7/7	0.97	0.21	66,66,66,66	0
91	MG	1	3848	1/1	0.97	0.36	34,34,34,34	0
90	OHX	1	3617	7/7	0.97	0.37	68,68,68,68	0
91	MG	5	3794	1/1	0.97	0.30	37,37,37,37	0
91	MG	5	4090	1/1	0.97	0.17	37,37,37,37	0
90	OHX	1	3468	7/7	0.97	0.13	56,56,56,56	0
90	OHX	1	3471	7/7	0.97	0.11	62,62,62,62	0
90	OHX	1	3623	7/7	0.97	0.23	81,81,81,81	0
90	OHX	1	3624	7/7	0.97	0.25	69,69,69,69	0
90	OHX	1	3474	7/7	0.97	0.14	51,51,51,51	0
90	OHX	1	3475	7/7	0.97	0.17	62,62,62,62	0
90	OHX	5	3443	7/7	0.97	0.16	51,51,51,51	0
91	MG	1	4116	1/1	0.97	0.21	76,76,76,76	0
90	OHX	5	3455	7/7	0.97	0.24	41,41,41,41	0
90	OHX	l5	301	7/7	0.97	0.20	77,77,77,77	0
90	OHX	5	3461	7/7	0.97	0.13	44,44,44,44	0
91	MG	5	4105	1/1	0.97	0.33	34,34,34,34	0
90	OHX	l9	201	7/7	0.97	0.24	60,60,60,60	0
90	OHX	M5	302	7/7	0.97	0.27	61,61,61,61	0
91	MG	1	4122	1/1	0.97	0.27	37,37,37,37	0
91	MG	5	4109	1/1	0.97	0.19	49,49,49,49	0
90	OHX	m0	304	7/7	0.97	0.37	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	5	3468	7/7	0.97	0.12	63,63,63,63	0
90	OHX	5	3470	7/7	0.97	0.14	53,53,53,53	0
90	OHX	5	3473	7/7	0.97	0.19	46,46,46,46	0
91	MG	3	214	1/1	0.97	0.45	59,59,59,59	0
90	OHX	1	3476	7/7	0.97	0.18	59,59,59,59	0
90	OHX	2	1990	7/7	0.97	0.29	99,99,99,99	0
90	OHX	1	3484	7/7	0.97	0.10	78,78,78,78	0
90	OHX	5	3477	7/7	0.97	0.14	56,56,56,56	0
90	OHX	5	3490	7/7	0.97	0.18	64,64,64,64	0
90	OHX	5	3494	7/7	0.97	0.19	57,57,57,57	0
90	OHX	2	1991	7/7	0.97	0.35	96,96,96,96	0
91	MG	5	4123	1/1	0.97	0.22	39,39,39,39	0
90	OHX	5	3498	7/7	0.97	0.17	50,50,50,50	0
90	OHX	5	3500	7/7	0.97	0.20	63,63,63,63	0
90	OHX	2	2029	7/7	0.97	0.34	79,79,79,79	0
90	OHX	O9	101	7/7	0.97	0.41	49,49,49,49	0
90	OHX	6	1902	7/7	0.97	0.13	91,91,91,91	0
90	OHX	5	3511	7/7	0.97	0.21	42,42,42,42	0
90	OHX	5	3515	7/7	0.97	0.20	47,47,47,47	0
90	OHX	6	1905	7/7	0.97	0.11	73,73,73,73	0
91	MG	5	3830	1/1	0.97	0.31	35,35,35,35	0
91	MG	1	3885	1/1	0.97	0.22	53,53,53,53	0
90	OHX	6	1907	7/7	0.97	0.14	77,77,77,77	0
90	OHX	5	3525	7/7	0.97	0.17	58,58,58,58	0
91	MG	1	3888	1/1	0.97	0.77	39,39,39,39	0
91	MG	5	4138	1/1	0.97	0.18	43,43,43,43	0
91	MG	5	3835	1/1	0.97	0.41	34,34,34,34	0
90	OHX	6	1914	7/7	0.97	0.14	61,61,61,61	0
90	OHX	6	1919	7/7	0.97	0.17	74,74,74,74	0
90	OHX	1	3638	7/7	0.97	0.32	67,67,67,67	0
90	OHX	6	1921	7/7	0.97	0.19	64,64,64,64	0
91	MG	5	3841	1/1	0.97	0.59	43,43,43,43	0
90	OHX	1	3639	7/7	0.97	0.38	63,63,63,63	0
91	MG	L4	401	1/1	0.97	0.37	37,37,37,37	0
90	OHX	5	3533	7/7	0.97	0.22	51,51,51,51	0
90	OHX	1	3640	7/7	0.97	0.31	70,70,70,70	0
90	OHX	2	1917	7/7	0.97	0.16	83,83,83,83	0
90	OHX	6	1928	7/7	0.97	0.16	105,105,105,105	0
90	OHX	5	3537	7/7	0.97	0.19	73,73,73,73	0
91	MG	5	3852	1/1	0.97	0.61	31,31,31,31	0
91	MG	L7	302	1/1	0.97	0.20	37,37,37,37	0
91	MG	5	4157	1/1	0.97	0.44	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	2	2079	1/1	0.97	0.41	85,85,85,85	0
90	OHX	2	1941	7/7	0.97	0.26	93,93,93,93	0
90	OHX	1	3644	7/7	0.97	0.36	61,61,61,61	0
90	OHX	6	1933	7/7	0.97	0.13	98,98,98,98	0
90	OHX	5	3547	7/7	0.97	0.28	61,61,61,61	0
90	OHX	5	3548	7/7	0.97	0.27	49,49,49,49	0
90	OHX	5	3549	7/7	0.97	0.15	79,79,79,79	0
91	MG	M7	206	1/1	0.97	0.63	37,37,37,37	0
90	OHX	5	3550	7/7	0.97	0.31	49,49,49,49	0
91	MG	5	3864	1/1	0.97	0.54	39,39,39,39	0
90	OHX	6	1935	7/7	0.97	0.17	68,68,68,68	0
90	OHX	1	3502	7/7	0.97	0.22	46,46,46,46	0
90	OHX	5	3555	7/7	0.97	0.32	55,55,55,55	0
90	OHX	5	3556	7/7	0.97	0.23	83,83,83,83	0
90	OHX	5	3557	7/7	0.97	0.20	78,78,78,78	0
91	MG	1	3917	1/1	0.97	0.60	32,32,32,32	0
90	OHX	5	3558	7/7	0.97	0.31	59,59,59,59	0
90	OHX	1	3504	7/7	0.97	0.17	64,64,64,64	0
91	MG	5	3875	1/1	0.97	0.43	34,34,34,34	0
90	OHX	6	1940	7/7	0.97	0.16	59,59,59,59	0
90	OHX	5	3568	7/7	0.97	0.23	62,62,62,62	0
91	MG	1	3924	1/1	0.97	0.30	42,42,42,42	0
90	OHX	1	3648	7/7	0.97	0.35	65,65,65,65	0
90	OHX	1	3650	7/7	0.97	0.22	57,57,57,57	0
90	OHX	5	3572	7/7	0.97	0.27	54,54,54,54	0
90	OHX	5	3575	7/7	0.97	0.35	65,65,65,65	0
91	MG	5	3883	1/1	0.97	0.43	32,32,32,32	0
90	OHX	6	1943	7/7	0.97	0.15	102,102,102,102	0
91	MG	7	222	1/1	0.97	0.31	35,35,35,35	0
90	OHX	5	3578	7/7	0.97	0.17	63,63,63,63	0
90	OHX	5	3579	7/7	0.97	0.34	53,53,53,53	0
91	MG	O7	106	1/1	0.97	0.14	46,46,46,46	0
90	OHX	5	3580	7/7	0.97	0.44	55,55,55,55	0
90	OHX	6	1946	7/7	0.97	0.16	79,79,79,79	0
90	OHX	1	3651	7/7	0.97	0.30	64,64,64,64	0
90	OHX	1	3508	7/7	0.97	0.12	67,67,67,67	0
91	MG	2	2107	1/1	0.97	0.34	81,81,81,81	0
90	OHX	5	3591	7/7	0.97	0.28	62,62,62,62	0
90	OHX	5	3592	7/7	0.97	0.22	54,54,54,54	0
90	OHX	1	3653	7/7	0.97	0.37	60,60,60,60	0
90	OHX	2	1942	7/7	0.97	0.28	84,84,84,84	0
90	OHX	1	3655	7/7	0.97	0.27	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	6	1954	7/7	0.97	0.12	116,116,116,116	0
90	OHX	6	1956	7/7	0.97	0.14	79,79,79,79	0
90	OHX	5	3599	7/7	0.97	0.17	83,83,83,83	0
90	OHX	1	3517	7/7	0.97	0.21	57,57,57,57	0
90	OHX	1	3522	7/7	0.97	0.18	58,58,58,58	0
90	OHX	1	3658	7/7	0.97	0.28	73,73,73,73	0
91	MG	l2	303	1/1	0.97	1.01	44,44,44,44	0
90	OHX	5	3605	7/7	0.97	0.29	61,61,61,61	0
90	OHX	1	3525	7/7	0.97	0.21	77,77,77,77	0
90	OHX	2	1963	7/7	0.97	0.27	73,73,73,73	0
90	OHX	6	1964	7/7	0.97	0.23	62,62,62,62	0
90	OHX	6	1965	7/7	0.97	0.27	77,77,77,77	0
90	OHX	6	1966	7/7	0.97	0.29	69,69,69,69	0
90	OHX	1	3662	7/7	0.97	0.28	71,71,71,71	0
91	MG	m0	301	1/1	0.97	0.32	36,36,36,36	0
90	OHX	2	1927	7/7	0.97	0.15	85,85,85,85	0
91	MG	5	3915	1/1	0.97	0.59	36,36,36,36	0
90	OHX	1	3664	7/7	0.97	0.31	66,66,66,66	0
90	OHX	5	3620	7/7	0.97	0.24	76,76,76,76	0
90	OHX	2	1965	7/7	0.97	0.18	84,84,84,84	0
90	OHX	5	3623	7/7	0.97	0.26	58,58,58,58	0
90	OHX	5	3624	7/7	0.97	0.35	53,53,53,53	0
90	OHX	2	1967	7/7	0.97	0.16	85,85,85,85	0
90	OHX	1	3536	7/7	0.97	0.29	61,61,61,61	0
91	MG	6	2090	1/1	0.97	0.27	56,56,56,56	0
91	MG	n0	201	1/1	0.97	0.49	37,37,37,37	0
90	OHX	2	1968	7/7	0.97	0.37	86,86,86,86	0
90	OHX	1	3669	7/7	0.97	0.27	60,60,60,60	0
91	MG	5	3926	1/1	0.97	0.77	32,32,32,32	0
90	OHX	5	3629	7/7	0.97	0.35	53,53,53,53	0
90	OHX	6	1978	7/7	0.97	0.26	90,90,90,90	0
90	OHX	6	1979	7/7	0.97	0.27	62,62,62,62	0
90	OHX	2	1944	7/7	0.97	0.18	83,83,83,83	0
91	MG	5	3932	1/1	0.97	0.76	41,41,41,41	0
90	OHX	1	3671	7/7	0.97	0.16	60,60,60,60	0
91	MG	1	3971	1/1	0.97	0.18	44,44,44,44	0
90	OHX	5	3635	7/7	0.97	0.33	46,46,46,46	0
90	OHX	2	1911	7/7	0.97	0.09	98,98,98,98	0
91	MG	5	3938	1/1	0.97	0.72	34,34,34,34	0
90	OHX	5	3637	7/7	0.97	0.30	41,41,41,41	0
91	MG	1	3975	1/1	0.97	0.20	53,53,53,53	0
91	MG	5	3941	1/1	0.97	0.17	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	6	1983	7/7	0.97	0.19	89,89,89,89	0
90	OHX	6	1986	7/7	0.97	0.27	77,77,77,77	0
91	MG	5	3944	1/1	0.97	0.49	35,35,35,35	0
90	OHX	2	2040	7/7	0.97	0.26	97,97,97,97	0
92	ZN	D9	101	1/1	0.97	0.07	90,90,90,90	0
90	OHX	1	3544	7/7	0.97	0.15	77,77,77,77	0
90	OHX	2	1931	7/7	0.97	0.33	95,95,95,95	0
90	OHX	1	3676	7/7	0.97	0.31	67,67,67,67	0
90	OHX	2	2006	7/7	0.97	0.32	98,98,98,98	0
90	OHX	6	1992	7/7	0.97	0.28	88,88,88,88	0
90	OHX	5	3652	7/7	0.97	0.32	59,59,59,59	0
90	OHX	5	3654	7/7	0.97	0.42	62,62,62,62	0
90	OHX	2	1921	7/7	0.97	0.26	97,97,97,97	0
90	OHX	6	1994	7/7	0.97	0.32	98,98,98,98	0
90	OHX	6	1995	7/7	0.97	0.36	79,79,79,79	0
90	OHX	6	1996	7/7	0.97	0.36	78,78,78,78	0
90	OHX	5	3660	7/7	0.97	0.43	58,58,58,58	0
90	OHX	1	3477	7/7	0.98	0.17	51,51,51,51	0
91	MG	6	2126	1/1	0.98	0.49	62,62,62,62	0
90	OHX	1	3584	7/7	0.98	0.21	80,80,80,80	0
90	OHX	1	3706	7/7	0.98	0.09	97,97,97,97	0
90	OHX	1	3585	7/7	0.98	0.20	74,74,74,74	0
90	OHX	1	3708	7/7	0.98	0.32	60,60,60,60	0
90	OHX	1	3586	7/7	0.98	0.23	46,46,46,46	0
90	OHX	1	3479	7/7	0.98	0.12	67,67,67,67	0
90	OHX	1	3711	7/7	0.98	0.36	58,58,58,58	0
90	OHX	6	2011	7/7	0.98	0.38	72,72,72,72	0
90	OHX	1	3480	7/7	0.98	0.12	48,48,48,48	0
90	OHX	2	1934	7/7	0.98	0.26	94,94,94,94	0
90	OHX	1	3482	7/7	0.98	0.14	57,57,57,57	0
90	OHX	2	2008	7/7	0.98	0.14	106,106,106,106	0
90	OHX	5	3639	7/7	0.98	0.29	58,58,58,58	0
90	OHX	5	3640	7/7	0.98	0.29	59,59,59,59	0
90	OHX	1	3592	7/7	0.98	0.20	86,86,86,86	0
90	OHX	5	3642	7/7	0.98	0.36	49,49,49,49	0
90	OHX	1	3485	7/7	0.98	0.14	69,69,69,69	0
90	OHX	1	3487	7/7	0.98	0.12	68,68,68,68	0
90	OHX	2	1910	7/7	0.98	0.10	89,89,89,89	0
90	OHX	5	3646	7/7	0.98	0.48	63,63,63,63	0
90	OHX	1	3489	7/7	0.98	0.18	51,51,51,51	0
90	OHX	1	3597	7/7	0.98	0.17	78,78,78,78	0
90	OHX	5	3649	7/7	0.98	0.28	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	5	3650	7/7	0.98	0.28	50,50,50,50	0
90	OHX	1	3491	7/7	0.98	0.15	66,66,66,66	0
90	OHX	1	3599	7/7	0.98	0.34	58,58,58,58	0
90	OHX	1	3600	7/7	0.98	0.24	63,63,63,63	0
90	OHX	2	2010	7/7	0.98	0.25	85,85,85,85	0
91	MG	1	4016	1/1	0.98	0.40	52,52,52,52	0
90	OHX	5	3656	7/7	0.98	0.35	64,64,64,64	0
90	OHX	2	1904	7/7	0.98	0.09	83,83,83,83	0
90	OHX	1	3496	7/7	0.98	0.14	53,53,53,53	0
90	OHX	1	3497	7/7	0.98	0.17	74,74,74,74	0
91	MG	6	2160	1/1	0.98	0.38	73,73,73,73	0
90	OHX	1	3605	7/7	0.98	0.14	63,63,63,63	0
90	OHX	1	3606	7/7	0.98	0.24	62,62,62,62	0
90	OHX	5	3662	7/7	0.98	0.29	47,47,47,47	0
90	OHX	3	201	7/7	0.98	0.10	60,60,60,60	0
90	OHX	1	3498	7/7	0.98	0.14	50,50,50,50	0
90	OHX	1	3608	7/7	0.98	0.28	71,71,71,71	0
90	OHX	1	3609	7/7	0.98	0.29	66,66,66,66	0
90	OHX	1	3500	7/7	0.98	0.16	62,62,62,62	0
90	OHX	2	1937	7/7	0.98	0.16	84,84,84,84	0
90	OHX	2	1992	7/7	0.98	0.20	95,95,95,95	0
90	OHX	1	3503	7/7	0.98	0.16	75,75,75,75	0
90	OHX	4	205	7/7	0.98	0.11	49,49,49,49	0
91	MG	5	4012	1/1	0.98	0.18	35,35,35,35	0
90	OHX	4	206	7/7	0.98	0.18	51,51,51,51	0
90	OHX	6	2041	7/7	0.98	0.34	79,79,79,79	0
90	OHX	4	207	7/7	0.98	0.23	46,46,46,46	0
90	OHX	5	3675	7/7	0.98	0.28	59,59,59,59	0
91	MG	1	3771	1/1	0.98	0.24	30,30,30,30	0
90	OHX	4	208	7/7	0.98	0.14	49,49,49,49	0
90	OHX	2	1949	7/7	0.98	0.11	94,94,94,94	0
90	OHX	1	3615	7/7	0.98	0.21	64,64,64,64	0
90	OHX	4	211	7/7	0.98	0.30	56,56,56,56	0
90	OHX	4	212	7/7	0.98	0.26	53,53,53,53	0
90	OHX	1	3505	7/7	0.98	0.22	66,66,66,66	0
90	OHX	4	214	7/7	0.98	0.29	50,50,50,50	0
90	OHX	1	3507	7/7	0.98	0.24	51,51,51,51	0
90	OHX	4	216	7/7	0.98	0.22	70,70,70,70	0
90	OHX	C8	202	7/7	0.98	0.13	80,80,80,80	0
91	MG	c8	201	1/1	0.98	0.08	86,86,86,86	0
90	OHX	5	3686	7/7	0.98	0.42	58,58,58,58	0
90	OHX	1	3619	7/7	0.98	0.30	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	5	3688	7/7	0.98	0.45	59,59,59,59	0
90	OHX	2	1962	7/7	0.98	0.22	86,86,86,86	0
90	OHX	1	3621	7/7	0.98	0.28	79,79,79,79	0
91	MG	1	3787	1/1	0.98	0.41	49,49,49,49	0
90	OHX	5	3691	7/7	0.98	0.29	64,64,64,64	0
90	OHX	1	3622	7/7	0.98	0.34	54,54,54,54	0
91	MG	1	4056	1/1	0.98	0.22	34,34,34,34	0
90	OHX	5	3693	7/7	0.98	0.29	63,63,63,63	0
90	OHX	5	3694	7/7	0.98	0.34	55,55,55,55	0
91	MG	1	4059	1/1	0.98	0.08	46,46,46,46	0
90	OHX	1	3510	7/7	0.98	0.22	58,58,58,58	0
90	OHX	1	3512	7/7	0.98	0.22	48,48,48,48	0
90	OHX	L3	402	7/7	0.98	0.24	65,65,65,65	0
90	OHX	s1	301	7/7	0.98	0.14	77,77,77,77	0
90	OHX	1	3513	7/7	0.98	0.18	52,52,52,52	0
90	OHX	1	3514	7/7	0.98	0.19	56,56,56,56	0
90	OHX	L6	202	7/7	0.98	0.35	62,62,62,62	0
90	OHX	1	3627	7/7	0.98	0.25	62,62,62,62	0
91	MG	5	4049	1/1	0.98	0.19	48,48,48,48	0
90	OHX	1	3628	7/7	0.98	0.25	79,79,79,79	0
90	OHX	M6	201	7/7	0.98	0.15	54,54,54,54	0
90	OHX	1	3516	7/7	0.98	0.15	73,73,73,73	0
90	OHX	5	3706	7/7	0.98	0.49	76,76,76,76	0
90	OHX	1	3631	7/7	0.98	0.35	88,88,88,88	0
90	OHX	5	3403	7/7	0.98	0.13	43,43,43,43	0
90	OHX	5	3420	7/7	0.98	0.13	44,44,44,44	0
90	OHX	5	3429	7/7	0.98	0.13	47,47,47,47	0
90	OHX	5	3432	7/7	0.98	0.20	45,45,45,45	0
90	OHX	5	3434	7/7	0.98	0.08	46,46,46,46	0
91	MG	1	3811	1/1	0.98	0.42	40,40,40,40	0
91	MG	1	3812	1/1	0.98	0.18	47,47,47,47	0
91	MG	1	4080	1/1	0.98	0.52	33,33,33,33	0
90	OHX	1	3632	7/7	0.98	0.23	72,72,72,72	0
91	MG	5	3776	1/1	0.98	0.51	40,40,40,40	0
90	OHX	5	3445	7/7	0.98	0.12	45,45,45,45	0
90	OHX	5	3448	7/7	0.98	0.14	48,48,48,48	0
90	OHX	5	3449	7/7	0.98	0.11	58,58,58,58	0
91	MG	1	4085	1/1	0.98	0.33	39,39,39,39	0
90	OHX	5	3451	7/7	0.98	0.12	63,63,63,63	0
90	OHX	5	3454	7/7	0.98	0.13	58,58,58,58	0
91	MG	1	3819	1/1	0.98	0.22	43,43,43,43	0
91	MG	5	4072	1/1	0.98	0.32	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	2	1928	7/7	0.98	0.18	79,79,79,79	0
90	OHX	5	3720	7/7	0.98	0.27	49,49,49,49	0
90	OHX	5	3456	7/7	0.98	0.10	58,58,58,58	0
90	OHX	5	3457	7/7	0.98	0.15	57,57,57,57	0
90	OHX	5	3458	7/7	0.98	0.15	64,64,64,64	0
90	OHX	5	3460	7/7	0.98	0.09	48,48,48,48	0
91	MG	5	3790	1/1	0.98	0.41	31,31,31,31	0
90	OHX	1	3634	7/7	0.98	0.25	57,57,57,57	0
90	OHX	1	3518	7/7	0.98	0.22	46,46,46,46	0
90	OHX	5	3467	7/7	0.98	0.12	70,70,70,70	0
91	MG	1	3829	1/1	0.98	0.68	38,38,38,38	0
90	OHX	1	3520	7/7	0.98	0.16	64,64,64,64	0
90	OHX	5	3469	7/7	0.98	0.14	48,48,48,48	0
90	OHX	1	3521	7/7	0.98	0.16	62,62,62,62	0
90	OHX	5	3471	7/7	0.98	0.11	66,66,66,66	0
90	OHX	5	3472	7/7	0.98	0.10	63,63,63,63	0
90	OHX	1	3418	7/7	0.98	0.15	52,52,52,52	0
91	MG	5	3801	1/1	0.98	0.25	32,32,32,32	0
90	OHX	1	3523	7/7	0.98	0.25	59,59,59,59	0
90	OHX	1	3524	7/7	0.98	0.30	57,57,57,57	0
90	OHX	5	3736	7/7	0.98	0.29	85,85,85,85	0
90	OHX	1	3422	7/7	0.98	0.10	55,55,55,55	0
90	OHX	1	3642	7/7	0.98	0.30	77,77,77,77	0
90	OHX	5	3478	7/7	0.98	0.12	58,58,58,58	0
90	OHX	5	3479	7/7	0.98	0.10	52,52,52,52	0
91	MG	5	4100	1/1	0.98	0.28	40,40,40,40	0
90	OHX	5	3480	7/7	0.98	0.11	49,49,49,49	0
90	OHX	5	3482	7/7	0.98	0.16	57,57,57,57	0
90	OHX	5	3486	7/7	0.98	0.14	53,53,53,53	0
90	OHX	5	3488	7/7	0.98	0.15	41,41,41,41	0
90	OHX	5	3489	7/7	0.98	0.12	53,53,53,53	0
90	OHX	6	1922	7/7	0.98	0.18	60,60,60,60	0
90	OHX	1	3526	7/7	0.98	0.16	69,69,69,69	0
90	OHX	5	3495	7/7	0.98	0.28	47,47,47,47	0
90	OHX	6	1924	7/7	0.98	0.10	63,63,63,63	0
90	OHX	7	204	7/7	0.98	0.15	45,45,45,45	0
90	OHX	7	205	7/7	0.98	0.14	55,55,55,55	0
90	OHX	7	206	7/7	0.98	0.17	56,56,56,56	0
90	OHX	1	3423	7/7	0.98	0.10	61,61,61,61	0
90	OHX	5	3499	7/7	0.98	0.12	72,72,72,72	0
91	MG	3	213	1/1	0.98	0.67	39,39,39,39	0
90	OHX	7	209	7/7	0.98	0.30	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	1	3528	7/7	0.98	0.14	79,79,79,79	0
90	OHX	1	3427	7/7	0.98	0.10	52,52,52,52	0
91	MG	1	3861	1/1	0.98	0.74	38,38,38,38	0
91	MG	5	4120	1/1	0.98	0.24	34,34,34,34	0
90	OHX	5	3502	7/7	0.98	0.18	44,44,44,44	0
90	OHX	8	206	7/7	0.98	0.22	58,58,58,58	0
90	OHX	6	1929	7/7	0.98	0.13	63,63,63,63	0
90	OHX	5	3504	7/7	0.98	0.09	52,52,52,52	0
91	MG	1	3866	1/1	0.98	0.57	40,40,40,40	0
90	OHX	5	3505	7/7	0.98	0.25	39,39,39,39	0
90	OHX	5	3506	7/7	0.98	0.24	52,52,52,52	0
90	OHX	5	3507	7/7	0.98	0.23	61,61,61,61	0
90	OHX	1	3647	7/7	0.98	0.38	55,55,55,55	0
91	MG	1	3871	1/1	0.98	0.26	41,41,41,41	0
90	OHX	5	3509	7/7	0.98	0.12	90,90,90,90	0
90	OHX	1	3530	7/7	0.98	0.17	89,89,89,89	0
91	MG	5	3840	1/1	0.98	0.20	35,35,35,35	0
90	OHX	5	3513	7/7	0.98	0.20	52,52,52,52	0
90	OHX	5	3514	7/7	0.98	0.13	85,85,85,85	0
90	OHX	1	3649	7/7	0.98	0.22	64,64,64,64	0
91	MG	1	3877	1/1	0.98	0.32	39,39,39,39	0
90	OHX	5	3517	7/7	0.98	0.15	55,55,55,55	0
90	OHX	l3	401	7/7	0.98	0.12	52,52,52,52	0
90	OHX	1	3531	7/7	0.98	0.21	55,55,55,55	0
91	MG	5	4142	1/1	0.98	0.39	34,34,34,34	0
90	OHX	5	3519	7/7	0.98	0.21	48,48,48,48	0
91	MG	5	3850	1/1	0.98	0.27	41,41,41,41	0
91	MG	5	3851	1/1	0.98	0.90	40,40,40,40	0
90	OHX	5	3520	7/7	0.98	0.20	60,60,60,60	0
90	OHX	5	3523	7/7	0.98	0.22	50,50,50,50	0
90	OHX	2	1929	7/7	0.98	0.15	83,83,83,83	0
91	MG	5	3855	1/1	0.98	0.51	31,31,31,31	0
90	OHX	6	1938	7/7	0.98	0.14	76,76,76,76	0
90	OHX	m6	202	7/7	0.98	0.12	48,48,48,48	0
90	OHX	1	3534	7/7	0.98	0.15	70,70,70,70	0
90	OHX	1	3432	7/7	0.98	0.15	55,55,55,55	0
90	OHX	o3	201	7/7	0.98	0.18	54,54,54,54	0
90	OHX	1	3433	7/7	0.98	0.13	52,52,52,52	0
91	MG	1	3891	1/1	0.98	0.46	33,33,33,33	0
90	OHX	1	3435	7/7	0.98	0.08	63,63,63,63	0
90	OHX	1	3538	7/7	0.98	0.17	54,54,54,54	0
90	OHX	5	3532	7/7	0.98	0.20	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	6	1945	7/7	0.98	0.18	72,72,72,72	0
90	OHX	1	3439	7/7	0.98	0.11	59,59,59,59	0
91	MG	1	3897	1/1	0.98	0.73	30,30,30,30	0
90	OHX	6	1947	7/7	0.98	0.18	71,71,71,71	0
91	MG	5	3870	1/1	0.98	0.39	33,33,33,33	0
90	OHX	2	1940	7/7	0.98	0.10	94,94,94,94	0
91	MG	5	3872	1/1	0.98	0.59	31,31,31,31	0
90	OHX	1	3659	7/7	0.98	0.36	70,70,70,70	0
90	OHX	5	3538	7/7	0.98	0.28	47,47,47,47	0
90	OHX	5	3539	7/7	0.98	0.21	55,55,55,55	0
90	OHX	2	1966	7/7	0.98	0.20	65,65,65,65	0
90	OHX	1	3543	7/7	0.98	0.15	72,72,72,72	0
91	MG	1	3905	1/1	0.98	0.41	35,35,35,35	0
90	OHX	1	3445	7/7	0.98	0.11	47,47,47,47	0
90	OHX	5	3543	7/7	0.98	0.26	45,45,45,45	0
90	OHX	5	3544	7/7	0.98	0.21	66,66,66,66	0
91	MG	1	3909	1/1	0.98	0.59	29,29,29,29	0
90	OHX	5	3545	7/7	0.98	0.27	49,49,49,49	0
90	OHX	5	3546	7/7	0.98	0.20	68,68,68,68	0
90	OHX	1	3545	7/7	0.98	0.22	68,68,68,68	0
90	OHX	1	3546	7/7	0.98	0.25	65,65,65,65	0
90	OHX	2	1914	7/7	0.98	0.12	78,78,78,78	0
91	MG	1	3915	1/1	0.98	0.54	34,34,34,34	0
90	OHX	1	3549	7/7	0.98	0.23	63,63,63,63	0
90	OHX	1	3449	7/7	0.98	0.12	56,56,56,56	0
90	OHX	5	3552	7/7	0.98	0.20	54,54,54,54	0
91	MG	1	3919	1/1	0.98	0.59	36,36,36,36	0
90	OHX	1	3450	7/7	0.98	0.11	62,62,62,62	0
90	OHX	5	3554	7/7	0.98	0.20	52,52,52,52	0
90	OHX	1	3451	7/7	0.98	0.10	65,65,65,65	0
91	MG	1	3923	1/1	0.98	0.24	41,41,41,41	0
90	OHX	6	1962	7/7	0.98	0.20	69,69,69,69	0
90	OHX	6	1963	7/7	0.98	0.16	78,78,78,78	0
90	OHX	1	3452	7/7	0.98	0.14	46,46,46,46	0
90	OHX	2	1907	7/7	0.98	0.12	93,93,93,93	0
91	MG	8	223	1/1	0.98	0.14	47,47,47,47	0
90	OHX	5	3561	7/7	0.98	0.25	60,60,60,60	0
90	OHX	1	3556	7/7	0.98	0.19	56,56,56,56	0
91	MG	5	3903	1/1	0.98	0.44	32,32,32,32	0
90	OHX	5	3563	7/7	0.98	0.24	72,72,72,72	0
90	OHX	5	3564	7/7	0.98	0.30	59,59,59,59	0
90	OHX	5	3567	7/7	0.98	0.28	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
91	MG	5	3907	1/1	0.98	0.19	31,31,31,31	0
90	OHX	1	3557	7/7	0.98	0.20	74,74,74,74	0
90	OHX	1	3558	7/7	0.98	0.16	69,69,69,69	0
91	MG	5	3910	1/1	0.98	0.43	34,34,34,34	0
90	OHX	1	3454	7/7	0.98	0.11	65,65,65,65	0
90	OHX	5	3571	7/7	0.98	0.25	61,61,61,61	0
90	OHX	1	3456	7/7	0.98	0.12	73,73,73,73	0
90	OHX	5	3573	7/7	0.98	0.21	60,60,60,60	0
90	OHX	5	3574	7/7	0.98	0.18	55,55,55,55	0
90	OHX	6	1971	7/7	0.98	0.25	55,55,55,55	0
91	MG	l7	301	1/1	0.98	0.41	34,34,34,34	0
90	OHX	6	1972	7/7	0.98	0.15	67,67,67,67	0
90	OHX	1	3458	7/7	0.98	0.09	72,72,72,72	0
90	OHX	1	3459	7/7	0.98	0.12	44,44,44,44	0
90	OHX	1	3460	7/7	0.98	0.10	58,58,58,58	0
90	OHX	5	3581	7/7	0.98	0.27	56,56,56,56	0
90	OHX	5	3582	7/7	0.98	0.18	71,71,71,71	0
90	OHX	5	3583	7/7	0.98	0.19	52,52,52,52	0
90	OHX	6	1976	7/7	0.98	0.26	58,58,58,58	0
90	OHX	5	3585	7/7	0.98	0.22	51,51,51,51	0
90	OHX	1	3564	7/7	0.98	0.19	50,50,50,50	0
90	OHX	1	3462	7/7	0.98	0.11	80,80,80,80	0
91	MG	5	3928	1/1	0.98	0.59	29,29,29,29	0
90	OHX	5	3589	7/7	0.98	0.34	47,47,47,47	0
90	OHX	5	3590	7/7	0.98	0.29	60,60,60,60	0
90	OHX	1	3566	7/7	0.98	0.18	71,71,71,71	0
90	OHX	1	3683	7/7	0.98	0.28	56,56,56,56	0
91	MG	5	3933	1/1	0.98	0.65	31,31,31,31	0
90	OHX	2	1969	7/7	0.98	0.09	87,87,87,87	0
90	OHX	1	3465	7/7	0.98	0.13	70,70,70,70	0
90	OHX	5	3595	7/7	0.98	0.29	48,48,48,48	0
90	OHX	1	3569	7/7	0.98	0.21	75,75,75,75	0
90	OHX	6	1984	7/7	0.98	0.41	87,87,87,87	0
90	OHX	6	1985	7/7	0.98	0.34	91,91,91,91	0
90	OHX	1	3687	7/7	0.98	0.42	58,58,58,58	0
90	OHX	2	2002	7/7	0.98	0.39	86,86,86,86	0
90	OHX	1	3571	7/7	0.98	0.20	64,64,64,64	0
90	OHX	5	3602	7/7	0.98	0.24	64,64,64,64	0
90	OHX	5	3603	7/7	0.98	0.30	57,57,57,57	0
90	OHX	1	3572	7/7	0.98	0.22	60,60,60,60	0
90	OHX	1	3692	7/7	0.98	0.29	69,69,69,69	0
90	OHX	1	3573	7/7	0.98	0.20	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	5	3610	7/7	0.98	0.31	45,45,45,45	0
92	ZN	D6	500	1/1	0.98	0.03	87,87,87,87	0
90	OHX	1	3469	7/7	0.98	0.16	82,82,82,82	0
90	OHX	5	3612	7/7	0.98	0.27	54,54,54,54	0
90	OHX	2	1916	7/7	0.98	0.11	84,84,84,84	0
91	MG	5	3952	1/1	0.98	0.39	41,41,41,41	0
92	ZN	d9	101	1/1	0.98	0.10	97,97,97,97	0
90	OHX	1	3576	7/7	0.98	0.14	60,60,60,60	0
90	OHX	1	3472	7/7	0.98	0.11	62,62,62,62	0
92	ZN	q3	501	1/1	0.98	0.12	55,55,55,55	0
90	OHX	1	3473	7/7	0.98	0.10	55,55,55,55	0
90	OHX	1	3579	7/7	0.98	0.18	67,67,67,67	0
90	OHX	2	1933	7/7	0.98	0.11	91,91,91,91	0
90	OHX	2	2005	7/7	0.98	0.22	84,84,84,84	0
90	OHX	5	3621	7/7	0.98	0.19	73,73,73,73	0
90	OHX	6	2000	7/7	0.98	0.22	69,69,69,69	0
90	OHX	1	3702	7/7	0.98	0.38	49,49,49,49	0
90	OHX	2	1987	7/7	0.98	0.19	94,94,94,94	0
90	OHX	q2	502	7/7	0.99	0.09	45,45,45,45	0
90	OHX	5	3630	7/7	0.99	0.25	65,65,65,65	0
91	MG	4	230	1/1	0.99	0.12	46,46,46,46	0
91	MG	1	3801	1/1	0.99	0.17	37,37,37,37	0
90	OHX	6	1917	7/7	0.99	0.09	55,55,55,55	0
90	OHX	6	1918	7/7	0.99	0.11	49,49,49,49	0
90	OHX	1	3483	7/7	0.99	0.15	72,72,72,72	0
90	OHX	1	3539	7/7	0.99	0.18	52,52,52,52	0
90	OHX	5	3481	7/7	0.99	0.09	49,49,49,49	0
90	OHX	2	1924	7/7	0.99	0.08	103,103,103,103	0
90	OHX	5	3483	7/7	0.99	0.16	43,43,43,43	0
90	OHX	5	3484	7/7	0.99	0.14	48,48,48,48	0
90	OHX	5	3485	7/7	0.99	0.20	52,52,52,52	0
90	OHX	1	3404	7/7	0.99	0.18	43,43,43,43	0
90	OHX	5	3487	7/7	0.99	0.12	47,47,47,47	0
90	OHX	1	3486	7/7	0.99	0.10	57,57,57,57	0
91	MG	sM	302	1/1	0.99	0.58	45,45,45,45	0
90	OHX	1	3405	7/7	0.99	0.13	43,43,43,43	0
90	OHX	1	3442	7/7	0.99	0.12	58,58,58,58	0
90	OHX	5	3492	7/7	0.99	0.12	48,48,48,48	0
90	OHX	5	3493	7/7	0.99	0.13	51,51,51,51	0
90	OHX	6	1926	7/7	0.99	0.19	67,67,67,67	0
90	OHX	1	3443	7/7	0.99	0.07	53,53,53,53	0
90	OHX	5	3496	7/7	0.99	0.20	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	1	3490	7/7	0.99	0.21	53,53,53,53	0
90	OHX	1	3547	7/7	0.99	0.20	58,58,58,58	0
90	OHX	6	1930	7/7	0.99	0.14	64,64,64,64	0
91	MG	1	3992	1/1	0.99	0.38	44,44,44,44	0
90	OHX	5	3653	7/7	0.99	0.36	54,54,54,54	0
91	MG	1	3994	1/1	0.99	0.18	46,46,46,46	0
90	OHX	1	3444	7/7	0.99	0.09	66,66,66,66	0
90	OHX	1	3406	7/7	0.99	0.15	52,52,52,52	0
90	OHX	1	3493	7/7	0.99	0.16	42,42,42,42	0
90	OHX	6	1934	7/7	0.99	0.14	68,68,68,68	0
90	OHX	1	3494	7/7	0.99	0.13	67,67,67,67	0
90	OHX	6	1936	7/7	0.99	0.12	74,74,74,74	0
90	OHX	1	3408	7/7	0.99	0.12	41,41,41,41	0
90	OHX	1	3447	7/7	0.99	0.12	54,54,54,54	0
90	OHX	1	3554	7/7	0.99	0.14	70,70,70,70	0
90	OHX	3	202	7/7	0.99	0.21	54,54,54,54	0
90	OHX	5	3510	7/7	0.99	0.07	35,35,35,35	0
90	OHX	1	3448	7/7	0.99	0.07	54,54,54,54	0
90	OHX	5	3512	7/7	0.99	0.16	60,60,60,60	0
90	OHX	1	3409	7/7	0.99	0.10	39,39,39,39	0
90	OHX	3	205	7/7	0.99	0.14	69,69,69,69	0
91	MG	5	4130	1/1	0.99	0.21	32,32,32,32	0
90	OHX	6	1944	7/7	0.99	0.21	71,71,71,71	0
90	OHX	5	3516	7/7	0.99	0.23	51,51,51,51	0
90	OHX	1	3499	7/7	0.99	0.11	40,40,40,40	0
91	MG	1	3843	1/1	0.99	0.48	36,36,36,36	0
90	OHX	1	3410	7/7	0.99	0.14	48,48,48,48	0
90	OHX	1	3411	7/7	0.99	0.08	43,43,43,43	0
90	OHX	1	3412	7/7	0.99	0.08	51,51,51,51	0
90	OHX	5	3521	7/7	0.99	0.17	47,47,47,47	0
90	OHX	5	3522	7/7	0.99	0.13	61,61,61,61	0
90	OHX	1	3413	7/7	0.99	0.08	45,45,45,45	0
90	OHX	6	1950	7/7	0.99	0.15	90,90,90,90	0
90	OHX	4	203	7/7	0.99	0.12	41,41,41,41	0
90	OHX	4	204	7/7	0.99	0.12	47,47,47,47	0
90	OHX	1	3415	7/7	0.99	0.11	53,53,53,53	0
91	MG	5	3966	1/1	0.99	0.11	49,49,49,49	0
90	OHX	5	3528	7/7	0.99	0.17	42,42,42,42	0
90	OHX	1	3455	7/7	0.99	0.10	50,50,50,50	0
91	MG	5	4148	1/1	0.99	0.26	34,34,34,34	0
90	OHX	6	1955	7/7	0.99	0.09	108,108,108,108	0
90	OHX	1	3506	7/7	0.99	0.22	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	1	3417	7/7	0.99	0.18	52,52,52,52	0
90	OHX	1	3457	7/7	0.99	0.11	53,53,53,53	0
90	OHX	2	1905	7/7	0.99	0.13	76,76,76,76	0
90	OHX	1	3420	7/7	0.99	0.11	59,59,59,59	0
90	OHX	1	3511	7/7	0.99	0.15	45,45,45,45	0
90	OHX	1	3421	7/7	0.99	0.12	57,57,57,57	0
90	OHX	1	3629	7/7	0.99	0.13	50,50,50,50	0
90	OHX	1	3461	7/7	0.99	0.10	43,43,43,43	0
90	OHX	1	3690	7/7	0.99	0.21	52,52,52,52	0
90	OHX	2	1912	7/7	0.99	0.07	93,93,93,93	0
90	OHX	1	3515	7/7	0.99	0.18	39,39,39,39	0
90	OHX	1	3463	7/7	0.99	0.11	54,54,54,54	0
90	OHX	2	1913	7/7	0.99	0.14	84,84,84,84	0
90	OHX	1	3424	7/7	0.99	0.12	55,55,55,55	0
90	OHX	1	3519	7/7	0.99	0.25	53,53,53,53	0
90	OHX	1	3466	7/7	0.99	0.14	43,43,43,43	0
90	OHX	1	3467	7/7	0.99	0.10	54,54,54,54	0
90	OHX	1	3425	7/7	0.99	0.10	50,50,50,50	0
90	OHX	1	3426	7/7	0.99	0.14	58,58,58,58	0
90	OHX	L6	201	7/7	0.99	0.16	44,44,44,44	0
90	OHX	1	3470	7/7	0.99	0.14	48,48,48,48	0
90	OHX	2	1919	7/7	0.99	0.07	73,73,73,73	0
90	OHX	M5	301	7/7	0.99	0.12	46,46,46,46	0
90	OHX	5	3404	7/7	0.99	0.14	36,36,36,36	0
90	OHX	5	3405	7/7	0.99	0.17	36,36,36,36	0
90	OHX	5	3406	7/7	0.99	0.13	38,38,38,38	0
90	OHX	5	3408	7/7	0.99	0.17	47,47,47,47	0
90	OHX	5	3409	7/7	0.99	0.12	43,43,43,43	0
90	OHX	5	3560	7/7	0.99	0.15	41,41,41,41	0
90	OHX	5	3410	7/7	0.99	0.14	45,45,45,45	0
90	OHX	5	3411	7/7	0.99	0.11	44,44,44,44	0
90	OHX	5	3413	7/7	0.99	0.14	47,47,47,47	0
90	OHX	5	3415	7/7	0.99	0.08	42,42,42,42	0
90	OHX	5	3565	7/7	0.99	0.19	55,55,55,55	0
90	OHX	5	3566	7/7	0.99	0.15	58,58,58,58	0
90	OHX	5	3416	7/7	0.99	0.11	43,43,43,43	0
90	OHX	5	3417	7/7	0.99	0.11	41,41,41,41	0
90	OHX	5	3419	7/7	0.99	0.09	50,50,50,50	0
90	OHX	1	3429	7/7	0.99	0.10	55,55,55,55	0
90	OHX	5	3421	7/7	0.99	0.09	44,44,44,44	0
90	OHX	5	3422	7/7	0.99	0.10	51,51,51,51	0
90	OHX	5	3423	7/7	0.99	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	5	3424	7/7	0.99	0.08	41,41,41,41	0
90	OHX	5	3426	7/7	0.99	0.12	51,51,51,51	0
90	OHX	5	3576	7/7	0.99	0.15	50,50,50,50	0
90	OHX	5	3427	7/7	0.99	0.06	41,41,41,41	0
90	OHX	5	3428	7/7	0.99	0.07	37,37,37,37	0
90	OHX	1	3430	7/7	0.99	0.11	43,43,43,43	0
90	OHX	5	3431	7/7	0.99	0.11	46,46,46,46	0
91	MG	5	3844	1/1	0.99	0.24	45,45,45,45	0
90	OHX	2	1920	7/7	0.99	0.07	76,76,76,76	0
90	OHX	2	1901	7/7	0.99	0.18	78,78,78,78	0
90	OHX	5	3435	7/7	0.99	0.09	64,64,64,64	0
90	OHX	5	3436	7/7	0.99	0.10	41,41,41,41	0
90	OHX	5	3437	7/7	0.99	0.09	46,46,46,46	0
90	OHX	5	3438	7/7	0.99	0.11	46,46,46,46	0
90	OHX	5	3587	7/7	0.99	0.19	44,44,44,44	0
90	OHX	5	3439	7/7	0.99	0.10	43,43,43,43	0
90	OHX	5	3440	7/7	0.99	0.08	45,45,45,45	0
90	OHX	5	3441	7/7	0.99	0.07	57,57,57,57	0
90	OHX	5	3745	7/7	0.99	0.10	70,70,70,70	0
90	OHX	5	3442	7/7	0.99	0.12	59,59,59,59	0
90	OHX	2	1922	7/7	0.99	0.07	83,83,83,83	0
90	OHX	5	3444	7/7	0.99	0.08	51,51,51,51	0
90	OHX	7	201	7/7	0.99	0.07	49,49,49,49	0
90	OHX	N9	101	7/7	0.99	0.10	42,42,42,42	0
90	OHX	5	3446	7/7	0.99	0.08	56,56,56,56	0
90	OHX	5	3447	7/7	0.99	0.09	41,41,41,41	0
90	OHX	O3	201	7/7	0.99	0.23	55,55,55,55	0
90	OHX	1	3434	7/7	0.99	0.12	58,58,58,58	0
90	OHX	5	3450	7/7	0.99	0.10	65,65,65,65	0
90	OHX	1	3532	7/7	0.99	0.15	48,48,48,48	0
90	OHX	5	3452	7/7	0.99	0.09	55,55,55,55	0
90	OHX	5	3453	7/7	0.99	0.07	91,91,91,91	0
90	OHX	1	3478	7/7	0.99	0.16	51,51,51,51	0
90	OHX	8	203	7/7	0.99	0.11	41,41,41,41	0
91	MG	1	3766	1/1	0.99	0.37	36,36,36,36	0
90	OHX	8	204	7/7	0.99	0.11	40,40,40,40	0
90	OHX	Q2	502	7/7	0.99	0.06	41,41,41,41	0
90	OHX	6	1901	7/7	0.99	0.16	59,59,59,59	0
90	OHX	2	1902	7/7	0.99	0.13	81,81,81,81	0
90	OHX	5	3607	7/7	0.99	0.23	40,40,40,40	0
90	OHX	5	3608	7/7	0.99	0.41	67,67,67,67	0
90	OHX	5	3609	7/7	0.99	0.15	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	6	1903	7/7	0.99	0.12	61,61,61,61	0
91	MG	1	4112	1/1	0.99	0.25	59,59,59,59	0
90	OHX	5	3459	7/7	0.99	0.10	46,46,46,46	0
90	OHX	6	1904	7/7	0.99	0.08	68,68,68,68	0
90	OHX	1	3436	7/7	0.99	0.10	52,52,52,52	0
91	MG	1	3945	1/1	0.99	0.10	39,39,39,39	0
90	OHX	5	3614	7/7	0.99	0.12	47,47,47,47	0
90	OHX	6	1906	7/7	0.99	0.12	60,60,60,60	0
90	OHX	5	3463	7/7	0.99	0.10	50,50,50,50	0
90	OHX	5	3464	7/7	0.99	0.06	57,57,57,57	0
90	OHX	5	3465	7/7	0.99	0.08	56,56,56,56	0
90	OHX	5	3466	7/7	0.99	0.14	45,45,45,45	0
90	OHX	1	3437	7/7	0.99	0.06	47,47,47,47	0
90	OHX	6	1908	7/7	0.99	0.12	65,65,65,65	0
90	OHX	6	1909	7/7	0.99	0.08	91,91,91,91	0
92	ZN	O7	103	1/1	0.99	0.06	39,39,39,39	0
92	ZN	Q0	500	1/1	0.99	0.11	47,47,47,47	0
92	ZN	Q2	501	1/1	0.99	0.05	51,51,51,51	0
92	ZN	Q3	501	1/1	0.99	0.06	55,55,55,55	0
92	ZN	d6	101	1/1	0.99	0.07	67,67,67,67	0
90	OHX	6	1910	7/7	0.99	0.12	62,62,62,62	0
90	OHX	m0	303	7/7	0.99	0.29	49,49,49,49	0
90	OHX	6	1911	7/7	0.99	0.08	57,57,57,57	0
92	ZN	o7	501	1/1	0.99	0.09	41,41,41,41	0
90	OHX	m5	301	7/7	0.99	0.11	48,48,48,48	0
90	OHX	m5	302	7/7	0.99	0.18	66,66,66,66	0
90	OHX	6	1912	7/7	0.99	0.10	74,74,74,74	0
90	OHX	6	1913	7/7	0.99	0.08	80,80,80,80	0
90	OHX	1	3438	7/7	0.99	0.12	56,56,56,56	0
90	OHX	n9	101	7/7	0.99	0.07	41,41,41,41	0
90	OHX	6	1915	7/7	0.99	0.08	62,62,62,62	0
90	OHX	o7	502	7/7	0.99	0.14	54,54,54,54	0
91	MG	6	2179	1/1	0.99	0.12	93,93,93,93	0
90	OHX	6	1916	7/7	0.99	0.07	70,70,70,70	0
90	OHX	1	3419	7/7	1.00	0.06	38,38,38,38	0
90	OHX	5	3418	7/7	1.00	0.11	40,40,40,40	0
90	OHX	5	3430	7/7	1.00	0.07	53,53,53,53	0
90	OHX	1	3403	7/7	1.00	0.14	37,37,37,37	0
90	OHX	1	3416	7/7	1.00	0.07	38,38,38,38	0
91	MG	5	4091	1/1	1.00	0.14	32,32,32,32	0
90	OHX	5	3433	7/7	1.00	0.05	39,39,39,39	0
92	ZN	q0	500	1/1	1.00	0.14	37,37,37,37	0

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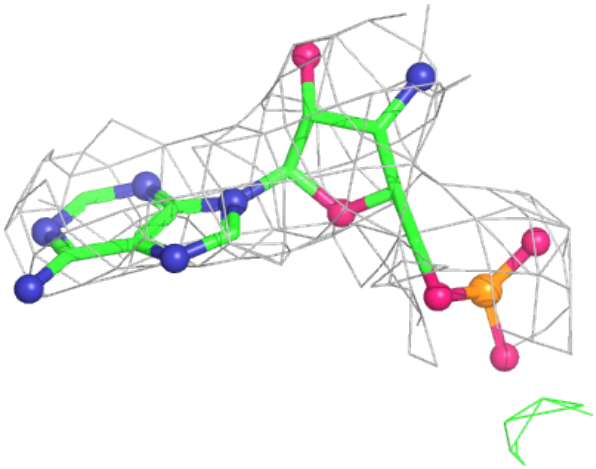
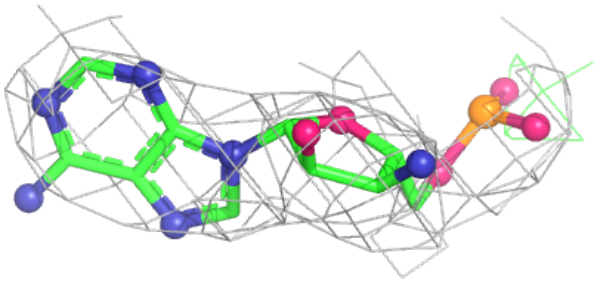
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	OHX	1	3407	7/7	1.00	0.10	41,41,41,41	0
91	MG	5	4094	1/1	1.00	0.11	32,32,32,32	0
90	OHX	5	3412	7/7	1.00	0.10	33,33,33,33	0
90	OHX	1	3428	7/7	1.00	0.07	47,47,47,47	0
90	OHX	5	3414	7/7	1.00	0.10	42,42,42,42	0
90	OHX	5	3425	7/7	1.00	0.06	52,52,52,52	0
90	OHX	5	3491	7/7	1.00	0.07	46,46,46,46	0
90	OHX	1	3414	7/7	1.00	0.07	47,47,47,47	0
90	OHX	5	3407	7/7	1.00	0.20	44,44,44,44	0
91	MG	5	4150	1/1	1.00	0.11	37,37,37,37	0

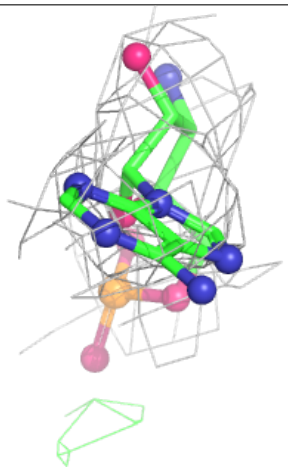
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8AN P 101:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

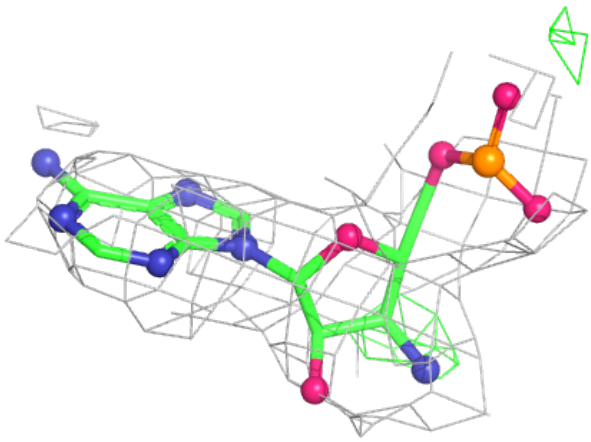


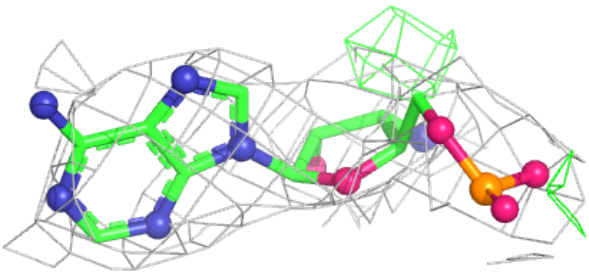


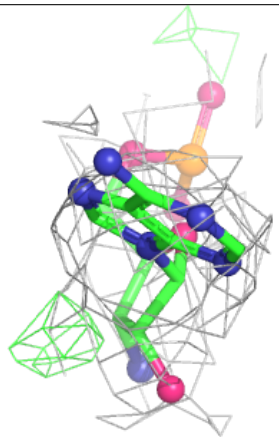


Electron density around 8AN p 101:

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

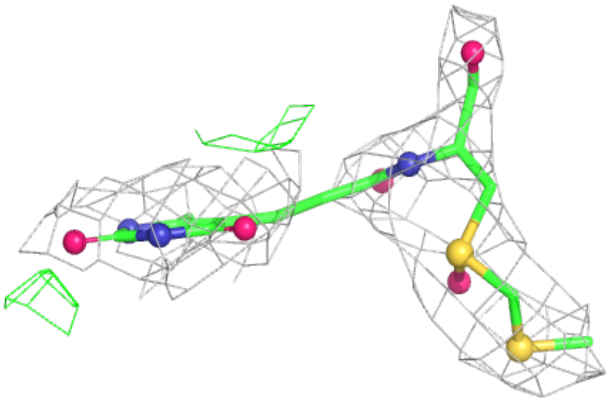


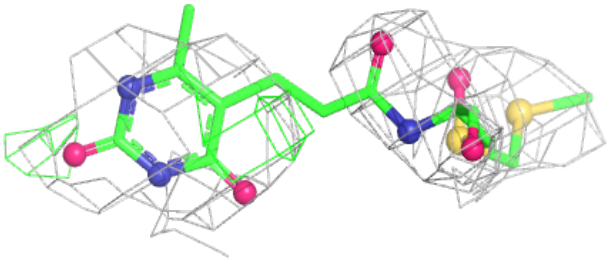


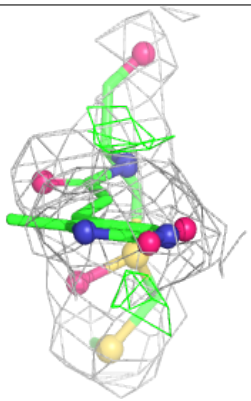


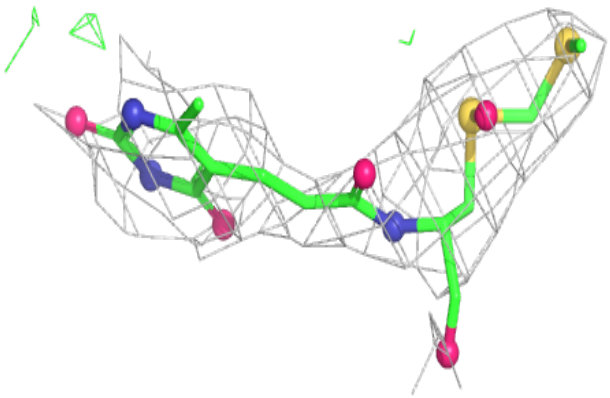
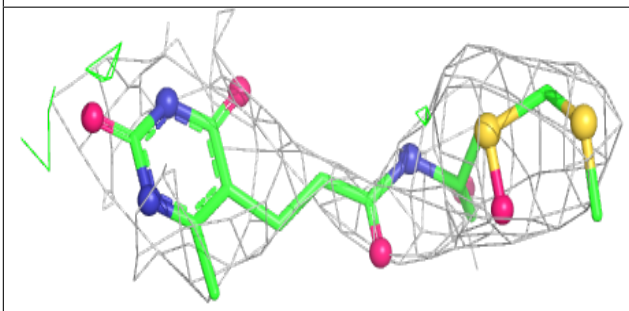
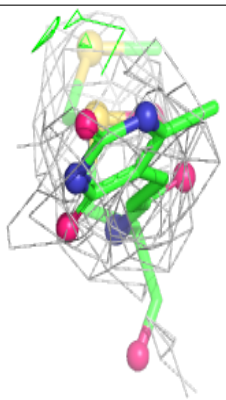
Electron density around SPS 1 4125:

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







Electron density around SPS 5 4176: 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

There are no such residues in this entry.